

## Supporting Information

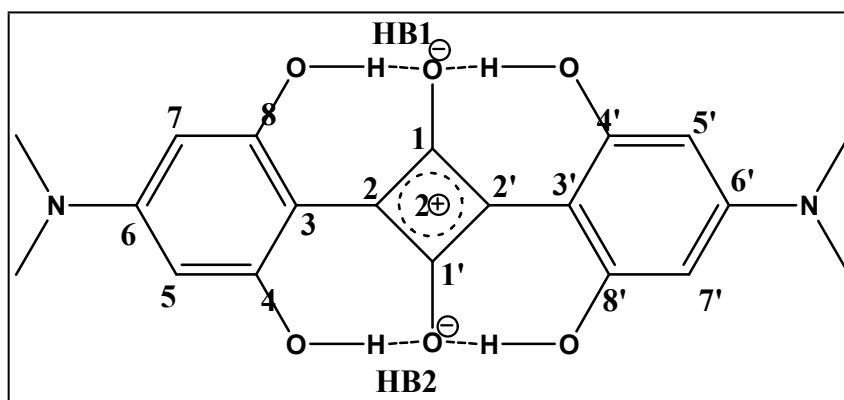
### A Computational Probe Granting Insight into Intra and Inter-Stacking Interactions in Squaraine Dye Derivatives

Krishna Chaitanya Gunturu<sup>a</sup>, Carola Schulzke<sup>b</sup>

<sup>a</sup> School of Chemical Sciences, SRTM University, Vishnupuri, Nanded-431606, India

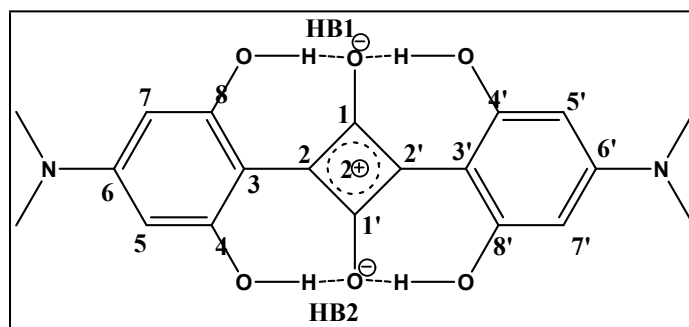
<sup>b</sup> Institute of Biochemistry, University of Greifswald, 17489 Greifswald, Germany

Table S1: Selected metrical parameters (bond lengths in Å and dihedral angles in °) of all motifs obtained from crystal structures.



Geometrical Indices	Motif-1	Motif-2	Motif-3	Motif-4
C1-O	1.25	1.252	1.252	1.248
C1-C2	1.459/1.452	1.457/1.463	1.463/1.460	1.454/1.438
C2-C3	1.400	1.399	1.407/1.406	1.379
C3-C4	1.441	1.436	1.444	1.434
C4-C5	1.370	1.365	1.371	1.349
C5-C6	1.417	1.419	1.422	1.402
C6-C7	1.419	1.414	1.424	1.426
C7-C8	1.370	1.367	1.372	1.356
C8-C3	1.439	1.434	1.440	1.419
C6-N	1.357	1.359	1.354	1.341
C4-O	1.351	1.361	1.360	1.359
C8-O	1.350	1.355	1.356	1.351
HB1	1.788	1.746	1.757	1.665
HB2	1.775	1.657	1.637	1.653
O-1-2-3	1.31	-1.33	0.74	1.26
O-1-2'-3'	-0.77	0.78	0.04	-0.25
1-2-3-8	0.57	-3.55	-0.31	-1.80
1'-2-3-4	-0.51	-3.03	-0.56	-1.13
5-6-N-C	2.49	0.04	6.64	8.49
7-6-N-C	1.35	0.77	-0.39	2.52

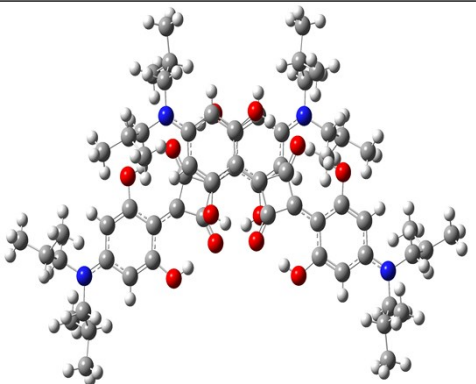
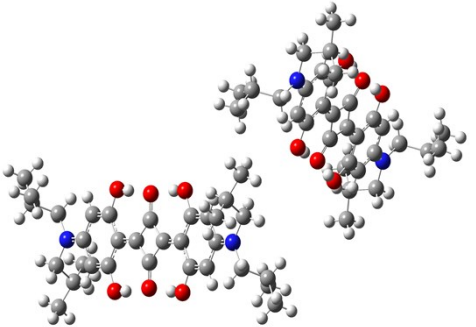
Table S2: Selected metrical parameters of neutral, cationic and anionic species (bond lengths in Å and dihedral angles in °) of all motifs obtained at the B3LYP/6-31G+(d,p) level of theory. Motif-1 and motif-2 have the same chemical structure and therefore the calculations are identical.

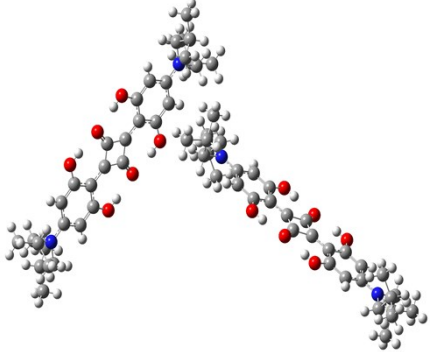
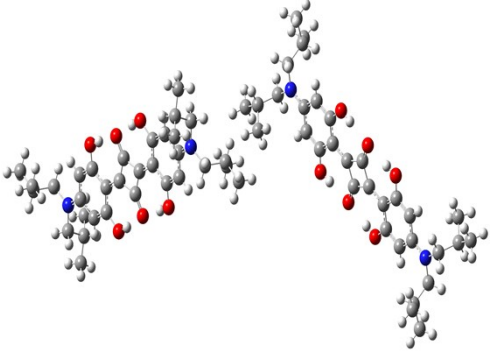
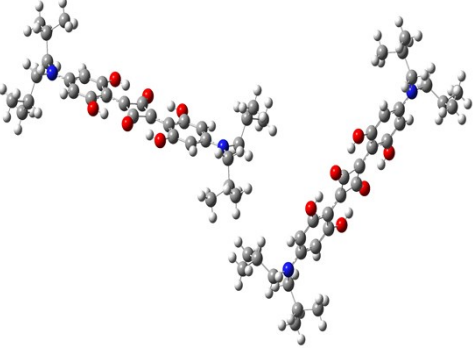


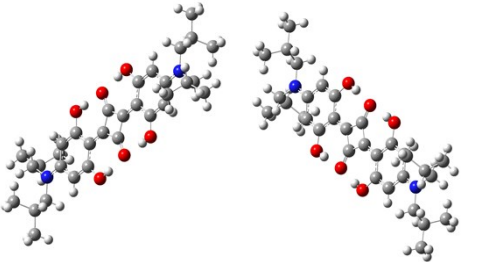
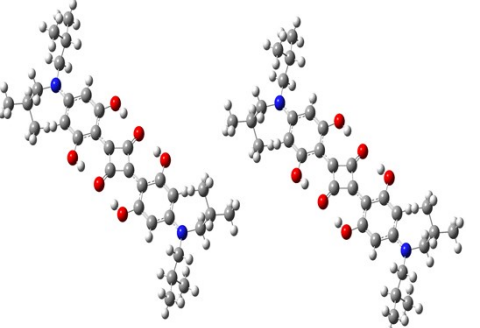
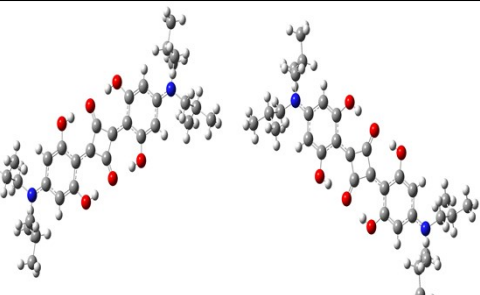
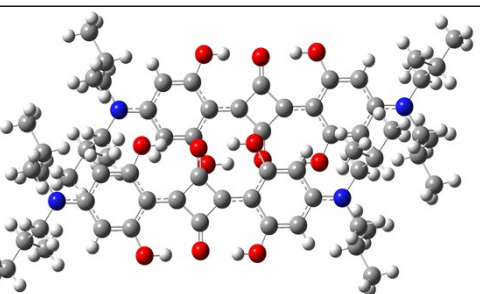
Motif-1(Motif-2)			
Geometrical Indices	Cation	Anion	Neutral
C1-O	1.244	1.262	1.254
C1-C2	1.470	1.459	1.460
C2-C3	1.395	1.431	1.404
C3-C4	1.463	1.428	1.448
C4-C5	1.375	1.396	1.383
C5-C6	1.430	1.410	1.420
C6-C7	1.429	1.410	1.419
C7-C8	1.375	1.395	1.383
C8-C3	1.463	1.430	1.448
C6-N	1.353	1.405	1.373
C4-O	1.337	1.358	1.344
C8-O	1.337	1.359	1.345
HB1	1.679	1.694	1.675
HB2	1.676	1.694	1.677
O-1-2-3	-0.02	-0.05	-0.01
O-1-2'-3'	0.05	-0.12	-0.02
1-2-3-8	-0.07	-0.09	-0.05
1'-2-3-4	0.13	-0.20	0.11
5-6-N-C	-2.28	-5.24	2.11
7-6-N-C	-3.40	-13.93	4.06
Motif-3			
Geometrical Indices	Cation	Anion	Neutral
C1-O	1.243	1.261	1.254
C1-C2	1.470	1.459	1.460
C2-C3	1.394	1.431	1.404

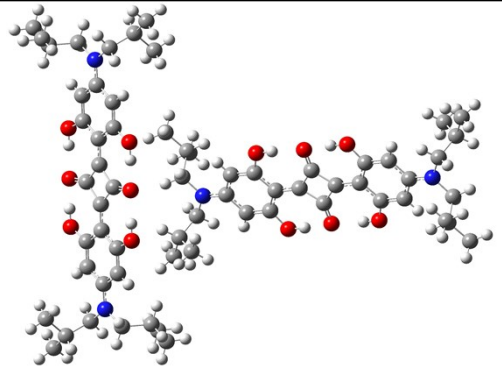
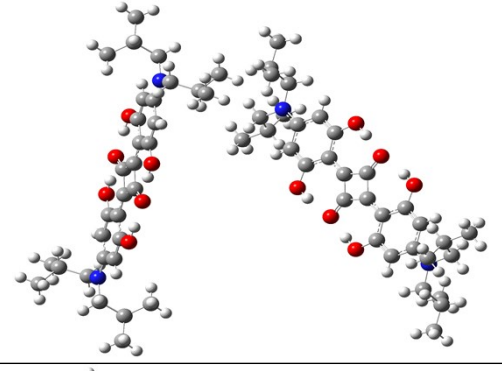
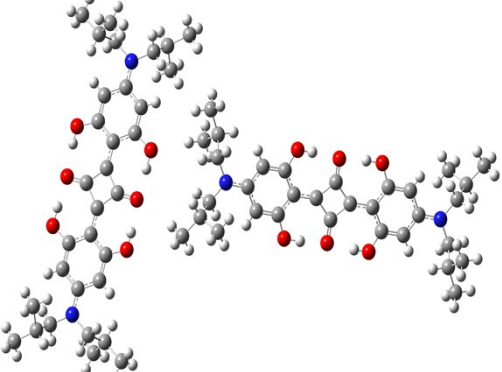
C3-C4	1.464	1.428	1.448
C4-C5	1.375	1.397	1.384
C5-C6	1.429	1.406	1.420
C6-C7	1.429	1.409	1.419
C7-C8	1.375	1.394	1.383
C8-C3	1.463	1.432	1.448
C6-N	1.352	1.413	1.373
C4-O	1.336	1.358	1.344
C8-O	1.337	1.358	1.345
HB1	1.676	1.691	1.674
HB2	1.679	1.692	1.676
O-1-2-3	-0.15	-0.07	0.10
O-1-2'-3'	0.03	-0.09	0.09
1-2-3-8	-0.14	-0.12	-0.13
1'-2-3-4	-0.19	-0.60	0.24
5-6-N-C	-5.14	-5.97	3.66
7-6-N-C	-7.79	-37.52	9.90
Motif-4			
Geometrical Indices	Cation	Anion	Neutral
C1-O	1.243	1.261	1.254
C1-C2	1.470	1.459	1.460
C2-C3	1.394	1.431	1.404
C3-C4	1.464	1.432	1.448
C4-C5	1.375	1.394	1.383
C5-C6	1.429	1.409	1.419
C6-C7	1.429	1.406	1.420
C7-C8	1.375	1.397	1.383
C8-C3	1.463	1.429	1.448
C6-N	1.352	1.412	1.373
C4-O	1.336	1.358	1.345
C8-O	1.337	1.358	1.344
HB1	1.676	1.692	1.676
HB2	1.679	1.691	1.674
O-1-2-3	0.17	-0.09	-0.08
O-1-2'-3'	-0.03	-0.08	-0.12
1-2-3-8	0.13	0.61	0.22
1'-2-3-4	0.18	0.12	-0.13
5-6-N-C	5.31	5.44	9.81
7-6-N-C	7.98	36.17	3.78

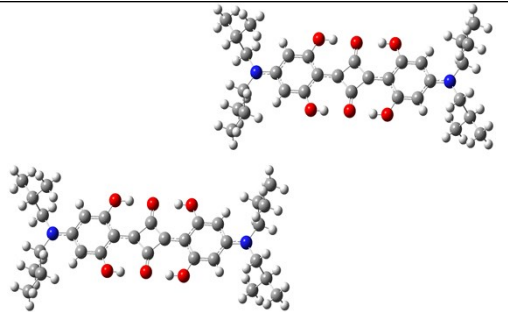
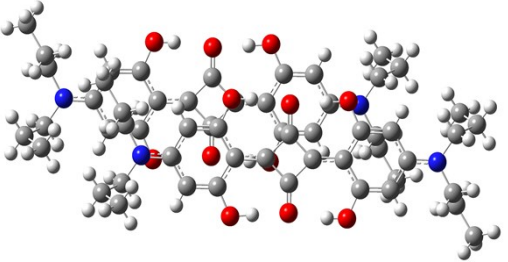
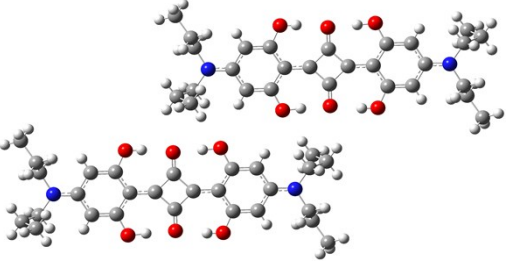
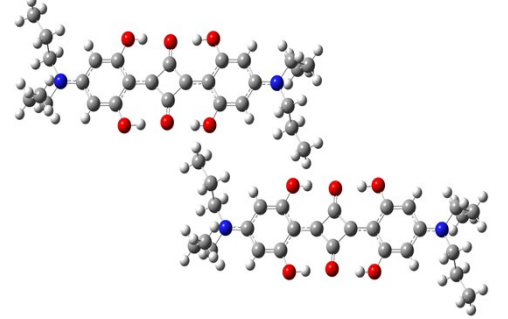
Table S3: At B3LYP/6-31G+(d,p) level of theory calculated interaction energies  $\Delta E_{int}^{CP}$  (kcal/mol), effective charge transfer integrals ( $(J_{eff})_{ij}$  in eV), rate constants (in  $S^{-1}$ ), and drift mobilities for hole and electron transfer ( $\mu$  in  $cm^2/V s$ ) of all motifs. The observed centroid-centroid distances are given as  $d_{cc}$  (in Å).

Motif	Interactions	$d_{cc}$	$J_+$	$J_-$	$K_+$	$K_-$	$\mu_+$	$\mu_-$
Motif-1-1		5.40	- $9.08 \times 10^{-02}$	$5.15 \times 10^{-02}$	$7.85 \times 10^{13}$	$3.65 \times 10^{12}$	1.1067	0.0514
Motif-1-2		11.81	- $2.38 \times 10^{-05}$	- $4.51 \times 10^{-04}$	$5.39 \times 10^{06}$	$2.8 \times 10^{08}$		

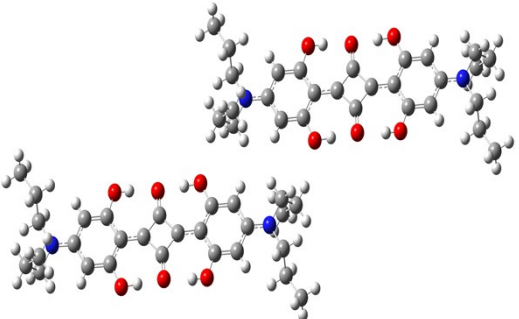
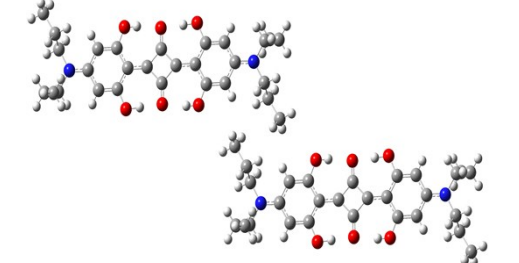
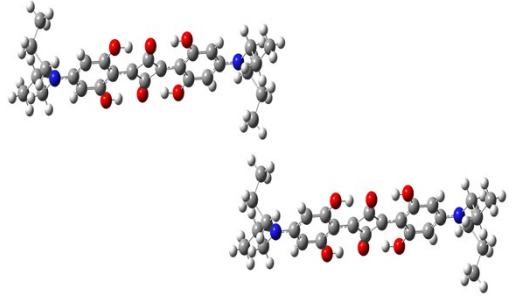
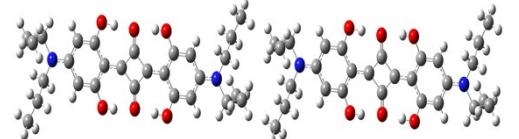
Motif-1-3		12.99	$1.21 \times 10^{-03}$	$1.05 \times 10^{-03}$	$1.40 \times 10^{10}$	$1.51 \times 10^{09}$		
Motif-1-4		15.98	$2.56 \times 10^{-04}$	$1.18 \times 10^{-04}$	$6.24 \times 10^{08}$	$1.93 \times 10^{07}$		
Motif-1-5		16.01	$3.11 \times 10^{-04}$	$1.00 \times 10^{-04}$	$9.18 \times 10^{08}$	$1.38 \times 10^{07}$		

Motif-1-6		16.20	- $9.93 \times 10^{-05}$	$9.04 \times 10^{-05}$	$9.38 \times 10^{07}$	$1.13 \times 10^{07}$		
Motif-1-7		18.52	- $1.31 \times 10^{-04}$	$1.34 \times 10^{-04}$	$1.64 \times 10^{08}$	$2.45 \times 10^{07}$		
Motif-1-8		22.11	- $7.01 \times 10^{-04}$	$4.05 \times 10^{-04}$	$4.68 \times 10^{09}$	$2.25 \times 10^{08}$		
Motif-2-1		6.20	- $3.31 \times 10^{-02}$	$2.37 \times 10^{-03}$	$1.04 \times 10^{13}$	$7.74 \times 10^{09}$	0.3099	0.0003

Motif-2-2		11.31	- $3.74 \times 10^{-04}$	$1.48 \times 10^{-03}$	$1.33 \times 10^{09}$	$3.02 \times 10^{09}$		
Motif-2-3		11.47	- $1.76 \times 10^{-04}$	- $2.90 \times 10^{-04}$	$2.94 \times 10^{08}$	$1.16 \times 10^{08}$		
Motif-2-4		14.18	- $1.50 \times 10^{-03}$	- $7.14 \times 10^{-04}$	$2.15 \times 10^{10}$	$7.02 \times 10^{08}$		

Motif-2-5		17.61	$2.78 \times 10^{-04}$	$1.72 \times 10^{-04}$	$7.33 \times 10^{08}$	$4.06 \times 10^{07}$		
Motif-3-1		5.22	$8.12 \times 10^{-03}$	$7.57 \times 10^{-02}$	$5.32 \times 10^{11}$	$2.2 \times 10^{12}$	0.0558	0.0332
Motif-3-2		11.18	$3.76 \times 10^{-03}$	$2.63 \times 10^{-03}$	$1.14 \times 10^{11}$	$2.65 \times 10^{09}$		
Motif-3-3		12.73	$2.81 \times 10^{-03}$	$8.75 \times 10^{-05}$	$6.38 \times 10^{10}$	$2.94 \times 10^{06}$		



Motif-3-4		13.63	$1.13 \times 10^{-02}$	$6.32 \times 10^{-03}$	$1.03 \times 10^{12}$	$1.53 \times 10^{10}$		
Motif-3-5		15.93	$1.65 \times 10^{-03}$	$8.82 \times 10^{-04}$	$2.19 \times 10^{10}$	$2.99 \times 10^{08}$		
Motif-3-6		17.54	$2.41 \times 10^{-04}$	$6.36 \times 10^{-05}$	$4.69 \times 10^{08}$	$1.55 \times 10^{06}$		
Motif-3-7		19.46	$4.27 \times 10^{-04}$	$1.39 \times 10^{-04}$	$1.47 \times 10^{09}$	$7.44 \times 10^{06}$		

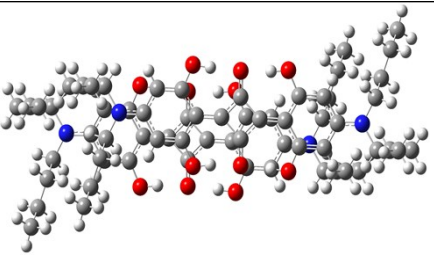
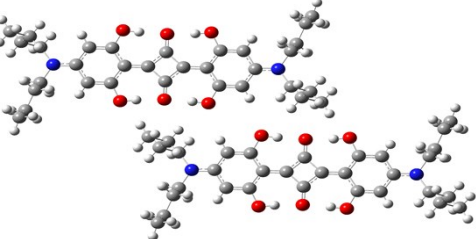
Motif-4-1		5.17	$8.61 \times 10^{-03}$	$5.56 \times 10^{-02}$	$6.14 \times 10^{11}$	$1.34 \times 10^{12}$	0.0300	0.0692
Motif-4-2		10.86	$3.24 \times 10^{-03}$	$2.48 \times 10^{-03}$	$8.68 \times 10^{10}$	$2.66 \times 10^{09}$		

Table S4: Hirshfeld contact surfaces ( $C_{XY}$ ) and random contacts ( $R_{XY}$ ) of the main intermolecular interactions for all motifs in this study.<sup>a</sup>

$C_{XY}$	Motif-1	Motif-2	Motif-3	Motif-4
H---H	0.05	0.03	0.03	0.01
C---H	0.24	0.45	0.52	0.38
C---C	1.18	0.34	1.63	1.17
C---N	0	0	0	0
O---H	0.27	0.04	0.07	0.03
O---C	0.71	1.21	1.42	1.14
O---N	0	0	0.02	0.02
HC---H	0.93	0.91	1.17	0.78
HC---C	3.27	4.44	3.77	3.01
HC---N	0.02	0	0	0
HC---O	2.6	2.45	3.31	2.44
HC---HC	7.05	6.9	6.77	7.31

$R_{XY}$	Motif-1	Motif-2	Motif-3	Motif-4
H---H	1.35	1.13	1.24	0.83
C---H	11.53	10.47	12.37	9.53
C---C	24.54	24.22	30.9	27.53
C---N	0.13	0.01	1.06	0.93
O---H	6.53	5.78	6.56	4.99
O---C	27.82	26.79	32.78	28.81
O---N	0.08	0	0.56	0.49
HC---H	36.64	33.33	29.63	28.56
HC---C	156.29	154.73	148.22	165.01
HC---N	0.43	0.02	2.52	2.78
HC---O	88.48	85.38	78.6	86.34
HC---HC	248.32	246.18	177.36	246.86

<sup>a</sup> The HC refers to H-C hydrogen atom.

Table S5: Optimized Cartesian coordinates of all motifs obtained at the B3LYP/6-31G+(d,p) level of theory. Motif-1 and motif-2 have the same chemical structure and therefore the coordinates are identical.

<b>Motif</b>		<b>Cartesian Coordinates</b>			
Motif-1/ Motif-2	Neutral	8	0.460390	-1.978538	1.003610
		8	-0.905087	-3.408983	-0.777626
		1	-0.379907	-2.945755	-0.074635
		8	-1.899382	0.865084	-2.948343
		1	-1.378160	1.351842	-2.258910
		7	-3.519344	-3.229477	-4.716018
		6	0.205591	-0.883517	0.448232
		6	-0.553628	-0.504309	-0.740089
		6	-1.292028	-1.177060	-1.726608
		6	-1.447027	-2.616226	-1.718683

		6	-2.174146	-3.267421	-2.698926
		1	-2.231586	-4.342148	-2.613580
		6	-2.805965	-2.557914	-3.754257
		6	-2.672560	-1.145073	-3.774016
		1	-3.137851	-0.530854	-4.529789
		6	-1.946167	-0.471784	-2.809035
		6	-3.611553	-4.695748	-4.708577
		1	-4.470940	-4.966523	-5.330730
		1	-3.850882	-5.041580	-3.696755
		6	-2.364406	-5.444608	-5.233307
		1	-1.508860	-5.150660	-4.613079
		6	-2.578354	-6.956790	-5.067936
		1	-3.430842	-7.303444	-5.666303
		1	-2.770277	-7.226916	-4.023266
		1	-1.695229	-7.513382	-5.398207
		6	-2.031324	-5.084690	-6.687913
		1	-1.841301	-4.013256	-6.805754
		1	-2.848528	-5.366437	-7.364809
		1	-1.132554	-5.616415	-7.018277
		6	-4.267910	-2.553189	-5.782619
		1	-4.121536	-3.132677	-6.700378
		1	-3.830834	-1.571827	-5.975218
		6	-5.786898	-2.412524	-5.527965
		1	-6.185629	-3.422383	-5.352330
		6	-6.461005	-1.855600	-6.791792
		1	-6.271351	-2.488986	-7.666157
		1	-6.094043	-0.847463	-7.021899
		1	-7.545530	-1.788239	-6.657163
		6	-6.116216	-1.556919	-4.297288
		1	-5.787534	-0.520109	-4.434643
		1	-5.636606	-1.942035	-3.392800
		1	-7.197623	-1.541482	-4.122458
		8	-0.460390	1.978538	-1.003610

		8	0.905087	3.408983	0.777626
		1	0.379907	2.945755	0.074635
		8	1.899382	-0.865084	2.948343
		1	1.378160	-1.351842	2.258910
		7	3.519344	3.229477	4.716018
		6	-0.205591	0.883517	-0.448232
		6	0.553628	0.504309	0.740089
		6	1.292028	1.177060	1.726608
		6	1.447027	2.616226	1.718683
		6	2.174146	3.267421	2.698926
		1	2.231586	4.342148	2.613580
		6	2.805965	2.557914	3.754257
		6	2.672560	1.145073	3.774016
		1	3.137851	0.530854	4.529789
		6	1.946167	0.471784	2.809035
		6	3.611553	4.695748	4.708577
		1	4.470940	4.966523	5.330730
		1	3.850882	5.041580	3.696755
		6	2.364406	5.444608	5.233307
		1	1.508860	5.150660	4.613079
		6	2.578354	6.956790	5.067936
		1	3.430842	7.303444	5.666303
		1	2.770277	7.226916	4.023266
		1	1.695229	7.513382	5.398207
		6	2.031324	5.084690	6.687913
		1	1.841301	4.013256	6.805754
		1	2.848528	5.366437	7.364809
		1	1.132554	5.616415	7.018277
		6	4.267910	2.553189	5.782619
		1	4.121536	3.132677	6.700378
		1	3.830834	1.571827	5.975218
		6	5.786898	2.412524	5.527965
		1	6.185629	3.422383	5.352330

		6	6.461005	1.855600	6.791792
		1	6.271351	2.488986	7.666157
		1	6.094043	0.847463	7.021899
		1	7.545530	1.788239	6.657163
		6	6.116216	1.556919	4.297288
		1	5.787534	0.520109	4.434643
		1	5.636606	1.942035	3.392800
		1	7.197623	1.541482	4.122458
	Cation	8	0.460860	-1.975064	1.003984
		8	-0.908023	-3.412222	-0.764950
		1	-0.379934	-2.958197	-0.061358
		8	-1.906544	0.867616	-2.944839
		1	-1.386317	1.362867	-2.264218
		7	-3.514706	-3.221426	-4.687596
		6	0.207884	-0.889713	0.452205
		6	-0.559116	-0.507812	-0.742002
		6	-1.295298	-1.177009	-1.719339
		6	-1.449897	-2.631831	-1.705113
		6	-2.175414	-3.275805	-2.679208
		1	-2.239808	-4.349911	-2.596417
		6	-2.810909	-2.559513	-3.740674
		6	-2.679132	-1.136784	-3.765491
		1	-3.145011	-0.529990	-4.526080
		6	-1.956852	-0.461857	-2.810302
		6	-3.611563	-4.697640	-4.690929
		1	-4.473857	-4.952080	-5.312181
		1	-3.846476	-5.041385	-3.679880
		6	-2.362569	-5.435258	-5.230893
		1	-1.507743	-5.156590	-4.601832
		6	-2.590139	-6.948300	-5.088637
		1	-3.438343	-7.280951	-5.699039
		1	-2.788549	-7.235824	-4.050250
		1	-1.706910	-7.500547	-5.423051

		6	-2.025393	-5.054154	-6.679064
		1	-1.811349	-3.985784	-6.786337
		1	-2.844502	-5.313635	-7.361232
		1	-1.137061	-5.598042	-7.014582
		6	-4.259441	-2.549894	-5.771580
		1	-4.101350	-3.148404	-6.672495
		1	-3.823306	-1.570917	-5.969269
		6	-5.780388	-2.418485	-5.513886
		1	-6.172912	-3.426993	-5.323356
		6	-6.448171	-1.886273	-6.792165
		1	-6.255860	-2.535579	-7.653151
		1	-6.086579	-0.880809	-7.038955
		1	-7.532133	-1.822763	-6.658742
		6	-6.114025	-1.540852	-4.300397
		1	-5.785116	-0.506375	-4.453692
		1	-5.652834	-1.911617	-3.379606
		1	-7.196298	-1.519941	-4.138801
		8	-0.460860	1.975064	-1.003984
		8	0.908023	3.412222	0.764950
		1	0.379934	2.958197	0.061358
		8	1.906544	-0.867616	2.944839
		1	1.386317	-1.362867	2.264218
		7	3.514706	3.221426	4.687596
		6	-0.207884	0.889713	-0.452205
		6	0.559116	0.507812	0.742002
		6	1.295298	1.177009	1.719339
		6	1.449897	2.631831	1.705113
		6	2.175414	3.275805	2.679208
		1	2.239808	4.349911	2.596417
		6	2.810909	2.559513	3.740674
		6	2.679132	1.136784	3.765491
		1	3.145011	0.529990	4.526080
		6	1.956852	0.461857	2.810302

		6	3.611563	4.697640	4.690929
		1	4.473857	4.952080	5.312181
		1	3.846476	5.041385	3.679880
		6	2.362569	5.435258	5.230893
		1	1.507743	5.156590	4.601832
		6	2.590139	6.948300	5.088637
		1	3.438343	7.280951	5.699039
		1	2.788549	7.235824	4.050250
		1	1.706910	7.500547	5.423051
		6	2.025393	5.054154	6.679064
		1	1.811349	3.985784	6.786337
		1	2.844502	5.313635	7.361232
		1	1.137061	5.598042	7.014582
		6	4.259441	2.549894	5.771580
		1	4.101350	3.148404	6.672495
		1	3.823306	1.570917	5.969269
		6	5.780388	2.418485	5.513886
		1	6.172912	3.426993	5.323356
		6	6.448171	1.886273	6.792165
		1	6.255860	2.535579	7.653151
		1	6.086579	0.880809	7.038955
		1	7.532133	1.822763	6.658742
		6	6.114025	1.540852	4.300397
		1	5.785116	0.506375	4.453692
		1	5.652834	1.911617	3.379606
		1	7.196298	1.519941	4.138801
	Anion	8	0.290927	-1.961158	1.098102
		8	-1.069987	-3.386048	-0.723197
		1	-0.558899	-2.910160	-0.017751
		8	-1.706628	0.841113	-3.084051
		1	-1.188355	1.307837	-2.377962
		7	-3.503208	-3.236371	-4.822051
		6	0.128807	-0.869300	0.486943



		6	-0.547648	-0.502810	-0.752926
		6	-1.289460	-1.183181	-1.770170
		6	-1.525990	-2.591073	-1.725829
		6	-2.251077	-3.249643	-2.720369
		1	-2.374918	-4.315823	-2.590088
		6	-2.787424	-2.554305	-3.823278
		6	-2.564073	-1.163780	-3.886417
		1	-2.939009	-0.547704	-4.691939
		6	-1.842189	-0.497599	-2.896617
		6	-3.607463	-4.689658	-4.795992
		1	-4.432947	-4.974697	-5.459972
		1	-3.895853	-5.037179	-3.793776
		6	-2.337228	-5.447924	-5.250196
		1	-1.510856	-5.124933	-4.605872
		6	-2.536057	-6.958110	-5.057905
		1	-3.366964	-7.329052	-5.673962
		1	-2.758925	-7.204151	-4.013098
		1	-1.637026	-7.514551	-5.346319
		6	-1.961116	-5.112398	-6.699613
		1	-1.814218	-4.035552	-6.827713
		1	-2.744895	-5.438066	-7.397785
		1	-1.030293	-5.614331	-6.988743
		6	-4.309391	-2.547540	-5.821022
		1	-4.211778	-3.090966	-6.770807
		1	-3.896308	-1.553078	-6.005615
		6	-5.818248	-2.419033	-5.493508
		1	-6.206938	-3.436574	-5.335038
		6	-6.558226	-1.818138	-6.698871
		1	-6.407487	-2.415893	-7.606393
		1	-6.204377	-0.800083	-6.907343
		1	-7.636557	-1.759866	-6.511210
		6	-6.083941	-1.610793	-4.216490
		1	-5.753882	-0.571570	-4.330349

		1	-5.552048	-2.029870	-3.358210
		1	-7.155747	-1.599831	-3.983031
		8	-0.290927	1.961158	-1.098102
		8	1.069987	3.386048	0.723197
		1	0.558899	2.910160	0.017751
		8	1.706628	-0.841113	3.084051
		1	1.188355	-1.307837	2.377962
		7	3.503208	3.236371	4.822051
		6	-0.128807	0.869300	-0.486943
		6	0.547648	0.502810	0.752926
		6	1.289460	1.183181	1.770170
		6	1.525990	2.591073	1.725829
		6	2.251077	3.249643	2.720369
		1	2.374918	4.315823	2.590088
		6	2.787424	2.554305	3.823278
		6	2.564073	1.163780	3.886417
		1	2.939009	0.547704	4.691939
		6	1.842189	0.497599	2.896617
		6	3.607463	4.689658	4.795992
		1	4.432947	4.974697	5.459972
		1	3.895853	5.037179	3.793776
		6	2.337228	5.447924	5.250196
		1	1.510856	5.124933	4.605872
		6	2.536057	6.958110	5.057905
		1	3.366964	7.329052	5.673962
		1	2.758925	7.204151	4.013098
		1	1.637026	7.514551	5.346319
		6	1.961116	5.112398	6.699613
		1	1.814218	4.035552	6.827713
		1	2.744895	5.438066	7.397785
		1	1.030293	5.614331	6.988743
		6	4.309391	2.547540	5.821022
		1	4.211778	3.090966	6.770807

		1	3.896308	1.553078	6.005615
		6	5.818248	2.419033	5.493508
		1	6.206938	3.436574	5.335038
		6	6.558226	1.818138	6.698871
		1	6.407487	2.415893	7.606393
		1	6.204377	0.800083	6.907343
		1	7.636557	1.759866	6.511210
		6	6.083941	1.610793	4.216490
		1	5.753882	0.571570	4.330349
		1	5.552048	2.029870	3.358210
		1	7.155747	1.599831	3.983031
Motif-3	Neutral	8	0.063339	2.264869	0.010131
		8	2.710142	2.372425	0.264235
		8	2.575992	-2.521599	0.230470
		7	6.676041	-0.175097	0.664761
		6	0.028237	1.011466	0.004484
		6	1.047611	-0.029681	0.100580
		1	1.723079	2.414194	0.172013
		6	2.444505	-0.069006	0.236343
		1	1.588462	-2.507532	0.138162
		6	3.240244	1.137984	0.312172
		6	4.616566	1.085684	0.443154
		1	5.126602	2.036148	0.493183
		6	5.310818	-0.150071	0.519563
		6	4.549066	-1.344745	0.438282
		1	5.006594	-2.322547	0.446708
		6	3.172878	-1.318857	0.303662
		6	7.460698	1.066429	0.664857
		1	8.426134	0.833050	1.124878
		1	6.982770	1.803519	1.321953
		6	7.703482	1.679356	-0.724880
		1	8.237806	0.952403	-1.347640
		1	6.742842	1.863088	-1.217777

		6	8.503765	2.983767	-0.638388
		1	8.678309	3.403449	-1.633932
		1	9.482097	2.824176	-0.169223
		1	7.972048	3.740058	-0.049242
		6	7.427176	-1.402995	0.957241
		1	6.734061	-2.175009	1.292145
		1	8.079175	-1.188308	1.814250
		6	8.288426	-1.931406	-0.203141
		1	9.019348	-1.163943	-0.488221
		1	8.873482	-2.774119	0.188830
		6	7.496507	-2.378238	-1.436172
		1	8.172059	-2.714653	-2.229466
		1	6.887382	-1.562658	-1.838615
		1	6.823299	-3.209549	-1.199726
		8	-0.063359	-2.264871	-0.010109
		8	-2.710121	-2.372421	-0.264174
		8	-2.575970	2.521582	-0.230496
		7	-6.676038	0.175086	-0.664774
		6	-0.028248	-1.011467	-0.004466
		6	-1.047621	0.029678	-0.100569
		1	-1.723061	-2.414167	-0.171899
		6	-2.444510	0.069000	-0.236326
		1	-1.588440	2.507495	-0.138173
		6	-3.240241	-1.137993	-0.312146
		6	-4.616564	-1.085693	-0.443140
		1	-5.126602	-2.036155	-0.493161
		6	-5.310816	0.150062	-0.519570
		6	-4.549064	1.344736	-0.438302
		1	-5.006594	2.322537	-0.446747
		6	-3.172875	1.318851	-0.303670
		6	-7.460698	-1.066439	-0.664846
		1	-8.426133	-0.833067	-1.124871
		1	-6.982773	-1.803545	-1.321927

		6	-7.703484	-1.679338	0.724904
		1	-8.237804	-0.952369	1.347649
		1	-6.742844	-1.863063	1.217805
		6	-8.503772	-2.983747	0.638439
		1	-8.678319	-3.403406	1.633992
		1	-9.482103	-2.824162	0.169269
		1	-7.972057	-3.740053	0.049310
		6	-7.427172	1.402978	-0.957287
		1	-6.734055	2.174985	-1.292204
		1	-8.079165	1.188272	-1.814296
		6	-8.288429	1.931414	0.203078
		1	-9.019351	1.163958	0.488172
		1	-8.873483	2.774118	-0.188916
		6	-7.496516	2.378277	1.436102
		1	-8.172072	2.714709	2.229385
		1	-6.887391	1.562708	1.838568
		1	-6.823308	3.209584	1.199639
	Cation	8	-0.063654	-2.261975	0.018656
		8	-2.707246	-2.376268	0.277123
		8	-2.572502	2.527506	0.231637
		7	-6.646404	0.176424	0.697077
		6	-0.028637	-1.019226	0.007783
		6	-1.053385	0.030357	0.104167
		1	-1.723134	-2.428652	0.183968
		6	-2.440256	0.070119	0.242388
		1	-1.587875	2.523860	0.134007
		6	-3.241052	-1.152305	0.325025
		6	-4.607679	-1.094558	0.462047
		1	-5.123342	-2.040859	0.522957
		6	-5.302703	0.151775	0.543199
		6	-4.538203	1.356492	0.460772
		1	-5.000325	2.331453	0.475190
		6	-3.171626	1.335332	0.313225

		6	-7.450767	-1.065862	0.673751
		1	-8.417593	-0.817583	1.117344
		1	-6.987443	-1.802816	1.337471
		6	-7.669365	-1.660573	-0.728352
		1	-8.164150	-0.916385	-1.361653
		1	-6.702585	-1.874773	-1.196322
		6	-8.514007	-2.938247	-0.662756
		1	-8.670320	-3.347105	-1.664878
		1	-9.500163	-2.746270	-0.225616
		1	-8.025431	-3.712768	-0.061078
		6	-7.413596	1.413570	0.958598
		1	-6.729728	2.197866	1.278231
		1	-8.058420	1.195872	1.817087
		6	-8.275817	1.896432	-0.220477
		1	-8.999400	1.117480	-0.487717
		1	-8.868248	2.738073	0.158529
		6	-7.486702	2.332953	-1.458502
		1	-8.168784	2.661934	-2.247940
		1	-6.880545	1.517137	-1.866172
		1	-6.817433	3.170510	-1.233689
		8	0.063643	2.261988	-0.018693
		8	2.707259	2.376289	-0.276881
		8	2.572498	-2.527494	-0.231948
		7	6.646410	-0.176371	-0.697070
		6	0.028632	1.019240	-0.007807
		6	1.053382	-0.030344	-0.104191
		1	1.723154	2.428671	-0.183648
		6	2.440255	-0.070101	-0.242412
		1	1.587864	-2.523864	-0.134393
		6	3.241055	1.152328	-0.324937
		6	4.607683	1.094591	-0.461952
		1	5.123349	2.040897	-0.522766
		6	5.302707	-0.151735	-0.543205

		6	4.538204	-1.356458	-0.460892
		1	5.000323	-2.331418	-0.475405
		6	3.171625	-1.335310	-0.313360
		6	7.450775	1.065911	-0.673622
		1	8.417603	0.817671	-1.117233
		1	6.987457	1.802929	-1.337275
		6	7.669368	1.660487	0.728539
		1	8.164151	0.916238	1.361771
		1	6.702587	1.874643	1.196526
		6	8.514012	2.938166	0.663069
		1	8.670320	3.346929	1.665231
		1	9.500170	2.746230	0.225917
		1	8.025440	3.712745	0.061462
		6	7.413601	-1.413495	-0.958699
		1	6.729736	-2.197760	-1.278411
		1	8.058435	-1.195718	-1.817161
		6	8.275810	-1.896467	0.220341
		1	8.999390	-1.117539	0.487662
		1	8.868246	-2.738072	-0.158737
		6	7.486681	-2.333103	1.458316
		1	8.168755	-2.662159	2.247731
		1	6.880521	-1.517324	1.866057
		1	6.817413	-3.170638	1.233418
	Anion	8	-0.025017	-2.248808	0.279370
		8	-2.696379	-2.375106	0.461405
		8	-2.642457	2.475984	-0.125797
		7	-6.766757	0.142561	0.431523
		6	-0.010982	-0.997212	0.123849
		6	-1.055670	0.020453	0.069605
		1	-1.705498	-2.389214	0.404417
		6	-2.483559	0.047409	0.165393
		1	-1.652730	2.451592	-0.193561
		6	-3.253258	-1.141072	0.354156

		6	-4.646815	-1.109144	0.451466
		1	-5.137142	-2.060207	0.609718
		6	-5.356186	0.101390	0.360446
		6	-4.618910	1.284396	0.157083
		1	-5.102603	2.243921	0.025624
		6	-3.228209	1.266461	0.070252
		6	-7.515156	-1.110370	0.471582
		1	-8.528334	-0.875051	0.815977
		1	-7.095320	-1.802717	1.221396
		6	-7.620977	-1.817280	-0.888550
		1	-8.134108	-1.146311	-1.589111
		1	-6.616647	-1.979551	-1.292923
		6	-8.367019	-3.152835	-0.793022
		1	-8.448870	-3.632524	-1.774459
		1	-9.384481	-3.018301	-0.403153
		1	-7.847214	-3.851481	-0.126495
		6	-7.423963	1.270237	1.096157
		1	-6.665402	2.005352	1.371584
		1	-7.873576	0.924314	2.043871
		6	-8.513455	1.947567	0.247227
		1	-9.272956	1.202786	-0.028247
		1	-9.025944	2.684134	0.882767
		6	-7.979958	2.628620	-1.017337
		1	-8.796548	3.048527	-1.615994
		1	-7.430429	1.915586	-1.639636
		1	-7.294113	3.446711	-0.768207
		8	0.025037	2.248790	-0.279677
		8	2.696355	2.375120	-0.461319
		8	2.642422	-2.475957	0.125688
		7	6.766783	-0.142529	-0.431329
		6	0.010991	0.997194	-0.124158
		6	1.055684	-0.020452	-0.069766
		1	1.705468	2.389148	-0.404410



		6	2.483576	-0.047394	-0.165446
		1	1.652694	-2.451503	0.193410
		6	3.253267	1.141098	-0.354114
		6	4.646833	1.109184	-0.451351
		1	5.137167	2.060253	-0.609548
		6	5.356198	-0.101350	-0.360330
		6	4.618922	-1.284370	-0.157041
		1	5.102626	-2.243889	-0.025574
		6	3.228215	-1.266444	-0.070294
		6	7.515162	1.110422	-0.471179
		1	8.528392	0.875152	-0.815453
		1	7.095420	1.802834	-1.220990
		6	7.620786	1.817202	0.889034
		1	8.133839	1.146174	1.589596
		1	6.616401	1.979414	1.293293
		6	8.366812	3.152782	0.793735
		1	8.448524	3.632375	1.775229
		1	9.384328	3.018309	0.403985
		1	7.847079	3.851484	0.127209
		6	7.423950	-1.270017	-1.096337
		1	6.665376	-2.005083	-1.371858
		1	7.873442	-0.923840	-2.044019
		6	8.513554	-1.947536	-0.247705
		1	9.273069	-1.202813	0.027888
		1	9.025994	-2.683921	-0.883495
		6	7.980210	-2.628942	1.016734
		1	8.796873	-3.048997	1.615187
		1	7.430739	-1.916083	1.639283
		1	7.294352	-3.446978	0.767459
Motif-4	Neutral	8	-0.088328	2.264044	-0.000225
		8	2.526774	2.548075	-0.412058
		1	1.547524	2.523587	-0.255907
		8	2.714373	-2.344437	-0.424074

		1	1.735864	-2.396224	-0.268031
		7	6.615820	0.244299	-1.099349
		6	-0.039415	1.011065	-0.000309
		6	1.038556	0.040423	-0.168491
		6	2.423197	0.094133	-0.394679
		6	3.131338	1.351420	-0.516998
		6	4.495345	1.391542	-0.741559
		1	4.940542	2.374086	-0.785812
		6	5.263813	0.204752	-0.865089
		6	4.590169	-1.038119	-0.735904
		1	5.106891	-1.983117	-0.813652
		6	3.226135	-1.104539	-0.514601
		6	7.331347	1.479548	-1.446188
		1	6.608871	2.238050	-1.748611
		1	7.935045	1.264255	-2.337581
		6	8.252089	2.033046	-0.344969
		1	9.005095	1.276111	-0.086254
		1	8.809077	2.873959	-0.781990
		6	7.536188	2.500632	0.928503
		1	6.940486	1.676073	1.338455
		1	6.822872	3.295513	0.673808
		6	8.507342	3.014184	1.997827
		1	7.971650	3.347424	2.892744
		1	9.096134	3.861761	1.627287
		1	9.211315	2.231113	2.304183
		6	7.414061	-0.988156	-1.140709
		1	8.344910	-0.746457	-1.663096
		1	6.903619	-1.735003	-1.761092
		6	7.751330	-1.586710	0.235282
		1	8.321653	-0.851246	0.816510
		1	6.826295	-1.772147	0.793506
		6	8.553880	-2.889542	0.119165
		1	9.474429	-2.702827	-0.451806

		1	7.976764	-3.621183	-0.462929
		6	8.913289	-3.494059	1.481377
		1	9.482438	-4.422501	1.366392
		1	8.012341	-3.724767	2.061260
		1	9.521678	-2.801272	2.074506
		8	0.088335	-2.264050	0.000092
		8	-2.526756	-2.548059	0.412124
		1	-1.547509	-2.523574	0.255946
		8	-2.714350	2.344440	0.423477
		1	-1.735877	2.396172	0.267194
		7	-6.615756	-0.244198	1.099451
		6	0.039419	-1.011070	0.000100
		6	-1.038551	-0.040427	0.168260
		6	-2.423185	-0.094125	0.394477
		6	-3.131321	-1.351396	0.516962
		6	-4.495313	-1.391489	0.741622
		1	-4.940512	-2.374026	0.786011
		6	-5.263766	-0.204682	0.865090
		6	-4.590127	1.038174	0.735716
		1	-5.106844	1.983183	0.813371
		6	-3.226110	1.104562	0.514302
		6	-7.331264	-1.479408	1.446470
		1	-6.608770	-2.237881	1.748921
		1	-7.934898	-1.264019	2.337883
		6	-8.252086	-2.033017	0.345374
		1	-9.005106	-1.276105	0.086632
		1	-8.809047	-2.873881	0.782523
		6	-7.536276	-2.500741	-0.928099
		1	-6.940599	-1.676228	-1.338179
		1	-6.822946	-3.295597	-0.673371
		6	-8.507508	-3.014401	-1.997300
		1	-7.971880	-3.347738	-2.892220
		1	-9.096278	-3.861936	-1.626630

		1	-9.211498	-2.231358	-2.303689
		6	-7.413988	0.988265	1.140742
		1	-8.344802	0.746624	1.663219
		1	-6.903500	1.735173	1.761012
		6	-7.751352	1.586681	-0.235286
		1	-8.321719	0.851159	-0.816400
		1	-6.826355	1.772056	-0.793595
		6	-8.553888	2.889528	-0.119246
		1	-9.474398	2.702875	0.451808
		1	-7.976728	3.621225	0.462734
		6	-8.913389	3.493908	-1.481494
		1	-9.482524	4.422366	-1.366564
		1	-8.012480	3.724552	-2.061463
		1	-9.521824	2.801065	-2.074510
	Cation	8	-0.086956	2.261292	0.015239
		8	2.524431	2.553999	-0.405016
		1	1.548301	2.539831	-0.243841
		8	2.709327	-2.348376	-0.444304
		1	1.733932	-2.410569	-0.287283
		7	6.583506	0.245204	-1.133268
		6	-0.039195	1.018834	0.006117
		6	1.043975	0.041202	-0.172568
		6	2.418530	0.095231	-0.400962
		6	3.129788	1.367819	-0.523373
		6	4.483292	1.403094	-0.760973
		1	4.933689	2.382568	-0.807381
		6	5.253606	0.206293	-0.890581
		6	4.579261	-1.047147	-0.759405
		1	5.100395	-1.987938	-0.851429
		6	3.225444	-1.118800	-0.531865
		6	7.316663	1.489752	-1.452424
		1	6.603362	2.262805	-1.732853
		1	7.906144	1.272371	-2.349893

		6	8.249062	1.993358	-0.337696
		1	8.993665	1.222249	-0.103178
		1	8.813009	2.832795	-0.764867
		6	7.545939	2.449631	0.947335
		1	6.954107	1.623552	1.362172
		1	6.833664	3.250391	0.707701
		6	8.533605	2.951418	2.007380
		1	8.009398	3.276595	2.911101
		1	9.116389	3.801784	1.636366
		1	9.240116	2.165243	2.297189
		6	7.402579	-0.987617	-1.155716
		1	8.335156	-0.730023	-1.662498
		1	6.905598	-1.733201	-1.784391
		6	7.717753	-1.570303	0.232494
		1	8.246585	-0.817622	0.828811
		1	6.785963	-1.791022	0.766044
		6	8.569921	-2.843914	0.130758
		1	9.498895	-2.619637	-0.410575
		1	8.036815	-3.592324	-0.471121
		6	8.908819	-3.438547	1.502383
		1	9.514417	-4.343761	1.397907
		1	8.001153	-3.707028	2.054459
		1	9.475414	-2.728152	2.114785
		8	0.086988	-2.261216	-0.015135
		8	-2.524375	-2.553916	0.405379
		1	-1.548245	-2.539759	0.244207
		8	-2.709381	2.348460	0.443619
		1	-1.734043	2.410632	0.286235
		7	-6.583474	-0.245060	1.133325
		6	0.039210	-1.018757	-0.006141
		6	-1.043966	-0.041125	0.172496
		6	-2.418522	-0.095146	0.400877
		6	-3.129758	-1.367726	0.523502

		6	-4.483255	-1.402981	0.761148
		1	-4.933635	-2.382454	0.807735
		6	-5.253582	-0.206170	0.890590
		6	-4.579262	1.047259	0.759174
		1	-5.100414	1.988056	0.851017
		6	-3.225454	1.118893	0.531576
		6	-7.316601	-1.489565	1.452722
		1	-6.603279	-2.262559	1.733259
		1	-7.906054	-1.272037	2.350175
		6	-8.249030	-1.993376	0.338113
		1	-8.993652	-1.222317	0.103486
		1	-8.812953	-2.832746	0.765449
		6	-7.545945	-2.449862	-0.946862
		1	-6.954137	-1.623847	-1.361862
		1	-6.833650	-3.250571	-0.707112
		6	-8.533638	-2.951846	-2.006787
		1	-8.009457	-3.277174	-2.910469
		1	-9.116399	-3.802156	-1.635606
		1	-9.240169	-2.165731	-2.296710
		6	-7.402564	0.987752	1.155589
		1	-8.335121	0.730231	1.662445
		1	-6.905575	1.733451	1.784120
		6	-7.717793	1.570196	-0.232711
		1	-8.246633	0.817405	-0.828881
		1	-6.786023	1.790836	-0.766329
		6	-8.569975	2.843812	-0.131165
		1	-9.498929	2.619615	0.410236
		1	-8.036859	3.592333	0.470569
		6	-8.908925	3.438206	-1.502881
		1	-9.514532	4.343429	-1.398541
		1	-8.001281	3.706605	-2.055032
		1	-9.475531	2.727698	-2.115143
	Anion	8	-0.023415	2.241019	0.336680

		8	2.629131	2.493041	0.033007
		1	1.645244	2.459046	0.157632
		8	2.680423	-2.341510	-0.675846
		1	1.694611	-2.364774	-0.561787
		7	6.728810	0.204521	-0.819181
		6	-0.010225	0.993739	0.149422
		6	1.049651	0.030624	-0.130338
		6	2.469254	0.071260	-0.308419
		6	3.210302	1.293248	-0.226526
		6	4.593428	1.324783	-0.394078
		1	5.076141	2.285436	-0.268190
		6	5.325777	0.152950	-0.668708
		6	4.619648	-1.060592	-0.748697
		1	5.105817	-2.003743	-0.958576
		6	3.234514	-1.105983	-0.571078
		6	7.348569	1.363819	-1.464606
		1	6.573655	2.101309	-1.681750
		1	7.761916	1.058628	-2.441906
		6	8.467134	2.018096	-0.635949
		1	9.239483	1.267926	-0.410860
		1	8.955678	2.777895	-1.264729
		6	7.988676	2.660792	0.671367
		1	7.439235	1.913439	1.255367
		1	7.268702	3.457555	0.440538
		6	9.134059	3.238848	1.510718
		1	8.760971	3.696909	2.433650
		1	9.686986	4.008439	0.957159
		1	9.850790	2.457747	1.793778
		6	7.480136	-1.041220	-0.944191
		1	8.468369	-0.787520	-1.343194
		1	7.017366	-1.711712	-1.688000
		6	7.672573	-1.788636	0.384589
		1	8.233075	-1.139993	1.071427

		1	6.695739	-1.962191	0.849760
		6	8.406997	-3.124009	0.211845
		1	9.377297	-2.950013	-0.276771
		1	7.833749	-3.767578	-0.469717
		6	8.631142	-3.863277	1.536522
		1	9.152899	-4.814936	1.382517
		1	7.677301	-4.081189	2.030635
		1	9.231747	-3.260941	2.229039
		8	0.023512	-2.240966	-0.336473
		8	-2.629182	-2.493065	-0.032786
		1	-1.645264	-2.459260	-0.157239
		8	-2.680583	2.341603	0.676056
		1	-1.694754	2.365064	0.562136
		7	-6.728851	-0.204520	0.819050
		6	0.010298	-0.993708	-0.149074
		6	-1.049605	-0.030580	0.130595
		6	-2.469234	-0.071215	0.308584
		6	-3.210291	-1.293219	0.226655
		6	-4.593429	-1.324753	0.394100
		1	-5.076133	-2.285408	0.268194
		6	-5.325806	-0.152932	0.668676
		6	-4.619695	1.060607	0.748718
		1	-5.105895	2.003748	0.958576
		6	-3.234549	1.106026	0.571207
		6	-7.348619	-1.363785	1.464526
		1	-6.573704	-2.101257	1.681725
		1	-7.761990	-1.058548	2.441803
		6	-8.467157	-2.018115	0.635876
		1	-9.239507	-1.267965	0.410724
		1	-8.955712	-2.777884	1.264684
		6	-7.988656	-2.660877	-0.671392
		1	-7.439204	-1.913549	-1.255413
		1	-7.268684	-3.457623	-0.440499



		6	-9.134011	-3.238983	-1.510747
		1	-8.760892	-3.697085	-2.433647
		1	-9.686946	-4.008554	-0.957167
		1	-9.850742	-2.457903	-1.793864
		6	-7.480197	1.041218	0.943976
		1	-8.468466	0.787515	1.342888
		1	-7.017502	1.711723	1.687820
		6	-7.672518	1.788616	-0.384831
		1	-8.232942	1.139957	-1.071716
		1	-6.695643	1.962184	-0.849911
		6	-8.406982	3.123978	-0.212170
		1	-9.377325	2.949970	0.276356
		1	-7.833810	3.767564	0.469440
		6	-8.631014	3.863228	-1.536876
		1	-9.152807	4.814877	-1.382932
		1	-7.677129	4.081157	-2.030897
		1	-9.231536	3.260872	-2.229447

Fig. S1: Finger print plots of all motifs broken down into contribution from specific pairs of atom types.

