

Supplementary Information

Inter and Intra-Stacking Influenced Charge Hopping Interactions in Core-Substituted Squarylium Dye Derivatives: A Computational Investigation

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Table S1: Selected geometrical parameters of all CSQs obtained from crystal structures.

CSQ-1		CSQ-2	
CSQ-3		CSQ-4	
CSQ-5		CSQ-6	
CSQ-7		CSQ-8	
CSQ-9		CSQ-10	

geometrical indices	CSQ-1	CSQ-2	CSQ-3	CSQ-4	CSQ-5	CSQ-6
C1-C2	1.494	1.492	1.489	1.494	1.461	1.467
C2-C3	1.439	1.443	1.439	1.444	1.449	1.444
C3-C4	1.433	1.446	1.444	1.450	1.450	1.449
O-C1	1.211	1.218	1.212	1.217	1.248	1.246
C1-C4	1.488	1.487	1.482	1.4921	1.464	1.470
C3-C5	1.390	1.391	1.385	1.396	1.378	1.381
C5-C6	1.419	1.425	1.424	1.427	1.417	1.422
C5-C7	1.420	1.428	1.426	1.429	1.420	1.427
C6-N	1.143	1.151	1.149	1.150	1.142	1.149
C7-N	1.144	1.154	1.145	1.146	1.145	1.153
C4-C8	1.399	1.395	1.395	1.394	1.384	1.389
C2-C8'	1.386	1.399	1.391	1.399	1.389	1.388
C8-C9	1.379/1.389	1.391/1.383	1.382/1.372	1.387/1.388	1.390/1.388	1.389/1.387
C9-C10	1.525	1.523/1.527	1.527/1.517	1.53/1.536	1.523/1.530	1.523
C10-C11	1.534/1.530	1.540/1.538	1.536/1.551	1.545/1.540	1.539/1.533	1.538/1.535
C10-C12	1.539/1.535	1.537/1.544	1.537/1.493	1.534/1.542	1.534/1.532	1.539/1.545
C10-C13	1.516/1.512	1.516/1.514	1.506/1.543	1.511/1.512	1.509/1.515	1.519/1.511
C13-C14	1.378/1.379	1.381/1.377	1.386/1.373	1.380/1.378	1.379/1.382	1.386/1.383
C14-C15	1.392/1.389	1.393/1.396	1.376/1.368	1.399/1.399	1.388/1.386	1.393/1.397
C15-X		1.745/1.742	1.895/1.898	2.097/2.099	1.363/1.361	
C15-C16	1.377/1.379	1.380/1.385	1.381/1.394	1.388/1.395	1.366/1.374	1.386/1.394
C16-C17	1.383/1.392	1.391/1.385	1.383/1.94	1.397/1.386	1.392/1.388	1.396/1.389
C17-C18	1.383/1.381	1.386/1.387	1.385/1.389	1.381/1.391	1.378/1.383	1.383/1.386
C18-C13	1.379/1.384	1.386/1.389	1.379/1.375	1.389/1.387	1.389/1.389	1.389/1.394
C18-N	1.408/1.409	1.416/1.406	1.405/1.383	1.411/1.407	1.406/1.400	1.408
N-C9	1.360/1.351	1.361/1.364	1.361/1.367	1.365/1.365	1.342/1.341	1.341/1.344
HB(NH-O)					1.899/1.824	1.957/1.988

geometric indices	CSQ-7	geometrical indices	CSQ-8	geometrical indices	CSQ-9	geometric indices	CSQ-10
C1-C2	1.501	C1-C2	1.490	C1-C2	1.496	C1-C2	1.484
C2-C3	1.453	C2-C3	1.441	C2-C3	1.433	C2-C3	1.438
C3-C4	1.439	C3-C4	1.437	C3-C4	1.439	C3-C4	1.399
O-C1	1.217	O-C1	1.220	O-C1	1.220	O-C1	1.223
C1-C4	1.493	C1-C4	1.457	C1-C4	1.495	C4-C5	1.408
C3-C5	1.393	C3-C5	1.394	C3-C5	1.402	C5-N	1.141
C5-C6	1.432	C5-C6	1.404	C5-C6	1.417	C2-C6	1.390
C5-C7	1.424	C5-C7	1.412	C5-C7	1.417	C6-C7	1.402

C6-N	1.148	C6-N	1.140	C6-N	1.152	C7-C8	1.405
C7-N	1.148	C7-N	1.146	C7-N	1.152	C8-C9	1.350
C4-C8	1.404	C4-C8	1.389	C4-C8	1.384	C9-N	1.353
C2-C8'	1.383	C2-C8'	1.381	C2-C8'	1.391	N-C10	1.385
C8-C9	1.383/1.405	C8-C9	1.379/1.382	C8-C9	1.409/1.405	C10-C11	1.409
C9-C10	1.527/1.519	C9-S	1.733/1.741	C9-C10	1.429/1.433	C11-C12	1.364
C10-C11	1.523/1.515	S-C10	1.739/1.734	C10-C11	1.349/1.343	C12-C13	1.375
C11-C12	1.385/1.382	C10-C11	1.389/1.377	C11-C12	1.425/1.426	C13-C14	1.365
C12-C13	1.396/1.394	C11-C12	1.382/1.383	C12-C13	1.405/1.400	C14-C15	1.405
C13-C14	1.390/1.381	C12-C13	1.366/1.374	C13-C14	1.373/1.370	C15-C7	1.457
C14-C15	1.392/1.388	C13-C14	1.368/1.374	C14-C15	1.394/1.383		
C15-C16	1.390	C14-C15	1.378/1.394	C15-C16	1.373/1.377		
C16-C11	1.395/1.373	C15-C10	1.373/1.391	C16-C17	1.403/1.398		
C16-N	1.406/1.405	N-C9	1.351/1.358	C17-C12	1.412/1.408		
N-C9	1.367/1.348	S-O(HB)	2.910/2.858	C17-N	1.401/1.403		
				C9-N	1.375/1.379		

Table S2: Selected geometrical parameters of neutral, cationic and anionic species of all CSQs obtained at the B3LYP/6-31G+(d,p) level of theory and only for CSQ-4 additional LANL2DZ for I atom.

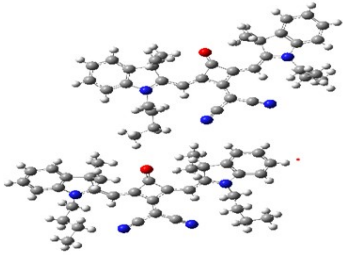
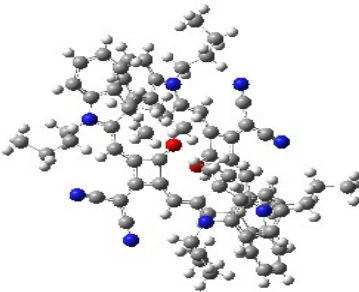
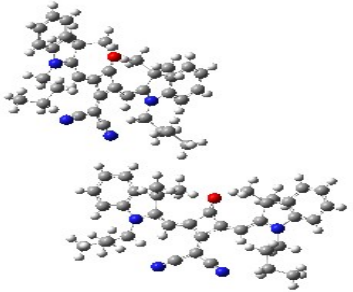
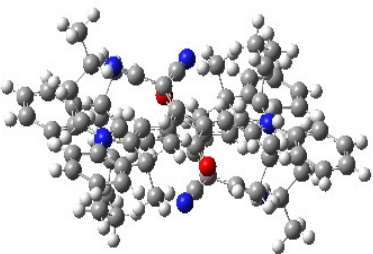
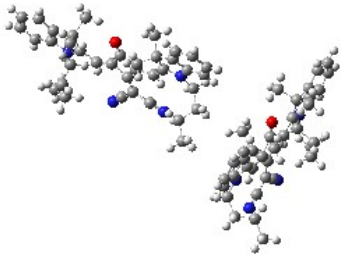
CSQ-1				CSQ-2			
Geometrical indices	Neutral	Cation	Anion	Geometrical indices	Neutral	Cation	Anion
C1-C2	1.484	1.502	1.485	C1-C2	1.484	1.501	1.485
C2-C3	1.453	1.461	1.451	C2-C3	1.454	1.461	1.451
C3-C4	1.453	1.461	1.451	C3-C4	1.454	1.461	1.451
O-C1	1.231	1.217	1.236	O-C1	1.231	1.218	1.230
C1-C4	1.484	1.502	1.485	C1-C4	1.484	1.501	1.485
C3-C5	1.395	1.388	1.408	C3-C5	1.395	1.388	1.407
C5-C6	1.422	1.423	1.420	C5-C6	1.423	1.423	1.420
C5-C7	1.422	1.423	1.420	C5-C7	1.423	1.423	1.420
C6-N	1.168	1.166	1.171	C6-N	1.168	1.166	1.170
C7-N	1.168	1.166	1.171	C7-N	1.168	1.166	1.170
C4-C8	1.400	1.383	1.416	C4-C8	1.400	1.383	1.415
C2-C8'	1.400	1.383	1.416	C2-C8'	1.400	1.383	1.415
C8-C9	1.393	1.416	1.377	C8-C9	1.392	1.414	1.377
C9-C10	1.535	1.529	1.537	C9-C10	1.535	1.530	1.537
C10-C11	1.549	1.551	1.548	C10-C11	1.549	1.551	1.548
C10-C12	1.549	1.551	1.548	C10-C12	1.549	1.551	1.548
C10-C13	1.519	1.516	1.524	C10-C13	1.519	1.516	1.524
C13-C14	1.388	1.389	1.385	C13-C14	1.387	1.386	1.384
C14-C15	1.403	1.401	1.407	C14-C15	1.400	1.401	1.403
C15-C16	1.398	1.401	1.397	C15-C1	1.757	1.743	1.771
C16-C17	1.400	1.397	1.401	C15-C16	1.396	1.401	1.392
C17-C18	1.394	1.395	1.401	C16-C17	1.399	1.395	1.401
C18-C13	1.398	1.397	1.408	C17-C18	1.394	1.395	1.400
C18-N	1.409	1.416	1.385	C18-C13	1.398	1.397	1.408
N-C9	1.369	1.349	1.411	C18-N	1.407	1.413	1.383
				N-C9	1.369	1.350	1.412
CSQ-3				CSQ-4			
Geometrical indices	Neutral	Cation	Anion	Geometrical indices	Neutral	Cation	Anion
C1-C2	1.483	1.501	1.485	C1-C2	1.484	1.501	1.485
C2-C3	1.453	1.46	1.451	C2-C3	1.453	1.461	1.451
C3-C4	1.454	1.46	1.45	C3-C4	1.453	1.461	1.451
O-C1	1.231	1.218	1.235	O-C1	1.231	1.218	1.230
C1-C4	1.484	1.500	1.485	C1-C4	1.484	1.501	1.485
C3-C5	1.395	1.387	1.400	C3-C5	1.395	1.388	1.407
C5-C6	1.422	1.424	1.421	C5-C6	1.423	1.424	1.420

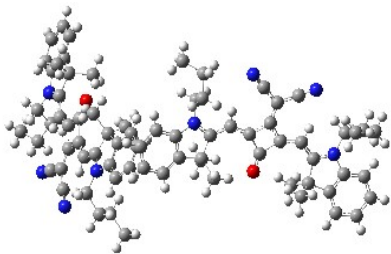
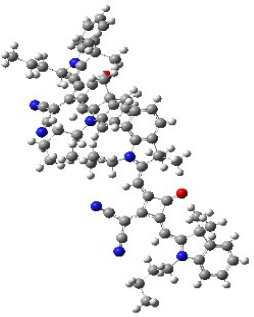
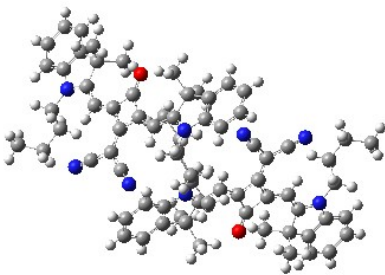
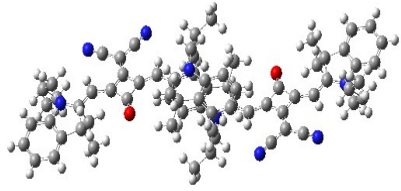
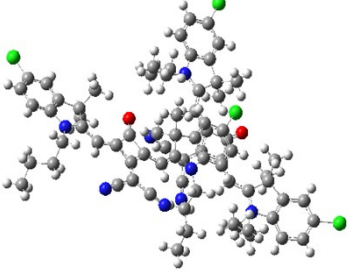
C5-C7	1.423	1.424	1.421	C5-C7	1.423	1.424	1.420
C6-N	1.168	1.166	1.170	C6-N	1.168	1.166	1.170
C7-N	1.168	1.166	1.170	C7-N	1.168	1.166	1.170
C4-C8	1.400	1.383	1.414	C4-C8	1.401	1.384	1.415
C2-C8'	1.400	1.383	1.415	C2-C8'	1.401	1.384	1.415
C8-C9	1.392	1.413	1.377	C8-C9	1.392	1.414	1.377
C9-C10	1.535	1.530	1.537	C9-C10	1.536	1.530	1.538
C10-C11	1.549	1.545	1.548	C10-C11	1.549	1.551	1.548
C10-C12	1.549	1.545	1.548	C10-C12	1.549	1.551	1.548
C10-C13	1.519	1.514	1.523	C10-C13	1.519	1.517	1.524
C13-C14	1.386	1.385	1.384	C13-C14	1.388	1.387	1.385
C14-C15	1.400	1.400	1.402	C14-C15	1.401	1.402	1.404
C15-Br	1.901	1.893	1.919	C15-I	2.134	2.120	2.147
C15-C16	1.395	1.400	1.392	C15-C16	1.396	1.402	1.393
C16-C17	1.399	1.396	1.401	C16-C17	1.401	1.396	1.402
C17-C18	1.394	1.393	1.400	C17-C18	1.394	1.395	1.400
C18-C13	1.398	1.397	1.408	C18-C13	1.398	1.397	1.408
C18-N	1.406	1.413	1.382	C18-N	1.406	1.412	1.382
N-C9	1.370	1.349	1.412	N-C9	1.370	1.351	1.412
CSQ-5				CSQ-6			
Geometrical indices	Neutral	Cation	Anion	Geometrical indices	Neutral	Cation	Anion
C1-C2	1.464	1.476	1.470	C1-C2	1.464	1.477	1.470
C2-C3	1.457	1.465	1.453	C2-C3	1.457	1.465	1.453
C3-C4	1.457	1.465	1.453	C3-C4	1.457	1.465	1.453
O-C1	1.257	1.245	1.256	O-C1	1.256	1.244	1.256
C1-C4	1.464	1.476	1.470	C1-C4	1.464	1.477	1.470
C3-C5	1.384	1.377	1.399	C3-C5	1.385	1.377	1.400
C5-C6	1.424	1.425	1.421	C5-C6	1.423	1.425	1.421
C5-C7	1.424	1.425	1.421	C5-C7	1.423	1.425	1.421
C6-N	1.167	1.165	1.170	C6-N	1.167	1.165	1.170
C7-N	1.167	1.165	1.170	C7-N	1.167	1.165	1.170
C4-C8	1.396	1.379	1.413	C4-C8	1.395	1.378	1.413
C2-C8'	1.396	1.379	1.413	C2-C8'	1.395	1.378	1.413
C8-C9	1.391	1.414	1.374	C8-C9	1.392	1.415	1.374
C9-C10	1.535	1.527	1.538	C9-C10	1.534	1.527	1.537
C10-C11	1.547	1.551	1.547	C10-C11	1.547	1.551	1.547
C10-C12	1.547	1.551	1.547	C10-C12	1.547	1.551	1.547
C10-C13	1.522	1.519	1.526	C10-C13	1.523	1.519	1.527
C13-C14	1.388	1.387	1.387	C13-C14	1.388	1.389	1.386
C14-C15	1.396	1.397	1.396	C14-C15	1.404	1.402	1.407

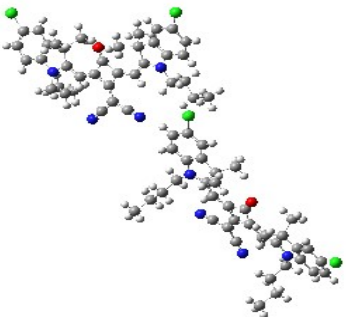
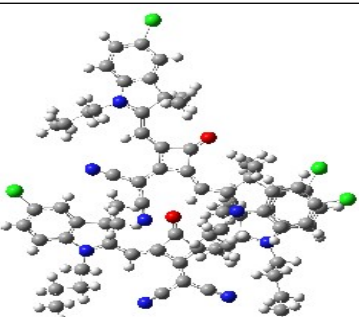
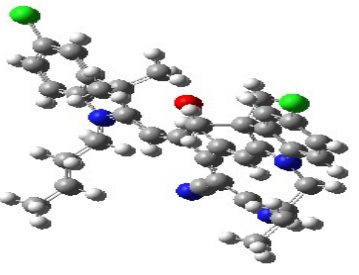
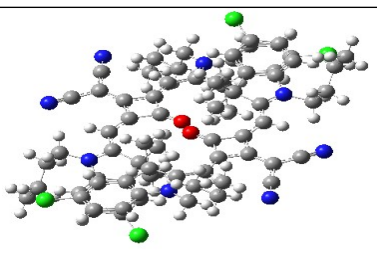
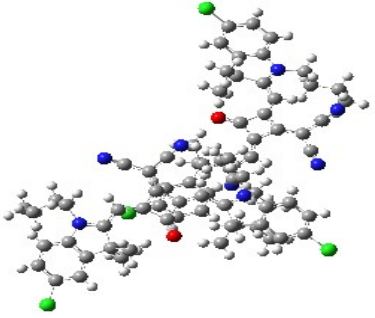
C15-F	1.360	1.346	1.374	C15-C16	1.399	1.402	1.399
C15-C16	1.391	1.396	1.388	C16-C17	1.400	1.397	1.400
C16-C17	1.400	1.395	1.402	C17-C18	1.392	1.392	1.399
C17-C18	1.392	1.393	1.398	C18-C13	1.402	1.401	1.411
C18-C13	1.402	1.402	1.411	C18-N	1.401	1.407	1.379
C18-N	1.402	1.405	1.380	N-C9	1.351	1.334	1.390
N-C9	1.351	1.334	1.390	HB(NH-O)	1.835	1.862	1.868
HB(NH-O)	1.831	1.858	1.863				
CSQ-7				CSQ-8			
Geometrical indices	Neutral	Cation	Anion	Geometrical indices	Neutral	Cation	Anion
C1-C2	1.485	1.500	1.484	C1-C2	1.483	1.497	1.487
C2-C3	1.453	1.460	1.452	C2-C3	1.449	1.458	1.446
C3-C4	1.453	1.464	1.452	C3-C4	1.449	1.458	1.446
O-C1	1.231	1.217	1.236	O-C1	1.228	1.218	1.230
C1-C4	1.485	1.507	1.487	C1-C4	1.483	1.497	1.487
C3-C5	1.396	1.389	1.408	C3-C5	1.396	1.386	1.410
C5-C6	1.422	1.424	1.420	C5-C6	1.421	1.423	1.418
C5-C7	1.422	1.422	1.419	C5-C7	1.421	1.423	1.418
C6-N	1.168	1.167	1.171	C6-N	1.169	1.166	1.171
C7-N	1.168	1.167	1.171	C7-N	1.169	1.166	1.171
C4-C8	1.401	1.382	1.416	C4-C8	1.394	1.376	1.409
C2-C8'	1.401	1.384	1.417	C2-C8'	1.394	1.376	1.409
C8-C9	1.393	1.421	1.378	C8-C9	1.394	1.418	1.376
C9-C10	1.535	1.528	1.537	C9-S	1.762	1.744	1.784
C10-C11	1.519	1.515	1.524	S-C10	1.761	1.753	1.768
C11-C12	1.388	1.390	1.385	C10-C11	1.394	1.397	1.389
C12-C13	1.403	1.402	1.407	C11-C12	1.396	1.391	1.404
C13-C14	1.398	1.403	1.397	C12-C13	1.400	1.406	1.396
C14-C15	1.400	1.397	1.401	C13-C14	1.396	1.391	1.401
C15-C16	1.394	1.395	1.401	C14-C15	1.400	1.402	1.402
C16-C11	1.398	1.395	1.407	C15-C10	1.406	1.406	1.413
C16-N	1.400	1.416	1.385	C15-N	1.397	1.400	1.383
N-C9	1.369	1.351	1.411	N-C9	1.375	1.359	1.408
				S-O	3.020	3.010	3.090
CSQ-9				CSQ-10			
Geometrical indices	Neutral	Cation	Anion	Geometrical indices	Neutral	Cation	Anion
C1-C2	1.484	1.499	1.487	C1-C2	1.486	1.498	1.490
C2-C3	1.452	1.461	1.450	C2-C3	1.454	1.462	1.452
C3-C4	1.452	1.461	1.450	C3-C4	1.364	1.384	1.404

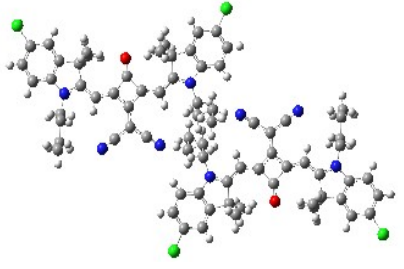
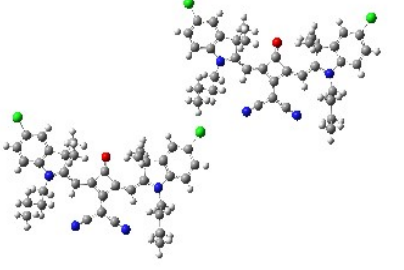
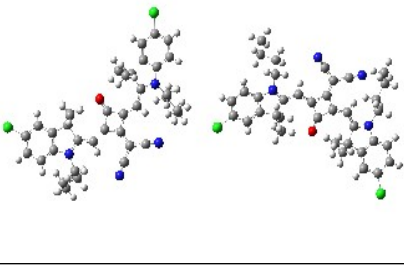
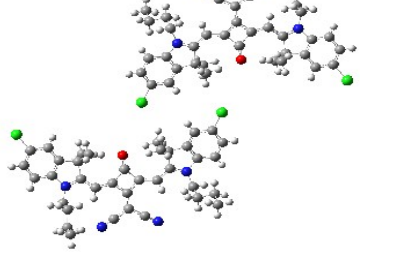
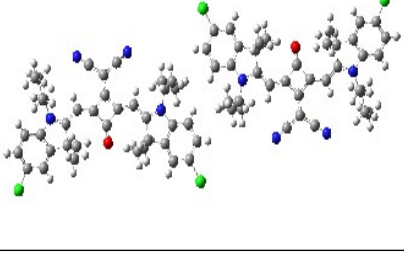
O-C1	1.234	1.223	1.236	O-C1	1.234	1.225	1.235
C1-C4	1.484	1.499	1.487	C4-C5	1.422	1.424	1.420
C3-C5	1.395	1.385	1.406	C5-N	1.168	1.166	1.170
C5-C6	1.422	1.424	1.420	C2-C6	1.394	1.377	1.400
C5-C7	1.422	1.424	1.420	C6-C7	1.405	1.431	1.404
C6-N	1.168	1.166	1.170	C7-C8	1.427	1.410	1.440
C7-N	1.168	1.166	1.170	C8-C9	1.363	1.376	1.354
C4-C8	1.395	1.377	1.402	C9-N	1.368	1.350	1.390
C2-C8'	1.395	1.377	1.402	N-C10	1.390	1.390	1.390
C8-C9	1.408	1.432	1.401	C10-C11	1.411	1.411	1.407
C9-C10	1.435	1.422	1.429	C11-C12	1.386	1.382	1.396
C10-C11	1.358	1.366	1.363	C12-C13	1.402	1.407	1.395
C11-C12	1.432	1.420	1.440	C13-C14	1.385	1.380	1.393
C12-C13	1.409	1.415	1.404	C14-C15	1.414	1.419	1.410
C13-C14	1.386	1.379	1.396	C15-C7	1.466	1.452	1.472
C14-C15	1.402	1.409	1.396				
C15-C16	1.390	1.385	1.399				
C16-C17	1.411	1.413	1.409				
C17-C12	1.422	1.426	1.427				
C17-N	1.399	1.398	1.394				
C9-N	1.390	1.376	1.420				

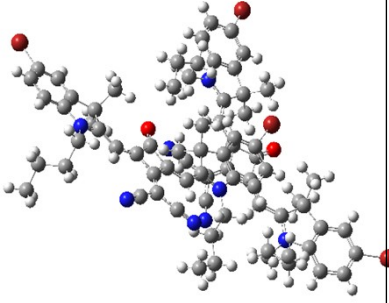
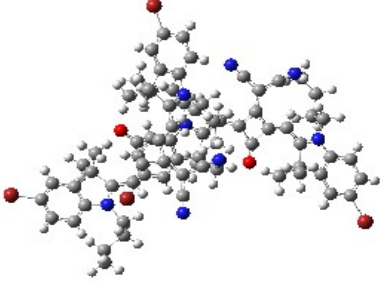
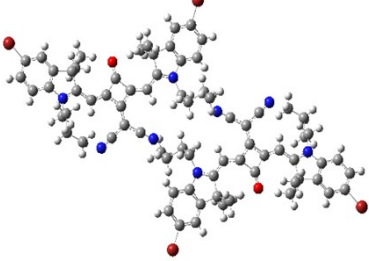
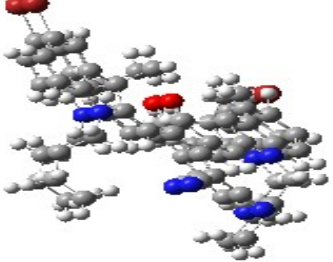
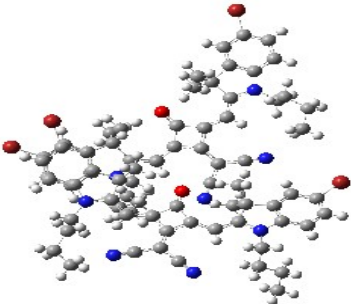
Table S3: At B3LYP/6-31G+(d,p) level of theory calculated interaction energies in kcal/mol), effective charge transfer integrals ΔE_{int}^{CP} ((Jeff)ij in eV), rate constants (in S-1), and drift mobilities for hole and electron transfer (μ in cm²/V s) of all motifs. The observed centroid-centroid distances are given as dcc (in Å).

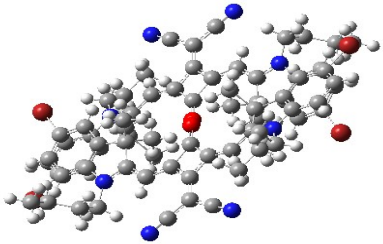
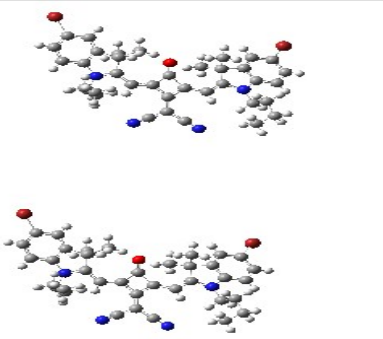
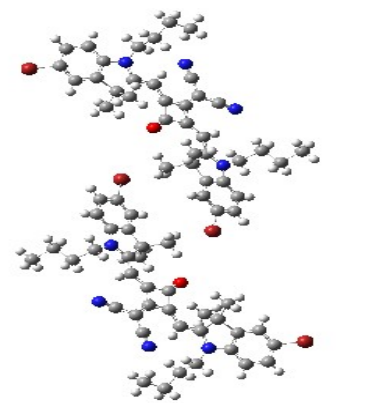
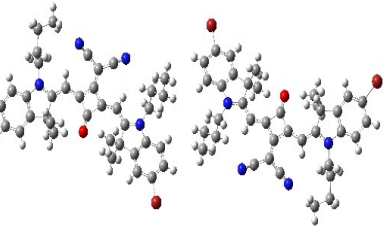
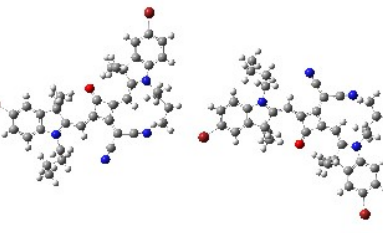
CSQs	Interactions	d_{cc}	ΔE_{int}^{CP}	J_+	J_-	K_+	K_-	μ_+	μ_-
CSQ-1-1		12.31	-6.07	5.69×10^{-05}	-9.28×10^{-04}	1.29×10^{06}	1.93×10^{09}	0.07	0.00
CSQ-1-2		9.24	-5.79	-8.76×10^{-04}	-6.75×10^{-03}	3.05×10^{08}	1.02×10^{11}		
CSQ-1-3		12.88	-4.12	1.44×10^{-04}	-1.55×10^{-04}	8.20×10^{06}	5.39×10^{07}		
CSQ-1-4		6.28	-19.43	-1.05×10^{-01}	-8.40×10^{-03}	4.39×10^{12}	1.58×10^{11}		
CSQ-1-5		14.9	-0.3	2.80×10^{-05}	6.91×10^{-05}	3.13×10^{05}	1.07×10^{07}		

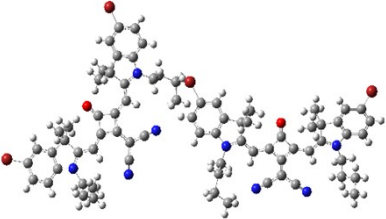
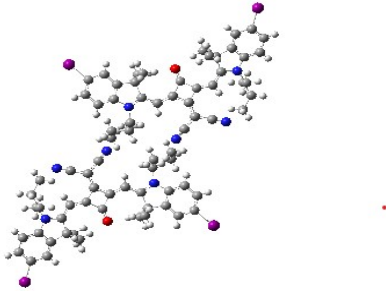
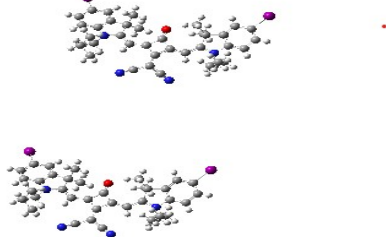
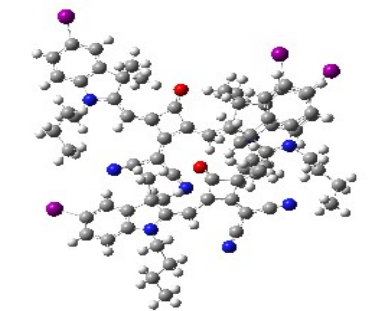
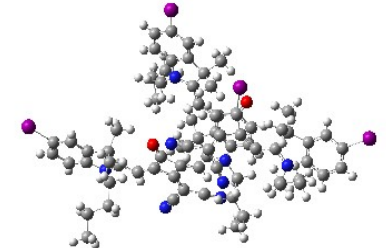
CSQ-1-6		14.82	-2.34	4.49×10^{-03}	-3.55×10^{-03}	8.03×10^{09}	2.82×10^{10}		
CSQ-1-7		13.59	-4.41	-1.97×10^{-03}	-1.63×10^{-03}	1.54×10^{09}	5.97×10^{09}		
CSQ-1-8		10.21	-8.31	7.07×10^{-03}	-1.84×10^{-03}	1.99×10^{10}	7.56×10^{09}		
CSQ-1-9		11.85	-9.09	-3.41×10^{-03}	4.40×10^{-04}	4.64×10^{09}	4.34×10^{08}		
CSQ-2-1		10.14	-10.4	-2.64×10^{-03}	-9.26×10^{-03}	2.90×10^{11}	1.95×10^{11}	0.10	0.01

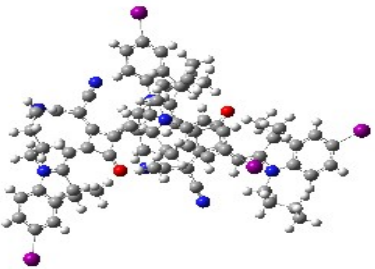
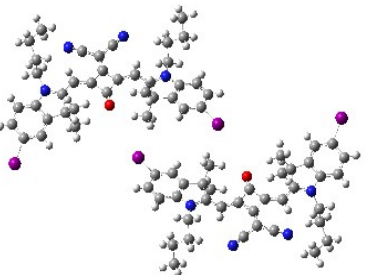
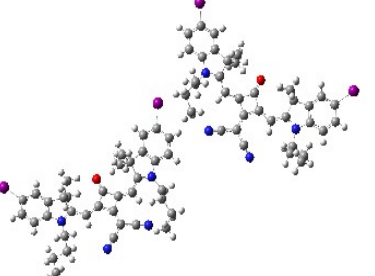
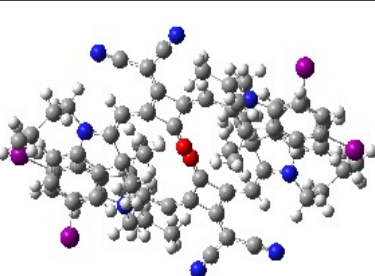
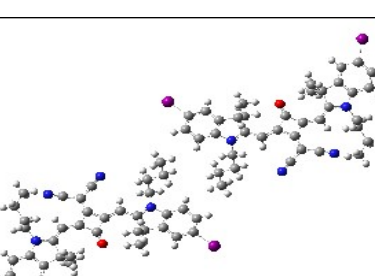
CSQ-2-2		15.76	-6.28	-2.45×10^{-03}	9.11×10^{-04}	2.49×10^{11}	1.88×10^{09}		
CSQ-2-3		10.95	-1.12	4.89×10^{-05}	-1.30×10^{-04}	9.99×10^{07}	3.81×10^{07}		
CSQ-2-4		9.01	-12.26	-1.04×10^{-02}	4.73×10^{-03}	4.51×10^{12}	5.06×10^{10}		
CSQ-2-5		8.02	-8.78	-9.28×10^{-03}	-2.36×10^{-03}	3.59×10^{12}	1.27×10^{10}		
CSQ-2-6		13.91	-2.69	6.35×10^{-04}	7.82×10^{-04}	1.68×10^{10}	1.39×10^{09}		

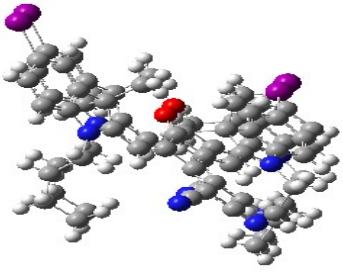
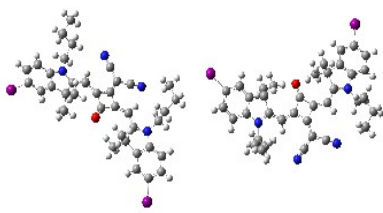
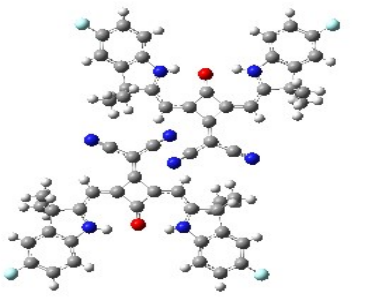
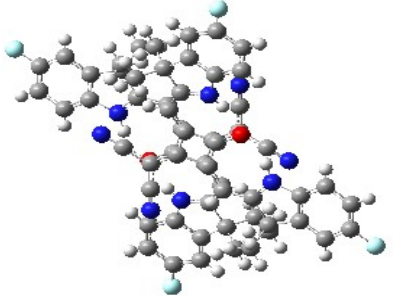
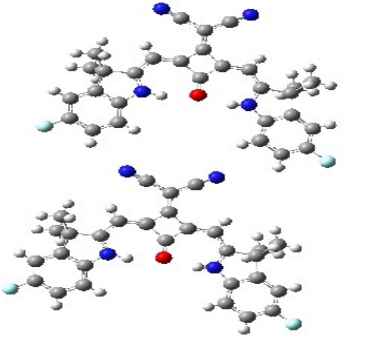
CSQ-2-7		13.22	-12.63	-9.87×10^{-04}	-2.70×10^{-03}	4.06×10^{10}	1.65×10^{10}		
CSQ-2-8		17.85	-0.38	-3.88×10^{-04}	-2.28×10^{-04}	6.27×10^{09}	1.18×10^{08}		
CSQ-2-9		19.7	-0.28	8.44×10^{-07}	-3.98×10^{-05}	2.97×10^{04}	3.59×10^{06}		
CSQ-2-10		13.95	-2.49	-1.82×10^{-03}	2.31×10^{-03}	1.38×10^{11}	1.21×10^{10}		
CSQ-2-11		17.47	-3.06	-8.15×10^{-05}	-5.53×10^{-04}	2.77×10^{08}	6.93×10^{08}		

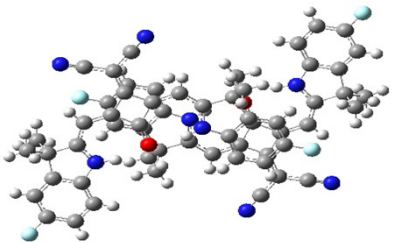
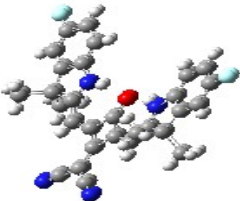
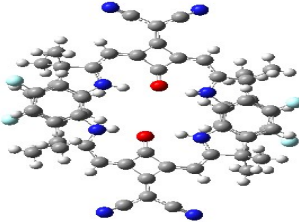
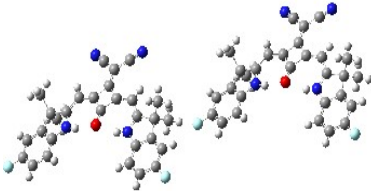
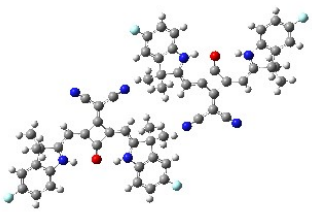
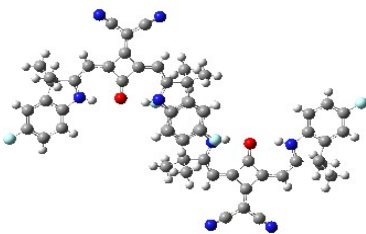
CSQ-3-1		10.67	-11.36	8.42×10^{-03}	1.16×10^{-02}	3.00×10^{12}	3.16×10^{11}	0.11	0.01
CSQ-3-2		13.45	-3.61	5.12×10^{-04}	-8.04×10^{-04}	1.11×10^{10}	1.52×10^{09}		
CSQ-3-3		13.93	-12.6	-5.18×10^{-04}	2.77×10^{-03}	1.13×10^{10}	1.80×10^{10}		
CSQ-3-4		9.13	-13.1	1.10×10^{-02}	2.55×10^{-03}	5.12×10^{12}	1.53×10^{10}		
CSQ-3-5		11.06	-1.35	-1.29×10^{-04}	9.76×10^{-05}	7.04×10^{08}	2.24×10^{07}		

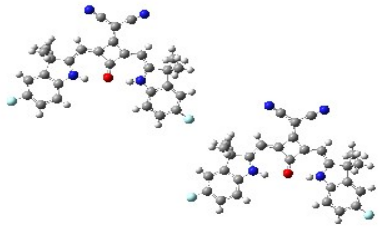
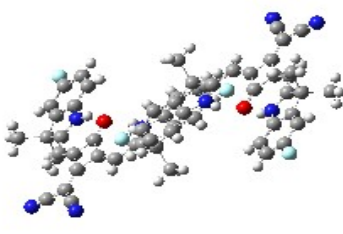
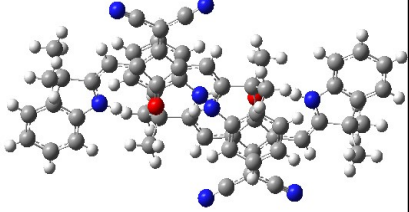
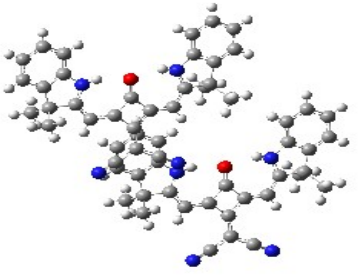
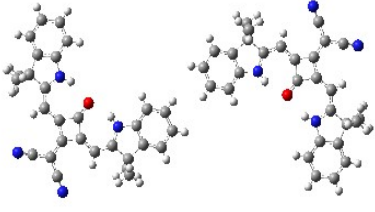
CSQ-3-6		7.10	-10.45	-8.65×10^{-03}	5.54×10^{-03}	3.16×10^{12}	7.20×10^{10}		
CSQ-3-7		18.76	-0.09	2.09×10^{-07}	-6.44×10^{-07}	1.84×10^{03}	9.74×10^{02}		
CSQ-3-8		13.24	-2.91	1.81×10^{-03}	2.31×10^{-03}	1.39×10^{11}	1.25×10^{10}		
CSQ-3-9		17.86	-2.72	-7.95×10^{-05}	4.07×10^{-04}	2.67×10^{08}	3.89×10^{08}		
CSQ-3-10		19.51	-0.75	-2.19×10^{-04}	3.00×10^{-04}	2.02×10^{09}	2.11×10^{08}		

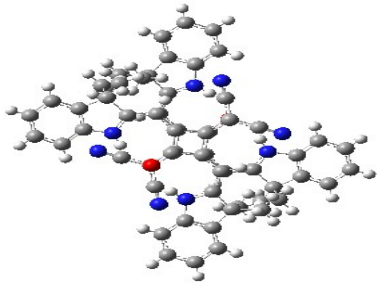
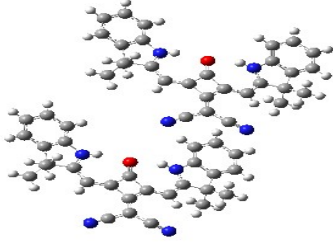
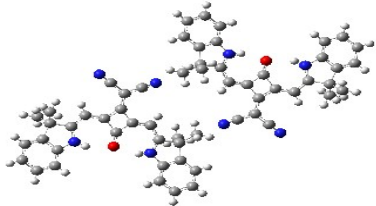
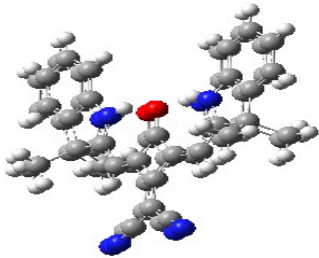
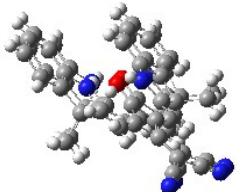
CSQ-3-11		16.49	-6.06	-2.12×10^{-03}	1.22×10^{-03}	1.90×10^{11}	3.48×10^{09}		
CSQ-4-1		14.69	-12.46	-2.84×10^{-04}	-2.42×10^{-03}	3.55×10^{07}	1.37×10^{10}	0.00	0.01
CSQ-4-2		19.30	-0.1	2.97×10^{-07}	2.11×10^{-06}	3.88×10^{01}	1.04×10^{04}		
CSQ-4-3		11.22	-1.36	1.83×10^{-04}	6.95×10^{-05}	1.48×10^{07}	1.13×10^{07}		
CSQ-4-4		11.19	-11.81	-1.49×10^{-02}	-1.15×10^{-02}	9.73×10^{10}	3.08×10^{11}		

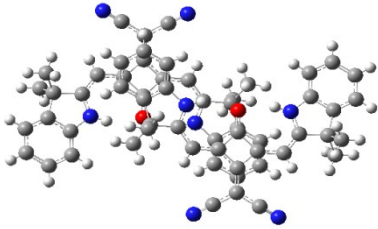
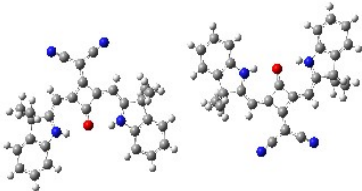
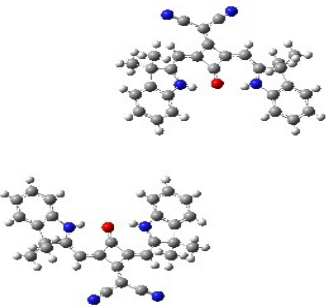
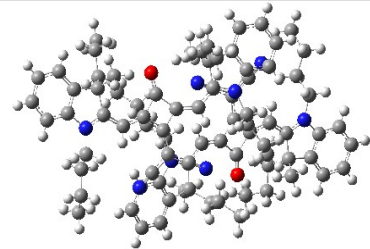
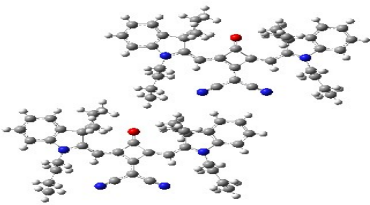
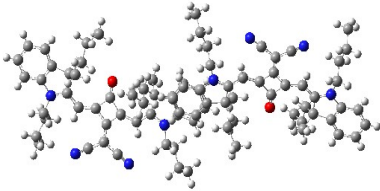
CSQ-4-5		13.68	-4.06	1.43×10^{-03}	3.34×10^{-04}	8.98×10^{08}	2.63×10^{08}		
CSQ-4-6		12.75	-3.23	2022×10^{-03}	2.20×10^{-03}	2.17×10^{09}	1.13×10^{10}		
CSQ-4-7		17.27	-5.15	-1.72×10^{-03}	1.04×10^{-03}	1.30×10^{09}	2.53×10^{09}		
CSQ-4-8		6.43	-11.1	-6.70×10^{-03}	6.16×10^{-03}	1.98×10^{10}	8.90×10^{10}		
CSQ-4-9		18.36	-2.69	-8.37×10^{-06}	2.77×10^{-04}	3.09×10^{04}	1.81×10^{08}		

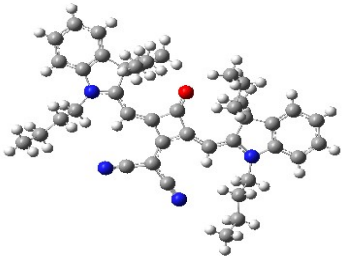
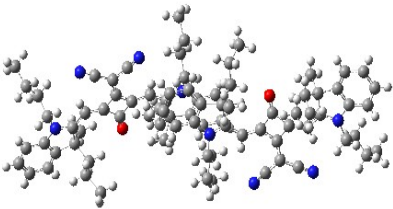
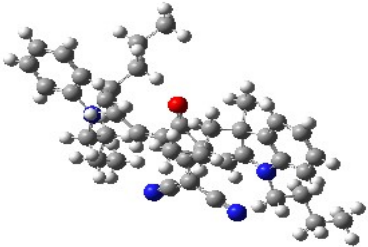
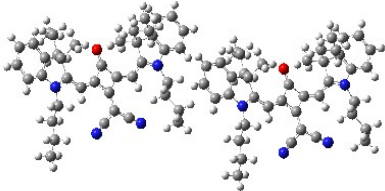
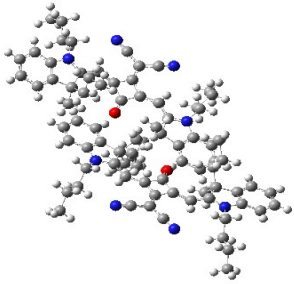
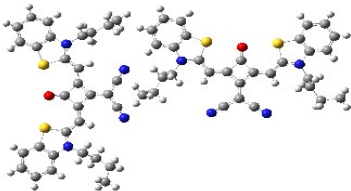
CSQ-4-10		9.32	-14.02	1.01×10^{-02}	9.90×10^{-04}	4.53×10^{10}	2.30×10^{09}		
CSQ-4-11		19.87	-0.58	-2.38×10^{-04}	4.33×10^{-04}	2.51×10^{07}	4.40×10^{08}		
CSQ-5-1		11.29	-6.28	-1.01×10^{-02}	-3.34×10^{-04}	4.59×10^{10}	2.16×10^{08}		
CSQ-5-2		7.05	-15.44	5.23×10^{-02}	6.44×10^{-03}	1.22×10^{12}	8.01×10^{10}		
CSQ-5-3		11.39	-7.17	-2.17×10^{-03}	2.68×10^{-04}	2.11×10^{09}	1.39×10^{08}	0.02	0.04

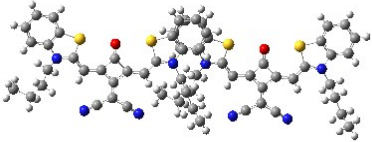
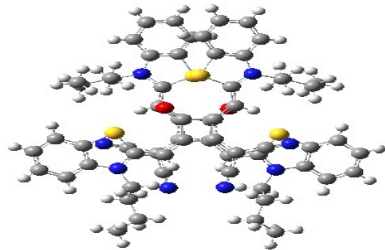
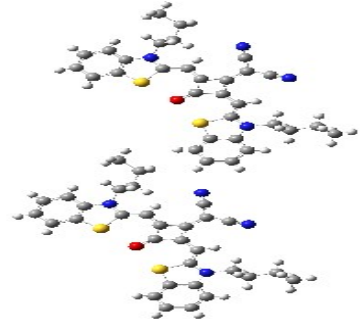
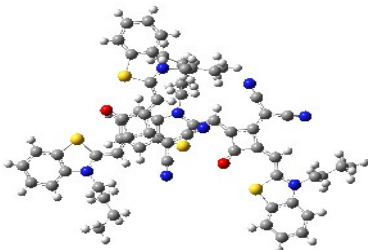
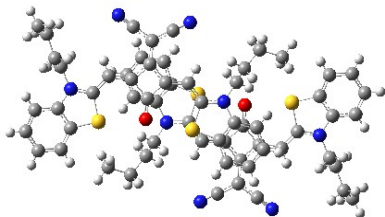
CSQ-5-4		6.16	-17.64	3.06×10^{-02}	4.34×10^{-02}	4.19×10^{11}	3.64×10^{12}		
CSQ-5-5		11.65	-0.46	1.27×10^{-03}	2.50×10^{-03}	7.18×10^{08}	1.21×10^{10}		
CSQ-5-6		6.68	-11.46	2.42×10^{-04}	-1.33×10^{-02}	2.61×10^{07}	3.39×10^{11}		
CSQ-5-7		16.46	-2.41	-4.15×10^{-04}	9.87×10^{-04}	7.69×10^{07}	1.88×10^{09}		
CSQ-5-8		12.44	-7.77	1.52×10^{-03}	9.71×10^{-04}	1.03×10^{09}	1.82×10^{09}		
CSQ-5-9		13.02	-4.55	-9.58×10^{-04}	7.84×10^{-04}	4.11×10^{08}	1.19×10^{09}		

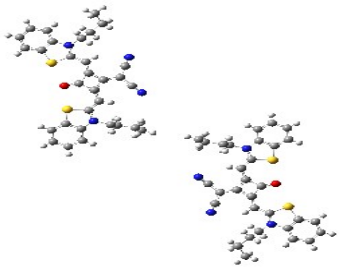
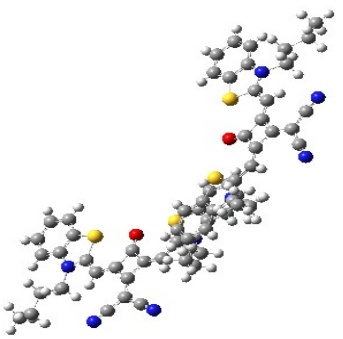
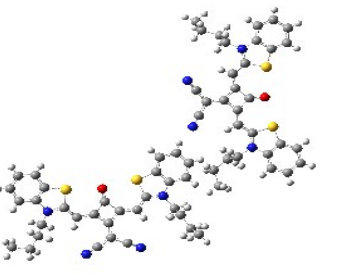
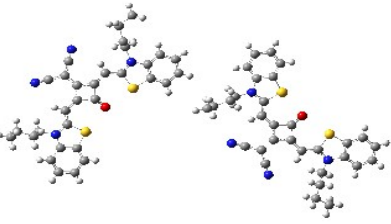
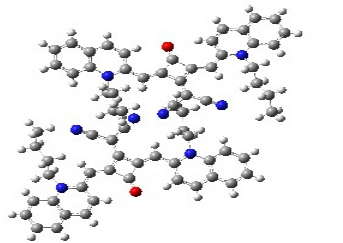
CSQ-5-10		17.21	-1.09	-2.64×10^{-04}	-5.28×10^{-04}	3.12×10^{07}	5.38×10^{08}		
CSQ-5-11		14.79	-2.66	1.01×10^{-03}	1.30×10^{-03}	4.54×10^{08}	3.28×10^{09}		
CSQ-6-1		7.02	-13.2	-4.55×10^{-02}	2.38×10^{-02}	9.23×10^{13}	1.22×10^{12}		
CSQ-6-2		10.61	-3.85	3.34×10^{-02}	-8.50×10^{-05}	4.96×10^{13}	1.55×10^{07}		
CSQ-6-3		16.44	-0.38	-5.76×10^{-04}	-3.75×10^{-04}	1.48×10^{10}	3.01×10^{08}		

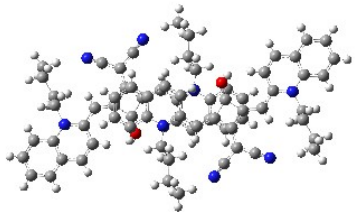
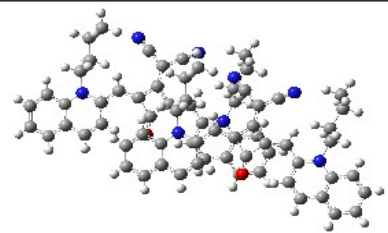
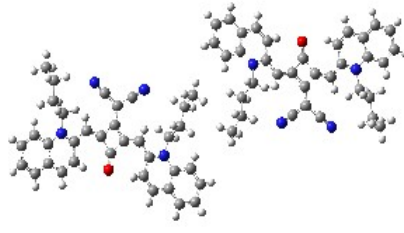
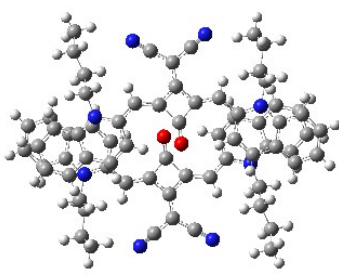
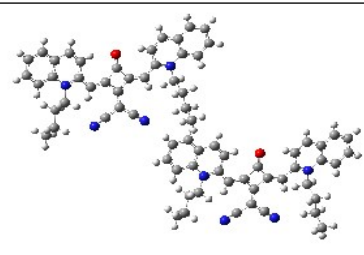
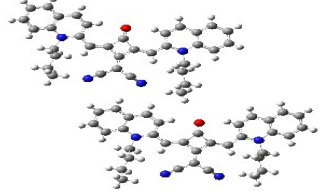
CSQ-6-4		7.32	-4.15	-2.63×10^{-03}	6.67×10^{-03}	3.08×10^{11}	9.52×10^{10}		
CSQ-6-5		12.66	-3.91	1.29×10^{-03}	5.63×10^{-05}	7.45×10^{10}	6.79×10^{06}		
CSQ-6-6		12.82	-7.97	7.90×10^{-03}	1.46×10^{-03}	2.78×10^{12}	4.55×10^{09}		
CSQ-6-7		11.54	-0.81	9.37×10^{-04}	-1.61×10^{-03}	3.91×10^{10}	5.53×10^{09}		
CSQ-6-8		13.29	-1.96	-6.62×10^{-04}	5.80×10^{-04}	1.95×10^{10}	7.19×10^{08}		

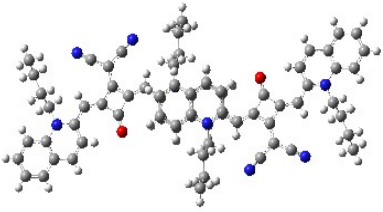
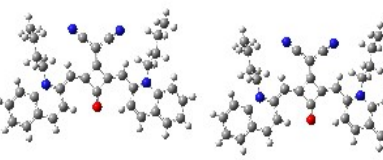
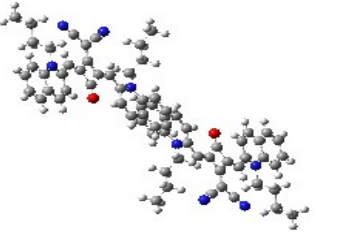
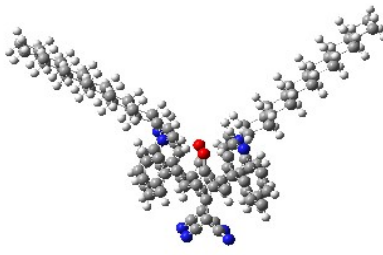
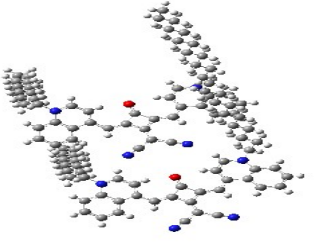
CSQ-6-9		5.91	-18.38	4.13×10^{-02}	2.38×10^{-02}	7.60×10^{13}	1.21×10^{12}		
CSQ-6-10		17.00	-0.46	1.27×10^{-05}	8.51×10^{-05}	7.23×10^{06}	1.55×10^{07}		
CSQ-6-11		16.58	0.18	-7.05×10^{-06}	2.67×10^{-06}	2.22×10^{06}	1.52×10^{04}		
CSQ-7-1		8.78	-17.41	1.48×10^{-03}	1.68×10^{-03}	8.50×10^{08}	6.26×10^{09}		
CSQ-7-2		12.52	-7.05	-2.66×10^{-04}	-1.14×10^{-04}	2.74×10^{07}	2.90×10^{07}		
CSQ-7-3		15.07	-3.41	-3.17×10^{-03}	-5.44×10^{-03}	3.90×10^{09}	6.56×10^{10}		

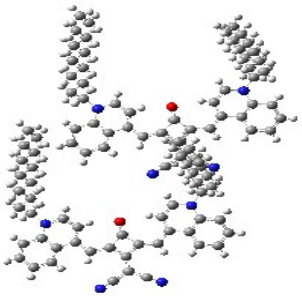
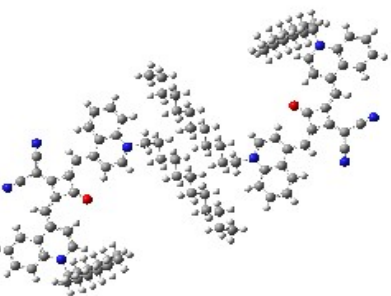
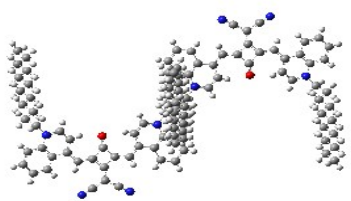
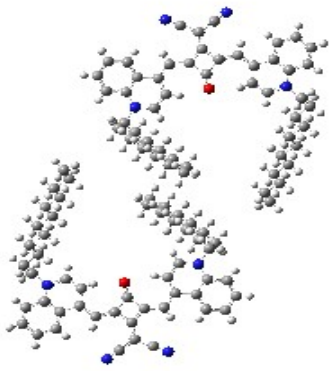
CSQ-7-4		8.19	-2.25	7.17×10^{-04}	1.41×10^{-03}	2.00×10^{08}	4.41×10^{09}		
CSQ-7-5		12.19	-12.13	1.15×10^{-02}	1.17×10^{-02}	5.13×10^{10}	3.01×10^{11}		
CSQ-7-6		14.96	-0.79	-5.37×10^{-05}	5.69×10^{-05}	1.12×10^{06}	7.16×10^{06}		
CSQ-7-7		18.35	-1.73	-5.55×10^{-04}	1.21×10^{-03}	1.19×10^{08}	3.25×10^{09}		
CSQ-7-8		12.06	-2.53	2.59×10^{-04}	1.31×10^{-03}	2.60×10^{07}	3.79×10^{09}		
CSQ-8-1		13.89	-7.46	3.91×10^{-03}	-3.89×10^{-04}	1.36×10^{11}	4.58×10^{08}		

CSQ-8-2		12.63	-8.11	-3.14×10^{-03}	-4.70×10^{-03}	8.82×10^{10}	6.70×10^{10}		
CSQ-8-3		3.71	-24.42	-1.18×10^{-01}	-1.62×10^{-02}	1.25×10^{14}	7.91×10^{11}		
CSQ-8-4		15.22	-5.01	5.27×10^{-03}	5.05×10^{-04}	2.48×10^{11}	7.71×10^{08}		
CSQ-8-5		10.43	-1.66	3.20×10^{-04}	-3.04×10^{-04}	9.11×10^{08}	2.80×10^{08}		
CSQ-8-6		7.10	-24.72	1.01×10^{-01}	5.04×10^{-02}	9.10×10^{13}	7.68×10^{12}		

CSQ-8-7		20.43	-0.66	1.36×10^{-04}	1.46×10^{-05}	1.64×10^{08}	6.45×10^{05}		
CSQ-8-8		15.63	-0.7	-1.66×10^{-04}	3.24×10^{-04}	2.47×10^{08}	3.17×10^{08}		
CSQ-8-9		15.67	-1.75	-1.09×10^{-03}	4.01×10^{-04}	1.05×10^{10}	4.86×10^{08}		
CSQ-8-10		17.65	-0.38	7.44×10^{-06}	7.48×10^{-06}	4.94×10^{05}	1.69×10^{05}		
CSQ-9-1		8.77	-12.4	2.13×10^{-02}	-3.24×10^{-04}	1.78×10^{13}	6.74×10^{08}		

CSQ-9-2		9.21	-15.66	-4.85×10^{-02}	8.06×10^{-02}	9.21×10^{13}	4.18×10^{13}		
CSQ-9-3		11.74	-2.15	2.28×10^{-05}	8.41×10^{-05}	2.05×10^{07}	4.56×10^{07}		
CSQ-9-4		16.36	-4.3	2.91×10^{-04}	3.85×10^{-04}	3.31×10^{09}	9.55×10^{08}		
CSQ-9-5		5.78	-16.95	4.22×10^{-02}	-9.84×10^{-02}	7.00×10^{13}	6.23×10^{13}		
CSQ-9-6		16.43	-3.72	9.87×10^{-04}	-1.33×10^{-04}	3.82×10^{10}	1.13×10^{08}		
CSQ-9-7		12.41	-7.46	1.21×10^{-03}	-7.64×10^{-05}	5.77×10^{10}	3.76×10^{07}		

CSQ-9-8		13.33	-7.72	-2.03×10^{-02}	-2.29×10^{-03}	1.62×10^{13}	3.38×10^{10}		
CSQ-9-9		19.99	-0.27	-1.96×10^{-03}	5.67×10^{-03}	1.51×10^{11}	2.07×10^{11}		
CSQ-9-10		18.94	-0.81	1.28×10^{-04}	6.85×10^{-04}	6.47×10^{08}	3.02×10^{09}		
CSQ-10-1		6.69	-22.04	-1.87×10^{-01}	-7.26×10^{-02}	1.37×10^{15}	6.35×10^{13}		
CSQ-10-2		9.61	-11.6	-1.04×10^{-02}	2.92×10^{-04}	4.26×10^{12}	1.03×10^{09}		

CSQ-10-3		11.71	-6.63	-4.27×10^{-03}	2.00×10^{-04}	7.17×10^{11}	4.81×10^{08}		
CSQ-10-4		19.23	-5.46	3.72×10^{-05}	3.33×10^{-05}	5.45×10^{07}	1.33×10^{07}		
CSQ-10-5		18.00	-9.42	7.39×10^{-06}	8.49×10^{-06}	2.15×10^{06}	8.68×10^{05}		
CSQ-10-6		22.55	-3.66	1.81×10^{-06}	-3.97×10^{-06}	1.29×10^{05}	1.90×10^{05}		

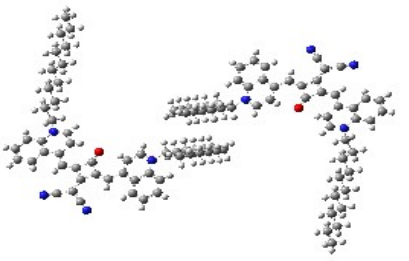
CSQ-10- 7		23.51	-1.21	-7.37×10^{-07}	2.64×10^{-06}	2.13×10^{04}	8.39×10^{04}		
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Table S4: Intermolecular interactions energies (in KJ mol⁻¹) calculated by the PIXEL method for different molecular pairs in all CSQs in this study

CSQ	dcc	Symmerty xode	Ecoul	Epol	Edisp	Erep	Etot	major interactions
CSQ-1-1	12.31	x+1/2, -y+1/2, -z	-11.2	-3.7	-20.1	7.8	-27.3	Inter-stack N---H, O---H
CSQ-1-2	9.24	-x+1/2, y+1/2, z	-5.7	-2.6	-34.4	17.4	-25.3	Slip stack C---C, C---N
CSQ-1-3	12.88	x+1/2, y, -z+1/2	-10.9	-4.8	-15.8	12	-19.5	Inter-stack N---H
CSQ-1-4	6.28	-x, -y, -z	-21.5	-20.1	-123.8	82	-83.4	Slip stack C---C, C---N, N---H
CSQ-1-6	14.82	-x+1/2, -y, z+1/2	-3.9	-2.5	-18.4	12.9	-12	Inter-stack C---C, C---H
CSQ-1-7	13.59	x, -y+1/2, z+1/2	-6.9	-3.6	-30.8	17.7	-23.6	Inter-stack C---C, C---H
CSQ-1-8	10.21	-x, y+1/2, -z+1/2	-8.9	-3.2	-37.2	11.5	-37.8	Inter-stack N---H, O---H
CSQ-1-9	11.85	-x, -y, -z	-18.8	-10.1	-56.2	51.1	-34	Slip stack C---C, C---N, N---H
CSQ-2-1	10.14	-x+1/2, y+1/2, -z+1/2	-15.3	-13.1	-84.5	56.8	-56.2	Inter-stack N---H, C---C, H---Cl, C---Cl
CSQ-2-2	15.76	-x+1/2, y+1/2, -z+1/2	-18.3	-6.7	-24.8	17.6	-32.1	Inter-stack N---H, H---Cl, C---Cl
CSQ-2-3	10.95	-x+1/2, y+1/2, -z+1/2	0.2	-0.1	-4.8	0.3	-4.4	Inter-stack C---H
CSQ-2-4	9.01	x, y, z	-20.1	-10.5	-77.5	49.5	-58.5	Intra-stack C---C
CSQ-2-5	8.02	-x, -y, -z	-13.6	-5.5	-58.8	37	-40.8	Slip stack C---C, C---Cl, H---Cl
CSQ-2-6	13.91	x+1/2, -y+1/2, z+1/2	-2.9	-2	-19	12.2	-11.7	Inter-stack C---H
CSQ-2-7	13.22	-x, -y, -z	-35.6	-13	-32	28.6	-52.1	Inter-stack N---H
CSQ-2-8	17.85	x, y, z	-2.2	-1	-8.6	7.6	-4.1	Inter-stack H---Cl, C---Cl
CSQ-2-9	19.7	x+1/2, -y+1/2, z+1/2	-0.1	-0.9	-6.7	3.9	-3.8	Inter-stack H---Cl
CSQ-2-10	13.95	-x, -y, -z	-5.6	-2.8	-19.9	10.4	-17.8	Inter-stack H---Cl, C---Cl
CSQ-2-11	17.47	-x, -y, -z	-2.9	-5.3	-32	21.6	-18.5	Inter-stack C---H
CSQ-3-1	10.67	-x+1/2, y+1/2, -z+1/2	-51.9	-35.9	-89.5	58.6	-118.8	Inter-stack N---H, C---C, H---Br
CSQ-3-2	13.45	x+1/2, -y+1/2, z+1/2	-6.5	-6.3	-23.3	15.8	-20.4	Inter-stack C---H
CSQ-3-3	13.93	-x, -y, -z	-57.8	-22.9	-31.9	34.9	-77.7	Inter-stack N---H
CSQ-3-4	9.13	x, y, z	-68.1	-44.4	-79.6	51.7	-140.4	Intra-stack C---C
CSQ-3-5	11.06	-x+1/2, y+1/2, -z+1/2	-0.3	-1.1	-7.3	2.4	-6.3	Inter- stack C---H
CSQ-3-6	7.1	-x, -y, -z	-38	-42.4	-71.7	39.3	-112.8	Slip stack C---C, C---Br, H---Br
CSQ-3-7	18.76	x, y, z	-65.7	-5.9	-8.9	8	-14.8	Inter-stack H---Br
CSQ-3-8	13.24	-x, -y, -z	-13.9	-9.6	-13.7	3.7	-33.6	Inter-stack H---Br, C---Br
CSQ-3-9	17.86	-x, -y, -z	-10.4	-10.7	-24.4	17.6	-27.8	Inter-stack C---H
CSQ-3-10	19.51	x+1/2, -y+1/2, z+1/2	-2	-6.8	-8	3.3	-13.4	Inter-stack H---Br
CSQ-3-11	16.49	-x+1/2, y+1/2, -z+1/2	-20	-17.7	-23.6	19.8	-41.5	Inter-stack H---Br, C---Br
CSQ-4-1	14.69	-x, -y, -z	3961.2	-1353	-35.6	27.8	2600.7	Inter-stack N---H
CSQ-4-2	19.3	x, y, z	-4367	-1118	-6	11.3	-5479.5	Inter-stack H---I
CSQ-4-3	11.22	-x+1/2, y+1/2, -z+1/2	3726.6	-736	-8.6	2.6	2984.6	Inter-stack C---H
CSQ-4-4	11.19	-x+1/2, y+1/2, -z+1/2	4613.4	5948.7	79.1	65.5	>9999.0	Inter-stack N---H, C---C, H---I
CSQ-4-5	13.68	x+1/2, -y+1/2, z+1/2	-1448	-1278	-32.4	19.9	-2737.9	Inter-stack C---H
CSQ-4-7	17.27	-x+1/2, y+1/2, -z+1/2	-1299	-109.3	-0.2	0	-1408.5	Inter-stack N---H, H---I
CSQ-4-8	6.43	-x, -y, -z	-1001	-8136	-72.3	49.2	-9159.9	Slip stack C---C, C---I, H---I

CSQ-4-9	18.36	-x, -y, -z	-4446	-843.8	-31.3	15.2	-5305.3	Inter-stack C---H
CSQ-4-10	9.32	x, y, z	1870	-6038	-81.6	57.8	-4191.4	Intra-stack C---C
CSQ-4-11	19.87	$x+1/2, -y+1/2, z+1/2$	-6236	-1020	-7.3	6.4	-7256.4	Inter-stack H---I, C---I
CSQ-5-1	11.29	-x, -y, -z	2.3	-0.6	-5.6	0.1	-3.8	Inter-stack N---H
CSQ-5-2	7.05	-x, -y, -z	-3.7	-7.2	-52.5	27.4	-36	Intra-stack C---C, C---N, C---O, N---O, N---H
CSQ-5-3	11.39	x, y, z	-22.7	-7.8	-15.4	15.4	-30.5	Inter-stack N---H
CSQ-5-4	6.16	-x, -y, -z	-674.9	-1099	-244.6	2673.9	655.7	Slip stack C---C, C---N, C---O, O---H, H---F, C---F
CSQ-5-6	6.68	-x, -y, -z	-431.7	-396.3	-131.2	1219	259.8	Slip stack C---C, H---F
CSQ-5-7	16.46	x, y, z	-6.1	-2.1	-9.4	7.5	-10.1	Inter-stack H---F, C---F
CSQ-5-8	12.44	-x, -y, -z	-11.7	-10.4	-48.5	52.7	-18	Inter-stack N---H
CSQ-5-9	13.02	-x, -y, -z	-9	-5.1	-12.8	12.1	-14.9	Inter-stack C---C, C---F, H---F
CSQ-5-10	17.21	x, y, z	-1.9	-0.3	-2.3	0.3	-4.2	Inter-stack H---F
CSQ-5-11	14.79	-x, -y, -z	3.5	-2.4	-12.7	5.8	-5.9	Inter-stack H---F
CSQ-6-1	7.02	-x, -y, -z	-20.5	-12.1	-105	77.1	-60.4	Slip stack C---C, C---O, C---N, O---H, N—H
CSQ-6-2	10.61	x, y, z	-5	-4.6	-28.8	20.3	-18.1	Intra-stack C---C
CSQ-6-4	7.32	-x, -y, -z	-4.4	-1.4	-12.8	1.7	-17	Intra-stack C---C, C---O, N---H
CSQ-6-5	12.66	x, y, z	-10.6	-4.2	-15.5	13.2	-17.1	Inter-stack N---H
CSQ-6-6	12.82	-x, -y, -z	-26.2	-9.6	-15.5	17.3	-33.9	Inter-stack N---H
CSQ-6-8	13.29	x, y, z	-0.9	-1	-10.5	3.7	-8.7	Intra-stack C---C
CSQ-6-9	5.91	-x, -y, -z	-39.2	-14.1	-115.1	90.5	-77.9	Slip stack C---C, C---N, O---H, N---H
CSQ-7-1	8.78	-x, $y+1/2, -z$	-28.6	-15.9	-96.4	66.5	-74.5	Slip stack C---C, N---H, O---H
CSQ-7-2	12.52	x, y, z	-17.1	-6.4	-30.4	20.2	-33.8	Inter-stack N---H, O---H
CSQ-7-3	15.07	-x, $y+1/2, -z$	-3.9	-2.9	-25.1	15.5	-16.4	Slip stack C---C
CSQ-7-4	8.19	x, y, z	0.2	-1.4	-17.1	9.5	-8.8	Intra-stack C---C
CSQ-7-5	12.19	-x, $y+1/2, -z$	-22.7	-12.3	-77	57.2	-54.8	Slip stack C---C, C---N, N---H
CSQ-7-6	14.96	x, y, z	-0.8	-0.2	-4.6	1.6	-4	Intra-stack C---C
CSQ-7-7	18.35	x, y, z	-1	-1.7	-13.8	6.9	-9.6	Inter-stack C---C, C---H
CSQ-7-8	12.06	-x, $y+1/2, -z$	12.058	-2.8	-3.2	-18.1	12.1	Inter-stack O---H
CSQ-8-1	13.89	$-x+1/2, y+1/2, -z+1/2$	-23.8	-10.3	-25.3	25.9	-33.4	Inter-stack N---H
CSQ-8-2	12.63	$x+1/2, y+1/2, z$	-9.7	-5.5	-46.6	27.3	-34.5	Slip stack C---C, C---N, C---S
CSQ-8-3	3.71	-x, y, $-z+1/2$	-48.7	-30.2	-146	123.2	-101.9	Intra-stack C---C, C---O, S---N, O---H
CSQ-8-4	15.22	x, y, z	-17.5	-8.5	-20.3	23	-23.3	Inter-stack N---H
CSQ-8-5	10.43	x, -y, $z+1/2$	2.1	-1.4	-10.1	1.7	-7.8	Inter-Stack C---C, O---H
CSQ-8-6	7.1	-x, -y, -z	-55.5	-20.4	-128.4	111.4	-92.9	Slip stack C---C, C---S, C---O, O---H, S---H, N---H
CSQ-8-8	15.63	x, -y, $z+1/2$	-0.7	-0.1	-2.6	0.1	-3.3	Inter-stack C--H
CSQ-8-9	15.67	-x, y, $-z+1/2$	-4.4	-3.6	-15.6	14.8	-8.8	Inter-stack N---H
CSQ-9-1	8.77	x, $-y+1/2, z+1/2$	-17.3	-8.9	-48	22.5	-51.6	Slip stack C---C, C---N, N---H

CSQ-9-2	9.21	-x, -y, -z	-21.7	-9.6	-91.5	57.3	-65.5	Slip stack C---C, C---N, N---H, O---H
CSQ-9-3	11.74	x, y, z	-0.9	-0.7	-10.5	2.7	-9.3	Intra-stack C---C
CSQ-9-4	16.36	x, -y+1/2, z+1/2	-9.5	-3.2	-25.6	16.9	-21.3	Inter-stack C---H
CSQ-9-5	5.78	-x, -y, -z	-17.2	-10.6	-123.6	84.7	-66.7	Slip stack C---C, C---N, C---O, O---H
CSQ-9-6	16.43	-x, y+1/2, -z+1/2	-10.9	-4.4	-19.8	16.8	-18.3	Inter-stack N---H, C---H
CSQ-9-7	12.41	-x, y+1/2, -z+1/2	-18.6	-7.1	-24.2	18	-31.9	Inter-stack N---H, O---H
CSQ-9-8	13.33	-x, -y, -z	-12.8	-5.1	-57	42.3	-32.5	Slip stack C---C, C---N
CSQ-9-9	19.99	x, y, z	2.1	-2.9	-11.2	8.8	-3.1	Inter-stack C---H
CSQ-9-10	18.94	-x, -y, -z	0.5	-0.3	-4	0.2	-3.6	Inter-stack C---C, C---H
CSQ-10-1	6.69	x, y, z	-81.3	-39.1	-162.5	103.2	-179.7	Intra -stack C---C
CSQ-10-2	9.61	x, y, z	-62.2	-38.3	-54.4	47	-107.9	Inter-stack N---H, N---O
CSQ-10-3	11.71	x, y, z	-12.2	-4.8	-19.1	5.2	-30.9	Inter-stack N---H
CSQ-10-4	19.23	-x, -y, -z	-15.9	-10.7	-39.6	21.2	-45.1	Inter-stack C---H
CSQ-10-5	18	-x, -y, -z	-30.8	-13.9	-74.4	42.9	-76.2	Inter-stack C---H

Table S5 Enrichment ratios (E_{xy}) of the main intermolecular interactions for all CSQs in this study^a

Interactions	CSQ-1	CSQ-2	CSQ-3	CSQ-4	CSQ-5	CSQ-6	CSQ-7	CSQ-8	CSQ-9	CSQ-10
C---C	0.83	1.95	1.82	1.74	1.70	1.38	1.21	2.13	1.57	2.34
C---N	1.46	0.53	0.55	0.61	1.26	1.37	1.15	0.41	1.08	0.52
HC---C	2.30	1.53	1.55	1.52	1.28	1.51	1.97	1.04	1.42	1.32
HC---N	2.29	3.24	3.33	3.48	2.98	2.88	2.39	2.99	2.89	2.38
HC---HC	0.90	0.99	0.98	1.01	1.01	1.07	0.98	1.15	1.13	1.09
HC---CO	1.69	0.08	0	0	0	0	2.45	0.47	1.11	0
HC---C=O	3.26	3.44	2.83	1.50	3.81	1.96	2.88	3.21	1.70	0.86
C=O---C	0	1.08	1.68	1.53	0.81	3.12	0	1.03	2.49	4.62
CO---C	0.11	0.14	0	0	5.86	6.25	1.18	6.02	3.37	9.07
C---X		1.72	2.12	2.36	1.59					
CH---X		2.42	2.38	2.25	3.28					
CO---X		16.73	14.06	11.56						
C=O---X		0.83	3.27	8.98						
CO---N	16.95		0		1.82	0.16		0.52		0.02
C=O---N					0.09	0.17				9.96
NH---C					2.77	3.62				
NH---HC					2.67	1.40				
HN---N					0.17	1.39				
C---S								1.89		
S---N								2.26		
S---S								0.49		
S---HC								2.26		

^a C=O -Ketonic oxygen CO- Ketonic carbon HC - Hydrogen X-Halogen atom

Table S6 Proportion of chemical type on the molecular surface (S_x %) of the main intermolecular interactions found for all CSQs in this study^a

Interactions	CSQ-1	CSQ-2	CSQ-3	CSQ-4	CSQ-5	CSQ-6	CSQ-7	CSQ-8	CSQ-9	CSQ-10
C---C	6.02	10.78	9.74	8.69	16.42	13.79	7.13	16.88	18.42	10.68
C---N	2.13	0.76	0.75	0.79	4.03	4.44	1.28	0.91	2.16	0.52
HC---C	40.85	20.68	19.96	18.16	18.11	24.99	33.44	15.49	27.38	20.21
HC---N	8.17	11.33	10.91	10.68	13.94	15.36	7.77	12.46	9.41	7.91
HC---HC	39.10	32.53	30.55	28.68	21.09	29.13	47.93	31.75	35.79	56.31
HC---CO	0.89	0.04	0	0	0	0	1.26	0.31	0.86	0
HC---C=O	2.01	1.18	0.64	0.29	3.49	1.94	0.86	3.14	2.15	0.75
C=O---C	0	0.15	0.16	0.12	0.51	1.89		0.54	1.92	1.21
CO---C	0.02	0.02	0	0	2.70	2.86	0.21	2.09	1.58	1.65
C---X		4.73	6.89	9.13	3.31					
CH---X		16.28	18.68	20.81	10.01					
CO---X		1.45	1.49	1.48	0					
C=O---X		0.06	0.19	0.56	0					
CO---N	0.74				0.27	0.02		0.05		0
C=O---N					0.02	0.03		0		0.56
NH---C					1.88	2.82				
NH---HC					2.67	1.80				
HN---N					0.03	0.35				
C---S								4.43		
S---N								1.50		
S---S								0.34		
S---HC								9.86		

^a C=O -Ketonic oxygen CO- Ketonic carbon HC - Hydrogen X-Halogen atom

Table S7: Optimized Cartesian coordinates of all CSQs obtained at the B3LYP/6-31G+(d,p) level of theory and only for CSQ-4 additional LANL2DZ for I atom.

CSQs		Cartesian Coordinates			
CSQ-1	Neutral	6	-5.73989900	-0.35195500	0.00003200
		6	-7.13220400	-0.26870400	0.00007300
		1	-7.65685500	0.68020700	0.00013000
		6	-7.85116200	-1.47050300	0.00004400
		1	-8.93637800	-1.43641500	0.00007500
		6	-7.19550400	-2.70572000	-0.00003100
		1	-7.77412100	-3.62410700	-0.00006100
		6	-5.79360300	-2.76358400	-0.00007800
		1	-5.28697000	-3.72463900	-0.00014100
		6	-5.06910400	-1.57926200	-0.00004400
		6	-3.56909500	-1.33774000	-0.00008800
		6	-3.50711400	0.19659300	-0.00002700
		6	-2.43303000	1.08423300	-0.00003300
		1	-2.71639900	2.12961100	-0.00000300
		6	-1.04361800	0.90569200	-0.00002600
		6	0.00000600	-0.14985800	-0.00012300
		6	0.00000400	1.91774600	0.00001900
		6	1.04362400	0.90569200	-0.00007100
		6	2.43303800	1.08422900	-0.00013000
		1	2.71641500	2.12960500	-0.00009800
		6	3.50712200	0.19659400	-0.00017500
		6	3.56911100	-1.33773500	0.00001100
		6	5.06912000	-1.57924900	0.00010200
		6	5.79361100	-2.76357500	0.00032800
		1	5.28697300	-3.72462600	0.00045600
		6	7.19551200	-2.70571900	0.00039700
		1	7.77412400	-3.62410900	0.00056900
		6	7.85117100	-1.47050300	0.00024800
		1	8.93638700	-1.43641800	0.00033200
		6	7.13222100	-0.26870100	0.00001500
		1	7.65688800	0.68019900	-0.00005100
		6	5.73991300	-0.35193800	-0.00007500
		6	-0.00000800	3.31358000	0.00010900
		6	-1.21338600	4.05690100	0.00020200
		6	1.21335300	4.05692900	0.00008900
		6	-2.92301400	-1.93085600	-1.27732700
		1	-3.36192200	-1.49143400	-2.17846800
		1	-3.10457600	-3.01031200	-1.30313500
		1	-1.84457500	-1.76918100	-1.27273100
		6	-2.92296800	-1.93092400	1.27710900
		1	-3.36189200	-1.49158900	2.17828600
		1	-1.84453600	-1.76920300	1.27252100
		1	-3.10447700	-3.01039100	1.30283300

		6	2.92305900	-1.93103700	-1.27715900
		1	3.36203000	-1.49178500	-2.17835400
		1	1.84462700	-1.76932100	-1.27264600
		1	3.10457500	-3.01050700	-1.30277800
		6	2.92294800	-1.93072500	1.27727400
		1	3.36183300	-1.49124600	2.17839800
		1	3.10445700	-3.01018800	1.30317100
		1	1.84451600	-1.76901400	1.27262300
		6	-5.12581400	2.10383900	0.00018600
		1	-4.72131300	2.59907900	0.88763200
		1	-6.20842200	2.21221600	0.00043000
		6	5.12577500	2.10385800	-0.00059500
		1	6.20838000	2.21227000	-0.00160500
		1	4.72224100	2.59915000	0.88726600
		7	-4.78600000	0.68507800	0.00004200
		7	-2.22082000	4.64910100	0.00026800
		7	2.22075700	4.64917900	0.00008500
		7	4.78599800	0.68509300	-0.00033600
		8	0.00001100	-1.38136700	-0.00018700
		1	4.72066600	2.59913800	-0.88773600
		1	-4.72169600	2.59918400	-0.88737600
	Cation	6	-5.75352500	-0.34252100	-0.00007900
		6	-7.14419700	-0.22968200	-0.00011600
		1	-7.65588200	0.72570500	-0.00031100
		6	-7.87640400	-1.41954300	0.00011800
		1	-8.96039800	-1.37439300	0.00010200
		6	-7.23312000	-2.66462600	0.00037800
		1	-7.82667200	-3.57302400	0.00056200
		6	-5.83446000	-2.75073200	0.00040500
		1	-5.34687100	-3.72079600	0.00060600
		6	-5.09454900	-1.57504900	0.00017400
		6	-3.59556200	-1.34754500	0.00012100
		6	-3.52528800	0.18052600	-0.00009900
		6	-2.42932600	1.07761700	-0.00012900
		1	-2.71870900	2.12128200	-0.00018300
		6	-1.05761000	0.90115600	-0.00006900
		6	0.00001000	-0.16583200	-0.00008200
		6	0.00000100	1.90980100	-0.00002000
		6	1.05758900	0.90115700	-0.00001100
		6	2.42932300	1.07759500	0.00008300
		1	2.71870700	2.12126100	0.00016600
		6	3.52527200	0.18051000	0.00006100
		6	3.59557100	-1.34756100	-0.00014700
		6	5.09456000	-1.57504300	-0.00012100
		6	5.83448200	-2.75071800	-0.00027500
		1	5.34689900	-3.72078600	-0.00045400
		6	7.23314000	-2.66460200	-0.00020400
		1	7.82670300	-3.57299300	-0.00032900

		6	7.87641100	-1.41951000	0.00002000
		1	8.96040500	-1.37434900	0.00007100
		6	7.14419400	-0.22965800	0.00017800
		1	7.65587200	0.72573300	0.00034200
		6	5.75352100	-0.34250400	0.00009800
		6	-0.00000500	3.29841300	0.00000500
		6	-1.22030800	4.03225700	-0.00000900
		6	1.22029800	4.03226100	0.00012400
		6	-2.95464000	-1.94117700	-1.28199400
		1	-3.40133800	-1.50996900	-2.18258800
		1	-3.13318300	-3.02008700	-1.29902300
		1	-1.87716000	-1.77891800	-1.29039200
		6	-2.95450500	-1.94090000	1.28227500
		1	-3.40104000	-1.50944500	2.18283000
		1	-1.87701100	-1.77871000	1.29048000
		1	-3.13310800	-3.01979500	1.29959800
		6	2.95459900	-1.94092800	-1.28233800
		1	3.40120700	-1.50949100	-2.18286600
		1	1.87710800	-1.77872700	-1.29062800
		1	3.13318800	-3.01982600	-1.29963600
		6	2.95458300	-1.94119700	1.28193300
		1	3.40117200	-1.50992500	2.18254900
		1	3.13320100	-3.02009400	1.29901300
		1	1.87709100	-1.77901000	1.29023100
		6	-5.11775100	2.11180000	-0.00057000
		1	-4.71506700	2.59953400	0.89006300
		1	-6.19924500	2.21702900	-0.00069600
		6	5.11769300	2.11180700	0.00041100
		1	6.19918100	2.21708600	0.00060400
		1	4.71475700	2.59923500	0.89110000
		7	-4.77715400	0.68362800	-0.00025300
		7	-2.24745000	4.58505900	-0.00001400
		7	2.24745400	4.58503800	0.00019100
		7	4.77714800	0.68362700	0.00019900
		8	0.00001000	-1.38375400	-0.00014600
		1	4.71505500	2.59944400	-0.89030100
		1	-4.71490700	2.59915600	-0.89133900
	Anion	6	-5.77424000	-0.33773000	0.00009100
		6	-7.17430500	-0.27750100	0.00026000
		1	-7.70649600	0.66813500	0.00045500
		6	-7.88773600	-1.48409600	0.00021400
		1	-8.97447500	-1.45200800	0.00033800
		6	-7.23112700	-2.71781300	0.00003400
		1	-7.80310200	-3.64113100	0.00000900
		6	-5.82397300	-2.75809500	-0.00009500
		1	-5.30765700	-3.71517000	-0.00021800
		6	-5.10248200	-1.57537100	-0.00006300
		6	-3.59661900	-1.34037300	-0.00016100

		6	-3.52342800	0.19562600	0.00001000
		6	-2.45891400	1.07048000	0.00008600
		1	-2.74408100	2.11731200	0.00027600
		6	-1.05223700	0.90759000	0.00005200
		6	-0.00000800	-0.14158900	-0.00013700
		6	-0.00000700	1.90714000	0.00014500
		6	1.05225800	0.90758500	0.00000200
		6	2.45891400	1.07049200	0.00004700
		1	2.74407400	2.11732500	0.00022900
		6	3.52346000	0.19564800	-0.00015800
		6	3.59663400	-1.34035700	-0.00003700
		6	5.10249400	-1.57536600	0.00014800
		6	5.82398800	-2.75808600	0.00044100
		1	5.30767800	-3.71516300	0.00057500
		6	7.23114400	-2.71779500	0.00057900
		1	7.80312100	-3.64111200	0.00081900
		6	7.88775000	-1.48407900	0.00044900
		1	8.97449000	-1.45198500	0.00060100
		6	7.17431400	-0.27748300	0.00016800
		1	7.70649700	0.66815600	0.00017900
		6	5.77425600	-0.33772600	-0.00003400
		6	-0.00002600	3.31554700	0.00024900
		6	-1.20306900	4.07102900	0.00041400
		6	1.20297500	4.07109700	0.00012300
		6	-2.95134800	-1.94762500	-1.27045400
		1	-3.38883900	-1.50999100	-2.17383600
		1	-3.12951100	-3.02967500	-1.29446700
		1	-1.87258200	-1.78123800	-1.26529100
		6	-2.95113700	-1.94791900	1.26988000
		1	-3.38851200	-1.51052900	2.17343900
		1	-1.87237700	-1.78150400	1.26459600
		1	-3.12924200	-3.02998400	1.29365300
		6	2.95142100	-1.94780700	-1.27028000
		1	3.38895700	-1.51030500	-2.17370500
		1	1.87265500	-1.78142000	-1.26518000
		1	3.12957600	-3.02986200	-1.29412000
		6	2.95110500	-1.94769900	1.27005800
		1	3.38842700	-1.51016200	2.17357200
		1	3.12922000	-3.02975800	1.29401000
		1	1.87234300	-1.78131400	1.26470600
		6	-5.17174700	2.10077900	-0.00010800
		1	-4.76286300	2.60195900	0.88524200
		1	-6.25481100	2.22349300	-0.00055400
		6	5.17181600	2.10077200	-0.00098300
		1	6.25489000	2.22343800	-0.00224400
		1	4.76358700	2.60212800	0.88457400
		7	-4.84520100	0.69044600	0.00009200
		7	-2.18926200	4.70259600	0.00044600

		7	2.18908900	4.70278500	-0.00004900
		7	4.84521400	0.69045000	-0.00038400
		8	-0.00001000	-1.37782600	-0.00036100
		1	4.76165200	2.60162200	-0.88590600
		1	-4.76218700	2.60177300	-0.88523900
CSQ-2	Neutral	17	-8.11011600	-3.70984500	-0.00037000
		17	8.11017700	-3.70977700	-0.00059200
		8	0.00004500	-0.90008400	0.00072200
		6	0.00003300	0.33139600	0.00038700
		7	4.78566200	1.16516300	0.00068000
		7	-4.78560000	1.16512700	0.00026200
		6	-2.43284100	1.56485200	0.00005700
		1	-2.71704600	2.61007900	-0.00002800
		6	2.43288400	1.56488500	0.00036300
		1	2.71708700	2.61010300	0.00050100
		6	-0.00001100	2.39972100	-0.00027300
		6	1.04327200	1.38690800	0.00011000
		6	-5.78063400	-2.28760300	-0.00016000
		1	-5.28261000	-3.25138300	-0.00026900
		6	7.85126800	-0.99413300	0.00038200
		1	8.93526100	-0.97411000	0.00057800
		6	-1.21453700	4.53667000	-0.00070800
		6	-7.17983400	-2.21816500	-0.00020900
		6	-7.85121600	-0.99420000	-0.00011900
		1	-8.93520900	-0.97418100	-0.00017000
		6	-3.50568500	0.67688000	0.00022100
		6	5.73704400	0.12854500	0.00046900
		7	-2.22438200	5.12448800	-0.00054500
		6	-1.04323500	1.38687500	0.00002100
		6	5.78069200	-2.28755600	-0.00038800
		1	5.28268600	-3.25134100	-0.00077900
		6	5.06616300	-1.09863900	-0.00006800
		7	2.22373900	5.12514700	-0.00174100
		6	-5.73699800	0.12850900	0.00010000
		6	-3.56583900	-0.85788900	0.00015700
		6	3.50573900	0.67692200	0.00033500
		6	-5.06611600	-1.09867800	0.00000000
		6	7.12918500	0.20472100	0.00071600
		1	7.66126000	1.14925200	0.00117200
		6	-0.00012400	3.79477900	-0.00067600
		6	2.92101400	-1.45168100	1.27750400
		1	3.10079600	-2.53137800	1.30279100
		1	1.84279300	-1.28876500	1.27237800
		1	3.35994700	-1.01288400	2.17888300
		6	-7.12914400	0.20465900	0.00002200
		1	-7.66124600	1.14918000	0.00002300
		6	1.21409400	4.53698800	-0.00080700
		6	3.56588700	-0.85785200	-0.00004500

		6	2.92084900	-1.45125300	-1.27764200
		1	3.35950700	-1.01204700	-2.17894500
		1	1.84261700	-1.28854100	-1.27221500
		1	3.10074700	-2.53091700	-1.30336800
		6	7.17988800	-2.21810000	-0.00018400
		6	-2.92067300	-1.45152200	-1.27728700
		1	-3.10044600	-2.53121200	-1.30278500
		1	-1.84245200	-1.28863700	-1.27186900
		1	-3.35935400	-1.01259300	-2.17871400
		6	-2.92104700	-1.45145600	1.27784600
		1	-3.36005700	-1.01250900	2.17911300
		1	-1.84284000	-1.28852000	1.27274900
		1	-3.10078900	-2.53115700	1.30329900
		6	5.12693200	2.58402700	0.00136600
		1	4.72259800	3.07977100	-0.88575800
		1	4.72353700	3.07864000	0.88956300
		1	6.20962900	2.69187900	0.00082600
		6	-5.12677300	2.58401400	0.00043300
		1	-4.72240600	3.07913300	0.88789600
		1	-4.72330900	3.07917900	-0.88742600
		1	-6.20945400	2.69196300	0.00099900
	Cation	17	-8.16724400	-3.65332900	0.00006000
		17	8.16734100	-3.65324400	-0.00004000
		8	0.00001500	-0.90955600	-0.00003600
		6	0.00001500	0.30862100	0.00004000
		7	4.77759000	1.15619900	-0.00000700
		7	-4.77758700	1.15617900	-0.00007700
		6	-2.42953100	1.55101200	0.00012400
		1	-2.71949900	2.59456100	0.00019900
		6	2.42955000	1.55100300	0.00000200
		1	2.71954100	2.59454400	0.00002900
		6	-0.00000600	2.38425600	0.00008700
		6	1.05721300	1.37528100	0.00005100
		6	-5.82153900	-2.28140100	0.00006300
		1	-5.34096500	-3.25362400	0.00013800
		6	7.87641700	-0.95045500	0.00005700
		1	8.95980200	-0.91801700	0.00009900
		6	-1.22101600	4.50553100	0.00003100
		6	-7.22030200	-2.18937700	-0.00000900
		6	-7.87637100	-0.95053600	-0.00012900
		1	-8.95975600	-0.91811600	-0.00020100
		6	-3.52380700	0.65396300	0.00004200
		6	5.75062100	0.13109300	0.00001800
		7	-2.24977000	5.05529600	0.00006600
		6	-1.05720500	1.37527200	0.00008300
		6	5.82161000	-2.28136100	-0.00006900
		1	5.34105900	-3.25359500	-0.00012800
		6	5.09219600	-1.10187500	-0.00004700

		7	2.24939000	5.05568200	-0.00010700
		6	-5.75059800	0.13105400	-0.00007400
		6	-3.59262500	-0.87486300	0.00008200
		6	3.52382300	0.65395800	-0.00002300
		6	-5.09214900	-1.10190000	0.00002700
		6	7.14200500	0.23561900	0.00007700
		1	7.66127800	1.18679800	0.00015700
		6	-0.00008100	3.77275100	0.00003500
		6	2.95290400	-1.46897700	1.28228500
		1	3.13021800	-2.54809500	1.29949400
		1	1.87559100	-1.30589800	1.28988700
		1	3.39917000	-1.03771000	2.18302600
		6	-7.14198200	0.23555300	-0.00016500
		1	-7.66127600	1.18672200	-0.00026100
		6	1.22072100	4.50575700	-0.00006100
		6	3.59266700	-0.87486700	-0.00006500
		6	2.95290300	-1.46894900	-1.28242000
		1	3.39919200	-1.03768400	-2.18315100
		1	1.87559500	-1.30585100	-1.29003200
		1	3.13018700	-2.54807100	-1.29962300
		6	7.22037000	-2.18930800	-0.00001900
		6	-2.95281800	-1.46894300	-1.28227100
		1	-3.13011400	-2.54806200	-1.29949800
		1	-1.87550600	-1.30583900	-1.28983400
		1	-3.39907000	-1.03766500	-2.18301200
		6	-2.95286000	-1.46893900	1.28242800
		1	-3.39916100	-1.03769100	2.18316300
		1	-1.87555500	-1.30582600	1.29004900
		1	-3.13013200	-2.54806600	1.29963400
		6	5.11959200	2.58435400	0.00008900
		1	4.71661400	3.07209700	-0.89036100
		1	4.71759100	3.07173400	0.89119000
		1	6.20120700	2.68921300	-0.00051500
		6	-5.11963900	2.58432400	-0.00013200
		1	-4.71754200	3.07184300	0.89084800
		1	-4.71680000	3.07195700	-0.89070800
		1	-6.20125900	2.68913900	-0.00059100
	Anion	17	-8.14172400	-3.72957500	-0.00138700
		17	8.14188100	-3.72943600	0.00086600
		8	-0.00000800	-0.89518700	0.00054000
		6	-0.00000300	0.34097200	0.00029100
		7	4.84381700	1.17282300	-0.00090300
		7	-4.84383500	1.17280300	0.00119900
		6	-2.45788200	1.55287300	0.00059000
		1	-2.74373500	2.59948400	0.00079500
		6	2.45789100	1.55284400	-0.00049400
		1	2.74377300	2.59944500	-0.00097300
		6	-0.00000600	2.39063300	0.00000900

	6	1.05166600	1.39019400	-0.00003000
	6	-5.81152100	-2.27957400	-0.00063800
	1	-5.30607200	-3.24004800	-0.00113000
	6	7.88874900	-1.00218400	-0.00060400
	1	8.97349100	-0.98489600	-0.00088800
	6	-1.20441100	4.55167700	-0.00001900
	6	-7.21368800	-2.22041800	-0.00064000
	6	-7.88868600	-1.00231500	-0.00007900
	1	-8.97342700	-0.98506600	-0.00013300
	6	-3.52142100	0.67763300	0.00064800
	6	5.77096100	0.14589000	-0.00067400
	7	-2.19379300	5.17787800	-0.00001300
	6	-1.05166600	1.39019600	0.00026800
	6	5.81163200	-2.27951600	0.00064100
	1	5.30621800	-3.24000900	0.00128100
	6	5.09918900	-1.09205100	0.00015800
	7	2.19325800	5.17845600	-0.00009200
	6	-5.77093700	0.14583000	0.00056900
	6	-3.59302200	-0.85866200	0.00014400
	6	3.52142600	0.67760000	-0.00037900
	6	-5.09911900	-1.09208300	-0.00004400
	6	7.17057600	0.20133300	-0.00109000
	1	7.70909100	1.14284600	-0.00174900
	6	-0.00008100	3.79795100	-0.00003600
	6	2.94943800	-1.46616500	1.27126500
	1	3.12641600	-2.54824900	1.29541300
	1	1.87083600	-1.29922300	1.26525100
	1	3.38643400	-1.02832300	2.17465000
	6	-7.17055300	0.20122700	0.00052600
	1	-7.70909700	1.14272400	0.00088700
	6	1.20412200	4.55187000	-0.00005900
	6	3.59308300	-0.85869200	0.00033400
	6	2.94907400	-1.46732700	-1.26987300
	1	3.38581700	-1.03029600	-2.17377700
	1	1.87047200	-1.30039800	-1.26369400
	1	3.12607300	-2.54942800	-1.29308600
	6	7.21379600	-2.22031300	0.00025900
	6	-2.94901400	-1.46634000	-1.27049100
	1	-3.12593400	-2.54843800	-1.29446700
	1	-1.87042100	-1.29934800	-1.26424300
	1	-3.38580400	-1.02871200	-2.17408100
	6	-2.94929600	-1.46702300	1.27064100
	1	-3.38633500	-1.02988200	2.17434500
	1	-1.87071300	-1.29994700	1.26471600
	1	-3.12617600	-2.54913900	1.29399000
	6	5.17140300	2.58361900	-0.00213200
	1	4.76269200	3.08329800	-0.88811000
	1	4.76225100	3.08493800	0.88268900

		1	6.25448100	2.70604200	-0.00194600
		6	-5.17154600	2.58357200	0.00142400
		1	-4.76187100	3.08410100	0.88645100
		1	-4.76347400	3.08411500	-0.88435800
		1	-6.25463900	2.70588200	0.00246000
CSQ-3	Neutral	35	-8.17904100	-3.39254000	-0.00255900
		35	8.17914700	-3.39244200	0.00142800
		7	-2.22442300	5.57486400	-0.00104100
		6	-3.50430300	1.12660200	0.00155500
		6	-1.21447000	4.98724400	-0.00094500
		6	-5.73463400	0.57646300	0.00213000
		6	2.91871300	-1.00049300	1.27866900
		1	3.09766800	-2.08028000	1.30427700
		1	1.84065900	-0.83682800	1.27463700
		1	3.35900500	-0.56157000	2.17929400
		6	-0.00006600	4.24537600	-0.00077600
		8	0.00002500	-0.44906700	0.00157000
		6	1.04308300	1.83767900	-0.00031800
		6	-2.43261000	2.01550400	0.00131000
		1	-2.71731100	3.06055500	0.00174600
		6	7.12682000	0.65080300	-0.00215800
		1	7.66051500	1.59440600	-0.00321500
		7	4.78481300	1.61371300	-0.00191400
		6	3.50430200	1.12655600	-0.00104700
		7	2.22411000	5.57517800	-0.00129700
		6	-5.06236700	-0.64984700	0.00040000
		6	-3.56281100	-0.40789000	0.00039800
		7	-4.78481900	1.61372700	0.00291700
		6	0.00000000	0.78235700	0.00091000
		6	-0.00001000	2.85056700	-0.00025600
		6	3.56287400	-0.40793900	0.00015500
		6	-5.77347300	-1.84031400	-0.00088500
		1	-5.27133400	-2.80155100	-0.00223100
		6	-1.04311000	1.83768300	0.00057400
		6	1.21426900	4.98736500	-0.00113600
		6	2.43258800	2.01545900	-0.00124000
		1	2.71730100	3.06049500	-0.00211800
		6	5.73466400	0.57645100	-0.00143500
		6	2.91827500	-1.00242100	-1.27722500
		1	3.35818200	-0.56483000	-2.17869400
		1	1.84021300	-0.83880500	-1.27305800
		1	3.09728100	-2.08223400	-1.30133200
		6	5.06236700	-0.64985300	-0.00002100
		6	7.17188700	-1.77182000	-0.00001400
		6	-2.91815500	-1.00093200	-1.27745300
		1	-3.35771400	-0.56202500	-2.17846400
		1	-3.09755200	-2.08063400	-1.30301500
		1	-1.84004500	-0.83771000	-1.27290200

		6	7.84576600	-0.54995000	-0.00135900
		1	8.92951000	-0.52826200	-0.00180600
		6	5.77356400	-1.84027500	0.00074100
		1	5.27150400	-2.80155600	0.00204700
		6	-7.84569900	-0.55005200	0.00148900
		1	-8.92944500	-0.52839400	0.00190200
		6	-7.17179800	-1.77191700	-0.00032900
		6	-2.91887500	-1.00173000	1.27854000
		1	-3.09769800	-2.08156900	1.30304500
		1	-3.35946300	-0.56373800	2.17947300
		1	-1.84082700	-0.83794900	1.27498500
		6	-7.12682000	0.65072700	0.00280300
		1	-7.66059700	1.59428500	0.00441900
		6	5.12775500	3.03219700	-0.00356100
		1	4.72475500	3.52667400	-0.89199000
		1	4.72442900	3.52884300	0.88349700
		1	6.21061400	3.13857800	-0.00345200
		6	-5.12788800	3.03217900	0.00454100
		1	-4.72341100	3.52704300	0.89205500
		1	-4.72616500	3.52849800	-0.88344500
		1	-6.21076400	3.13842900	0.00636200
	Cation	35	-8.23876900	-3.34280000	-0.00018100
		35	8.23876700	-3.34280200	0.00011800
		7	-2.24969500	5.49991500	0.00003000
		6	-3.52229800	1.09754200	0.00002900
		6	-1.22091300	4.95018800	-0.00000500
		6	-5.74820600	0.57263500	0.00010000
		6	2.95031500	-1.02483100	1.28288100
		1	3.12677900	-2.10409500	1.29966100
		1	1.87314400	-0.86094900	1.29166800
		1	3.39792600	-0.59418800	2.18327100
		6	-0.00001100	4.21737600	-0.00001600
		8	0.00001300	-0.46457300	0.00035100
		6	1.05698000	1.82002400	0.00002500
		6	-2.42931800	1.99546200	-0.00013800
		1	-2.71984900	3.03886300	-0.00035600
		6	7.13962200	0.67493700	-0.00043000
		1	7.66084100	1.62508900	-0.00072100
		7	4.77680400	1.59853600	-0.00019600
		6	3.52230100	1.09755600	-0.00010200
		7	2.24967500	5.49990700	0.00013700
		6	-5.08826300	-0.65938700	-0.00002900
		6	-3.58950800	-0.43108700	-0.00000600
		7	-4.77679800	1.59852900	0.00012500
		6	0.00000700	0.75367700	0.00019100
		6	-0.00000200	2.82907200	-0.00001700
		6	3.58950700	-0.43108200	0.00012900
		6	-5.81447000	-1.84040000	-0.00011300

		1	-5.32934900	-2.81005800	-0.00021900
		6	-1.05697800	1.82001700	0.00007000
		6	1.22087200	4.95021700	0.00005400
		6	2.42932200	1.99547900	-0.00032800
		1	2.71984800	3.03887900	-0.00073700
		6	5.74821000	0.57264300	-0.00020000
		6	2.95016500	-1.02521700	-1.28236600
		1	3.39767200	-0.59485100	-2.18294100
		1	1.87299400	-0.86133800	-1.29108200
		1	3.12663800	-2.10448500	-1.29884000
		6	5.08827200	-0.65937800	0.00004800
		6	7.21240700	-1.75038900	-0.00001300
		6	-2.95014400	-1.02501400	-1.28259200
		1	-3.39758900	-0.59445100	-2.18310300
		1	-3.12665500	-2.10427100	-1.29928100
		1	-1.87296600	-0.86116500	-1.29121600
		6	7.87058600	-0.51338900	-0.00033000
		1	8.95376800	-0.47908100	-0.00050800
		6	5.81446600	-1.84039600	0.00016600
		1	5.32932800	-2.81004600	0.00039400
		6	-7.87058600	-0.51338500	0.00007700
		1	-8.95376900	-0.47907100	0.00013200
		6	-7.21241200	-1.75038200	-0.00006200
		6	-2.95031300	-1.02506900	1.28265100
		1	-3.12678000	-2.10433600	1.29921200
		1	-3.39795400	-0.59461000	2.18311600
		1	-1.87314700	-0.86117200	1.29148900
		6	-7.13961700	0.67493800	0.00015700
		1	-7.66083000	1.62509300	0.00026500
		6	5.12044800	3.02619400	-0.00039900
		1	4.71989600	3.51378400	-0.89204900
		1	4.71730600	3.51465800	0.88958000
		1	6.20221300	3.12970300	0.00119800
		6	-5.12044100	3.02618700	0.00033700
		1	-4.71831000	3.51413800	0.89106300
		1	-4.71888000	3.51428900	-0.89056900
		1	-6.20220700	3.12969700	0.00067600
	Anion	35	8.21284100	-3.40588600	0.00043300
		35	-8.21281600	-3.40590700	-0.00091600
		7	2.19407100	5.62726700	-0.00100700
		6	3.52021300	1.12770100	-0.00036100
		6	1.20438000	5.00162000	-0.00073700
		6	5.76901200	0.59616700	-0.00056400
		6	-2.94811600	-1.01629400	-1.27049500
		1	-3.12487300	-2.09838800	-1.29384600
		1	-1.86954600	-0.84925200	-1.26526200
		1	-3.38578100	-0.57915700	-2.17389200
		6	-0.00002100	4.24800500	-0.00038300

		8	0.00000400	-0.44472600	0.00057300
		6	-1.05142700	1.84048500	0.00016800
		6	2.45735800	2.00331700	-0.00050900
		1	2.74336600	3.04986600	-0.00097700
		6	-7.16871000	0.65105400	0.00044400
		1	-7.70806400	1.59208800	0.00052100
		7	-4.84279000	1.62269700	0.00133200
		6	-3.52021000	1.12770100	0.00073200
		7	-2.19418800	5.62715100	0.00020900
		6	5.09671300	-0.64161600	0.00001100
		6	3.59116600	-0.40825800	0.00016500
		7	4.84278900	1.62270000	-0.00076300
		6	-0.00000400	0.79134300	0.00027900
		6	-0.00001100	2.84105700	-0.00016500
		6	-3.59115400	-0.40826000	0.00043100
		6	5.80646200	-1.82994200	0.00031500
		1	5.29813300	-2.78847600	0.00076200
		6	1.05142200	1.84049400	-0.00016000
		6	-1.20444300	5.00159000	-0.00013100
		6	-2.45736700	2.00331300	0.00044200
		1	-2.74337400	3.04986700	0.00036200
		6	-5.76900300	0.59615500	0.00069900
		6	-2.94821700	-1.01678000	1.27116000
		1	-3.38596900	-0.58002600	2.17470300
		1	-1.86964900	-0.84968900	1.26608100
		1	-3.12492700	-2.09889500	1.29407400
		6	-5.09670000	-0.64162500	0.00028800
		6	-7.20786400	-1.76982200	-0.00026400
		6	2.94837400	-1.01610500	1.27128600
		1	3.38624500	-0.57889700	2.17455000
		1	3.12505600	-2.09821400	1.29473300
		1	1.86980800	-0.84901600	1.26626600
		6	-7.88481700	-0.55332300	-0.00000900
		1	-8.96929700	-0.53380400	-0.00021800
		6	-5.80644700	-1.82995300	-0.00015000
		1	-5.29811300	-2.78848400	-0.00040700
		6	7.88482900	-0.55330400	-0.00055900
		1	8.96930800	-0.53378300	-0.00077900
		6	7.20787800	-1.76980400	0.00002500
		6	2.94800400	-1.01697900	-1.27036700
		1	3.12475800	-2.09908600	-1.29315900
		1	3.38557100	-0.58032600	-2.17404700
		1	1.86943500	-0.84991800	-1.26509800
		6	7.16871400	0.65106900	-0.00087000
		1	7.70806700	1.59210500	-0.00134500
		6	-5.17080700	3.03353700	0.00177200
		1	-4.75972800	3.53399200	0.88610200
		1	-4.76429500	3.53378700	-0.88483500

		1	-6.25389700	3.15560900	0.00467600
		6	5.17077500	3.03354800	-0.00108600
		1	4.76244000	3.53361100	-0.88694300
		1	4.76147800	3.53417300	0.88399400
		1	6.25386400	3.15564400	-0.00051300
CSQ-4	Neutral	53	8.31158500	-3.18253700	0.00025900
		53	-8.31157900	-3.18254000	-0.00034200
		6	-1.04322300	2.23880200	0.00023000
		8	0.00001100	-0.04851200	0.00036000
		6	0.00000900	1.18316300	0.00025400
		7	4.78625900	2.01722500	-0.00063900
		6	-5.78240500	-1.43613000	-0.00011500
		1	-5.27236100	-2.39357400	-0.00032600
		6	5.73735100	0.98065100	-0.00049200
		7	-4.78625200	2.01722100	0.00051800
		6	-3.50599200	1.52870300	0.00036300
		7	-2.22472500	5.97632200	-0.00004300
		6	-2.92102500	-0.59946500	-1.27776000
		1	-3.10057900	-1.67931300	-1.30346600
		1	-1.84273300	-0.43636000	-1.27277700
		1	-3.36017700	-0.16058300	-2.17912400
		6	2.43309300	2.41688000	-0.00026700
		1	2.71730200	3.46223600	-0.00051000
		6	-2.92113700	-0.59981900	1.27793900
		1	-3.36040300	-0.16122400	2.17938400
		1	-1.84284700	-0.43668400	1.27311300
		1	-3.10065700	-1.67968100	1.30330400
		6	7.85108300	-0.14452700	-0.00057700
		1	8.93473200	-0.11141100	-0.00078700
		6	-1.21459100	5.38883900	-0.00002800
		6	3.56618300	-0.00612600	0.00003100
		6	-7.18255900	-1.37085200	-0.00005200
		6	5.12773800	3.43611700	-0.00056200
		1	4.72420500	3.93167600	-0.88839300
		1	6.21067000	3.54375600	-0.00028100
		6	0.00000700	3.25159400	0.00008300
		6	-7.12931900	1.05628900	0.00040400
		1	-7.66271400	2.00039200	0.00058400
		6	-3.56618300	-0.00613300	0.00014500
		6	1.21456900	5.38885900	-0.00022900
		6	5.06696600	-0.24644200	-0.00008200
		7	2.22465900	5.97641600	-0.00038600
		6	-5.12773500	3.43611300	0.00081700
		1	-6.21066800	3.54374600	0.00100000
		1	-4.72411500	3.93182200	-0.88689200
		6	3.50599500	1.52870900	-0.00030000
		6	-0.00000700	4.64692700	-0.00001100
		6	1.04323200	2.23880400	0.00001300

		6	2.92119900	-0.59932500	1.27809600
		1	3.10071100	-1.67917600	1.30384900
		1	1.84291500	-0.43617900	1.27325200
		1	3.36051300	-0.16038600	2.17934500
		6	-5.73735000	0.98065000	0.00033900
		6	-7.85108300	-0.14452700	0.00020300
		1	-8.93473100	-0.11140300	0.00024800
		6	-5.06696600	-0.24644500	0.00007600
		6	2.92095200	-0.59995500	-1.27759900
		1	3.36006500	-0.16144200	-2.17916700
		1	1.84265900	-0.43682000	-1.27263600
		1	3.10049700	-1.67981500	-1.30290200
		6	-2.43308200	2.41686600	0.00039800
		1	-2.71729000	3.46222000	0.00049200
		6	5.78240600	-1.43612900	0.00011600
		1	5.27235400	-2.39357100	0.00041700
		6	7.12932300	1.05628700	-0.00079500
		1	7.66271400	2.00039300	-0.00122700
		6	7.18255600	-1.37085600	-0.00011200
		1	4.72373800	3.93164400	0.88707800
		1	-4.72383600	3.93149300	0.88858400
	Cation	53	8.37531000	-3.13632600	0.00001700
		53	-8.37529800	-3.13633300	-0.00054800
		6	-1.05696000	2.21503300	0.00013800
		8	0.00000400	-0.07015600	0.00119900
		6	-0.00000300	1.14846800	0.00051100
		7	4.77821000	1.99638900	-0.00029100
		6	-5.82390800	-1.44143400	-0.00024600
		1	-5.33030900	-2.40725000	-0.00062000
		6	5.75076100	0.97142400	-0.00031800
		7	-4.77818600	1.99637800	0.00066700
		6	-3.52377300	1.49391100	0.00032300
		7	-2.25010400	5.89529300	-0.00063900
		6	-2.95251200	-0.62913300	-1.28206500
		1	-3.12973300	-1.70842800	-1.29936800
		1	-1.87505700	-0.46590400	-1.28960200
		1	-3.39882100	-0.19803400	-2.18306100
		6	2.42976700	2.39095500	-0.00004700
		1	2.71963900	3.43471700	-0.00027800
		6	-2.95303800	-0.62884700	1.28291000
		1	-3.39981200	-0.19754000	2.18356600
		1	-1.87559800	-0.46550000	1.29086100
		1	-3.13021800	-1.70814300	1.30036300
		6	7.87544800	-0.11339400	-0.00055500
		1	8.95841600	-0.06702400	-0.00080800
		6	-1.22110600	5.34577400	-0.00056000
		6	3.59285400	-0.03497400	0.00040800
		6	-7.22397300	-1.35567700	-0.00006600

		6	5.12010300	3.42447500	-0.00065400
		1	4.71794000	3.91209800	-0.89181100
		1	6.20194400	3.52938900	-0.00013200
		6	-0.00001300	3.22409900	-0.00020200
		6	-7.14194900	1.07510500	0.00071400
		1	-7.66256800	2.02590600	0.00105100
		6	-3.59284100	-0.03500200	0.00014300
		6	1.22101300	5.34581700	-0.00078600
		6	5.09288800	-0.26158800	0.00010500
		7	2.24989900	5.89554200	-0.00095300
		6	-5.12002400	3.42447400	0.00120300
		1	-6.20185800	3.52945400	0.00111300
		1	-4.71732700	3.91277800	-0.88932900
		6	3.52378100	1.49394000	-0.00002600
		6	-0.00003400	4.61291700	-0.00053400
		6	1.05695400	2.21504800	0.00002900
		6	2.95314700	-0.62842200	1.28336700
		1	3.13033500	-1.70771000	1.30115000
		1	1.87570500	-0.46509300	1.29131700
		1	3.39994700	-0.19682700	2.18387200
		6	-5.75074500	0.97142300	0.00050600
		6	-7.87543600	-0.11340200	0.00042200
		1	-8.95840300	-0.06702800	0.00057600
		6	-5.09287900	-0.26159800	0.00006600
		6	2.95243300	-0.62953300	-1.28160100
		1	3.39871500	-0.19874800	-2.18276000
		1	1.87498200	-0.46627500	-1.28912800
		1	3.12965500	-1.70883000	-1.29854300
		6	-2.42978000	2.39091800	0.00025400
		1	-2.71966500	3.43467400	0.00024000
		6	5.82391800	-1.44142400	0.00019200
		1	5.33031800	-2.40724000	0.00049600
		6	7.14196000	1.07511300	-0.00066400
		1	7.66256700	2.02592200	-0.00105500
		6	7.22398400	-1.35566900	-0.00013000
		1	4.71711300	3.91275600	0.88974600
		1	-4.71751300	3.91203100	0.89222600
	Anion	53	8.34061300	-3.19655900	0.00160400
		53	-8.34060300	-3.19656800	-0.00183500
		6	-1.05159500	2.24510400	0.00059000
		8	-0.00000600	-0.04060400	0.00033300
		6	-0.00000500	1.19572700	0.00015700
		7	4.84418700	2.02799600	-0.00318400
		6	-5.81239100	-1.42494900	-0.00029900
		1	-5.29606900	-2.37947000	-0.00143000
		6	5.77098600	1.00155500	-0.00215500
		7	-4.84419400	2.02799800	0.00359800
		6	-3.52150600	1.53243000	0.00198300

		7	-2.19450800	6.03219000	0.00153700
		6	-2.94936800	-0.61112600	-1.27045700
		1	-3.12601000	-1.69336800	-1.29484200
		1	-1.87067000	-0.44396400	-1.26459700
		1	-3.38661100	-0.17331900	-2.17388600
		6	2.45798500	2.40784600	-0.00143900
		1	2.74391500	3.45460900	-0.00195700
		6	-2.94913100	-0.61293200	1.27118600
		1	-3.38626500	-0.17644300	2.17530800
		1	-1.87044400	-0.44565500	1.26536600
		1	-3.12571000	-1.69521900	1.29405500
		6	7.88922200	-0.14787400	-0.00136600
		1	8.97359100	-0.11831700	-0.00155300
		6	-1.20465800	5.40661600	0.00069900
		6	3.59305800	-0.00395500	-0.00053900
		6	-7.21532600	-1.36735100	-0.00001000
		6	5.17163900	3.43910200	-0.00468300
		1	4.75962500	3.93917800	-0.88903800
		1	6.25486200	3.56175000	-0.00845300
		6	-0.00000400	3.24559900	-0.00010000
		6	-7.17061100	1.05673100	0.00248400
		1	-7.71043700	1.99784700	0.00333700
		6	-3.59305800	-0.00395000	0.00083800
		6	1.20464100	5.40662500	-0.00128800
		6	5.09979800	-0.23650600	-0.00068400
		7	2.19449000	6.03220100	-0.00220000
		6	-5.17165200	3.43910100	0.00496200
		1	-6.25487300	3.56174400	0.00950400
		1	-4.76611400	3.93987600	-0.88205700
		6	3.52150200	1.53242500	-0.00173300
		6	-0.00000600	4.65306000	-0.00024000
		6	1.05158800	2.24510100	-0.00055400
		6	2.94952200	-0.61107100	1.27086800
		1	3.12613200	-1.69331800	1.29526800
		1	1.87082900	-0.44386600	1.26514100
		1	3.38690200	-0.17324700	2.17422400
		6	-5.77099000	1.00155300	0.00235000
		6	-7.88922200	-0.14788100	0.00132700
		1	-8.97359100	-0.11832900	0.00140900
		6	-5.09979700	-0.23650500	0.00084400
		6	2.94898500	-0.61300800	-1.27077400
		1	3.38599800	-0.17656000	-2.17497300
		1	1.87029600	-0.44575300	-1.26483400
		1	3.12557800	-1.69529400	-1.29360800
		6	-2.45799200	2.40785100	0.00147500
		1	-2.74392000	3.45461600	0.00183100
		6	5.81239500	-1.42494800	0.00035600
		1	5.29607500	-2.37947000	0.00145900

		6	7.17060700	1.05673600	-0.00241400
		1	7.71043200	1.99785300	-0.00331100
		6	7.21533000	-1.36734600	-0.00003000
		1	4.76547200	3.94005800	0.88193800
		1	-4.75901800	3.93936200	0.88891600
CSQ-5	Neutral	9	7.39420600	-3.75879600	-0.00021400
		9	-7.39419900	-3.75880600	-0.00010600
		8	0.00002000	-0.67169400	0.00005400
		7	2.25056300	5.31102400	-0.00005000
		7	2.80203200	-0.77875100	0.00040700
		7	-2.25069400	5.31096400	0.00034000
		7	-2.80201500	-0.77877800	-0.00000500
		6	1.03806200	1.61842700	0.00005900
		6	0.00000000	2.64186600	0.00004100
		6	-1.03804700	1.61841600	0.00007800
		6	0.00001700	0.58575700	0.00007100
		6	-0.00003800	4.02653100	0.00005400
		6	1.22619800	4.75141300	-0.00001200
		6	-1.22631500	4.75136700	0.00018300
		6	2.43393700	1.63757700	-0.00009900
		6	3.23713200	0.50094100	0.00002400
		6	4.77222300	0.50706400	-0.00023400
		6	5.31708900	1.20433800	1.26952800
		6	5.31687400	1.20432200	-1.27004500
		6	5.07317900	-0.98545500	-0.00013200
		6	6.28038700	-1.67148400	-0.00029200
		6	6.22317400	-3.06637700	-0.00003400
		6	5.02962700	-3.78080600	0.00038000
		6	3.81340900	-3.08626300	0.00055100
		6	3.86350900	-1.69483300	0.00026300
		6	-2.43392300	1.63756300	-0.00002900
		6	-3.23712000	0.50091100	-0.00007000
		6	-4.77220600	0.50704000	-0.00008700
		6	-5.31688300	1.20426500	1.26977100
		6	-5.31701800	1.20435600	-1.26981200
		6	-5.07316600	-0.98547300	-0.00008100
		6	-6.28037600	-1.67149900	-0.00011300
		6	-6.22316500	-3.06639200	-0.00009200
		6	-5.02961800	-3.78082400	-0.00005800
		6	-3.81339800	-3.08628300	-0.00003200
		6	-3.86349700	-1.69485400	-0.00002900
		1	2.93122900	2.60074100	-0.00029700
		1	4.93315100	0.73193400	2.17810300
		1	5.03481300	2.26106400	1.28170500
		1	6.40979700	1.14228900	1.28572500
		1	4.93289300	0.73185300	-2.17856700

		1	6.40958500	1.14238800	-1.28634200
		1	5.03452300	2.26102800	-1.28223600
		1	7.24304600	-1.17080600	-0.00064000
		1	5.05789100	-4.86472000	0.00056400
		1	2.86965300	-3.62159700	0.00088600
		1	1.79820700	-1.01853000	0.00048400
		1	-2.93121100	2.60073000	-0.00007300
		1	-5.03451400	2.26096600	1.28199400
		1	-4.93289600	0.73176700	2.17827600
		1	-6.40959400	1.14231300	1.28607200
		1	-5.03466700	2.26106300	-1.28199100
		1	-4.93314200	0.73192800	-2.17840000
		1	-6.40973100	1.14241700	-1.28598700
		1	-7.24303500	-1.17082000	-0.00013000
		1	-5.05788800	-4.86473700	-0.00006500
		1	-2.86964200	-3.62161700	-0.00001300
		1	-1.79817400	-1.01856000	0.00002400
	Cation	9	-7.38859200	3.75025200	-0.00014500
		9	7.38858500	3.75025900	0.00039300
		8	-0.00001700	0.65800100	0.00001800
		7	-2.27590000	-5.26210700	0.00043000
		7	-2.82303100	0.77397500	-0.00004300
		7	2.27590800	-5.26210900	-0.00000100
		7	2.82302900	0.77397700	-0.00025600
		6	-1.04913800	-1.62617100	0.00000100
		6	-0.00000500	-2.64944900	-0.00011300
		6	1.04915100	-1.62617300	-0.00013800
		6	-0.00000500	-0.58708800	-0.00006600
		6	0.00000600	-4.02657700	0.00011500
		6	-1.23339000	-4.74140500	0.00032900
		6	1.23342100	-4.74136400	0.00012500
		6	-2.42843300	-1.63880900	-0.00022800
		6	-3.25302300	-0.48981500	-0.00013400
		6	-4.78076700	-0.50807000	-0.00000500
		6	-5.31760900	-1.21232300	1.27377000
		6	-5.31816900	-1.21274700	-1.27322500
		6	-5.08863400	0.98028300	-0.00005500
		6	-6.29542300	1.66516900	-0.00010300
		6	-6.23176000	3.06100000	-0.00008600
		6	-5.03418200	3.78019300	-0.00001800
		6	-3.82160800	3.08967100	0.00002300
		6	-3.88326200	1.69733800	-0.00000100
		6	2.42843500	-1.63880900	-0.00046100
		6	3.25302500	-0.48980100	-0.00032200
		6	4.78076800	-0.50806500	-0.00018200
		6	5.31772600	-1.21275200	1.27325800
		6	5.31805500	-1.21232000	-1.27373700
		6	5.08863400	0.98028700	0.00008000

		6	6.29542000	1.66517500	0.00021000
		6	6.23175200	3.06100800	0.00026700
		6	5.03417500	3.78019900	0.00017600
		6	3.82160100	3.08967400	0.00002800
		6	3.88326300	1.69734500	0.00001500
		1	-2.93334200	-2.59878500	-0.00041500
		1	-4.93748200	-0.74160600	2.18449200
		1	-5.03952100	-2.26979900	1.28100000
		1	-6.40921700	-1.15052300	1.28650900
		1	-4.93835900	-0.74245400	-2.18430400
		1	-6.40978000	-1.15085100	-1.28557000
		1	-5.04023400	-2.27027000	-1.28016000
		1	-7.26056200	1.17016000	-0.00016000
		1	-5.06742600	4.86369000	-0.00000700
		1	-2.87721000	3.62352700	0.00007400
		1	-1.82203200	1.02269600	0.00004600
		1	2.93335500	-2.59878000	-0.00077800
		1	5.03973300	-2.27025800	1.28011800
		1	4.93762500	-0.74241900	2.18419100
		1	6.40933200	-1.15087800	1.28596100
		1	5.04004800	-2.26981900	-1.28104100
		1	4.93820400	-0.74165500	-2.18460300
		1	6.40966600	-1.15047700	-1.28612600
		1	7.26056300	1.17017300	0.00028600
		1	5.06741300	4.86369700	0.00021200
		1	2.87720400	3.62353200	-0.00003000
		1	1.82203300	1.02269600	-0.00012900
	Anion	9	-7.45158800	-3.75938900	-0.00016700
		9	7.45156100	-3.75941000	-0.00011400
		8	0.00001100	-0.67729100	-0.00011200
		7	-2.21640400	5.36040700	0.00016600
		7	-2.82895700	-0.79833800	-0.00002600
		7	2.21655900	5.36014700	0.00028000
		7	2.82894800	-0.79833600	-0.00000600
		6	-1.04797900	1.61066500	0.00006300
		6	-0.00000100	2.61801500	0.00003900
		6	1.04797900	1.61067100	-0.00000100
		6	0.00000300	0.57947400	-0.00001900
		6	0.00000000	4.01751900	0.00006600
		6	-1.21414400	4.75675700	0.00017500
		6	1.21414100	4.75676100	0.00013800
		6	-2.46120600	1.62698800	0.00010800
		6	-3.27426000	0.51924300	0.00009600
		6	-4.81226200	0.51280300	0.00021200
		6	-5.37889600	1.20035700	-1.26457000
		6	-5.37862500	1.20003500	1.26534600
		6	-5.10185900	-0.98597000	0.00009600
		6	-6.30886600	-1.67083100	0.00002500

		6	-6.26404300	-3.06676200	-0.00013800
		6	-5.07404400	-3.78190000	-0.00025900
		6	-3.85319300	-3.09151100	-0.00022100
		6	-3.88043000	-1.69293600	-0.00003000
		6	2.46120400	1.62699000	-0.00006500
		6	3.27425500	0.51924400	-0.00010100
		6	4.81225800	0.51279600	-0.00016100
		6	5.37873900	1.20018000	-1.26511700
		6	5.37878300	1.20018800	1.26479800
		6	5.10184700	-0.98598000	-0.00014300
		6	6.30884900	-1.67084800	-0.00016300
		6	6.26401800	-3.06677800	-0.00010200
		6	5.07401700	-3.78191100	-0.00003400
		6	3.85316800	-3.09151500	-0.00001400
		6	3.88041400	-1.69294100	-0.00004000
		1	-2.94670900	2.59810800	0.00021100
		1	-4.99328100	0.72694500	-2.17224300
		1	-5.09588900	2.25777800	-1.28369900
		1	-6.47379600	1.13646400	-1.27966900
		1	-4.99270900	0.72642200	2.17278800
		1	-6.47352000	1.13602500	1.28073200
		1	-5.09568900	2.25746600	1.28465200
		1	-7.26786900	-1.16144800	0.00009300
		1	-5.10273900	-4.86662200	-0.00039600
		1	-2.91323900	-3.63426200	-0.00031400
		1	-1.82902500	-1.03305300	-0.00008800
		1	2.94671500	2.59811000	-0.00013400
		1	5.09570000	2.25758800	-1.28438200
		1	4.99304200	0.72661600	-2.17267700
		1	6.47363900	1.13630800	-1.28031800
		1	5.09578000	2.25760200	1.28404500
		1	4.99306100	0.72664700	2.17235700
		1	6.47368600	1.13626600	1.28000000
		1	7.26785400	-1.16147000	-0.00022900
		1	5.10270400	-4.86663300	-0.00003600
		1	2.91321200	-3.63426100	-0.00001200
		1	1.82900400	-1.03305500	-0.00005100
CSQ-6	Neutral	8	0.00000500	-0.93045000	0.00066900
		7	-2.80541000	-1.03733800	0.00050100
		1	-1.80235200	-1.27861900	0.00069500
		7	2.80540000	-1.03734500	0.00037400
		1	1.80234700	-1.27862400	0.00059400
		7	-2.24819200	5.05629800	-0.00005400
		6	-5.07675400	-1.24257500	-0.00029000
		6	-3.81437000	-3.34348800	0.00057500
		1	-2.86795300	-3.87491100	0.00103700
		6	-3.23897000	0.24302500	0.00002600
		6	-6.27884300	-1.93724100	-0.00060400

		1	-7.22914100	-1.41030900	-0.00105200
		6	-4.77356500	0.24994600	-0.00039100
		6	-3.86750700	-1.95219900	0.00028000
		6	0.00002200	3.76756200	0.00020100
		6	3.23896900	0.24301800	0.00005600
		6	1.03825600	1.35934600	0.00042500
		6	-5.03482600	-4.03076200	0.00024900
		1	-5.03251600	-5.11657100	0.00045700
		6	4.77356200	0.24993200	-0.00034100
		6	0.00000800	2.38224500	0.00028700
		6	3.86749200	-1.95221000	0.00017800
		6	-2.43409100	1.37879300	-0.00003400
		1	-2.93081200	2.34227800	-0.00035400
		6	-5.31617900	0.94946300	-1.26983300
		1	-6.40892400	0.88754200	-1.28660400
		1	-5.03348600	2.00625400	-1.28223100
		1	-4.93248400	0.47646300	-2.17825500
		6	0.00000100	0.32623500	0.00052800
		6	-6.25262600	-3.34140300	-0.00033600
		1	-7.18533300	-3.89664700	-0.00058800
		6	5.31673500	0.94962900	1.26878700
		1	4.93342900	0.47675300	2.17743700
		1	6.40948500	0.88770300	1.28509900
		1	5.03404700	2.00642100	1.28116500
		6	3.81434800	-3.34349700	0.00036600
		1	2.86792800	-3.87491600	0.00071200
		6	5.07674300	-1.24259100	-0.00025500
		7	2.24823800	5.05627600	0.00028500
		6	-5.31669500	0.94958900	1.26880200
		1	-4.93336000	0.47666300	2.17741300
		1	-5.03399300	2.00637800	1.28121800
		1	-6.40944500	0.88766500	1.28514900
		6	6.27882700	-1.93726300	-0.00051200
		1	7.22912900	-1.41033800	-0.00084700
		6	2.43409300	1.37879100	0.00006200
		1	2.93081100	2.34228000	-0.00013700
		6	5.31612400	0.94939500	-1.26985000
		1	5.03342100	2.00618300	-1.28228500
		1	6.40886800	0.88747500	-1.28666100
		1	4.93239400	0.47634800	-2.17823100
		6	-1.03825500	1.35935000	0.00038900
		6	5.03480100	-4.03077900	0.00009800
		1	5.03248400	-5.11658800	0.00023100
		6	-1.22548900	4.49343400	0.00011200
		6	6.25260300	-3.34142500	-0.00033700
		1	7.18530800	-3.89667200	-0.00054300
		6	1.22556100	4.49337200	0.00027400

Cation	8	-0.00009300	-0.91641000	0.00107700
	7	-2.82595200	-1.03184400	0.00042400
	1	-1.82587700	-1.28242700	0.00065600
	7	2.82598400	-1.03188900	0.00051800
	1	1.82591800	-1.28251600	0.00099300
	7	-2.27377600	5.00729200	-0.00013300
	6	-5.09206400	-1.23654100	-0.00034000
	6	-3.82373900	-3.34598100	0.00070700
	1	-2.87711800	-3.87648500	0.00126700
	6	-3.25468800	0.23167300	-0.00010900
	6	-6.29524100	-1.93063600	-0.00066200
	1	-7.24754600	-1.40913800	-0.00117000
	6	-4.78162000	0.25133600	-0.00051200
	6	-3.88854500	-1.95491100	0.00029900
	6	-0.00000600	3.76769200	0.00022600
	6	3.25466100	0.23164700	0.00004900
	6	1.04948100	1.36746700	0.00046300
	6	-5.04267600	-4.02934800	0.00039200
	1	-5.04594100	-5.11432400	0.00069800
	6	4.78159400	0.25137200	-0.00052900
	6	-0.00001500	2.39024400	0.00029200
	6	3.88861600	-1.95491200	0.00029400
	6	-2.42843400	1.38069500	-0.00022700
	1	-2.93304500	2.34081400	-0.00071000
	6	-5.31610600	0.95850900	-1.27375100
	1	-6.40773000	0.89738000	-1.28660500
	1	-5.03707600	2.01588400	-1.28098800
	1	-4.93678300	0.48712900	-2.18450200
	6	-0.00005500	0.32775100	0.00075700
	6	-6.26019600	-3.33312700	-0.00030000
	1	-7.19163200	-3.88985900	-0.00057300
	6	5.31675500	0.95890100	1.27223300
	1	4.93814500	0.48760600	2.18332500
	1	6.40840300	0.89804400	1.28440700
	1	5.03748200	2.01621300	1.27948800
	6	3.82386200	-3.34598600	0.00062200
	1	2.87726000	-3.87652200	0.00116400
	6	5.09210400	-1.23649300	-0.00036600
	7	2.27367100	5.00749600	0.00093100
	6	-5.31661900	0.95875200	1.27240000
	1	-4.93781100	0.48743400	2.18339700
	1	-5.03741900	2.01608400	1.27966900
	1	-6.40825900	0.89780700	1.28476900
	6	6.29530600	-1.93054200	-0.00073100
	1	7.24759300	-1.40901100	-0.00124400
	6	2.42837300	1.38064700	0.00002700
	1	2.93296900	2.34077400	-0.00026200
	6	5.31585100	0.95846800	-1.27392500

		1	5.03673200	2.01582000	-1.28123300
		1	6.40747800	0.89742600	-1.28692800
		1	4.93644200	0.48696900	-2.18457600
		6	-1.04954900	1.36750400	0.00032800
		6	5.04282400	-4.02930500	0.00024300
		1	5.04613400	-5.11428100	0.00046800
		6	-1.23278100	4.48348900	0.00013500
		6	6.26031600	-3.33303500	-0.00042800
		1	7.19177600	-3.88972800	-0.00071800
		6	1.23278500	4.48347200	0.00048200
	Anion	8	-0.00009300	-0.91641000	0.00107700
		7	-2.82595200	-1.03184400	0.00042400
		1	-1.82587700	-1.28242700	0.00065600
		7	2.82598400	-1.03188900	0.00051800
		1	1.82591800	-1.28251600	0.00099300
		7	-2.27377600	5.00729200	-0.00013300
		6	-5.09206400	-1.23654100	-0.00034000
		6	-3.82373900	-3.34598100	0.00070700
		1	-2.87711800	-3.87648500	0.00126700
		6	-3.25468800	0.23167300	-0.00010900
		6	-6.29524100	-1.93063600	-0.00066200
		1	-7.24754600	-1.40913800	-0.00117000
		6	-4.78162000	0.25133600	-0.00051200
		6	-3.88854500	-1.95491100	0.00029900
		6	-0.00000600	3.76769200	0.00022600
		6	3.25466100	0.23164700	0.00004900
		6	1.04948100	1.36746700	0.00046300
		6	-5.04267600	-4.02934800	0.00039200
		1	-5.04594100	-5.11432400	0.00069800
		6	4.78159400	0.25137200	-0.00052900
		6	-0.00001500	2.39024400	0.00029200
		6	3.88861600	-1.95491200	0.00029400
		6	-2.42843400	1.38069500	-0.00022700
		1	-2.93304500	2.34081400	-0.00071000
		6	-5.31610600	0.95850900	-1.27375100
		1	-6.40773000	0.89738000	-1.28660500
		1	-5.03707600	2.01588400	-1.28098800
		1	-4.93678300	0.48712900	-2.18450200
		6	-0.00005500	0.32775100	0.00075700
		6	-6.26019600	-3.33312700	-0.00030000
		1	-7.19163200	-3.88985900	-0.00057300
		6	5.31675500	0.95890100	1.27223300
		1	4.93814500	0.48760600	2.18332500
		1	6.40840300	0.89804400	1.28440700
		1	5.03748200	2.01621300	1.27948800
		6	3.82386200	-3.34598600	0.00062200
		1	2.87726000	-3.87652200	0.00116400
		6	5.09210400	-1.23649300	-0.00036600

		7	2.27367100	5.00749600	0.00093100
		6	-5.31661900	0.95875200	1.27240000
		1	-4.93781100	0.48743400	2.18339700
		1	-5.03741900	2.01608400	1.27966900
		1	-6.40825900	0.89780700	1.28476900
		6	6.29530600	-1.93054200	-0.00073100
		1	7.24759300	-1.40901100	-0.00124400
		6	2.42837300	1.38064700	0.00002700
		1	2.93296900	2.34077400	-0.00026200
		6	5.31585100	0.95846800	-1.27392500
		1	5.03673200	2.01582000	-1.28123300
		1	6.40747800	0.89742600	-1.28692800
		1	4.93644200	0.48696900	-2.18457600
		6	-1.04954900	1.36750400	0.00032800
		6	5.04282400	-4.02930500	0.00024300
		1	5.04613400	-5.11428100	0.00046800
		6	-1.23278100	4.48348900	0.00013500
		6	6.26031600	-3.33303500	-0.00042800
		1	7.19177600	-3.88972800	-0.00071800
		6	1.23278500	4.48347200	0.00048200
CSQ-7	Neutral	6	-1.04524400	1.19300100	-0.15292700
		6	-0.01084400	2.21082000	-0.11328300
		6	1.05831800	1.22987600	-0.08709200
		6	0.02534400	0.16266900	-0.14471500
		6	2.46204900	1.41915300	-0.05981600
		1	2.72779500	2.47061600	-0.09192600
		6	3.54301700	0.56713400	0.00374700
		6	3.64166200	-0.96499800	0.11489200
		6	5.14641800	-1.15908200	0.28836100
		6	5.89249800	-2.29872800	0.55110300
		1	5.40244400	-3.25915500	0.68058000
		6	7.29306700	-2.21109400	0.66523200
		1	7.87828900	-3.10320300	0.86855000
		6	7.92438000	-0.97308200	0.52487700
		1	9.00543100	-0.90441100	0.61757700
		6	7.18807600	0.19443300	0.28260600
		1	7.69472200	1.15060400	0.20308700
		6	5.79594000	0.08680000	0.16966300
		6	-2.45353200	1.33419200	-0.20176800
		1	-2.75303800	2.37689600	-0.21661500
		6	-3.50659400	0.44559700	-0.22698100
		6	-3.56259400	-1.09123300	-0.21761200
		6	-5.06532300	-1.34298600	-0.26125700
		6	-5.75029500	-0.11350500	-0.29910900
		6	-7.14983700	-0.06903400	-0.35363200
		1	-7.69193400	0.87045000	-0.38414900
		6	-7.84949000	-1.28352900	-0.36840000
		1	-8.93570000	-1.26389000	-0.41031600

		6	-7.17973200	-2.50964700	-0.33104400
		1	-7.74105700	-3.43938300	-0.34340400
		6	-5.77329900	-2.53384100	-0.27790900
		1	-5.24672000	-3.48490600	-0.24884200
		6	2.87215200	-1.50614400	1.34245100
		1	3.16230800	-0.95471100	2.24251000
		1	3.10932600	-2.56285100	1.50679800
		1	1.79504200	-1.41751000	1.19114200
		6	3.12348400	-1.58765000	-1.22482600
		1	2.09345400	-1.24655100	-1.35851800
		1	3.72095900	-1.16332000	-2.04352000
		6	3.13613300	-3.11793700	-1.33859200
		1	4.15649700	-3.50390400	-1.22488600
		1	2.53503800	-3.55366800	-0.53162400
		6	2.57049600	-3.58907300	-2.68569800
		1	2.57711500	-4.68313900	-2.76166800
		1	3.15918100	-3.19305700	-3.52273200
		1	1.53698900	-3.24912500	-2.81563900
		6	5.16340800	2.49084800	-0.16532700
		1	6.23312700	2.61457900	-0.33748000
		1	4.88084200	3.05254900	0.73467300
		6	-2.88657100	-1.68742800	-1.47880000
		1	-3.31752000	-1.25526100	-2.38791300
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		1	-3.09443500	-2.80048800	1.00797400
		1	-1.83587000	-1.57574200	0.98961200
		6	-3.44080100	-1.18023600	2.39486900
		1	-4.53025100	-1.30557800	2.45101100
		1	-3.24625600	-0.10210600	2.45216300
		6	-2.78599500	-1.87705100	3.59459700
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		1	-3.15943300	-1.47435000	4.54367300
		6	-5.17543500	2.33171100	-0.30315600
		1	-4.79070300	2.85098500	0.58230200
		1	-6.25957200	2.44169400	-0.32682900
		6	-0.03539300	3.61882100	-0.10987400
		6	-1.25086100	4.35362700	-0.14108600
		6	1.15385600	4.39545600	-0.08001100
		7	4.85521900	1.08204500	-0.03947000
		7	-4.83307400	0.92525600	-0.27395300
		7	2.12824400	5.04462900	-0.05828400
		7	-2.24735800	4.96824800	-0.16576000
		8	0.04857600	-1.07289100	-0.18745100
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		1	-4.75366000	2.82424900	-1.18749800

Cation	6	-1.04597500	1.17420400	-0.15374500
	6	-0.00647000	2.20088600	-0.12055900
	6	1.06773800	1.21108700	-0.06801500
	6	0.02929100	0.12533200	-0.11497600
	6	2.43473400	1.41467000	-0.01629700
	1	2.70200400	2.46416800	-0.02110300
	6	3.55050300	0.54380400	0.05583100
	6	3.65217100	-0.98063200	0.12747100
	6	5.15214800	-1.16861400	0.26979200
	6	5.92319800	-2.30855900	0.47236200
	1	5.46530700	-3.28711000	0.56442400
	6	7.31489500	-2.17648900	0.57062600
	1	7.92630100	-3.05934300	0.72662000
	6	7.92720100	-0.92023800	0.47713800
	1	9.00611100	-0.83903600	0.55748300
	6	7.16633600	0.23705600	0.29653300
	1	7.64967300	1.20580500	0.24721400
	6	5.78362900	0.07865600	0.20174500
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	6	-3.56416400	-1.10559800	-0.18773200
	6	-5.05936800	-1.34624500	-0.24967800
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	6	-7.83886200	-1.21728900	-0.40362400
	1	-8.92161600	-1.18235600	-0.46314300
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	6	-5.78967200	-2.52800500	-0.24856100
	1	-5.29509200	-3.49271200	-0.18825800
	6	2.90563000	-1.54798600	1.35988900
	1	3.22054700	-1.03380700	2.27274000
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	1	4.17391300	-3.45117600	-1.31678300
	1	2.57112300	-3.54756700	-0.58835600
	6	2.56122300	-3.50871300	-2.74587200
	1	2.58388700	-4.59771300	-2.85121900
	1	3.12892300	-3.08233300	-3.58062300
	1	1.51952100	-3.18487100	-2.84777200
	6	5.10136800	2.50734000	-0.03872800
	1	6.17702900	2.62803400	-0.13572600

		1	4.76102000	3.03707200	0.85477900
		6	-2.87619400	-1.71970200	-1.43843100
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		6	-2.94305400	-1.68827800	1.12069200
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		1	-3.30538300	-0.04829700	2.49345700
		6	-2.87664700	-1.81253900	3.66057100
		1	-1.78827800	-1.68508700	3.67863700
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		6	-5.11037600	2.33688400	-0.38990200
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		6	-1.26087100	4.30298500	-0.19310300
		6	1.17655500	4.34506900	-0.10215700
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		7	-4.75949200	0.91327000	-0.31572700
		7	2.19239500	4.91777100	-0.07433900
		7	-2.29520600	4.84026500	-0.23979000
		8	0.05174800	-1.09220600	-0.13098400
		1	-4.66555700	2.79332600	-1.27704100
		1	4.62066500	2.93935100	-0.91825500
	Anion	6	-1.04524400	1.19300100	-0.15292700
		6	-0.01084400	2.21082000	-0.11328300
		6	1.05831800	1.22987600	-0.08709200
		6	0.02534400	0.16266900	-0.14471500
		6	2.46204900	1.41915300	-0.05981600
		1	2.72779500	2.47061600	-0.09192600
		6	3.54301700	0.56713400	0.00374700
		6	3.64166200	-0.96499800	0.11489200
		6	5.14641800	-1.15908200	0.28836100
		6	5.89249800	-2.29872800	0.55110300
		1	5.40244400	-3.25915500	0.68058000
		6	7.29306700	-2.21109400	0.66523200
		1	7.87828900	-3.10320300	0.86855000
		6	7.92438000	-0.97308200	0.52487700
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		1	-2.75303800	2.37689600	-0.21661500

		6	-3.50659400	0.44559700	-0.22698100
		6	-3.56259400	-1.09123300	-0.21761200
		6	-5.06532300	-1.34298600	-0.26125700
		6	-5.75029500	-0.11350500	-0.29910900
		6	-7.14983700	-0.06903400	-0.35363200
		1	-7.69193400	0.87045000	-0.38414900
		6	-7.84949000	-1.28352900	-0.36840000
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		6	-7.17973200	-2.50964700	-0.33104400
		1	-7.74105700	-3.43938300	-0.34340400
		6	-5.77329900	-2.53384100	-0.27790900
		1	-5.24672000	-3.48490600	-0.24884200
		6	2.87215200	-1.50614400	1.34245100
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		6	2.57049600	-3.58907300	-2.68569800
		1	2.57711500	-4.68313900	-2.76166800
		1	3.15918100	-3.19305700	-3.52273200
		1	1.53698900	-3.24912500	-2.81563900
		6	5.16340800	2.49084800	-0.16532700
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		1	4.88084200	3.05254900	0.73467300
		6	-2.88657100	-1.68742800	-1.47880000
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		1	-4.79070300	2.85098500	0.58230200
		1	-6.25957200	2.44169400	-0.32682900
		6	-0.03539300	3.61882100	-0.10987400
		6	-1.25086100	4.35362700	-0.14108600

		6	1.15385600	4.39545600	-0.08001100
		7	4.85521900	1.08204500	-0.03947000
		7	-4.83307400	0.92525600	-0.27395300
		7	2.12824400	5.04462900	-0.05828400
		7	-2.24735800	4.96824800	-0.16576000
		8	0.04857600	-1.07289100	-0.18745100
		1	4.62550600	2.92655000	-1.01324600
		1	-4.75366000	2.82424900	-1.18749800
CSQ-8	Neutral	6	-5.50199800	-0.76248000	0.00000100
		6	-6.89929900	-0.85132300	-0.00005500
		1	-7.52483900	0.03363200	-0.00007900
		6	-7.48768800	-2.11734000	-0.00010000
		1	-8.57031300	-2.19456100	-0.00013600
		6	-6.70754700	-3.28098000	-0.00010900
		1	-7.18601900	-4.25493400	-0.00015400
		6	-5.31359100	-3.19522300	-0.00007800
		1	-4.70111800	-4.09127200	-0.00010100
		6	-4.72240200	-1.93276300	-0.00001800
		6	-3.35622700	0.16980000	0.00003700
		6	-2.42907300	1.21139800	0.00004200
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		6	0.00000600	2.12754200	-0.00001300
		6	0.00000900	0.05618200	-0.00011300
		6	1.03800100	1.11610600	-0.00008600
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		6	3.35623700	0.16981600	-0.00013500
		6	5.50199800	-0.76249100	-0.00006800
		6	6.89929800	-0.85135400	-0.00002900
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		6	7.48767300	-2.11737500	0.00013800
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		6	6.70751300	-3.28100700	0.00028200
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		6	5.31355900	-3.19523200	0.00026800
		1	4.70107500	-4.09127100	0.00039500
		6	4.72238600	-1.93276400	0.00008900
		6	-1.22309400	4.24783200	0.00012500
		6	-0.00000100	3.52411200	0.00004200
		6	1.22308500	4.24784500	-0.00000800
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		7	-2.25304500	4.80083300	0.00032700
		8	0.00001100	-1.17247100	-0.00012800
		16	-3.00113000	-1.55640400	-0.00001400
		16	3.00111600	-1.55637700	0.00004900
		7	2.25304400	4.80083200	-0.00001300

		6	5.26014300	1.74910900	-0.00034800
		1	4.93126600	2.29293100	-0.89015900
		1	4.93169500	2.29296800	0.88960400
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		1	-6.34604400	1.69905900	0.00048900
	Cation	6	-5.48711500	-0.77318500	0.00001900
		6	-6.88592700	-0.86943100	0.00002700
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		6	-7.45571600	-2.13846400	-0.00003100
		1	-8.53661900	-2.23055900	-0.00001800
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		6	-4.69572000	-1.93631800	-0.00006200
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		1	2.84378200	2.23019500	-0.00011300
		6	3.36294800	0.16517800	-0.00009600
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		6	6.88592600	-0.86945100	0.00004700
		1	7.52110200	0.00802400	0.00004300
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		1	4.65419000	-4.10071300	0.00019600
		6	4.69570700	-1.93631400	0.00001900
		6	-1.23028400	4.25509100	0.00008900
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		6	1.23026100	4.25510900	0.00002400
		7	4.70367800	0.38768100	-0.00018600
		7	-4.70366500	0.38767500	0.00008600
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		16	-2.98779700	-1.53810100	-0.00008000
		16	2.98778900	-1.53807800	0.00001900
		7	2.27686000	4.77001700	-0.00006200

		6	5.27353900	1.74501500	-0.00031600
		1	4.95552800	2.28711300	-0.89348900
		1	4.95644800	2.28692500	0.89330800
		1	6.35725800	1.67428900	-0.00091900
		6	-5.27350400	1.74501500	0.00021300
		1	-4.95564700	2.28704900	0.89348200
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		6	-6.82414600	-3.24070200	0.17053300
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		6	-5.42160300	-3.16811200	0.15181200
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		6	-4.80516500	-1.92596200	0.05664400
		6	-3.38843500	0.16656200	-0.06767900
		6	-2.45307800	1.17686300	-0.06275800
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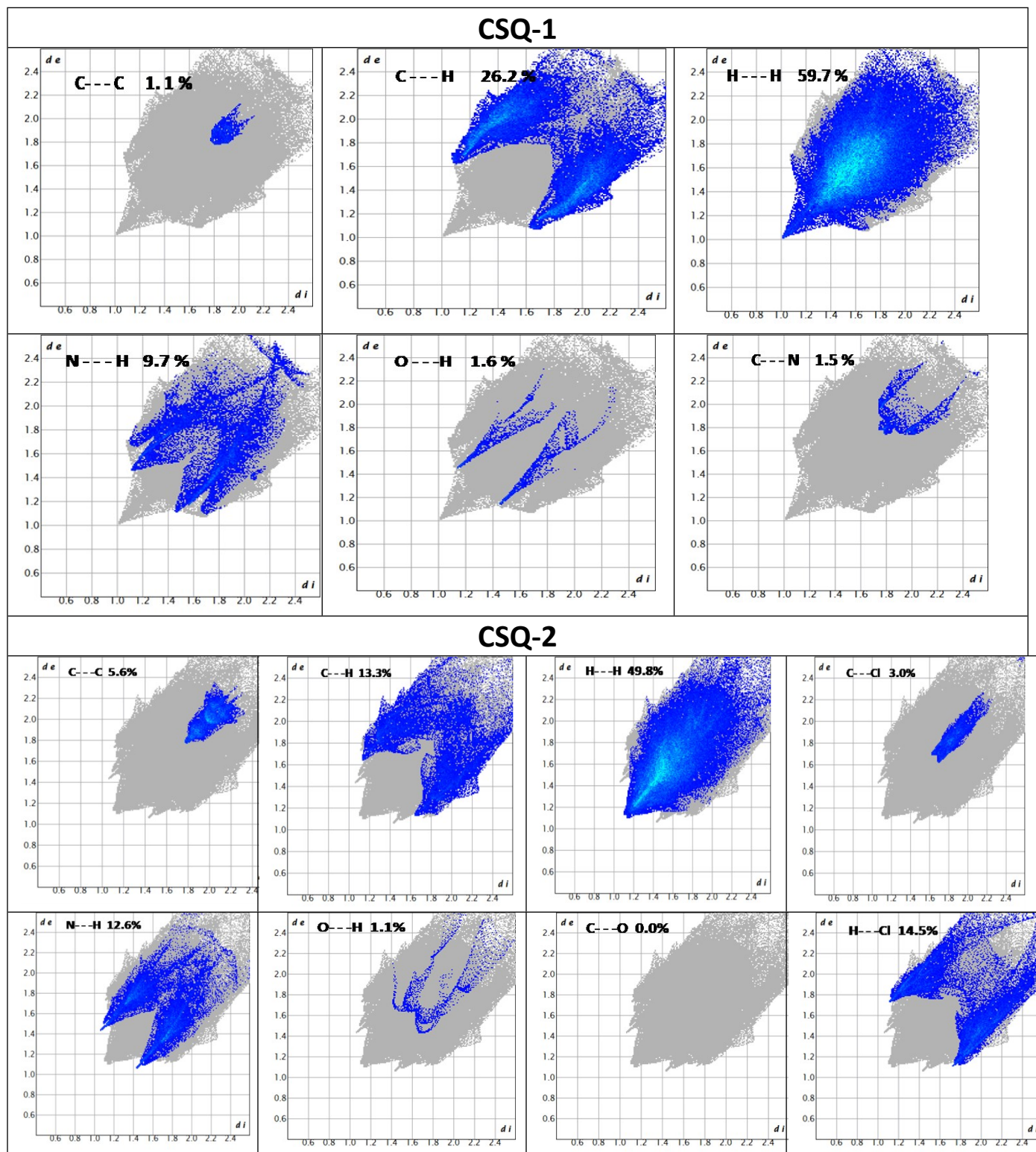
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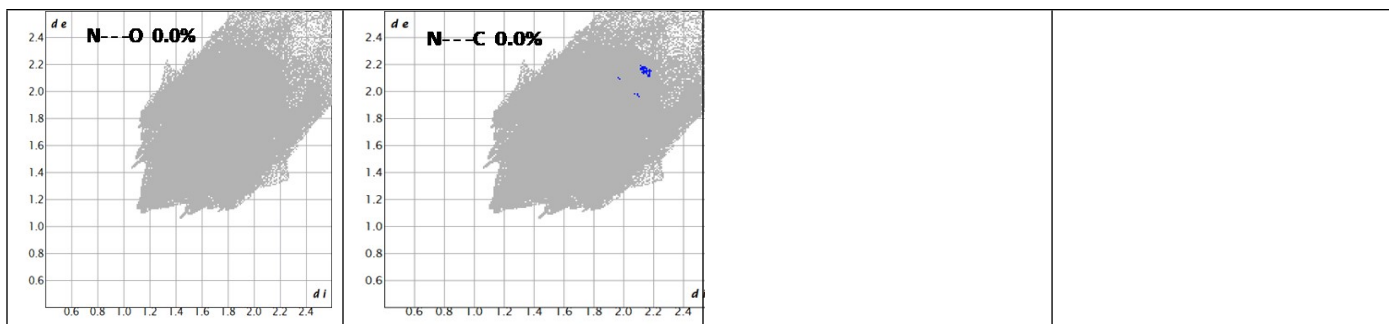
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		1	-5.85952600	4.39611600	0.00049200
		6	6.39216000	3.44660200	-0.00056100
		1	7.01884200	3.39068300	0.89265400
		1	7.01869600	3.39088400	-0.89389500
		1	5.85952700	4.39611600	-0.00042900
	Anion	6	-0.00000800	0.49986100	-0.00011600
		6	-1.05230800	-0.55512700	-0.00009000
		6	0.00000000	-1.55630000	-0.00007400
		6	0.00000500	-2.96125600	-0.00007000
		6	-1.20673100	-3.71125700	0.00021900
		6	-2.44733600	-0.67839100	0.00012400
		1	-2.78780000	-1.70691200	0.00034700
		6	-3.43481600	0.31606700	-0.00006400
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		1	-2.07982500	2.03441400	-0.00030500

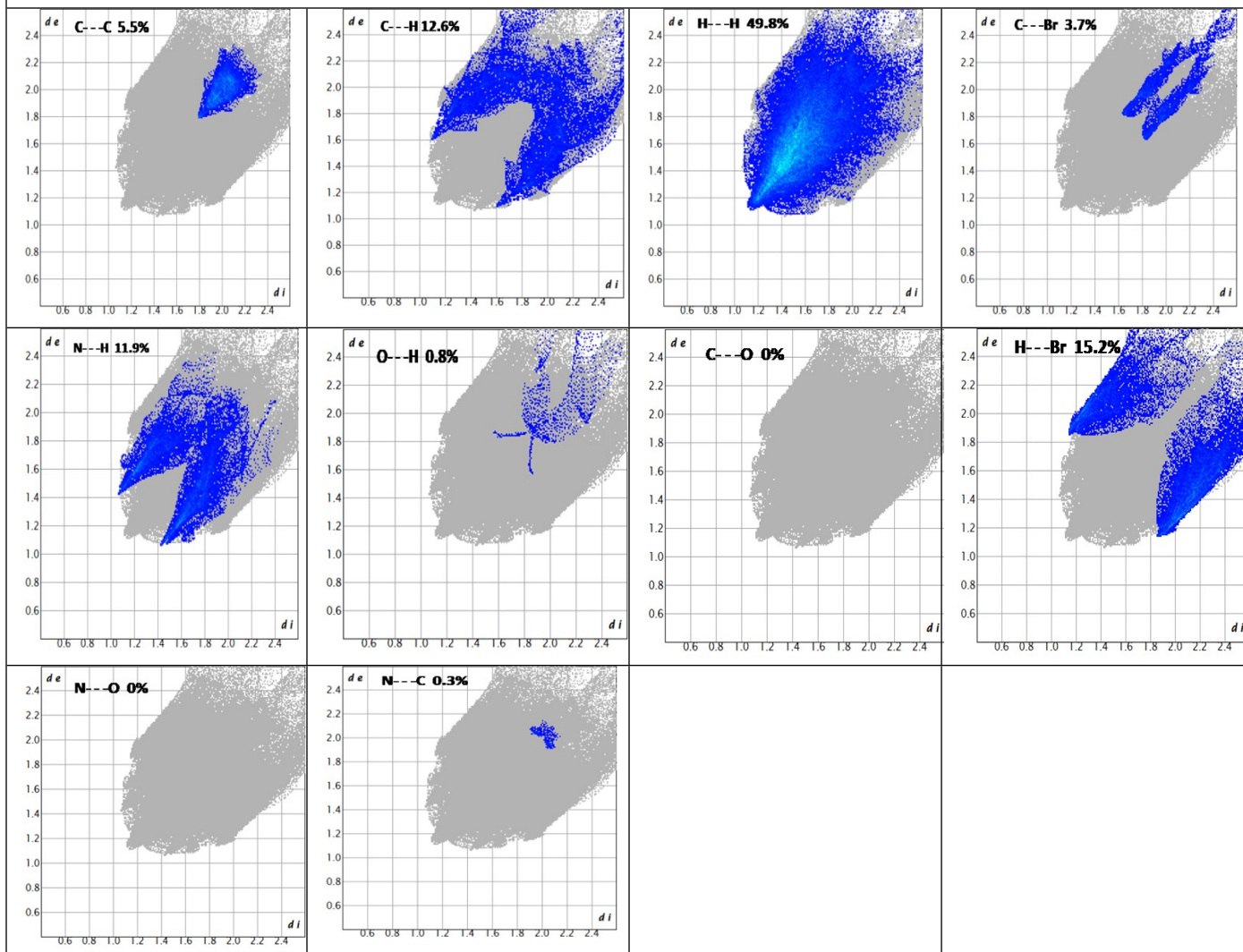
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		6	-7.22291100	0.70858100	0.00000200
		1	-7.96430500	1.49857800	-0.00016600
		6	-7.65185800	-0.62022500	0.00031100
		1	-8.71593600	-0.84043400	0.00041600
		6	-6.70965200	-1.64899500	0.00051400
		1	-7.02476100	-2.68841200	0.00075200
		6	-5.34995100	-1.34292600	0.00039900
		1	-4.64128500	-2.16259000	0.00058300
		6	-4.86935600	-0.01632700	0.00006900
		7	-2.19946500	-4.33177400	0.00039900
		7	-5.44405600	2.36442600	-0.00055800
		8	-0.00001500	1.73570900	-0.00008300
		6	1.05230200	-0.55512000	-0.00002900
		6	1.20674700	-3.71124800	-0.00035800
		6	2.44733000	-0.67837800	-0.00016700
		1	2.78779600	-1.70689800	-0.00033100
		6	3.43481300	0.31607900	0.00003200
		6	3.11935800	1.72157700	0.00022100
		1	2.07983200	2.03443400	0.00012300
		6	4.08617500	2.66989400	0.00039000
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		6	5.85182800	1.02701700	0.00022800
		6	7.22291000	0.70857100	0.00019000
		1	7.96430900	1.49856400	0.00038900
		6	7.65184900	-0.62023700	-0.00003800
		1	8.71592500	-0.84045200	-0.00005900
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Fig. S1: Finger print plots of all CSQs broken down into contribution from specific pairs of atom types.

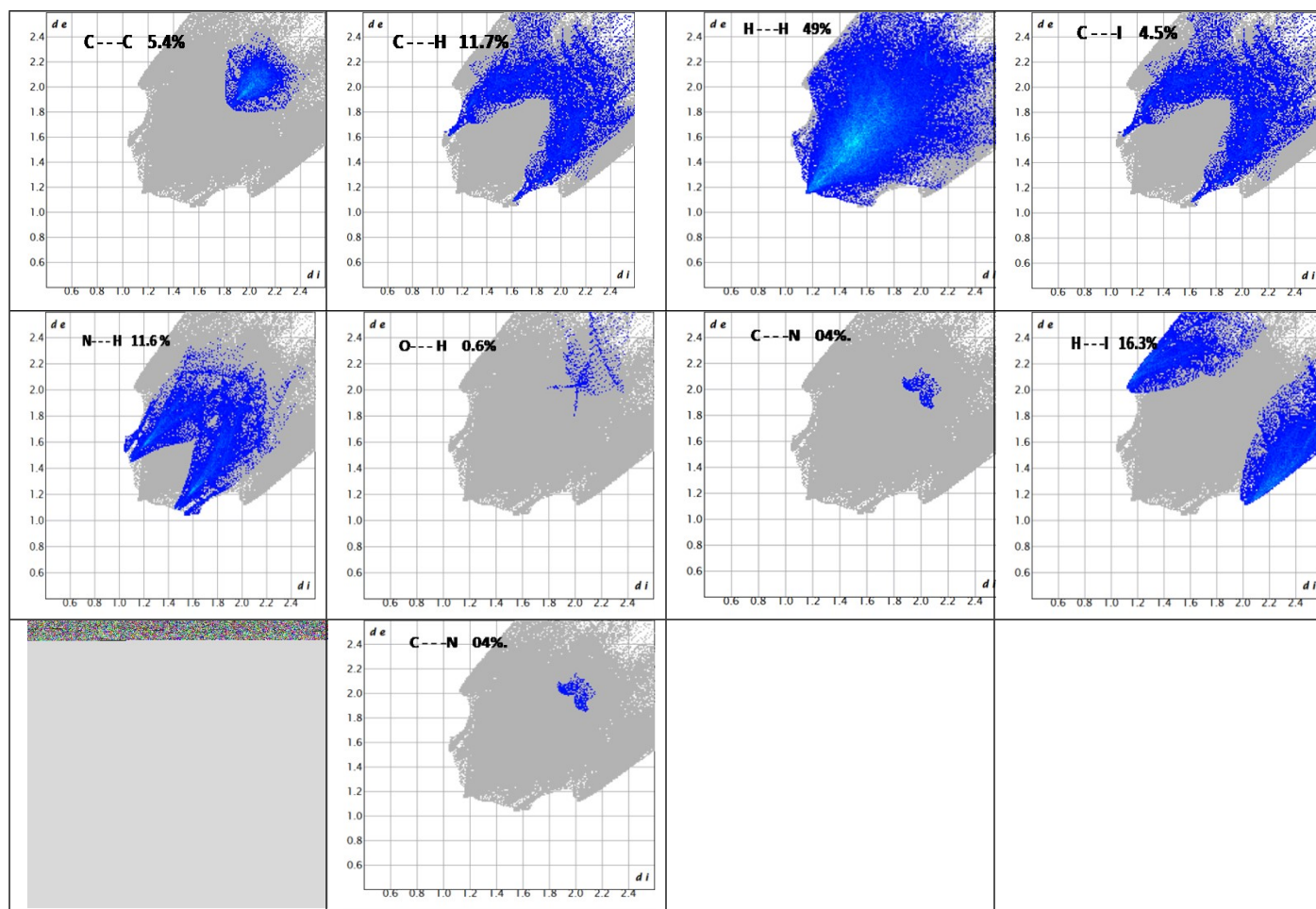




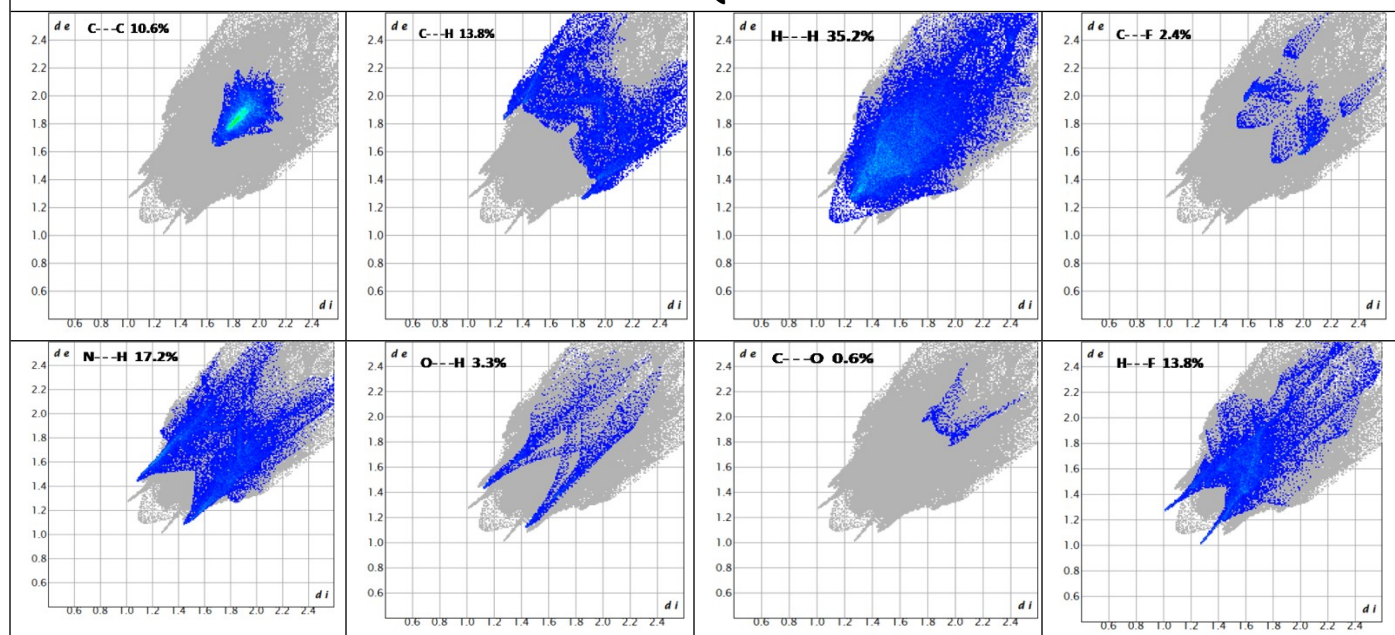
CSQ-3

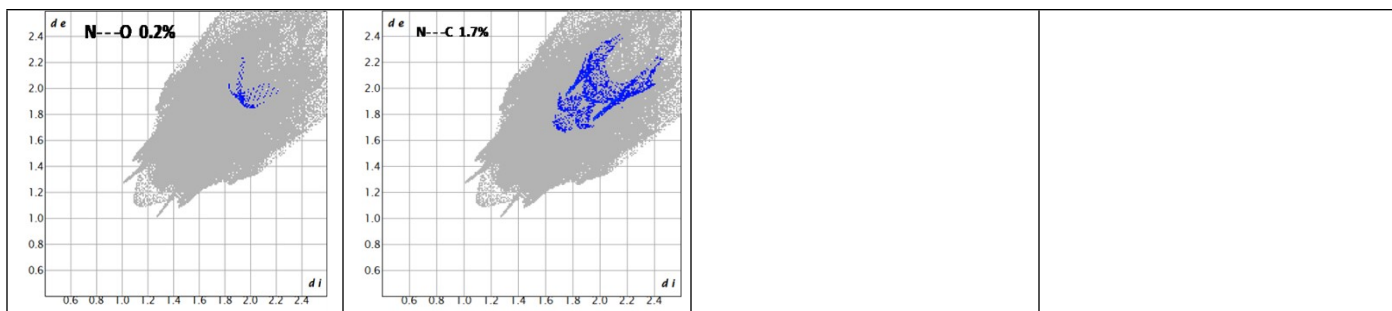


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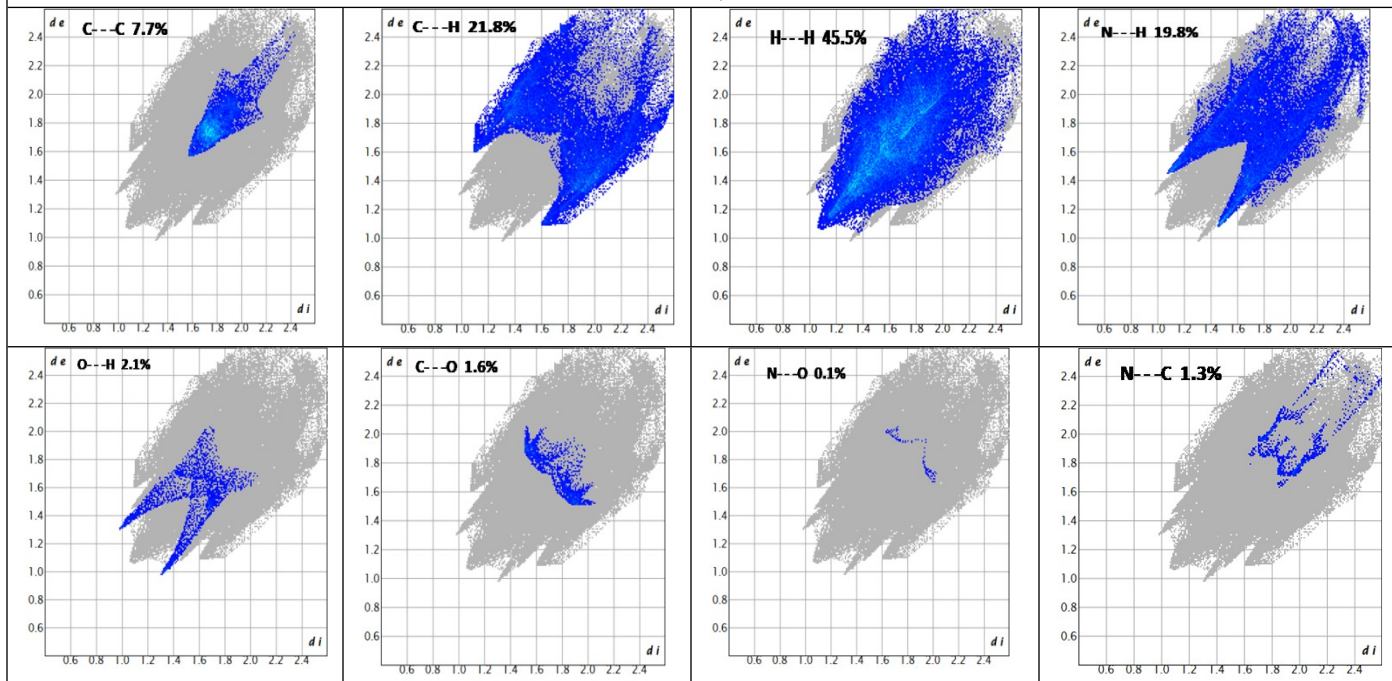


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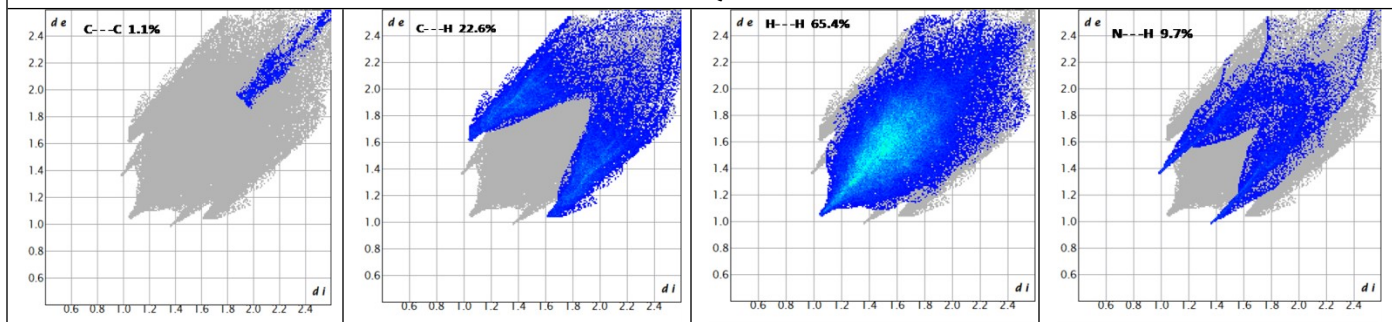


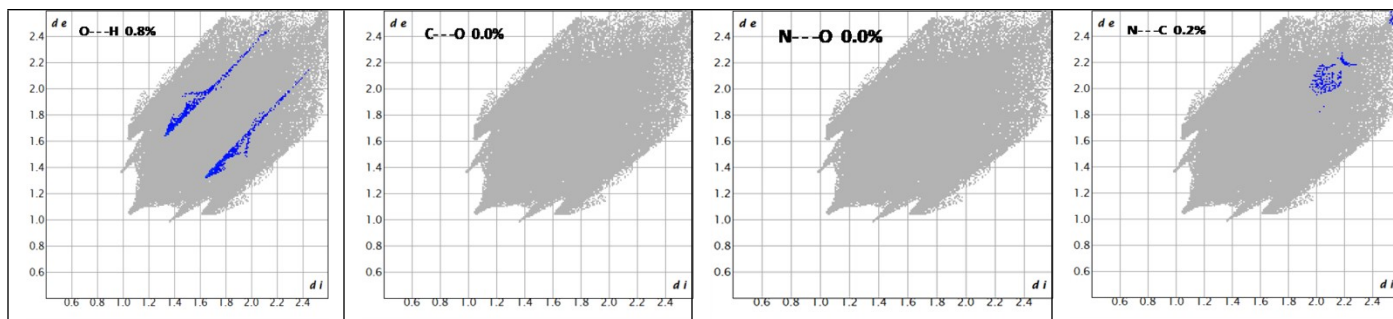


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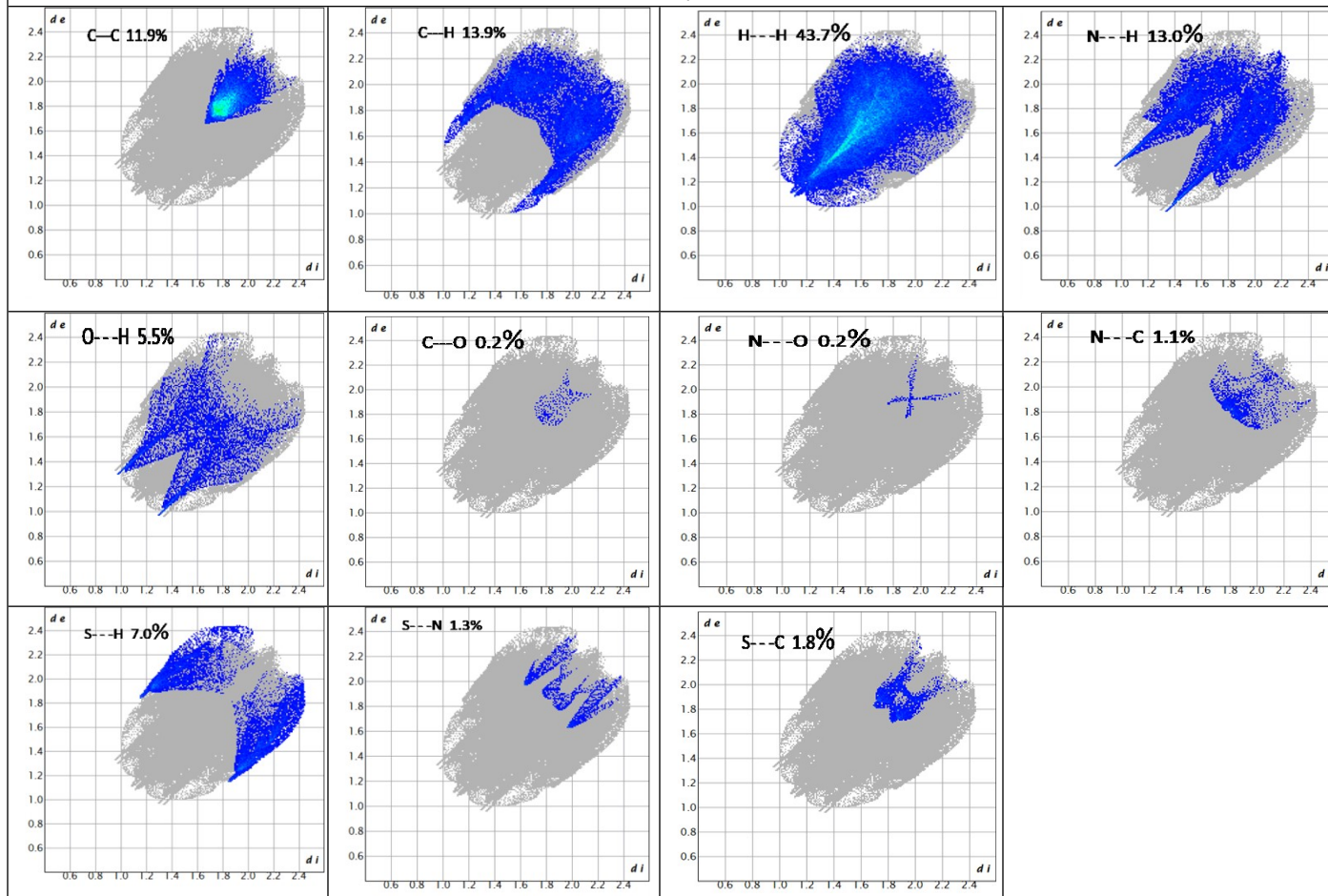


CSQ-7

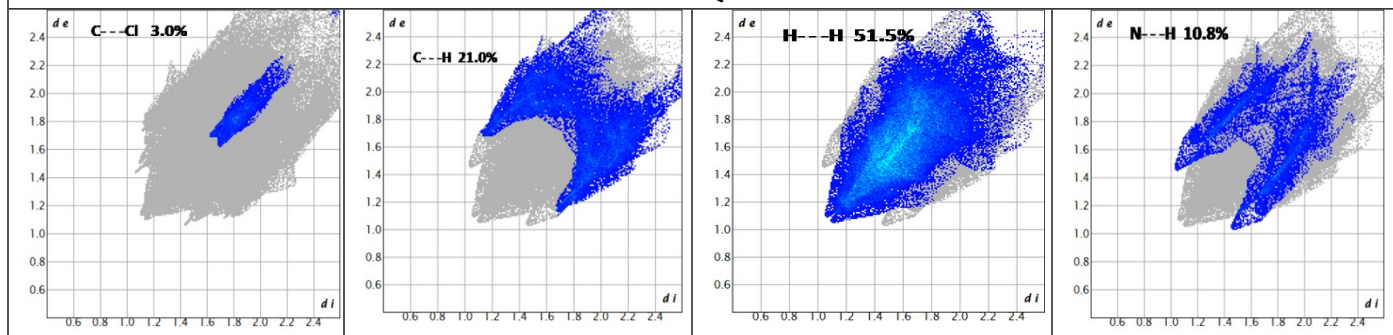


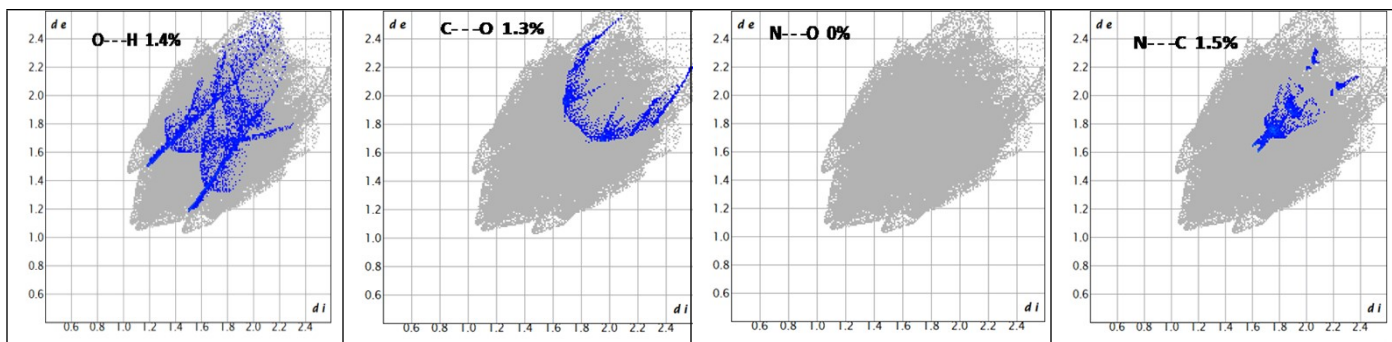


CSQ-8



CSQ-9





CSQ-10

