# Lipophilicity determination of antifungal isoxazolo[3,4-*b*]pyridin-3(1*H*)-ones and their N1-substituted derivatives with chromatographic and computational methods

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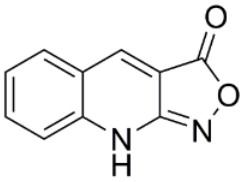
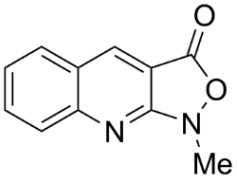
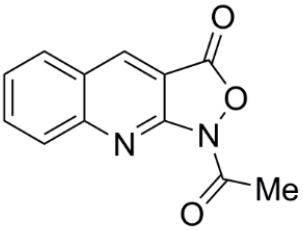
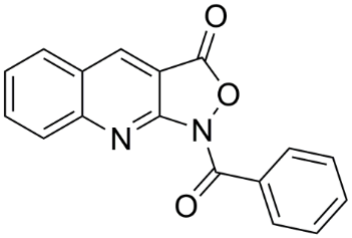
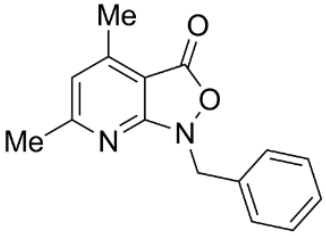
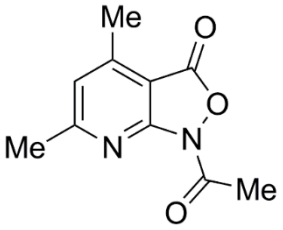
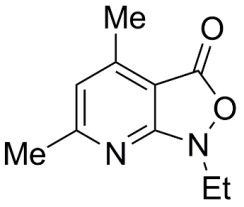
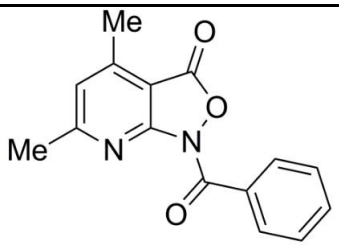
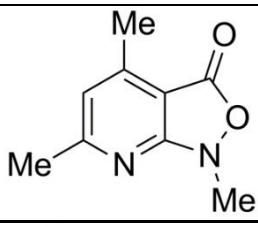
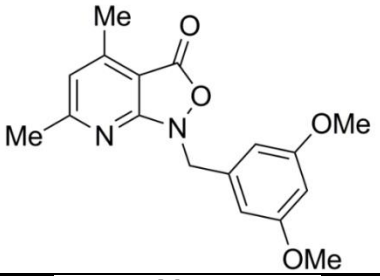
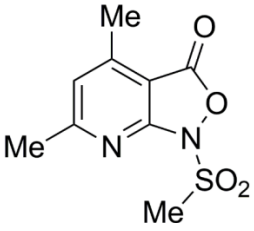
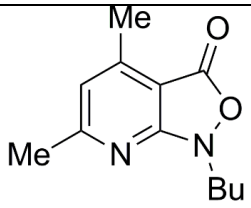
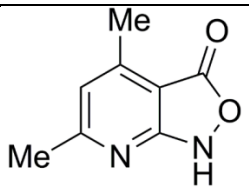
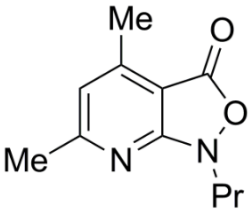
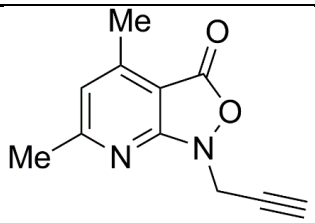
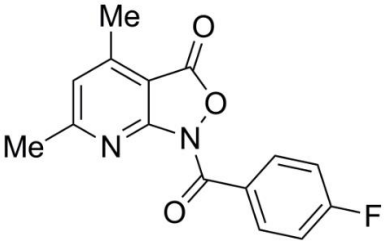
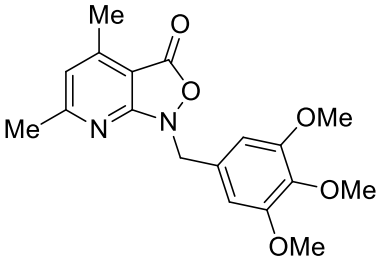
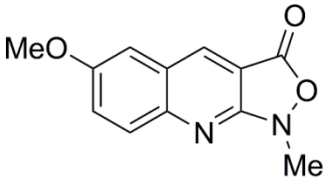
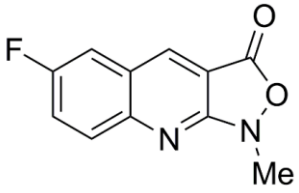
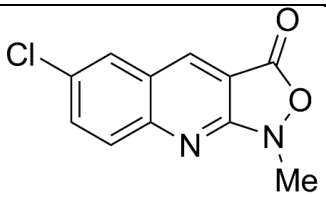
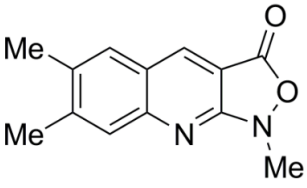
**Table 1S**. Chemical names and structural formulas of the studied of pyrido- and quinolino-isoxazolones

| No. | Chemical name | Chemical structure |
|---|---|---|
| **1** | isoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **2** | 1-benzylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **3** | 1-methylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **4** | 1-acetylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **5** | 1-benzoylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **6** | 1-benzyl-4,6-dimethylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |

| | | |
|---|---|---|
| **7** | 1-acetyl-4,6-dimethylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **8** | 1-ethyl-4,6-dimethylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **9** | 1-benzoyl-4,6-dimethylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **10** | 1,4,6-trimethylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **11** | 1-(3,5-dimethoxybenzyl)-4,6-dimethylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **12** | 4,6-dimethyl-1-(methylsulfonyl)isoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **13** | 1-butyl-4,6-dimethylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **14** | 4,6-dimethylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |

| | | |
|---|---|---|
| **15** | 4,6-dimethyl-1-propylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **16** | 4,6-dimethyl-1-(prop-2-yn-1-yl)isoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **17** | 1-(4-fluorobenzoyl)-4,6-dimethylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **18** | 1-(3,4,5-trimethoxybenzyl)-4,6-dimethylisoxazolo[3,4-*b*]pyridin-3(1*H*)-one |  |
| **19** | 6-methoxy-1-methylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **20** | 6-fluoro-1-methylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **21** | 6-chloro-1-methylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **22** | 1,6,7-trimethylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |

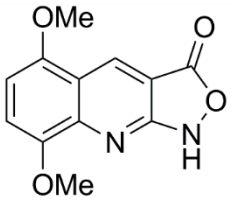
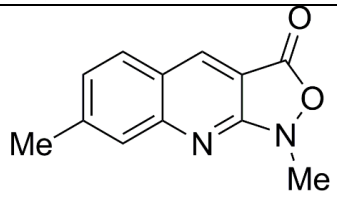
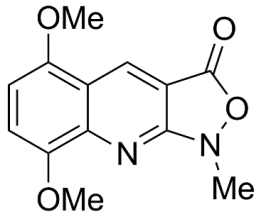
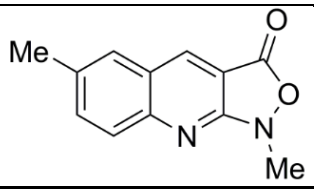
| | | |
|---|---|---|
| **23** | 5,8-dimethoxyisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **24** | 1,7-dimethylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **25** | 5,8-dimethoxy-1-methylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |
| **26** | 1,6-dimethylisoxazolo[3,4-*b*]quinolin-3(1*H*)-one |  |

**Table 2S**. Minimum, maximum and mean value of log*P*-s calculated by different software

| | mean log P | minimal log P | maximal log P |
|---|---|---|---|
| log P Chem Draw | 1.88 | -0.42 | 3.10 |
| Clog P Chem Draw | 2.44 | 0.11 | 4.10 |
| vlogp | 2.45 | 0.95 | 3.43 |
| LogPC Spartan | 2.65 | 0.69 | 4.47 |
| LogPV Spartan | 0.76 | -0.71 | 4.72 |
| miLogP | 1.95 | 0.54 | 3.16 |
| log KOWWIN | 2.29 | -0.04 | 3.94 |
| AlogPs | 2.26 | 0.72 | 3.67 |
| AClogP | 2.46 | 1.24 | 3.52 |
| AlopgP | 2.56 | 0.96 | 3.95 |
| MlogGP | 2.51 | 1.02 | 3.70 |
| XlogP2 | 2.11 | 0.72 | 3.44 |
| XlogP3 | 2.58 | 0.92 | 3.96 |

**Table 3S**. Retention data for the investigated pyrido- and quinolino-isoxazolones obtained from the Soczewiński–Wachtmeister's with statistical parameters

**Stationary phase: $C_8$ bonded silica gel**
**Mobile phase: MeOH-Water**

| No | $R_M^0$ | $\sigma R_M^0$ | $m$ | $\sigma m$ | $R$ | $R^2$ | $F$ | $s$ |
|---|---|---|---|---|---|---|---|---|
| 1 | 1.496 | 0.102 | -2.198 | 0.151 | 0.991 | 0.981 | 210.480 | 0.063 |
| 2 | 3.120 | 0.146 | -3.730 | 0.217 | 0.993 | 0.987 | 296.732 | 0.091 |
| 3 | 2.162 | 0.092 | -2.805 | 0.137 | 0.995 | 0.991 | 418.648 | 0.057 |
| 4 | 1.893 | 0.067 | -2.593 | 0.100 | 0.997 | 0.994 | 672.229 | 0.042 |
| 5 | 2.929 | 0.096 | -3.592 | 0.144 | 0.997 | 0.994 | 626.162 | 0.060 |
| 6 | 3.293 | 0.214 | -4.063 | 0.318 | 0.988 | 0.976 | 163.499 | 0.133 |
| 7 | 1.791 | 0.121 | -2.477 | 0.180 | 0.990 | 0.979 | 189.270 | 0.075 |
| 8 | 2.175 | 0.089 | -2.772 | 0.132 | 0.995 | 0.991 | 438.375 | 0.055 |
| 9 | 2.834 | 0.156 | -3.539 | 0.231 | 0.992 | 0.983 | 233.815 | 0.097 |
| 10 | 1.919 | 0.094 | -2.558 | 0.140 | 0.994 | 0.988 | 334.492 | 0.059 |
| 11 | 3.477 | 0.106 | -4.192 | 0.158 | 0.997 | 0.994 | 706.077 | 0.066 |
| 12 | 2.238 | 0.164 | -2.094 | 0.244 | 0.973 | 0.949 | 73.798 | 0.101 |
| 13 | 2.988 | 0.065 | -3.555 | 0.096 | 0.999 | 0.997 | 1357.867 | 0.040 |
| 14 | 0.991 | 0.058 | -1.831 | 0.086 | 0.996 | 0.991 | 455.085 | 0.036 |
| 15 | 2.722 | 0.103 | -3.391 | 0.153 | 0.996 | 0.992 | 489.391 | 0.064 |
| 16 | 1.951 | 0.075 | -2.734 | 0.111 | 0.997 | 0.993 | 602.508 | 0.047 |
| 17 | 2.864 | 0.133 | -3.579 | 0.198 | 0.994 | 0.988 | 326.728 | 0.083 |
| 18 | 2.808 | 0.097 | -3.476 | 0.144 | 0.997 | 0.993 | 583.604 | 0.060 |
| 19 | 2.421 | 0.049 | -3.023 | 0.072 | 0.999 | 0.998 | 1746.354 | 0.030 |
| 20 | 2.123 | 0.040 | -2.780 | 0.059 | 0.999 | 0.998 | 2223.849 | 0.025 |
| 21 | 2.568 | 0.079 | -3.182 | 0.118 | 0.997 | 0.995 | 732.630 | 0.049 |
| 22 | 2.907 | 0.058 | -3.498 | 0.087 | 0.999 | 0.998 | 1632.503 | 0.036 |
| 23 | 2.123 | 0.027 | -2.664 | 0.041 | 1.000 | 0.999 | 4242.300 | 0.017 |
| 24 | 2.431 | 0.031 | -3.033 | 0.046 | 1.000 | 0.999 | 4333.181 | 0.019 |
| 25 | 2.557 | 0.036 | -3.026 | 0.054 | 0.999 | 0.999 | 3161.924 | 0.023 |
| 26 | 2.461 | 0.089 | -2.990 | 0.133 | 0.996 | 0.992 | 508.969 | 0.055 |

Table 3S. (continued)

| Stationary phase: $C_{18}$ bonded silica gel<br>Mobile phase: MeOH-Water | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **No** | $R_M^0$ | $\sigma R_M^0$ | $m$ | $\sigma m$ | $R$ | $R^2$ | $F$ | $s$ |
| 1 | 2.771 | 0.163 | -3.153 | 0.200 | 0.999 | 0.997 | 1183.611 | 0.019 |
| 2 | 3.702 | 0.213 | -4.031 | 0.262 | 0.994 | 0.987 | 236.093 | 0.083 |
| 3 | 2.045 | 0.060 | -2.414 | 0.074 | 0.999 | 0.997 | 1056.838 | 0.023 |
| 4 | 1.935 | 0.035 | -2.440 | 0.043 | 1.000 | 0.999 | 3170.983 | 0.014 |
| 5 | 3.143 | 0.117 | -3.561 | 0.144 | 0.998 | 0.995 | 609.047 | 0.046 |
| 6 | 3.012 | 0.142 | -3.363 | 0.175 | 0.996 | 0.992 | 367.840 | 0.055 |
| 7 | 1.616 | 0.053 | -2.087 | 0.066 | 0.999 | 0.997 | 1013.956 | 0.021 |
| 8 | 2.098 | 0.041 | -2.465 | 0.050 | 0.999 | 0.999 | 2383.061 | 0.016 |
| 9 | 2.901 | 0.056 | -3.345 | 0.069 | 0.999 | 0.999 | 2359.717 | 0.022 |
| 10 | 1.775 | 0.071 | -2.186 | 0.088 | 0.998 | 0.995 | 620.512 | 0.028 |
| 11 | 3.041 | 0.132 | -3.324 | 0.162 | 0.996 | 0.993 | 419.007 | 0.051 |
| 12 | 3.017 | 0.669 | -3.633 | 0.823 | 0.931 | 0.867 | 19.491 | 0.260 |
| 13 | 3.175 | 0.084 | -3.457 | 0.104 | 0.999 | 0.997 | 1108.349 | 0.033 |
| 14 | 0.945 | 0.263 | -1.841 | 0.323 | 0.957 | 0.915 | 32.394 | 0.102 |
| 15 | 2.770 | 0.058 | -3.111 | 0.071 | 0.999 | 0.998 | 1927.377 | 0.022 |
| 16 | 1.948 | 0.056 | -2.641 | 0.068 | 0.999 | 0.998 | 1494.420 | 0.022 |
| 17 | 3.158 | 0.038 | -3.649 | 0.047 | 1.000 | 0.999 | 5987.251 | 0.015 |
| 18 | 3.151 | 0.052 | -3.743 | 0.064 | 1.000 | 0.999 | 3382.991 | 0.020 |
| 19 | 2.509 | 0.094 | -2.888 | 0.116 | 0.998 | 0.995 | 618.312 | 0.037 |
| 20 | 2.314 | 0.104 | -2.778 | 0.128 | 0.997 | 0.994 | 473.594 | 0.040 |
| 21 | 2.412 | 0.171 | -2.718 | 0.210 | 0.991 | 0.982 | 167.234 | 0.066 |
| 22 | 3.028 | 0.131 | -3.319 | 0.161 | 0.996 | 0.993 | 425.171 | 0.051 |
| 23 | 2.066 | 0.101 | -2.569 | 0.125 | 0.996 | 0.993 | 425.453 | 0.039 |
| 24 | 2.731 | 0.131 | -3.107 | 0.162 | 0.996 | 0.992 | 369.059 | 0.051 |
| 25 | 2.664 | 0.137 | -2.980 | 0.169 | 0.995 | 0.990 | 310.187 | 0.054 |
| 26 | 2.771 | 0.163 | -3.153 | 0.200 | 0.994 | 0.988 | 247.242 | 0.063 |

*R* the coefficient of correlation, $R^2$ the coefficient of determination, *F* the value of the Snedecor's *F*-test, *s* the standard estimation error, *p* value < 0.05.

**Table 4S.** Antifungal activity toward references *Candida* species [1–3]

| *No.* | Candida albicans ATCC 10231 | Candida glabrata ATCC 66032 | Candida lusitaniae ATCC 34499 | Candida parapsilosis ATCC 22019 | Candida tropicalis ATCC 750 |
|---|---|---|---|---|---|
| 1 | >128 | >128 | >128 | >128 | >128 |
| 2 | >128 | >128 | >128 | >128 | >128 |
| 3 | >128 | >128 | >128 | >128 | >128 |
| 4 | >128 | >128 | >128 | >128 | >128 |
| 5 | >128 | >128 | >128 | >128 | >128 |
| 6 | 100 | >200 | 100 | >200 | >200 |
| 7 | >200 | >200 | 100 | >200 | >200 |
| 8 | >200 | >200 | >200 | >200 | >200 |
| 9 | 50 | 50 | 50 | 50 | 50 |
| 10 | >200 | >200 | >200 | >200 | >200 |
| 11 | >200 | >200 | >200 | 100 | >200 |
| 12 | 100 | >200 | 100 | >200 | >200 |
| 13 | *nt* | *nt* | *nt* | *nt* | *nt* |
| 14 | >200 | >200 | 50 | >200 | 100 |
| 15 | 100 | >200 | 50 | <6.2 | 25 |
| 16 | 100 | >200 | >200 | <6.2 | >200 |
| 17 | 50 | 100 | 25 | <6.2 | 100 |
| 18 | >200 | >200 | >200 | 100 | >200 |
| 19 | >128 | >128 | >128 | >128 | >128 |
| 20 | >128 | >128 | >128 | >128 | >128 |
| 21 | >128 | >128 | >128 | >128 | >128 |
| 22 | >128 | >128 | >128 | >128 | >128 |
| 23 | >128 | >128 | >128 | >128 | >128 |
| 24 | >128 | >128 | >128 | >128 | >128 |
| 25 | >128 | >128 | >128 | >128 | >128 |
| 26 | >128 | >128 | >128 | >128 | >128 |

nt – not tested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2. Saczewski, J.; Fedorowicz, J.; Kedzia, A.; Ziolkowska-Klinkosz, M.; Jalinska, A. Synthesis and Antifungal Activity of Some 4,6-Dimethylisoxazolo[3,4- b]pyridin-3(1H)-one Derivatives. *Med. Chem. (Los. Angeles).* **2016**, *12*, 640–646.

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**Table 5S.** Cross-validation – analysis of variance summary for the TLC $C_8$ QSRR model.

| Source of ariance | *SS* | *df* | *MS* | *F* | Prob. > *F* |
|---|---|---|---|---|---|
| Total | 16.512 | 17 | 0.971 | 49.44 | 4.66E-6 |
| Fit | 16.121 | 8 | 2.015 | | |
| Residual | 0.391 | 9 | 0.0408 | | |

*SS* – sum of squares, *df* – degrees of freedom, *MS* – median square, *F* – Fisher test statistic.

**Table 6S.** Cross-validation – analysis of variance summary for the TLC $C_{18}$ QSRR model.

| Source of ariance | *SS* | *df* | *MS* | *F* | Prob. > *F* |
|---|---|---|---|---|---|
| Total | 16.463 | 17 | 0.968 | 244.26 | 8.60E-9 |
| Fit | 16.354 | 8 | 2.044 | | |
| Residual | 0.109 | 9 | 0.008 | | |

*SS* – sum of squares, *df* – degrees of freedom, *MS* – median square, *F* – Fisher test statistic.

**Table 7S.** Cross-validation – analysis of variance summary for the HPLC log$k_w$ QSRR model.

| Source of ariance | *SS* | *df* | *MS* | *F* | Prob. > *F* |
|---|---|---|---|---|---|
| Total | 16.429 | 17 | 0.966 | 31.56 | 2.62E-5 |
| Fit | 15.979 | 8 | 1.997 | | |
| Residual | 0.451 | 9 | 0.063 | | |

*SS* – sum of squares, *df* – degrees of freedom, *MS* – median square, *F* – Fisher test statistic.

**Table 8S.** Cross-validation – analysis of variance summary for the MEKC log*k* QSRR model.

| Source of variance | *SS* | *df* | *MS* | *F* | Prob. > *F* |
|---|---|---|---|---|---|
| Total | 16.731 | 17 | 0.984 | 19.54 | 4.47E-5 |
| Fit | 16.185 | 10 | 1.619 | | |
| Residual | 0.546 | 7 | 0.083 | | |

*SS* – sum of squares, *df* – degrees of freedom, *MS* – median square, *F* – Fisher test statistic.

**Table 9S.** List of molecular descriptors with coefficients values in PLS models built for RP-LC and MEKC.

| TLC $C_8$ QSRR model | | | | |
|---|---|---|---|---|
| No. | Name | Coefficients | Descriptor full name | Block |
| 1 | PJI2 | 0.09 | 2D Petitjean shape index | Topological indices |
| 2 | X5Av | 0.12 | average valence connectivity index of order 5 | Connectivity indices |
| 3 | MATS7i | -0.03 | Moran autocorrelation of lag 7 weighted by ionization potential | 2D autocorrelations |
| 4 | GATS3p | 0.08 | Geary autocorrelation of lag 3 weighted by polarizability | 2D autocorrelations |
| 5 | GATS5p | -0.21 | Geary autocorrelation of lag 5 weighted by polarizability | 2D autocorrelations |
| 6 | JGI2 | -0.12 | mean topological charge index of order 2 | 2D autocorrelations |
| 7 | SpMax2_ Bh(s) | -0.11 | largest eigenvalue n. 2 of Burden matrix weighted by I-state | Burden eigenvalues |
| 8 | SpMax3_ Bh(s) | 0.11 | largest eigenvalue n. 3 of Burden matrix weighted by I-state | Burden eigenvalues |
| 9 | Mor19s | -0.01 | signal 19 / weighted by I-state | 3D-MoRSE descriptors |
| 10 | E2u | -0.24 | 2nd component accessibility directional WHIM index / unweighted | WHIM descriptors |
| 11 | E1i | 0.24 | 1st component accessibility directional WHIM index / weighted by ionization potential | WHIM descriptors |
| 12 | HATS4u | -0.30 | leverage-weighted autocorrelation of lag 4 / unweighted | GETAWAY descriptors |
| 13 | HATS4v | -0.26 | leverage-weighted autocorrelation of lag 4 / weighted by van der Waals volume | GETAWAY descriptors |
| 14 | R3p | 0.20 | R autocorrelation of lag 3 / weighted by polarizability | GETAWAY descriptors |
| 15 | R4p | 0.27 | R autocorrelation of lag 4 / weighted by polarizability | GETAWAY descriptors |
| 16 | R7p+ | 0.42 | R maximal autocorrelation of lag 7 / weighted by polarizability | GETAWAY descriptors |
| 17 | CATS3D_ 08_AL | 0.15 | CATS3D Acceptor-Lipophilic at lag 08 | CATS 3D |
| TLC $C_{18}$ QSRR model | | | | |
| No | Name | Coefficients | | |
| 1 | PJI2 | 0.04 | 2D Petitjean shape index | Topological indices |
| 2 | X5Av | 0.27 | average valence connectivity index of order 5 | Connectivity indices |
| 3 | MATS2s | -0.06 | Moran autocorrelation of lag 2 weighted by I-state | 2D autocorrelations |
| 4 | SpMax3_B h(s) | 0.19 | largest eigenvalue n. 3 of Burden matrix weighted by I-state | Burden eigenvalues |
| 5 | DISPp | -0.11 | displacement value / weighted by polarizability | Geometrical descriptors |
| 6 | Mor10v | 0.15 | signal 10 / weighted by van der Waals volume | 3D-MoRSE descriptors |
| 7 | Mor10p | 0.11 | signal 10 / weighted by polarizability | 3D-MoRSE descriptors |
| 8 | E1e | 0.08 | 1st component accessibility directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |
| 9 | E2p | -0.20 | 2nd component accessibility directional WHIM index / weighted by polarizability | WHIM descriptors |

**Table 8S.** (continued)

| | | | | |
|---|---|---|---|---|
| 10 | Kv | 0.18 | K global shape index / weighted by van der Waals volume | WHIM descriptors |
| 11 | HATS1e | -0.18 | leverage-weighted autocorrelation of lag 1 / weighted by Sanderson electronegativity | GETAWAY descriptors |
| 12 | HATS4i | -0.10 | leverage-weighted autocorrelation of lag 4 / weighted by ionization potential | GETAWAY descriptors |
| 13 | R4v+ | -0.08 | R maximal autocorrelation of lag 4 / weighted by van der Waals volume | GETAWAY descriptors |
| 14 | R3p | 0.24 | R autocorrelation of lag 3 / weighted by polarizability | GETAWAY descriptors |
| 15 | R4p | 0.15 | R autocorrelation of lag 4 / weighted by polarizability | GETAWAY descriptors |
| 16 | CATS3D_03_DL | 0.01 | CATS3D Donor-Lipophilic at lag 03 | CATS 3D |
| 17 | CATS3D_08_AL | 0.08 | CATS3D Acceptor-Lipophilic at lag 08 | CATS 3D |
| | | | HPLC | |
| No | Label | Coefficients | | |
| 1 | ATSC3p | 0.29 | Centred Broto-Moreau autocorrelation of lag 3 weighted by polarizability | 2D autocorrelations |
| 2 | MATS7i | -0.11 | Moran autocorrelation of lag 7 weighted by ionization potential | 2D autocorrelations |
| 3 | MATS2s | -0.03 | Moran autocorrelation of lag 2 weighted by I-state | 2D autocorrelations |
| 4 | SpMax2_Bh(s) | -0.19 | largest eigenvalue n. 2 of Burden matrix weighted by I-state | Burden eigenvalues |
| 5 | SpMax3_Bh(s) | 0.18 | largest eigenvalue n. 3 of Burden matrix weighted by I-state | Burden eigenvalues |
| 6 | DISPi | -0.15 | displacement value / weighted by ionization potential | Geometrical descriptors |
| 7 | E2u | -0.14 | 2nd component accessibility directional WHIM index / unweighted | WHIM descriptors |
| 8 | Ki | 0.04 | K global shape index / weighted by ionization potential | WHIM descriptors |
| 9 | HATS4u | -0.13 | leverage-weighted autocorrelation of lag 4 / unweighted | GETAWAY descriptors |
| 10 | HATS4v | -0.05 | leverage-weighted autocorrelation of lag 4 / weighted by van der Waals volume | GETAWAY descriptors |
| 11 | R4v+ | -0.13 | R maximal autocorrelation of lag 4 / weighted by van der Waals volume | GETAWAY descriptors |
| 12 | R3p | 0.21 | R autocorrelation of lag 3 / weighted by polarizability | GETAWAY descriptors |
| 13 | R4p | 0.28 | R autocorrelation of lag 4 / weighted by polarizability | GETAWAY descriptors |
| 14 | R7p+ | 0.18 | R maximal autocorrelation of lag 7 / weighted by polarizability | GETAWAY descriptors |
| 15 | R4s | 0.05 | R autocorrelation of lag 4 / weighted by I-state | GETAWAY descriptors |
| 16 | R6s+ | 0.19 | R maximal autocorrelation of lag 6 / weighted by I-state | GETAWAY descriptors |
| 17 | CATS3D_08_AL | 0.20 | CATS2D Acceptor-Lipophilic at lag 08 | CATS 3D |

**Table 9S.** (continued)

| MECK | | | | |
|---|---|---|---|---|
| No | Label | Coefficients | | |
| 1 | VE1_Dz(p) | 0.14 | coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability | 2D matrix-based descriptors |
| 2 | Mor24s | -0.24 | signal 24 / weighted by I-state | 3D-MoRSE descriptors |
| 3 | E2u | 0.52 | 2nd component accessibility directional WHIM index / unweighted | WHIM descriptors |
| 4 | E1e | 0.24 | 1st component accessibility directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |
| 5 | HATS1e | -0.56 | leverage-weighted autocorrelation of lag 1 / weighted by Sanderson electronegativity | GETAWAY descriptors |
| 6 | HATS7p | 0.06 | leverage-weighted autocorrelation of lag 7 / weighted by polarizability | GETAWAY descriptors |
| 7 | R4v+ | 0.33 | R maximal autocorrelation of lag 4 / weighted by van der Waals volume | GETAWAY descriptors |
| 8 | R4p | 0.16 | R autocorrelation of lag 4 / weighted by polarizability | GETAWAY descriptors |
| 9 | R4p+ | 0.17 | R maximal autocorrelation of lag 4 / weighted by polarizability | GETAWAY descriptors |
| 10 | R6s+ | 0.31 | R maximal autocorrelation of lag 6 / weighted by I-state | GETAWAY descriptors |
| 11 | CATS3D_08_AA | -0.49 | CATS3D Acceptor-Acceptor at lag 08 | CATS 3D |
| 12 | CATS3D_03_LL | -0.33 | CATS3D Lipophilic-Lipophilic at lag 03 | CATS 3D |

**Figure 1S.** Optimization of the number of latent variables (LVs) for the consensus GA-PLS models for **A)** TLC with the $C_8$ plate, **B)** TLC with the $C_{18}$ plate, **C)** HPLC log$k_w$, and **D)** MEKC log$k$ parameters. The optimal number of LVs is denoted in pink.

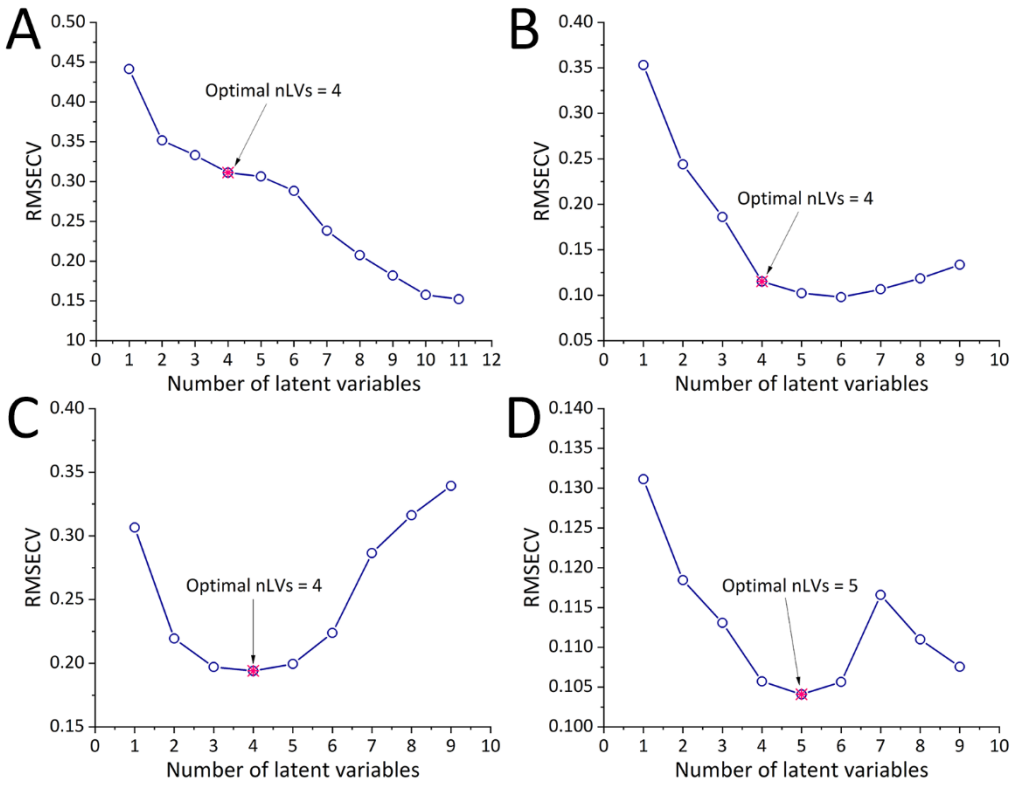

**Figure 2S.** Leave one out-cross validation (LOO-CV) predictive ability (on the training set) for **A)** TLC with the $C_8$ plate, **B)** TLC with the $C_{18}$ plate, **C)** HPLC log$k_w$, and **D)** MEKC log$k$ parameters.