## Supplementary material for

Designing High-refractive Index Polymers using Materials Informatics

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 $Table \ S1: \ List \ of \ molecular \ descriptors \ used \ in \ this \ study.$ 

| Namo                      | Decemintion   |
|---------------------------|---|
|                           | Description   |
| CDCA DDCA 9               | partial positive surface area   |
| CDSA_FF5A-2               | partial positive surface area - total positive charge on the molecule |
| CPSA_PPSA-3               | charge weighted partial positive surface area                         |
| CPSA_PNSA-1               | partial negative surface area   |
| CPSA_PNSA-2               | partial negative surface area * total negative charge on the molecule |
| CPSA_PNSA-3               | charge weighted partial negative surface area                         |
| CPSA_DPSA-1               | difference of PPSA-1 and PNSA-1                                       |
| CPSA_DPSA-2               | difference of FPSA-2 and PNSA-2                                       |
| CPSA_DPSA-3               | difference of PPSA-3 and PNSA-3                                       |
| CPSA_FPSA-1               | PPSA-1/total molecular surface area                                   |
| CPSA_FFSA-2               | PPSA-2/total molecular surface area                                   |
| CPSA_FPSA-3               | PPSA-3/total molecular surface area                                   |
| CPSA_FNSA-1               | PNSA-1/total molecular surface area                                   |
| CPSA_FNSA-2               | PNSA-2/total molecular surface area                                   |
| CPSA_FNSA-3               | PNSA-3/total molecular surface area                                   |
| CPSA_WPSA-1               | PPSA-1 * total molecular surface area/1000                            |
| CPSA_WPSA-2               | PPSA-2 * total molecular surface area /1000                           |
| CPSA_WPSA-3               | PPSA-3 * total molecular surface area/1000                            |
| CPSA_WNSA-1               | PNSA-1 $*$ total molecular surface area /1000                         |
| CPSA_WNSA-2               | PNSA-2 * total molecular surface area/1000                            |
| CPSA_WNSA-3               | PNSA-3 * total molecular surface area/1000                            |
| CPSA_RPCG                 | relative positive charge  |
| CPSA_RNCG                 | relative negative charge  |
| CPSA_RPCS                 | relative positive charge surface area                                 |
| CPSA_RNCS                 | relative negative charge surface area                                 |
| CPSA_PPSA-4               | additional CPSA descriptors [1]                                       |
| CPSA_PPSA-5               | additional CPSA descriptors   |
| CPSA_PNSA-4               | additional CPSA descriptors   |
| CPSA_PNSA-5               | additional CPSA descriptors   |
| CPSA_SPMX                 | additional CPSA descriptors   |
| CPSA_SNMX                 | additional CPSA descriptors   |
| MOPAC COSMO AREA          | Area of the solvent accessible surface                                |
| MOPAC COSMO VOLUME        | Volume included in the COSMO surface                                  |
| MOPAC HOMO                | Highest occupied molecular orbital                                    |
| MOPAC LUMO                | Lowest unoccupied molecular orbital                                   |
| MOPAC_HLGAP               | Difference between HOMO-LUMO energies                                 |
| MOPAC HLFRACTION          | ratio of HOMO/LUMO energies   |
| MOPAC CHARGE DIPOLE       | Dipole moment is calculated from the atomic charges                   |
| MOPAC HYBRID DIPOLE       | hybrid dipole moment  |
| MOPAC TOTAL DIPOLE        | total dipole moment   |
| MOPAC HOF                 | Heat of formation   |
| MOPAC ABSOLUTE HABDNESS   | Part and Polla absolute hardness                                      |
| MOPAC TOTAL SOFTNESS      | Inverse of the hardness   |
| MOPAC CORE-CORE REPULSION | corescore repulsion energy  |
| MOPAC TOTAL ENERGY        | total energy  |
| MOPAC ELEC NUC ATTR       | ELECTRON-NUCLEAR ATTRACTION   |
| MOPAC ELEC ELEC BEPL      | ELECTRON ELECTRON REPUI SION  |
| MOPAC ELEC ENERGY         | TOTAL OF FLECTRONIC AND NUCLEAR ENERGIES                              |
| MOPAC RESONANCE ENERGY    |   |
| MOPAC EXCHC ENERGY        | exchange energy   |
| MOPAC TOTAL ELEC INTRN    | total electronic interaction  |
| MOPAC TOTAL EPHIL DELOC   | total electronhilic delocalizability                                  |
| MOPAC TOTAL NPHIL DELOC   | total neutrophilic delocalizability                                   |
| MOPAC TOTAL SPOI          | total solf polarizability   |
| MODAC EI ECTRODUII ICITV  |   |
| MODAC DIMY                | Dringing moments of inertia   |
| MOPAC DIMY                | r incipal moments of mertia   |
| MOPAC DIM7                | r incipal moments of mertia   |
|                           | r micipal moments of mertia   |
| MOPAC-MW                  | Morecular weight  |
| MOPAC_FILLEDLEVELS        | Number of filled levels   |
| MOPAC_MIN_DNR             | minimum nucleophilic delocalizability                                 |

| Name Description   |           |
|--|-----------|
| MOPAC_MIN_DER minimum electrophilic delocalizability   |           |
| MOPAC_MIN_SPOL minimum self polarizability   |           |
| MOPAC_MAX_DNR maximum nucleophilic delocalizability  |           |
| MOPAC_MAX_DER maximum electrophilic delocalizability   |           |
| MOPAC_MAX_SPOL maximum self polarizability   |           |
| MOPAC_AVG_POLARIZABILITY average polarizability  |           |
| MOPAC_POLARANISOTROPY polar anisotropy   |           |
| MOPAC-VIB_ENTHALPY vibrational ENTHALPY  |           |
| MOPAC-VIB_HEATCAP vibrational HEATCAP  |           |
| MOPAC_VIB_ENTROPY vibrational ENTROPY  |           |
| MOPAC_ROT_ENTHALPY rotational ENTHALPY   |           |
| MOPAC_ROT_HEATCAP rotational HEATCAP   |           |
| MOPAC_ROT_ENTROPY rotational ENTROPY   |           |
| MOPAC_TRANS_ENTHALPY translational ENTHALPY  |           |
| MOPAC_TRANS_HEATCAP translational HEATCAP  |           |
| MOPAC_TRANS_ENTROPY translational ENTROPY  |           |
| MOPAC_POL_ALPHA ALPHA polarizability   |           |
| MOPAC_POL_BETA BETA polarizability   |           |
| MOPAC_POL_GAMMA GAMMA polarizability   |           |
| CHG_MAXPOSCHG maximum positive charge  |           |
| CHG_MINNEGCHG maximum negative charge  |           |
| CHG_TOTABSCHG Total absolute charge  |           |
| CHG_TOTNEGCHG Total negative charge  |           |
| CHG_TOTPOSCHG Total positive charge  |           |
| CHG_TOTSQCHG total squared charge  |           |
| CHG_CHGPOL charge polarization   |           |
| CHG_LOCDIPOLEINDX local dipole index   |           |
| CHG_DP second-order submolecular polarity Parameter  |           |
| CHG_SPP submolecular polarity Parameter  |           |
| CHG_TEIATOMS topological electronic index for atoms  |           |
| CHG_TEIBONDS topological electronic index for bonds  |           |
| CHG_ECDCI Electronic charge density connectivity index   |           |
| GEOM_Wiener3D 3D Wiener index  |           |
| GEOM_RadGyration Radius of gyration  |           |
| GEOM_InertialSF inertial shape factor  |           |
| GEOM_MolEccentricity Molecular eccentricity  |           |
| GEOM_Asphericity Asphericity index   |           |
| GEOM.Spherosity Spherosity index   |           |
| GEOM.Globularity Globularity index   |           |
| GEOM_Ovality Ovality index   |           |
| GRAPH_GEIGGE_PROPERTY Graph energy from the weighted (charge,self-polarizability,delocalizability) adjacen | cy matrix |
| Radial Distribution Function 1 weighted by charge, self-polarizability, delocalizability                   |           |
| Radial Distribution Function 1.1 weighted by charge, self-polarizability, delocalizability                 |           |
| Radial Distribution Function 1.2 weighted by charge, self-polarizability, delocalizability                 |           |
| Radial Distribution Function 1.3 weighted by charge, self-polarizability, delocalizability                 |           |
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| Radial Distribution Function 1.5 weighted by charge, self-polarizability, delocalizability                 |           |
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| Radial Distribution Function 1.7 Weighted by charge, self-polarizability, delocalizability                 |           |
| Radial Distribution Function 1.8 Weighted by charge, self-polarizability, delocalizability                 |           |
| Radial Distribution Function 1.9 Weighted by charge, self-polarizability, delocalizability                 |           |
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| Radial Distribution Function 2.1 weighted by charge, self-polarizability, delocalizability                 |           |
| Radial Distribution Function 2.2 weighted by charge, self-polarizability, delocalizability                 |           |
| Padial Distribution Function 2.5 weighted by charge, self-polarizability, delocalizability                 |           |
| Padial Distribution Function 2.4 weighted by charge, self-polarizability, delocalizability                 |           |
| Padial Distribution Function 2.6 weighted by charge, self-polarizability, delocalizability                 |           |
| Radial Distribution Function 2.7 weighted by charge, self-polarizability, delocalizability                 |           |
| Radial Distribution Function 2.8 weighted by charge self-polarizability, delocalizability                  |           |
| Radial Distribution Function 2.9 weighted by charge self-polarizability delocalizability                   |           |
| Radial Distribution Function 3 weighted by charge self-polarizability delocalizability                     |           |
| Radial Distribution Function 3.1 weighted by charge, self-polarizability, delocalizability                 |           |

|                                  | Table S1 – Continued from previous page                   |
|----------------------------------|---|
| Name                             | Description   |
| Radial Distribution Function 3.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 3.3 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 3.4 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 3.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 3.0 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 3.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 3.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 4   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 4.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 4.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 4.3 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 4.4 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 4.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 4.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 4.7 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 4.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 4.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 5   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 5.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 5.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 5.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 5.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 5.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 5.7 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 5.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 5.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 6   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 6.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 6.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 6.3 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 6.4 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 6.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 6.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 6.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 6.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 7   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 7.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 7.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 7.3 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 7.4 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 7.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 7.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 7.7 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 7.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 7.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 8   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 8.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 8.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 8.4 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 8.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 8.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 8.7 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 8.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 8.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 9   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 9.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 9.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 9.3 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 9.4 | weighted by charge, self-polarizability, delocalizability |

|                                   | Table S1 – Continued from previous page                   |
|-----------------------------------|---|
| Name                              | Description   |
| Radial Distribution Function 9.5  | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 9.6  | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 9.7  | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 9.8  | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 9.9  | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 10   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 10.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 10.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 10.3 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 10.4 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 10.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 10.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 10.7 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 10.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 10.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 11   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 11.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 11.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 11.3 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 11.4 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 11.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 11.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 11.7 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 11.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 11.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 12   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 12.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 12.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 12.3 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 12.4 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 12.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 12.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 12.7 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 12.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 12.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 13   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 13.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 13.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 13.3 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 13.4 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 13.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 13.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 13.7 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 13.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 13.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 14   | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 14.1 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 14.2 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 14.3 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 14.4 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 14.5 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 14.6 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 14.7 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 14.8 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 14.9 | weighted by charge, self-polarizability, delocalizability |
| Radial Distribution Function 15   | weighted by charge, self-polarizability, delocalizability |

Table S2: Summary of the regression model performances for the refractive index (n), glass transition temperatures  $(T_g)$  and decomposition temperatures  $(T_d)$ . Here, NVAR is the number of variables used used in the model,  $N_{LV}$  the number of latent variables in the PLSR model, mtry the number of predictors sampled for splitting at each node in the RF model, MAE is the mean absolute error, RMSE is the root mean squared error and  $R^2$  the squared correlation between the observed and predicted values.

| <br>N/[]_]    |            |       | N. /          | Calibration |                 | Testing |                 |
|---------------|------------|-------|---------------|-------------|-----------------|---------|-----------------|
| Model         | Property   | INVAR | $N_{LV}/mtry$ | $R_{cv}^2$  | RMSE (MAE)      | $R^2$   | RMSE (MAE)      |
|               | n          | 61    | 4             | 0.79        | $0.04 \ (0.03)$ | 0.79    | $0.04 \ (0.03)$ |
| PLSR          | $T_q$ (°C) | 175   | 5             | 0.81        | 52(34)          | 0.83    | 49(38)          |
|               | $T_d$ (°C) | 218   | 4             | 0.61        | 49(24)          | 0.62    | 51 (41)         |
|               | n          | 5     | 3             | 0.83        | 0.03 (0.01)     | 0.88    | 0.03 (0.02)     |
| $\mathbf{RF}$ | $T_g$ (°C) | 16    | 4             | 0.86        | 44(14)          | 0.88    | 40 (30)         |
|               | $T_d$ (°C) | 11    | 4             | 0.80        | 35(12)          | 0.72    | 45(30)          |
|               | ho         | 7     | 3             | 0.64        | $0.13\ (0.04)$  | 0.66    | $0.14\ (0.08)$  |

| MONOMER   | $n^{exp}$ | $n_{PLSR}^{pred}$ | $n_{RF}^{pred}$ | Ref        |
|---|-----------|-------------------|-----------------|------------|
|   | 1.34      | $1.33 \pm 0.02$   | $1.36 \pm 0.04$ | [6, 14, 4] |
|   | 1.35      | $1.36 \pm 0.02$   | $1.37\pm0.03$   | [6, 14, 4] |
|   | 1.35      | $1.37 \pm 0.02$   | $1.36 \pm 0.03$ | [6, 14, 4] |
| $\mathbf{E} \qquad \mathbf{E}$                            | 1.35      | $1.44 \pm 0.05$   | $1.4 \pm 0.05$  | [6, 14, 4] |
|   |           |                   |                 |            |
|   |           |                   |                 |            |
| F F<br>SHLAZZ   | 1.36      | $1.36 \pm 0.02$   | $1.36 \pm 0.03$ | [6, 14, 4] |
|   | 1.36      | $1.38 \pm 0.01$   | $1.37\pm0.03$   | [6, 14, 4] |
|   | 1.36      | $1.39 \pm 0.02$   | $1.37\pm0.03$   | [6, 14, 4] |
| ° · · · · · · · · · · · · · · · · · · ·                   | 1.36      | $1.41 \pm 0.01$   | $1.39 \pm 0.05$ | [6, 14, 4] |
|   |           |                   |                 |            |
|   | 1.37      | $1.39 \pm 0.01$   | $1.37 \pm 0.03$ | [6, 14, 4] |
|   | 1.38      | $1.42 \pm 0.01$   | $1.39 \pm 0.04$ | [6, 14, 4] |
|   |           |                   |                 |            |
|   | 1.38      | $1.4 \pm 0.01$    | $1.38 \pm 0.03$ | [6, 14, 4] |
|   | 1.38      | $1.38 \pm 0.02$   | $1.39 \pm 0.03$ | [6, 14, 4] |
| F Sir o   |           |                   |                 |            |
|   | 1.39      | $1.4 \pm 0.01$    | $1.38\pm0.03$   | [6, 14, 4] |
|   | 1.39      | $1.38 \pm 0.02$   | $1.37 \pm 0.04$ | [6, 14, 4] |
| $\sim \lambda_{\circ} \sim \sim \chi_{r} t_{r}^{r}$       | 1.39      | $1.4 \pm 0.01$    | $1.4 \pm 0.03$  | [6, 14, 4] |
|   |           |                   |                 |            |
|   | 1.4       | $1.35 \pm 0.04$   | $1.43 \pm 0.06$ | [6, 14, 4] |
| Si  | 1.4       | $1.44 \pm 0.03$   | $1.42 \pm 0.05$ | [6, 14, 4] |
| Si  |           |                   |                 |            |
|   |           |                   |                 |            |
|   | 1.41      | $1.42 \pm 0.01$   | $1.41 \pm 0.04$ | [6, 14, 4] |
|   | 1.41      | $1.42 \pm 0.01$   | $1.41 \pm 0.03$ | [6, 14, 4] |
| ≫ <sup>Ĭ</sup> o~° <sub>F</sub> <sup>Í</sup> <sub>F</sub> | 1.40      | 1 45 1 0 0-       | 1 40 1 0 00     |            |
|   | 1.42      | $1.45 \pm 0.01$   | $1.42 \pm 0.03$ | [6, 14, 4] |
|   |           |                   |                 |            |

Table S3: The table lists the experimental and predicted ( $\pm$  uncertainty) refractive indices for different polymers. Predictions for both PLSR and RF models are reported.

| Table S3 – Continued from pr  | evious page      |                                       |                                   |             |
|---|------------------|---------------------------------------|-----------------------------------|-------------|
| MONOMER   | n <sup>exp</sup> | $\frac{n_{PLSR}^{prea}}{1.42 + 0.01}$ | $\frac{n_{RF}^{prea}}{1.41+0.02}$ | Ref         |
| S <sup>0</sup> <sub>µ</sub> <sub>0</sub> ∼ <sup>p</sup> <sup>F</sup> <sub>F</sub> | 1.42             | $1.42 \pm 0.01$                       | $1.41 \pm 0.03$                   | [6, 14, 4]  |
| N F   | 1.42             | 1.40 ± 0.02                           | 1.40 ± 0.07                       | [0, 14, 4]  |
|   |                  |                                       |                                   |             |
|   |                  |                                       |                                   |             |
| Ē   |                  |                                       |                                   |             |
|   | 1.43             | $1.44\pm0.05$                         | $1.46\pm0.06$                     | [6, 14, 4]  |
|   |                  |                                       |                                   |             |
|   |                  |                                       |                                   |             |
|   |                  |                                       |                                   |             |
|   | 1.44             | $1.44 \pm 0.01$                       | $1.42 \pm 0.03$                   | [6, 14, 4]  |
|   |                  |                                       |                                   | ., , ,      |
| Υ F   |                  |                                       |                                   |             |
| 0   | 1.44             | $1.46\pm0.02$                         | $1.45\pm0.03$                     | [6, 14, 4]  |
| Si o  |                  |                                       |                                   |             |
| ······································  | 1.44             | $1.47 \pm 0.02$                       | $1.46 \pm 0.03$                   | [6, 14, 4]  |
|   | 1.45             | $1.5 \pm 0.02$                        | $1.48 \pm 0.03$                   | [6, 14, 4]  |
|   | 1.45             | $1.42\pm0.02$                         | $1.46 \pm 0.03$                   | [6, 14, 4]  |
|   |                  |                                       |                                   |             |
| $\mathbf{}$   |                  |                                       |                                   |             |
|   | 1.45             | $1.5\pm0.01$                          | $1.46 \pm 0.03$                   | [6, 14, 4]  |
| $\mathbb{N}^{0}$  |                  |                                       |                                   |             |
|   | 1.45             | $1.45\pm0.02$                         | $1.46\pm0.03$                     | [6, 14, 4]  |
|   | 1.45             | $1.49 \pm 0.01$                       | $1.46 \pm 0.03$                   | [6, 14, 4]  |
|   | 1.46             | $1.46 \pm 0.02$                       | $1.46 \pm 0.03$                   | [6, 14, 4]  |
| ~~~~~ <sup>s</sup> o  | 1.46             | $1.41 \pm 0.03$                       | $1.46 \pm 0.04$                   | [6, 14, 4]  |
| $\sim$ 0  |                  |                                       |                                   | [0,, -]     |
|   | 1.46             | $1.48 \pm 0.01$                       | $1.46 \pm 0.02$                   | [6 14 4]    |
| <b>√√</b>   | 1.40             | 1.40 ± 0.01                           | 1.40 ± 0.02                       | [0, 14, 4]  |
|   | 1.40             | $1.44 \pm 0.01$                       | $1.47 \pm 0.03$                   | [0, 14, 4]  |
| × • • • • • • • • • • • • • • • • • • •   | 1.46             | $1.43\pm0.01$                         | $1.47 \pm 0.03$                   | [6, 14, 4]  |
|   | 1.46             | $1.48 \pm 0.01$                       | $1.46 \pm 0.02$                   | [6, 14, 4]  |
|   | 1.46             | $1.48 \pm 0.01$                       | $1.46 \pm 0.02$                   | [6, 14, 4]  |
|   | 1.46             | $1.5 \pm 0.02$                        | $1.52 \pm 0.09$                   | [6, 14, 4]  |
| F V   |                  |                                       |                                   |             |
|   |                  |                                       |                                   |             |
|   |                  |                                       |                                   |             |
|   | 1.46             | $1.48\pm0.01$                         | $1.46\pm0.02$                     | [6, 14, 4]  |
|   | 1.46             | $1.53 \pm 0.01$                       | $1.46\pm0.02$                     | [6, 14, 4]  |
|   |                  |                                       |                                   |             |
|   | 1.46             | $1.49 \pm 0.01$                       | $1.47 \pm 0.03$                   | [6, 14, 4]  |
| <u> </u>  | 1.46             | $1.42 \pm 0.02$                       | 1.41 ± 0.04                       | [0, 14, 4]  |
| $\sim$  |                  |                                       |                                   |             |
|   | 1.46             | $1.49\pm0.01$                         | $1.48 \pm 0.03$                   | [6, 14, 4]  |
| $\mathcal{O} \to \mathcal{A}$   |                  |                                       |                                   |             |
|   | 1.46             | $1.44\pm0.02$                         | $1.45\pm0.05$                     | [6, 14, 4]  |
|   |                  |                                       |                                   |             |
| ö   | 1.46             | $1.53 \pm 0.01$                       | $1.51 \pm 0.04$                   | [6, 14, 4]  |
|   |                  |                                       |                                   |             |
| $\sim$  |                  |                                       |                                   |             |
|   | 1.46             | $1.49 \pm 0.01$                       | $1.48\pm0.03$                     | [6, 14, 4]  |
| · · · · · · · · · · · · · · · · · · ·   |                  |                                       | Continued or                      | i next page |

|  | Table S3 – Continued from previous page |                  |   | ,                                  |                          |
|--|---|------------------|---|------------------------------------|--------------------------|
| MONOMER                                |   | n <sup>exp</sup> | $\frac{n_{PLSR}^{pred}}{1.50 \pm 0.00}$ | $\frac{n_{RF}^{prea}}{1.49}$       | Ref                      |
|  |   | 1.47             | $1.52 \pm 0.02$                         | $1.48 \pm 0.03$                    | [0, 14, 4]               |
| $\wedge$                               |   |                  |   |                                    |                          |
|  |   | 1.47             | $1.48\pm0.04$                           | $1.48 \pm 0.02$                    | [6, 14, 4]               |
| $\sim \sim ~ $                         |   |                  |   |                                    |                          |
| <b>~~~</b> ⁰ <b>√</b> <                |   | 1.47             | $1.49 \pm 0.01$                         | $1.47 \pm 0.03$                    | [6, 14, 4]               |
|  |   | 1 47             | $1.5 \pm 0.01$                          | $1.47 \pm 0.03$                    | [6 14 4]                 |
| ∕ <mark>√</mark> ⁰ ∕∕                  |   | 1.47             | 1.5 ± 0.01                              | 1.47 ± 0.05                        | [0, 14, 4]               |
|  |   |                  |   |                                    |                          |
| 0                                      |   | 1.47             | $1.49 \pm 0.01$                         | $1.47 \pm 0.03$                    | [6, 14, 4]               |
|  |   |                  |   |                                    |                          |
|  |   | 1.47             | 15 001                                  | 1 47 1 0 00                        | [0 14 4]                 |
| 0.//                                   |   | 1.47             | $1.5 \pm 0.01$                          | $1.47 \pm 0.02$                    | [6, 14, 4]               |
|  |   | 1.47             | $1.5 \pm 0.01$                          | $1.48 \pm 0.04$                    | [6, 14, 4]               |
| $\sim^{\circ}$                         |   |                  |   |                                    | ., , ,                   |
| 0                                      |   | 1 47             | 1 42 . 0.00                             | 1.46 . 0.02                        | [6 14 4]                 |
| ~~~~ <sub>0</sub>                      |   | 1.47             | $1.43 \pm 0.02$<br>$1.49 \pm 0.02$      | $1.40 \pm 0.02$<br>$1.49 \pm 0.03$ | [0, 14, 4]<br>[6, 14, 4] |
|  |   | 1.47             | $1.48 \pm 0.02$                         | $1.47 \pm 0.02$                    | [6, 14, 4]               |
| , , , μ <sup>ο</sup>                   |   | a 7=             | 1                                       | 1 45 1 0 01                        | [0 14 ···                |
| ∕₀∼⁰γ∕∾                                |   | 1.47             | $1.5 \pm 0.01$                          | $1.47 \pm 0.01$                    | [6, 14, 4]               |
|  |   | 1.47             | $1.49 \pm 0.02$                         | $1.47 \pm 0.01$                    | [6, 14, 4]               |
|  |   | 1.47             | $1.51\pm0.02$                           | $1.49 \pm 0.03$                    | [6, 14, 4]               |
|  |   |                  |   |                                    |                          |
| $\sim$                                 |   | 1.47             | $1.53 \pm 0.01$                         | $1.49 \pm 0.06$                    | [6, 14, 4]               |
| $\sim$                                 |   |                  |   |                                    |                          |
| A .                                    |   | 1.47             | $1.5 \pm 0.01$                          | $1.48 \pm 0.02$                    | [6, 14, 4]               |
| ~~~~~ <sup>j</sup> r                   |   |                  | 1 45 1 0 01                             | 1 44 1 0 05                        | [0 14 4]                 |
| ₀∼⁰┰∽∞₀                                |   | 1.47             | $1.45 \pm 0.01$                         | $1.44 \pm 0.05$                    | [0, 14, 4]               |
| 0                                      |   | 1.47             | $1.5\pm0.01$                            | $1.48\pm0.02$                      | [6, 14, 4]               |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ |   | 1.48             | $1.54 \pm 0.02$                         | $1.49 \pm 0.03$                    | [6, 14, 4]               |
|  |   | 1.48             | $1.52 \pm 0.01$                         | $1.51 \pm 0.03$                    | [6, 14, 4]               |
| N ~ ~ ~ H ~ ~ ~                        |   | 1.48             | $1.5 \pm 0.02$                          | $1.47 \pm 0.03$                    | [6, 14, 4]               |
| ~~~~.Å                                 |   | 1.48             | $1.44 \pm 0.01$                         | $1.47 \pm 0.04$                    | [6, 14, 4]               |
|  |   |                  | ±                                       |                                    | [0,, -]                  |
|  |   |                  |   |                                    |                          |
|  |   |                  |   |                                    |                          |
|  |   | 1.48             | $1.49\pm0.02$                           | $1.47\pm0.03$                      | [6, 14, 4]               |
|  |   | 1.48             | $1.48 \pm 0.04$                         | $1.51 \pm 0.04$                    | [6, 14, 4]               |
|  |   | 1.48             | $1.49 \pm 0.02$                         | $1.48 \pm 0.04$                    | [6, 14, 4]               |
| $\sim^{\circ}$                         |   |                  |   |                                    | [0,, -]                  |
|  |   |                  |   |                                    |                          |
| 0                                      |   | 1.48             | $1.49\pm0.01$                           | $1.46 \pm 0.04$                    | [6, 14, 4]               |
|  |   |                  |   |                                    |                          |
|  |   | 1                | 1 50 1 0 0.                             |                                    | [0 1 · · ·]              |
|  |   | 1.48             | $1.52 \pm 0.01$                         | $1.5 \pm 0.03$                     | [6, 14, 4]               |
| $\sim$                                 |   |                  |   |                                    |                          |
| 0                                      |   | 1.48             | $1.46\pm0.02$                           | $1.47\pm0.03$                      | [6, 14, 4]               |
|  |   |                  |   |                                    | -                        |
|  |   |                  |   |                                    |                          |
|  |   | 1 40             | 1.95 - 0.02                             | 1.46 - 0.04                        | [6 14 4]                 |
| -0                                     |   | 1.48             | $1.35 \pm 0.06$                         | $1.40 \pm 0.04$                    | [0, 14, 4]               |
|  |   |                  |   | Continued o                        | n next page              |

| Table S3 - Contin   | nued from previous page | pred                             | pred                           | Pof         |
|---|-------------------------|----------------------------------|--------------------------------|-------------|
| II  | 1.48                    | $\frac{"_{PLSR}}{1.52 \pm 0.01}$ | $\frac{n_{RF}}{1.49 \pm 0.02}$ | [6, 14, 4]  |
|   |                         |                                  |                                |             |
| - 0<br>~~~°n  | 1.48                    | $1.5\pm0.01$                     | $1.49\pm0.02$                  | [6, 14, 4]  |
| $\sim$  | 1.48                    | $1.49 \pm 0.01$                  | $1.5 \pm 0.02$                 | [6, 14, 4]  |
| ة<br>لمروح م  | 1.48                    | $1.5\pm0.06$                     | $1.49\pm0.03$                  | [6, 14, 4]  |
|   | 1.48                    | $1.51\pm0.01$                    | $1.48 \pm 0.02$                | [6, 14, 4]  |
|   | 1.48                    | $1.5\pm0.01$                     | $1.49\pm0.03$                  | [6, 14, 4]  |
|   | 1.48                    | $1.47\pm0.02$                    | $1.48 \pm 0.05$                | [6, 14, 4]  |
| $\sim$ $\gamma$ $\sim$   | 1 49                    | $1.51 \pm 0.01$                  | $1.5 \pm 0.03$                 | [6 14 4]    |
| ∼° <mark>∥</mark>   |                         | 101 ± 0101                       | 110 1 0100                     | [0, 11, 1]  |
| 0<br>~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   | 1.49                    | $1.46 \pm 0.02$                  | $1.48 \pm 0.02$                | [6, 14, 4]  |
|   | 1.49                    | $153 \pm 0.01$                   | $1.5 \pm 0.03$                 | [6 14 4]    |
| $\sim$  | 1.43                    | 1.55 ± 0.01                      | 1.5 ± 0.05                     | [0, 14, 4]  |
|   | 1.49                    | $1.53\pm0.01$                    | $1.5 \pm 0.03$                 | [6, 14, 4]  |
| $\prod_{n=0}^{n} \sqrt{n} < 0$  | 1.49                    | $1.51 \pm 0.01$                  | $1.5 \pm 0.03$                 | [6, 14, 4]  |
| $\rightarrow$   |                         |                                  |                                |             |
|   | 1.49                    | $1.44 \pm 0.01$                  | $1.45 \pm 0.04$                | [6, 14, 4]  |
|   | 1.49                    | $1.52\pm0.01$                    | $1.5 \pm 0.02$                 | [6, 14, 4]  |
| Ϋ́Ϋ́Ϋ́Υ, Ϋ́Ϋ́Υ, Ϋ́Υ`, Υ`, Ϋ́Υ`, Υ`, Ϋ́Υ`, Υ`, Υ`, Υ`, Υ`, Υ`, Υ`, Υ`, Υ`, Υ`, | 1.5                     | $1.53\pm0.01$                    | $1.49 \pm 0.02$                | [6, 14, 4]  |
| $\sim$ , $\beta$ , $\beta$  | 1.5                     | $1.47 \pm 0.02$                  | $1.45 \pm 0.04$                | [6, 14, 4]  |
|   |                         |                                  |                                | . , , ,     |
|   | 1.5                     | $1.51 \pm 0.01$                  | $1.5\pm0.02$                   | [6, 14, 4]  |
|   | 1.5                     | $1.46\pm0.03$                    | $1.49\pm0.03$                  | [6, 14, 4]  |
|   | 1.5                     | $1.54\pm0.02$                    | $1.5 \pm 0.03$                 | [6, 14, 4]  |
| $\sum_{n} = C =$  | 1.5                     | $1.52\pm0.01$                    | $1.52 \pm 0.03$                | [6, 14, 4]  |
| ۵ <sup>۲</sup> ۳ <sup>۲</sup>   |                         |                                  |                                |             |
|   |                         |                                  | Continued or                   | n next page |

|                           | Table S3 – Continued from previous page | and d                                   |                                       |                          |
|---------------------------|---|---|---------------------------------------|--------------------------|
| MONOMER                   | n <sup>ea</sup>                         | $\frac{p}{2} n \frac{pred}{PLSR}$       | $\frac{n_{RF}^{pred}}{1.48 \pm 0.02}$ | Ref                      |
|                           | 1.                                      | $5 1.40 \pm 0.02$                       | $1.40 \pm 0.03$                       | [0, 14, 4]               |
| 0                         | 1.                                      | 5 $1.51 \pm 0.01$                       | $1.5 \pm 0.03$                        | [6, 14, 4]               |
|                           | 1.                                      | $5 	1.5 \pm 0.02$<br>$5 	1.55 \pm 0.01$ | $1.48 \pm 0.03$<br>$1.52 \pm 0.07$    | [6, 14, 4]<br>[6, 14, 4] |
| F<br>F                    |   | 2                                       |                                       | [*,, -]                  |
|                           | 1.                                      | 5 $1.51 \pm 0.01$                       | $1.51 \pm 0.02$                       | [6, 14, 4]               |
|                           | 1.                                      | 5 $1.53 \pm 0.01$                       | $1.49 \pm 0.02$                       | [6, 14, 4]               |
|                           | 1.                                      | $5 	1.56 \pm 0.02$                      | $1.5 \pm 0.04$                        | [6, 14, 4]               |
|                           | 1.5                                     | $1 153 \pm 0.01$                        | $151 \pm 0.03$                        | [6 14 4]                 |
| Je m Je                   |   | 1 150 4 0.01                            | 151 - 0.00                            |                          |
| <sup>⊥</sup> <sup>™</sup> | 1.3                                     | 1 1.52 ± 0.01                           | $1.51 \pm 0.02$                       | [0, 14, 4]               |
|                           | 1.5                                     | 1 $1.51 \pm 0.01$                       | $1.49\pm0.03$                         | [6, 14, 4]               |
| $\mathcal{L}$             | 1.5                                     | 1 $1.53 \pm 0.01$                       | $1.52 \pm 0.03$                       | [6, 14, 4]               |
|                           | 1.5                                     | 1 $1.5 \pm 0.01$                        | $1.48\pm0.03$                         | [6, 14, 4]               |
|                           | 1.5                                     | 1 $1.5 \pm 0.02$                        | $1.5\pm0.03$                          | [6, 14, 4]               |
| ×° ↓↓                     | 1.5                                     | 1 $1.54 \pm 0.01$                       | $1.54 \pm 0.04$                       | [6, 14, 4]               |
|                           | 1.5                                     | 1 $1.49 \pm 0.01$                       | $1.52\pm0.03$                         | [6, 14, 4]               |
| ö<br>∽∽~∾y↓               | 1.5                                     | $1  1.54 \pm 0.01$                      | $1.52\pm0.03$                         | [6, 14, 4]               |
|                           | 1.5                                     | 2 $1.51 \pm 0.01$                       | $1.5 \pm 0.03$                        | [6, 14, 4]               |
|                           | 1.5                                     | $2 1.52 \pm 0.01$                       | $1.51 \pm 0.03$                       | [6, 14, 4]               |
|                           | 1.5                                     | $2 1.55 \pm 0.01$                       | $1.57\pm0.04$                         | [6, 14, 4]               |
|                           |   |   |                                       | -                        |
| `                         |   |   | Continued of                          | n next page              |

| Table S3 – Continued from previous page |                  |                                    |                                    |                          |
|---|------------------|------------------------------------|------------------------------------|--------------------------|
| MONOMER                                 | n <sup>exp</sup> | $n_{PLSR}^{pred}$                  | $n_{RF}^{pred}$                    | Ref                      |
|   | 1.02             | $1.03 \pm 0.01$                    | 1.40 ± 0.04                        | [0, 14, 4]               |
|   | 1.52             | $1.52 \pm 0.01$                    | $1.52 \pm 0.02$                    | [6, 14, 4]               |
|   | 1.52             | $1.52 \pm 0.02$                    | $1.51 \pm 0.03$                    | [6, 14, 4]               |
|   | 1.52             | $1.57 \pm 0.02$                    | $1.52 \pm 0.03$                    | [6, 14, 4]               |
|   | 1.52             | $1.55\pm0.01$                      | $1.52\pm0.03$                      | [6, 14, 4]               |
|   | 1.52             | $1.56 \pm 0.02$                    | $1.57 \pm 0.07$                    | [6, 14, 4]               |
|   | 1.52             | $1.58 \pm 0.02$                    | $1.55 \pm 0.06$                    | [6, 14, 4]               |
|   | 1.52             | $1.53 \pm 0.01$                    | $1.53 \pm 0.03$                    | [6, 14, 4]               |
|   | 1.53             | $1.49 \pm 0.01$                    | $1.5 \pm 0.04$                     | [6, 14, 4]               |
|   | 1.53             | $1.52 \pm 0.01$                    | $1.51\pm0.03$                      | [6, 14, 4]               |
|   | 1.53             | $1.53\pm0.02$                      | $1.51 \pm 0.04$                    | [6, 14, 4]               |
|   | 1.53             | $1.51\pm0.02$                      | $1.52\pm0.03$                      | [6, 14, 4]               |
|   | 1.53             | $1.55 \pm 0.01$                    | $1.55 \pm 0.04$                    | [6, 14, 4]               |
|   | 1.53             | $1.5 \pm 0.01$                     | $1.48 \pm 0.03$                    | [6, 14, 4]               |
|   | 1 59             | $1.47 \pm 0.01$                    | 1 51 ± 0.02                        | [6 14 4]                 |
|   | 1.53             | $1.47 \pm 0.01$<br>$1.46 \pm 0.02$ | $1.31 \pm 0.03$<br>$1.49 \pm 0.02$ | [0, 14, 4]<br>[6, 14, 4] |
| ال<br>۱۱                                | 1.53<br>1.53     | $1.51 \pm 0.01$<br>$1.53 \pm 0.01$ | $1.51 \pm 0.03$<br>$1.52 \pm 0.02$ | [6, 14, 4]<br>[6, 14, 4] |
|   | 1.53             | $1.5 \pm 0.01$                     | $1.52 \pm 0.02$                    | [6, 14, 4]               |
|   | 1.54             | $1.53 \pm 0.01$                    | $1.53 \pm 0.03$                    | [6, 14, 4]               |
|   |                  |                                    |                                    |                          |

| MONOMER   | Table S3 – Continued from $\gamma$ | n <sup>exp</sup> | n <sup>pred</sup>                | npred                          | Ref            |
|---|------------------------------------|------------------|----------------------------------|--------------------------------|----------------|
| 0   |                                    | 1.54             | $\frac{n_{PLSR}}{1.53 \pm 0.01}$ | $\frac{R_{RF}}{1.57 \pm 0.03}$ | [6, 14, 4]     |
| $\sim$  |                                    |                  |                                  |                                |                |
|   |                                    | 1.54             | $1.49 \pm 0.02$                  | $1.52 \pm 0.04$                | [6, 14, 4]     |
|   |                                    |                  |                                  |                                |                |
|   |                                    | 1.54             | $1.59 \pm 0.01$                  | $1.57 \pm 0.03$                | [6, 14, 4]     |
| o- <del>√</del>   |                                    |                  |                                  |                                |                |
|   |                                    |                  |                                  |                                |                |
| N //  |                                    | 1.54             | $1.55 \pm 0.01$                  | $1.53 \pm 0.02$                | [6, 14, 4]     |
| >— </td <td></td> <td></td> <td></td> <td></td> <td></td> |                                    |                  |                                  |                                |                |
| 0 N   |                                    | 1 54             | 1 55   0.01                      | 1 52   0.02                    | [C 14 4        |
|   |                                    | 1.54             | $1.55 \pm 0.01$                  | $1.52 \pm 0.02$                | [0, 14, 4      |
| Ϋ́ΎΎΎΎΎΎΎΎΎΎΎΎΎΎΎΎΎΎ                                      |                                    |                  |                                  |                                | To             |
|   |                                    | 1.54             | $1.55 \pm 0.01$                  | $1.53 \pm 0.02$                | [6, 14, 4]     |
| Ϊ ( )   |                                    |                  |                                  |                                |                |
|   |                                    | 1.54             | $1.53 \pm 0.01$                  | $1.51\pm0.03$                  | [6, 14, 4]     |
| <sup>™</sup> <sup>™</sup> <sup>™</sup> <sup>™</sup>       |                                    |                  |                                  |                                |                |
| U II  |                                    | 1.55             | $1.55 \pm 0.01$                  | $1.54 \pm 0.03$                | [6, 14, 4]     |
| $\sim \sqrt{1}$   |                                    |                  |                                  |                                |                |
| 0   |                                    | 1.55             | $1.55 \pm 0.01$                  | $1.56 \pm 0.03$                | [6, 14, 4]     |
|   |                                    |                  |                                  |                                |                |
|   |                                    | 1.55             | $1.57 \pm 0.01$                  | $1.57 \pm 0.03$                | [6, 14, 4]     |
| $\sim $   |                                    |                  |                                  |                                |                |
| - <u></u>   |                                    | 1 55             | $1.51 \pm 0.01$                  | $15 \pm 0.04$                  | [6 14 <i>4</i> |
|   |                                    | 1.00             | 1.01 ± 0.01                      | 1.0 ± 0.04                     | [0, 14, 4      |
| <b>○</b> _/   |                                    |                  | 1 50 1 0 01                      | 1 50 1 0 00                    | 6 14           |
| 0   |                                    | 1.55             | $1.52 \pm 0.01$                  | $1.53 \pm 0.03$                | [0, 14, 4      |
| $\Upsilon$  |                                    |                  |                                  |                                |                |
|   |                                    | 1.55             | $1.55 \pm 0.01$                  | $1.57 \pm 0.03$                | [6, 14, 4]     |
| Q   |                                    |                  |                                  |                                |                |
|   |                                    | 1.55             | $1.58\pm0.02$                    | $1.57\pm0.03$                  | [6, 14, 4]     |
| -0-   |                                    | 1.50             | 1 50 1 0 01                      | 1 55 1 0 00                    | [0.14.         |
|   |                                    | 1.50             | $1.50 \pm 0.01$                  | $1.57 \pm 0.03$                | [0, 14, 4      |
|   |                                    |                  |                                  |                                |                |
| ,0<br>,0  |                                    | 1.56             | $1.54\pm0.01$                    | $1.57\pm0.03$                  | [6, 14, 4]     |
| °-O-C   |                                    | 1.50             | 1 50 1 0 00                      |                                | [0.14          |
| CI  |                                    | 1.56             | $1.56 \pm 0.02$                  | $1.57 \pm 0.06$                | [6, 14, 4      |
|   |                                    |                  |                                  |                                |                |
| $\sim$ $\sim$   |                                    | 1.56             | $1.53 \pm 0.01$                  | $1.57\pm0.03$                  | [6, 14, 4]     |
| ¥°∽∕∩   |                                    |                  |                                  |                                |                |
|   |                                    | 1.56             | $1.56 \pm 0.01$                  | $1.58\pm0.03$                  | [6, 14, 4]     |
| ↓↓ <mark>↓</mark> ↓                                       |                                    |                  |                                  |                                |                |
| · •   |                                    |                  |                                  |                                |                |

|   | Table S3 – Continued from previous page | nnod                                    | mod                                   |             |
|---|---|---|---------------------------------------|-------------|
| MONOMER   | $n^{exp}$                               | $\frac{n_{PLSR}^{prea}}{1.58 \pm 0.01}$ | $\frac{n_{RF}^{prea}}{1.56 \pm 0.03}$ | Ref         |
| -<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>- | 1.00                                    | 1.58 ± 0.01                             | 1.50 ± 0.05                           | [0, 14, 4]  |
|   | 1.57                                    | $1.58 \pm 0.01$                         | $1.57 \pm 0.02$                       | [6, 14, 4]  |
|   | 1.57                                    | $1.54 \pm 0.01$                         | $1.52 \pm 0.03$                       | [6, 14, 4]  |
| O Br  | 1.57                                    | $1.53 \pm 0.01$                         | $1.57 \pm 0.03$                       | [6, 14, 4]  |
|   | 1.57                                    | $1.57 \pm 0.06$                         | $1.55 \pm 0.05$                       | [6, 14, 4]  |
| D.L   | 1.57                                    | $1.55 \pm 0.01$                         | $1.57 \pm 0.02$                       | [6, 14, 4]  |
|   | 1.57                                    | $1.57 \pm 0.01$                         | $1.57 \pm 0.02$                       | [6, 14, 4]  |
|   | 1.57                                    | $1.55 \pm 0.01$                         | $1.57 \pm 0.02$                       | [6, 14, 4]  |
|   | 1.57                                    | $1.55 \pm 0.01$                         | $1.57 \pm 0.02$                       | [6, 14, 4]  |
| "<br>"  | 1.57                                    | $1.54 \pm 0.01$                         | $1.57\pm0.04$                         | [6, 14, 4]  |
|   | 1.57                                    | $1.52 \pm 0.01$                         | $1.51 \pm 0.03$                       | [6, 14, 4]  |
|   | 1.57                                    | $1.54 \pm 0.02$                         | $1.56 \pm 0.06$                       | [6, 14, 4]  |
| °°<br>>   | 1.57                                    | $1.58 \pm 0.02$                         | $1.58 \pm 0.06$                       | [6, 14, 4]  |
| $\rightarrow \bigcirc$  | 1.58                                    | $1.55 \pm 0.01$                         | $1.58 \pm 0.02$                       | [6, 14, 4]  |
| ∕~° <sup>⊥</sup> O  | 1.50                                    | 1 50 4 0 01                             | 1 52 4 0 00                           |             |
|   | 1.58                                    | 1.09 ± 0.01                             | $1.58 \pm 0.02$                       | [0, 14, 4]  |
| $\sim$  | 1.58                                    | $1.54 \pm 0.01$                         | $1.58\pm0.03$                         | [6, 14, 4]  |
| ↓<br>↓<br>↓<br>↓<br>↓<br>↓  | 1.58                                    | $1.55 \pm 0.01$                         | $1.56 \pm 0.04$                       | [6, 14, 4]  |
|   |   |   | Continued o                           | n next page |

|              | Table S3 – Continued from previous page |                                    |                                     |                          |
|--------------|---|------------------------------------|-------------------------------------|--------------------------|
| MONOMER      | n <sup>exp</sup>                        | $\frac{n_{PLSR}^{pred}}{1.50}$     | $\frac{n_{RF}^{pred}}{1.50 + 0.02}$ | Ref                      |
|              | 1.59                                    | $1.56 \pm 0.01$<br>$1.57 \pm 0.01$ | $1.58 \pm 0.03$<br>$1.6 \pm 0.03$   | [0, 14, 4]<br>[6, 14, 4] |
| °-\$\        | 1.50                                    | 1.6 ± 0.02                         | 1 50 ± 0.02                         | [6 14 4]                 |
|              | 1.59                                    | 1.0 ± 0.02                         | 1.59 ± 0.05                         | [0, 14, 4]               |
|              | 1.59                                    | $1.6 \pm 0.02$                     | $1.6\pm0.03$                        | [6, 14, 4]               |
|              | 1.59                                    | $1.6 \pm 0.01$                     | $1.59 \pm 0.04$                     | [6, 14, 4]               |
|              | 1.59                                    | $1.59 \pm 0.02$                    | $1.58 \pm 0.05$                     | [6, 14, 4]               |
|              |   |                                    |                                     |                          |
|              | 1.6                                     | $1.61 \pm 0.02$                    | $1.57\pm0.07$                       | [6, 14, 4]               |
| S<br>X       | 1.6                                     | $1.58 \pm 0.01$                    | $1.57 \pm 0.02$                     | [6, 14, 4]               |
|              | 1.6                                     | $1.57\pm0.01$                      | $1.57\pm0.03$                       | [6, 14, 4]               |
|              | 1.6                                     | $1.57 \pm 0.01$                    | $1.6\pm0.03$                        | [6, 14, 4]               |
| Š, ČI        | 1.6                                     | $1.53 \pm 0.03$                    | $1.57 \pm 0.05$                     | [6, 14, 4]               |
| CI<br>↓ 。↓ 。 | 1.61                                    | $1.56 \pm 0.01$                    | $1.59\pm0.04$                       | [6, 14, 4]               |
|              | 1.61                                    | $1.59 \pm 0.02$                    | $1.6 \pm 0.03$                      | [6, 14, 4]               |
|              |   |                                    |                                     |                          |
|              | 1.61                                    | $1.56 \pm 0.01$                    | $1.59 \pm 0.03$                     | [6, 14, 4]               |
|              | 1.61                                    | $1.61 \pm 0.02$                    | $1.62\pm0.02$                       | [6, 14, 4]               |
|              | 1.62                                    | $1.59 \pm 0.02$                    | $1.62\pm0.04$                       | [6, 14, 4]               |
|              |   |                                    | Continued or                        | n next page              |

| Table S3 – Continued j                 | rom previous page      |   |                                       |                          |
|--|------------------------|---|---------------------------------------|--------------------------|
| MONOMER                                | $\frac{n^{exp}}{1.62}$ | $\frac{n_{PLSR}^{pred}}{1.58 \pm 0.02}$ | $\frac{n_{RF}^{pred}}{1.61 \pm 0.03}$ | Ref                      |
|  | 1.02                   | 1.55 ± 0.02                             | 7.01 <u>-</u> 0.03                    | [0, 14, 4]               |
|  | 1.63                   | $1.56 \pm 0.02$                         | $1.59\pm0.06$                         | [6, 14, 4]               |
| JOI                                    | 1.63                   | $1.58 \pm 0.01$                         | $1.62 \pm 0.03$                       | [6, 14, 4]               |
| , OO                                   | 1.63                   | $1.58 \pm 0.01$                         | $1.62 \pm 0.04$                       | [6, 14, 4]               |
| $\gamma^{i} \sim O$                    |                        |   |                                       | [*,, -]                  |
|  | 1.63                   | $1.66 \pm 0.06$<br>$1.65 \pm 0.02$      | $1.62 \pm 0.03$<br>$1.62 \pm 0.03$    | [6, 14, 4]<br>[6, 14, 4] |
|  |                        |   |                                       | [*,, -]                  |
|  | 1.64                   | $1.58 \pm 0.01$                         | $1.63 \pm 0.03$                       | [6, 14, 4]               |
|  | 1.66                   | $1.7\pm0.02$                            | $1.65 \pm 0.02$                       | [6, 14, 4]               |
|  | 1.67                   | $1.55 \pm 0.02$                         | $1.6 \pm 0.07$                        | [6, 14, 4]               |
|  | 1.68                   | $1.63 \pm 0.02$                         | $1.67 \pm 0.02$                       | [6, 14, 4]               |
|  | 1.68                   | $1.65 \pm 0.01$                         | $1.67 \pm 0.02$                       | [6, 14, 4]               |
|  |                        |   |                                       |                          |
|  | 1.71                   | $1.62 \pm 0.01$                         | $1.6 \pm 0.05$                        | [6, 14, 4]               |
|  | 1 61                   | $1.61 \pm 0.02$                         | $1.63 \pm 0.03$                       | [60]                     |
|  | 1.63                   | $1.59 \pm 0.02$                         | $1.61 \pm 0.03$                       | [60]                     |
|  | 1.65                   | $1.67 \pm 0.05$                         | $1.65 \pm 0.02$                       | [60]                     |
| ·~~·~;~<br>•^@\$@,                     | 1.68                   | $1.65 \pm 0.01$                         | $1.68 \pm 0.02$                       | [45]                     |
|  | 1.7                    | $1.66 \pm 0.01$                         | $1.68 \pm 0.02$                       | [45]                     |
|  | 1.68                   | $1.67 \pm 0.02$                         | $1.68 \pm 0.01$                       | [45]                     |
|  | 1.68                   | $1.68 \pm 0.01$                         | $1.68 \pm 0.01$                       | [45]                     |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ | 1.68                   | $1.7\pm0.02$                            | $1.67\pm0.02$                         | [45]                     |
|  |                        |   |                                       |                          |

| Table S3 – Continued from  | n previous page        | nred                                    | nred                                  |      |
|--|------------------------|---|---------------------------------------|------|
| MONOMER  | $\frac{n^{exp}}{1.49}$ | $\frac{n_{PLSR}^{preu}}{1.55 \pm 0.01}$ | $\frac{n_{RF}^{preu}}{1.56 \pm 0.02}$ | [29] |
| $\sim \sim $  | 1.43                   | 1.55 ± 0.01                             | 1.50 ± 0.02                           | [23] |
|  | 1.51                   | $1.52 \pm 0.01$                         | $1.51 \pm 0.03$                       | [29] |
|  | 1.51                   | $1.54 \pm 0.01$                         | $1.57\pm0.03$                         | [29] |
|  | 1.69                   | $1.64 \pm 0.06$                         | $1.64 \pm 0.02$                       | [42] |
|  | 1.6                    | $1.75 \pm 0.03$                         | $1.67\pm0.02$                         | [46] |
|  | 1.65                   | $1.69 \pm 0.09$                         | $1.64 \pm 0.05$                       | [46] |
|  | 1.64                   | $1.6\pm0.02$                            | $1.63 \pm 0.03$                       | [46] |
|  |                        |   |                                       |      |
|  | 1.64                   | $1.61 \pm 0.01$                         | $1.63\pm0.02$                         | [46] |
|  |                        |   |                                       |      |
| ~. <del></del> .   | 1.66                   | $1.64 \pm 0.02$                         | $1.66 \pm 0.02$                       | [46] |
|  | 1.64                   | $1.64 \pm 0.01$                         | $1.65 \pm 0.04$                       | [46] |
| Q2k  | 1.65                   | $1.64 \pm 0.01$                         | $1.65\pm0.03$                         | [46] |
| ~~~ <sup>6</sup> 6~~~~ <sup>4</sup>  | 1.62                   | $1.61 \pm 0.02$                         | $1.65 \pm 0.04$                       | [42] |
|  | 1.05                   | $1.04 \pm 0.02$                         | $1.03 \pm 0.04$                       | [42] |
| $\mathcal{I}_{\mathcal{A}}^{\circ} \mathcal{I}_{\mathcal{A}}^{\circ} \mathcal{I}_{\mathcal{A}}^$ | 1.62                   | $1.61 \pm 0.01$                         | $1.62 \pm 0.04$                       | [42] |
| $\mathcal{Y}_{0}\sim \mathcal{I}_{0}^{\mathcal{I}}$  | 1.61                   | $1.61 \pm 0.02$                         | $1.61 \pm 0.04$                       | [42] |
| $ \int_{\mathbb{R}^{n}} \int_$   | 1.59                   | $1.6\pm0.02$                            | $1.61 \pm 0.06$                       | [50] |
| N slows frights o  | 1.64                   | $1.6\pm0.02$                            | $1.63\pm0.03$                         | [50] |
| $\sim \gamma_{1}^{2}$  | 1.61                   | $1.65 \pm 0.05$                         | $1.64\pm0.04$                         | [12] |
|  | 1.62                   | $1.68\pm0.1$                            | $1.65\pm0.04$                         | [12] |
| Q  | 1.69                   | $1.64 \pm 0.01$                         | $1.66\pm0.03$                         | [12] |
|  |                        |   |                                       |      |
| -≺<br>©  | 1.62                   | $1.63 \pm 0.01$                         | $1.62\pm0.02$                         | [12] |
| 4°~~~~,00°.  | 1.60                   | 1.65 - 0.01                             | 1.62 4 0.02                           | [19] |
| Q<br>~~~~~,QQ,.  | 1.62                   | 1.00 ± 0.01                             | $1.02 \pm 0.02$                       | [12] |
|  | 1.61                   | $1.63\pm0.01$                           | $1.61\pm0.02$                         | [12] |
| y ······   | 1.63                   | $1.65 \pm 0.01$                         | $1.62\pm0.02$                         | [12] |
|  |                        |   |                                       |      |
|  |                        |   |                                       |      |

| Table $S3 - Continued$ from previous page |           |                   |                 |      |  |  |
|---|-----------|-------------------|-----------------|------|--|--|
| MONOMER                                   | $n^{exp}$ | n <sup>pred</sup> | $n_{BE}^{pred}$ | Ref  |  |  |
|   | 1.61      | $1.63 \pm 0.01$   | $1.63 \pm 0.03$ | [44] |  |  |
| \$<br>,                                   | 1.62      | $1.64 \pm 0.01$   | $1.63\pm0.02$   | [44] |  |  |
| 4,~~~,0<br>20 <sup>1,~</sup> ~0.0         | 1.65      | $1.66 \pm 0.01$   | $1.65 \pm 0.02$ | [44] |  |  |
|   | 1.66      | $1.6 \pm 0.01$    | $1.63 \pm 0.03$ | [44] |  |  |
| 20 <sup>0</sup>                           | 1.64      | $1.63\pm0.01$     | $1.65 \pm 0.02$ | [44] |  |  |
|   | 1.66      | $1.66 \pm 0.01$   | $1.67\pm0.02$   | [44] |  |  |
|   | 1.66      | $1.65 \pm 0.01$   | $1.66 \pm 0.02$ | [44] |  |  |
|   |           |                   |                 |      |  |  |

| MONOMER               | $T_g^{exp}$ | $T_g^{\widehat{PLSR}}$     | $\widehat{T_g^{RF}}$         | Ref        |
|-----------------------|-------------|----------------------------|------------------------------|------------|
|                       | -143        | $-27\pm 32$                | $15 \pm 76$                  | [4]        |
|                       |             |                            |                              |            |
| $\sim$ .0             | -121        | $-87\pm 30$                | $1\pm79$                     | [4]        |
| Si                    |             |                            |                              |            |
|                       |             |                            |                              |            |
|                       | -102        | -11± 10                    | $-71 \pm 55$                 | [4]        |
|                       | -100        | $-27 \pm 16$               | $-65 \pm 46$                 | [4]        |
|                       |             |                            |                              |            |
| Ĭ                     |             |                            |                              |            |
|                       | -86         | $-14 \pm 21$               | -25+75                       | [4]        |
|                       | -00         | -14_ 21                    | -20110                       | [.#]       |
|                       |             |                            |                              |            |
|                       | -85         | -61± 14                    | -71±37                       | [4]        |
|                       | -83         | -97± 15                    | -75±23                       | [4]        |
| $\sim$ N              | -82         | $-53 \pm 31$               | $-14 \pm 79$                 | [4]        |
| Si                    |             |                            |                              |            |
|                       |             |                            |                              |            |
|                       | -81         | $-15 \pm 12$               | $-51 \pm 50$                 | [4]        |
| ∽∽∽∽°∕                | -79<br>-79  | $-31\pm 12$<br>$-62\pm 13$ | $-46\pm 36$<br>$-66\pm 47$   | [4]<br>[4] |
| ∼∽o ∼ <sub>C</sub> o  | 78          | $16 \pm 26$                | 16+50                        | [4]        |
| $\blacksquare$        | -78         | $-98 \pm 17$               | $-77\pm20$                   | [4]        |
| $\sim^{\circ}$        |             |                            |                              |            |
|                       | -77         | $-10\pm 11$<br>$-31\pm 12$ | $-49\pm57$<br>$-40\pm41$     | [4]<br>[4] |
|                       | -76         | $-7\pm 10$                 | $-40 \pm 41$<br>$-44 \pm 58$ | [4]        |
| F F                   | -74         | -137 $\pm$ 35              | $13 \pm 81$                  | [4]        |
| • Si ~ K <sup>F</sup> |             |                            |                              |            |
| Ĩ                     | -74         | $9\pm 16$                  | $-59 \pm 65$                 | [4]        |
| $\overline{1}$        |             |                            |                              |            |
| Ý                     |             |                            |                              |            |
|                       |             |                            |                              |            |
|                       | -70         | -42± 13                    | $-58 \pm 36$                 | [4]        |
| → Si                  |             |                            |                              |            |
| ~~~~_0                | -70<br>-70  | $-92\pm 16$<br>57 $\pm 10$ | $-72\pm33$<br>$-40\pm61$     | [4]<br>[4] |
|                       | 10          | 5.1 10                     | 10-01                        | [#]        |
|                       |             |                            |                              |            |
| ~~~ <sup>0</sup>      | -69         | -97± 15                    | -72±31                       | [4]        |
| ₀∽∽₀بُلُمی ہ          | -68         | -10± 14                    | -47±59                       | [4]        |
| $\sim$ 0              | -67         | -103± 27                   | $-69 \pm 14$                 | [4]        |
|                       |             |                            |                              |            |

Table S4: The table lists the experimental and predicted ( $\pm$  uncertainty) glass transition temperatures for different monomers. Predictions for both PLSR and RF models are reported.

| Table S4 - Continued from previous page                              |             |              |              |                     |
|--|-------------|--------------|--------------|---------------------|
| MONOMER  | $T_g^{exp}$ | $T_g^{PLSR}$ | $T_g^{RF}$   | Ref                 |
|  | -67         | -62± 19      | -69±29       | [4]                 |
|  |             |              |              |                     |
| 0  | -66         | $-29\pm 12$  | $-52\pm30$   | [4]                 |
|  | -66         | $20\pm 13$   | $-33\pm60$   | [4]                 |
|  |             |              |              |                     |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~                               | -65         | $-22\pm 10$  | $-53 \pm 22$ | [4]                 |
|  | -64         | $-30\pm~11$  | $-55 \pm 27$ | [4]                 |
| .0   | -62         | $-60 \pm 12$ | $-68 \pm 45$ | [4]                 |
| $\sim$   |             |              |              |                     |
|  | -60         | $59\pm~11$   | $-14 \pm 69$ | [4]                 |
|  | 20          |              | ~ ~ ~        | 141                 |
| $\tilde{a}_0$  | -60         | -19± 10      | $-55\pm15$   | [4]                 |
|  | -60         | $-23 \pm 11$ | $-12\pm54$   | [4]                 |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~                               | -58         | $-24 \pm 11$ | $-49 \pm 28$ | [4]                 |
|  | -57         | -16± 9       | $-50 \pm 33$ | [4]                 |
|  | -56         | -9± 19       | $-35 \pm 57$ | [4]                 |
|  | -55         | -140± 49     | $-68 \pm 30$ | [4]                 |
| —0   | -55         | $-31\pm 15$  | $-23\pm53$   | [4]                 |
| Ţ <sup>1</sup> ,~~~~~  | E 4         | 0 1 7        | 49   41      | [4]                 |
| <i>∞</i> ↓ <sup>0</sup> <i>· · · · · · · · · · · · · · · · · · ·</i> | -34         | -o± /        | -48±41       | [4]                 |
|  | -53         | $-20\pm$ 11  | $-18 \pm 47$ | [4]                 |
|  | -53         | -19± 9       | $-25 \pm 48$ | [4]                 |
|  |             |              |              |                     |
|  | -52         | $-28 \pm 13$ | -44+35       | [4]                 |
| <b>√√</b> <sup>0</sup> <i>∉</i>                                      | -50         | $-21 \pm 10$ | -18+47       | [4]                 |
| $\sim$   | 50          | 10± 12       | ±<br>28±47   | [4]                 |
| $\sim$   | -50         | -15 12       | -20141       | [.#]                |
|  | -48         | $80 \pm 13$  | $-38\pm62$   | [4]                 |
|  |             |              |              |                     |
|  | -47         | $19 \pm 15$  | -35+66       | [4]                 |
|  | -11         | 10 10        | -00100       | [*]                 |
|  |             |              |              |                     |
|  | -45         | $-16\pm 15$  | $-27 \pm 43$ | [4]                 |
|  |             |              |              |                     |
| °~°¥~~~~°  | -45         | -11± 15      | $-43\pm57$   | [4]                 |
| $\sim$   | -45         | -8± 11       | $-20 \pm 51$ | [4]                 |
|  | -44         | -3± 7        | $-42 \pm 48$ | [4]                 |
| ×Y × ×   |             |              |              |                     |
| Ň.   | -7          | -12± 20      | $-17 \pm 51$ | [4]                 |
| $\sim$   |             |              |              |                     |
| E E  | -40         | $33\pm\ 27$  | $-28 \pm 58$ | [4]                 |
|  |             |              |              |                     |
|  |             |              |              |                     |
| II   | -40         | -14+ 13      | -47+57       | [4]                 |
| °~°ų~~~°   | -40         | -1-1 10      | -11-101      | []                  |
| <pre>~/~~</pre>  | -38         | $2\pm 10$    | $-26 \pm 47$ | $\lfloor 4 \rfloor$ |
| 0 '  |             | Cont         | inued on ne: | xt page             |

| Table S4 – Continued j | rom previous page |                            | ~            |               |
|------------------------|-------------------|----------------------------|--------------|---------------|
| MONOMER                | $T_g^{exp}$       | $T_g^{PLSR}$               | $T_g^{RF}$   | Ref           |
| $\downarrow$           | -34               | -9± 10                     | -20±53       | [4]           |
|                        | -33               | -23± 9                     | -26±47       | [4]           |
| ·~°Y~~~~~              | -30               | -9± 16                     | $-29 \pm 59$ | [4]           |
|                        | -24               | 8± 9                       | $-36 \pm 38$ | [4]           |
| $\sim$                 | -99               | -11+ 9                     | -17+43       | [4]           |
|                        | -22               | -11_ 0                     | -11_40       | [*]           |
| ✓ <sup>°</sup> ✓       | -22               | $10\pm 9$                  | $-25\pm62$   | [4]           |
| 0<br>↓                 | -20               | -22± 11                    | -11±42       | [4]           |
|                        | -20               | $6\pm 10$                  | -15±52       | [4]           |
|                        | -20               | $14\pm 11$                 | -18±48       | [4]           |
|                        | -19               | -18± 12                    | -30±38       | [4]           |
|                        | -17               | -6± 33                     | -5±77        | [4]           |
| $\mathbf{T}$           |                   |                            |              |               |
|                        | -16               | $35\pm$ 13                 | $-6\pm 58$   | [4]           |
| ≈ <sup>μ</sup> , √     |                   |                            |              |               |
|                        | -14               | -12± 11                    | $2{\pm}65$   | [4]           |
|                        | -8                | -5± 14                     | $30{\pm}75$  | [4]           |
| $\rightarrow$          |                   |                            |              |               |
| o CI                   |                   |                            | 00 1 50      | [4]           |
| SI CIN                 | -6                | 67± 9                      | $23\pm 56$   | [4]           |
|                        | -5                | -15± 9                     | $-3 \pm 40$  | [4]           |
|                        | -3                | -5± 10                     | $-27 \pm 45$ | [4]           |
|                        | 1                 | 6+ 13                      | 44+60        | [4]           |
| °~°y~~°                | -1                | $-0 \pm 13$<br>32 $\pm 17$ | -44±00       | [4]           |
| - <sup>S</sup>         | -1                | 87+ 49                     | 120+64       | [4]           |
|                        | 0                 | 011 44                     | 120104       | [. <b>z</b> ] |
| ✓ ° ✓                  | 5                 | -12± 7                     | $38\pm52$    | [4]           |
|                        | 5                 | $54\pm 9$                  | $40 \pm 34$  | [4]           |
|                        | 6                 | $81{\pm}~8$                | $35 \pm 45$  | [4]           |
|                        |                   |                            |              |               |

| Table S4 -  | - Continued from previous page |             |               |                    |      |
|---|--------------------------------|-------------|---------------|--------------------|------|
| MONOMER   |                                | $T_g^{exp}$ | $T_g^{PLSR}$  | $T_g^{R\tilde{F}}$ | Ref  |
| ∕∕ <mark>``</mark>  |                                | 8           | $20\pm 10$    | $2\pm 64$          | [4]  |
| o<br>∕√°≪   |                                | 10          | $4\pm$ 8      | $22 \pm 46$        | [4]  |
|   |                                | 11          | $7\pm~10$     | $26\pm42$          | [4]  |
|   |                                | 13          | 55+ 9         | 32+32              | [4]  |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~  |                                | 20          | -10+ 7        | 10+45              | [4]  |
| <sup>⊥</sup> ,°~~   |                                | 20          | 101 1         | 10-40              | [*]  |
|   |                                | 20          | -6± 8         | $11 \pm 67$        | [4]  |
|   |                                | 22          | $68\pm8$      | 34±31              | [4]  |
|   |                                | 25          | $75\pm 10$    | $68 \pm 45$        | [4]  |
| I)  |                                |             |               |                    |      |
| F<br>F  |                                | 27          | $20\pm$ 13    | -8±63              | [4]  |
| $\times$  |                                | 28          | 0+11          | 24+55              | [4]  |
|   |                                |             |               |                    |      |
|   |                                | 29          | -2± 10        | $6\pm65$           | [4]  |
|   |                                | 31          | $20\pm$ 18    | $32 \pm 69$        | [4]  |
| and a state of the state of th |                                | 31          | $25\pm 9$     | $30{\pm}50$        | [4]  |
|   |                                | 33          | $10\pm$ 9     | $42 \pm 51$        | [4]  |
|   |                                | 35          | -5± 7         | $11 \pm 55$        | [4]  |
| <sup>⊥</sup> ,°~  |                                |             |               |                    |      |
| Å.  |                                | 37          | -18± 14       | $36\pm35$          | [4]  |
| riO   |                                | 40          | $0 \pm 12$    | $46\pm75$          | [4]  |
| $\sum_{i=1}^{n}$  |                                | 41          | $29 \pm 14$   | $27 \pm 61$        | [4]  |
|   |                                |             |               |                    | r +1 |
| F F .   |                                | 42          | -17± 13       | $36\pm36$          | [4]  |
|   |                                | 42          | $27 \pm \ 11$ | $24\pm60$          | [4]  |
| $\sim \sim \sim$  |                                | 42          | $59\pm$ 7     | $53 \pm 42$        | [4]  |
|   |                                |             |               |                    |      |

| Table S4 – Continued from previous page |             |                |                        |     |
|---|-------------|----------------|------------------------|-----|
| MONOMER                                 | $T_g^{exp}$ | $T_g^{PLSR}$   | $T_g^{RF}$             | Ref |
| W F                                     | 42          | $35\pm 13$     | $43 \pm 41$            | [4] |
|   |             |                |                        |     |
|   | 43          | -14± 12        | $33{\pm}40$            | [4] |
|   | 45          | $1\pm 9$       | $34\pm51$              | [4] |
|   | 46          | 20   16        | 24   44                | [4] |
|   | 40<br>46    | $-2\pm 8$      | $34\pm44$<br>$47\pm42$ | [4] |
|   | 40          | 45   14        | 54 50                  | [4] |
|   | 40          | 45 <u>±</u> 14 | $54\pm50$              | [4] |
|   | 47          | $68 \pm 8$     | $54 \pm 33$            | [4] |
| ~~°Q_                                   | 40          |                | 22 41                  | [4] |
|   | 48          | 2± 8           | 33±41                  | [4] |
|   | 50          | $6\pm$ 13      | $23\pm63$              | [4] |
|   |             |                |                        |     |
|   | 51          | -18± 11        | $33 \pm 39$            | [4] |
|   | 51          | -16± 11        | $34{\pm}41$            | [4] |
|   | 51          | $-37 \pm \ 16$ | $29\pm76$              | [4] |
|   |             |                |                        |     |
|   | 51          | 96± 9          | 74±77                  | [4] |
|   | 51          | $5\pm$ 7       | $27 \pm 54$            | [4] |
|   |             |                |                        |     |
|   | 52          | $139 \pm\ 14$  | $69\pm53$              | [4] |
|   | 54          | $6\pm$ 9       | $44 \pm 35$            | [4] |
| <sup>™</sup> T°                         |             |                |                        |     |
|   | 55          | $70\pm$ 10     | $75\pm48$              | [4] |
| <u>μ</u>                                |             |                |                        |     |
|   | 57          | $19\pm 9$      | $61 \pm 41$            | [4] |
|   | 57          | 14 1 11        | 20-11                  | [4] |
| N ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~  | 57          | -14± 11        | 59±41                  | [4] |
|   | 57          | 12± 10         | J3 <u>∓</u> 43         | [4] |
|   | 57          | -10± 11        | $28 \pm 48$            | [4] |
| ~~~*j~~*.<br>~~~°~~                     | 57          | $70\pm 8$      | $54 \pm 28$            | [4] |
|   | 58          | $40\pm$ 18     | $13 \pm 59$            | [4] |
|   |             |                |                        |     |
| F Γ                                     |             |                |                        |     |

| Table S4 – Continu   | ned from previous page |                    |                          |     |
|----------------------|------------------------|--------------------|--------------------------|-----|
| MONOMER              | $T_g^{exp}$            | $T_g^{PLSR}$       | $T_g^{RF}$               | Ref |
|                      | 58                     | $137 \pm 13$       | 89±42                    | [4] |
|                      | 60                     | $59\pm~10$         | $64 \pm 50$              | [4] |
|                      | 60                     | $0\pm$ 10          | $31\pm63$                | [4] |
|                      | 60                     | $63\pm~7$          | $64 \pm 36$              | [4] |
| N~~~~~°              | 62                     | -13± 11            | $34{\pm}58$              | [4] |
|                      | 70                     | $73\pm 8$<br>21+ 8 | $60\pm 27$<br>$64\pm 38$ | [4] |
|                      |                        | 212 0              | 01200                    | [*] |
|                      | 72                     | 90± 10             | $112 \pm 80$             | [4] |
|                      | 74                     | $33\pm 9$          | $60 \pm 45$              | [4] |
|                      | 75                     | -3± 22             | $33 \pm 63$              | [4] |
|                      | 75                     | $9\pm$ 11          | $50\pm75$                | [4] |
|                      | 75                     | $7\pm~12$          | $4{\pm}67$               | [4] |
|                      | 76                     | 8± 7               | 47±58                    | [4] |
| $\sim$               | 77                     | 76± 7              | 66±48                    | [4] |
|                      | 80                     | 77± 9              | $62\pm 62$               | [4] |
|                      | 80                     | 73± 10             | $76 \pm 60$              | [4] |
| Br                   |                        |                    |                          |     |
|                      | 82                     | 40± 7              | $50 \pm 57$              | [4] |
| $\sim$               | 85                     | -18± 35            | -30±64                   | [4] |
|                      | 85                     | $59\pm$ 13         | $53 \pm 66$              | [4] |
|                      | 86                     | 92± 9              | $61 \pm 51$              | [4] |
| $\sim^{\circ}$       | 86                     | 78± 8              | $70\pm36$                | [4] |
| <b>以</b> , <i>//</i> |                        |                    |                          |     |

| Table S4 – Cont    | tinued from previous page |               |               |         |
|--------------------|---------------------------|---------------|---------------|---------|
| MONOMER            | $T_g^{exp}$               | $T_g^{PLSR}$  | $T_g^{RF}$    | Ref     |
|                    | 86                        | $21\pm 8$     | $47 \pm 59$   | [4]     |
| s – (              | 87                        | 69± 9         | 74±69         | [4]     |
|                    | 87                        | $95\pm 8$     | 80±44         | [4]     |
|                    | 87                        | $114{\pm}~13$ | $69 \pm 43$   | [4]     |
|                    | 89                        | $94\pm 8$     | 90±28         | [4]     |
|                    | 90                        | $27\pm 9$     | $54 \pm 48$   | [4]     |
|                    |                           |               |               | ſ-]     |
|                    | 90                        | 93± 7         | 85±43         | [4]     |
|                    | 137                       | $11\pm 14$    | 80±71         | [4]     |
|                    | 90                        | $101 \pm 19$  | $102 \pm 46$  | [4]     |
|                    |                           |               |               |         |
|                    | 90                        | $73 \pm \ 11$ | $82 \pm 46$   | [4]     |
|                    | 90                        | $118\pm 10$   | $114 \pm 32$  | [4]     |
|                    | 92                        | -1± 10        | $65 \pm 55$   | [4]     |
|                    | 93                        | 26± 9         | $54 \pm 53$   | [4]     |
| ~° <sup>™</sup> /≈ |                           |               |               |         |
| Si                 | 93                        | -21± 13       | 52±73         | [4]     |
| $\sum_{i=1}^{n}$   | 97                        | $100\pm 11$   | $107 \pm 36$  | [4]     |
|                    | 100                       | 78± 11        | 90±43         | [4]     |
|                    | 100                       | $77\pm 12$    | $76 \pm 54$   | [4]     |
|                    |                           | -             | _             |         |
| CI F               | 100                       | $106 \pm 11$  | $104 \pm 40$  | [4]     |
|                    |                           |               |               |         |
| ¥                  |                           | Cont          | tinued on ne: | ct page |

| MONOMER                               | $T^{exp}_{-}$ | $T_a^{\widehat{PLSR}}$ | $\widehat{T_c^{RF}}$ | Ref         |
|---------------------------------------|---------------|------------------------|----------------------|-------------|
|                                       | 19<br>101     | $\frac{-g}{99\pm 9}$   | $100\pm33$           | [4]         |
|                                       |               |                        |                      |             |
|                                       | 101           | $131\pm 10$            | $126 \pm 41$         | [4]         |
|                                       |               |                        |                      |             |
| F                                     |               |                        |                      |             |
|                                       | 103           | $106{\pm}~12$          | $107 \pm 38$         | [4]         |
| $\geq \langle$                        |               |                        |                      |             |
|                                       |               |                        |                      | <b>F</b> 13 |
| $\chi \propto $                       | 104           | $106 \pm 11$           | $105 \pm 41$         | [4]         |
|                                       |               |                        |                      |             |
|                                       | 104           | $12\pm 10$             | $89 \pm 48$          | [4]         |
| <sup>↓</sup> <sup>●</sup> <sup></sup> |               |                        |                      |             |
|                                       |               |                        | 101100               |             |
| N N                                   | 104           | $113 \pm 11$           | $104 \pm 26$         | [4]         |
|                                       |               |                        |                      |             |
| $\sim$                                | 105           | $20\pm$ 8              | $70\pm 64$           | [4]         |
|                                       |               |                        |                      |             |
|                                       | 105           | 44 - 04                | 14 69                | [4]         |
| λ                                     | 105           | $44\pm 24$             | 14±62                | [4]         |
| <u>∿_</u> ∎N                          | 105           | 42 1 16                | 48177                | [4]         |
| $\checkmark$                          | 105           | -43± 10                | 40±11                | [4]         |
|                                       |               |                        |                      |             |
| ,<br>T                                | 105           | $123 \pm\ 11$          | $124 \pm 41$         | [4]         |
| $\geq$                                |               |                        |                      |             |
|                                       |               |                        |                      |             |
|                                       | 105           | $168 \pm\ 14$          | $192 \pm 77$         | [4]         |
|                                       |               |                        |                      |             |
|                                       |               |                        |                      |             |
| F F                                   | 106           | 24 1 14                | 56460                | [4]         |
| 0                                     | 100           | 34 <u>±</u> 14         | 20±09                | [4]         |
| 1/1                                   |               |                        |                      |             |
|                                       | 106           | $109\pm 9$             | $112 \pm 32$         | [4]         |
| $\prec$                               |               |                        |                      |             |
|                                       | 107           | $24{\pm}~11$           | $86 {\pm} 44$        | [4]         |
| $\sim 0.00$                           |               |                        |                      |             |
|                                       | 111           | $101\pm 9$             | $101 \pm 34$         | [4]         |
|                                       |               |                        |                      |             |
|                                       | 111           | $118\pm 10$            | $113 \pm 38$         | [4]         |
| $\gamma$                              |               |                        |                      |             |
|                                       |               |                        |                      |             |
|                                       |               |                        |                      |             |

| Table S4 - Continued from previous page |             |              |              |     |
|---|-------------|--------------|--------------|-----|
| MONOMER                                 | $T_g^{exp}$ | $T_g^{PLSR}$ | $T_g^{RF}$   | Ref |
|   | 112         | 97± 10       | $105 \pm 41$ | [4] |
|   | 113         | 97± 8        | 90±40        | [4] |
|   | 114         | 106± 8       | 120±51       | [4] |
|   | 114         | 43± 11       | 61±46        | [4] |
|   | 115         | $67\pm~12$   | $95 \pm 38$  | [4] |
|   | 116         | $111\pm 11$  | $123 \pm 32$ | [4] |
|   | 117         | $52\pm~10$   | $25 \pm 67$  | [4] |
|   | 119         | $124 \pm 11$ | 122±31       | [4] |
|   |             |              |              |     |
|   | 120         | $121\pm 10$  | $124 \pm 30$ | [4] |
|   | 120         | $56\pm 8$    | $104 \pm 36$ | [4] |
|   | 120         | 44± 20       | $25 \pm 66$  | [4] |
|   | 122         | 116± 9       | $124\pm31$   | [4] |
|   | 125         | $99\pm 11$   | $109 \pm 41$ | [4] |
|   | 128         | $115\pm 10$  | 120±31       | [4] |
|   | 129         | 98± 9        | 76±47        | [4] |
|   | 130         | $106 \pm 12$ | 113±41       | [4] |
|   | 133         | $124 \pm 11$ | 128±33       | [4] |
|   | 136         | $101\pm 11$  | $126\pm34$   | [4] |
|   |             |              |              |     |

|                   | Table S4 – Continued from previous page |                 | ~              | $\sim$         |     |
|-------------------|---|-----------------|----------------|----------------|-----|
| MONOMER           | T                                       | $\frac{exp}{g}$ | $T_g^{PLSR}$   | $T_g^{RF}$     | Ref |
| $\rightarrow$     |   | 136             | 93± 9          | 112±38         | [4] |
|                   | 1                                       | 138             | 181± 18        | $139 \pm 66$   | [4] |
|                   |   |                 |                |                |     |
|                   | 1                                       | 138             | $150\pm 11$    | $135 \pm 42$   | [4] |
| •                 | 1                                       | 140             | 90± 8          | $100 \pm 45$   | [4] |
|                   | 1                                       | 142             | $106\pm 11$    | $126 \pm 37$   | [4] |
| $\sim$            | 1                                       | 143             | $103\pm11$     | $118 {\pm} 40$ | [4] |
|                   |   |                 |                |                |     |
|                   | 1                                       | 138             | $151\pm12$     | $115 \pm 54$   | [4] |
|                   | 1                                       | 144             | $112 \pm \ 10$ | $125 \pm 33$   | [4] |
|                   | 1                                       | 145             | $101\pm 9$     | $123 \pm 48$   | [4] |
|                   | 1                                       | 145             | $51\pm 13$     | 33±62          | [4] |
|                   |   |                 |                |                |     |
|                   | 1                                       | 145             | $124\pm~12$    | $141\pm35$     | [4] |
|                   |   |                 |                |                |     |
|                   | 1                                       | 146             | $126 \pm 13$   | $111 \pm 58$   | [4] |
|                   | I                                       | 146             | $107\pm 9$     | $116 \pm 39$   | [4] |
|                   | 1                                       | 146             | $132\pm 8$     | $157 \pm 61$   | [4] |
|                   | 1                                       | 147             | $95\pm~11$     | $124 \pm 53$   | [4] |
|                   | 1                                       | 148             | $143\pm$ 15    | $134\pm51$     | [4] |
| .O                | 1                                       | 149             | $109\pm 10$    | $117 \pm 63$   | [4] |
| .0 <sup>1</sup> 0 | 1                                       | 150             | $180 \pm 14$   | $141 \pm 45$   | [4] |
|                   |   |                 |                |                |     |
|                   |   |                 |                |                |     |

| Table S               | S4 – Continued from previous page |             | ~             | ~            |     |
|-----------------------|-----------------------------------|-------------|---------------|--------------|-----|
| MONOMER               |                                   | $T_g^{exp}$ | $T_g^{PLSR}$  | $T_g^{RF}$   | Ref |
|                       |                                   | 152         | 70± 18        | $126 \pm 62$ | [4] |
|                       |                                   | 159         | 182± 13       | $144 \pm 30$ | [4] |
| °                     |                                   | 160         | $105\pm$ 12   | $116 \pm 35$ | [4] |
|                       |                                   | 160         | $71\pm~21$    | $104 \pm 69$ | [4] |
|                       |                                   | 171         | $191{\pm}~14$ | $257 \pm 99$ | [4] |
|                       |                                   | 194         | 190± 19       | 214±96       | [4] |
|                       |                                   | 202         | $136\pm 12$   | $169 \pm 53$ | [4] |
|                       |                                   | 209         | 79± 11        | 89±56        | [4] |
|                       |                                   | 220         | 141± 9        | 178±74       | [4] |
| Toporotor V           |                                   | 220         | $232 \pm 13$  | $248 \pm 69$ | [4] |
|                       |                                   | 225         | 193± 13       | $257 \pm 94$ | [4] |
|                       |                                   | 272         | 197± 20       | $197 \pm 98$ | [4] |
|                       |                                   | 275         | 197± 20       | 190±89       | [4] |
|                       |                                   | 277         | $189\pm10$    | $296 \pm 58$ | [4] |
|                       |                                   | 318         | 238± 17       | 299±62       | [4] |
| Ny CP <sup>û</sup> NY |                                   | 327         | 260± 59       | 192±106      | [4] |
|                       |                                   | 372         | 295± 21       | 332±68       | [4] |
|                       |                                   | 376         | 243± 17       | $306 \pm 82$ | [4] |

|  | Table S4 – Continued from previous page |                            |                      |      |
|--|---|----------------------------|----------------------|------|
| MONOMER  | $T_g^{ex}$                              | $p = T_g^{\widehat{PLSR}}$ | $\widehat{T_g^{RF}}$ | Ref  |
|  |   | $285 \pm 13$               | $360 \pm 61$         | [4]  |
| · · · · · · · · · · · · · · · · · · ·  | 111                                     | $103\pm 10$                | $147 \pm 92$         | [4]  |
|  | 100                                     | $84\pm 9$                  | $89 \pm 36$          | [4]  |
|  | 327                                     | $7 284 \pm 23$             | $333 \pm 25$         | [3]  |
| p.p. p.p   |   |                            |                      |      |
|  |   |                            |                      |      |
|  | 332                                     | $22282\pm 22$              | $332\pm23$           | [3]  |
| ĭ°<br>Q  |   |                            |                      |      |
| er.<br>Gr  | 356                                     | $5 	264 \pm 37$            | $332 \pm 35$         | [3]  |
| a a protoco  |   |                            |                      |      |
|  | 371                                     | $299\pm 32$                | $334{\pm}29$         | [3]  |
| A Charles Contraction  |   |                            |                      | [0]  |
| à.   | 333                                     | 3 290± 37                  | $331 \pm 19$         | [3]  |
| al and a set of a set | 362                                     | $304\pm 42$                | $336 \pm 32$         | [3]  |
| A Constraints  |   |                            |                      |      |
|  | 301                                     | $226\pm 25$                | $317 \pm 40$         | [3]  |
| y g <sup>i y y y</sup> qi  |   |                            |                      |      |
|  | 303                                     | $216\pm 25$                | $315\pm44$           | [3]  |
| ind<br>ind   | 319                                     | 241 + 30                   | $318 \pm 34$         | [3]  |
| A a protoco  |   |                            |                      | [*]  |
| 13-2-3-9-10-10-  | 345                                     | $261\pm 28$                | $339 \pm 34$         | [3]  |
| 2 Protein an   | 304                                     | 4 281± 33                  | $323\pm33$           | [3]  |
| the state  | 336                                     | $3295\pm 41$               | $328 \pm 35$         | [3]  |
| A Contraction  |   |                            |                      |      |
|  | 121                                     | 1 88± 8                    | $97 \pm 44$          | [4]  |
|  | 223                                     | $230 \pm 17$               | $226\pm22$           | [16] |
|  |   |                            |                      |      |
|  | 212                                     | $220\pm 18$                | $225\pm26$           | [16] |
|  |   |                            |                      |      |
|  | 228                                     | $235\pm 20$                | $230\pm28$           | [16] |
|  |   |                            |                      |      |
|  | 203                                     | $3226\pm 20$               | $213\pm27$           | [16] |
|  |   |                            |                      |      |
| Ö  |   |                            |                      |      |

|  | Table S4 – Continued from previous page |             |                        |                      |      |
|--|---|-------------|------------------------|----------------------|------|
| MONOMER  |   | $T_g^{exp}$ | $T_g^{\widehat{PLSR}}$ | $\widehat{T_g^{RF}}$ | Ref  |
|  |   | 194         | 254± 46                | 238±38               | [16] |
| Barrag   |   | 194         | $205\pm$ 33            | $193 \pm 34$         | [38] |
| ag an ag   |   | 125         | 141± 19                | $165 {\pm} 48$       | [38] |
| ar an ar   |   | 120         | $148 \pm 17$           | $181 \pm 53$         | [38] |
| joan.o.  |   | 174         | 176± 19                | $214 \pm 33$         | [38] |
|  |   | 220         | 198± 11                | $216 \pm 30$         | [15] |
|  |   | 208         | $182 \pm\ 12$          | $211 \pm 40$         | [15] |
|  |   | 217         | $207 \pm \ 11$         | $216\pm38$           | [15] |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   |   | 205         | $190\pm 12$            | $217 \pm 34$         | [15] |
|  |   | 181         | $268 \pm 28$           | $196 \pm 25$         | [15] |
|  |   | 181         | 2001 20                | 190±25               | [13] |
|  |   | 239         | $208 \pm \ 18$         | $206\pm 26$          | [15] |
|  |   | 228         | $217 \pm\ 14$          | $205 \pm 29$         | [15] |
|  |   | 235         | $218\pm12$             | $216 \pm 29$         | [15] |
|  |   |             |                        |                      | ( 1  |
|  |   | 226         | 192± 16                | 218±24               | [15] |
|  |   | 197         | 273± 29                | $200\pm 28$          | [15] |
|  |   | 252         | $261 \pm 11$           | 243±21               | [25] |
| por ma   |   | 229         | $250 \pm 10$           | $233 \pm 22$         | [25] |
| రి, భరిరాష్ సర్వారా<br>రి, భరిరాష్ స్ట్రా  |   | 240         | $245 \pm 11$           | $232\pm23$           | [25] |
| . A. John Stranger, Strang |   | 201         | $168\pm 17$            | $211 \pm 31$         | [25] |
|  |   | 57          | 58± 9                  | 75±63                | [62] |
|  |   | -35         | $45\pm\ 27$            | $16\pm69$            | [62] |

| Table 54 – Continuea from previous page                  |             | $\sim$       | $\sim$       |      |
|--|-------------|--------------|--------------|------|
| MONOMER  | $T_g^{exp}$ | $T_g^{PLSR}$ | $T_g^{RF}$   | Ref  |
|  | 180         | 87± 25       | $138 \pm 93$ | [62] |
|  | 147         | $75\pm$ 15   | $129\pm55$   | [62] |
|  | -26         | $48\pm15$    | -9±47        | [62] |
|  | -57         | -15± 8       | $-48\pm37$   | [62] |
| $\sim$   | -3          | $32\pm 9$    | $24 \pm 38$  | [62] |
|  | 24          | -37+ 17      | 5+43         | [62] |
|  | -40         | $-24\pm 24$  | $-15\pm58$   | [62] |
| ×ũ ~ ∞ <sup>×</sup> ·                                    | -22         | -4± 23       | $5{\pm}55$   | [62] |
|  | -10         | $23\pm 17$   | $6\pm48$     | [62] |
|  | -38         | -11± 21      | 8±53         | [62] |
| $\sim 1_{\circ} \sim \circ \downarrow k_{\rm F}^{\circ}$ | 15          | $42\pm$ 13   | $24 \pm 44$  | [62] |
| ×i (   |             |              |              |      |
| ∽µ° Y Y  | -15         | $19\pm 12$   | -25±39       | [62] |
| ₹°~~~~~  | -3          | -31± 14      | $-16 \pm 39$ | [62] |
|  | 30          | 109± 18      | 86±64        | [62] |
| $\sim$   | -50         | -9± 8        | $-18 \pm 51$ | [62] |
| × <sup>°</sup> / <sub>1</sub> °~~°~                      | -55         | -12± 9       | $-22\pm50$   | [62] |
|  | -50         | $10\pm 10$   | -36±46       | [62] |
|  | 15          | $26\pm$ 11   | $18 \pm 55$  | [62] |
|  | -30         | $43\pm~24$   | -8±52        | [62] |
| $F \xrightarrow{F} F$                                    | -45         | $6\pm$ 30    | $13 \pm 57$  | [62] |
|  | -55         | $33\pm 39$   | $21\pm58$    | [62] |
| F F  | 10          | $63\pm33$    | $11 \pm 53$  | [62] |
|  |             |              |              |      |
|  | 35          | -42± 19      | -18±47       | [62] |
|  | -22         | 24± 22       | -19±50       | [62] |
|  | -56         | $1\pm7$      | -38±43       | [62] |

| Table S4 - Continued from previous page   |             |                              |                        |      |
|---|-------------|------------------------------|------------------------|------|
| MONOMER   | $T_g^{exp}$ | $T_g^{PLSR}$                 | $T_g^{RF}$             | Ref  |
|   | 46          | $107 \pm 12$                 | $86{\pm}52$            | [62] |
| <pre>~;°<pre>~;°</pre></pre>  | 38          | $67\pm 10$                   | $68 \pm 51$            | [62] |
| T° CLI°   | 67          | $69\pm 10$                   | 73±50                  | [62] |
| $\sim$ $\sim$ $\sim$ $\sim$ $\sim$  | -50         | -1± 8                        | -33±45                 | [62] |
|   | -32         | $64\pm 9$<br>$7\pm 9$        | $-28\pm27$             | [62] |
|   | 45          | 67 8                         | 42-24                  | [62] |
| ° m <sup>°</sup> | -43         | $6\pm 9$                     | $-34\pm40$             | [62] |
| $\sim$  | 85          | 116± 9                       | $96 {\pm} 48$          | [62] |
|   | 6           | 38± 7                        | $28 \pm 44$            | [62] |
|   | 72          | $98\pm 14$                   | $89{\pm}36$            | [62] |
|   |             |                              |                        |      |
|   | 71          | $61\pm~7$                    | $75 \pm 29$            | [62] |
|   | 46          | $31\pm 16$                   | $23 \pm 60$            | [62] |
|   | 53          | 77± 9                        | $66 \pm 34$            | [62] |
| <sup>™</sup> <sup>°</sup>   | 59          | 564 12                       | 79119                  | [69] |
|   | 50<br>60    | $50\pm 12$                   | 72+43                  | [62] |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~  |             |                              |                        | [+-] |
|   | 138         | $186\pm\ 26$                 | $234 \pm 26$           | [11] |
|   | 142<br>146  | $165 \pm 13$<br>$143 \pm 12$ | $201 \pm 43$<br>189+47 | [11] |
|   | 150         | $228 \pm 17$                 | 208±28                 | [11] |
| .0,0,0,0  | 165         | 191+ 21                      | $100 \pm 64$           | [11] |
|   | 100         | -vi <u>r</u> 21              | 100704                 | [++] |
|   | 168         | 128± 25                      | 194±43                 | [11] |

|  | Table S4 – Continued from previous page |             |                 |              |         |
|--|---|-------------|-----------------|--------------|---------|
| MONOMER  |   | $T_g^{exp}$ | $T_g^{PLSR}$    | $T_g^{RF}$   | Ref     |
|  |   | 171         | 198± 31         | 178±34       | [11]    |
|  |   | 176         | $179 \pm\ 12$   | $184\pm56$   | [11]    |
|  |   | 178         | $211 \pm\ 13$   | $186\pm50$   | [11]    |
|  |   | 180         | $153 \pm\ 15$   | $196{\pm}45$ | [11]    |
| ,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0   |   | 180         | $170\pm 11$     | $202 \pm 46$ | [11]    |
|  |   | 186         | $179\pm$ 15     | $195 \pm 42$ | [11]    |
|  |   | 188         | $218{\pm}~28$   | $186\pm51$   | [11]    |
|  |   | 190         | $242 \pm \ 15$  | $210\pm33$   | [11]    |
| in a contraction of the contract |   | 195         | $230{\pm}~24$   | $226\pm25$   | [11]    |
| 70.00  |   |             |                 |              |         |
|  |   | 195         | $232 \pm \ 18$  | $207 \pm 37$ | [11]    |
|  |   | 197         | $220 \pm \ 16$  | $185 \pm 36$ | [11]    |
|  |   |             |                 |              |         |
|  |   | 200         | $194\pm$ 13     | $194 \pm 28$ | [11]    |
| 1 Q. Q.  |   | 200         | $225 \pm 14$    | $200 \pm 30$ | [11]    |
| 0,0,0  |   | 2005        | 242   14        | 201   24     | [11]    |
| ga o o   |   | 205         | 242 <u>±</u> 14 | 201±34       | [11]    |
|  |   | 205         | $235 \pm \ 18$  | $204\pm29$   | [11]    |
|  |   | 210         | $150\pm$ 18     | $181 \pm 56$ | [11]    |
|  |   | 210         | $180{\pm}~12$   | $200 \pm 40$ | [11]    |
| · ()   |   | 215         | $185\pm~10$     | $200\pm51$   | [11]    |
|  |   | 216         | $159\pm$ 15     | $180{\pm}65$ | [11]    |
|  |   | 220         | $188 \pm 11$    | $194{\pm}44$ | [11]    |
|  |   | 220         | $205\pm~16$     | $213\pm21$   | [11]    |
|  |   | 221         | $250 \pm 41$    | $112 \pm 65$ | [11]    |
|  |   |             |                 |              | L1      |
|  |   | 221         | $182 \pm \ 10$  | $200 \pm 47$ | [11]    |
|  |   | 222         | $282 \pm ~ 39$  | $223\pm29$   | [11]    |
|  |   |             | Cont            | inued on ne  | rt page |
|   | Table S4 - Continued from previous page | <u> </u>                                      |                      | <u> </u>                     |              |
|---|---|---|----------------------|------------------------------|--------------|
| MONOMER   | $T_g^{ex}$                              | $\frac{T_{P}^{P}}{5} = \frac{T_{g}^{P}}{134}$ | $\frac{LSR}{+15}$    | $\frac{T_g^{RF}}{194\pm 45}$ | Ref          |
|   | 22:                                     | 5 134   | T 19                 | 194±40                       | [11]         |
|   | 22                                      | 5 142   | $\pm$ 21             | $205 \pm 38$                 | [11]         |
| °Ç  | 22'                                     | 7 191   | ± 19                 | 210±36                       | [11]         |
|   | 22'                                     | 7 168   | $\pm$ 12             | $200\pm50$                   | [11]         |
|   | 224                                     | 8 180   | $\pm$ 12             | $187 \pm 48$                 | [11]         |
| A HA  | 228                                     | 8 226   | $\pm 15$             | $207 \pm 41$                 | [11]         |
|   | 230                                     | ) 266   | ± 21                 | $208 \pm 33$                 | [11]         |
|   | 23-                                     | 4 117   | ± 26                 | $206 \pm 64$                 | [11]         |
| o-w   |   |   |                      |                              |              |
| oforpa.ara.at   | 26                                      | 3 242<br>3 238                                | $\pm 19$ + 25        | $244\pm27$<br>$234\pm27$     | [53]<br>[53] |
| orogo orogo   | 22:                                     | 3 207   | $\pm 23$<br>$\pm 21$ | $234\pm27$<br>$230\pm37$     | [53]         |
| al<br>al<br>hu mu al al <sup>da</sup> la  | 27:                                     | 2 277   | $\pm 31$             | $251 \pm 31$                 | [53]         |
| 60.070 000 000 000 000 000 000 000 000 00   | 22                                      | 9 214   | ± 21                 | $234\pm34$                   | [53]         |
|   | 94                                      | 61  | $\pm 21$             | $117 \pm 40$                 | [59]         |
| ~~~.Q`Q`~~~~  | 14                                      | 3 91:   | ± 27                 | 134±30                       | [59]         |
|   | 26                                      | 9 230   | ± 16                 | $250 \pm 22$                 | [48]         |
| ritin ton   | 250                                     | ) 233   | ± 14                 | 252±13                       | [48]         |
|   | 25                                      | 5 232   | ± 15                 | $251 \pm 18$                 | [48]         |
| in the second | 23                                      | 3 220   | ± 17                 | 241±17                       | [48]         |
| A A A A A A A A A A A A A A A A A A A   | 26                                      | 1 261   | $\pm 17$             | 253±19                       | [48]         |
| ġ<br>Alananan   | 44                                      | 5.8-  | + 16                 | 81+52                        | [28]         |
|   |   |   |                      | 01102                        | [=0]         |

| Table S4 - Continued from previous page                        |             |              | ~            |       |
|--|-------------|--------------|--------------|-------|
| MONOMER  | $T_g^{exp}$ | $T_g^{PLSR}$ | $T_g^{RF}$   | Ref   |
|  | 51          | $29\pm 17$   | $42\pm53$    | [28]  |
|  | 4           | $10\pm 16$   | $15\pm62$    | [28]  |
|  | 85          | $9\pm~17$    | $79 \pm 57$  | [28]  |
|  | 90          | $74\pm 19$   | $78 \pm 52$  | [28]  |
|  |             |              |              |       |
|  | 24          | $73 \pm 18$  | $51 \pm 66$  | [28]  |
|  | -58         | -4± 20       | $15 \pm 73$  | [28]  |
|  | -75         | -8± 8        | $-36 \pm 41$ | [28]  |
|  | -60         | $12\pm 12$   | $-30 \pm 58$ | [28]  |
|  | -70         | -1± 12       | $-16 \pm 58$ | [28]  |
| "<br>~°∽₅~   | -71         | -2± 12       | -14±67       | [28]  |
| °<br>~r°~s~∕*″   | -50         | $4\pm~20$    | $29 \pm 74$  | [28]  |
| °°©₊.~~  | 13          | $46\pm$ 11   | $80 \pm 55$  | [28]  |
| <u>لا م</u>  | -40         | -3± 16       | -22±59       | [28]  |
| $\sqrt{n}$ $\sqrt{n}$ $\sqrt{n}$                               | -23         | -6± 17       | -11±55       | [28]  |
| ≤ <sup>™</sup> o <sup>−</sup> λ⊂ <sup>™</sup> / <sub>µ</sub> ∕ | 47          | $83 \pm 10$  | $90 \pm 55$  | [28]  |
|  | 37          | $74\pm\ 16$  | $52 \pm 49$  | [28]  |
|  | 0           | 11 - 0       | 04   45      | [00]  |
| ✓ Y° Y   | -3          | 11± 9        | -24±47       | [28]  |
| م <sup>⊥</sup> <sup>0</sup> ,,,,,,,, .                         | -76         | -4± 13       | -13±68       | [28]  |
| ≈ <sup>1</sup> <sup>0</sup> ···· <sup>s</sup>                  | -65         | $4\pm 12$    | $-25\pm52$   | [28]  |
| 0<br>~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~                      | -59         | -17 $\pm$ 20 | $14\pm72$    | [28]  |
|  | 116         | -1± 17       | $82 \pm 56$  | [28]  |
| N<br>N<br>N  | 98          | $135\pm 8$   | $100 \pm 36$ | [28]  |
|  | 66          | $85 \pm 6$   | 86+29        | [28]  |
| $\sim$   |             |              |              | L - J |
|  | 76          | $84\pm~7$    | $81 \pm 36$  | [28]  |
|  | 74          | $96\pm~7$    | $73 \pm 35$  | [28]  |
|  | 102         | $103 \pm 9$  | $96 \pm 28$  | [28]  |
|  |             |              |              |       |

|                   | Table S4 – Continued from previous page |             |                             |                      |         |
|-------------------|---|-------------|-----------------------------|----------------------|---------|
| MONOMER           |   | $T_g^{exp}$ | $T_g^{PLSR}$                | $T_g^{RF}$           | Ref     |
|                   |   | 94          | 90± 8                       | 84±38                | [28]    |
|                   |   | 74          | 87± 9                       | 74±29                | [28]    |
|                   |   | 86          | 72± 7                       | 49±43                | [28]    |
|                   |   | 66          | $80\pm$ 8                   | $69\pm28$            | [28]    |
| ~~~.i£            |   | 45          | $69\pm~7$                   | 79±28                | [28]    |
|                   |   | 66          | $74\pm\ 8$                  | 77±33                | [28]    |
|                   |   | 46          | $75\pm 8$                   | $54{\pm}39$          | [28]    |
| $\sim$            |   | 90          | $93\pm 6$                   | $91{\pm}43$          | [28]    |
|                   |   | 68          | 81± 6                       | 81±28                | [28]    |
|                   |   | 78          | 72± 7                       | 70±32                | [28]    |
| <u></u> ↓.↓       |   | 95          | 94± 7                       | 78±35                | [28]    |
|                   |   | 88          | 89± 9                       | $80{\pm}25$          | [28]    |
|                   |   | 50          | $68\pm 10$                  | 72±22                | [28]    |
|                   |   | 78          | $117{\pm}~8$                | $108 \pm 54$         | [28]    |
| , V<br>V          |   | 92          | 92± 7                       | 85±20                | [28]    |
|                   |   | 70          | 84± 7                       | 72±36                | [28]    |
|                   |   | 103         | $131\pm 8$                  | $109 \pm 41$         | [28]    |
| ~UU               |   | 91          | $94\pm$ 13                  | $91{\pm}34$          | [28]    |
|                   |   | 75          | $107{\pm}~10$               | 94±42                | [28]    |
| $\langle \rangle$ |   | 100         | 104 - 0                     | 115 50               | [00]    |
| ()°Q_             |   | 235         | $124 \pm 9$<br>$202 \pm 17$ | $115\pm52$<br>208+51 | [28]    |
|                   |   | 230         | 202± 17                     | 200±01               | [41]    |
|                   |   | 237         | 217± 23                     | $185 \pm 56$         | [41]    |
| $\sim M$          |   |             | Con                         | tinued on ne:        | xt page |

|  | Table S4 – Continued from previous page |             |                | ~            |      |
|--|---|-------------|----------------|--------------|------|
| MONOMER  |   | $T_g^{exp}$ | $T_g^{PLSR}$   | $T_g^{RF}$   | Ref  |
|  |   | 269         | $267 \pm 15$   | 261±17       | [48] |
|  |   | 250         | 262± 14        | $254 \pm 15$ | [48] |
|  |   | 255         | $255 \pm 16$   | $252 \pm 14$ | [48] |
|  |   | 233         | 251± 15        | $244\pm25$   | [48] |
| no.<br>Antono a  |   | 261         | 273± 17        | 260±21       | [48] |
|  |   | 227         | $225 \pm \ 13$ | $234 \pm 17$ | [26] |
|  |   | 227         | $221 \pm\ 11$  | $233\pm24$   | [26] |
| And and a second |   | 196         | $230{\pm}~16$  | $234\pm23$   | [26] |
| മന്മണ<br><sub>പറ</sub> ക്താനും   |   | 179         | $168\pm$ 18    | $211\pm31$   | [26] |
| 6<br>  |   | 192         | $167{\pm}~15$  | $210{\pm}35$ | [26] |
| n ata  |   | 252         | $211\pm~13$    | $249{\pm}16$ | [27] |
| tono - motoria - moto  |   | 251         | $235 \pm \ 10$ | $246{\pm}16$ | [27] |
| the constant   |   | 201         | $147{\pm}~21$  | $204 \pm 27$ | [27] |
| an and some  |   | 189         | $217 \pm\ 20$  | $189\pm23$   | [58] |
| 6<br>  |   | 181         | $203 \pm \ 18$ | $190\pm27$   | [58] |
|  |   | 244         | $233 \pm\ 25$  | $245\pm23$   | [18] |
|  |   | 229         | 222± 22        | 231±23       | [18] |
|  |   | 242         | 217± 24        | 243±20       | [18] |
|  |   | 219         | 198± 24        | 227±20       | [18] |
| \$<br>\$<br>\$   |   | 210         | $233\pm31$     | 229±28       | [18] |
|  |   |             |                |              |      |

|  | Table S4 – Continued from previous page |                              |                    |      |
|--|---|------------------------------|--------------------|------|
| MONOMER  | $T_g^{exp}$                             | $T_g^{PLSR}$                 | $T_g^{R\tilde{F}}$ | Ref  |
| $\bigcirc$   | 253                                     | $196 \pm 20$                 | $188 \pm 91$       | [46] |
|  |   |                              |                    |      |
| •~• << <>>   | 150                                     | 160 + 17                     | 169 + 92           | [46] |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   | 100                                     | 1001 11                      | 100 102            | [10] |
|  |   |                              |                    |      |
| $\sim$   | 148                                     | $148{\pm}~26$                | $120{\pm}81$       | [46] |
|  |   |                              |                    |      |
|  | 89                                      | $126\pm\ 26$                 | $124 \pm 73$       | [46] |
|  |   |                              |                    |      |
| r° <sup>-0</sup> <sup>-0</sup> <sup>-1</sup> √ <sup>−</sup> ~  |   |                              |                    |      |
| ××·····  | 60                                      | $116\pm 26$                  | $91 \pm 52$        | [46] |
|  |   |                              |                    |      |
| ~0   | 48                                      | $89\pm\ 29$                  | $125\pm60$         | [46] |
| · · · · · · · · · · · · · · · · · · ·  |   |                              |                    |      |
| یر.<br>مرد   | 16                                      | 81± 39                       | $106 \pm 56$       | [46] |
| ·r   |   |                              |                    |      |
| لمسمس  |   |                              |                    |      |
| , Guora a de Cara de C | 212                                     | $237\pm78$                   | $200 \pm 40$       | [61] |
| 550 S  | 247                                     | $268 \pm\ 79$                | $215\pm41$         | [61] |
| r Halgo  |   |                              |                    |      |
|  | 266                                     | $292\pm 82$                  | $224 \pm 41$       | [61] |
| and<br>A. O'antarian   | 143                                     | $148 \pm 20$                 | 144+46             | [51] |
|  | 149                                     | $140 \pm 20$<br>$151 \pm 17$ | 197+44             | [51] |
|  | 142                                     | 101 17                       | 121 1 44           | [01] |
|  | 145                                     | $178 \pm 18$                 | $133 \pm 30$       | [51] |
| s the state  | 193                                     | $148 \pm 18$                 | $187 \pm 29$       | [63] |
| s-()-i-()- N   |   |                              |                    | [00] |
|  | 202                                     | $144\pm\ 20$                 | $197 \pm 32$       | [63] |
|  |   |                              |                    |      |
|  | 110                                     | $98\pm$ 31                   | $107\pm53$         | [60] |
| °⇒s, s, s   | 65                                      | E   9E                       | 60   47            | [60] |
|  | 60                                      | $5\pm 35$                    | 60±47              | [60] |
|  | 47                                      | $10\pm~56$                   | $58\pm48$          | [60] |
|  | 331                                     | $218 \pm 23$                 | $300 \pm 74$       | [45] |
|  | 001                                     | 2101 20                      | 000111             | [10] |
|  | 346                                     | $232 \pm 23$                 | $325 \pm 52$       | [45] |
|  | Urti                                    | _01_ 10                      | 220102             | [10] |
|  | 970                                     | 224⊥ 2F                      | <u>980⊥ 79</u>     | [45] |
| A. C. C.   | 302                                     | 204 <u>T</u> 20              | 200±12             | [40] |
|  | 340                                     | $227 \pm 23$                 | $322 \pm 64$       | [45] |
|  | 015                                     |                              |                    | [-~] |
|  | 177                                     | $192{\pm}~36$                | $203 \pm 46$       | [45] |
|  |   |                              |                    |      |
| < { < < < < < < < < < < < < < < < < < <  |   |                              |                    |      |

|   | Table S4 – Continued from previous page |             | ~              |                |      |
|---|---|-------------|----------------|----------------|------|
| MONOMER   |   | $T_g^{exp}$ | $T_g^{PLSR}$   | $T_g^{RF}$     | Ref  |
| $\langle \rangle$   |   | 90          | $158 \pm 16$   | $125 \pm 84$   | [12] |
|   |   |             |                |                |      |
|   |   |             |                |                |      |
| -\\<br>   |   | 52          | $139\pm$ 15    | $171 \pm 93$   | [12] |
| 1°  |   |             |                |                |      |
| Ū.  |   | 58          | $126 \pm 16$   | $151 \pm 88$   | [12] |
| Â   |   | 00          | 1201 10        | 101200         | [12] |
| ~;~~~   |   |             |                |                |      |
| Lancet  |   | 64          | $96\pm 17$     | $89 \pm 52$    | [12] |
|   |   | 73          | $132 \pm 14$   | $180 \pm 107$  | [12] |
|   |   | 10          | 1021 14        | 100±101        | [12] |
|   |   |             |                |                |      |
| Ŷ   |   | 58          | $93\pm$ 15     | $124 \pm 91$   | [12] |
| $\downarrow$ ,, $\Box_{i}$ ,  |   | <b>F</b> 0  | 1011 12        | 100 - 00       | [10] |
| $\bigcirc$  |   | 59          | $104 \pm 16$   | $168 \pm 92$   | [12] |
| L   |   |             |                |                |      |
|   |   | 193         | $226 \pm 21$   | $200 \pm 51$   | [44] |
| s<br>A  |   | 100         | 2201 21        | 200101         | [**] |
| -90, 08   |   |             |                |                |      |
|   |   | 109         | $217\pm 30$    | $187 \pm 47$   | [44] |
| Brive CO  |   |             |                |                |      |
| Xni~n0  |   | 161         | $243\pm\ 23$   | $184 {\pm} 43$ | [44] |
| -0 <u>-</u>   |   |             |                |                |      |
| <<br>(  |   | 217         | $238 \pm \ 19$ | $215\pm69$     | [44] |
| - and |   |             |                |                |      |
|   |   | 007         | 000   10       | 024   10       | [10] |
| 20.0°00   |   | 221         | 206± 10        | 234±19         | [13] |
| bardo.  |   | 230         | $211\pm 11$    | $232 \pm 20$   | [13] |
|   |   | 231         | $226 \pm \ 11$ | $230\pm27$     | [13] |
|   |   | 266         | $228{\pm}~21$  | $235\pm22$     | [13] |
| 11.0°0;-0;-0  |   | 205         | $209 \pm \ 16$ | $236\pm26$     | [13] |
| jalandio. 0   |   | 275         | $295\pm~11$    | $287 \pm 31$   | [5]  |
|   |   |             |                |                |      |
| - ""  |   | 296         | $305{\pm}~13$  | $283 \pm 30$   | [5]  |
|   |   | ~~ .        | 082            | 0001.55        | [    |
|   |   | 251         | $273 \pm 12$   | $282 \pm 40$   | [5]  |
|   |   | 281         | $322\pm 16$    | $271 \pm 41$   | [5]  |
|   |   |             |                |                |      |
| - ~,  |   | 299         | $283 \pm\ 24$  | $283 \pm 43$   | [5]  |
|   |   |             |                |                |      |
| Q'A M   |   | 287         | $315\pm$ 15    | $286{\pm}30$   | [5]  |
| r L L. L. L   |   |             |                |                |      |

| Table S   | 54 – Continued from previous page |                         |                |      |
|---|-----------------------------------|-------------------------|----------------|------|
| MONOMER   | $T_g^{exp}$                       | $T_g^{PLSR}$<br>324± 17 | $T_g^{RF}$     | [5]  |
| بې مې د.  | 323                               | 024 <u>⊤</u> 1/         | 201 ± 30       | [9]  |
|   | 283                               | 294± 14                 | 278±37         | [5]  |
|   | 328                               | $320\pm~21$             | $289 \pm 47$   | [5]  |
| Śń  | 303                               | $289 \pm\ 23$           | $285 \pm 40$   | [5]  |
|   | 208                               | $189\pm~20$             | $214 \pm 20$   | [49] |
| وموري بردين   | 238                               | $259\pm~86$             | $249 \pm 38$   | [49] |
| - and a de  | 235                               | $228 \pm 19$            | $224 \pm 24$   | [49] |
| or open and   | 85                                | $32\pm~28$              | 89±37          | [42] |
| $\mathcal{A}^{h}_{o} \sim \mathcal{M}^{h}_{e}$  | 105                               | 42+ 28                  | $100 \pm 48$   | [42] |
| \Long <sup>1</sup> <sup>1</sup> · Λ <sup>2</sup> <sup>1</sup> L <sup>2</sup> ≥ 0                    | 105                               | 421 20                  | 100740         | [*2] |
| $\sqrt{\hat{L}_0} \sim \sqrt{\hat{L}_0} \sqrt{\hat{L}_0} \sqrt{\hat{L}_0} = 0$                      | 44                                | 41± 28                  | $99{\pm}70$    | [42] |
| $\mathcal{L}_{\alpha}^{\alpha} \sim \mathcal{L}_{\alpha}^{\beta} \sim \mathcal{L}_{\alpha}^{\beta}$ | 109                               | $28\pm 35$              | 93±28          | [42] |
|   | 74                                | $50\pm 46$              | $82 \pm 55$    | [50] |
| Vitoria and   | 113                               | $20\pm 85$              | $109 \pm 69$   | [50] |
|   | 105                               | $58\pm 23$              | 95±29          | [30] |
|   | 98                                | $140{\pm}~14$           | $109 \pm 30$   | [30] |
|   | 140                               | 87± 27                  | $126 \pm 37$   | [30] |
|   | 99                                | $118{\pm}~22$           | $110\pm30$     | [30] |
|   | 124                               | $106{\pm}~24$           | $121 \pm 38$   | [30] |
|   |                                   |                         |                |      |
| 0 <sup>1</sup> 0,0 <sup>1,0</sup>   | 112                               | $152\pm\ 22$            | $139 \pm 59$   | [30] |
|   | 123                               | $187 \pm\ 12$           | $166 \pm 48$   | [30] |
|   | 214                               | $166 \pm ~34$           | $199 \pm 42$   | [30] |
|   |                                   |                         |                |      |
|   | 208                               | $158\pm$ 39             | $164 \pm 55$   | [30] |
| °°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°  |                                   |                         | <b>75</b> - 40 | [20] |
|   | 59                                | 75± 20                  | 75±42          | [30] |
|   | 85                                | $64\pm~21$              | 88±48          | [30] |
|   |                                   |                         |                |      |

| Table S4 - Continued from pre-   | evious page | ~                            | ~                            |              |
|--|-------------|------------------------------|------------------------------|--------------|
| MONOMER  | $T_g^{exp}$ | $T_g^{PLSR}$                 | $T_g^{RF}$                   | Ref          |
|  | 81          | $79\pm 24$                   | $130 \pm 50$                 | [30]         |
|  | 127         | 94± 17                       | $121 \pm 61$                 | [40]         |
|  | 77          | $96\pm 17$                   | $98\pm52$                    | [40]         |
|  | 129         | $121 \pm\ 13$                | $123 \pm 36$                 | [40]         |
|  |             |                              |                              |              |
| $\overset{\sim}{\longrightarrow} \overset{\sim}{\prod} \overset{\sim}{\underset{\sim}{\longrightarrow}} \overset{\sim}{\longrightarrow} \overset{\sim}{\underset{\sim}{\longrightarrow}}$  | 75          | $122 \pm 16$                 | $98 \pm 42$                  | [40]         |
|  | 93<br>247   | $147 \pm 19$<br>$228 \pm 11$ | $105\pm 56$<br>$238\pm 20$   | [40]<br>[8]  |
| E a a a a  |             |                              |                              | [-]          |
| and and a set of the s | 215         | $214 \pm 10$                 | $224 \pm 19$                 | [8]          |
| andahanan  | 153         | $162 \pm 18$                 | $176 \pm 32$                 | [57]         |
| and the second sec   | 188         | $223 \pm 15$                 | $230 \pm 33$                 | [57]         |
| Jane .   | 230         | $246 \pm \ 15$               | $242{\pm}29$                 | [57]         |
|  | 259         | $230{\pm}~24$                | $247 \pm 35$                 | [55]         |
| ora to to to   | 292         | $200\pm$ 18                  | $272 \pm 53$                 | [55]         |
| ta at-ol   | 238         | $211\pm 19$                  | $246 \pm 28$                 | [55]         |
| opponenter a   | 273         | $280\pm 20$                  | $256 \pm 19$                 | [19]         |
|  |             |                              |                              |              |
|  | 255         | $288 \pm ~17$                | $256 \pm 18$                 | [19]         |
| Chille -   |             |                              |                              |              |
|  | 261         | $281\pm18$                   | $258 \pm 14$                 | [19]         |
|  |             |                              |                              |              |
|  | 027         | 020   24                     | 062   20                     | [10]         |
| official and the second second   | 231         | 232± 34                      | 203±32                       | [19]         |
|  | 264         | $295\pm\ 25$                 | $263 \pm 22$                 | [19]         |
| -OFO-YOT-O-O-O-O-O-O-O-O-O-O-O-O-O-O-O-O-O-  |             |                              |                              |              |
|  | 206         | $202\pm 24$<br>$203\pm 21$   | $245 \pm 36$<br>$233 \pm 26$ | [35]<br>[35] |
|  | 233         | $203\pm21$<br>$239\pm12$     | $233\pm 20$<br>$233\pm 37$   | [24]         |
|  | 248         | $253 \pm 12$                 | $248 \pm 30$                 | [24]         |
| a.o. o.   | 250         | 219+14                       | 243+20                       | [24]         |
| a.a. a.   | 200         | 210 <u>1</u> 17              | 210 T 20                     | [= -]        |

|  | Table S4 – Continued from previous page |             |                              |                             |      |
|--|---|-------------|------------------------------|-----------------------------|------|
| MONOMER  |   | $T_g^{exp}$ | $T_g^{\widehat{PLSR}}$       | $\widehat{T_g^{RF}}$        | Ref  |
|  |   | 221         | $218 \pm 17$                 | $228 \pm 46$                | [17] |
|  |   | 248         | $215 \pm \ 18$               | 215±45                      | [17] |
|  |   | 250         | $225{\pm}~18$                | $245 \pm 36$                | [17] |
|  |   | 265         | $219 \pm \ 19$               | $245 \pm 39$                | [17] |
|  |   | 243         | 276± 29                      | $228 \pm 45$                | [17] |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~  |   |             |                              |                             |      |
| <sup>°</sup> گ، نہ، <sup>۵</sup>   |   | 235         | $253\pm\ 25$                 | 207±33                      | [20] |
| °۵۵،~۰<br>«۹۹»، ۵۰۰۰   |   | 199         | 229± 17                      | 203±33                      | [20] |
|  |   | 231         | 241± 15                      | 210±28                      | [20] |
| .0° 0.1  |   | 211         | $242 \pm 19$<br>$279 \pm 23$ | $194\pm 28$<br>213 $\pm 23$ | [20] |
|  |   | 245         | $262\pm12$                   | 247±14                      | [52] |
|  |   | 244         | $291 \pm 19$                 | $245\pm25$                  | [52] |
|  |   | 000         | 070 - 00                     | 0.40   05                   | [70] |
| and the second s |   | 220         | 279± 20                      | 240±25                      | [52] |
| v<br>.o <sup>r</sup> .totor  |   | 239         | 270± 28                      | 248±34                      | [52] |
|  |   | 257         | 248± 28                      | $230\pm38$                  | [52] |
| juli (   |   | 278         | $272 \pm 14$                 | $269\pm27$                  | [52] |
| do to to to  |   | 306         | $295 \pm 19$                 | 259±32                      | [52] |
| joraj o o  |   |             |                              |                             |      |

| Table S4 – Continued from  | previous page |                        |                      |       |
|--|---------------|------------------------|----------------------|-------|
| MONOMER  | $T_g^{exp}$   | $T_g^{\widehat{PLSR}}$ | $\widehat{T_g^{RF}}$ | Ref   |
| $\overline{\mathbb{Q}}$  | 227           | $265 \pm 15$           | $235 \pm 17$         | [52]  |
|  |               |                        |                      |       |
|  |               |                        |                      |       |
|  | 243           | $290\pm\ 21$           | $245 \pm 39$         | [52]  |
|  |               |                        |                      |       |
|  | 226           | $197 \pm 26$           | $237 \pm 21$         | [64]  |
| on <sup>ora</sup> ta charan  | *             |                        |                      | [* -] |
| , cr<br>, cro <sub>ves</sub> ,   | 248           | $217 \pm\ 34$          | $253 \pm 19$         | [64]  |
| · Ara-   | 245           | $178{\pm}~26$          | $241{\pm}22$         | [64]  |
| we have a second |               |                        |                      |       |
|  | 278           | $211\pm\ 21$           | $261\pm28$           | [64]  |
|  | 220           | $256 \pm \ 13$         | $224{\pm}19$         | [7]   |
| in all the   |               |                        |                      |       |
| J. J. C. L.  | 177           | $176\pm~29$            | $189\pm25$           | [7]   |
| 2 Second   | 150           | 005 1 05               | 000 1 05             | []    |
| A A A A A A A A A A A A A A A A A A A  | 157           | $205 \pm 25$           | $223 \pm 35$         | [7]   |
| y and y  | 229           | $190\pm14$             | $223 \pm 16$         | [65]  |
|  | 261           | $226 \pm \ 19$         | $254{\pm}28$         | [65]  |
| all and a second and   |               |                        |                      |       |
| ralatan a  | 227           | $193 \pm 15$           | $228 \pm 16$         | [65]  |
| ano and  | 262           | $214 \pm 20$           | $259 \pm 30$         | [65]  |
| A A A A A A A A A A A A A A A A A A A  | 178           | $192\pm$ 15            | $192 \pm 32$         | [9]   |
| 12 <sup>040</sup> 01   | 207           | $203\pm~30$            | $242\pm33$           | [9]   |
|  | 203           | $210{\pm}~19$          | $218 \pm 35$         | [9]   |
|  | 207           |                        | 007 1 00             | [0]   |
| glado an   | 205           | $202\pm\ 20$           | $207 \pm 20$         | [9]   |
|  | 134           | $87\pm~28$             | $119 \pm 58$         | [21]  |
|  |               |                        |                      |       |
|  |               |                        |                      |       |
|  | 132           | $102 \pm 12$           | $122 \pm 39$         | [37]  |
|  | 201           | $241{\pm}~24$          | $193{\pm}46$         | [37]  |
|  | 143           | $180\pm 24$            | $192\pm63$           | [37]  |
|  |               |                        |                      | []    |
|  |               |                        |                      |       |
|  | 165           | 204+ 22                | $177 \pm 43$         | [37]  |
|  | 105           | 2041 22                | 111 143              | [31]  |
|  | 264           | $173\pm~14$            | $244 {\pm} 56$       | [56]  |
| ju-ja.j.   |               |                        |                      |       |
| í í<br>Stí ísi   | 228           | $175 \pm\ 24$          | $221\!\pm\!29$       | [56]  |
|  |               |                        |                      |       |

|  | Table S4 – Continued from previous page | ~                      | ~                    |      |
|--|---|------------------------|----------------------|------|
| MONOMER  | $T_g^{exp}$                             | $T_g^{\widehat{PLSR}}$ | $\widehat{T_g^{RF}}$ | Ref  |
| to of the  | 255                                     | 225± 17                | 250±34               | [56] |
| E. S.  | 227                                     | 223± 27                | 228±22               | [56] |
| to a transfer to | 246                                     | $204\pm\ 27$           | $245 \pm 35$         | [56] |
| - the south of the   | 229                                     | 208± 26                | 234±32               | [56] |
| Solomon  | 217                                     | $197\pm\ 20$           | $204 \pm 38$         | [36] |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   | 237                                     | $229 \pm\ 23$          | $199{\pm}45$         | [36] |
|  | 327                                     | 342± 21                | 327±23               | [3]  |
| 0- <del>;</del> 0 <sup>, 0</sup> ;6<br>;-,   | 332                                     | 338± 22                | $334\pm28$           | [3]  |
|  | 356                                     | $352\pm~21$            | 343±27               | [3]  |
|  | 371                                     | 374± 25                | $351 \pm 25$         | [3]  |
|  | 333                                     | $354\pm52$             | 337±28               | [3]  |
| and the second s | 362                                     | $350\pm$ 48            | $350\pm26$           | [3]  |
| 0-20 <sup>1.0.1</sup> 0  | 301                                     | $284 \pm\ 14$          | $314 \pm 35$         | [3]  |
| , ini.Qia  | 303                                     | $283{\pm}~14$          | $311\pm39$           | [3]  |
|  | 319                                     | $289 \pm ~17$          | $310\pm32$           | [3]  |
| o o por mage   | 349                                     | $306\pm$ 29            | 313±39               | [3]  |
| · Painiain   | 304                                     | $318 \pm ~32$          | $313\pm32$           | [3]  |
| Soforger De  | 336                                     | $307\pm$ 33            | $316{\pm}32$         | [3]  |
|  | 264                                     | $296 \pm \ 17$         | $314 \pm 27$         | [2]  |
|  | 259                                     | $281 \pm\ 17$          | $318\pm28$           | [2]  |
|  |   |                        |                      |      |

|  | Table S4 – Continued from previous page |             |                              |                              |              |
|--|---|-------------|------------------------------|------------------------------|--------------|
| MONOMER  |   | $T_g^{exp}$ | $T_g^{\widehat{PLSR}}$       | $\widehat{T_g^{RF}}$         | Ref          |
| 100.001.001.00   |   | 301         | $322\pm 19$                  | $310 \pm 24$                 | [2]          |
| ون.<br>منابع   |   | 305         | 348± 17                      | $324 \pm 31$                 | [2]          |
|  |   | 317         | $350\pm16$                   | $319\pm32$                   | [2]          |
| jogonni<br>oralini soli  |   | 306         | $306\pm~20$                  | 307±28                       | [2]          |
|  |   | 328         | $311\pm$ 18                  | $320\pm26$                   | [2]          |
|  |   | 331         | $335\pm$ 18                  | $325\pm27$                   | [2]          |
|  |   | 353         | $383\pm~21$                  | $344\pm22$                   | [2]          |
| and the form   |   | 291         | $296 \pm 15$                 | $255 \pm 30$                 | [47]         |
| na hogo h  |   | 284<br>245  | $287 \pm 17$<br>$333 \pm 23$ | $256 \pm 29$<br>$261 \pm 34$ | [47]<br>[47] |
| And the second s |   | 255         | $293 \pm\ 23$                | $258 \pm 38$                 | [47]         |
| or a proton  |   | 263         | $286 \pm 19$                 | 268±34                       | [47]         |
|  |   | 208<br>251  | $290\pm 21$<br>$296\pm 21$   | $250\pm32$<br>$256\pm36$     | [47]         |
|  |   | 334         | $276 \pm 45$                 | $263 \pm 88$                 | [45]         |

| MONOMER   | $T_D^{exp}$ | $T_D^{pred}$    | Ref  |
|---|-------------|-----------------|------|
|   | 443         | $415 \pm 68$    | [61] |
|   | 391         | $401\pm60$      | [61] |
| - Malero  | 494         | $410 \pm 60$    | [61] |
| A B B B B B B B B B B B B B B B B B B B   | 424         | 410 ± 09        | [01] |
|   | 563         | $546\pm32$      | [25] |
| 10 000 00 00 00 00 00 00 00 00 00 00 00   | 546         | $536\pm30$      | [25] |
| - 0-0-4<br>   | 527         | $531\pm21$      | [25] |
|   | 508         | $480 \pm 36$    | [25] |
| of the second | 508         | 469 <u>1</u> 50 | [20] |
|   | 442         | $453 \pm 25$    | [15] |
|   |             |                 |      |
|   | 435         | $451 \pm 26$    | [15] |
|   |             |                 |      |
|   | 436         | $468\pm47$      | [15] |
|   |             |                 |      |
|   | 430         | $460\pm34$      | [15] |
|   |             |                 |      |
|   | 415         | $477~\pm~45$    | [15] |
|   |             |                 |      |
|   | 450         | $453 \pm 15$    | [15] |
|   |             |                 |      |
|   | 447         | $448 \pm 17$    | [15] |
|   |             |                 |      |
|   | 448         | $457\pm29$      | [15] |
|   |             |                 |      |
|   | 445         | $448 \pm 34$    | [15] |
|   |             |                 |      |
|   | 426         | $458\pm44$      | [15] |
|   |             |                 |      |
|   |             |                 |      |
|   | 125         | $300 \pm 75$    | [22] |
|   | 235         | $273\pm66$      | [22] |
|   |             |                 |      |

Table S5: The table lists the experimental and predicted ( $\pm$  uncertainty) 10% thermal decomposition temperatures for different polymers. Predictions for only the RF model are reported.

|  | Table S5 – Continued from previous page |    |              |       |
|--|---|----|--------------|-------|
| MONOMER  | $T_r^e$                                 | xp | $T_D^{pred}$ | Ref   |
| °. //  | 23                                      | 37 | $284 \pm 68$ | [22]  |
|  |   |    |              |       |
|  |   |    |              |       |
|  |   |    |              |       |
| s.   |   |    |              |       |
| $\bigtriangleup$   |   |    |              |       |
| "×".   | 51                                      | 13 | $499 \pm 36$ | [16]  |
|  |   |    |              |       |
|  |   |    |              |       |
|  |   |    |              |       |
| N FN FN  | 50                                      | 01 | $489 \pm 40$ | [16]  |
|  |   |    |              |       |
|  |   |    |              |       |
| Q  | -                                       | 07 | 405 1 90     | [1.6] |
| ,  | 50                                      | 07 | $495 \pm 30$ | [10]  |
|  |   |    |              |       |
|  |   |    |              |       |
|  | 40                                      | 96 | $493 \pm 40$ | [16]  |
|  |   | 00 | 100 1 10     | [10]  |
|  |   |    |              |       |
|  |   |    |              |       |
|  | 47                                      | 78 | $475 \pm 47$ | [16]  |
|  |   |    |              | 1 - 1 |
|  |   |    |              |       |
|  |   |    |              |       |
|  | 40                                      | 97 | $499 \pm 19$ | [53]  |
| afa-ba ara as  | 7.                                      | 51 | 400 1 10     | [55]  |
| /  | 49                                      | 94 | $487 \pm 49$ | [53]  |
| ana ang ang ang ang ang ang ang ang ang  |   |    |              | []    |
| 04 <u>0</u>  | 49                                      | 96 | $501 \pm 39$ | [53]  |
| tararanaf-a- <sub>tara</sub>   |   |    |              | []    |
| 640  | 53                                      | 32 | $516 \pm 34$ | [53]  |
| A CARACTER AND A CARACTER ANTE ANTE ANTE ANTE ANTE ANTE ANTE ANTE |   |    |              |       |
| An ho  |   |    |              |       |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   |   |    |              |       |
| 29   | 51                                      | 13 | $491 \pm 58$ | [53]  |
| to and of  |   |    |              |       |
|  | 24                                      | GE | 200 1 50     | [FO]  |
| $\gamma \sim 0^{\circ} $   | 50                                      | 05 | 380 T 38     | [59]  |
| 8 8  | 36                                      | 65 | $355~\pm~65$ | [59]  |
| ~~~ <sup>0,0</sup> ,0'~~~  |   |    |              |       |
| N = 1  | 51                                      | 10 | $506 \pm 20$ | [48]  |
|  |   |    |              |       |
|  |   |    |              |       |
|  |   |    |              |       |
| o text   | 49                                      | 96 | $499 \pm 25$ | [48]  |
|  |   |    |              |       |
|  |   |    |              |       |
|  |   |    |              |       |
|  |   |    |              |       |
| Lad  | 50                                      | 03 | $502 \pm 30$ | [48]  |
|  |   |    |              |       |
|  |   |    |              |       |
| J "U"  |   |    |              |       |
| ¥  | 48                                      | 82 | $491\pm36$   | [48]  |
| E Pro  |   |    |              |       |
|  |   |    |              |       |
| K-Y i  |   |    |              |       |
| As i   | 50                                      | 07 | $441 \pm 65$ | [48]  |
| Noto-  |   |    |              |       |
| ×.   |   |    |              |       |
|  | 52                                      | 29 | $528\pm19$   | [26]  |
| Poten an a   |   |    |              |       |

| MONOMER  | Table 55 – Continued from previous page | $T_D^{exp}$ | $T_D^{pred}$                 | Ref                |
|--|---|-------------|------------------------------|--------------------|
| . <u>8.</u> 9.0,0,0,0  |   | 536         | $521 \pm 27$                 | [26]               |
| a a a a a  |   | 532         | $534 \pm 23$                 | [26]               |
| ararata <sub>aan</sub>   |   | 500         | $497 \pm 35$                 | [26]               |
| ං<br>- ඉතින කිරීම  |   | 504         | $510\pm32$                   | [26]               |
| and and a set of the s |   | 456.2       | $504\pm31$                   | 10.1002/pola.23497 |
| 6<br>  |   | 453.3       | $474\pm61$                   | 10.1002/pola.23497 |
|  |   | 510         | $506\pm20$                   | [48]               |
|  |   |             |                              |                    |
|  |   | 496         | $400 \pm 25$                 | [48]               |
|  |   | 430         | 433 1 23                     | [40]               |
|  |   |             |                              |                    |
| il and the second secon |   | 503         | $502\pm30$                   | [48]               |
|  |   |             |                              |                    |
|  |   | 482         | $491\pm36$                   | [48]               |
| North Control of the second seco   |   |             |                              |                    |
|  |   | 507         | $441 \pm 65$                 | [48]               |
|  |   |             |                              |                    |
| Y. A.  |   | 557.6       | $528\pm34$                   | [27]               |
| Janin para   |   | 549.7       | $539 \pm 35$                 | [27]               |
| 0,000,000,0  |   | 506.3       | $497 \pm 30$                 | [27]               |
| ന്നുക്കുന്നത്  |   | 429         | $436\pm40$                   | [44]               |
| · ~  |   |             |                              |                    |
| ~~~~~~   |   | 407         | $411\pm30$                   | [44]               |
| gu.~. ye   |   |             |                              |                    |
| Xa'~aA   |   | 408         | $418\pm31$                   | [44]               |
|  |   |             |                              |                    |
|  |   | 486         | $442 \pm 41$                 | [44]               |
|  |   |             |                              |                    |
| 10.0°000   |   | 533         | $520 \pm 31$                 | [13]               |
| , a. a. a. a.  |   | 543         | $519 \pm 35$                 | [13]               |
| à.a.a.a. <sup>2</sup>  |   | 540         | $527~\pm~39$                 | [13]               |
| à.o.o.o.o.   |   | 508         | $491 \pm 63$                 | [13]               |
| 00 <sup>1</sup> 00   |   | 503         | $518 \pm 54$<br>$540 \pm 20$ | [13]               |
|  |   | 002         | J40 T 29                     | [3]                |

| MONOMER   | Table S5 – Continued from previous page $T_D^{exp}$ | $T_D^{pred}$ | Ref  |
|---|---|--------------|------|
|   | 500   | $507 \pm 22$ | [5]  |
|   | 554   | $539~\pm~33$ | [5]  |
|   |   | 510 L 00     | [-]  |
| Joseph Colorado   | 523   | $513 \pm 38$ | [5]  |
|   | 517   | $505\pm51$   | [5]  |
| She was a first of the  |   | 510 50       | [-]  |
|   | 539   | $512 \pm 56$ | [5]  |
|   | 563   | $550\pm38$   | [5]  |
| i i i i i i i i i i i i i i i i i i i   | 484   | $500 \pm 36$ | [5]  |
| to the second |   | 000 ± 00     | [0]  |
| that the  | 537   | $536 \pm 35$ | [5]  |
|   | 531   | $510\pm46$   | [5]  |
| · · · · · · · · · · · · · · · · · · ·   | 540   | $523 \pm 37$ | [5]  |
| de la trada   | 049   | 525 ± 51     | [0]  |
|   | 357   | $421\pm65$   | [30] |
|   |   |              |      |
|   | 433   | $430 \pm 45$ | [30] |
|   | 327   | $423\pm63$   | [30] |
|   | 242   | $391 \pm 92$ | [30] |
|   |   |              |      |
| $(\mathbf{Q}, \mathbf{Q})$  | 241   | $422 \pm 63$ | [30] |
|   | 430   | $430 \pm 51$ | [30] |
|   |   |              | [~~] |
|   | 471   | $405 \pm 88$ | [30] |
|   | 484   | $465\pm39$   | [30] |
|   |   |              |      |
|   | 414   | $428\pm51$   | [30] |
|   |   |              |      |
|   | 405   | $422 \pm 62$ | [30] |
|   |   |              |      |
| d V   | 433   | $425\pm60$   | [30] |
|   |   |              |      |
|   | 443   | $422\pm62$   | [30] |
|   | 540   | $527 \pm 34$ | [8]  |
| Exa a a   |   |              |      |

|   | Table S5 - | <ul> <li>Continued from previous page</li> </ul> |             |                    |                |
|---|------------|--|-------------|--------------------|----------------|
| MONOMER                                     |            |  | $T_D^{exp}$ | $T_D^{pred}$       | $\mathbf{Ref}$ |
| °   |            |  | 529         | $524 \pm 21$       | [8]            |
|   |            |  |             |                    |                |
| / U,D U                                     |            |  | 478         | $448 \pm 58$       | [57]           |
| a dia ana ana ana ana ana ana ana ana ana a |            |  | 110         | 110 ± 00           | [01]           |
|   |            |  | 409         | $477 \pm 51$       | [57]           |
|   |            |  |             |                    | [*.]           |
|   |            |  |             |                    |                |
|   |            |  | 521         | $480 \pm 50$       | [57]           |
| and a                                       |            |  |             |                    | [···]          |
|   |            |  |             |                    |                |
|   |            |  | 522         | $502 \pm 21$       | [19]           |
| ~Q(   |            |  |             |                    | [-~]           |
| i r. C                                      |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  | 507         | $501 \pm 24$       | [19]           |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
| °' 🔽 'n-<                                   |            |  |             |                    |                |
|   |            |  | 510         | $503 \pm 24$       | [19]           |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
| n N   |            |  | 490         | $489 \pm 52$       | [19]           |
| ЧС <sub>2</sub> .                           |            |  |             |                    |                |
| ann i Ato                                   |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  | 518         | $495 \pm 28$       | [19]           |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~      |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  |             | <b>F</b> ( 0 ) 0 0 | [a. i]         |
|   |            |  | 542         | $540 \pm 30$       | [24]           |
|   |            |  |             |                    |                |
|   |            |  | 545         | $516 \pm 33$       | [24]           |
|   |            |  |             |                    |                |
| K-67.                                       |            |  | 501         | E10   20           | [94]           |
| a a)0'0.4                                   |            |  | 021         | $312 \pm 38$       | [24]           |
| V.V   |            |  |             |                    |                |
| N > N                                       |            |  | 542         | $479 \pm 46$       | [17]           |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
| . D   |            |  |             |                    |                |
| N N   |            |  | 545         | $478 \pm 44$       | [17]           |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
| NN  |            |  | 521         | $488 \pm 53$       | [17]           |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
| " D   |            |  |             |                    |                |
| N <sub>N 10</sub>                           |            |  | 556         | $481 \pm 49$       | [17]           |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  | 536         | $507 \pm 36$       | [17]           |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
| <u></u>                                     |            |  | 423         | $445~\pm~34$       | [20]           |
| ¥.~°  |            |  |             |                    |                |
|   |            |  |             |                    |                |
| La La                                       |            |  | 10.1        | 417 00             | [00]           |
|   |            |  | 404         | $417 \pm 80$       | [20]           |
|   |            |  |             |                    |                |
|   |            |  |             |                    |                |
| °~~a  |            |  | 421         | $450\pm36$         | [20]           |
| "QQ_~~"                                     |            |  |             |                    |                |
|   |            |  |             |                    |                |

|  | Table S5 – Continued from previous page |                              |             |
|--|---|------------------------------|-------------|
| MONOMER  | $T_D^{exp}$                             | $T_D^{pred}$                 | Ref         |
|  | 401                                     | $428 \pm 76$                 | [20]        |
|  | 410                                     | $465\pm44$                   | [20]        |
|  | 498                                     | $506\pm22$                   | [52]        |
|  |   |                              | [***]       |
|  | 507                                     | $519 \pm 34$                 | [52]        |
|  | 495                                     | $497 \pm 44$                 | [52]        |
|  |   |                              | [- ]        |
|  | 506                                     | $503\pm34$                   | [52]        |
|  | 467                                     | $459\pm49$                   | [52]        |
|  |   |                              |             |
|  | 509                                     | $513\pm18$                   | [52]        |
| -6,04-0-0  | 510                                     | E12   20                     | [50]        |
| á<br>ciricia ciricia   | 312                                     | $513 \pm 32$                 | [52]        |
|  | 501                                     | $510 \pm 40$                 | [52]        |
|  |   |                              |             |
|  | 505                                     | $516\pm32$                   | [52]        |
|  |   |                              |             |
| langeralan.<br>J   | 427                                     | $440\pm37$                   | [64]        |
| .or. <sub>ov.ov.ov.ov.</sub> or.   | 439                                     | $477 \pm 48$                 | [64]        |
| -o <sup>doro</sup> do  | 431                                     | $438 \pm 35$                 | [64]        |
| anaravarara  | 439<br>443                              | $473 \pm 44$<br>$469 \pm 45$ | [64]<br>[7] |
| a poros  |   | 100                          |             |
| word along the second s | 374                                     | $432 \pm 74$                 | [7]         |
| ann <sup>a</sup> rada  | 354                                     | $419 \pm 66$                 | [7]         |
| arean area ar  | 511 404                                 | $473 \pm 63$<br>500 + 34     | [9]         |
| re da  | 506                                     | $494 \pm 38$                 | [9]         |
| a,<br>alanda para  |   |                              |             |

|  | Table S5 – Continued from previous page |             |                 |       |
|--|---|-------------|-----------------|-------|
| MONOMER  |   | $T_D^{exp}$ | $T_D^{pred}$    | Ref   |
| ala afa an   |   | 498         | $459 \pm 64$    | [a]   |
| -Q' '''o   |   | 262.0       | $372 \pm 31$    | [33]  |
| auto to the second second  |   | 503.9       | 012 1 01        | [33]  |
|  |   | 369         | $372\pm30$      | [33]  |
| antototo   |   | 262.0       | 200   20        | [99]  |
| anorthetechar  |   | 303.2       | $380 \pm 30$    | [33]  |
| Addition and   |   | 357         | $406\pm86$      | [31]  |
| - At A TO  |   | 250         | 262 ± 55        | [91]  |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   |   | 350         | $302 \pm 35$    | [31]  |
|  |   | 350         | $376 \pm 49$    | [32]  |
| Ži pod-c   |   |             |                 |       |
| 0,9  |   | 340         | $385 \pm 63$    | [32]  |
| ,,   |   |             |                 | L- J  |
| 09   |   | 312.5       | $365 \pm 85$    | [21]  |
| 7,   |   | 01210       | 000 <u>T</u> 00 | [=+]  |
| s v s  |   |             |                 |       |
| s s  |   | 460         | $442 \pm 52$    | [56]  |
|  |   |             |                 |       |
|  |   | 445         | $436\pm42$      | [56]  |
|  |   |             |                 |       |
| (i   |   | 439         | $466~\pm~44$    | [56]  |
| the action   |   |             |                 |       |
| a alut o   |   | 499         | 440   97        | [= c] |
| ¢.   |   | 433         | 440 ± 27        | [50]  |
| A CALL   |   |             |                 |       |
| 4.0<br>  |   | 450         | $461\pm35$      | [56]  |
| to at the  |   |             |                 |       |
|  |   | 110         | 110 1 00        | [= 0] |
| The country of   |   | 440         | $440 \pm 22$    | [00]  |
| Land Of the  |   |             |                 |       |
| <u></u>  |   | 516         | $512 \pm 21$    | [3]   |
| , <b>.</b>   |   |             |                 |       |
|  |   |             |                 |       |
| ° - C  |   | 520         | $508\pm23$      | [3]   |
| Q <sup>r</sup>   |   |             |                 |       |
| o-ioi i  |   |             |                 |       |
|  |   | 528         | $510\pm25$      | [3]   |
| or official official   |   |             |                 |       |
| ****   |   |             |                 |       |
| -<br>  |   | 529         | $501 \pm 30$    | [3]   |
| Q  |   |             |                 |       |
| ot of of   |   |             | FO( 1           | [0]   |
|  |   | 543         | $524 \pm 32$    | [3]   |
| and the second sec |   |             |                 |       |

| MONOMER                        | Table S5 | - Continued from previous page | $T_D^{exp}$ | $T_D^{pred}$ | Ref  |
|--------------------------------|----------|--------------------------------|-------------|--------------|------|
| or contraction                 |          |                                | 539         | $514 \pm 30$ | [3]  |
| ٠٠<br>٥-;٥ <sup>:,٥,:</sup> ٩. |          |                                | 506         | $506\pm34$   | [3]  |
| o-;o <sup>i,O,i</sup> q.       |          |                                | 508         | $509\pm24$   | [3]  |
| o o joi. O. iq.                |          |                                | 513         | $503 \pm 36$ | [3]  |
| a joi a joi                    |          |                                | 516         | $502 \pm 27$ | [3]  |
| ogoiolog.                      |          |                                | 522         | $514\pm36$   | [3]  |
| opolaig.                       |          |                                | 518         | $515 \pm 25$ | [3]  |
|                                |          |                                | 455         | $466 \pm 25$ | [2]  |
|                                |          |                                | 461         | $465\pm25$   | [2]  |
| 0.101.01.<br>0.101.01.         |          |                                | 473         | $466 \pm 29$ | [9]  |
| a. of of                       |          |                                | 110         | 100 1 20     | [-]  |
|                                |          |                                | 477         | $464\pm26$   | [2]  |
|                                |          |                                | 458         | $464\pm24$   | [2]  |
| 20-30-1.004<br>0               |          |                                | 451         | $454 \pm 20$ | [9]  |
| o'a tat a                      |          |                                | 401         | 404 1 25     | [2]  |
|                                |          |                                | 460         | $464\pm27$   | [2]  |
|                                |          |                                | 468         | $465\pm24$   | [2]  |
|                                |          |                                | 482         | 474 + 29     | [9]  |
|                                |          |                                | 102         | 111 ± 20     | [-]  |
| or<br>. militari               |          |                                | 396         | $415\pm41$   | [47] |
| an when                        |          |                                | 440         | $423\pm30$   | [47] |
|                                |          |                                | 383         | $406\pm38$   | [47] |
| wayeter                        |          |                                | 412         | $425 \pm 45$ | [47] |

| Table $S5 - Continued$ from previous page   |             |              |      |  |  |
|---|-------------|--------------|------|--|--|
| MONOMER                                     | $T_D^{exp}$ | $T_D^{pred}$ | Ref  |  |  |
| a a h b f b h b h b h b h b h b h b h b h b | 425         | $408 \pm 38$ | [47] |  |  |
| o Price                                     | 389         | $398\pm41$   | [47] |  |  |
|   | 375         | $390\pm49$   | [47] |  |  |
|   | 250         | $270\pm50$   | [10] |  |  |
|   | 055         | 068   46     | [10] |  |  |
|   | 200         | $208 \pm 40$ | [10] |  |  |
|   | 300         | $290\pm56$   | [10] |  |  |
|   | 318         | $298\pm57$   | [10] |  |  |
|   | 300         | $299 \pm 53$ | [10] |  |  |
|   |             |              |      |  |  |
|   | 280         | $311 \pm 68$ | [10] |  |  |
|   |             |              |      |  |  |

| MONOMER                          | $\rho_{exp}$ | $\rho_{pred}$   |
|----------------------------------|--------------|-----------------|
| -0                               | 1.42         | $1.22 \pm 0.18$ |
| ~~~ <sup>\$</sup> .              | 1.11         | $1.09 \pm 0.17$ |
|                                  | 1.06         | $1.14 \pm 0.27$ |
| S Si o                           | 1.10         | $1.17 \pm 0.20$ |
|                                  |              |                 |
|                                  | 1.11         | $1.09 \pm 0.09$ |
|                                  |              |                 |
|                                  | 1.30         | $1.30 \pm 0.25$ |
|                                  |              |                 |
|                                  | 1.09         | $1.15 \pm 0.20$ |
|                                  | 0.91         | $0.93 \pm 0.08$ |
|                                  | 0.91         | $0.98 \pm 0.16$ |
| sit o                            | 0.89         | $0.92 \pm 0.10$ |
|                                  | 0.88         | $0.93 \pm 0.13$ |
| $\sim$                           | 1.12         | $1.14 \pm 0.17$ |
|                                  | 0.89         | $0.98 \pm 0.13$ |
|                                  | 1.14         | $1.18 \pm 0.12$ |
|                                  | 1.39         | $1.38 \pm 0.16$ |
| $\rightarrow$                    |              |                 |
|                                  |              |                 |
|                                  | 0.98         | $1.03 \pm 0.17$ |
| ~~~ <sup>0</sup>                 | 0.93         | $1.01 \pm 0.14$ |
|                                  | 2.10         | $1.93 \pm 0.33$ |
| $\mathbf{O}$                     |              |                 |
| Br → Br<br><sup>°</sup> ~°∩∩ ∩∩° | 1.20         | $1.18 \pm 0.10$ |
|                                  | 1.30         | $1.25 \pm 0.09$ |
|                                  |              |                 |
|                                  | 1.66         | $1.48 \pm 0.23$ |
| $\sim$                           |              |                 |
|                                  |              |                 |
|                                  | Continued    | d on next page  |

Table S6: The table lists the experimental and predicted ( $\pm$  uncertainty) densities for different polymers. Predictions for only the RF model are reported. The experimental values are taken from multiple references[23, 4, 34]

| Table S6 - Continued from previous page |                           |                                     |
|---|---------------------------|-------------------------------------|
| MONOMER                                 | $\frac{\rho_{exp}}{1.60}$ | $\frac{\rho_{pred}}{1.46 \pm 0.20}$ |
|   |                           |                                     |
| $\mathbf{v}$                            |                           |                                     |
|   |                           |                                     |
| F                                       |                           |                                     |
| s, <sup>Si</sup>                        | 0.98                      | $1.01 \pm 0.09$                     |
|   | 1.20                      | $1.17 \pm 0.11$                     |
|   |                           |                                     |
|   |                           |                                     |
| $\sim$                                  | 0.95                      | $0.95 \pm 0.14$                     |
|   |                           |                                     |
| $\sim$                                  | 1.20                      | 1 40 1 0 14                         |
|   | 1.38                      | $1.40 \pm 0.14$                     |
|   | 1.00                      |                                     |
| F /                                     | 1.38                      | $1.39 \pm 0.15$                     |
|   |                           |                                     |
| 0                                       | 1.25                      | $1.18 \pm 0.09$                     |
|   |                           |                                     |
| N - N                                   |                           |                                     |
|   |                           |                                     |
|   | 1.26                      | $1.02 \pm 0.15$                     |
|   |                           |                                     |
| 0 P                                     | 1.10                      | $1.17\pm0.13$                       |
|   |                           |                                     |
|   |                           |                                     |
| -0 //                                   | 1.17                      | $1.13 \pm 0.05$                     |
|   |                           |                                     |
|   |                           |                                     |
|   | 0.99                      | $1.01\pm0.04$                       |
|   |                           |                                     |
|   |                           |                                     |
| F II                                    | 1.34                      | $1.37 \pm 0.20$                     |
|   |                           |                                     |
| ≣ <mark>0</mark>                        | 1.02                      | $1.03 \pm 0.11$                     |
|   |                           |                                     |
|   |                           |                                     |
|   | 1.03                      | $1.05 \pm 0.09$                     |
|   |                           |                                     |
|   |                           |                                     |
| õ l                                     | 1.27                      | $1.33 \pm 0.17$                     |
|   |                           |                                     |
|   |                           |                                     |
| ▼                                       | 1.13                      | $1.12\pm0.08$                       |
|   |                           |                                     |
|   | 1.07                      | 1.05   0.00                         |
|   | 1.05                      | $1.05 \pm 0.06$                     |
| $\gamma \gamma$                         |                           |                                     |
|   | 1.17                      | $1.19 \pm 0.08$                     |
|   |                           |                                     |
| Ϋ́́, Ϋ́, Ϋ́, Ϋ́, Ϋ́, Ϋ́, Ϋ́, Ϋ́,        |                           |                                     |
| $\bigcirc$                              |                           |                                     |
| ¥                                       | a i                       | , ,                                 |

| Table S6 – Continued from previous page                            | 2                         |                                     |
|--|---------------------------|-------------------------------------|
|  | $\frac{\rho_{exp}}{1.00}$ | $\frac{\rho_{pred}}{1.02 \pm 0.05}$ |
| <sup>⊥</sup> <sup>µ</sup> <sup>°</sup> ° <sup>⊥</sup> <sup>−</sup> | 1.15                      | 1 16   0.07                         |
|  | 1.15                      | $1.16 \pm 0.07$                     |
|  | 1.02                      | $1.04 \pm 0.06$                     |
|  | 1.03                      | 1.04 ± 0.00                         |
|  | 1.01                      | $1.02 \pm 0.05$                     |
|  | 1.12                      | $1.14 \pm 0.07$                     |
|  | 1.21                      | $1.17 \pm 0.09$                     |
|  | 1.10                      | $1.03 \pm 0.07$                     |
|  |                           |                                     |
| ~°, ⊥⊥́  | 1.11                      | $1.10 \pm 0.06$                     |
|  | 0.99                      | $1.04 \pm 0.07$                     |
|  | 1.04                      | $1.05 \pm 0.05$                     |
|  |                           |                                     |
|  | 1.04                      | $1.03 \pm 0.06$                     |
|  | 1.18                      | $1.10\pm0.09$                       |
|  | 1.08                      | $1.06 \pm 0.09$                     |
| $\sim$   |                           |                                     |
| ~k   | 1.00                      | $1.02 \pm 0.05$                     |
|  | 1.03                      | $1.04 \pm 0.05$                     |
|  | 1.05                      | $1.03\pm0.04$                       |
|  | 1.01                      | $1.03\pm0.04$                       |
| ~ ~ ~ ¥ ~  | 0.97                      | $1.01\pm0.06$                       |
|  | 0.93                      | $1.02 \pm 0.05$                     |
|  | 1.32                      | $1.30\pm0.18$                       |
|  | 1.15                      | $1.11\pm0.06$                       |
| ×, √, √, √,  |                           |                                     |

| Table S6 – Continued from previous page |                           |                                     |
|---|---------------------------|-------------------------------------|
| MONOMER                                 | $\frac{\rho_{exp}}{1.15}$ | $\frac{\rho_{pred}}{1.15 \pm 0.14}$ |
|   |                           |                                     |
|   | 1.10                      | $1.06 \pm 0.13$                     |
|   | 0.93                      | $0.99 \pm 0.10$                     |
|   | 1.00                      | $1.10\pm0.17$                       |
|   | 1.19                      | $1.12 \pm 0.09$                     |
| $\mathbb{A}_{\circ}$                    | 0.95                      | $1.05 \pm 0.10$                     |
|   | 0.92                      | $0.98 \pm 0.12$                     |
|   | 0.02                      | 0.06   0.10                         |
|   | 0.92                      | $0.96 \pm 0.10$                     |
|   | 1.14                      | $0.96 \pm 0.10$<br>$1.11 \pm 0.10$  |
|   |                           |                                     |
|   | 0.95                      | $0.99\pm0.12$                       |
|   | 1.27                      | $1.26 \pm 0.09$                     |
|   | 1.30                      | $1.25 \pm 0.14$                     |
| N                                       | 1.41                      | $1.20 \pm 0.21$                     |
|   |                           |                                     |
|   | 1.22                      | $1.18 \pm 0.12$                     |
|   | 1.00                      | $1.07 \pm 0.11$                     |
|   | 1.08                      | $1.09 \pm 0.06$                     |
|   | 1.12                      | $1.10 \pm 0.08$                     |
|   | 1.06                      | $1.09 \pm 0.05$                     |
| $\sim$                                  | 1.11                      | $1.04 \pm 0.12$                     |
| $\sim \sim ^{\circ} \chi \sim$          | 1.09                      | $1.09 \pm 0.06$                     |
| O                                       | Continue                  | l on next page                      |

| MONOMER                | Table S6 | - Continued from previous page |                           |                                     |
|------------------------|----------|--------------------------------|---------------------------|-------------------------------------|
| MONOMER                |          |                                | $\frac{\rho_{exp}}{1.18}$ | $\frac{\rho_{pred}}{1.17 \pm 0.10}$ |
| $\mathbf{N}$           |          |                                | 1110                      | 1111 ± 0.110                        |
|                        |          |                                |                           |                                     |
| IN                     |          |                                | 1.26                      | $1.25 \pm 0.09$                     |
| $\sim$ , $\sim$        |          |                                |                           |                                     |
| Q                      |          |                                | 1.31                      | $1.26 \pm 0.21$                     |
|                        |          |                                |                           |                                     |
| <b>○</b> 0 //          |          |                                | 1.02                      | $1.06 \pm 0.08$                     |
|                        |          |                                |                           |                                     |
| Ö                      |          |                                | 0.02                      | 0.00   0.11                         |
| <b>√√</b>              |          |                                | 0.93                      | $0.96 \pm 0.11$                     |
| × ~ . <sup>8</sup> .// |          |                                | 0.98                      | $1.09 \pm 0.14$                     |
|                        |          |                                | 1.04                      | $0.98\pm0.14$                       |
|                        |          |                                | 0.92                      | $0.94 \pm 0.13$                     |
|                        |          |                                | 0.99                      | $1.05 \pm 0.11$                     |
| N                      |          |                                | 0.01                      | $0.05 \pm 0.17$                     |
| ∽∽∽∽°∕∕                |          |                                | 0.91                      | $0.95 \pm 0.17$<br>0.98 + 0.12      |
|                        |          |                                | 1.04                      | $1.08 \pm 0.11$                     |
|                        |          |                                |                           |                                     |
| ∽∽∽∽∽°∕∕               |          |                                | 0.89                      | $0.95 \pm 0.14$                     |
| ~~~~~ <sup>6</sup> .~  |          |                                | 1.00                      | $1.12 \pm 0.10$                     |
|                        |          |                                | 1.01                      | $1.04 \pm 0.12$                     |
|                        |          |                                | 0.97                      | $1.03 \pm 0.14$                     |
| °~~~°0                 |          |                                | 1 36                      | $1.33 \pm 0.15$                     |
| 0                      |          |                                | 1.50                      | 1.35 ± 0.15                         |
| /''''<                 |          |                                |                           |                                     |
|                        |          |                                |                           |                                     |
|                        |          |                                | 1.60                      | $1.22 \pm 0.15$                     |
| 0                      |          |                                |                           |                                     |
|                        |          |                                |                           |                                     |
|                        |          |                                |                           |                                     |
|                        |          |                                | 0.99                      | $1.12 \pm 0.21$                     |
| Si o Si o Si           |          |                                |                           |                                     |
| $\sim$ /               |          |                                | 0.91                      | $0.92 \pm 0.07$                     |
| Si                     |          |                                |                           |                                     |
|                        |          |                                | 1.06                      | $1.16 \pm 0.12$                     |
| $\sqrt{-\nabla}$       |          |                                |                           |                                     |
|                        |          |                                |                           |                                     |
| \\ //                  |          |                                |                           |                                     |
|                        |          |                                | 1.36                      | $1.22 \pm 0.12$                     |
| $\sqrt{-\nabla}$       |          |                                |                           |                                     |
|                        |          |                                |                           |                                     |
| \\ //                  |          |                                |                           |                                     |
|                        |          |                                | 0.85                      | $0.91\pm0.10$                       |
|                        |          |                                | 0.91                      | $0.94 \pm 0.10$                     |
| Λ                      |          |                                | 0.31                      | 2.04 T 0.10                         |
| $\sum C \equiv$        |          |                                |                           |                                     |
|                        |          |                                | 0.85                      | $0.88 \pm 0.10$                     |
|                        |          |                                |                           |                                     |
| $\sim$                 |          |                                | 0.01                      | $0.95 \pm 0.11$                     |
|                        |          |                                | 0.91                      | 0.30 ± 0.11                         |
|                        |          |                                |                           |                                     |
| $\sim$                 |          |                                |                           | 0.00 1.5 15                         |
| ~ //                   |          |                                | 0.89                      | $0.98 \pm 0.12$                     |
| 1/1/                   |          |                                |                           |                                     |
| ·                      |          |                                | 1.05                      | $1.02\pm0.10$                       |
| $\ll$ Y $\sim$         |          |                                |                           |                                     |
| L J                    |          |                                |                           |                                     |
| $\sim$                 |          |                                |                           |                                     |

| MONOMER |
|---------|
|         |

| MONOMER                                | Table 50 Continued from previous page | $\rho_{exp}$                                | $\rho_{pred}$   |
|--|---------------------------------------|---|---|
|  |                                       | 1.04  | $1.03 \pm 0.10$   |
| $\overline{}$                          |                                       | 0.86  | $0.90\pm0.08$   |
|  |                                       | 0.89  | $0.92\pm0.10$   |
| $\sim$                                 |                                       | 1.05  | $1.04 \pm 0.10$   |
|  |                                       | 0.85  | $0.90\pm0.10$   |
|  |                                       | 0.86  | $0.90\pm0.07$   |
| ······································ |                                       | $\begin{array}{c} 0.86 \\ 1.14 \end{array}$ | $\begin{array}{c} 0.93  \pm  0.10 \\ 1.25  \pm  0.22 \end{array}$ |
|  |                                       |   |   |
| 0 0                                    |                                       |   |   |
|  |                                       | 1.04  | $1.06 \pm 0.11$   |
|  |                                       | 1.05  | $1.05 \pm 0.11$   |
|  |                                       | 1.34  | $1.26\pm0.22$   |
|  |                                       |   |   |
|  |                                       | 1.97  | 1.92   0.12   |
|  |                                       | 1.27  | $1.23 \pm 0.13$   |
|  |                                       |   |   |
|  |                                       | 1.34  | $1.25 \pm 0.22$   |
|  |                                       |   |   |
| 0'                                     |                                       | 1.02  | $1.03 \pm 0.07$   |
|  |                                       |   |   |
|  |                                       | 1.18  | $1.13\pm0.09$   |
|  |                                       |   |   |
| 0× ° F°                                |                                       | 1.18  | $1.07 \pm 0.10$   |
|  |                                       |   |   |
| ° × ° ~ °                              |                                       | 1.08  | $1.07 \pm 0.10$   |
| <pre>&gt;°</pre>                       |                                       |   |   |
|  |                                       | 1.07  | $1.21 \pm 0.09$   |
|  |                                       |   |   |
|  |                                       | 1.00  | $1.23 \pm 0.12$   |
| 0                                      |                                       | Continued                                   | on next page  |
|  |                                       |   | page  |

| MONOMER        | $\rho_{exp}$ | Ppred 1         |
|----------------|--------------|-----------------|
|                | 1.15         | $1.20 \pm 0.10$ |
|                | 1.06         | $1.04 \pm 0.11$ |
|                | 1.21         | $1.21\pm0.11$   |
| $\sim$         |              |                 |
|                | 1.08         | $1.13 \pm 0.16$ |
| $\tilde{\rho}$ | 1.23         | $1.11\pm0.18$   |
|                | 1.07         | $1.03 \pm 0.10$ |
| $\rightarrow$  | 1.07         | 1.05 ± 0.10     |
|                | 1.12         | $1.13\pm0.11$   |
|                | 1.10         | 1.04   0.12     |
|                | 1.10         | $1.04 \pm 0.12$ |
|                | 0.94         | 0.00   0.07     |
| $\checkmark$   | 0.84         | 0.89 ± 0.07     |
|                | 1.06         | $1.03 \pm 0.12$ |
| Ly o the       | 1100         | 100 ± 0112      |
|                | 1.20         | $1.20 \pm 0.09$ |
|                | 0.84         | $0.91 \pm 0.07$ |
| $\sim$         | 1.03         | $1.02 \pm 0.10$ |
|                |              |                 |
|                | 1.06         | $1.10\pm0.18$   |
|                |              |                 |
|                | 1.07         | $1.08 \pm 0.15$ |
| $\bowtie$      |              |                 |
|                | 1.07         | $1.14 \pm 0.12$ |
| >→             |              |                 |
| ° ~ ~ ~ °      | 1.00         | 1.00 1.0.00     |
|                | 1.30         | $1.20 \pm 0.09$ |
| 0              | C + :        |                 |

| Table S6 -  | Continued from previous page |                                   |
|---|------------------------------|-----------------------------------|
| MONOMER   | ρexp<br>1.07                 | $\frac{\rho_{pred}}{1.11 + 0.15}$ |
| $\sim$ N  | 1.07                         | <u>-</u> 0.10                     |
|   | 1.06                         | $1.07 \pm 0.08$                   |
|   | 1.39                         | $1.35 \pm 0.12$                   |
|   | 1.15                         | $1.07 \pm 0.12$                   |
| ~°ŋ~~~ <sup>4</sup> °                                       | 1.24                         | $1.43 \pm 0.16$                   |
|   |                              |                                   |
| CI F  | 1.92                         | $1.37 \pm 0.18$                   |
|   |                              |                                   |
| F F   | 1.27                         | $1.28 \pm 0.09$                   |
|   |                              |                                   |
|   | 1.24                         | $1.28 \pm 0.09$                   |
|   | 1.25                         | $1.29 \pm 0.10$                   |
|   |                              |                                   |
|   | 1.24                         | $1.29 \pm 0.13$                   |
|   | 1.45                         | $1.40 \pm 0.18$                   |
|   | 1.05                         | $1.03 \pm 0.16$                   |
| S //  | 1.18                         | $1.17 \pm 0.14$                   |
| F F   | 2.00                         | $1.38 \pm 0.20$                   |
| $\succ$   |                              |                                   |
| F F   | 1.32                         | $1.37 \pm 0.21$                   |
| F<br>F  |                              |                                   |
|   | 1.58                         | $1.44 \pm 0.21$                   |
| <i></i> <sup>↓</sup> <sup>↓</sup> <sup>↓</sup> <sup>↓</sup> |                              |                                   |
| F F<br>F  | 1.91                         | $1.38 \pm 0.20$                   |
|   | 1.43                         | $1.38 \pm 0.20$                   |
|   |                              |                                   |
| <i>I I I I I I I I I I</i>                                  | 1.20                         | $1.27 \pm 0.22$                   |
|   | C                            | l on next page                    |
|   | Continued                    | i on next page                    |

| Table S6 – Continued from previous page   |                           | 0.1                              |
|---|---------------------------|----------------------------------|
|   | $\frac{\rho_{exp}}{1.30}$ | $\frac{p_{pred}}{1.27 \pm 0.18}$ |
|   | 1 48                      | $1.14 \pm 0.12$                  |
| $\neg$ $\overset{\sim}{\sim}$   | 1.40                      | 1.14 ± 0.12                      |
|   |                           |                                  |
|   | 1.04                      | $1.09 \pm 0.13$                  |
|   | 1.14                      | $1.14 \pm 0.10$                  |
|   | 0.98                      | $0.96 \pm 0.09$                  |
| Si  |                           |                                  |
|   |                           |                                  |
|   | 1.46                      | $1.17\pm0.11$                    |
|   | 1.14                      | $1.10 \pm 0.10$                  |
|   |                           |                                  |
|   | 1.36                      | $1.37 \pm 0.28$                  |
|   |                           |                                  |
|   | 1.42                      | $1.21 \pm 0.10$                  |
| o ta a a a a a a a a a a a a a a a a a a  | 1.27                      | $1.23 \pm 0.09$                  |
|   | 1.20                      | $1.18\pm0.12$                    |
|   | 1.18                      | $1.13 \pm 0.07$                  |
|   | 1.12                      | $1.14 \pm 0.11$                  |
|   | 1.99                      | $1.96 \pm 0.26$                  |
| $ \sum_{m=1}^{n} \frac{1}{m} \sum_{r=1}^{n} \frac{1}{r} \sum_{r=1}^{n} \frac{1}{m} \sum_{$ |                           |                                  |
|   | 1.95                      | $1.88 \pm 0.34$                  |
|   | 1.08                      | $1.12 \pm 0.10$                  |
|   |                           |                                  |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   | 1.42                      | $1.35 \pm 0.12$                  |
|   | 1 44                      | $1.34 \pm 0.13$                  |
| $\circ - \bigcirc - \checkmark \circ$   |                           | 1101 1 0110                      |
|   | 1.24                      | $1.21\pm0.09$                    |
|   | 1.36                      | $1.32\pm0.09$                    |
|   | 1.07                      | $1.20\pm0.13$                    |
|   | 1.33                      | $1.21 \pm 0.10$                  |
|   | 1.31                      | $1.15 \pm 0.11$                  |
|   |                           |                                  |
| , ×, · · · · · · · · · · · · · · · · · ·  | 1.14                      | $1.20 \pm 0.14$                  |
|   | 1.17                      |                                  |
|   |                           |                                  |

| Table S6 – Continued from previous page |              |                 |
|---|--------------|-----------------|
| MONOMER                                 | $\rho_{exp}$ | $\rho_{pred}$   |
|   | 1.39         | $1.27 \pm 0.15$ |
|   | 1.24         | $1.20 \pm 0.09$ |
|   | 1.19         | $1.17 \pm 0.11$ |
|   | 1.23         | $1.16 \pm 0.12$ |
|   | 1.16         | $1.16 \pm 0.10$ |
| °~°, <sup>l</sup> imoro                 | 1.36         | $1.22 \pm 0.10$ |
|   | 1.13         | $1.18 \pm 0.11$ |

Table S7: Summary of the classification model performances for the polymer solubilities in different solvents (NMP, THF,  $CHCl_3$ , DMSO and DMAC). The solubility classes include: S - soluble, PS - partially soluble/swelling/soluble on heating and I - insoluble. Here, mtry is the number of predictors sampled for splitting at each node in the RF model, while accuracy and kappa coefficient are used as the performance metrics.

| Solvent             | I/PS/S   | ACCURACY | KAPPA | mtry | I/PS/S   | ACCURACY | KAPPA |
|---------------------|----------|----------|-------|------|----------|----------|-------|
| $\overline{CHCl_3}$ | 27/17/24 | 0.71     | 0.56  | 8    | 26/17/24 | 0.75     | 0.61  |
| DMAC                | 4/21/28  | 0.74     | 0.52  | 15   | 4/20/28  | 0.73     | 0.48  |
| DMSO                | 10/28/40 | 0.73     | 0.53  | 8    | 9/28/39  | 0.75     | 0.57  |
| NMP                 | 5/21/47  | 0.83     | 0.62  | 42   | 5/21/46  | 0.72     | 0.36  |
| THF                 | 8/30/23  | 0.72     | 0.49  | 51   | 7/29/23  | 0.78     | 0.62  |

| MONOMER  | Experimental | Predicted      | Ref     |
|--|--------------|----------------|---------|
|  | PS           | I              | [63]    |
|  | Ι            | Ι              | [63]    |
|  | S            | S              | [60]    |
|  | S            | S              | [60]    |
|  | S            | S              | [60]    |
|  | S            | S              | [45]    |
|  | S            | S              | [45]    |
|  |              |                |         |
|  | S            | S              | [45]    |
|  | S            | S              | [45]    |
|  | S            | S              | [45]    |
|  |              |                |         |
|  | S            | S              | [45]    |
|  | S            | Ι              | [43]    |
|  | S            | S              | [16]    |
| Contraction of the second seco | PS           | PS             | [16]    |
|  |              |                | [ · ]   |
|  | PS           | $_{\rm PS}$    | [16]    |
|  |              |                |         |
|  | PS           | $_{\rm PS}$    | [16]    |
|  |              |                |         |
|  | PS           | PS             | [16]    |
|  | C            | S              | [90]    |
|  | 5            | 5              | [38]    |
| jour.ora   | S            | S              | [38]    |
| מיייים <u>מ</u> י<br>מייידים   | S            | S              | [38]    |
| <u> </u>   | Co           | ntinued on nex | ct page |

Table S8: The table lists the experimental and predicted solubility classes (S - soluble, PS - partially soluble/swelling/soluble on heating, I - insoluble) for different polymers in  $CHCl_3$ . Predictions for the RF model are reported.

| MONOMER                                  | ble S8 – Continued from previous page<br>Experiment | al Predicted | Ref  |
|--|---|--------------|------|
| na n | S   | I            | [38] |
|  | I   | Ι            | [48] |
|  |   |              |      |
| ý ma                                     | Ţ   | т            | [49] |
|  | 1   | 1            | [40] |
|  |   |              |      |
|  | Ι   | Ι            | [48] |
|  |   |              |      |
|  | PS  | PS           | [48] |
| A A A A A A A A A A A A A A A A A A A    |   |              | [ -] |
|  | Ţ   | т            | [48] |
| je to to to to                           |   | Ĩ            | [40] |
|  | I   | $_{\rm PS}$  | [18] |
|  |   |              |      |
|  | PS  | PS           | [18] |
|  | 15  | 15           | [10] |
|  |   |              |      |
|  | S   | S            | [18] |
| ·~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   |   |              |      |
|  | PS  | $_{\rm PS}$  | [18] |
|  |   |              |      |
|  | PS  | PS           | [18] |
|  |   |              |      |
|  | S   | S            | [46] |
|  |   |              |      |
| ·*··*·                                   | S   | S            | [46] |
| ·*·*                                     |   |              |      |
|  | S   | S            | [46] |
| È a a ~ . <sup>i</sup>                   |   | 2            | [10] |
|  | 2   | S            | [46] |
| °*°~~°                                   | 5   | 2            | [10] |
|  | S   | S            | [46] |
| ·*-~~~.<br>, -5~~                        |   |              |      |
| r <sup>o</sup>                           |   |              |      |

| MONOMER  | Table S8 - Continued from previous page           Experimen | tal Predicted | Ref  |
|--|---|---------------|------|
| ۲······  | 5   | 5             | [46] |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~         | S   | S             | [46] |
| المكري م                                       | S   | S             | [46] |
| ·······  | 5   | 5             | [40] |
| متع <sub>ا</sub> م متعام                       | Ι   | Ι             | [65] |
| . anora la | Ι   | Ι             | [65] |
| ioloriaio.or                                   | I   | Ι             | [65] |
| anayan manan                                   | Ι   | Ι             | [65] |
| A Contractor                                   | PS  | I             | [52] |
|  | PS  | $_{\rm PS}$   | [52] |
|  |   |               |      |
|  | Ι   | Ι             | [52] |
| de para  |   |               |      |
|  | Ι   | Ι             | [52] |
|  | Ι   | S             | [52] |
|  |   |               |      |
|  | Ι   | Ι             | [52] |
|  |   |               |      |
|  | Ι   | I             | [52] |
| j<br>Antop                                     |   |               |      |
|  | 1   | PS            | [52] |
|  |   |               |      |
|  | Ι   | PS            | [52] |
| °, °, °, °, °, °, °, °, °, °, °, °, °, °       | Т   | Т             | [64] |
| madala <sup>lana</sup> ng<br>d<br>ta           | -   |               | [v=] |
| araharanahara.                                 | 1   | l<br>T        | [64] |
| -of Croade                                     | 1   | 1             | [04] |
| John Martin Martin                             | I   | Ι             | [64] |

| MONOMER   | Table S8 – Continued from previous page | Experimental | Predicted | Ref  |
|---|---|--------------|-----------|------|
| $\int_{-1}^{\infty} \int_{-1}^{\infty} \int_{-1}^{0$ |   | S            | S         | [40] |
| _ i<br>   |   | S            | S         | [40] |
|   |   | S            | S         | [40] |
|   |   | 5            | 5         | [40] |
| <sup>I</sup> s<br>∽∽ <sup>s</sup> Υ <sup>N</sup> Υ <sup>s</sup> Υ <sup>s</sup> Υ  |   | S            | S         | [40] |
|   |   | S            | S         | [40] |
|   |   | Ι            | Ι         | [19] |
| 1150<br>  |   |              |           |      |
|   |   | S            | S         | [19] |
|   |   |              |           |      |
|   |   |              |           |      |
|   |   | PS           | PS        | [19] |
|   |   |              |           |      |
| ۰<br>۳  |   | PS           | Ι         | [19] |
| or and a second   |   |              |           |      |
|   |   | Ι            | Ι         | [19] |
|   |   |              |           |      |
| . Charlen and the second se   |   | Ι            | Ι         | [35] |
| and and a second and   |   | I            | I         | [35] |
|   |   | 1            | 1         | [17] |
|   |   | PS           | T         | [17] |
|   |   | 15           | Ĩ         | [11] |
|   |   | т            | T         | [17] |
|   |   | I            | 1         | [17] |
|   |   | PS           | PS        | [17] |
|   |   |              |           |      |
|   |   | PS           | PS        | [17] |
|   |   |              |           |      |
|   |   | Ι            | Ι         | [20] |
| "↓, • • • • • • • • • • • • • • • • • • •   |   |              |           |      |
| °Ω  |   | PS           | PS        | [20] |
|   |   |              |           |      |
|   |   | Ι            | Ι         | [20] |
| <sup>∞</sup> ″~°∕∩  |   |              |           |      |
| PS         I         [01]           I         I         I         I01           S         S         I42         I         I           I         I         I         I         I01           I         I         I         I         I01           I         I         I         I01         I01           I         I         I         I00         S         I01           I         I         I         I00         S         I00           I         I         I00         S         I00         I00           I         I         I00         S         I00         I00         I00           I         I         I00         S         I00  | MONOMER  | Table S8 – Continued from previous page | Experimental | Predicted | Ref  |
|--|--|---|--------------|-----------|------|
| 、 、 、 、 、 、 、 、 、 、 、 、 、 、 、 、 、 、  |  |   | PS           | Ι         | [20] |
| 1 1   1 1 <  |  |   | Ι            | Ι         | [20] |
| 「「」」」」         「」」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」」         「」」」」           「」」」」         「」」」」         「」」」」           「」」」」         「」」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」」         「」」」」           「」」」」         「」」」」         「」」」」           「」」」」         「」」」」         「」」」」           「」」」」         「」」」」         「」」」」           「」」」」         「」」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」」         「」」」           「」」」」         「」」」         「」」」           「」」」」         「」」」         「」」」           「」」」         「」」  | <ul> <li>√, √, ∘ ∅,</li> <li>(<sup>1</sup>)<sup>5</sup> ≽<sup>0</sup></li> </ul> |   | S            | S         | [42] |
| 「日本の日本の日本の日本の日本の日本の日本の日本の日本の日本の日本の日本の日本の日  | $\chi_{s}^{s}$   |   | I            | I         | [50] |
| 内国         内国         月         月           日         日         日         日         日           日         日         日         日         日           日         日         日         日         日           日         日         日         日         日           日         日         日         日         日           日         日         日         日         日           日         日         日         日         日           日         日         日         日         日           日         日         日         日         日           日         日         日         日         日         日           日         日         日         日         日         日           日         日         日         日         日         日           日         日         日         日         日         日           日         日         日         日         日         日           日         日         日         日         日         日           日         日         日         日         日         日 <td></td> <td></td> <td>I</td> <td>I</td> <td>[50]</td>  |  |   | I            | I         | [50] |
| S        |  |   | S            | S         | [54] |
| S        | °Q_Q°  |   |              |           |      |
| S       S       S       [54]         S       S       S       [30]         S       S       S       [30]         S       S       S       [30]         S       S       S       [41]         S       S       [  |  |   |              |           |      |
| S       S       S       [90]         S       S       [30]         S       S       [41]         S       S       [41]         S       S       [41]         S       S       [41]         S       S   | •  |   | S            | S         | [54] |
| S        |  |   |              |           |      |
| s       s       (30)         s       s       (31)         s       s       (32)  |  |   |              |           |      |
| S       S       S       [4]         S       S       S       [4]      S       S       S       [4]         S       S       S       [4]         S       S       S       [3]         S       S       S       [3]         S       S       [3]       [3]         S       S       [3]       [3]   | a a di a a a a a a a a a a a a a a a a a   |   | S            | S         | [39] |
| Formation       S       S       [4]         S       S       S <t< td=""><td></td><td></td><td>S</td><td>S</td><td>[39]</td></t<>   |  |   | S            | S         | [39] |
| s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s       s         s       s       s       s       s       s       s       s         s  | Falaiaia <sup>7</sup>  |   | S            | S         | [44] |
| s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s         s       s       s       s       s       s       s         s       s       s       s       s       s       s       s         s       s       s       s       s       s       s       s       s       s       s       s       s       s       s       s       s <t< td=""><td>, da<sup>r</sup> ~ af</td><td></td><td></td><td></td><td></td></t<>  | , da <sup>r</sup> ~ af   |   |              |           |      |
| S       S       S       [4]         ス       S       S       [3]         ス       S       S       [3]<   | QLinous S  |   | S            | S         | [44] |
| <ul> <li>たびていいい</li> <li>ち</li> <li>ち</li> <li>ち</li> <li>ち</li> <li>たびていい</li> <li>ち</li> <li>ち</li> <li>たびていい</li> <li>ち</li> <li>ち</li> <li>たびていい</li> <li>ち</li> <li>ち</li> <li>た</li> <li>た<td></td><td></td><td>S</td><td>S</td><td>[44]</td></li></ul>  |  |   | S            | S         | [44] |
| <ul> <li>よのでもない</li> <li>よのでもない<td>en ser</td><td></td><td></td><td></td><td></td></li></ul>   | en ser   |   |              |           |      |
| s        |  |   | S            | S         | [44] |
| S       S       S       [4]         S       S       S       [3]         S       S       S       [3]         S       S       S       [3]         S       S       S       [3]  |  |   |              |           |      |
| S = S = [44] $S = S = [44]$ $S = S = [37]$ $S = S = [37]$  | i.<br>i.   |   | S            | S         | [44] |
| $ \begin{array}{cccc} & & & & & & \\ & & & & \\ & & & & & \\ & & &$ |  |   | S            | S         | [44] |
| $ \begin{array}{cccc} S & S & [4] \\ S & S & [5] \\ S & S$  |  |   |              |           |      |
| は、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、  |  |   | S            | S         | [44] |
| 、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、   | 8  |   | g            | q         | [44] |
| s s [4]  | Ba <sup>-ia</sup> to,  |   | 5            | 5         | [44] |
| درجه درجه درجه درجه درجه درجه درجه درجه  |  |   | S            | S         | [44] |
| ່<br>ເວັດເຊັ່ນ<br>ໂດຍ ເພີ້ອງ ເພີ່ອງ ເພີ່ອງ ເພີ່ອງ ເພີ່ອງ ເພີ່ອງ ເພື່ອງ ເພື່ອງ ເພື່ອງ ເພື່ອງ ເພື່ອງ ເພື່ອງ ເພື່ອງ ເພື່ອງ ເພື່ອງ ເພ  | -aprilation  |   |              |           |      |
| s s [37]   |  |   | S            | S         | [37] |
|  |  |   | S            | S         | [37] |

| MONOMER  | Table S8 | - Continued from previous page | Experimental | Predicted   | Ref  |
|--|----------|--------------------------------|--------------|-------------|------|
| Ô  |          |                                | S            | S           | [37] |
|  |          |                                |              |             |      |
|  |          |                                |              |             |      |
|  |          |                                | S            | S           | [37] |
|  |          |                                | Ŧ            | т           | [10] |
|  |          |                                | 1            | 1           | [10] |
|  |          |                                | т            | т           | [10] |
| "Ĵ¦poġ,_"  |          |                                | 1            | 1           | [10] |
| -* * * * •   |          |                                | т            | т           | [10] |
|  |          |                                | 1            | 1           | [10] |
|  |          |                                | т            | T           | [10] |
|  |          |                                | -            | -           | [10] |
|  |          |                                | I            | I           | [10] |
| \$ <b>0</b> \$   |          |                                |              |             |      |
|  |          |                                | Ι            | Ι           | [10] |
|  |          |                                |              |             |      |
| 279<br>* "L  |          |                                | PS           | $_{\rm PS}$ | [3]  |
|  |          |                                |              |             |      |
|  |          |                                |              |             |      |
| °  |          |                                | PS           | PS          | [3]  |
|  |          |                                |              |             |      |
|  |          |                                | Ŧ            | т           | [0]  |
| orai di  |          |                                | 1            | 1           | [3]  |
|  |          |                                |              |             |      |
| ۲.<br>۲.   |          |                                | PS           | $_{\rm PS}$ | [3]  |
|  |          |                                |              |             |      |
|  |          |                                | PS           | PS          | [3]  |
| and the second s |          |                                |              |             |      |
|  |          |                                | PS           | PS          | [3]  |
| a da da  |          |                                | 10           | 15          | [0]  |
|  |          |                                |              |             |      |
| 0-10 <sup>1.Q.1</sup> 0.   |          |                                | PS           | Ι           | [3]  |
|  |          |                                | Ι            | Ι           | [3]  |
|  |          |                                | т            | Т           | [3]  |
| 0-0-201.0.10.  |          |                                | 1            | 1           | [0]  |
| R. Laidin  |          |                                | PS           | $_{\rm PS}$ | [3]  |
| 0-50Q  |          |                                | PS           | Ι           | [3]  |
| ogojaia.g.   |          |                                | DC           | DC          | [0]  |
| o joi. O. io.  |          |                                | PS           | PS          | [3]  |
|  |          |                                |              |             |      |

|                              | Table S8 – Continued from previous page |              |                |             |
|------------------------------|---|--------------|----------------|-------------|
| MONOMER                      |   | Experimental | Predicted<br>S | Ref<br>[66] |
| یھ، م <sup>ن</sup> ، شر<br>ک |   |              |                | [**]        |
| 900                          |   | Ι            | S              | [66]        |
|                              |   | Ι            | Ι              | [66]        |
| °O. O', L',                  |   | T            | т              | [47]        |
| oon to fait                  |   | T            | T              | [47]        |
| monthing of the              |   | I            | T              | [47]        |
|                              |   | 1            | 1              | [47]        |
|                              |   | Ι            | Ι              | [47]        |
| ovo rotor                    |   | Ι            | I              | [47]        |
| ola woter                    |   | Ι            | I              | [47]        |
| "O, \$10 HO4.                |   | Т            | т              | [47]        |
|                              |   | 1            | 1              | [11]        |
|                              |   | PS           | PS             | [2]         |
|                              |   |              |                |             |
|                              |   | Ι            | $_{\rm PS}$    | [2]         |
|                              |   |              |                |             |
|                              |   | Ι            | PS             | [2]         |
|                              |   | DC           | DG             | [0]         |
|                              |   | P5           | PS             | [2]         |
|                              |   |              |                |             |
|                              |   | PS           | PS             | [2]         |
|                              |   | PS           | PS             | [2]         |
| 10.101.010.                  |   | 10           | 10             | [=]         |
| ·                            |   | PS           | PS             | [2]         |
| -00. oc. oc.                 |   |              |                |             |
| *0                           |   | PS           | PS             | [2]         |
|                              |   |              |                |             |
|                              |   | $_{\rm PS}$  | PS             | [2]         |
|                              |   |              |                |             |

| MONOMER   | Experimental | Predicted | Ref  |
|---|--------------|-----------|------|
| $(\alpha, \alpha, \alpha)$  | I            | S         | [51] |
|   | I            | S         | [51] |
|   | 1            | 5         | [51] |
|   | S            | S         | [63] |
|   | S            | S         | [63] |
|   | PS           | PS        | [45] |
|   | DS           | DC        | [45] |
|   | 15           | 15        | [40] |
|   | PS           | PS        | [45] |
|   | S            | S         | [45] |
| n an  | S            | S         | [45] |
|   |              |           |      |
|   | PS           | PS        | [45] |
|   | S            | S         | [43] |
|   | PS           | S         | [15] |
|   | S            | q         | [15] |
|   | 5            | 5         | [10] |
|   | S            | S         | [15] |
| and the second |              |           |      |
|   | S            | S         | [15] |
|   | S            | S         | [15] |
|   |              |           |      |
|   | PS           | S         | [15] |
|   | S            | S         | [15] |
|   | U.           | U         | [10] |
|   | S            | S         | [15] |
| je provenské  |              |           |      |

Table S9: The table lists the experimental and predicted solubility classes (S - soluble, PS - partially soluble/swelling/soluble on heating, I - insoluble) for different polymers in N-methylpyrrolidone (NMP). Predictions for the RF model are reported.

| Table S9 - Continued from previous page  |                |             |      |
|--|----------------|-------------|------|
| MONOMER  | S Experimental | S Predicted | [15] |
|  | 2              |             | []   |
|  | S              | S           | [15] |
|  | S              | S           | [16] |
|  | S              | S           | [16] |
|  | g              | S           | [16] |
|  | 5              | 5           | [10] |
|  | S              | S           | [16] |
|  | S              | S           | [16] |
|  | S              | S           | [38] |
|  | S              | S           | [38] |
| and the second of the second o | S              | S           | [38] |
| and the second sec   | S              | S           | [38] |
|  | PS             | S           | [48] |
|  | S              | S           | [48] |
|  | 2              |             | [10] |
|  | 5              | 5           | [48] |
|  | S              | S           | [48] |
|  | S              | S           | [48] |
|  | S              | S           | [41] |
| , a. a. b.   | S              | S           | [41] |
|  |                |             |      |

| Table S9 – Continued from previous page |              |                 |         |
|---|--------------|-----------------|---------|
| MONOMER                                 | Experimental | Predicted       | Ref     |
|   | 5            | د               | [10]    |
|   | S            | S               | [18]    |
|   | S            | S               | [46]    |
|   | S            | S               | [46]    |
|   | PS           | s               | [46]    |
|   | s            | S               | [46]    |
|   | PS           | S               | [46]    |
|   | PS           | PS              | [46]    |
|   | PS           | PS              | [46]    |
|   | PS           | PS              | [46]    |
|   | S            | S               | [65]    |
| aranananan ar                           | S            | S               | [65]    |
|   | s            | S               | [65]    |
| warana aa                               | S            | 5               | [65]    |
| jo ci o ci                              | PS           | PS              | [52]    |
| <u></u> <u>γ</u>                        | Ca           | ontinued on ne: | rt page |

|  | Table S9 – Continued from previous page |                    |                |       |
|--|---|--------------------|----------------|-------|
| MONOMER  |   | Experimental<br>PS | Predicted<br>I | [52]  |
| طْ<br>ا  |   | 10                 | -              | [02]  |
| rt.d.s   |   |                    |                |       |
|  |   |                    |                |       |
|  |   | -                  | -              | [* 0] |
|  |   | 1                  | 1              | [52]  |
|  |   |                    |                |       |
|  |   |                    |                |       |
|  |   | Ι                  | Ι              | [52]  |
| al <sup>ĝ</sup>  |   |                    |                | . ,   |
|  |   |                    |                |       |
|  |   | Т                  | т              | [52]  |
| °D   |   | 1                  | -              | [02]  |
| , <u>4</u> 0   |   |                    |                |       |
|  |   |                    |                |       |
|  |   | Ι                  | I              | [52]  |
|  |   |                    |                | L- 1  |
| <u>_</u> Q'Q{-Q-Q  |   |                    |                |       |
|  |   |                    |                |       |
| ~  |   | I                  | I              | [52]  |
|  |   |                    |                |       |
| " Terling and the second se  |   |                    |                |       |
| $\bigcirc$   |   |                    |                |       |
| $\langle \nabla \rangle$   |   | I                  | I              | [52]  |
|  |   |                    |                |       |
| ",,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,   |   |                    |                |       |
|  |   |                    |                |       |
| \_/<br>  |   | Ι                  | Ι              | [52]  |
| V. O   |   |                    |                |       |
|  |   |                    |                |       |
|  |   |                    |                |       |
|  |   | PS                 | S              | [64]  |
| gir rabaar.  |   |                    |                |       |
| ί <b>α</b> ,   |   | PS                 | $\mathbf{PS}$  | [64]  |
| -arayararararararara   |   |                    |                |       |
| 19-10-1  |   | PS                 | S              | [64]  |
|  |   |                    |                |       |
| 1-Gr.  |   | PS                 | $_{\rm PS}$    | [64]  |
| ~ molalalanara.  |   |                    |                |       |
| · CH' - D  |   | S                  | S              | [19]  |
|  |   |                    |                |       |
|  |   |                    |                |       |
|  |   | C                  | q              | [10]  |
|  |   | U U                | U U            | [19]  |
| ~ <sup>*</sup> <sup>*</sup> <sup>*</sup> <sup>*</sup> <sup>*</sup>   |   |                    |                |       |
|  |   |                    |                |       |
|  |   |                    |                |       |
|  |   | S                  | S              | [19]  |
| r Liter it has   |   |                    |                |       |
| () - Li  |   |                    |                |       |
| ·≁⊖→v,́_<  |   |                    |                |       |
| ν<br>N   |   | S                  | S              | [19]  |
|  |   |                    |                | -     |
| O'DING O   |   |                    |                |       |
| کر یہ  |   | S                  | S              | [19]  |
| - Of you   |   |                    |                | r - 1 |
|  |   |                    |                |       |
|  |   | S                  | PS             | [35]  |
| un and a standard and a standard and a standard a st |   | 5                  |                | [00]  |
| and marking and  |   | S                  | S              | [35]  |
| 11 (n. a)**  |   |                    |                |       |

| Table S9 - Continued from previous page  |                   | D 1: ( 1 |      |
|--|-------------------|----------|------|
| NONOMER  | Experimental<br>S | S        | [17] |
|  |                   |          |      |
|  | S                 | S        | [17] |
|  | S                 | S        | [17] |
|  |                   |          |      |
|  | S                 | S        | [17] |
|  | S                 | S        | [17] |
|  | S                 | S        | [20] |
|  | -                 | -        | [=0] |
|  | S                 | S        | [20] |
|  | PS                | S        | [5]  |
|  | S                 | S        | [5]  |
| - केंक्स् <del>क</del>   | S                 | S        | [5]  |
| ्र के कर   | S                 | S        | [5]  |
| a the second sec | S                 | S        | [5]  |
|  | S                 | S        | [5]  |
| or the second se | S                 | S        | [50] |
|  | S                 | S        | [50] |

| Table S9 – Continued from previous page  | Experimental | Predicted      | Ref     |
|--|--------------|----------------|---------|
|  | S            | S              | [39]    |
|  | S            | S              | [39]    |
| fa.aca.af  | S            | S              | [44]    |
| en antiparte a series and a s |              | _              |         |
| gin  | S            | S              | [44]    |
| Bar-rate   | S            | S              | [44]    |
|  | S            | S              | [44]    |
| -ccp-rofo  |              |                |         |
|  | S            | S              | [44]    |
|  | S            | S              | [44]    |
|  | S            | S              | [44]    |
|  |              |                |         |
| Bar-tat-   | S            | S              | [44]    |
|  | S            | S              | [44]    |
|  | PS           | $\mathbf{PS}$  | [10]    |
|  |              |                |         |
|  | PS           | PS             | [10]    |
|  | PS           | $\mathbf{PS}$  | [10]    |
|  | PS           | PS             | [10]    |
|  | PS           | PS             | [10]    |
|  | PS           | S              | [10]    |
|  | S            | S              | [3]     |
|  |              |                |         |
|  | S            | S              | [3]     |
| or<br>A hailei   |              |                |         |
|  | Co           | ntinued on new | ct page |

| MONOMER  | Table S9 - | - Continued from previous page | Experimental | Predicted   | Ref  |
|--|------------|--------------------------------|--------------|-------------|------|
| متعبيصيع   |            |                                | PS           | S           | [3]  |
|  |            |                                | S            | S           | [3]  |
|  |            |                                | S            | S           | [3]  |
|  |            |                                | S            | S           | [3]  |
| in the second of |            |                                | PS           | s           | [3]  |
| o-joi.Q.iq.  |            |                                |              | 2           | [0]  |
| o-joi.Q.iq.  |            |                                | S            | 8           | [3]  |
| 0 <sup>-0-}0<sup>i.0.i</sup>g.</sup>   |            |                                | PS           | PS          | [3]  |
| 0  |            |                                | 5            | 5           | [3]  |
| o Bobolo in  |            |                                | PS           | S           | [3]  |
| opolaig.   |            |                                | S            | S           | [3]  |
|  |            |                                | S            | S           | [56] |
| kri sz.<br>huhara  |            |                                | PS           | PS          | [56] |
| ,  |            |                                | S            | PS          | [56] |
| to of the  |            |                                | S            | s           | [56] |
| a compro   |            |                                | S            | q           | [56] |
| ~d   |            |                                | 5            | 5           | [50] |
| to the second  |            |                                | S            | S           | [56] |
|  |            |                                | PS           | $_{\rm PS}$ | [66] |
| °×<br>Soro, cr   |            |                                | PS           | S           | [66] |
|  |            |                                | PS           | PS          | [66] |
|  |            |                                | PS           | PS          | [2]  |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   |            |                                | Þ¢           | PS          | [0]  |
| 0.101-01-01-01-01-01-01-01-01-01-01-01-01-   |            |                                | 10           |             | ["]  |

| Table S9 – Continued from previous page |              |           |     |
|---|--------------|-----------|-----|
| MONOMER                                 | Experimental | Predicted | Ref |
|   | PS           | PS        | [2] |

| MONOMER | Experimental | Predicted      | Ref     |
|---------|--------------|----------------|---------|
|         | S            | S              | [45]    |
|         | Ι            | PS             | [15]    |
|         | PS           | PS             | [15]    |
|         | PS           | PS             | [15]    |
|         | PS           | PS             | [15]    |
|         | S            | S              | [15]    |
|         |              |                |         |
|         | PS           | PS             | [15]    |
|         |              |                |         |
|         | S            | S              | [15]    |
|         | PS           | PS             | [16]    |
|         |              |                |         |
|         | Cc           | ntinued on new | ct page |

Table S10: The table lists the experimental and predicted solubility classes (S - soluble, PS - partially soluble/swelling/soluble on heating, I - insoluble) for different polymers in THF. Predictions for the RF model are reported.

|  | Table S10 $-$ Continued from previous page |              |             |      |
|--|--|--------------|-------------|------|
| MONOMER  |  | Experimental | Predicted   | Ref  |
|  |  | PS           | P5          | [16] |
|  |  | PS           | PS          | [16] |
|  |  | S            | S           | [16] |
|  |  | S            | S           | [16] |
|  |  |              |             |      |
|  |  | S            | S           | [38] |
| 90   |  | S            | S           | [38] |
| 900.0.<br>J. 600.0.  |  | S            | S           | [38] |
| agoma/a.   |  | PS           | PS          | [48] |
|  |  |              | Pa          | [10] |
|  |  | PS           | PS          | [48] |
|  |  | $_{\rm PS}$  | PS          | [48] |
| fro of the of th |  | PS           | PS          | [48] |
| K Korona   |  | PG           | PS          | [48] |
| A A A A A A A A A A A A A A A A A A A  |  | 15           | 15          | [40] |
|  |  | PS           | PS          | [18] |
|  |  | PS           | $_{\rm PS}$ | [18] |
|  |  | PS           | PS          | [18] |
| ~0~,~¢~0<br>.~0~,~¢~0  |  | e            | Þç          | [10] |
|  |  | 3            | 19          | [10] |

| MONOMER  | Table S10 - Continued from previous page | Experimental | Predicted | Ref  |
|--|--|--------------|-----------|------|
|  |  | 5            | 5         | [16] |
|  |  | S            | S         | [46] |
|  |  | S            | S         | [46] |
| , O.R  |  | S            | S         | [46] |
|  |  | S            | S         | [46] |
| ·r·~··   |  | PS           | S         | [46] |
|  |  | S            | S         | [46] |
| · · · · · · · · · · · · · · · · · · ·                          |  | S            | S         | [46] |
| ·*·····  |  | S            | S         | [46] |
|  |  | PS           | PS        | [19] |
|  |  |              |           |      |
|  |  | PS           | PS        | [19] |
|  |  | PS           | PS        | [19] |
|  |  | S            | c         | [10] |
| orité  |  | 5            | 5         | [19] |
| 010-010-010-   |  | PS           | PS        | [19] |
| °-O-("-("I'-")<br>"-(D)-("-(")-(")-(")-(")-(")-(")-(")-(")-(") |  | PS           | PS        | [17] |
|  |  | PS           | PS        | [17] |
|  |  | PS           | S         | [17] |
|  |  |              |           |      |

| MUNUALIT         Production         Productio  |   | Table S10 – Continued from previous page |                    |                 |          |
|--|---|--|--------------------|-----------------|----------|
| S      | MONOMER   |  | Experimental<br>PS | Predicted<br>PS | [17] Ref |
| 入してしてしてしてしてしてしてしてしてしてしてしてしてしてしてしてしてしてして  |   |  |                    |                 |          |
| 3         5         17           PS         P8         201           PS         P8         101           PS         P8<  |   |  |                    |                 |          |
| PS       PS <td< td=""><td></td><td></td><td>S</td><td>S</td><td>[17]</td></td<>   |   |  | S                  | S               | [17]     |
| 内S         DS         DS <thds< th="">         DS         DS         D</thds<>  |   |  |                    |                 |          |
| PS       PS       PS       PS       PS       PS  | · ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~   |  |                    |                 |          |
| <ul> <li>みみない</li> <li>からいていていていていていていていていていていていていていていていていていていて</li></ul>  | °Q.~~   |  | PS                 | PS              | [20]     |
| 内容         内容         内容         内容         内容           1   |   |  |                    |                 |          |
| No. Control (1) (2) (2) (2) (2) (2) (2) (2) (2) (2) (2   |   |  | PS                 | $_{\rm PS}$     | [20]     |
| <ul> <li>Note of the second second</li></ul>  |   |  |                    |                 |          |
| <ul> <li>、、、、、、、、、、、、、、、、、、、、、、、、、、、、、、、、、、、、</li></ul>  |   |  | PS                 | $_{\rm PS}$     | [20]     |
| <ul> <li>みののです。</li> <li>ろのです。</li> <li>ろので</li></ul>  |   |  |                    |                 |          |
| <ul> <li>P3 P3 月3</li> <li>P3 P3 P3</li> <li>P3 P3</li></ul>   | ° ►1  |  | S                  | S               | [20]     |
| PS         PS         [0]           1         PS         [5]           20100000000000000000000000000000000000  |   |  |                    |                 |          |
| <ul> <li>「「「」」」」」</li> <li>「」」」</li> <li>「」」</li> <li>」</li></ul>   | ``û., ``Q.~.  |  | PS                 | $_{\rm PS}$     | [20]     |
| 小         ドラ         ドラ         ドラ           こうちんか         PS         PS         (5)           こうちんか         PS         PS         (5)           こうちんか         PS         PS         (5)           こうちんか         S         PS         (5)           こうちんか         S         PS         (5)           こうちんか         S         S         (5)           こうしのか         S         S         (5)           こうしのか         S         S         (5)           こうしのか         S         S         (5)   |   |  | Ţ                  | DC              | [#]      |
| <ul> <li>PS PS 月</li> <li>PS PS 10</li> <li>PS 10<td></td><td></td><td>1</td><td>PS</td><td>[5]</td></li></ul>  |   |  | 1                  | PS              | [5]      |
| control       PS       PS       (5)         control       PS       PS       (5)         control       S       PS       (5)         control       S       S       (5)         control   |   |  | PS                 | PS              | [5]      |
| <ul> <li>PS</li> <l< td=""><td></td><td></td><td></td><td>- ~</td><td>[*]</td></l<></ul>   |   |  |                    | - ~             | [*]      |
| みううろう         PS         PS         PS         (5)           ひううろう         S         PS         (5)           ひううろう         S         S         (5)           ひううう         S         S         (5)           ひうう         S         S         (5)   |   |  | PS                 | $_{\rm PS}$     | [5]      |
| PS         P   |   |  |                    |                 |          |
| みのようない         S         PS         (5)           ひううない         S         S         (5)           ひううない         PS         S         (5)           ひうかいい         S         S         (5)           ひうかいい         I         I         (5)           ひうかいい         I         I         (5)           ひういい         S         S         (5)           ひういい         I         I         (5)           ひういい         S         S         (5)           ひういい         I         I         (5)           ひろいい         S         S         (5)           ひろいい         S         S         (5)           ひろいい         S         S         (5)           ひろいい         S         S         (5)           ひろいい </td <td></td> <td></td> <td>PS</td> <td><math>_{\rm PS}</math></td> <td>[5]</td>  |   |  | PS                 | $_{\rm PS}$     | [5]      |
| S       FS       FS       FS         S       S       S       S       S         S       S       S       S       S       S         S       S       S       S       S       S       S         S       S       S       S       S       S       S       S         S   | Q- , , , , , , , , , , , , , , , , , , ,  |  |                    |                 |          |
| $ \begin{array}{c c} S & S & S \\ PS & S & S \\ S & S & S \\ S & S & S \\ S & S &$   | a'å i i   |  | S                  | PS              | [5]      |
| $ \begin{array}{cccc} & & & & & & & & & & & & & & & & & $  |   |  | G                  | G               | [#]      |
| PS       S       5         ようたいで       S       S       5         ようたいで       I       I       50         よういで       S       S       54         よういで       S       S       54         よういで       S       S       54  |   |  | 5                  | 5               | [5]      |
| $\begin{array}{cccc} S & S & S & S \\ S & S & S & S \\ S & S &$  |   |  | PS                 | S               | [5]      |
| S = S = [5] $S = S = [5]$ $S = [5]$ $S$  |   |  |                    |                 |          |
| S = S = S $S = S$  | ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~  |  | S                  | S               | [5]      |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$   | 9. p. joʻq.   |  |                    |                 |          |
| $S \qquad S \qquad [5]$  |   |  | S                  | S               | [5]      |
| S = S = [5] $S = S = [5]$ $T = T = [50]$ $T = T = [50]$ $S = S = [54]$ $S = S = [54]$  |   |  | S                  | S               | [5]      |
| $ \begin{array}{c} S & S & [5] \\ \hline \\ $  |   |  |                    |                 |          |
| $ \begin{array}{c} & I & I & [50] \\ \hline & & & \\ \hline & & \\ \hline & & & \\ \hline \\ \hline$ |   |  | S                  | S               | [5]      |
| $I \qquad I \qquad [50]$ $I \qquad I \qquad [50]$ $I \qquad I \qquad [50]$ $S \qquad S \qquad [54]$  |   |  |                    |                 |          |
| $I \qquad I \qquad [50]$ $S \qquad S \qquad [54]$  |   |  | Ι                  | Ι               | [50]     |
|  | or supplies   |  | I                  | I               | [50]     |
|  | in the second |  | -                  | q               | [54]     |
|  |   |  | 0                  | 5               | [o.a]    |
|  |   |  |                    |                 |          |
|  |   |  |                    |                 |          |

| MONOMER                                | Table S10 - Continued from previous page | Experimental | Predicted | Ref    |
|--|--|--------------|-----------|--------|
| •                                      |  | S            | S         | [54]   |
|  |  |              |           |        |
|  |  |              |           |        |
| ° C °                                  |  | q            | q         | [44]   |
| \$                                     |  | 6            | 5         | [44]   |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ |  | g            | S         | [44]   |
| gli~do                                 |  | 5            | 6         | [.1.1] |
|  |  | S            | S         | [44]   |
| -00 -20                                |  |              |           |        |
|  |  | S            | S         | [44]   |
|  |  |              |           |        |
| °`-,; O                                |  | S            | S         | [44]   |
| fo                                     |  |              | _         |        |
| 5                                      |  | S            | S         | [44]   |
| '90,~08                                |  | S            | S         | [44]   |
| gli~yj                                 |  | 5            | 5         | [11]   |
| 300 V                                  |  | S            | S         | [44]   |
|  |  |              |           |        |
| {<br>Q                                 |  | S            | S         | [44]   |
| -do. do                                |  |              |           |        |
|  |  | Ι            | Ι         | [37]   |
|  |  | S            | S         | [37]   |
|  |  | S            | S         | [37]   |
|  |  |              |           |        |
|  |  |              |           |        |
| à.~                                    |  | S            | S         | [37]   |
|  |  | PS           | PS        | [3]    |
| ý.                                     |  |              |           |        |
|  |  | 50           | D.C.      | [0]    |
| ۍ<br>کې                                |  | PS           | PS        | [3]    |
|  |  |              |           |        |
| ora, di                                |  | Ι            | Ι         | [3]    |
|  |  |              |           |        |
| ÷.                                     |  | PS           | PS        | [3]    |
|  |  |              |           |        |

| MONOMER  | Table S10 $-$ Continued from previous page | Experimental | Predicted   | Ref   |
|--|--|--------------|-------------|-------|
| 0.00   |  | PS           | PS          | [3]   |
|  |  |              |             |       |
| φ  |  | PS           | $_{\rm PS}$ | [3]   |
| o a da ta ta ta  |  |              |             |       |
|  |  | PS           | I           | [3]   |
|  |  |              |             |       |
| 0-70 <sup>1.0.1</sup> 0,.  |  | PS           | $_{\rm PS}$ | [3]   |
| -0-20 <sup>1.0.1</sup> 0.  |  | Ι            | $_{\rm PS}$ | [3]   |
|  |  | PS           | $_{\rm PS}$ | [3]   |
|  |  | PS           | PS          | [3]   |
| 0-28-0-20 <sup>1.0.1</sup> 9.  |  | PS           | PS          | [3]   |
| Soportalia.  |  |              |             | [0]   |
| ď.   |  | $_{\rm PS}$  | $_{\rm PS}$ | [56]  |
| ji-ja.b  |  |              |             |       |
| KX E   |  | Ι            | PS          | [56]  |
|  |  | I            | I           | [56]  |
| d. d. tr   |  |              |             |       |
| 2<br>2   |  | Ι            | Ι           | [56]  |
| B. And   |  |              |             |       |
|  |  | PS           | $_{\rm PS}$ | [56]  |
| to at the  |  |              |             |       |
|  |  | PS           | PS          | [56]  |
| The strate the state of the sta |  |              |             |       |
|  |  | PS           | $_{\rm PS}$ | [47]  |
| o <sup>o</sup> toto  |  | PS           | PS          | [47]  |
| no o tribitotico   |  |              |             | []    |
|  |  | PS           | PS          | [47]  |
| A. J. Part   |  | DC           | DC          | [477] |
| man projection   |  | F5           | FS          | [47]  |
| a onistria   |  | PS           | PS          | [47]  |
| A  |  | PS           | $_{\rm PS}$ | [47]  |
|  |  |              |             |       |
|  |  | PS           | PS          | [47]  |
|  |  | PS           | Ι           | [2]   |
|  |  |              |             |       |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   |  |              |             |       |

| I PS [2]   | MONOMER         | Experimental | Predicted | Ref |
|--|-----------------|--------------|-----------|-----|
| I       I       I       I       [2]         I       I       I       [2]         I       I<   |                 | I            | PS        | [2] |
| $I \qquad I \qquad$  |                 | I            | Ι         | [2] |
| PS       I       [2]         PS       PS       PS       [2]         No       I       I       [3]         No       I       I <t< td=""><td></td><td>Ι</td><td>Ι</td><td>[2]</td></t<>  |                 | Ι            | Ι         | [2] |
| $\begin{array}{c} & & & & & \\ & & & \\$ |                 | PS           | Ι         | [2] |
| I       I       I       [2]         I       I       I       [2]         I       I       I       [2]         I       I </td <td>6"<br/>oraiotagi</td> <td>PS</td> <td>PS</td> <td>[2]</td>  | 6"<br>oraiotagi | PS           | PS        | [2] |
| I I [2]  |                 | Ι            | Ι         | [2] |
| PS PS [2]  |                 | I            | Ι         | [2] |
|  |                 | PS           | PS        | [2] |

| MONOMER | Experimental | Predicted      | Ref     |
|---------|--------------|----------------|---------|
|         | PS           | PS             | [45]    |
|         | PS           | PS             | [45]    |
|         | PS           | $_{\rm PS}$    | [45]    |
| jan ga. | PS           | $_{\rm PS}$    | [45]    |
|         | S            | S              | [45]    |
|         | PS           | S              | [45]    |
|         | S            | S              | [15]    |
|         | S            | S              | [15]    |
|         | q            | g              | [15]    |
|         | 5            | 5              | [10]    |
|         | S            | S              | [15]    |
|         | S            | S              | [15]    |
|         | q            | q              | [1 ]    |
|         | 5            | 5              | [15]    |
|         | S            | S              | [15]    |
|         | S            | S              | [15]    |
|         | s            | S              | [15]    |
|         |              |                |         |
|         | S            | S              | [15]    |
|         | S            | S              | [16]    |
|         |              |                |         |
|         | Co           | ntinued on new | ct page |

Table S11: The table lists the experimental and predicted solubility classes (S - soluble, PS - partially soluble/swelling/soluble on heating, I - insoluble) for different polymers in N,N-Dimethylacetamide (DMAc). Predictions for the RF model are reported.

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|   | Table S11 $-$ Continued from previous page |              |           |       |
|---|--|--------------|-----------|-------|
| MONOMER   |  | Experimental | Predicted | Ref   |
|   |  | S            | S         | [16]  |
|   |  | S            | S         | [16]  |
|   |  |              |           |       |
|   |  | S            | S         | [16]  |
|   |  | S            | S         | [16]  |
|   |  |              |           |       |
| 3. 2. 0. 0. 2. 2. 2. 2. C.  |  | S            | S         | [38]  |
| joan ora  |  | S            | S         | [38]  |
| jour.org.   |  | S            | S         | [38]  |
| no alla   |  | S            | S         | [38]  |
|   |  | PS           | PS        | [48]  |
|   |  | PS           | S         | [48]  |
| A. A. C.  |  |              |           |       |
|   |  | PS           | S         | [48]  |
| $\sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{i$ |  | S            | S         | [48]  |
| to a contraction of   |  |              |           | []    |
| n na harana   |  | PS           | PS        | [48]  |
|   |  | S            | S         | [18]  |
|   |  | 2            |           | [1 0] |
|   |  | S            | S         | [18]  |
| ~   |  | S            | S         | [18]  |
|   |  |              |           |       |
|   |  | S            | S         | [18]  |
| " ) () · · · · · · · · · · · · · · · · ·  |  |              |           |       |

|  | Table S11 – Continued from previous page |              |             |        |
|--|--|--------------|-------------|--------|
| MONOMER                                |  | Experimental | Predicted   | Ref    |
| °~ 0                                   |  | S            | S           | [18]   |
|  |  |              |             |        |
|  |  |              |             |        |
|  |  |              |             |        |
| $\bigcirc$ " $\lor$ $\bigcirc$         |  | c            | q           | [46]   |
|  |  | 5            | 5           | [40]   |
| Y II                                   |  |              |             |        |
|  |  |              |             |        |
| °~°~                                   |  |              |             |        |
|  |  | S            | S           | [46]   |
|  |  |              |             |        |
| TO LE                                  |  |              |             |        |
|  |  |              |             |        |
|  |  | S            | S           | [46]   |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ |  |              |             |        |
| <u> </u>                               |  |              |             |        |
|  |  |              |             |        |
|  |  | S            | S           | [46]   |
| °×°~                                   |  |              |             |        |
|  |  |              |             |        |
|  |  | S            | $_{\rm PS}$ | [46]   |
|  |  |              |             |        |
| -55                                    |  |              |             |        |
| ~ °                                    |  |              |             |        |
| $\sim$                                 |  | PS           | $_{\rm PS}$ | [46]   |
| ······································ |  |              |             |        |
|  |  |              |             |        |
| 7                                      |  | PS           | S           | [46]   |
| ·*·~·~·~·                              |  |              |             |        |
| ° ,                                    |  |              |             |        |
| ° <sup>ر</sup> °                       |  | DC           | DC          | [40]   |
| ·····                                  |  | PS           | PS          | [46]   |
| 1                                      |  |              |             |        |
| مس میں                                 |  |              |             |        |
|  |  | PS           | PS          | [52]   |
| × . ×                                  |  |              |             |        |
|  |  |              |             |        |
| ° ź                                    |  |              |             |        |
|  |  | PS           | Ι           | [52]   |
|  |  |              |             |        |
| ~~~~~                                  |  |              |             |        |
|  |  |              |             |        |
| ~~. <                                  |  | _            |             | 6      |
|  |  | 1            | $_{\rm PS}$ | [52]   |
|  |  |              |             |        |
|  |  |              |             |        |
| $\bigcirc$                             |  | т            | т           | [52]   |
| A. P.                                  |  | 1            | 1           | [02]   |
| at Quillering                          |  |              |             |        |
|  |  |              |             |        |
| °~~                                    |  | Ι            | Ι           | [52]   |
|  |  |              |             |        |
|  |  |              |             |        |
| TH. D                                  |  |              |             |        |
| 8                                      |  | Ι            | PS          | [52]   |
|  |  | -            | ~           | r - =1 |
|  |  |              |             |        |
|  |  |              |             |        |
| ~ <b>_</b> /                           |  | Ι            | $_{\rm PS}$ | [52]   |
| $\Diamond$                             |  |              |             |        |
|  |  |              |             |        |
| i-i-i                                  |  |              |             |        |
| < <u>_</u> >                           |  |              |             |        |

| MONOMER              | Table S11 - Continued from previous page | Emponimental | Prodicted   | Pof    |
|----------------------|--|--------------|-------------|--------|
|                      |  | I            | S           | [52]   |
|                      |  |              |             |        |
|                      |  |              |             |        |
|                      |  |              |             |        |
|                      |  | Ι            | I           | [52]   |
|                      |  | -            | -           | []     |
|                      |  |              |             |        |
|                      |  |              |             |        |
| 0<br>0               |  | S            | $_{\rm PS}$ | [42]   |
| \                    |  |              |             |        |
| $\sim$               |  | S            | S           | [42]   |
|                      |  |              |             | []     |
| ∼, Åo, ,             |  | G            | g           | [40]   |
| , DI⊁°               |  | 5            | Б           | [42]   |
| X°~~ J               |  | G            | G           | [ 4 4] |
| Š                    |  | 5            | Б           | [44]   |
|                      |  |              |             |        |
| 24.000               |  | G            | G           | [ 4 4] |
| الله الم             |  | 8            | 5           | [44]   |
| Hi~ de               |  |              |             |        |
|                      |  | q            | q           | [44]   |
| Lo <sup>i</sup> ~ nA |  | 5            | 5           | [44]   |
| -00                  |  |              |             |        |
| 2                    |  | q            | q           | [44]   |
|                      |  | 5            | 5           | [44]   |
|                      |  |              |             |        |
|                      |  |              |             |        |
| °~                   |  | S            | S           | [44]   |
| 20                   |  |              |             |        |
|                      |  | s            | S           | [44]   |
| Ś                    |  | ~            | -           | []     |
| ion 20               |  |              |             |        |
| Xxxh.~~ ()           |  | S            | S           | [44]   |
|                      |  |              |             | []     |
| Sec Of               |  |              |             |        |
|                      |  | S            | S           | [44]   |
| stor ~ al            |  |              |             |        |
|                      |  |              |             |        |
|                      |  | S            | S           | [44]   |
|                      |  |              |             |        |
|                      |  |              |             |        |
|                      |  | т            | т           | [37]   |
|                      |  | 1            | 1           | [37]   |
| 0, ~ ~ 0, N.         |  | S            | S           | [37]   |
|                      |  |              |             |        |
|                      |  | S            | S           | [37]   |
| -Y.                  |  |              |             |        |
|                      |  |              |             |        |
|                      |  |              |             |        |
| o <u>``</u> ``       |  | S            | S           | [37]   |
| 20° 0° ° ° ° 0       |  |              |             |        |
| ₩-O                  |  | ÞS           | PG          | [10]   |
|                      |  | 1.0          | 10          | [10]   |
|                      |  |              |             |        |

| MONOMER  | Table S11 - Continued from previous page | Experimental | Predicted | Ref          |
|--|--|--------------|-----------|--------------|
|  |  | PS           | PS        | [10]         |
|  |  | PS           | PS        | [10]         |
|  |  | PS           | PS        | [10]         |
| -Q ** * **<br>∴-book-c."   |  | PS           | PS        | [10]         |
|  |  | PS           | PS        | [10]         |
| 0.0  |  | S            | S         | [3]          |
|  |  |              |           |              |
|  |  | S            | S         | [3]          |
|  |  |              |           |              |
| ora-jot-o  |  | PS           | S         | [3]          |
| -76<br>}7**  |  | S            | S         | [3]          |
|  |  | G            | G         | [9]          |
| a construction of the second s |  | 5            | 5         | [3]          |
| adan Jak   |  | S            | S         | [3]          |
| aialain  |  | S            | S         | [3]          |
| otoilaia.  |  | S            | S         | [3]          |
| o-o-joi.o.jo.  |  | PS           | S         | [3]          |
| A poilaig.   |  | 5            | 5         | [3]          |
| ogo pointe   |  | S            | s         | [3]          |
| opioining.   |  | PS           | PS        | [66]         |
| .۵.۵ <sup>°</sup> . ک.   |  | . S          |           | [00]         |
| °da.a'.X   |  | PS<br>PS     | 5<br>PS   | [66]         |
| <sup>م</sup> گر ب <sup>ش</sup> گر م<br>م   |  | 15           | 10        | [00]         |
| oontotot   |  | PS           | PS<br>PS  | [47]<br>[47] |
| and the state  |  | • •          |           | L-,1         |

| Table S11 - Con  | tinued from previous page Experimental | Predicted   | Ref  |
|--|--|-------------|------|
| *  | PS                                     | PS          | [47] |
| To the second  |  |             |      |
| 20 A B B B B B B B B B B B B B B B B B B   | PS                                     | $_{\rm PS}$ | [47] |
| a a the second s | PS                                     | PS          | [47] |
|  | PS                                     | $_{\rm PS}$ | [47] |
|  | PS                                     | PS          | [47] |
|  |  | DC          | [0]  |
|  | P5                                     | PS          | [2]  |
|  |  |             |      |
| ×  | PS                                     | $_{\rm PS}$ | [2]  |
|  |  |             |      |
| Data 201   | PS                                     | PS          | [2]  |
|  | PS                                     | PS          | [2]  |
|  |  |             |      |
|  | Pg                                     | PS          | [0]  |
| in the second se | 15                                     | 15          | [2]  |
|  | PS                                     | $_{\rm PS}$ | [2]  |
| o to   |  |             |      |
|  | PS                                     | PS          | [2]  |
| -00-104-0 <u>4</u>   |  |             |      |
|  | PS                                     | $_{\rm PS}$ | [2]  |
|  |  |             |      |
| - 10   | PS                                     | $_{\rm PS}$ | [2]  |
|  |  |             |      |

| MONOMER   | Experimental | Predicted | Ref  |
|---|--------------|-----------|------|
| Q,Q,Q,Q,  | I            | Ι         | [51] |
|   | Ι            | Ι         | [51] |
|   | Ι            | Ι         | [51] |
| $s^{*} \sim s^{*} \sim s^{*$ | S            | S         | [63] |
|   | S            | S         | [63] |
|   | PS           | PS        | [45] |
|   | PS           | PS        | [45] |
|   |              | 10        | [10] |
|   | PS           | PS        | [45] |
|   | PS           | PS        | [45] |
|   | PS           | PS        | [45] |
|   |              |           |      |
|   | $_{\rm PS}$  | S         | [45] |
|   | S            | S         | [15] |
|   | S            | S         | [15] |
|   |              |           |      |
|   | S            | S         | [15] |
|   | S            | S         | [15] |
|   |              |           |      |
|   | S            | S         | [15] |
|   |              |           |      |
|   | S            | S         | [15] |
|   | S            | S         | [15] |
|   |              |           |      |
|   | S            | S         | [15] |
|   |              |           |      |

Table S12: The table lists the experimental and predicted solubility classes (S - soluble, PS - partially soluble/swelling/soluble on heating, I - insoluble) for different polymers in DMSO. Predictions for the RF model are reported.

| MONOMER                                  | Table S12 – Continued from previous page $($ | Fanonimental | Prodicted | Pof  |
|--|--|--------------|-----------|------|
| MONOMER                                  |  | S            | S         | [15] |
|  |  |              |           |      |
|  |  | S            | S         | [15] |
|  |  | S            | S         | [16] |
|  |  | S            | S         | [16] |
|  |  | S            | S         | [16] |
|  |  | S            | S         | [16] |
|  |  |              |           | [ ]  |
|  |  | S            | S         | [16] |
| 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1 |  | S            | S         | [38] |
|  |  | PS           | PS        | [38] |
| joau.o.a.                                |  | S            | S         | [38] |
| damara.                                  |  | PS           | S         | [48] |
|  |  | PS           | S         | [48] |
|  |  | 10           | 5         | [40] |
|  |  | S            | S         | [48] |
|  |  | S            | S         | [48] |
|  |  | PS           | S         | [48] |
| Kingero-                                 |  | S            | S         | [18] |
| O-("-Q<br>D-0                            |  | ~            |           | r ~1 |

| MONOMER   | Table S12 – Continued from previous page | Experimental | Predicted | Ref  |
|---|--|--------------|-----------|------|
|   |  | 5            | 5         | [18] |
|   |  | S            | S         | [18] |
|   |  | S            | S         | [18] |
|   |  | S            | S         | [18] |
|   |  | S            | S         | [46] |
| .i.0  |  | S            | S         | [46] |
| ;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;  |  | 5            | 5         | [10] |
|   |  | PS           | PS        | [46] |
| ·*·~·~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~  |  | PS           | S         | [46] |
|   |  | PS           | PS        | [46] |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~  |  | PS           | PS        | [46] |
|   |  | PS           | PS        | [46] |
| مر<br>چر  |  | PS           | PS        | [46] |
| میں<br>چانہ میں میں میں   |  | S            | S         | [65] |
| in the second |  | S            | S         | [65] |
| <u>, o tata, ara</u> .<br>'''.  |  | S            | S         | [65] |
| analam analana  |  | S            | S         | [65] |
| مېمېمون<br>م  |  | PS           | PS        | [52] |
| , ¢   |  | PS           | Ι         | [52] |
| 12 02 0   |  | Ŧ            | DC        | [#0] |
| a a point and a |  | 1            | 42        | [52] |

| MONOMER  | Table S12 – Continued from previous page | Experimental | Predicted   | Ref   |
|--|--|--------------|-------------|-------|
|  |  | I            | Ι           | [52]  |
| .₽ <sup>, u</sup> ło <u>‡</u> q.   |  |              |             |       |
| Ŭ.   |  | I            | Ι           | [52]  |
|  |  |              |             |       |
|  |  | I            | Ι           | [52]  |
|  |  |              |             |       |
|  |  | Ŧ            |             | [50]  |
|  |  | 1            | 1           | [52]  |
| piaj de  |  |              |             |       |
|  |  | I            | Ι           | [52]  |
|  |  |              |             |       |
| "herd" and the   |  |              |             |       |
| < <u>&lt;</u> _>   |  | Ι            | Ι           | [52]  |
|  |  |              |             |       |
| °+{-}-,<br>°+{-}-,<br>°  |  | DG           | DC          | [0.4] |
| on <sup>oral</sup> alatalan<br>K   |  | PS           | PS          | [64]  |
| ີອ.<br>  |  | PS           | $_{\rm PS}$ | [64]  |
| · malaar malaa   |  | PS           | $_{\rm PS}$ | [64]  |
| -0-10-10-0-0-0-0-0-0-0-0-0-0-0-0-0-0-0-  |  |              |             |       |
|  |  | PS           | PS          | [64]  |
|  |  | PS           | PS          | [19]  |
| A A A A  |  |              |             |       |
|  |  | S            | S           | [19]  |
|  |  |              |             |       |
|  |  |              |             |       |
|  |  | S            | S           | [19]  |
|  |  |              |             |       |
|  |  |              |             |       |
| N<br>ČÇşe  |  | S            | S           | [19]  |
| of Jupping   |  |              |             |       |
| ~Q.,   |  | S            | S           | [19]  |
| -ninter -0   |  |              |             |       |
| and the second s |  | S            | $_{\rm PS}$ | [35]  |
| ······································   |  | S            | S           | [35]  |
| ">"  |  | S            | S           | [17]  |
|  |  |              |             |       |
| ")<br>", = ",  |  | S            | S           | [17]  |
|  |  |              |             |       |
|  |  |              |             |       |

| Table S<br>MONOMER  | 512 – Continued from previous page | Experimental | Predicted | Ref        |
|---|------------------------------------|--------------|-----------|------------|
|   |                                    | 5            | 5         | [17]       |
|   |                                    | S            | S         | [17]       |
|   |                                    | S            | S         | [17]       |
|   |                                    | S            | S         | [20]       |
|   |                                    | S            | S         | [20]       |
|   |                                    | S            | S         | [20]       |
|   |                                    | S            | S         | [20]       |
| lonaluta.<br>Tal. 19.~  |                                    | S            | S         | [20]       |
|   |                                    | Ι            | S         | [5]        |
| to the second   |                                    | S            | S         | [5]        |
|   |                                    | S            | S         | [5]        |
| a jajat at  |                                    | S            | S         | [5]        |
| a pita  |                                    | S            | S         | [5]        |
|   |                                    | I            | I         | [5]<br>[5] |
| the second se   |                                    | S            | S         | [5]        |
| topologe and the second s  |                                    | S            | S         | [5]        |
| plater and the second   |                                    | S            | S         | [5]        |
| ditatat   |                                    | S            | S         | [5]        |
| $\sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{i$ |                                    | S            | S         | [42]       |
| $\mathcal{N}_{0}^{\mu}$ $\sim$ $^{a}\mathcal{D}_{0}^{\mu}$ $\neq$ $^{o}$  |                                    | S            | S         | [42]       |
| And a start for the start for   |                                    | s            | S         | [42]       |
|   |                                    | S            | S         | [50]       |

| MONOMER                                  | Table S12 - Continued from previous page | Experimental | Predicted | Ref  |
|--|--|--------------|-----------|------|
| i an Ar                                  |  | 1            | 1         | [50] |
| Qin to                                   |  | S            | S         | [44] |
| Arrise C                                 |  | I            | I         | [44] |
|  |  |              |           |      |
| - A                                      |  | S            | Ι         | [44] |
| ^ <sup>*</sup> ,                         |  | S            | S         | [44] |
|  |  | I            | I         | [44] |
| - 90                                     |  |              |           |      |
| giu ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ |  | S            | S         | [44] |
| tai~al                                   |  | Ι            | Ι         | [44] |
|  |  | S            | T         | [44] |
| -op-ofo                                  |  |              |           | []   |
| , O <sup>°</sup> O, O                    |  | Ι            | S         | [44] |
|  |  | I            | PS        | [37] |
|  |  | 1            | 1         | [37] |
|  |  | PS           | т         | [37] |
|  |  | 15           | 1         | [37] |
|  |  | P5           | PS        | [37] |
|  |  | PS           | PS        | [10] |
| ب<br>۲-۲-۲-۲                             |  | PS           | PS        | [10] |
|  |  | PS           | PS        | [10] |
|  |  | PS           | PS        | [10] |
| -2-00C                                   |  | PS           | PS        | [10] |
|  |  | гэ           | гð        | [10] |
|  |  | S            | PS        | [10] |
|  |  |              |           |      |

| Sec. 1  | PS |             | [0]   |
|---|----|-------------|-------|
|   |    | гЪ          | [3]   |
| 0-j0 <sup>1</sup> .0 <sup>1</sup> .0  | PS | PS          | [3]   |
| orovie pot<br>Potenti<br>Att  |    |             |       |
|   | S  | PS          | [3]   |
|   | S  | S           | [3]   |
| Tation and the second sec  |    |             |       |
| oo da ja ja ja  | S  | S           | [3]   |
| o <sup>l Q</sup> iodo   | PS | PS          | [3]   |
|   | PS | PS          | [3]   |
|   | PS | $_{\rm PS}$ | [3]   |
|   | PS | PS          | [3]   |
| o Bo jai a ia   | S  | S           | [3]   |
| Jarta Andra   | S  | $_{\rm PS}$ | [3]   |
|   | S  | S           | [3]   |
| ju jo jo  | S  | PS          | [56]  |
|   | PS | PS          | [56]  |
| to of the   |    |             |       |
| a starter and   | S  | S           | [56]  |
| the set of | S  | S           | [56]  |
|   | S  | S           | [56]  |
| - The second  | 20 | D.C.        | [= 0] |
|   | PS | PS          | [56]  |
| Sa.o.   | PS | PS          | [66]  |
|   | PS | PS          | [66]  |
|   | PS | PS          | [66]  |
| on when   | PS | $_{\rm PS}$ | [47]  |

| Table S12 – Continued from previo  |                    | Dradit-1-1  | D - f |
|--|--------------------|-------------|-------|
|  | Experimental<br>PS | Preatcted   | [47]  |
|  |                    |             |       |
| and the factor   | PS                 | S           | [47]  |
| a a the second sec | PS                 | PS          | [47]  |
|  | PS                 | $_{\rm PS}$ | [47]  |
|  | PS                 | PS          | [47]  |
|  | DC                 | ÞS          | [47]  |
|  | F3                 | го          | [47]  |
|  | PS                 | PS          | [2]   |
|  |                    |             |       |
|  | PS                 | PS          | [2]   |
|  | PS                 | PS          | [2]   |
|  |                    |             |       |
|  | PS                 | PS          | [2]   |
|  |                    |             |       |
|  | PS                 | PS          | [2]   |
| a construction of the second  |                    |             |       |
| .00. ini.  | PS                 | PS          | [2]   |
|  | PS                 | $_{\rm PS}$ | [2]   |
|  |                    |             |       |
|  | PS                 | PS          | [2]   |
|  |                    |             |       |
|  |                    |             |       |

Table S13: The table lists the experimental and predicted refractive indices measured at given wavelengths for different polymers. Refractive indices for polymers at wavelengths other than 589 nm were taken from multiple references [51, 21, 16, 8, 57, 55, 19, 35, 42, 24, 54]. Here, the the refractive indices are predicted using the polarizabilities derived from DFT calculations and densities predicted using a QSPR model.

| MONOMER   | n <sub>DFT</sub> | $\frac{\lambda}{500}$ | n <sub>pred</sub> |
|---|------------------|-----------------------|-------------------|
| $\bigwedge_{i} \circ \bigvee_{i} \circ \bigvee_{i} \circ \bigvee_{i} \circ \bigvee_{i} \circ \circ$   | 1.34             | 589<br>589            | 1.27              |
| $ \bigotimes_{r}^{M} \circ \bigvee_{r}^{M} \circ \bigvee_{$ | 1.35             | 589                   | 1.29              |
|   | 1.35             | 589                   | 1.21              |
|   |                  |                       |                   |
| F F   |                  |                       |                   |
| $\sim \tilde{H}_{o} \sim r_{p} r_{p} r_{p} r_{p} r_{p}$   | 1.36             | 589                   | 1.28              |
|   | 1.36             | 589                   | 1.29              |
| ۲۹ <sup>°</sup> <sup>۲</sup> <sup>°</sup> <sup>۲</sup> <sup>°</sup> <sup>۲</sup> <sup>°</sup>   | 1.36             | 589                   | 1.30              |
|   | 1.36             | 589                   | 1.30              |
|   | 1.37             | 589                   | 1.31              |
|   | 1.38             | 589                   | 1.34              |
|   |                  |                       |                   |
|   | 1.38             | 589                   | 1.31              |
|   | 1.38             | 589                   | 1.41              |
|   | 1.00             | 500                   | 1.04              |
|   | 1.39             | 589                   | 1.34              |
| $ \begin{array}{c} F \ F \\ \overset{P}{\underset{o}{\overset{P}}} & \overset{P}{\underset{o}{\overset{P}}} \\ \overset{P}{\underset{o}{\overset{P}}} & \overset{P}{\underset{o}{\overset{P}}} \\ \end{array} $   | 1.39             | 589                   | 1.35              |
|   | 1.39             | 589                   | 1.33              |
|   | 1.40             | 589                   | 1.53              |
| Si  | 1.40             | 589                   | 1.42              |
| Si  |                  |                       |                   |
|   | 1.41             | 589                   | 1.38              |
|   |                  |                       |                   |
| $\circ$   | 1.41             | 589                   | 1.38              |
| E F   | Contin           | ued on r              | next page         |

| Table S13 - Continued from previous page |                     |                       |                         |
|--|---------------------|-----------------------|-------------------------|
|  | <u>nDFT</u><br>1.42 | $\frac{\lambda}{589}$ | $\frac{n_{pred}}{1.44}$ |
|  |                     |                       |                         |
|  | 1.42                | 589                   | 1.42                    |
| <b>S F</b>                               | 1.42                | 589                   | 1.36                    |
|  |                     |                       |                         |
| F  | 1 49                | 590                   | 1.96                    |
|  | 1.45                | 269                   | 1.20                    |
|  |                     |                       |                         |
|  | 1.44                | 589                   | 1.41                    |
|  |                     | 500                   |                         |
| Stop Stop                                | 1.44                | 589                   | 1.47                    |
| k<br>I                                   | 1.44<br>1.45        | $589 \\ 589$          | 1.51                    |
|  | 1.45                | 589                   | 1.55                    |
|  |                     |                       |                         |
|  | 1.45                | 589                   | 1.53                    |
|  | 1.45                | 589<br>589            | 1.52                    |
|  | 1.46                | 589                   | 1.51                    |
|  | 1.46                | 589                   | 1.48                    |
|  | 1.46                | 589                   | 1.59                    |
|  | 1.46                | 589                   | 1.56                    |
|  | 1.46                | 589                   | 1.59                    |
|  | $1.46 \\ 1.46$      | 589<br>589            | 1.60<br>1.61            |
|  | 1.46                | 589                   | 1.51                    |
|  |                     |                       |                         |
| // ₩<br>~~~~~°≪                          | 1.46                | 589                   | 1.62                    |
|  | 1.46                | 589                   | 1.54                    |
|  | $1.46 \\ 1.46$      | $589 \\ 589$          | $1.61 \\ 1.48$          |
|  |                     |                       |                         |
| ~° <i>γ</i> ≈                            | 1.46                | 589                   | 1.52                    |
|  | 1.46                | 589                   | 1.48                    |
|  | 1.46                | 589                   | 1.51                    |
| $\sim 10^{10} \times$                    |                     |                       |                         |

| Table S13 – Continued from previous page  |                  |            |       |
|---|------------------|------------|-------|
| MONOMER   | n <sub>DFT</sub> | λ          | npred |
| ~~~~°⁄  | 1.40             | 589<br>589 | 1.61  |
|   |                  | 000        | 1.01  |
| $\wedge$  |                  |            |       |
|   | 1.47             | 589        | 1.56  |
|   |                  |            |       |
| $\sim \sim \sim \sim$   | 1.47             | 589        | 1.54  |
|   |                  |            |       |
| ~ 9 <i>//</i>   | 1.47             | 589        | 1.49  |
| $\gamma \uparrow \gamma$  |                  |            |       |
| 0   | 1 47             | 589        | 1 49  |
| 0   |                  | 000        | 1110  |
|   |                  |            |       |
|   | 1.47             | 580        | 1 49  |
| 0 //  | 1.47             | 589        | 1.40  |
|   | 1 47             | 589        | 1.52  |
| $\searrow^{0}$  |                  | 000        | 1.02  |
|   |                  |            |       |
|   | 1.47             | 589        | 1.55  |
|   | 1.47             | 589        | 1.59  |
| ~°~~~° <sub>1</sub> ~   | 1.47             | 589        | 1.51  |
| 0   | 1.47             | 589        | 1.52  |
| $\sim \sim $ |                  |            |       |
|   | 1.47             | 589        | 1.59  |
|   | 1.47             | 589        | 1.40  |
| о ~ Å ~.0   |                  |            |       |
| ·~~~·'i   | 1.48             | 589        | 1.58  |
| "~~~~ <sup>n</sup> Ă~~~~ <sup>0</sup>   | 1.48             | 589        | 1.55  |
| °~~   | 1.48             | 589        | 1.44  |
|   |                  |            |       |
|   |                  |            |       |
| , L   |                  |            |       |
|   | 1.48             | 589        | 1.50  |
|   |                  |            |       |
|   |                  |            |       |
|   | 1.48             | 589        | 1.47  |
|   |                  |            |       |
|   |                  |            |       |
| ) , <mark>°</mark>  | 1 48             | 589        | 1 48  |
|   |                  |            |       |
| ∧ Å × .º  |                  |            |       |
| 0   | 1.49             | 589        | 1.41  |
| $\sim \sqrt{2}$   |                  |            |       |
| 0   | 1.50             | 589        | 1.46  |
|   |                  |            |       |
|   |                  |            |       |
|   | 1.50             | 589        | 1.49  |
|   |                  |            |       |
|   |                  |            |       |
|   | 1.50             | 589        | 1.50  |
|   |                  |            |       |
| <b>▼</b>  | 1.50             | 589        | 1.70  |
|   |                  |            |       |
| <u>∽c</u> −   |                  | FOO        | 1 50  |
|   | 1.50             | 589        | 1.53  |
|   |                  |            |       |
|   |                  |            |       |

| $\begin{array}{c c} \hline MONOMER & n_{DFT} \\ \hline & & 1.50 \\ \hline & & 0 \\ \hline & & 1.50 \end{array}$ | $\frac{\lambda}{589}$ | <u>n<sub>pred</sub></u><br>1.48 |
|---|-----------------------|---------------------------------|
|   | 589                   | -                               |
| 1.50  | 589                   |                                 |
|   |                       | 1.56                            |
| 1.50  | 589                   | 1.54                            |
|   | 589                   | 1.61                            |
|   | 589                   | 1.52                            |
|   | 589                   | 1.49                            |
|   | 589                   | 1.56                            |
| 1.51  | 589                   | 1.51                            |
|   | 589                   | 1.47                            |
|   | 589                   | 1.48                            |
|   | 589                   | 1.50                            |
|   | 589                   | 1.49                            |
|   | 589                   | 1.56                            |
|   | 589                   | 1.55                            |
|   | 589                   | 1.58                            |
| 1.54  | 589                   | 1.43                            |
| 0<br>1.55   | 589                   | 1.61                            |
|   | 589                   | 1.55                            |
|   | 589                   | 1.60                            |
| Table S13 - Continued from previous page  |                          |                       |                         |
|---|--------------------------|-----------------------|-------------------------|
| MONOMER   | n <sub>DFT</sub><br>1.55 | $\frac{\lambda}{589}$ | $\frac{n_{pred}}{1.53}$ |
|   | 1.00                     | 000                   | 1100                    |
|   | 1.55                     | 589                   | 1.48                    |
|   | 1.55                     | 589                   | 1.55                    |
|   | 1.55                     | 589                   | 1.69                    |
|   | 1.56                     | 589                   | 1.63                    |
|   | 1.56                     | 589                   | 1.65                    |
|   | 1.56                     | 589                   | 1.62                    |
|   | 1.56                     | 589                   | 1.59                    |
|   | 1.56                     | 589                   | 1.55                    |
| ↓ ny O <sup>l</sup>   | 1.57                     | 589                   | 1.63                    |
|   | 1.57                     | 589                   | 1.46                    |
| O Br  | 1.57                     | 589                   | 1.61                    |
|   | 1.57                     | 589                   | 1.56                    |
| ,<br>М.<br>М.<br>М.<br>М.<br>М.<br>С  | 1.57                     | 589                   | 1.62                    |
|   | 1.57                     | 589                   | 1.59                    |
|   | 1.57                     | 589                   | 1.60                    |
|   | 1.57                     | 589                   | 1.60                    |
| ° ↓<br><sup>↓</sup> <sup>↓</sup> <sup>↓</sup> <sup>↓</sup> <sup>↓</sup> <sup>↓</sup> <sup>↓</sup> | 1.57                     | 589                   | 1.59                    |
|   | Contin                   | ued on a              | next page               |

| Table S13 - Continued from previous page   |                          |                       |                         |
|--|--------------------------|-----------------------|-------------------------|
| MONOMER  | n <sub>DFT</sub><br>1.57 | $\frac{\lambda}{589}$ | $\frac{n_{pred}}{1.52}$ |
| $ \underset{O}{\overset{Br}{\longrightarrow}} \circ \overset{Br}{\overset{Br}{\longrightarrow}} Br $ | 1.01                     |                       | 1.02                    |
| • عرفی او م  | 1.58                     | 589                   | 1.51                    |
|  | 1.58                     | 589                   | 1.56                    |
| $-\langle \bigcirc \rangle$  | 1.58                     | 589                   | 1.64                    |
|  | 1.58                     | 589                   | 1.64                    |
|  |                          |                       |                         |
| $\langle \rangle$  | 1.58                     | 589                   | 1.60                    |
| $\gamma^{i} \sim Q$  | 1.63                     | 589                   | 1.69                    |
|  | 1.63                     | 589                   | 1.68                    |
|  | 1.64                     | 589                   | 1.72                    |
| $\downarrow^{\circ}$   | 1.64                     | 589                   | 1.69                    |
|  | 1.66                     | 589                   | 1.73                    |
|  | 1.67                     | 589                   | 1.57                    |
|  | 1.68                     | 589                   | 1.81                    |
|  | 1.68                     | 589                   | 1.81                    |
|  | 1.71                     | 589                   | 1.52                    |
|  |                          |                       |                         |
|  | 1.79                     | 633                   | 1.75                    |
|  | 1.51                     | 589                   | 1.60                    |
|  | 1.64                     | 637                   | 1.65                    |
|  |                          |                       |                         |

Continued on next page

|   | Table S13 · | <ul> <li>Continued from previous page</li> </ul> |                     |          |                         |
|---|-------------|--|---------------------|----------|-------------------------|
| MONOMER   |             |  | <u>nDFT</u><br>1.76 | λ<br>633 | $\frac{n_{pred}}{1.85}$ |
|   |             |  |                     |          |                         |
|   |             |  |                     |          |                         |
| 0.5 M O'  |             |  | 1.75                | 633      | 1.78                    |
|   |             |  |                     |          |                         |
| já-Ó  |             |  |                     |          |                         |
|   |             |  | 1.76                | 633      | 1.81                    |
|   |             |  |                     |          |                         |
| <u>6</u>  |             |  |                     |          |                         |
| 0,0'0.  |             |  | 1.71                | 633      | 1.80                    |
| ·*·Q0 <sup>2</sup> .  |             |  | 1 76                | 622      | 1 91                    |
| م <sup>بغ</sup> ره مرم <sup>ب</sup> ه ک   |             |  | 1.70                | 035      | 1.81                    |
|   |             |  | 1.75                | 633      | 1.81                    |
| 0.4-0-0   |             |  |                     |          |                         |
| °~<br>*↓*Å.   |             |  | 1.58                | 1324     | 1.62                    |
|   |             |  |                     |          |                         |
|   |             |  | 1.51                | 1324     | 1.61                    |
|   |             |  |                     |          |                         |
|   |             |  | 1.74                | 633      | 1.78                    |
| ) <u> </u>  |             |  |                     |          |                         |
| ~0 <sup>4</sup> , 0   |             |  |                     | 400      | 1 50                    |
|   |             |  | 1.74                | 633      | 1.78                    |
|   |             |  |                     |          |                         |
|   |             |  |                     |          |                         |
|   |             |  | 1.74                | 633      | 1.78                    |
|   |             |  |                     |          |                         |
|   |             |  |                     |          |                         |
| ·~O <sup>4</sup> .~O  |             |  |                     |          |                         |
| 10 00 00 00   |             |  | 1.74                | 633      | 1.75                    |
| 2,0 1 1 1 0,0   |             |  |                     |          |                         |
|   |             |  | 1.75                | 633      | 1.74                    |
| -2  |             |  |                     |          |                         |
| ~0 <sup>4</sup> .0  |             |  | 1 50                | 400      | 1.00                    |
|   |             |  | 1.73                | 033      | 1.80                    |
| کو  |             |  | 1 57                | 1294     | 1.62                    |
| کې بغر مړه کې   |             |  | 1.57                | 1524     | 1.03                    |
| 0.0'0.0   |             |  | 1.70                | 1310     | 1.77                    |
| ·~~VO-4.  |             |  | 1 59                | 589      | 1.58                    |
| , <sup>k</sup> α~"1 <sup>°</sup> ~" <sup>(C<sup>1</sup>)</sup> <sup>(2)</sup> <sup>(2)</sup> <sup>(2)</sup> |             |  | 1.00                |          |                         |
| <<br>入<br>。<br>"<br>一<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、<br>、                      |             |  | 1.64                | 589      | 1.58                    |
| Xys~sk1s~   |             |  |                     |          |                         |
|   |             |  | 1.61                | 589      | 1.61                    |
| 5   |             |  | 1.62                | 589      | 1.55                    |
| ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~  |             |  | 1.02                |          |                         |
|   |             |  | 1.65                | 1324     | 1.62                    |
|   |             |  |                     |          |                         |
| -<br>   |             |  | 1.72                | 1310     | 1.77                    |
| o a a a'r   |             |  |                     |          |                         |

Continued on next page

|          | Table S13 – Continued from previous page |                   |      |
|----------|--|-------------------|------|
| MONOMER  | n <sub>DFT</sub>                         | $\lambda$ $n_{j}$ | pred |
|          | 1.60                                     | 633 1             | .66  |
|          | 1.60                                     | 633 1             | 66   |
| io or    | 1.71                                     | 633 1             | 75   |
|          | 1.73                                     | 633 1             | 77   |
| NOCON-O  | 1.69 1                                   | 1320 1            | 58   |
| ° ° F    | 1.52                                     | 589 1             | 33   |
|          |  |                   |      |
| °∽°°°°°© | 1.58                                     | 589 1             | .64  |
| \N       | 1.52                                     | 500 1             | .00  |
| <u> </u> | 1.45                                     | 009 1             |      |



Figure S1: Plot shows the histogram of the predicted refractive indices for the different monomers emerging from the de novo runs.



Figure S2: Plot shows the scatter plot of the molecular weights vs the experimental refractive indices (taken from literature) of various polymers.



Figure S3: Plot shows the scatter plot of the molecular weights vs the predicted refractive indices of different monomers emerging from the de novo runs.



Figure S4: Plot shows the histogram of the synthetic accessibility scores for the different monomers emerging from the de novo runs.



Figure S5: Calculated UV-VIS spectra for different polymers (see main article).

| MONOMER              | $n_{exp}$ | $\rho_{qspr}$ | $\rho_{exp}$ | $n_{pred}$ |
|----------------------|-----------|---------------|--------------|------------|
|                      | 1.34      | 1.40          | 1.42         | 1.27       |
|                      | 1.35      | 1.37          | 0.91         | 1.14       |
|                      |           |               |              |            |
| $\bowtie$            |           |               |              |            |
| F F                  | 1.40      | 0.06          | 0.80         | 1 20       |
| 0. /                 | 1.40      | 0.90          | 0.89         | 1.39       |
| Si                   |           |               |              |            |
|                      |           |               |              |            |
| e F II               | 1.42      | 1.38          | 0.88         | 1.27       |
|                      |           |               |              |            |
|                      | 1.42      | 1.44          | 1.13         | 1.27       |
|                      |           |               |              |            |
|                      |           |               |              |            |
| F                    |           |               |              |            |
| CI F                 | 1.43      | 1.36          | 1.66         | 1.32       |
| $\rightarrow$        |           |               |              |            |
|                      |           |               |              |            |
|                      | 1.44      | 0.94          | 1.60         | 1.93       |
| Ś.                   | 1.45      | 1.25          | 1 39         | 1.62       |
|                      | 1.40      | 1.20          | 1.00         | 1.02       |
|                      |           |               |              |            |
|                      | 1.45      | 1.03          | 1.25         | 1.67       |
| ≫° ∕∕                | 1.45      | 0.97          | 1.26         | 1.73       |
|                      | 1.45      | 1.03          | 1.17         | 1.59       |
|                      | 1.46      | 0.95          | 1.34         | 1.79       |
|                      | 1.46      | 1.11          | 1.02         | 1.44       |
| $\sim$ 0             |           |               |              |            |
| <b>∽∽</b> ⁰ <i>∅</i> | 1.46      | 1.13          | 1.03         | 1.53       |
|                      | 1.40      | 1.13          | 1.13         | 1.61       |
| F F                  | 1.46      | 1.38          | 1.17         | 1.42       |
| F - X                |           |               |              |            |
| F F                  |           |               |              |            |
|                      | 1.46      | 1.13          | 1.15         | 1.63       |
|                      | 1.46      | 1.10          | 1.12         | 1.62       |
|                      | 1.40      | 1.09          | 1.41         | 1.00       |
|                      |           |               |              |            |
|                      | 1.46      | 1.10          | 1.10         | 1.62       |
|                      | 1.41      | 0.95          | 1.11         | 1.00       |
| $\wedge$             |           |               |              |            |

Table S14: The table lists the experimental  $(n_{exp})$  and predicted refractive indices  $(n_{pred})$  for different polymers. The n were estimated using DFT-based polarizability values at 589 nm and reported experimental densities.

Continued on next page

|                | Table S14 - Continued from previous page |               |              |                   |
|----------------|--|---------------|--------------|-------------------|
| MONOMER        | <i>n<sub>exp</sub></i>                   | $\rho_{qspr}$ | $\rho_{exp}$ | n <sub>pred</sub> |
| ~~°∦≈          | 1.47                                     | 1.15          | 1.05         | 1.48              |
| ∧_v° ∕∕∕       | 1.47                                     | 1.13          | 1.18         | 1.51              |
| Ö              | 1.47                                     | 1.20          | 1.08         | 1.44              |
|                |  |               |              |                   |
| 0.1            | 1.47                                     | 1.03          | 1.06         | 1.50              |
|                | 1.47                                     | 1.18          | 1.01         | 1.43              |
|                | 1.47                                     | 0.99          | 0.93         | 1.54              |
| °~°Å~~°        | 1.47                                     | 1.10          | 1.10         | 1.39              |
| N~~~~~NH~~~~0  | 1.48                                     | 1.14          | 0.93         | 1.43              |
| 0 //           | 1.50                                     | 1.13          | 1.30         | 1.40              |
| $\mathbf{v}$   | 1.50                                     | 1.07          | 1.04         | 1.68              |
| $\leq_{c} =$   | 1.50                                     | 1.15          | 0.93         | 1.43              |
|                |  |               |              |                   |
|                | 1.50                                     | 1.37          | 0.91         | 1.33              |
|                |  |               |              |                   |
|                | 1.51                                     | 0.94          | 0.88         | 1.52              |
| $\mathbf{i}$   |  |               |              |                   |
|                |  | 1.01          | 0.00         | 1.41              |
| <sup>⊥</sup> , | 1.51                                     | 1.01          | 0.89         | 1.41              |
|                | 1.51                                     | 1.18          | 0.85         | 1.34              |
|                |  |               |              |                   |
|                | 1.51                                     | 0.93          | 0.91         | 1.54              |
|                | 1.55                                     | 1.09          | 1.03         | 1.51              |
|                |  |               |              |                   |
|                | 1.55                                     | 1.04          | 1.07         | 1.49              |
|                |  |               |              |                   |
| CI             | 1.56                                     | 1.31          | 1.24         | 1.61              |
| $\sim$         |  | 1.00          | 1.02         | 0.04              |
|                | 1.56                                     | 1.26          | 1.92         | 2.04              |
| •              | 1.57                                     | 1.19          | 1.25         | 1.65              |
|                |  |               |              |                   |
| ¥              |  | Conti         | nued on n    | ext page          |

|   | Table S14 – Continued from previous page |           |               |              |            |
|---|--|-----------|---------------|--------------|------------|
| MONOMER   |  | $n_{exp}$ | $\rho_{qspr}$ | $\rho_{exp}$ | $n_{pred}$ |
| ,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>,<br>, |  | 1.57      | 1.18          | 1.45         | 1.78       |
|   |  | 1.57      | 1.23          | 1.05         | 1.49       |
|   |  | 1.58      | 1.07          | 2.00         | 2.38       |
|   |  | 1.58      | 1.19          | 1.43         | 1.82       |
|   |  | 1.45      | 1.16          | 1.01         | 1.39       |
|   |  | 1.34      | 1.45          | 2.03         | 1.33       |
|   |  | 1.48      | 0.91          | 0.85         | 1.76       |
| $\overline{\checkmark}$   |  | 1.47      | 0.91          | 0.85         | 1.88       |

Table S15: Cases where large deviations between QSPR and DFT estimates for n are observed.



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