

Electronic supplementary material for manuscript:

Radical...radical chalcogen bonds: CSD analysis and DFT calculations

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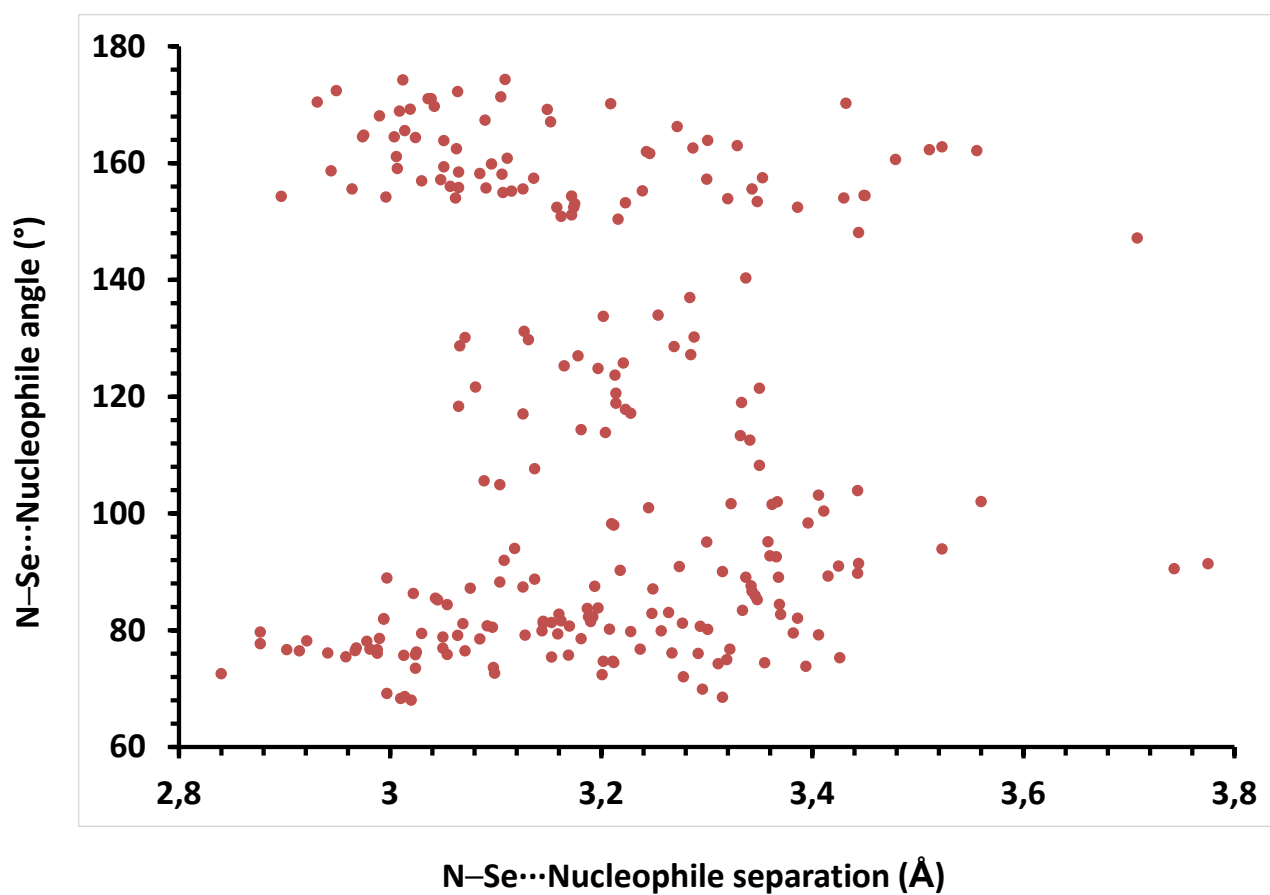


Figure S1 Scatterplot of the N–Se···nucleophile short contacts in DSDA derivatives present in the CSD.

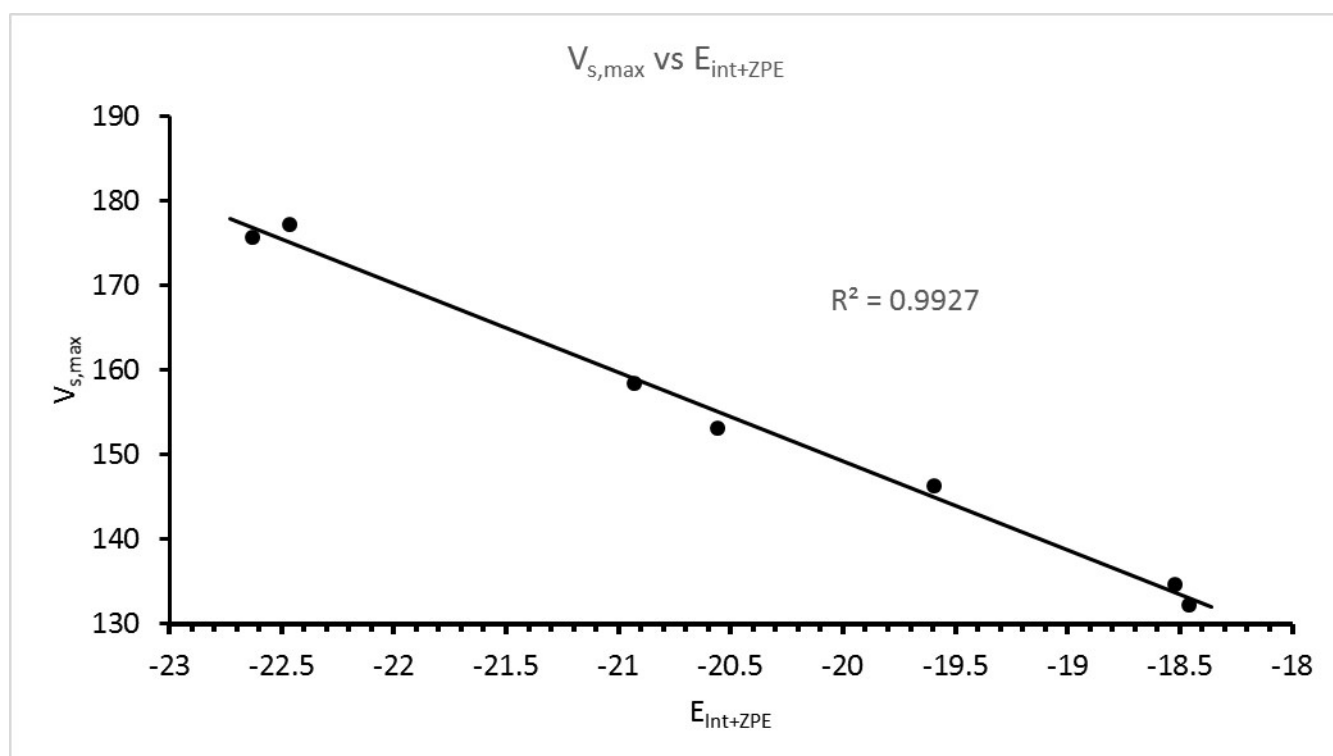


Figure S2. Regression plot of $V_{s,max}$ (KJ/mol) vs $E_{int+ZPE}$ (KJ/mol) for the S-complexes

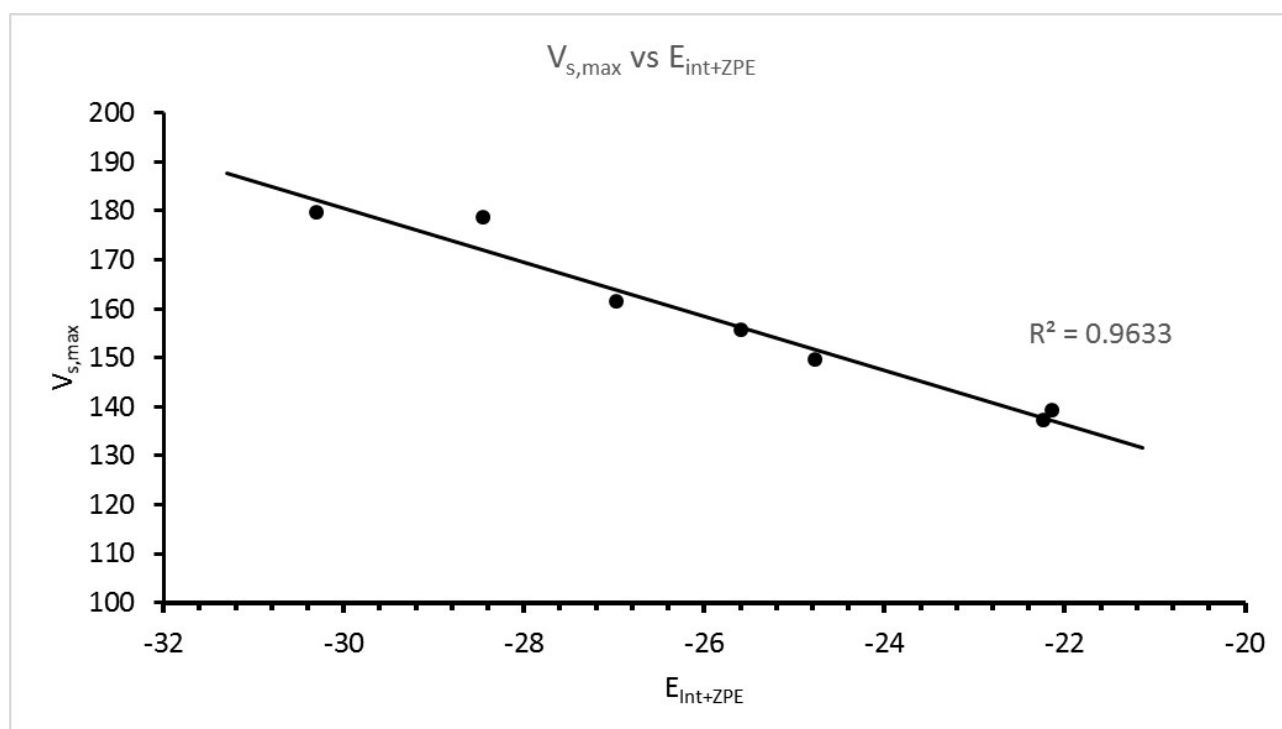


Figure S3. Regression plot of $V_{s,max}$ (KJ/mol) vs E_{int} (KJ/mol) for the Se-complexes

Cartesian coordinates

1

S	0.7443305	3.0927071	-2.6854462
S	1.3238361	3.8622733	-0.8154713
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N	0.9553465	2.5025181	-0.0124939
F	-1.2622675	1.3713507	1.4519875
F	-1.9404572	-0.9358533	2.6169329
F	0.6714776	-3.2902149	-0.4855008
F	1.3844659	-0.9909755	-1.6462846
C	0.4641527	1.5349057	-0.7741788
C	0.0826520	0.2590708	-0.1309999
C	-0.7628242	0.2420786	0.9728010
C	-1.1225460	-0.9546152	1.5698999
C	-0.6485418	-2.1564731	1.0866045
C	0.1927818	-2.1470363	-0.0065583
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H	-0.9316981	-3.0893358	1.5559986

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F	-1.9362323	-0.9331488	2.6177536
F	0.6715143	-3.2869501	-0.4875099
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C	0.2820775	-1.8736792	-0.1530147
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N	-1.2174542	-4.1023788	2.0830184

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F	-1.7778483	-0.3205739	2.2876262
F	0.8785558	-2.6686652	-0.7874787
F	1.5790324	-0.3773549	-1.9420647
C	0.6500003	2.1575214	-1.0877170
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C	-0.5899192	0.8487898	0.6505170
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F	-1.8411776	-0.5274611	2.3885545
F	0.7876670	-2.8770500	-0.6939209
F	1.5340589	-0.5749686	-1.8335538
C	0.6428486	1.9764717	-0.9578790
C	0.2381656	0.6958771	-0.3290145
C	-0.6191777	0.6629495	0.7654706
C	-0.9963025	-0.5276133	1.3509789
C	-0.5337087	-1.7533558	0.8800424
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C	0.6964825	-0.5271548	-0.8064355
N	-0.8640594	-2.9305366	1.4948983
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Se	0.9533169	3.6050078	-3.0089842

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F	2.2898680	0.4178958	-1.8539884
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C	0.6616341	1.6733024	-0.7067888
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C	-0.3217689	-0.8028204	0.3372139
C	0.7668100	-0.7400731	-0.5432737
C	1.2274475	0.4544480	-1.0594389
N	-0.7941220	-1.9866349	0.8379472
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H	-0.0729307	-3.9072957	0.3085696
H	-1.8278414	-3.6645143	0.1851070
C	-1.2580439	-2.1111916	2.1976790

H	-0.9300375	-1.2631735	2.7951699
H	-2.3502791	-2.1788433	2.2625076
H	-0.8310871	-3.0178580	2.6399564
Se	2.0867234	5.4191896	-1.0119732
Se	1.9241502	4.5624528	-3.1993492

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F	0.1480435	-4.9524866	0.3137522
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C	-1.0971659	-3.6906195	1.8651811
C	-1.9120031	-3.6998745	2.9909037
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C	-1.8174753	-6.0995452	3.1034512
C	-1.0072685	-6.0977322	1.9870801
C	-0.6515482	-4.9101813	1.3696274
C	1.2899891	4.4592965	-1.4818388
C	1.2146181	3.8500588	-2.7374357
C	1.4488677	4.5875331	-3.8930259
C	1.7576658	5.9315392	-3.7771389
C	1.8341598	6.5382798	-2.5258898
C	1.6017406	5.8101949	-1.3721792
H	1.3901878	4.1155561	-4.8665176
H	1.9419581	6.5148334	-4.6710555
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H	1.6611847	6.2824737	-0.3988605
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H	-2.0951975	-7.0293867	3.5817883

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C	1.2527947	4.1433318	-2.8640253
C	1.3612786	4.8959164	-4.0285719
C	1.6959251	6.2350382	-3.9296233
C	1.9207010	6.8220567	-2.6866942
C	1.8139034	6.0788114	-1.5242450
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H	1.7832325	6.8302349	-4.8303775
H	2.1820124	7.8714602	-2.6258879
H	1.9879343	6.5360781	-0.5575972
N	0.9051588	2.2643401	-1.1310152
S	1.2922069	3.6245586	-0.2906080
S	0.8469816	2.4566936	-2.7639568
C	-2.2624618	-7.0159757	3.5192543
N	-2.6206893	-7.9975251	4.0008930

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S	-0.3375771	-0.3246840	-0.9440808
S	0.1917920	0.4636724	0.9226117
N	-0.7582482	-1.7747643	-0.3469274
N	-0.1665921	-0.8968329	1.7330884
F	-2.3483799	-2.0934955	3.1857411
F	-2.9674147	-4.3987500	4.3532237
F	-0.2791705	-6.6944870	1.2494209
F	0.3750022	-4.3867488	0.1066729
C	-0.6123286	-1.8798102	0.9653009
C	-0.9664428	-3.1650633	1.6084503
C	-1.8102535	-3.2035551	2.7123297
C	-2.1400396	-4.4005506	3.3257093
C	-1.6355073	-5.5884113	2.8213867
C	-0.7989401	-5.5758504	1.7169139
C	-0.4650586	-4.3685855	1.1264997
O	-2.4317977	-7.7184816	2.7340434
O	-1.8004588	-6.9387379	4.6461975
N	-1.9866196	-6.8593947	3.4557765
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C	1.2819335	4.3863829	-2.9915055
C	1.5355470	5.1106802	-4.1513519

C	1.9745785	6.4182757	-4.0397052
C	2.1603117	7.0020075	-2.7888327
C	1.9097474	6.2867588	-1.6310165
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H	2.1753719	6.9911467	-4.9367948
H	2.5041967	8.0267046	-2.7182187
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N	0.6560677	2.5683548	-1.2719884
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S	0.7288449	2.7411541	-2.9063760

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S	-0.1299192	-0.1405044	-1.0503215
S	0.3889955	0.6394760	0.8231526
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F	-2.2622239	-1.8525744	3.0495331
F	-2.9676473	-4.1379589	4.2011252
F	-0.2715409	-6.5087059	1.1793016
F	0.4640876	-4.2292409	0.0332236
C	-0.4760829	-1.6867527	0.8595956
C	-0.8745535	-2.9585157	1.4992404
C	-1.7452990	-2.9802102	2.5817401
C	-2.1182853	-4.1741091	3.1736568
C	-1.6402696	-5.3966142	2.7282614
C	-0.7713306	-5.3650819	1.6485770
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C	1.3961027	4.6182833	-3.1044663
C	1.5747855	5.3606030	-4.2669075
C	1.9545554	6.6872420	-4.1611762
C	2.1549139	7.2721955	-2.9132320
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H	1.4200572	4.9054546	-5.2378482
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H	-2.9253509	-7.1013424	2.8683285
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N	-0.7185438	-1.8102758	-0.3537339
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F	-2.2651745	-2.1022047	3.2622755
F	-2.8954227	-4.4137853	4.4403336
F	-0.3928328	-6.7543406	1.2497929
F	0.2791431	-4.4561504	0.0680125
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C	-0.9711683	-3.1830166	1.6117708
C	-1.7755978	-3.2210277	2.7475153
C	-2.1157737	-4.4127703	3.3528727
C	-1.6710720	-5.6372259	2.8627789
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C	1.5444478	5.1089630	-4.1804239
C	1.9194705	6.4370334	-4.0752644
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C	1.8313405	6.3216121	-1.6665896
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H	2.3560199	8.0793619	-2.7614590
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S	1.1180905	3.9109435	-0.4422825
S	0.8342657	2.7138721	-2.9241129
H	-1.4843094	-7.6229826	3.2164822
H	-2.3842538	-6.7737523	4.3806775
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N	-0.6041293	-0.4808263	-0.9742297
N	0.1941385	0.3324187	1.0605202
F	-1.8669702	-0.8651920	2.6998328
F	-2.4775735	-3.1644600	3.8332920
F	-0.0366363	-5.4414114	0.4927823
F	0.4821592	-3.1511168	-0.6750346
C	-0.3447166	-0.6272482	0.3191574
C	-0.6702649	-1.9142776	0.9625318
C	-1.3966108	-1.9756054	2.1472317
C	-1.7123872	-3.1794618	2.7416386
C	-1.2983506	-4.4094443	2.2127817
C	-0.5464067	-4.3327808	1.0365246
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H	2.5507706	8.2871348	-5.5210883
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N	0.8235116	3.8859963	-1.9216900
S	1.1920657	5.2332544	-1.0536806
S	1.0003155	4.0451689	-3.5488074
N	-1.6690285	-5.5908436	2.8295980
C	-1.2610545	-5.8095598	4.2009798
H	-0.2568059	-6.2547019	4.2589271
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H	-1.9652095	-6.4910211	4.6845102
C	-1.8141958	-6.8005401	2.0549250
H	-2.2189892	-6.5714253	1.0701405
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N	-1.7766475	-1.8302651	0.5948527
N	0.4886280	-2.0513299	1.2940742
F	-2.4139848	-2.6141606	3.4901274
F	-3.0149626	-4.9296464	4.7044324

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C	-1.9279942	-3.7467131	2.9985014
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C	-1.7353768	-6.1374206	3.1520001
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C	-0.6067408	-4.9281711	1.4084268
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C	2.0365184	5.9097751	-3.7323229
C	1.8451356	6.5638183	-2.5175351
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H	1.9068901	4.0522123	-4.8051810
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H	2.0684475	7.6204217	-2.4335486
H	1.2228383	6.3876391	-0.4681186
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Se	0.8698601	-0.5150903	0.4783733
Se	-1.3623037	-0.2903810	-0.1962748

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N	-1.4682722	-2.1250175	0.1748661
N	0.2213671	-1.7672100	1.8150055
F	-2.3117961	-2.6402505	3.5881036
F	-2.9432781	-4.9783480	4.7664238
F	-0.5827191	-7.2961348	1.4391952
F	0.0492551	-4.9588785	0.2584208
C	-0.7601006	-2.4451875	1.2442997
C	-1.1142238	-3.7400952	1.8937750
C	-1.8749785	-3.7708156	3.0505306
C	-2.2081194	-4.9663787	3.6645112
C	-1.7689399	-6.1599531	3.1144036
C	-1.0057502	-6.1528426	1.9579051
C	-0.6892107	-4.9449241	1.3593331
C	1.1664362	4.5698818	-1.5295584

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C	1.6721504	4.5876433	-3.8960966
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H	1.3869027	6.4417106	-0.4886564
N	0.4999733	2.1247917	-1.0531411
S	0.6407932	3.5424971	-0.2301850
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N	0.5937938	-1.7785506	1.1898095
F	-2.3305517	-2.3090565	3.3353471
F	-2.9801190	-4.6121119	4.5303233
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F	0.2257075	-4.6683520	0.1799998
C	-0.6688832	-2.1470991	1.0643408
C	-1.0347465	-3.4313405	1.7290284
C	-1.8627620	-3.4443563	2.8412574
C	-2.1991196	-4.6313895	3.4653511
C	-1.7166501	-5.8458309	2.9818817
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C	1.2184238	4.7985986	-1.6657704
C	1.4187800	4.1397338	-2.8821056
C	1.8518462	4.8431399	-4.0011883
C	2.0808895	6.2027647	-3.8876081
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H	2.0670982	7.9239626	-2.6024897
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N	0.4237074	-1.2835412	1.5222419
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C	-0.6069850	-1.9159156	0.9909546
C	-0.9723099	-3.2113510	1.6368187
C	-1.6995241	-3.2356653	2.8150883
C	-2.0383235	-4.4318682	3.4245853
C	-1.6568648	-5.6273326	2.8350809
C	-0.9356035	-5.6245396	1.6510800
C	-0.5933373	-4.4160563	1.0684151
O	-2.5850482	-7.7051303	2.7730366
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C	1.2902257	5.0665871	-1.7865031
C	1.4958683	4.3792183	-2.9859202
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C	2.1627401	6.4177759	-4.0372347
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N	0.4653109	-1.0446245	1.4735916
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C	-1.6478916	-3.0268911	2.7023498
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C	-1.6275115	-5.4489829	2.7432196
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C	1.6026157	4.6233664	-3.1121822
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H	1.4148595	7.2118027	-0.9096349
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S	0.8393198	4.2763876	-0.6238769
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C	-2.0867503	-4.4804923	3.4183762
C	-1.6845922	-5.7033656	2.8891611
C	-0.9212110	-5.6603373	1.7261705
C	-0.5884045	-4.4646779	1.1232888
C	1.3668904	5.0926935	-1.8172391
C	1.4120995	4.4369226	-3.0506176
C	1.7577369	5.1313183	-4.2050153
C	2.0605039	6.4782243	-4.1093983
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C	1.6756833	6.4457981	-1.7274586
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N	0.7126290	2.6446499	-1.3315773
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N	-0.6152029	-0.5905804	-0.9292274
N	0.2724636	0.2228845	1.1244717
F	-2.2117253	-0.9081919	2.4452570
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C	-0.3118194	-0.6843638	0.3562745
C	-0.6685816	-1.9658023	1.0196014
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C	-1.3424704	-4.4255673	2.3000870
C	-0.3945562	-4.3550658	1.2751799
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C	1.8506547	5.6574482	-3.7113055
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N	1.0028558	3.8945605	-2.0293090
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C	-1.5334160	-5.7105656	4.3513679
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H	-1.7019011	-4.7551921	4.8431454
H	-2.2426452	-6.4322579	4.7638421
C	-1.6616915	-6.8539579	2.2150260
H	-1.9069479	-6.7091070	1.1638027
H	-0.6758795	-7.3322018	2.2791792
H	-2.4014676	-7.5348633	2.6450041
Se	0.7045152	1.7454491	0.3123882
Se	-0.1814564	0.9508387	-1.7038041

BDTA

C	-0.6988738	0.0000000	-0.8113868
C	0.6988738	0.0000000	-0.8113868
C	1.4020932	0.0000000	0.3882758
C	0.6961358	0.0000000	1.5792729
C	-0.6961358	0.0000000	1.5792729
C	-1.4020932	0.0000000	0.3882758
H	2.4856229	0.0000000	0.3888063
H	1.2354818	0.0000000	2.5188339
H	-1.2354818	0.0000000	2.5188339
H	-2.4856229	0.0000000	0.3888063
N	0.0000000	0.0000000	-3.3036131
S	-1.3807207	0.0000000	-2.4119956
S	1.3807207	0.0000000	-2.4119956