

SUPPLEMENTARY MATERIAL for Cramer *et al.*,
 "Prospective Identification .. By Topomeric Similarity Searching"

Chi-squared tests of significance for the dependence of frequency of biological activity (A-II Displacement) on topomeric shape similarity to various active compounds, for various activity ranges.

		Chi-Squared Values ^a				n ^b Signif	Wgt n ^c Signif
Compound	Activity (%Displ)	40%- >75%	30%- 75%	20%- 40%	30%- 30%		
BC A							
A 1	99	23.77	37.27	13.25	4.2	3	12
A 2	86	10.86	16.54	1.77	6.37	2	7
A 3	85	8.3	22.72	12.39	6.65	3	8
A 4	83	41.54	29.67	13.09	2.69	3	13
A 5	83	38.82	67.05	14.64	6.88	3	16
A 6	77	6.97	1.38	4.13	3.58	0	0
A 7	76	3.27	4.47	7.9	7.46	1	1
A 8	69	14.62	19.5	6.19	5.51	2	8
A 9	46	12.39	26.29	11.94	5.57	3	9
A 10	39	2.41	2.22	4.73	4.52	0	0
A 11	34	1.68	2.73	6.32	4.52	0	0
A 12	32	3.2	4.58	9.63	7.93	2	3
A 13	27	1.26	5.04	9.2	8.56	2	2
B 1	35	27.69	13.73	9.05	5.95	3	9
B 2	34	1.45	4.4	1.05	4.06	0	0
B 3	37	35.08	55.19	27.46	18.35	4	19
B 4	39	7.46	2.51	3.56	9.04	1	1
B 17	36	2.81	2.35	3.72	3.61	0	0
B 25	23	2.88	4.74	13.72	10.62	2	5
B 26	31	3.85	6.12	1.7	2.41	0	0
B 27	24	2.75	2.28	3.39	3.41	0	0
B 28	30	2.62	2.33	3.4	3.36	0	0
B 30	38	1.08	4.11	10.38	10.79	2	4
B 31	31	2.57	2.41	3.29	3.01	0	0
C 1	38	6.78	17.95	19.8	12.8	3	11
C 3	54	3.12	11.3	17.45	12.83	3	7
C 4	36	6.32	2.85	9.02	3.36	0	0
C 5	51	3.91	15.55	8.46	9.9	3	6
C 6	40	2.27	2.44	3.6	7.47	0	0
C 7	45	3.35	9.36	12.61	12.54	3	5
C 8	32	10.07	18.7	9.87	7.19	3	9
C 9	38	6.8	16.38	9.18	7.76	2	5
C 11	31	1.38	2.28	7.18	8.23	1	1
C 12	32	2.88	13.28	18.33	15.54	3	11
C 14	34	0.56	0.63	6.49	8.44	1	1
C 16	42	0.88	0.47	5.31	7.73	0	0
C 20	27	0.83	0.55	3.69	6.03	0	0
C 22	34	1.09	0.36	6.25	9.85	1	2
C 26	30	2.89	7.32	1.67	4.21	0	0
C 27	59	0.47	1.11	6.21	7.44	0	0
C 33	35	2.09	0.4	6.75	7.21	0	0
D 1	34	20.79	16.91	4.58	2.71	2	9

D 3	34	3.63	2.38	3.98	5.02	0	0
D 7	31	0.97	0.94	1.17	0.91	0	0
D 14	53	4.37	3.22	1.64	2.09	0	0
D 21	31	1.85	5.27	4.8	2.7	0	0
D 22	34	2.76	2.98	2.51	2.42	0	0
D 25	32	2.26	2.15	3.24	2.18	0	0
D 40	47	3.51	5.49	3.32	4.11	0	0
E 3	38	4.12	5.75	12.08	7.56	1	2
E 4	31	6.33	1.36	5.76	2.31	0	0
E 5	33	3.19	19.07	6.03	1.1	1	5
E 7	36	0.42	0.39	11.11	6.35	1	2
E 8	47	5.58	5.67	7.53	0.97	0	0
E 9	30	3.12	13.32	5.97	2.58	1	3
E 10	36	1.71	0.1	4.55	2.45	0	0
E 12	33	0.57	0.22	13.67	5.16	1	3
E 14	42	3.38	3.07	10.03	7.1	1	2
E 18	49	0.43	2.12	12.02	4.77	1	2
E 19	34	0.22	2.07	6.46	6.45	0	0
E 20	38	1.67	0.97	9.56	3.85	1	2
E 21	32	1.22	3.26	12.19	10.14	2	4
E 24	35	4.47	0.92	5.71	4.45	0	0
E 27	36	1.76	0.84	7.06	3.21	0	0
E 29	31	1.22	2.94	13.21	9.06	2	3
E 30	34	2.12	10.49	6.24	7.51	1	2
E 33	36	3.39	0.63	6.19	7.73	0	0
F 6	35	3.64	2.75	6.05	4.58	0	0
F 7	35	1.97	2.03	0.82	1.93	0	0
F 14	37	2.83	1.67	2.12	2.15	0	0
F 15	28	3.51	2.7	3.5	0.78	0	0
F 19	30	3.33	2.44	2.38	2.64	0	0
F 23	30	2.5	3.12	3.31	1.34	0	0
F 24	37	5.46	2.58	3.34	4.58	0	0
F 25	37	3.39	3.23	3.19	2.17	0	0
F 35	36	4.31	3.72	5.13	3.11	0	0
G 16	23	5.21	4.69	6.4	2.39	0	0
H 10	34	0.96	1.02	0.46	2.04	0	0
H 17	37	0.95	0.5	1.55	9.04	1	1
H 18	33	1.07	4.94	6.77	4.13	0	0
H 22	21	0.97	0.84	1.96	1.52	0	0
H 29	23	1.16	5.33	4.35	1.13	0	0
H 30	23	1.17	4.43	1.09	2.66	0	0
H 33	26	1.6	1.01	1.46	0.88	0	0
H 35	34	13.32	4.5	5.98	4.75	1	3
I 17	35	1.57	1.35	2	2.08	0	0
I 25	34	3.54	1.21	5.19	5.77	0	0
J 14	25	3.41	2.24	8.22	2.52	1	1
J 17	31	1.92	1.75	1.07	0.77	0	0
J 22	32	3.16	1.01	6.84	1.42	0	0
J 24	32	6.4	2.09	2.04	1.32	0	0
K 28	20	0.94	1.42	4.77	3.47	0	0
K 32	31	1.16	5.33	4.35	1.13	0	0
M 27	28	2.04	3.41	5.68	3.23	0	0

N 13	22	1.15	1.19	3.32	2.91	0	0
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^aEach chi-squared value tests the probability that the distribution of the stated range of activity among all 425 structures is related to their topomeric shape dissimilarity from the indicated compound. In other words, each line of this table corresponds to any sixth line of data in each block of Table 4.

^bThe number of chi-squared values in this row which are statistically significant ($P < .10$).

^cThe number of chi-squared values in this row which are statistically significant, weighted by the degree of significance (weights are: $P < .10$, 1; $P < .05$, 2; $P < .025$, 3; $P < .01$, 4; $P < .005$, 5; $P < .001$, 6).