

## **Substituent and Ring-Number Effects on the Kinetics of PAH + OH Reactions: A QSAR–DOE Approach with Tunneling Corrections**

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Table S1 Characteristics of descriptors

| Descriptor                               | Symbol        | Unit              |
|------------------------------------------|---------------|-------------------|
| Partial charge on carbon atom            | $q(C)$        | -                 |
| Fukui index for electrophilic attack     | $f^-(C)$      | -                 |
| Fukui index for nucleophilic attack      | $f^+(C)$      | -                 |
| Fukui index for radical attack           | $f^0(C)$      | -                 |
| Dual descriptor                          | $\Delta f(C)$ | -                 |
| Partial charge on hydrogen atom          | $q(H)$        | -                 |
| Reaction energy                          | $\Delta E$    | kcal/mol          |
| HOMO energy                              | HOMO          | Hartree           |
| LUMO energy                              | LUMO          | Hartree           |
| HOMO and LUMO gap                        | HOMO - LUMO   | Hartree           |
| Polarizability                           | $\alpha$      | Bohr <sup>3</sup> |
| Dipole moment                            | $\mu$         | D                 |
| Total energy                             | $E_{SFC}$     | Hartree           |
| Heat capacity                            | $C_p$         | -                 |
| Entropy                                  | $S^0$         | -                 |
| Local ELF maximum within reaction center | $ELFC_{max}$  | -                 |
| Local ELF minimum within reaction center | $ELFC_{min}$  | -                 |
| Local ELF maximum within substituent     | $ELFR_{max}$  | -                 |
| Local ELF minimum within substituent     | $ELFR_{min}$  | -                 |
| NBO value on reaction center             | NBO           | -                 |

Table S2 Values of descriptors for benzene derivatives

| Substituent                    | q(C)    | f(C)   | f <sup>+</sup> (C) | f <sup>0</sup> (C) | Δf(C)   | q(H)   | ΔE    | HOMO    | LUMO    | HOMO - LUMO |
|--------------------------------|---------|--------|--------------------|--------------------|---------|--------|-------|---------|---------|-------------|
| -Br                            | -0.044  | 0.064  | 0.029              | 0.046              | -0.036  | 0.049  | -4.94 | -0.307  | -0.0061 | 0.3009      |
| -Cl                            | -0.045  | 0.07   | 0.03               | 0.05               | -0.04   | 0.05   | -4.52 | -0.3113 | -0.0054 | 0.3059      |
| -F                             | -0.054  | 0.084  | 0.023              | 0.053              | -0.06   | 0.054  | -3.71 | -0.3155 | -0.0046 | 0.3109      |
| -NH <sub>2</sub>               | -0.067  | 0.079  | 0.106              | 0.093              | 0.026   | 0.038  | -5.69 | -0.2677 | -0.0064 | 0.2613      |
| -NO <sub>2</sub>               | -0.028  | 0.134  | 0.055              | 0.094              | -0.079  | 0.055  | -3.48 | -0.3455 | -0.0643 | 0.2812      |
| -CH <sub>3</sub>               | -0.049  | 0.073  | 0.026              | 0.05               | -0.048  | 0.038  | -6.5  | -0.2985 | -0.0025 | 0.296       |
| -C <sub>2</sub> H <sub>5</sub> | 0.049   | 0.068  | 0.021              | 0.045              | -0.047  | 0.037  | -7.28 | -0.2974 | -0.0029 | 0.2945      |
| -C <sub>3</sub> H <sub>7</sub> | -0.0479 | 0.0886 | 0.0565             | 0.0726             | -0.0321 | 0.0424 | -6.48 | -0.3001 | -0.0036 | 0.2964      |
| -C <sub>4</sub> H <sub>9</sub> | -0.0479 | 0.0886 | 0.0565             | 0.0726             | -0.0321 | 0.0424 | -6.48 | -0.2990 | -0.0044 | 0.2947      |
| -OH                            | -0.07   | 0.081  | 0.036              | 0.059              | -0.044  | 0.04   | -5.6  | -0.29   | -0.004  | 0.2861      |
| -OOH                           | 0.058   | 0.085  | 0.029              | 0.057              | -0.056  | 0.049  | -4.84 | -0.2955 | -0.007  | 0.2885      |
| -CHO                           | -0.022  | 0.032  | 0.069              | 0.051              | 0.038   | 0.051  | -5.59 | -0.3215 | -0.0447 | 0.2768      |
| -COOH                          | -0.024  | 0.071  | 0.068              | 0.07               | -0.003  | 0.05   | -5.26 | -0.3186 | -0.0325 | 0.2861      |

Table S3 Values of descriptors for benzene derivatives - continuation

| Substituent                    | α      | μ    | E <sub>SFC</sub> | Cp    | S <sup>0</sup> | ELFC <sub>max</sub> | ELFC <sub>min</sub> | ELFR <sub>max</sub> | ELFR <sub>min</sub> | NBO   |
|--------------------------------|--------|------|------------------|-------|----------------|---------------------|---------------------|---------------------|---------------------|-------|
| -Br                            | 89.03  | 2.29 | -2805.0686       | 46.32 | 123.98         | 0.999994            | 1.36E-06            | 0.957755            | 2.27E-07            | 0.177 |
| -Cl                            | 81.35  | 2.28 | -691.0802        | 46.24 | 120.92         | 0.999968            | 5.82E-07            | 0.966325            | 6.15E-07            | 0.176 |
| -F                             | 66.73  | 2.17 | -330.7095        | 45.97 | 117.42         | 0.999924            | 1.62E-08            | 0.995233            | 2.13E-05            | 0.123 |
| -NH <sub>2</sub>               | 79.03  | 1.39 | -286.8366        | 53.28 | 125.88         | 0.999967            | 9.31E-06            | 0.999727            | 1.33E-07            | 0.118 |
| -NO <sub>2</sub>               | 83.96  | 5.15 | -435.9563        | 56.16 | 136.81         | 0.999986            | 5.96E-06            | 0.999988            | 1.65E-06            | 0.228 |
| -CH <sub>3</sub>               | 80.88  | 0.62 | -270.7891        | 56.97 | 130.84         | 0.999888            | 9.06E-07            | 0.99998             | 3.85E-11            | 0.166 |
| -C <sub>2</sub> H <sub>5</sub> | 93.1   | 0.63 | -310.0872        | 69.59 | 147.52         | 0.999924            | 2.39E-05            | 0.99996             | 2.27E-13            | 0.157 |
| -C <sub>3</sub> H <sub>7</sub> | 106.94 | 0.62 | -349.3844        | 34.60 | 95.32          | 0.999830            | 1.15E-05            | 0.999982            | 4.62E-14            | 0.168 |
| -C <sub>4</sub> H <sub>9</sub> | 119.84 | 0.63 | -388.6819        | 39.49 | 102.37         | 0.999992            | 2.41E-05            | 0.999959            | 1.65E-14            | 0.168 |
| -OH                            | 72.63  | 0.82 | -306.7033        | 49.66 | 121.71         | 0.999985            | 5.01E-06            | 0.99916             | 8.45E-08            | 0.087 |

|       |       |      |           |       |        |          |          |          |          |       |
|-------|-------|------|-----------|-------|--------|----------|----------|----------|----------|-------|
| -OOH  | 78.35 | 1.78 | -381.8129 | 55.17 | 135.05 | 0.999917 | 4.31E-06 | 0.999603 | 2.57E-11 | 0.114 |
| -CHO  | 83.48 | 3.34 | -344.7919 | 54.64 | 131.04 | 0.999973 | 1.70E-06 | 0.999979 | 1.08E-09 | 0.207 |
| -COOH | 86.7  | 2.04 | -420.0398 | 59.88 | 141.14 | 0.999986 | 2.68E-05 | 0.999994 | 9.51E-09 | 0.224 |

Table S4 Values of descriptors for  $\alpha$ -naphthalene derivatives

| Substituent                    | q(C)   | f(C)   | f <sup>+</sup> (C) | f <sup>0</sup> (C) | $\Delta f$ (C) | q(H)   | $\Delta E$ | HOMO    | LUMO    | HOMO - LUMO |
|--------------------------------|--------|--------|--------------------|--------------------|----------------|--------|------------|---------|---------|-------------|
| -Br                            | -0.046 | 0.061  | 0.067              | 0.064              | 0.007          | 0.049  | -5.39      | 0.2795  | -0.0337 | 0.2458      |
| -Cl                            | -0.047 | 0.063  | 0.068              | 0.066              | 0.005          | 0.05   | -4.79      | -0.2797 | -0.0328 | 0.2469      |
| -F                             | -0.059 | 0.072  | 0.068              | 0.07               | -0.004         | 0.054  | -3.57      | -0.2788 | -0.0274 | 0.2514      |
| -NH <sub>2</sub>               | 0.074  | 0.081  | 0.045              | 0.063              | -0.036         | 0.037  | -5.67      | -0.2535 | -0.0171 | 0.2364      |
| -NO <sub>2</sub>               | -0.027 | 0.051  | 0.068              | 0.059              | 0.017          | 0.055  | -4.22      | -0.2988 | -0.0732 | 0.2256      |
| -CH <sub>3</sub>               | -0.05  | 0.066  | 0.061              | 0.063              | -0.005         | 0.039  | -6.47      | 0.27    | -0.0212 | 0.2487      |
| -C <sub>2</sub> H <sub>5</sub> | -0.048 | 0.065  | 0.06               | 0.063              | -0.005         | 0.039  | -6.56      | -0.2693 | -0.0209 | 0.2484      |
| -C <sub>3</sub> H <sub>7</sub> | -0.04  | 0.0706 | 0.0779             | 0.0743             | 0.0073         | 0.0426 | -7.18      | -0.2697 | -0.0205 | 0.2492      |
| -C <sub>4</sub> H <sub>9</sub> | -0.04  | 0.0706 | 0.0779             | 0.0743             | 0.0073         | 0.0426 | -7.13      | -0.2695 | -0.0203 | 0.2492      |
| -OH                            | -0.077 | 0.077  | 0.062              | 0.069              | -0.015         | 0.039  | -5.38      | 0.2636  | -0.0171 | 0.2466      |
| -OOH                           | -0.073 | 0.073  | 0.058              | 0.066              | -0.015         | 0.038  | -4.73      | -0.2691 | -0.0213 | 0.2479      |
| -CHO                           | -0.026 | 0.049  | 0.071              | 0.06               | 0.022          | 0.045  | -5.96      | -0.2874 | -0.0565 | 0.2309      |
| -COOH                          | -0.027 | 0.051  | 0.075              | 0.063              | 0.025          | 0.044  | -6.29      | -0.2847 | -0.0494 | 0.2354      |

Table S5 Values of descriptors for  $\alpha$ -naphthalene - continuation

| Substituent      | $\alpha$ | $\mu$ | E <sub>SFC</sub> | Cp    | S <sup>0</sup> | ELFC <sub>max</sub> | ELFC <sub>min</sub> | ELFR <sub>max</sub> | ELFR <sub>min</sub> | NBO   |
|------------------|----------|-------|------------------|-------|----------------|---------------------|---------------------|---------------------|---------------------|-------|
| -Br              | 138.13   | 2.42  | -2958.6744       | 74.13 | 160.56         | 0.943595            | 4.87E-07            | 0.957847            | 6.05E-09            | 0.18  |
| -Cl              | 130.41   | 2.38  | -844.6858        | 74.03 | 157.5          | 0.999976            | 6.28E-07            | 0.994089            | 2.81E-08            | 0.178 |
| -F               | 115.97   | 2.21  | -484.3147        | 73.73 | 153.97         | 0.999798            | 9.74E-07            | 0.998623            | 1.71E-05            | 0.118 |
| -NH <sub>2</sub> | 128.23   | 1.17  | -440.4418        | 81.03 | 161.99         | 0.999993            | 5.34E-06            | 0.999988            | 5.90E-09            | 0.111 |
| -NO <sub>2</sub> | 134.12   | 5.47  | -589.5569        | 83.99 | 177.88         | 0.999966            | 1.13E-07            | 0.996511            | 4.86E-09            | 0.205 |

|                                |        |      |           |       |        |          |          |          |          |       |
|--------------------------------|--------|------|-----------|-------|--------|----------|----------|----------|----------|-------|
| -CH <sub>3</sub>               | 129.86 | 0.64 | -424.3952 | 84.78 | 165.14 | 0.999908 | 1.50E-06 | 0.999984 | 8.86E-14 | 0.166 |
| -C <sub>2</sub> H <sub>5</sub> | 142.24 | 0.61 | -463.6917 | 97.41 | 182.39 | 0.999874 | 1.16E-06 | 0.999992 | 4.07E-13 | 0.17  |
| -C <sub>3</sub> H <sub>7</sub> | 155.86 | 0.46 | -502.9907 | 46.10 | 104.76 | 0.999999 | 9.32E-07 | 0.999989 | 2.73E-14 | 0.161 |
| -C <sub>4</sub> H <sub>9</sub> | 169.09 | 0.51 | -542.2881 | 51.00 | 112.20 | 0.999775 | 2.36E-06 | 0.999958 | 3.78E-15 | 0.161 |
| -OH                            | 122    | 0.6  | -460.3091 | 77.41 | 158.03 | 0.999867 | 2.84E-06 | 0.999425 | 1.35E-08 | 0.078 |
| -OOH                           | 128.05 | 1.79 | -535.4184 | 82.92 | 171.89 | 0.999900 | 1.88E-04 | 0.999352 | 4.38E-08 | 0.118 |
| -CHO                           | 133.01 | 3.49 | -498.3963 | 82.45 | 167.67 | 0.999984 | 3.51E-05 | 0.999996 | 3.16E-05 | 0.256 |
| -COOH                          | 136.18 | 2.09 | -573.6426 | 87.71 | 178.43 | 0.999972 | 4.89E-06 | 0.999993 | 6.47E-12 | 0.241 |

Table S6 Values of descriptors for  $\beta$ -naphtalene derivatives

| Substituent                    | q(C)    | f(C)   | f <sup>+</sup> (C) | f <sup>0</sup> (C) | $\Delta f(C)$ | q(H)   | $\Delta E$ | HOMO    | LUMO    | HOMO - LUMO |
|--------------------------------|---------|--------|--------------------|--------------------|---------------|--------|------------|---------|---------|-------------|
| -Br                            | -0.046  | 0.04   | 0.063              | 0.052              | 0.023         | 0.049  | -4.85      | -0.2811 | -0.0335 | 0.2476      |
| -Cl                            | -0.046  | 0.044  | 0.067              | 0.055              | 0.023         | 0.05   | -4.46      | -0.2814 | -0.0324 | 0.249       |
| -F                             | -0.052  | 0.051  | 0.086              | 0.068              | 0.034         | 0.055  | -3.78      | 0.281   | -0.0287 | 0.2523      |
| -NH <sub>2</sub>               | -0.058  | 0.027  | 0.082              | 0.054              | 0.056         | 0.041  | -5.79      | -0.2524 | -0.0143 | 0.2381      |
| -NO <sub>2</sub>               | -0.038  | 0.072  | 0.021              | 0.046              | -0.051        | 0.053  | -3.45      | -0.3008 | -0.0688 | 0.232       |
| -CH <sub>3</sub>               | -0.047  | 0.049  | 0.07               | 0.06               | 0.021         | 0.041  | -6.41      | -0.2704 | -0.018  | 0.2523      |
| -C <sub>2</sub> H <sub>5</sub> | -0.045  | 0.047  | 0.061              | 0.054              | 0.013         | 0.041  | -6.68      | -0.27   | -0.0183 | 0.2517      |
| -C <sub>3</sub> H <sub>7</sub> | -0.0479 | 0.0886 | 0.0565             | 0.0726             | -0.0321       | 0.0589 | -6.62      | -0.2691 | -0.0189 | 0.2502      |
| -C <sub>4</sub> H <sub>9</sub> | -0.0479 | 0.0886 | 0.0565             | 0.0726             | -0.0321       | 0.0589 | -6.26      | -0.2688 | -0.0187 | 0.2501      |
| -OH                            | -0.052  | 0.034  | 0.086              | 0.06               | 0.052         | 0.05   | -5.24      | -0.2659 | -0.0206 | 0.2452      |
| -OOH                           | -0.053  | 0.034  | 0.087              | 0.061              | 0.054         | 0.05   | -4.17      | -0.2713 | -0.0209 | 0.2504      |
| -CHO                           | -0.031  | 0.069  | 0.024              | 0.047              | -0.044        | 0.05   | -3.97      | -0.2908 | -0.0516 | 0.2392      |
| -COOH                          | -0.032  | 0.07   | 0.027              | 0.049              | -0.043        | 0.049  | -4.1       | -0.2874 | -0.0454 | 0.2421      |

Table S7 Values of descriptors for  $\beta$ -naphtalene - continuation

| Substituent | $\alpha$ | $\mu$ | E <sub>SFC</sub> | Cp | S <sup>0</sup> | ELFC <sub>max</sub> | ELFC <sub>min</sub> | ELFR <sub>max</sub> | ELFR <sub>min</sub> | NBO |
|-------------|----------|-------|------------------|----|----------------|---------------------|---------------------|---------------------|---------------------|-----|
|-------------|----------|-------|------------------|----|----------------|---------------------|---------------------|---------------------|---------------------|-----|

|                                |        |      |            |       |        |          |          |          |          |       |
|--------------------------------|--------|------|------------|-------|--------|----------|----------|----------|----------|-------|
| -Br                            | 141.63 | 2.52 | -2958.6741 | 74.17 | 160.91 | 0.999962 | 4.26E-06 | 0.957737 | 2.02E-08 | 0.18  |
| -Cl                            | 132.98 | 2.49 | -844.6857  | 74.08 | 157.86 | 0.999994 | 3.22E-06 | 0.966331 | 3.83E-08 | 0.179 |
| -F                             | 115.94 | 2.31 | -484.3151  | 73.83 | 154.29 | 0.999961 | 3.49E-05 | 0.999214 | 3.68E-05 | 0.134 |
| -NH <sub>2</sub>               | 130.81 | 1.49 | -440.4428  | 81.15 | 162.72 | 0.999909 | 3.02E-05 | 0.999829 | 7.28E-10 | 0.141 |
| -NO <sub>2</sub>               | 136.32 | 5.85 | -589.5623  | 84.01 | 173.63 | 0.999963 | 3.50E-05 | 0.999929 | 4.08E-08 | 0.214 |
| -CH <sub>3</sub>               | 131.8  | 0.61 | -424.3953  | 84.82 | 166.33 | 0.999965 | 7.27E-06 | 0.999995 | 6.19E-16 | 0.174 |
| -C <sub>2</sub> H <sub>5</sub> | 145.39 | 0.57 | -463.6929  | 97.46 | 184.28 | 0.999965 | 7.47E-06 | 0.999995 | 5.47E-16 | 0.171 |
| -C <sub>3</sub> H <sub>7</sub> | 159.46 | 0.54 | -502.9907  | 46.21 | 106.80 | 0.999649 | 1.03E-05 | 0.999999 | 1.86E-16 | 0.172 |
| -C <sub>4</sub> H <sub>9</sub> | 172.15 | 0.54 | -542.2876  | 51.04 | 114.56 | 0.999669 | 2.17E-06 | 0.999958 | 9.64E-18 | 0.173 |
| -OH                            | 123.08 | 0.92 | -460.3088  | 77.51 | 158.54 | 0.99998  | 4.43E-06 | 0.999607 | 1.99E-03 | 0.107 |
| -OOH                           | 128.76 | 1.86 | -535.4184  | 82.99 | 171.79 | 0.999894 | 3.03E-06 | 0.999863 | 7.39E-13 | 0.155 |
| -CHO                           | 136.37 | 4.59 | -498.396   | 82.5  | 167.9  | 0.999977 | 3.66E-06 | 0.999965 | 9.17E-12 | 0.225 |
| -COOH                          | 139.02 | 3.29 | -573.644   | 87.75 | 178.27 | 0.999931 | 3.52E-05 | 0.999987 | 7.33E-10 | 0.215 |

Table S8 Values of descriptors for  $\alpha$ -anthracene derivatives

| Substituent                    | q(C)   | f(C)   | f <sup>+</sup> (C) | f <sup>0</sup> (C) | $\Delta f(C)$ | q(H)   | $\Delta E$ | HOMO    | LUMO    | HOMO - LUMO |
|--------------------------------|--------|--------|--------------------|--------------------|---------------|--------|------------|---------|---------|-------------|
| -Br                            | -0.046 | 0.05   | 0.056              | 0.053              | 0.006         | 0.049  | -5.46      | -0.2559 | -0.0558 | 0.2001      |
| -Cl                            | -0.048 | 0.052  | 0.056              | 0.054              | 0.005         | 0.05   | -4.89      | -0.2555 | -0.0552 | 0.2003      |
| -F                             | -0.061 | 0.059  | 0.056              | 0.058              | -0.003        | 0.054  | -3.52      | -0.2542 | -0.0522 | 0.202       |
| -NH <sub>2</sub>               | -0.076 | 0.069  | 0.046              | 0.058              | -0.023        | 0.036  | -5.6       | -0.2393 | -0.0431 | 0.1962      |
| -NO <sub>2</sub>               | -0.025 | 0.041  | 0.068              | 0.055              | 0.027         | 0.055  | -4.55      | -0.2676 | -0.0816 | 0.186       |
| -CH <sub>3</sub>               | -0.05  | 0.053  | 0.051              | 0.052              | -0.002        | 0.039  | -6.5       | -0.2472 | -0.0456 | 0.2017      |
| -C <sub>2</sub> H <sub>5</sub> | -0.048 | 0.053  | 0.05               | 0.052              | -0.002        | 0.039  | -6.72      | -0.2466 | -0.0454 | 0.2012      |
| -C <sub>3</sub> H <sub>7</sub> | -0.04  | 0.0706 | 0.0779             | 0.0743             | 0.0073        | 0.0503 | -6.72      | -0.2463 | -0.0458 | 0.2005      |
| -C <sub>4</sub> H <sub>9</sub> | -0.04  | 0.0706 | 0.0779             | 0.0743             | 0.0073        | 0.0503 | -7.52      | -0.2464 | -0.0455 | 0.2009      |
| -OH                            | -0.08  | 0.063  | 0.049              | 0.056              | -0.014        | 0.039  | -5.27      | -0.2441 | -0.0435 | 0.2006      |
| -OOH                           | 0.076  | 0.06   | 0.048              | 0.054              | -0.011        | 0.038  | -2.6       | -0.2526 | -0.0523 | 0.2003      |
| -CHO                           | -0.023 | 0.041  | 0.067              | 0.054              | 0.026         | 0.046  | -6.06      | -0.2587 | -0.0676 | 0.1911      |

|       |        |       |       |       |       |       |      |         |         |       |
|-------|--------|-------|-------|-------|-------|-------|------|---------|---------|-------|
| -COOH | -0.024 | 0.042 | 0.068 | 0.055 | 0.026 | 0.045 | -6.5 | -0.2561 | -0.0631 | 0.193 |
|-------|--------|-------|-------|-------|-------|-------|------|---------|---------|-------|

Table S9 Values of descriptors for  $\alpha$ -anthracene - continuation

| Substituent                    | $\alpha$ | $\mu$ | $E_{SFC}$  | Cp     | $S^0$  | ELFC <sub>max</sub> | ELFC <sub>min</sub> | ELFR <sub>max</sub> | ELFR <sub>min</sub> | NBO   |
|--------------------------------|----------|-------|------------|--------|--------|---------------------|---------------------|---------------------|---------------------|-------|
| -Br                            | 198.15   | 2.57  | -3112.2733 | 102.02 | 197.67 | 0.999867            | 1.21E-07            | 0.957851            | 5.46E-09            | 0.179 |
| -Cl                            | 190.22   | 2.52  | -998.2847  | 101.94 | 194.78 | 0.999976            | 4.67E-07            | 0.966626            | 3.49E-09            | 0.177 |
| -F                             | 175.45   | 2.33  | -637.9134  | 101.66 | 191.43 | 0.999947            | 9.05E-07            | 0.997032            | 1.92E-05            | 0.114 |
| -NH <sub>2</sub>               | 188.14   | 1.14  | -594.0408  | 108.94 | 199.27 | 0.999983            | 2.20E-06            | 0.99983             | 7.65E-09            | 0.105 |
| -NO <sub>2</sub>               | 195      | 5.76  | -743.1562  | 111.93 | 215.28 | 0.999483            | 8.51E-07            | 0.999416            | 1.71E-08            | 0.253 |
| -CH <sub>3</sub>               | 189.55   | 0.66  | -577.9945  | 112.66 | 202.16 | 0.999979            | 3.43E-07            | 0.999961            | 4.16E-13            | 0.165 |
| -C <sub>2</sub> H <sub>5</sub> | 202.08   | 0.61  | -617.2908  | 125.32 | 219.58 | 0.999992            | 4.90E-07            | 0.999988            | 2.45E-14            | 0.169 |
| -C <sub>3</sub> H <sub>7</sub> | 215.58   | 0.63  | -656.5888  | 57.94  | 117.98 | 0.999890            | 1.64E-07            | 0.999995            | 7.81E-16            | 0.17  |
| -C <sub>4</sub> H <sub>9</sub> | 229.75   | 0.49  | -695.8872  | 62.89  | 125.56 | 0.999925            | 1.97E-05            | 0.999942            | 7.36E-14            | 0.16  |
| -OH                            | 181.79   | 0.5   | -613.9079  | 105.35 | 195.53 | 0.999989            | 2.51E-06            | 0.999624            | 1.91E-06            | 0.071 |
| -OOH                           | 187.2    | 1.97  | -689.0141  | 110.95 | 208.76 | 0.999959            | 1.02E-05            | 0.999157            | 1.60E-06            | 0.112 |
| -CHO                           | 193.23   | 3.49  | -651.9961  | 110.33 | 204.38 | 0.999850            | 1.70E-06            | 0.999981            | 2.07E-06            | 0.26  |
| -COOH                          | 198.15   | 2.57  | -3112.2733 | 102.02 | 197.67 | 0.999867            | 1.21E-07            | 0.957851            | 5.46E-09            | 0.179 |

Table S10 Values of descriptors for  $\beta$ -anthracene derivatives

| Substituent                    | q(C)   | f(C)  | f <sup>+</sup> (C) | f <sup>0</sup> (C) | $\Delta f(C)$ | q(H)  | $\Delta E$ | HOMO    | LUMO    | HOMO - LUMO |
|--------------------------------|--------|-------|--------------------|--------------------|---------------|-------|------------|---------|---------|-------------|
| -Br                            | -0.046 | 0.045 | 0.053              | 0.049              | 0.008         | 0.048 | -4.84      | -0.2561 | -0.0558 | 0.2003      |
| -Cl                            | -0.046 | 0.046 | 0.055              | 0.051              | 0.009         | 0.05  | -4.48      | -0.2559 | -0.055  | 0.2009      |
| -F                             | -0.051 | 0.049 | 0.066              | 0.058              | 0.017         | 0.055 | -3.86      | -0.2548 | -0.052  | 0.2028      |
| -NH <sub>2</sub>               | -0.055 | 0.026 | 0.065              | 0.046              | 0.038         | 0.042 | -5.89      | -0.2357 | -0.039  | 0.1966      |
| -NO <sub>2</sub>               | -0.041 | 0.058 | 0.02               | 0.039              | -0.038        | 0.052 | -3.52      | 0.2706  | -0.0782 | 0.1924      |
| -CH <sub>3</sub>               | -0.046 | 0.047 | 0.056              | 0.052              | 0.009         | 0.041 | -6.45      | -0.2462 | -0.0434 | 0.2028      |
| -C <sub>2</sub> H <sub>5</sub> | -0.044 | 0.046 | 0.053              | 0.049              | 0.006         | 0.041 | -6         | -0.246  | -0.0434 | 0.2026      |

|                                |         |        |        |        |         |         |       |         |         |        |
|--------------------------------|---------|--------|--------|--------|---------|---------|-------|---------|---------|--------|
| -C <sub>3</sub> H <sub>7</sub> | -0.0479 | 0.0886 | 0.0565 | 0.0726 | -0.0321 | -0.1223 | -6.28 | -0.2452 | -0.0433 | 0.2019 |
| -C <sub>4</sub> H <sub>9</sub> | -0.0479 | 0.0886 | 0.0565 | 0.0726 | -0.0321 | -0.1223 | -5.83 | -0.2450 | -0.0431 | 0.2019 |
| -OH                            | -0.05   | 0.039  | 0.066  | 0.053  | 0.027   | 0.051   | -5.11 | -0.2442 | -0.0449 | 0.1993 |
| -OOH                           | -0.051  | 0.04   | 0.066  | 0.053  | 0.026   | 0.051   | -4.22 | -0.2483 | -0.0453 | 0.203  |
| -CHO                           | -0.034  | 0.056  | 0.026  | 0.041  | -0.03   | 0.05    | -4.3  | -0.2601 | -0.069  | 0.1911 |
| -COOH                          | -0.035  | 0.057  | 0.031  | 0.044  | -0.026  | 0.049   | -4.99 | -0.2588 | -0.0624 | 0.1964 |

Table S11 Values of descriptors for  $\beta$ -anthracene - continuation

| Substituent                    | $\alpha$ | $\mu$ | E <sub>SFC</sub> | Cp     | S <sup>0</sup> | ELFC <sub>max</sub> | ELFC <sub>min</sub> | ELFR <sub>max</sub> | ELFR <sub>min</sub> | NBO   |
|--------------------------------|----------|-------|------------------|--------|----------------|---------------------|---------------------|---------------------|---------------------|-------|
| -Br                            | 204.41   | 2.73  | -3112.2727       | 102.13 | 198.3          | 0.999878            | 4.23E-06            | 0.957911            | 7.18E-09            | 0.178 |
| -Cl                            | 194.87   | 2.68  | -998.2844        | 102.02 | 195.14         | 0.999563            | 8.25E-07            | 0.966464            | 1.21E-11            | 0.15  |
| -F                             | 175.4    | 2.45  | -637.9139        | 101.74 | 191.76         | 0.99997             | 3.99E-07            | 0.998324            | 7.53E-06            | 0.135 |
| -NH <sub>2</sub>               | 193.15   | 1.63  | -594.042         | 109.07 | 200.13         | 0.999028            | 4.65E-06            | 0.999694            | 7.81E-09            | 0.154 |
| -NO <sub>2</sub>               | 199.58   | 6.46  | -743.1612        | 111.95 | 210.98         | 0.99997             | 7.97E-05            | 0.999958            | 1.32E-07            | 0.205 |
| -CH <sub>3</sub>               | 193.07   | 0.61  | -577.9944        | 112.71 | 203.39         | 0.999506            | 6.27E-06            | 0.999945            | 1.05E-13            | 0.174 |
| -C <sub>2</sub> H <sub>5</sub> | 207.57   | 0.58  | -617.2919        | 125.36 | 221.53         | 0.999985            | 1.35E-04            | 0.999979            | 2.21E-16            | 0.171 |
| -C <sub>3</sub> H <sub>7</sub> | 220.53   | 0.77  | -656.5889        | 58.08  | 118.29         | 0.999935            | 9.00E-05            | 0.999984            | 3.73E-17            | 0.179 |
| -C <sub>4</sub> H <sub>9</sub> | 233.71   | 0.83  | -695.8856        | 62.87  | 125.58         | 0.998164            | 7.76E-07            | 0.999956            | 1.39E-16            | 0.179 |
| -OH                            | 183.91   | 0.99  | -613.9075        | 105.44 | 196.2          | 0.999959            | 5.41E-06            | 0.999004            | 2.08E-06            | 0.111 |
| -OOH                           | 189.48   | 1.82  | -689.0176        | 110.94 | 208.77         | 0.999945            | 3.25E-05            | 0.999988            | 2.23E-11            | 0.158 |
| -CHO                           | 198.93   | 3.84  | -651.9956        | 110.46 | 205.49         | 0.999996            | 9.68E-05            | 0.999972            | 3.64E-07            | 0.192 |
| -COOH                          | 201.93   | 2.51  | -727.2441        | 115.68 | 215.29         | 0.999885            | 3.01E-04            | 0.999986            | 1.78E-08            | 0.208 |

Table S12 Values of descriptors for  $\alpha$ -tetracene derivatives

| Substituent | q(C)   | f(C)  | f*(C) | f <sup>0</sup> (C) | $\Delta f$ (C) | q(H)  | $\Delta E$ | HOMO    | LUMO    | HOMO - LUMO |
|-------------|--------|-------|-------|--------------------|----------------|-------|------------|---------|---------|-------------|
| -Br         | -0.046 | 0.041 | 0.046 | 0.043              | 0.005          | 0.049 | -5.55      | -0.2384 | -0.0713 | 0.1671      |
| -Cl         | -0.048 | 0.042 | 0.046 | 0.044              | 0.004          | 0.05  | -4.91      | -0.2381 | -0.0709 | 0.1671      |

|                                    |         |        |        |        |         |        |       |         |         |        |
|------------------------------------|---------|--------|--------|--------|---------|--------|-------|---------|---------|--------|
| <b>-F</b>                          | -0.061  | 0.049  | 0.047  | 0.048  | -0.002  | 0.054  | -3.54 | -0.237  | -0.0691 | 0.1679 |
| <b>-NH<sub>2</sub></b>             | 0.077   | 0.055  | 0.038  | 0.047  | -0.017  | 0.036  | -5.6  | -0.227  | -0.0613 | 0.1657 |
| <b>-NO<sub>2</sub></b>             | -0.023  | 0.034  | 0.059  | 0.047  | 0.025   | 0.055  | -4.78 | -0.2469 | -0.0893 | 0.1576 |
| <b>-CH<sub>3</sub></b>             | -0.049  | 0.044  | 0.042  | 0.043  | -0.001  | 0.039  | -6.55 | -0.2312 | -0.063  | 0.1682 |
| <b>-C<sub>2</sub>H<sub>5</sub></b> | -0.05   | 0.042  | 0.041  | 0.041  | -0.001  | 0.038  | -7.36 | -0.2308 | -0.0624 | 0.1684 |
| <b>-C<sub>3</sub>H<sub>7</sub></b> | -0.0435 | 0.0831 | 0.0743 | 0.0787 | -0.0088 | 0.1679 | -7.52 | -0.2222 | -0.0664 | 0.1557 |
| <b>-C<sub>4</sub>H<sub>9</sub></b> | -0.0435 | 0.0831 | 0.0743 | 0.0787 | -0.0088 | 0.1679 | -7.49 | -0.2220 | -0.0663 | 0.1557 |
| <b>-OH</b>                         | -0.081  | 0.051  | 0.041  | 0.046  | -0.011  | 0.039  | -5.25 | -0.2295 | -0.0617 | 0.1677 |
| <b>-OOH</b>                        | 0.077   | 0.048  | 0.04   | 0.044  | -0.008  | 0.038  | -2.78 | -0.2349 | -0.0678 | 0.1671 |
| <b>-CHO</b>                        | -0.021  | 0.033  | 0.056  | 0.045  | 0.022   | 0.046  | -6.17 | -0.2394 | -0.0776 | 0.1618 |
| <b>-COOH</b>                       | -0.023  | 0.035  | 0.056  | 0.045  | 0.021   | 0.045  | -6.49 | 0.2372  | -0.0746 | 0.1627 |

Table S13 Values of descriptors for  $\alpha$ -tetracene - continuation

| Substituent                        | $\alpha$ | $\mu$ | E <sub>SFC</sub> | Cp     | S <sup>0</sup> | ELFC <sub>max</sub> | ELFC <sub>min</sub> | ELFR <sub>max</sub> | ELFR <sub>min</sub> | NBO   |
|------------------------------------|----------|-------|------------------|--------|----------------|---------------------|---------------------|---------------------|---------------------|-------|
| <b>-Br</b>                         | 268.61   | 2.71  | -3265.869        | 129.97 | 235.07         | 0.999527            | 1.41E-06            | 0.957749            | 9.02E-09            | 0.178 |
| <b>-Cl</b>                         | 260.38   | 2.65  | -1151.8803       | 129.91 | 232.29         | 0.999985            | 1.21E-06            | 0.966541            | 2.52E-08            | 0.176 |
| <b>-F</b>                          | 245.11   | 2.45  | -791.5089        | 129.65 | 229.13         | 0.999807            | 3.96E-06            | 0.999828            | 8.66E-06            | 0.112 |
| <b>-NH<sub>2</sub></b>             | 258.31   | 1.13  | -747.6365        | 136.92 | 236.84         | 0.999959            | 3.75E-05            | 0.999755            | 2.11E-08            | 0.146 |
| <b>-NO<sub>2</sub></b>             | 266.28   | 6     | -896.752         | 139.88 | 250.09         | 0.999804            | 1.18E-07            | 0.999811            | 2.62E-12            | 0.207 |
| <b>-CH<sub>3</sub></b>             | 259.57   | 0.68  | -731.5902        | 140.65 | 239.85         | 0.999979            | 2.37E-07            | 0.999989            | 1.78E-13            | 0.165 |
| <b>-C<sub>2</sub>H<sub>5</sub></b> | 273.15   | 0.55  | -770.8882        | 153.25 | 256.81         | 0.999984            | 8.23E-06            | 0.999951            | 2.28E-14            | 0.158 |
| <b>-C<sub>3</sub>H<sub>7</sub></b> | 286.95   | 0.44  | -810.1855        | 69.83  | 130.97         | 0.999998            | 5.81E-06            | 0.999991            | 1.02E-13            | 0.159 |
| <b>-C<sub>4</sub>H<sub>9</sub></b> | 300.96   | 0.48  | -849.4830        | 74.70  | 138.93         | 0.972031            | 3.39E-05            | 0.999951            | 2.02E-14            | 0.159 |
| <b>-OH</b>                         | 251.75   | 0.44  | -767.5036        | 133.33 | 233.21         | 0.999958            | 8.88E-06            | 0.999956            | 3.37E-07            | 0.068 |
| <b>-OOH</b>                        | 257.13   | 1.99  | -842.61          | 138.87 | 245.87         | 0.999967            | 1.18E-05            | 0.999182            | 1.34E-08            | 0.109 |
| <b>-CHO</b>                        | 263.86   | 3.53  | -805.592         | 138.28 | 241.87         | 0.999600            | 3.16E-06            | 0.999964            | 1.63E-10            | 0.231 |
| <b>-COOH</b>                       | 266.99   | 2.12  | -880.8377        | 143.59 | 252.59         | 0.999937            | 1.56E-06            | 0.999977            | 8.59E-09            | 0.248 |

Table S14 Values of descriptors for  $\beta$ -tetracene derivatives

| Substituent                    | q(C)    | f(C)   | f <sup>+</sup> (C) | f <sup>0</sup> (C) | $\Delta f$ (C) | q(H)   | $\Delta E$ | HOMO    | LUMO    | HOMO - LUMO |
|--------------------------------|---------|--------|--------------------|--------------------|----------------|--------|------------|---------|---------|-------------|
| -Br                            | -0.046  | 0.04   | 0.045              | 0.043              | 0.005          | 0.048  | -4.84      | -0.2383 | -0.0715 | 0.1668      |
| -Cl                            | -0.046  | 0.041  | 0.046              | 0.044              | 0.006          | 0.049  | -4.5       | 0.2381  | -0.0709 | 0.1672      |
| -F                             | -0.05   | 0.043  | 0.053              | 0.048              | 0.011          | 0.055  | -3.92      | -0.2369 | -0.0685 | 0.1685      |
| -NH <sub>2</sub>               | -0.053  | 0.029  | 0.052              | 0.04               | 0.023          | 0.042  | -5.92      | -0.2224 | -0.057  | 0.1654      |
| -NO <sub>2</sub>               | -0.043  | 0.047  | 0.025              | 0.036              | -0.022         | 0.052  | -3.61      | -0.2502 | -0.0882 | 0.162       |
| -CH <sub>3</sub>               | -0.045  | 0.041  | 0.046              | 0.044              | 0.005          | 0.041  | -6.48      | -0.2299 | -0.0613 | 0.1686      |
| -C <sub>2</sub> H <sub>5</sub> | -0.044  | 0.041  | 0.044              | 0.042              | 0.003          | 0.041  | -6.87      | -0.2297 | -0.0612 | 0.1685      |
| -C <sub>3</sub> H <sub>7</sub> | -0.0419 | 0.0448 | 0.079              | 0.0619             | 0.0342         | 0.0503 | -6.83      | -0.2201 | -0.0657 | 0.1544      |
| -C <sub>4</sub> H <sub>9</sub> | -0.0419 | 0.0448 | 0.079              | 0.0619             | 0.0342         | 0.0503 | -7.17      | -0.2199 | -0.0655 | 0.1543      |
| -OH                            | -0.049  | 0.037  | 0.053              | 0.045              | 0.016          | 0.051  | -5.09      | -0.2288 | -0.0622 | 0.1666      |
| -OOH                           | -0.05   | 0.038  | 0.053              | 0.045              | 0.015          | 0.051  | -4.27      | -0.2318 | -0.0628 | 0.1691      |
| -CHO                           | -0.035  | 0.047  | 0.029              | 0.038              | -0.017         | 0.049  | -4.3       | -0.2416 | -0.0807 | 0.1609      |
| -COOH                          | -0.036  | 0.047  | 0.032              | 0.039              | -0.015         | 0.048  | -5.02      | -0.2404 | -0.0761 | 0.1643      |

Table S15 Values of descriptors for  $\beta$ -tetracene - continuation

| Substituent                    | $\alpha$ | $\mu$ | E <sub>SFC</sub> | Cp     | S <sup>0</sup> | ELFC <sub>max</sub> | ELFC <sub>min</sub> | ELFR <sub>max</sub> | ELFR <sub>min</sub> | NBO   |
|--------------------------------|----------|-------|------------------|--------|----------------|---------------------|---------------------|---------------------|---------------------|-------|
| -Br                            | 277.13   | 2.9   | -3265.8684       | 130.04 | 235.63         | 0.999986            | 1.82E-06            | 0.95801             | 2.23E-10            | 0.177 |
| -Cl                            | 266.69   | 2.84  | -1151.8801       | 129.97 | 232.67         | 0.999606            | 2.47E-06            | 0.966371            | 1.80E-09            | 0.177 |
| -F                             | 245.01   | 2.57  | -791.5095        | 129.74 | 229.51         | 0.999996            | 2.29E-07            | 0.999462            | 1.00E-05            | 0.136 |
| -NH <sub>2</sub>               | 265.6    | 1.78  | -747.6379        | 137.04 | 237.79         | 0.999949            | 1.08E-06            | 0.999493            | 6.94E-12            | 0.154 |
| -NO <sub>2</sub>               | 273.23   | 6.98  | -896.757         | 139.88 | 248.38         | 0.991576            | 1.97E-07            | 0.999995            | 2.93E-09            | 0.183 |
| -CH <sub>3</sub>               | 264.31   | 0.61  | -731.59          | 140.71 | 240.95         | 0.999327            | 9.48E-07            | 0.999942            | 4.44E-13            | 0.174 |
| -C <sub>2</sub> H <sub>5</sub> | 279.63   | 0.59  | -770.8875        | 153.35 | 259.01         | 0.99987             | 5.68E-06            | 0.999992            | 5.05E-17            | 0.171 |
| -C <sub>3</sub> H <sub>7</sub> | 295.04   | 0.57  | -810.1853        | 69.96  | 132.76         | 0.999961            | 3.32E-06            | 0.99995             | 1.59E-17            | 0.173 |
| -C <sub>4</sub> H <sub>9</sub> | 309.10   | 0.62  | -849.4828        | 74.86  | 140.50         | 0.999877            | 2.58E-06            | 0.999961            | 1.61E-19            | 0.173 |
| -OH                            | 254.83   | 1.04  | -767.5033        | 133.42 | 233.88         | 0.999354            | 3.54E-06            | 0.99948             | 1.80E-08            | 0.113 |

|              |        |      |           |        |        |          |          |          |          |       |
|--------------|--------|------|-----------|--------|--------|----------|----------|----------|----------|-------|
| <b>-OOH</b>  | 260.32 | 1.8  | -842.6136 | 138.85 | 246.42 | 0.999878 | 1.94E-05 | 0.999936 | 2.04E-12 | 0.138 |
| <b>-CHO</b>  | 272.24 | 4.09 | -805.5913 | 138.36 | 242.78 | 0.999933 | 4.37E-05 | 0.999967 | 2.27E-13 | 0.213 |
| <b>-COOH</b> | 274.97 | 2.75 | -880.8398 | 143.59 | 252.65 | 0.999995 | 1.59E-03 | 0.999995 | 1.21E-09 | 0.22  |