**Quantum Chemical (QC) Calculations and Linear Solvation Energy Relationships (LSER). Hydrogen-Bonding Calculations with New QC-LSER Molecular Descriptors**

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SUPPLEMENTARY INFORMATION FILE

This file provides with additional information on the new QC-LSER molecular descriptors in terms of graphs and tables. The COSMO-RS calculations are done at the DFT/ TZVPB-Fine level [1, 2].

Distribution curves of σi2AI are not always as symmetric as in in figure 2 of the main text for water. Corresponding curves for carbon tetrachloride and propanal, which are significantly more asymmetric, are shown in figures S1 and S2, respectively. As shown, CCl4 has only polarizability non-zero QC-LSER descriptors while propanal, in addition to polarizability descriptors it has a hydrogen-bonding basicity (HBA) descriptor.



Figure s1: The distribution function of the product *σi2Ai* of charge densities *σi* with the molecular charges *σiAi* of carbon tetrachloride and the definition areas of the QC-LSER molecular descriptors. CCl4 has only polarizability non-zero QC-LSER descriptors.



Figure S2: The distribution function of the product *σi2Ai* of **propanal** and the definition areas of the QC-LSER molecular descriptors. Propanal has one basic (hydrogen-bonding acceptor) and two polarizability non-zero QC-LSER descriptors.

It should be stressed that all new QC-LSER descriptors are positive, as is the case with Abraham’s LSER descriptors. One could use, alternatively, the distribution of the charge σiAi for an analogous definition leading to positive and negative descriptors.



Figure S3: The distribution function of the molecular charges *σiAi* of water and the areas) for alternative definition of analogous to QC-LSER molecular descriptors. *Ah* and *Bh* would correspond, approximately, to the regions of definition of Dohnal’s [3] *αcosm* and *βcosm* descriptors, respectively.

Klamt cosmoments [1,2] were based on distributions analogous to figure 1 of the main text. Dohnal cosmoments are based on distributions analogous to figure S3. Klamt’s regions of definitions of acidity and basicity cosmoments *HB­\_doni* and *HB\_acci* correspond to regions *Ah* and *Bh,* respectively, of figure 2 of the main text. In Table S1 are compared the hydrogen-bonding descriptors, Ah and Bh, with the corresponding Dohnal [3] descriptors. As seen, the two sets of descriptors are, in general, close although there are cases with significant differences.

TABLE S1: Comparison of hydrogen-bonding QC-LSER molecular descriptors, Ah and Bh, with the corresponding αcosmo and βcosmo Dohnal’s [3] descriptors for some common solutes.

|  |  |  |
| --- | --- | --- |
|  | This Work | Dohnal [5] |
| **SOLUTE** | **Ah** | **Bh** | **αcosmo** | **βcosmo** |
|  |  |  |  |  |
| 1-OCTENE | 0.00 | 0.05 | 0.0 | 0.2 |
| DICHLOROMETHANE | 0.94 | 0.00 | 1.3 | 0.0 |
| CHLOROFORM | 1.14 | 0.00 | 1.2 | 0.0 |
| DIETHYL ETHER | 0.00 | 1.81 | 0.0 | 1.8 |
| TETRAHYDROFURAN | 0.00 | 2.15 | 0.0 | 2.2 |
| 1,4-DIOXANE | 0.00 | 3.12 | 0.0 | 3.3 |
| TETRAHYDROPYRAN | 0.00 | 1.97 | 0.0 | 1.7 |
| ETHYL ACETATE | 0.00 | 2.81 | 0.0 | 2.8 |
| n-PROPYL ACETATE | 0.00 | 2.80 | 0.0 | 2.8 |
| n-BUTYL ACETATE | 0.00 | 2.81 | 0.0 | 2.8 |
| ETHYL PROPIONATE | 0.00 | 2.66 | 0.0 | 2.7 |
| ETHYL n-BUTYRATE | 0.00 | 2.65 | 0.0 | 2.8 |
| ACETONE | 0.02 | 2.95 | 0.0 | 2.8 |
| METHYL ETHYL KETONE | 0.00 | 2.78 | 0.0 | 2.7 |
| 2-PENTANONE | 0.00 | 2.81 | 0.0 | 2.7 |
| 3-PENTANONE | 0.00 | 2.58 | 0.0 | 2.5 |
| METHANOL | 1.39 | 2.39 | 1.4 | 2.4 |
| ETHANOL | 1.23 | 2.46 | 1.3 | 2.5 |
| 1-PROPANOL | 1.23 | 2.44 | 1.2 | 2.5 |
| 1-BUTANOL | 1.22 | 2.47 | 1.3 | 2.5 |
| 1-PENTANOL | 1.22 | 2.46 | 1.3 | 2.5 |
| ISOPROPANOL | 1.18 | 2.52 | 1.2 | 2.5 |
| 2-BUTANOL | 0.91 | 2.46 | 1.2 | 2.2 |
| 2-PENTANOL | 1.14 | 2.22 | 1.0 | 2.5 |
| GLYCEROL | 2.98 | 5.26 | 3.0 | 5.3 |
| ETHYLENE GLYCOL, c0 | 2.13 | 3.87 | 2.9 | 4.2 |
| 2-METHOXYETHANOL c0 | 0.77 | 3.13 | 1.5 | 3.6 |
| 2-ETHOXYETHANOL c0 | 0.63 | 3.13 | 1.5 | 3.7 |
| PHENOL | 2.03 | 0.88 | 2.1 | 1.0 |
| n-BUTYLAMINE | 0.43 | 2.73 | 0.7 | 2.5 |
| ANILINE | 1.62 | 0.78 | 1.7 | 1.0 |
| PYRIDINE | 0.00 | 2.11 | 0.0 | 2.1 |
| FORMAMIDE | 3.03 | 4.23 | 3.1 | 3.7 |
| DIMETHYL SULFOXIDE | 0.10 | 5.24 | 0.6 | 4.6 |
| ACETONITRILE | 0.31 | 2.00 | 1.0 | 2.3 |
| ACRYLONITRILE | 0.43 | 1.52 | 1.0 | 1.7 |
| PROPIONITRILE | 0.08 | 2.02 | 0.3 | 2.4 |
| N,N-DIMETHYLFORMAMIDE | 0.00 | 4.17 | 0.1 | 3.7 |
| N-METHYL FORMAMIDE | 1.58 | 4.20 | 1.5 | 3.7 |
| WATER | 2.89 | 2.99 | 3.0 | 2.9 |

Below are shown the σ-profiles and the sigma surfaces of various conformers of glycols and alkoxyethanols. Conformers c0 are the most stable facilitating intramolecular hydrogen-bonding. Deep blue in sigma-surfaces indicate donor sites and deep red acceptor sites.





Figure S4: The σ-profiles and σ-surfaces of conformer c0 (upper) and c6 (lower) of ethylene glycol. Data from [1].







Figure S5: The σ-profiles and σ-surfaces of conformer c0 (upper), c1 (middle) and c9 (lower) of 2-ethoxyethanol Data from [1].

**References**

1. Klamt, A. 2005. *COSMO-RS from Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design*; Amsterdam: Elsevier.
2. COSMObase, ver. 2019, COSMOlogic GmbH &CoKG (now, BIOVIA Dassault Systemes)
3. Dohnal, V. 2024, New QSPR molecular descriptors based on low-cost quantum chemistry computations using DFT/COSMO approach, *J. Mol. Liq*. 125256, [https://doi.org/10.1016/ j.molliq](https://doi.org/10.1016/%20j.molliq).2024.125256.