Supplementary Materials

Table S1.

L.p.	Polar surface area	Polar volume	Surface area	Volume	Acceptor count (sybyl)	Atom count	Bond count	Donor count (sybyl)	Hydrophobe count	Rotatable Bond count	Acceptor Mount (Lipinski)	ClogP	Donor Mount (Lipinski)	Lipinski violations	Molecular weight
1	49.446	148.212	605.397	1006.661	3	44	46	1	3	6	5	4.1632	1	0	324.3737
2a	51.491	160.579	648.635	1063.791	4	48	50	1	3	7	6	3.6486	1	0	354.3997
2b	61.506	165.704	653.223	1083.814	4	48	50	1	3	7	6	4.2386	1	0	354.3997
2c	61.876	148.051	653.419	1073.462	4	48	50	1	3	7	6	4.2386	1	0	354.3997
3a	45.255	141.705	623.038	1038.938	3	47	49	1	3	6	5	4.0122	1	0	338.4003
3b	49.460	129.946	636.949	1050.936	3	47	49	1	3	6	5	4.6622	1	0	338.4003
3c	49.466	132.090	637.767	1050.962	3	47	49	1	3	6	5	4.6622	1	0	338.4003
4a	48.435	144.032	610.640	1018.047	3	44	46	1	3	6	5	3.9638	1	0	342.3642
4b	49.474	131.146	614.901	1012.274	3	44	46	1	3	6	5	4.5638	1	0	342.3642
4c	49.441	144.623	614.922	1021.213	3	44	46	1	3	6	5	4.5638	1	0	342.3642
5a	48.725	135.310	618.371	1030.333	3	44	46	1	3	6	5	4.2838	1	0	358.8188
5b	49.486	134.686	628.707	1042.689	3	44	46	1	3	6	5	5.1338	1	1	358.8188
5c	49.435	133.841	628.664	1038.846	3	44	46	1	3	6	5	5.1338	1	1	358.8188
6a	49.183	137.829	621.311	1038.864	3	44	46	1	3	6	5	4.4038	1	0	403.2698
6b	49.440	137.166	633.526	1053.128	3	44	46	1	3	6	5	5.2838	1	1	403.2698
6c	49.462	133.509	633.536	1046.658	3	44	46	1	3	6	5	5.2838	1	1	403.2698
7a	42.920	142.558	636.372	1076.084	3	47	49	1	4	6	5	4.0470	1	0	392.3717
7b	49.450	118.742	659.789	1088.469	3	47	49	1	4	6	5	5.4970	1	1	392.3717
7c	49.438	124.821	660.914	1079.248	3	47	49	1	4	6	5	5.4970	1	1	392.3717
8a	110.799	195.483	623.940	1045.108	5	46	48	1	3	7	8	0.8712	1	0	369.3713
8b	134.854	207.158	641.084	1063.287	5	46	48	1	3	7	8	0.8712	1	0	369.3713
8c	134.702	209.563	641.602	1057.242	5	46	48	1	3	7	8	0.8712	1	0	369.3713
9a	93.856	164.611	614.104	1021.122	4	45	47	2	3	6	6	3.7262	2	0	340.3731
9b	105.477	172.921	619.746	1034.721	4	45	47	2	3	6	6	3.4962	2	0	340.3731
9c	105.171	173.231	619.497	1023.670	4	45	47	2	3	6	6	3.4962	2	0	340.3731