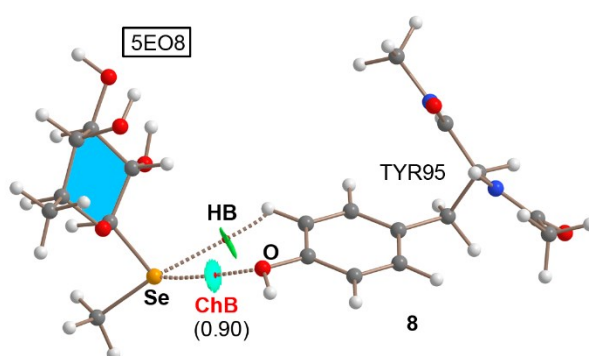


# Selenium Chalcogen bonds are involved in protein-carbohydrate recognition: A combined PDB and theoretical study.

Jose A. Fernández Riveras,<sup>a</sup> Antonio Frontera<sup>a</sup> and Antonio Bauzá<sup>a,\*</sup>

<sup>a</sup>Department of Chemistry, Universitat de les Illes Balears  
Ctra. de Valldemossa km 7.5, 07122 Palma de Mallorca (Spain)  
E-mail: [antonio.bauza@uib.es](mailto:antonio.bauza@uib.es)



**FigS1.** Distribution of critical points and bond paths in complex **8**. Intermolecular bond critical points (BCPs) are denoted by red dots. The bond paths connecting bond critical points are also represented. The value of the density at the BCP ( $\rho \cdot 10^2$ , a.u.) is also indicated for the ChB interaction (highlighted in red). NCIplot surfaces involving only intermolecular contacts between the Se-pyranose ligand and TYR95 are also shown. NCIplot colour range  $-0.002$  a.u.  $\leq (\text{sign}\lambda^2)\rho \leq -0.002$  a.u.

## Cartesian coordinates of PDB models

### 5 (1@SER)

C	-7.6551448	-0.0994732	-1.4148618
C	-6.2933048	-0.6162732	-0.9513318
O	-5.9999148	-1.8143932	-1.0208718
N	-5.4652548	0.2948268	-0.4775018
C	-4.1579448	-0.0613732	0.0349782
C	-3.6877048	1.0930368	0.9120182
O	-4.5038148	1.8673068	1.3979382
C	-3.1869648	-0.3478932	-1.1276918
O	-1.9543348	-0.8952632	-0.6213518
N	-2.3956748	1.1912068	1.1813982
C	-1.8980648	2.2817868	2.0004382
C	1.7550252	-0.5063132	-0.6977118
C	2.4722752	-0.4561132	0.6583482
C	2.9107152	0.9942268	0.9659882

C	3.7245652	1.5960568	-0.1885918
C	2.9271752	1.4507768	-1.4966218
C	3.7261752	1.9881068	-2.7087918
C	1.7526852	-1.9639732	2.4926582
C	2.9890252	-2.7578532	2.1712882
C	2.9146152	-3.0312432	-1.1084118
N	1.5568152	-0.8969632	1.7369582
O	3.7038552	1.0045468	2.1799582
O	3.9453452	2.9765968	0.0835982
O	2.6735652	0.0512468	-1.6954618
O	4.8922452	1.2228668	-2.8629718
O	1.0184852	-2.2695232	3.4810182
Se	1.2886552	-2.2465932	-1.1607918
H	-7.8376560	0.9702760	-1.1918100
H	-3.6738712	-1.0455324	-1.8410801
H	-2.9291852	0.5894244	-1.6603339
H	-2.1201712	-1.8137055	-0.3350287
H	-4.2401673	-0.9917210	0.6455225
H	-2.2757686	3.2545564	1.6265804
H	0.7992547	0.0678029	-0.6708619
H	3.3772587	-1.0759459	0.6425667
H	2.0016602	1.6380493	1.0828399
H	4.6776580	1.0299724	-0.3164666
H	1.9666200	2.0154952	-1.4034447
H	4.0170844	3.0347921	-2.4907605
H	3.0685784	1.9764856	-3.6124688
H	3.0938564	-3.5207030	2.9635972
H	3.9074233	-2.1381834	2.1689897
H	2.9078581	-3.2836606	1.2088604
H	2.8346666	-4.0586541	-0.7002715
H	3.6562303	-2.4910065	-0.4940957
H	3.3707910	-3.1231037	-2.1165749
H	3.1207831	0.6714050	2.8893783
H	4.3762969	3.0093462	0.9598486
H	4.5962920	0.2937598	-2.9305155
H	-5.7916506	1.2171310	-0.1623778
H	-1.7712896	0.4843241	0.7681104
H	0.7146073	-0.3426313	1.9189843
H	-8.4439584	-0.7154997	-0.9419733
H	-7.7358575	-0.2545210	-2.5093623
H	-2.2301029	2.1841177	3.0555280
H	-0.7914654	2.2853565	1.9716155

## 5 (1@SER) -Relaxed geometry

C	-7.7970453	-0.4649794	-1.0117067
C	-6.3501360	-0.8228472	-0.6961972
O	-5.9555299	-1.9910046	-0.6478125
N	-5.5072653	0.2384624	-0.4796183
C	-4.1527490	0.0361591	-0.0186790
C	-3.6458633	1.3871329	0.5427650
O	-4.4053153	2.3502278	0.6908044
C	-3.2374556	-0.5239720	-1.1374911
O	-1.9489576	-0.8937770	-0.6265057
N	-2.3205168	1.3967826	0.8507918
C	-1.6329323	2.5834096	1.3178127
C	1.8048620	-0.4309948	-0.6875915
C	2.4633890	-0.4107192	0.7075366
C	2.9281211	1.0113502	1.0311197
C	3.8000985	1.5787663	-0.0840985
C	3.0675087	1.4759461	-1.4296959
C	3.9664794	1.8464223	-2.6105716
C	1.5781119	-2.0971967	2.4307394
C	2.8520420	-2.9226120	2.3408985
C	3.1099097	-2.8854148	-1.5814050
N	1.5621924	-0.8954770	1.7318043
O	3.6690730	1.0734045	2.2380451
O	4.0970854	2.9448742	0.1442410
O	2.6544780	0.1161560	-1.6704411
O	5.0734402	0.9696666	-2.7157591
O	0.6062978	-2.4358072	3.0974999
Se	1.2940324	-2.2451070	-1.1659457
H	-7.9905371	0.6230889	-1.0777024
H	-3.7522326	-1.3906318	-1.6004198
H	-3.0679185	0.2497164	-1.9132924
H	-2.0356333	-1.7571312	-0.1775560
H	-4.1481631	-0.7211966	0.8033471
H	-1.2371761	3.2029438	0.4822066
H	0.8046319	0.0692891	-0.6760158
H	3.3630610	-1.0547733	0.6783862
H	2.0070374	1.6395355	1.0776860
H	4.7260222	0.9579305	-0.1628483
H	2.1776348	2.1515314	-1.4029342
H	4.3590343	2.8686537	-2.4401860
H	3.3436956	1.8578780	-3.5381084
H	2.7983885	-3.7160537	3.1067582
H	3.7629110	-2.3101406	2.4969400

H	2.9173426	-3.3972567	1.3407242
H	3.0115884	-3.9448824	-1.8841443
H	3.7817360	-2.8195130	-0.7033032
H	3.5218969	-2.2943720	-2.4192194
H	3.1049838	0.6790926	2.9328204
H	4.4665401	2.9919491	1.0474951
H	4.6928230	0.0697288	-2.7426878
H	-5.8536758	1.1960457	-0.3358050
H	-1.7892595	0.5694075	0.5391548
H	0.6501756	-0.4287443	1.7929645
H	-8.4459415	-0.9041401	-0.2279390
H	-8.0784167	-0.9455172	-1.9691766
H	-2.3376784	3.2087162	1.8983163
H	-0.7860882	2.2868427	1.9664616

## 6 (1@ASP)

C	-3.6993175	1.3561952	2.4701106
C	-4.0063175	1.9561952	1.1101106
O	-5.1033175	2.4051952	0.8551106
N	-3.0143175	1.9371952	0.2311106
C	-3.2003175	2.5011952	-1.1188894
C	-3.9843175	1.5571952	-2.0258894
O	-4.9963175	1.9631952	-2.6058894
C	-1.8633175	2.8841952	-1.7448894
C	-1.1993175	4.0821952	-1.0488894
O	-1.9083175	4.9841952	-0.5798894
O	0.0476825	4.1261952	-1.0378894
N	-3.5403175	0.3021952	-2.1258894
C	-4.1313175	-0.6278048	-3.0718894
C	2.3506825	-0.9048048	-0.1528894
C	1.6536825	-0.9678048	1.2201106
C	2.5506825	-1.9308048	2.0301106
C	2.4096825	-3.3228048	1.4071106
C	2.9516825	-3.2388048	-0.0208894
C	2.8596825	-4.5968048	-0.7098894
C	0.5536825	1.1991952	1.7191106
C	0.7086825	2.3921952	2.2341106
C	3.2156825	0.7681952	-2.5118894
N	1.6216825	0.3981952	1.7621106
O	2.2956825	-2.0548048	3.4181106
O	3.1016825	-4.3218048	2.1851106
O	2.2476825	-2.2158048	-0.7518894
O	3.1086825	-4.4808048	-2.1128894
O	-0.5183175	0.9131952	1.2191106

Se	1.6496825	0.5711952	-1.3088894
H	-3.8633697	2.1314957	3.2459710
H	-2.6706100	0.9533663	2.5633871
H	-1.1594623	2.0219705	-1.7688016
H	-2.0517117	3.1709139	-2.8027339
H	-3.8074240	3.4220864	-1.0271543
H	-5.0105501	-0.1112066	-3.5038110
H	3.4310739	-0.6569575	-0.0060943
H	0.6068023	-1.3137758	1.1138584
H	3.6107957	-1.5850467	1.8815592
H	1.3438207	-3.6270944	1.4055691
H	4.0354245	-2.9472036	0.0324658
H	3.6117906	-5.2787038	-0.2658332
H	1.8516070	-5.0407926	-0.5074759
H	1.6398877	2.5948832	2.8041370
H	0.6681007	3.1337529	1.3881365
H	4.1374592	0.9613430	-1.9278510
H	2.9813684	1.6586021	-3.1261229
H	3.3463207	-0.1181431	-3.1610796
H	2.5391962	-2.9839904	3.6194920
H	4.0585191	-4.1322385	2.1025960
H	2.6335099	-3.6656163	-2.3775221
H	-3.4272307	-0.8960301	-3.8920172
H	-4.4665814	-1.5675457	-2.5796455
H	-4.4310497	0.5464628	2.6671492
H	-2.0615313	1.6810375	0.5303739
H	-2.6961958	0.0466394	-1.6098801
H	2.4680056	0.7395644	2.2144510
H	-0.1537145	2.6808011	2.8667861

**7 (2@ASP)**

C	-5.4400517	-1.4886800	1.5574788
C	-4.2769317	-0.5517100	1.2524388
O	-3.9347417	0.3150300	2.0580388
N	-3.6765417	-0.7320800	0.0805488
C	-2.5502817	0.0889600	-0.3424912
C	-2.9536517	1.5540700	-0.4741312
O	-2.2432717	2.4463200	-0.0144512
C	-1.9831317	-0.4169800	-1.6700912
C	-1.4768417	-1.8437900	-1.5845112
O	-2.2223617	-2.7208300	-1.0951812
O	-0.3276817	-2.0909000	-2.0049912
N	-4.0962717	1.7947600	-1.1093912
C	-4.5933017	3.1516200	-1.3008412

Se	0.8165283	-1.6775900	1.3430888
C	2.6717383	-1.2454600	0.8424588
C	2.6834683	-1.4850500	-0.6658412
O	2.8320983	-2.8802000	-0.8758112
C	3.9170683	-0.7920500	-1.2672612
O	3.8757483	-0.8628200	-2.6776712
C	3.8523683	0.6818600	-0.8376012
O	4.8653783	1.4279700	-1.4806012
C	4.0514583	0.7040100	0.6843288
O	2.9073783	0.0727500	1.2882988
C	4.1279783	2.1276300	1.2281088
O	5.3733983	2.2744200	1.8855988
C	0.7431983	-0.8891500	3.1306888
H	-6.3620617	-0.8812109	1.6539502
H	-2.7644155	-0.3548460	-2.4614996
H	-1.1299143	0.2080815	-1.9799950
H	-1.7528713	0.0751577	0.4317842
H	-3.7553868	3.8423466	-1.0944617
H	3.3786306	-1.9655669	1.3185775
H	1.7766278	-1.0777001	-1.1619508
H	2.0898364	-3.1532545	-1.4460433
H	4.8375370	-1.2699656	-0.8477891
H	4.4882142	-0.1595236	-2.9749872
H	2.8350705	1.0753708	-1.0713415
H	4.5805498	2.3565155	-1.5277346
H	4.9992202	0.1804184	0.9507267
H	4.0032383	2.8746196	0.4028742
H	3.2570106	2.2669401	1.9128531
H	5.4005009	3.1604928	2.2899265
H	1.2160388	0.1092653	3.0917581
H	-0.3299769	-0.7796480	3.3786670
H	-3.8967604	-1.5697379	-0.4591662
H	-4.7120600	1.0068122	-1.3204136
H	1.2437553	-1.5258674	3.8853608
H	-5.6133373	-2.2825270	0.8029350
H	-5.2616137	-1.9579716	2.5442627
H	-4.9519186	3.2965093	-2.3401950
H	-5.4209098	3.3898002	-0.5985002
H	-1.7206483	-3.5700934	-1.0724749

**8 (3@TYR)**

C	5.4322761	-0.8276306	2.0810306
C	4.2922761	-1.7116306	1.5380306
O	3.4132761	-2.1326306	2.2860306

N	4.3372761	-1.9846306	0.2380306
C	3.3392761	-2.8476306	-0.3729694
C	3.9852761	-3.8516306	-1.3029694
O	5.0292761	-3.5896306	-1.9169694
C	2.3262761	-2.0426306	-1.1809694
C	1.4932761	-1.1686306	-0.3059694
C	0.3232761	-1.7026306	0.2440306
C	1.8232761	0.1683694	-0.0369694
C	-0.4947239	-0.9426306	1.0380306
C	0.9882761	0.9003694	0.8300306
C	-0.1517239	0.3393694	1.3150306
O	-1.0517239	1.0833694	2.1480306
N	3.3912761	-5.0436306	-1.3989694
C	3.7612761	-6.0426306	-2.4159694
O	-1.7627239	3.6623694	1.4770306
C	-2.6257239	4.0843694	0.4280306
C	-1.9937239	3.6673694	-0.9029694
O	-0.6687239	4.2033694	-1.0079694
C	-2.1707239	2.1673694	-1.1399694
C	-4.0167239	3.4663694	0.5660306
C	-4.6197239	3.8033694	1.9060306
O	-3.9847239	2.0383694	0.3850306
C	-3.6237239	1.7663694	-0.9639694
Se	-3.6727239	-0.2106306	-1.0479694
C	-5.5927239	-0.1246306	-1.1389694
H	6.1713153	-0.5128622	1.3174446
H	1.6775022	-2.7474721	-1.7441364
H	2.8832223	-1.4553730	-1.9418264
H	0.0481693	-2.7452396	0.0146215
H	2.7329389	0.6175818	-0.4619707
H	-1.4409053	-1.3304798	1.4407820
H	1.2367034	1.9408826	1.0924986
H	-1.1371557	2.0057953	1.8089680
H	2.8145267	-3.3483736	0.4687796
H	4.7323906	-5.7308868	-2.8418977
H	-2.0592941	4.0466509	2.3213176
H	-2.7121660	5.1961439	0.4378513
H	-2.5743449	4.1991666	-1.6910204
H	-0.1971966	3.8907288	-0.2096701
H	-1.5752720	1.6009633	-0.3961375
H	-4.6517313	3.9231629	-0.2377231
H	-4.6415794	4.9004161	2.0630843
H	-4.0380949	3.3260911	2.7219835
H	-5.6554911	3.4200704	1.9860686

H	-4.3304652	2.2158496	-1.7004551
H	-5.9578433	0.4972984	-0.2989495
H	-6.0193287	-1.1417542	-1.0359162
H	-5.9307210	0.3000451	-2.1049047
H	4.9777248	0.0712540	2.5412321
H	5.9490778	-1.3839273	2.8868065
H	3.8649732	-7.0451984	-1.9555036
H	3.0059522	-6.0929423	-3.2287903
H	2.5376344	-5.2085145	-0.8621440
H	5.1437277	-1.7587508	-0.3510008
H	-1.7881341	1.9078831	-2.1476152

**9 (4@TYR)**

C	24.4470000	30.4900000	3.2470000
C	22.9640000	30.8080000	3.1310000
O	22.5780000	31.9550000	2.9060000
H	24.5370000	29.5380000	3.4120000
N	22.1400000	29.7750000	3.2650000
C	20.6950000	29.9490000	3.3270000
C	20.3270000	30.7400000	4.5760000
O	20.9770000	30.6110000	5.6110000
C	19.9890000	28.5950000	3.3370000
C	20.1600000	27.7850000	2.0740000
C	21.2470000	26.9430000	1.9110000
C	19.2190000	27.8470000	1.0520000
C	21.4010000	26.1900000	0.7640000
C	19.3650000	27.1000000	-0.0960000
C	20.4580000	26.2730000	-0.2360000
O	20.6020000	25.5240000	-1.3810000
H	22.5022894	28.9202546	3.6895384
H	20.3945982	30.5199500	2.4203333
H	20.3469019	28.0270971	4.2244388
H	18.9109932	28.7853771	3.5184072
H	21.9913123	26.8432262	2.7173458
H	18.3370366	28.4987621	1.1635582
H	22.2638799	25.5129899	0.6542221
H	18.6230516	27.1408199	-0.9073506
H	21.3672761	24.9319736	-1.2640761
N	19.2840000	31.5560000	4.4830000
C	18.8700000	32.3690000	5.6180000
H	18.8974674	31.7693822	3.5624445



H	19.4607257	33.3082128	5.6889640
C	18.8660000	21.1280000	2.4100000
C	18.4000000	21.4640000	3.8270000
O	17.1210000	22.1140000	3.7980000
C	18.2460000	20.1860000	4.6430000
O	17.9470000	20.5190000	6.0020000
C	19.5030000	19.3330000	4.5840000
O	20.5570000	20.0500000	5.2320000
C	19.8400000	19.0690000	3.1250000
C	21.0490000	18.1510000	2.9690000
O	20.0540000	20.3270000	2.4880000
Se	19.3450000	22.6860000	1.3370000
C	17.7370000	23.7760000	1.0920000
H	18.0522034	20.5606169	1.8954279
H	19.1773244	22.1138842	4.2995333
H	16.8322765	22.1110997	4.7343089
H	17.3714108	19.6263554	4.2451117
H	18.8227364	20.7538119	6.3804348
H	19.3516392	18.3878227	5.1463911
H	20.8969911	20.6762067	4.5572408
H	18.9548048	18.5733292	2.6505752
H	20.8034312	17.1521649	3.3784490
H	21.3277113	18.0437875	1.9030740
H	21.9163041	18.5530630	3.5280758
H	17.2416668	23.9548664	2.0632931
H	17.0314915	23.3131982	0.3759681
H	18.1352788	24.7226709	0.6779573
H	24.9538371	30.7869842	2.3102250
H	17.7959754	32.6237313	5.5313853
H	19.0436064	31.7941238	6.5466265
H	24.8762402	31.0856417	4.0740036

**10 (4@MET)**

C	1.2969620	0.3559035	5.9555643
C	1.7909620	-0.5380965	4.8325643
O	1.4909620	-1.7320965	4.8145643
H	1.7616552	1.3622642	5.9815471
N	2.5339620	0.0279035	3.8885643
C	2.8919620	-0.7280965	2.6965643
C	4.3329620	-0.5410965	2.2685643
O	4.9589620	0.4829035	2.5435643
C	1.9629620	-0.3460965	1.5455643
C	2.0059620	1.1159035	1.1715643
S	0.8109620	1.4649035	-0.1344357

C	1.2249620	3.1609035	-0.5214357
H	2.9407277	0.9607798	3.9851943
H	2.6967617	-1.7888626	2.9618522
H	2.2039120	-0.9645860	0.6525905
H	0.9288759	-0.6301089	1.8400583
H	1.7752359	1.7458287	2.0591102
H	3.0240959	1.4063824	0.8299947
H	0.5518449	3.4668117	-1.3471589
H	1.0639386	3.8440498	0.3395596
H	2.2746483	3.2631962	-0.8698759
N	4.8419620	-1.5690965	1.6015643
C	6.1619620	-1.5460965	0.9945643
H	4.2578905	-2.3935889	1.4526542
H	6.6347769	-0.5840378	1.2675545
C	-2.5230380	0.4659035	-2.9424357
C	-3.0510380	0.8839035	-1.5704357
O	-3.3940380	2.2799035	-1.5554357
C	-4.2970380	0.0819035	-1.1984357
O	-4.6320380	0.3349035	0.1705643
C	-4.0790380	-1.4120965	-1.3784357
O	-3.1550380	-1.8740965	-0.3824357
C	-3.5340380	-1.6700965	-2.7764357
C	-3.2970380	-3.1530965	-3.0384357
O	-2.3160380	-0.9480965	-2.9314357
Se	-0.8470380	1.3719035	-3.3724357
C	-1.3780380	2.1379035	-5.0824357
H	-3.2599960	0.7677920	-3.7278548
H	-2.2665257	0.6401774	-0.8147232
H	-2.5482372	2.7491379	-1.7198749
H	-5.1252655	0.4136331	-1.8753430
H	-4.4946864	1.2945215	0.3005206
H	-5.0689333	-1.9260763	-1.2733315
H	-3.4097770	-1.3721711	0.4206155
H	-4.2946012	-1.2844490	-3.5054874
H	-2.5995574	-3.5550220	-2.2786039
H	-4.2537061	-3.7061412	-2.9707530
H	-2.8612723	-3.3046328	-4.0448806
H	-2.2520450	2.8062150	-4.9631068
H	-1.6029575	1.3396922	-5.8156263
H	-0.5183415	2.7307702	-5.4504739
H	0.2007305	0.4773228	5.8427095
H	1.4699383	-0.1578392	6.9199945
H	6.1035166	-1.6204236	-0.1119458
H	6.7934678	-2.3760367	1.3739569

**11 (4@TYR)**

C	2.5787493	-5.7163520	3.7477997
C	3.2567493	-4.3683520	3.9637997
O	4.4537493	-4.2993520	4.2417997
H	1.4819265	-5.6607552	3.6004893
N	2.4767493	-3.2983520	3.8377997
C	3.0007493	-1.9413520	3.9557997
C	1.8757493	-0.9773520	4.3127997
O	0.7127493	-1.3713520	4.3597997
C	3.6767493	-1.5123520	2.6497997
C	2.7317493	-1.4493520	1.4717997
C	2.3887493	-2.5973520	0.7677997
C	2.1897493	-0.2403520	1.0567997
C	1.5227493	-2.5413520	-0.3082003
C	1.3277493	-0.1753520	-0.0102003
C	0.9987493	-1.3243520	-0.6942003
O	0.1337493	-1.2463520	-1.7612003
H	1.4614968	-3.3515354	3.7058211
H	3.7723335	-1.9510252	4.7590039
H	4.1767492	-0.5294567	2.7883806
H	4.4922247	-2.2421825	2.4642268
H	2.8227133	-3.5640163	1.0667962
H	2.4525648	0.6841338	1.5959576
H	1.2597215	-3.4581017	-0.8614902
H	0.9018492	0.7819546	-0.3503941
H	0.0352138	-2.1288330	-2.1612552
N	2.2227493	0.2826480	4.5637997
C	1.2227493	1.3056480	4.8557997
H	3.2064936	0.5513352	4.5280505
H	0.2325239	0.8173816	4.8103392
C	-1.6992507	2.1736480	-3.4322003
C	-1.9602507	2.6146480	-1.9942003
O	-0.8642507	3.4396480	-1.5802003
C	-3.2972507	3.3506480	-1.9972003
O	-3.6562507	3.7846480	-0.6832003
C	-4.3812507	2.4396480	-2.5602003
O	-4.6022507	1.3756480	-1.6332003
C	-3.9582507	1.8816480	-3.9212003
C	-4.9532507	0.8966480	-4.5232003
O	-2.7032507	1.2286480	-3.7862003
Se	0.0657493	1.3936480	-3.6402003
C	0.4127493	2.2766480	-5.3472003
H	-1.7288680	3.0665593	-4.1029422

H	-2.0515318	1.6968765	-1.3674479
H	-1.1604596	3.8658357	-0.7509248
H	-3.1680319	4.2386166	-2.6649725
H	-4.3458122	4.4668565	-0.7784320
H	-5.3166102	3.0463090	-2.7089948
H	-4.5545176	1.8058905	-0.7538570
H	-3.8523800	2.7628483	-4.6088686
H	-5.0979829	0.0478625	-3.8278486
H	-4.5663682	0.5129443	-5.4863167
H	-5.9321482	1.3864549	-4.6945099
H	0.4723583	3.3759466	-5.2232370
H	1.3879345	1.9081878	-5.7212918
H	-0.3708325	2.0150413	-6.0845484
H	1.3691184	1.7360846	5.8685191
H	1.2591283	2.1268652	4.1096166
H	2.8016421	-6.3657032	4.6162077
H	3.0351162	-6.1969859	2.8592219