GM \ GC	[.0,.1[	[.1,.2[	[.2,.3[	[.3,.4[	[.4,.5[	[.5,.6[	[.6,.7[	[.7,.8[	[.8,.9[	[.9,1.0[	= 1.0
[.0,.1[	2035	911	314	197	64	82	2	68	0	0	0
[.1,.2[	3647	4336	1506	697	127	343	16	344	1	0	141
[.2,.3[	5537	6542	1943	919	204	445	22	337	3	0	131
[.3,.4[	6429	6886	2266	1178	191	435	25	374	1	0	120
[.4,.5[	4103	4562	1748	919	110	228	4	331	0	0	104
[.5,.6[	1369	1579	718	601	42	137	11	237	0	0	70
[.6,.7[	233	336	223	232	33	49	14	138	0	0	105
[.7,.8[	11	30	33	55	11	20	2	73	2	0	67
[.8,.9[	0	7	1	43	0	14	5	9	1	0	66
[.9,1.0[	0	0	0	1	0	0	0	0	0	0	14
= 1.0	0	0	0	0	0	0	0	0	0	0	69

TABLE 1: Confusion matrix of similarity with Molecular graphs (MG) and Graph Cycles(GC)

TC \ GC	[.0,.1[	[.1,.2[	[.2,.3[	[.3,.4[	[.4,.5[	[.5,.6[	[.6,.7[	[.7,.8[	[.8,.9[	[.9,1.0[	= 1.0
[.0,.1[	5437	3165	1695	1000	196	280	36	240	0	0	88
[.1,.2[	21074	19395	6815	3194	696	1131	68	948	7	0	389
[.2,.3[	20000	12962	5938	1986	572	649	64	449	5	0	140
[.3,.4[	4373	2811	1598	591	159	172	17	173	0	0	65
[.4,.5[	1116	788	618	247	68	101	5	112	2	0	67
[.5,.6[	386	286	352	197	49	92	15	115	1	0	55
[.6,.7[	153	85	151	117	47	49	12	126	4	0	61
[.7,.8[	50	45	78	56	36	38	11	63	4	0	45
[.8,.9[	10	13	12	22	11	24	6	55	0	0	34
[.9,1.0[	1	5	1	4	3	5	2	22	0	0	31
= 1.0	0	1	0	0	0	1	0	1	0	0	5

TABLE 2: Confusion matrix of similarity with Tanimoto Coefficient (TC) and Graph Cycles(GC)

GM \ TC	[.0,.1[	[.1,.2[	[.2,.3[	[.3,.4[	[.4,.5[	[.5,.6[	[.6,.7[	[.7,.8[	[.8,.9[	[.9,1.0[	= 1.0
[.0,.1[	1678	1731	259	5	0	0	0	0	0	0	0
[.1,.2[	2433	6499	2157	63	6	0	0	0	0	0	0
[.2,.3[	1399	9638	4642	343	50	7	4	0	0	0	0
[.3,.4[	593	8343	7187	1379	274	90	26	5	8	0	0
[.4,.5[	190	3932	5091	1834	652	269	97	34	6	3	1
[.5,.6[	53	974	1544	1032	486	366	186	91	30	2	0
[.6,.7[	10	150	245	236	242	175	161	101	37	6	0
[.7,.8[	2	6	15	30	26	50	62	58	39	16	0
[.8,.9[	0	1	10	7	8	21	31	35	22	10	1
[.9,1.0[	0	0	1	0	0	0	7	5	1	1	0
= 1.0	0	0	9	0	0	8	5	4	15	23	5

TABLE 3: Confusion matrix of similarity on Molecular graphs (MG) and Tanimoto Coefficient (TC)