

Table 1. The Solvation Free Energy for basic structural units in different solvent media at three basis sets

Free Energy				$\Delta G(\text{solvation})$ kcal/mol		
Solvent	631g**	631+g**	6311++g**	631g**	631+g**	6311++g**
Gas Phase	-839,8128710	-839,8412890	-840,0126460	0	0	0
Toluene ($\epsilon=2.37$)	-839,8181500	-839,8475340	-840,0188940	3,312623	3,918797	3,920679
Chloroform ($\epsilon=4.71$)	-839,8212430	-839,8511650	-840,0224960	5,25351	6,197284	6,180969
Chlorobenzene ($\epsilon=5.70$)	-839,8218920	-839,8519280	-840,0232560	5,660763	6,676074	6,657876
Dichloromethane ($\epsilon=8.93$)	-839,8231140	-839,8533680	-840,0246920	6,42758	7,579687	7,558979
quinoline ($\epsilon=9.16$)	-839,8231720	-839,8534350	-840,0247580	6,463975	7,62173	7,600395
Ethanol ($\epsilon=24.85$)	-839,8246750	-839,8552120	-840,0265310	7,407122	8,736815	8,712969
Methanol ($\epsilon=32.61$)	-839,8249000	-839,8554790	-840,0267990	7,548312	8,90436	8,881142
Acetonitrile ($\epsilon=36.69$)	-839,8249630	-839,8555540	-840,0268740	7,587845	8,951423	8,928205
DMSO ($\epsilon=46.83$)	-839,8251240	-839,8557440	-840,0270650	7,688874	9,07065	9,048059
Water ($\epsilon=78.36$)	-839,8253350	-839,8560900	-840,0273160	7,821278	9,287768	9,205564

Table 2. The Solvation Free Energy for each substituted structures in different dielectric media at 6-31G(dP) basis set

	A	B	C	D	E
Toluene	3,822	3,276	3,748	4,484	4,100
Chloroform	6,030	5,377	6,008	7,101	6,291
Chlorobenzene	6,506	5,841	6,495	7,647	6,761
Dichloromethane	7,421	6,749	7,321	8,663	7,666
quinoline	7,464	6,793	7,357	8,707	7,709
Ethanol	8,631	7,938	8,360	9,797	8,860
Methanol	8,811	8,108	8,521	9,965	9,033
Acetonitrile	8,860	8,155	8,563	10,013	9,082
DMSO	8,989	8,275	8,671	10,136	9,207
Water	9,157	8,437	8,817	10,299	9,370

Table 3. The Solvation Free Energy for each substituted structures in different dielectric media at 6-31+G(dP) basis set

	A	B	C	D	E
Toluene	4,334	3,960	4,731	5,593	4,480
Chloroform	6,890	6,354	6,756	7,949	7,038
Chlorobenzene	7,444	6,886	7,226	8,357	7,567
Dichloromethane	8,505	7,931	8,183	9,389	8,607
quinoline	8,564	7,981	8,229	9,442	8,655
Ethanol	9,926	9,340	9,495	10,868	9,981
Methanol	10,139	9,551	9,694	11,091	10,186
Acetonitrile	10,194	9,611	9,748	11,154	10,243
DMSO	10,345	9,761	9,895	11,314	10,391
Water	10,540	9,959	10,085	11,524	10,586

Table 4 The Solvation Free Energy for each substituted structures in different dielectric media at 6-311++G(dP) basis set

	A	B	C	D	E
Toluene	4,332	4,168	4,886	5,046	4,586
Chloroform	6,869	6,467	6,797	8,429	7,048
Chlorobenzene	7,422	6,985	7,245	8,500	7,585
Dichloromethane	8,489	7,997	8,165	9,408	8,611
quinoline	8,539	8,045	8,211	9,457	8,660
Ethanol	9,900	9,401	9,465	10,826	9,982
Methanol	10,109	9,607	9,662	11,042	10,171
Acetonitrile	10,168	9,667	9,718	11,103	10,245
DMSO	10,318	9,814	9,861	11,254	10,395
Water	10,517	10,007	10,051	11,466	10,588