

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)

