Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# *Supporting Information*

## *"New Journal of Chemistry"*

# New relationship models for solvent- pyrene solubility based on molecular structure and empirical properties

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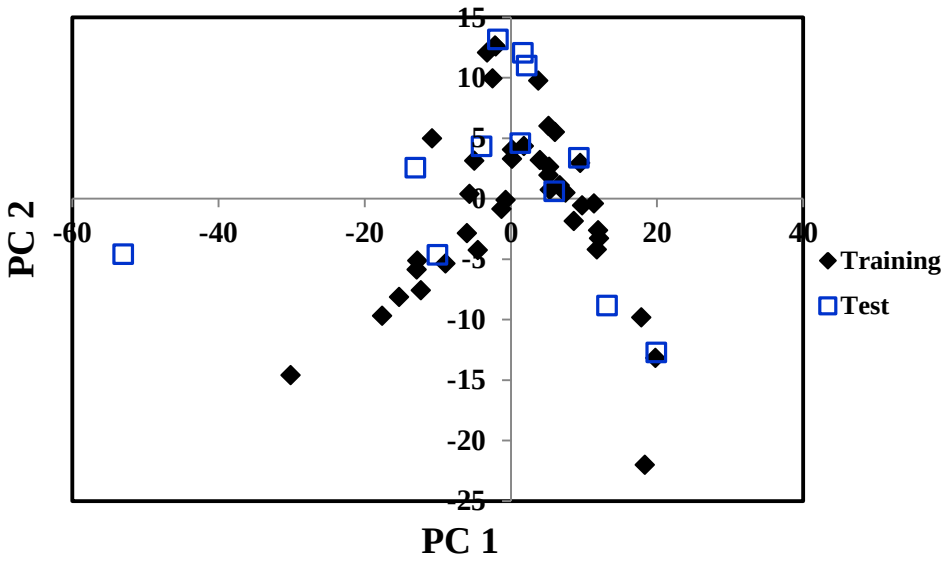


**Fig S1.** Distribution of 52 solvents in PCA space of total descriptors of model 1 (QSPR). It is clear that 12 test compounds were randomly selected from different situations of this 2D plot (PC1 vs. PC2)

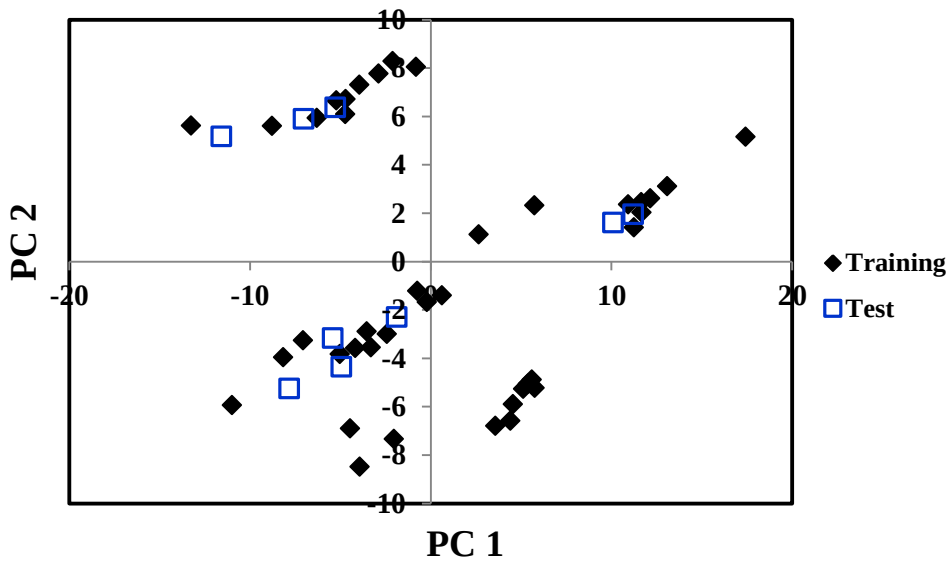


**Fig S2.** Distribution of 49 solvents in PCA space of total descriptors of model 2 (LSER). It is clear that 9 test compounds were randomly selected from different situations of this 2D plot (PC1 vs. PC2)

**Table S1**. Unstandardized and standardized coefficients of the model 1 (QSPR), and their statistical t and p-values (Eq. (2) in the main article).

| Model | Unstandardized Coefficients | Standardized Coefficients | t | p-value |
|---|---|---|---|---|
| Intercept | 11.61(±0.395) | | 29.377 | 0.000 |
| GATS1m | -56.66(±5.757) | -0.941(±0.096) | -9.841 | 0.000 |
| Ms | -0.772(±0.098) | -0.948(±0.121) | -7.844 | 0.000 |
| AAC | 0.652(±0.238) | 0.243(±0.089) | 2.741 | 0.010 |
| Mor26u | 0.955(±0.304) | 0.267(±0.085) | 3.146 | 0.003 |
| Mor12u | 0.768(±0.206) | 0.456(±0.122) | 3.727 | 0.001 |

**Table S2**. Numerical value of five descriptors uses in proposed QSPR model for pyrene solubility (Eq. (3) ).

| No. | Solvent name | GATS1m | Ms | AAC | Mor26u | Mor12u |
|---|---|---|---|---|---|---|
| **S 1** | hexane | 0.037 | 1.67 | 0.881 | 0.259 | -0.523 |
| **S 2** | heptane | 0.036 | 1.64 | 0.887 | 0.271 | -0.578 |
| **S 3** | octane | 0.035 | 1.63 | 0.89 | 0.237 | -0.604 |
| **S 4** | nonane | 0.035 | 1.61 | 0.894 | 0.253 | -0.668 |
| **S 5** | decane | 0.034 | 1.6 | 0.896 | 0.257 | -0.714 |
| **S 6** | hexadecane | 0.033 | 1.56 | 0.904 | 0.262 | -1.105 |
| **S 7** | cyclohexane | 0.028 | 1.5 | 0.918 | -0.007 | -1.023 |
| **S 8** | methylcyclohexane | 0.029 | 1.55 | 0.918 | -0.021 | -1.094 |
| **S 9** | 2,2,4-trimethylpentane | 0.035 | 1.76 | 0.89 | 0.008 | -0.695 |
| **S 10** † | squalane | 0.023 | 1.77 | 0.954 | 0.033 | -3.404 |
| **S 11** | carbon tetrachloride | 0.004 | 3.54 | 0.722 | 0.042 | 0.13 |
| **S 12** | benzene | 0.011 | 2 | 1 | -0.203 | -0.548 |
| **S 13** † | toluene | 0.013 | 1.95 | 0.997 | -0.073 | -0.506 |
| **S 14** † | o-xylene | 0.015 | 1.92 | 0.991 | -0.026 | -0.299 |
| **S 15** | m-xylene | 0.015 | 1.92 | 0.991 | -0.082 | -0.575 |
| **S 16** | p-xylene | 0.015 | 1.92 | 0.991 | -0.022 | -0.659 |
| **S 17** | ethylbenzene | 0.015 | 1.9 | 0.991 | -0.142 | -0.647 |
| **S 18** | dibutyl ether | 0.029 | 1.83 | 1.086 | 0.245 | -0.892 |
| **S 19** † | methyl t-buthyl ether | 0.028 | 2.13 | 1.135 | 0.101 | -0.938 |
| **S 20** | methanol | 0.029 | 4 | 1.252 | 0.107 | -0.023 |
| **S 21** | ethanol | 0 | 4.83 | 0.918 | 0.003 | 0.112 |
| **S 22** | 1-propanol | 0.029 | 2.75 | 1.189 | 0.124 | -0.379 |
| **S 23** | 2-propanol | 0.029 | 2.83 | 1.189 | 0.091 | -0.302 |
| **S 24** | 2-butanol | 0.03 | 2.57 | 1.159 | 0.103 | -0.296 |
| **S 25** | 2-methyl-1-propanol | 0.03 | 2.57 | 1.159 | -0.006 | -0.559 |
| **S 26** | 2-methyl-2-butanol | 0.03 | 2.46 | 1.135 | -0.047 | -0.477 |
| **S 27** | 3-methyl-1-butanol | 0.03 | 2.39 | 1.135 | -0.072 | -0.669 |
| **S 28** | 1-pentanol | 0.03 | 2.33 | 1.135 | 0.167 | -0.542 |
| **S 29** † | 4-methyl-2-pentanol | 0.03 | 2.31 | 1.116 | 0.144 | -0.547 |
| **S 30** | 1-hexanol | 0.03 | 2.21 | 1.116 | 0.185 | -0.652 |
| **S 31** † | 2-ethyl-1-hexanol | 0.03 | 2.09 | 1.086 | 0.068 | -0.892 |
| **S 32** † | 1-heptanol | 0.03 | 2.13 | 1.099 | 0.197 | -0.695 |
| **S 33** | 1-octanol | 0.03 | 2.06 | 1.086 | 0.216 | -0.688 |
| **S 34** | ethylene glycol | 0.02 | 3.75 | 1.371 | 0.046 | -0.288 |
| **S 35** † | 1,2-dichloroethane | 0.011 | 2.81 | 1.5 | 0.034 | 0.011 |
| **S 36** | tetrahydrofuran | 0.019 | 1.9 | 1.239 | -0.104 | -0.223 |
| **S 37** | 1,4-dioxane | 0.014 | 2.17 | 1.379 | -0.008 | -0.697 |
| **S 38** | methyl acetate | 0.013 | 3.23 | 1.435 | 0.13 | -0.042 |
| **S 39** | ethyl acetate | 0.015 | 2.94 | 1.379 | 0.189 | -0.126 |
| **S 40** | butyl acetate | 0.018 | 2.58 | 1.295 | 0.193 | -0.581 |
| **S 41** † | acetonitrile | 0.004 | 5 | 1.585 | 0.002 | -0.069 |

| | | | | | | |
|---|---|---|---|---|---|---|
| **S 42** | 1-propanenitrile | 0.015 | 3 | 1.352 | 0.018 | -0.14 |
| **S 43 †** | 1-butanenitrile | 0.017 | 2.7 | 1.281 | 0.026 | -0.273 |
| **S 44 †** | benzonitrile | 0.006 | 2.52 | 1.296 | -0.29 | -0.24 |
| **S 45 †** | N,N-dimethylformamide | 0.016 | 3 | 1.551 | 0.238 | -0.093 |
| **S 46** | N,N-dimethylacetamide | 0.018 | 2.78 | 1.472 | 0.084 | 0.041 |
| **S 47** | acetone | 0.018 | 3.17 | 1.295 | 0.257 | -0.165 |
| **S 48** | 2-butanone | 0.02 | 2.83 | 1.239 | 0.192 | -0.238 |
| **S 49** | cyclohexanone | 0.017 | 2.31 | 1.221 | -0.089 | -0.537 |
| **S 50** | acetophenone | 0.009 | 2.48 | 1.264 | -0.076 | -0.15 |
| **S 51** | dimethyl sulfoxide | 0.024 | 3.06 | 1.571 | 0.223 | 0.184 |
| **S 52** | aniline | 0.012 | 2.24 | 1.296 | -0.348 | -0.458 |

† Compounds of the test set (random selection #1)

**Table S3**. Unstandardized and standardized coefficients of the model 2 (LSER), and their statistical t and p-values (Eq. (4) in the main article).

| parameter | Unstandardized Coefficients | Standardized Coefficients | t-value | p-value |
|---|---|---|---|---|
| intercept | 10.825 (±0.147) | | 73.392 | 0.000 |
| $logk_{Dc}$ | 0.1030 (±0.025) | 0.282(±0.067) | 4.206 | 0.000 |
| $\Delta H^0_{BF3}$ | -0.012 (±0.001) | -0.690(±0.065) | -10.642 | 0.000 |
| *pKBH+* | 0.221 (±0.027) | 0.546(±0.066) | 8.253 | 0.000 |

**Table S4**. Numerical value of Three empirical parameters uses in the proposed LSER model for pyrene solubility (Eq. (6) ).

| No. | Solvent name | $Logk_{Dc}$ | $\Delta H^0_{BF3}$ | pKBH+ |
|---|---|---|---|---|
| **S1** | hexane | -1.51747 | 116.104 | -3.5194 |
| **S2** ‡ | heptane | -1.2401 | 116.234 | -3.49872 |
| **S3** | octane | -0.97099 | 116.101 | -3.48838 |
| **S4** | nonane | -0.70752 | 116.234 | -3.48493 |
| **S5** | decane | -0.4493 | 116.1 | -3.48321 |
| **S6** | hexadecane | 1.01935 | 116.1 | -3.32642 |
| **S7** | cyclohexane | -1.59117 | 115.386 | -3.26439 |
| **S8** ‡ | methylcyclohexane | -1.31471 | 115.652 | -3.06624 |
| **S9** | 2,2,4-trimethylpentane | -0.95016 | 115.706 | -3.37811 |
| **S10** | squalane | --- | --- | --- |
| **S11** | carbon tetrachloride | -2.82 | 7.02286 | -5.749 |
| **S12** | benzene | -2.32 | 107.227 | -1.05201 |
| **S13** | toluene | -0.85521 | 111.351 | -0.49719 |
| **S14** | o-xylene | -0.13679 | 111.826 | -0.24391 |
| **S15** | m-xylene | -0.22912 | 111.271 | -0.27837 |
| **S16** | p-xylene | -0.36216 | 110.888 | -0.03542 |
| **S17** | ethylbenzene | -0.24569 | 111.973 | -0.58334 |
| **S19** | dibutyl ether | 0.205419 | 78.57 | -2.32016 |
| **S19** | methyl t-buthyl ether | -0.53683 | 86.2905 | -2.39425 |
| **S20**‡ | methanol | -3.6 | 124.739 | -3.60727 |
| **S21** | ethanol | -3 | 125.122 | -3.161 |
| **S22** ‡ | 1-propanol | -2.56586 | 123.936 | -3.10931 |
| **S23** | 2-propanol | -2.4277 | 134.333 | -3.19374 |
| **S24** | 2-butanol | -1.81569 | 135.588 | -3.20063 |
| **S25** ‡ | 2-methyl-1-propanol | -1.92346 | 129.829 | -3.15756 |
| **S26** | 2-methyl-2-butanol | --- | --- | --- |
| **S27** | 3-methyl-1-butanol | -2.09908 | 134.11 | -3.12999 |
| **S28** | 1-pentanol | -2.02899 | 124.104 | -3.11104 |
| **S29** | 4-methyl-2-pentanol | --- | --- | --- |
| **S30** | 1-hexanol | -1.69296 | 125.365 | -3.11104 |
| **S31** | 2-ethyl-1-hexanol | -0.6116 | 137.932 | -2.90772 |
| **S32** | 1-heptanol | -1.42091 | 124.834 | -3.11276 |
| **S33** | 1-octanol | -1.15492 | 125.402 | -3.11448 |
| **S34** | ethylene glycol | -4.51351 | 153.49 | -3.07658 |
| **S35** | 1,2-dichloroethane | -1.56792 | 14.5266 | -4.09144 |
| **S36** | tetrahydrofuran | 0.6 | 90.40 | -1.96349 |
| **S37** | 1,4-dioxane | -1.39 | 74.09 | -2.00485 |
| **S38** | methyl acetate | 0.552858 | 72.79 | -3.9 |
| **S39** ‡ | ethyl acetate | 0.92134 | 75.550 | -3.80197 |
| **S40** | butyl acetate | 1.51638 | 65.6006 | -3.67964 |

| | | | | |
|---|---|---|---|---|
| **S41** ‡ | acetonitrile | 0.46 | 60.40 | -5.89718 |
| **S42** ‡ | 1-propanenitrile | -0.01383 | 60.95 | -5.07702 |
| **S43** | 1-butanenitrile | 0.338946 | 61.18 | -4.67383 |
| **S44** | benzonitrile | 0.4 | 55.40 | -1.68781 |
| **S45** | N,N-dimethylformamide | 1.56 | 110.490 | -1.09 |
| **S46** | N,N-dimethylacetamide | 2.2 | 112.140 | -0.21 |
| **S47** | acetone | 1.38 | 76.03 | -3.06 |
| **S48** | 2-butanone | 0.370113 | 76.10 | -2.58379 |
| **S49** | cyclohexanone | 1.02161 | 76.36 | -2.17543 |
| **S50** | acetophenone | 1.1463 | 74.50 | -1.53963 |
| **S51** | dimethyl sulfoxide | 1 | 105.340 | -1.54 |
| **S52** ‡ | aniline | -0.9957 | 113.498 | 1.42744 |

‡ Compounds of the test set (random selection #1)