Table S1. Correlation matrix (R^2 values).

	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}
D_1	1.00													
D_2	0.99	1.00												
D_3	0.89	0.86	1.00											
D_4	0.00	0.00	0.00	1.00										
D_5	0.03	0.01	0.00	0.01	1.00									
D_6	0.40	0.43	0.31	0.15	0.00	1.00								
D_7	0.41	0.46	0.38	0.05	0.05	0.44	1.00							
D_8	0.04	0.07	0.04	0.04	0.25	0.16	0.64	1.00						
D_9	0.10	0.07	0.02	0.03	0.56	0.01	0.01	0.20	1.00					
D_{10}	0.13	0.09	0.04	0.02	0.57	0.01	0.00	0.18	0.97	1.00				
D_{11}	0.00	0.01	0.02	0.04	0.81	0.03	0.13	0.37	0.60	0.59	1.00			
D_{12}	0.03	0.01	0.00	0.02	0.85	0.00	0.05	0.31	0.74	0.75	0.87	1.00		
D_{13}	0.00	0.00	0.03	0.03	0.81	0.00	0.12	0.36	0.53	0.47	0.77	0.74	1.00	
D_{14}	0.64	0.59	0.61	0.03	0.02	0.42	0.13	0.00	0.02	0.02	0.00	0.01	0.01	1.00

Table S2. Descriptor intercorrelations (R^2 values)

Equation (table/number)	Descriptors			
2-2	D_1	D_5		
	0.026	0.026		
2-3	D_3	D_9	D_8	
	0.113	0.255	0.273	
2-4	D_{14}	D_{12}	D_{10}	D_7
	0.161	0.793	0.781	0.269
3-2	D_6	D_{13}		
	0.002	0.002		
3-3	D_5	D_6	D_4	
	0.014	0.157	0.162	

Description for Tables S1 and S2

D_1 - Structural Information content (order 0)

D_2 - Bonding Information content (order 0)

D_3 - Structural Information content (order 1)

D_4 - Molecular volume / XYZ Box

D_5 - HACA-1 [Zefirov's PC]

D_6 - Min net atomic charge

D_7 - Tot dipole of the molecule

D_8 - Image of the Onsager-Kirkwood solvation energy

D_9 - HASA H-acceptors surface area [Semi-MO PC]

D_{10} - HBSA H-bonding surface area [Semi-MO PC]

D_{11} - HA dependent HDSA-1/TMSA [Semi-MO PC]

D_{12} - HACA-2/TMSA [Semi-MO PC]

D_{13} - RT:1 number of H-acceptors

D_{14} - CSA-2 of H atoms