NEW SOLVATION MODEL: SM8

Truhlar and Cramer have updated their Solvation Model to *SM8*.[1] This model allows for any solvent to be utilized (both water and organic solvents) and treats both neutral and charged solutes. While there are some small theoretical changes to the model, the major change is in how the parameters are selected, the number of parameters, and a much more extensive data set is used for the fitting procedure.

Of note is how well this new model works. Table 1 compares the errors in solvation free energies computed using the new *SM8* model against some other popular continuum methods. Clearly, *SM8*provides much better results. As they point out, what is truly discouraging is the performance of the 3PM model against the continuum methods. 3PM stands for “three-parameter model”, where the solvation energies of all the neutral solute in water is set to their average experimental value (-2.99 kcal mol^{-1}), and the same for the neutral solutes in organic solvents (-5.38 kcal mol^{-1}), and for ions (-65.0 kcal mol^{-1}). The 3PM outperforms *most of the continuum methods*!

Table 1. Mean unsigned error (kcal mol^{-1}) for the solvation free energies computed with different methods.[1]

Method	Aqueous neutral[a]	Organic neutrals[b]	Ions[c]
SM8[d]	0.55	0.61	4.31
IEF-PCM/UA0[e]	4.87	5.99	9.73
IEF-PCM/UAHF[f]	1.18	3.94	8.15
C-PCM/*GAMESS*[g]	1.57	2.78	8.39
PB/*Jaguar*[h]	0.86	2.28	6.72
3PM	2.65	1.49	8.60

[a]274 data points. [b]666 data points spread among 16 solvents. [c]332 data points spread among acetonitrile, water, DMSO, and methanol. [d]Using mPW1PW/6-31G(d). [e]Using mPW1PW/6-31G(d) and the UA0 atomic radii in *Gaussian*. [f]Using mPW1PW/6-31G(d) and the UAHF atomic radii in*Gaussian*. [g]Using B3LYP/6-31G(d) and conductor-PCM in *GAMESS*. [h]Using B3LYP/6-31G(d) and the PB method in *Jaguar*.

Source: http://comporgchem.com/blog/?p=46