Electronic Supplementary Material (ESI) for Green Chemistry

Towards Rational Molecular Design for Reduced Chronic Aquatic Toxicity

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Contents

Data Diversity Analysis

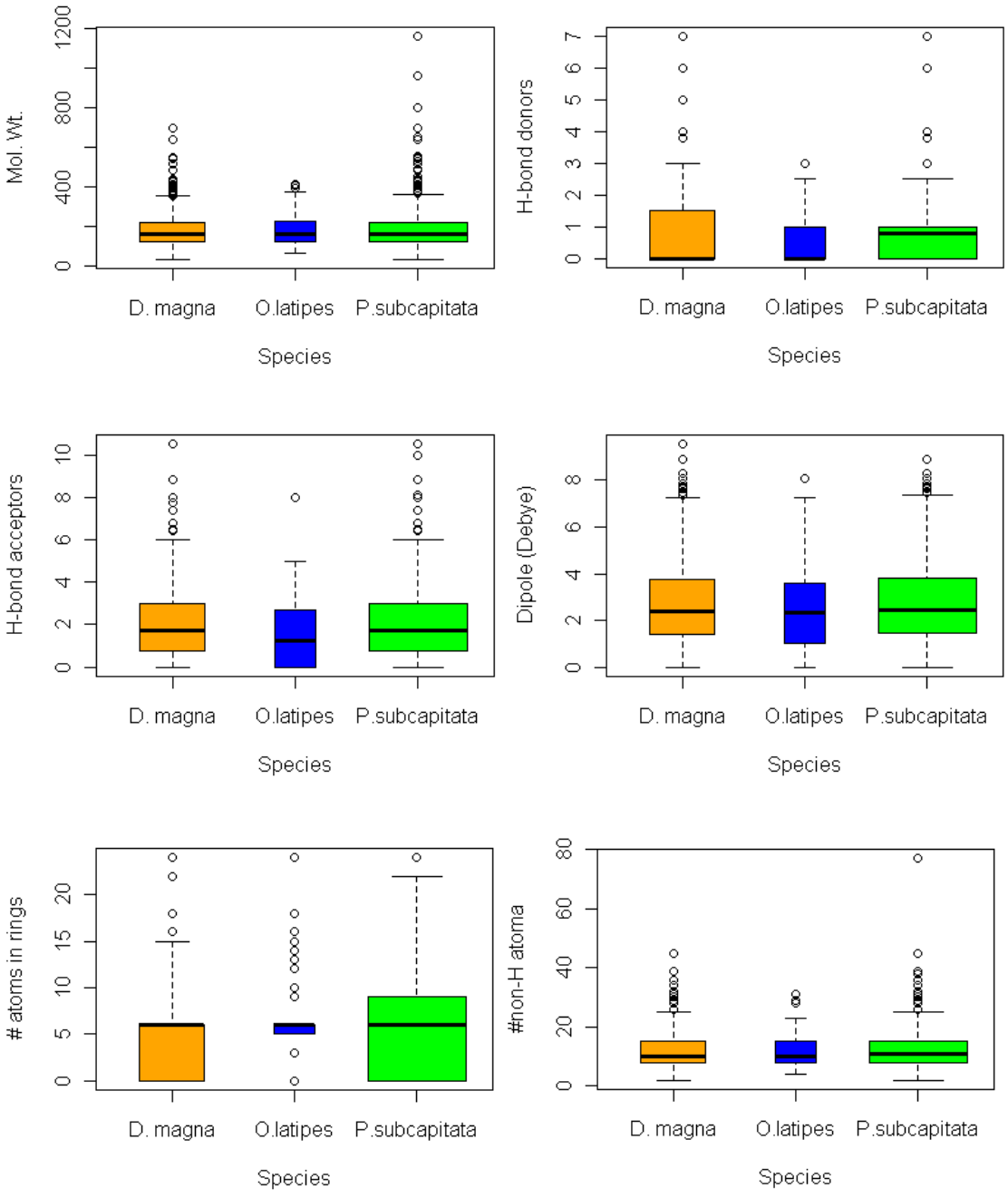

Figure SI-1. Box plots showing ranges of values of key physicochemical properties of the data set.

2. Experimental values of ionization energies

Table SI-1. Experimental values of ionization energies used to verify computationally obtained values by semi-empirical PM3, AM1 and DFT B3LYP methods.

CAS	Experimental Ionization Energy (PE), eV	Reference
91667	6.95	Maier, J.P.; Turner, D.W., *Steric inhibition of resonance studied by molecular photoelectron spectroscopy Part 3. Anilines, Phenols and Related Compounds*, **J. Chem. Soc. Faraday Trans. 2**, 1973, 69, 521
91598	7.03	Klasinc, L.; Kovac, B.; Gusten, H., *Photoelectron spectra of acenes. Electronic structure and substituent effects*, **Pure Appl. Chem.**, 1983, 55, 289.
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92842	7.26	Pozharskii, A.F.; Kashparov, I.S.; Holls, P.J.; Zaletov, V.G., *Hetrocyclic pleiadiene analogs. VI. Electronic properties of perimidine*, **Chem. Heterocycl. Compd.**, 1971, 4, 503, In original 543.
87627	7.30	Maier, J.P.; Turner, D.W., *Steric inhibition of resonance studied by molecular photoelectron spectroscopy Part 3. Anilines, Phenols and Related Compounds*, **J. Chem. Soc. Faraday Trans. 2**, 1973, 69, 521.
95534	7.45	Maier, J.P.; Turner, D.W., *Steric inhibition of resonance studied by molecular photoelectron spectroscopy Part 3. Anilines, Phenols and Related Compounds*, **J. Chem. Soc. Faraday Trans. 2**, 1973, 69, 521.
90040	7.50	Hunter, E.P.; Lias, S.G., *Evaluated Gas Phase Basicities and Proton Affinities of Molecules: An Update*, **J. Phys. Chem. Ref. Data**, 1998, 27, 3, 413-656.
83341	7.54	Hager, J.W.; Wallace, S.C., *Two-laser photoionization supersonic jet mass spectrometry of aromatic molecules*, **Anal. Chem.**, 1988, 60, 5.
95647	7.68	Szepes, L.; Distefano, G.; Pignataro, S., *Steric inhibition of resonance in acetanilides by UV photoelectron spectroscopy*, **Ann. Chim.**, 1974, 64, 159.
62533	7.73	Meek, J.T.; Sekreta, E.; Wilson, W.; Viswanathan, K.S.; Reilly, J.P., *The laser photoelectron spectrum of gas phase aniline*, **J. Chem. Phys.**, 1985, 82, 1741.
83329	7.73	Dewar, M.J.S.; Haselbach, E.; Worley, S.D., Calculated and observed ionization potentials of unsaturated polycyclic hydrocarbons; calculated heats of formation by several semiempirical s.c.f. m.o. methods, Proc. Roy. Soc. (London), 1970, A315, 431
87592	7.77	Szepes, L.; Distefano, G.; Pignataro, S., *Steric inhibition of resonance in acetanilides by UV photoelectron spectroscopy*, **Ann. Chim.**, 1974, 64, 159. [

90153	7.78	Potapov, V.K.; Kardash, I.E.; Sorokin, V.V.; Sokolov, S.A.; Evlasheva, T.I., *Photoionization of heteroaromatic compounds*, **Khim. Vys. Energ.**, 1972, 6, 392.
90437	7.80	Maier, J.P.; Turner, D.W., *Steric inhibition of resonance studied by molecular photoelectron spectroscopy. Part I. Biphenyls*, **Faraday Discuss. Chem. Soc.**, 1972, 54, 149.
91576	7.80	Klasinc, L.; Kovac, B.; Gusten, H., *Photoelectron spectra of acenes. Electronic structure and substituent effects*, **Pure Appl. Chem.**, 1983, 55, 289.
60800	7.86	Vondrak, T.; Bastl, Z.; Bohm, S., *Gas-phase tautomerism in 2,4-dihydropyrazol-3-ones: An ultraviolet photoelectron spectroscopic study and MNDO molecular orbital calculations*, **J. Am. Chem. Soc.**, 1988, 641
92068	7.90	Kobayashi, T., Conformational analysis of terphenyls by photoelectron spectroscopy, **Bull. Chem. Soc. Jpn**., 1983, 56, 3224.
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90131	8.13	Klasinc, L.; Kovac, B.; Gusten, H., *Photoelectron spectra of acenes. Electronic structure and substituent effects*, **Pure Appl. Chem.**, 1983, 55, 289.
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91225	8.62	Schafer, W.; Schweig, A.; Markl, G.; Heier, K.-H., *Zur elektronenstruktur der lambda$_3$- und lambda$_5$-phosphanaphthaline--ungewohnlich grosse MO destabilisierungen*, **Tetrahedron Lett.**, 1973, 3743.
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71556	11.00	Katsumata, S.; Kimura, K., *Photoelectron spectra and sum rule consideration. Effect of chlorine substitution on ionization energies for chloroethanes, chloroacetaldehydes and chloroacetyl chlorides*, **J. Electron Spectrosc. Relat. Phenom.**, 1975, 6, 309.
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67721	11.10	Kimura, K.; Katsumata, S.; Achiba, Y.; Yamazaki, T.; Iwata, S., *Ionization energies, Ab initio assignments, and valence electronic structure for 200 molecules* in **Handbook of HeI Photoelectron Spectra of Fundamental Organic Compounds**, Japan Scientific Soc. Press, Tokyo, 1981.

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