

Kinetic enantioselectivity of a protonated bis(diamido)- bridged basket resorcin[4]arene towards alanine peptides.

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Supplementary Information

Figure S1. Kinetic plots of the gas-phase reaction between $\mathbf{B}^R$ and $[\mathbf{1}\cdot\mathbf{H}\cdot\mathbf{AP}]^+$ (AP = L-Ala-L-Phe; $\mathbf{B}^R$ = (R)-(-)-2-aminobutane(1.7×10^{-7} mbar)).

Figure S2 . B3LYP/6-31G*-calculated structures of the $\mathbf{II}_{\text{het}}\text{-IV}_{\text{het}}$ isomers of Table 2 of the main text.

Figure S3 . B3LYP/6-31G*-calculated structures of the $\mathbf{II}_{\text{hom}}\text{-IV}_{\text{hom}}$ isomers of Table 2 of the main text.

Table S1. Cartesian Coordinates for the B3LYP/6-31G*-calculated structures of Figure 3 of main text and Figures S2 and S3.

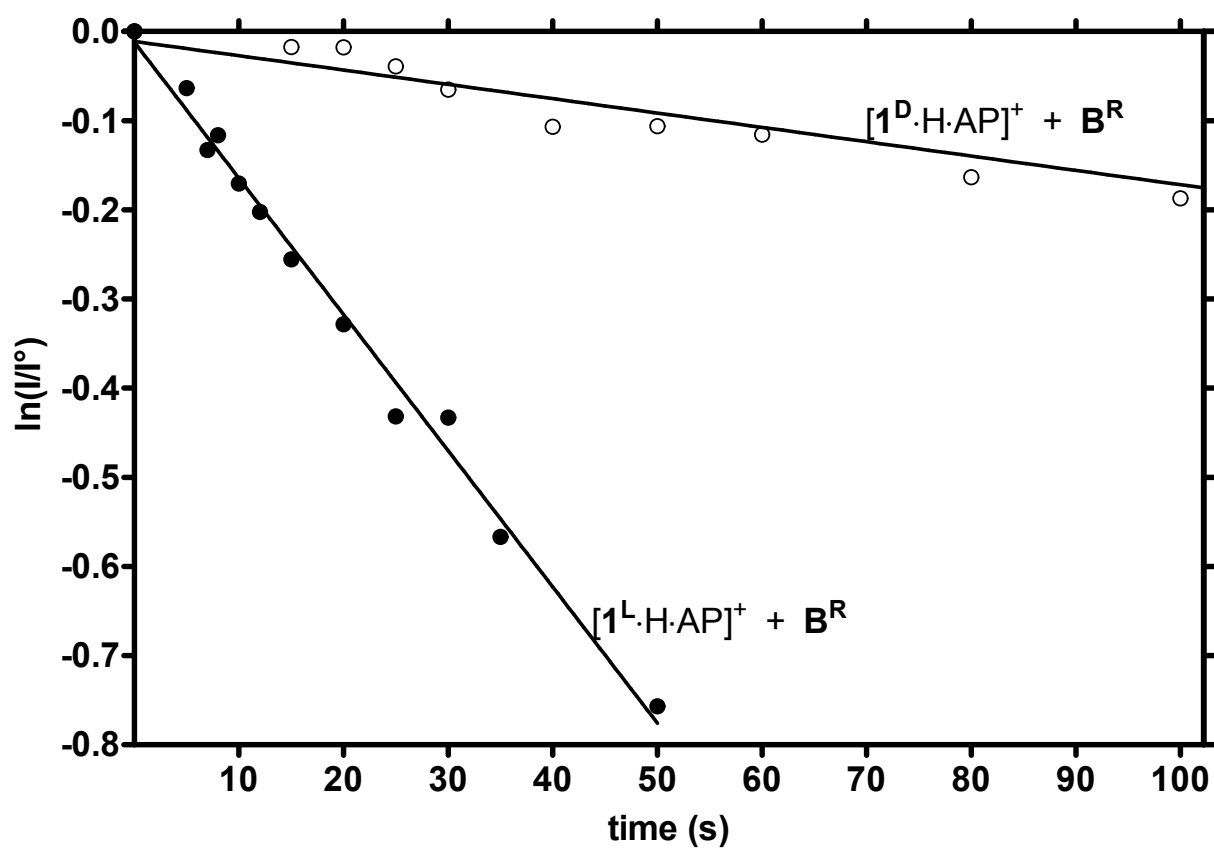


Figure S1. Kinetic plots of the gas-phase reaction between B^R and $[1\cdot H\cdot AP]^+$ (AP = L-Ala-L-Phe (1.7×10^{-7} mbar); B^R = (R)-(-)-2-aminobutane).

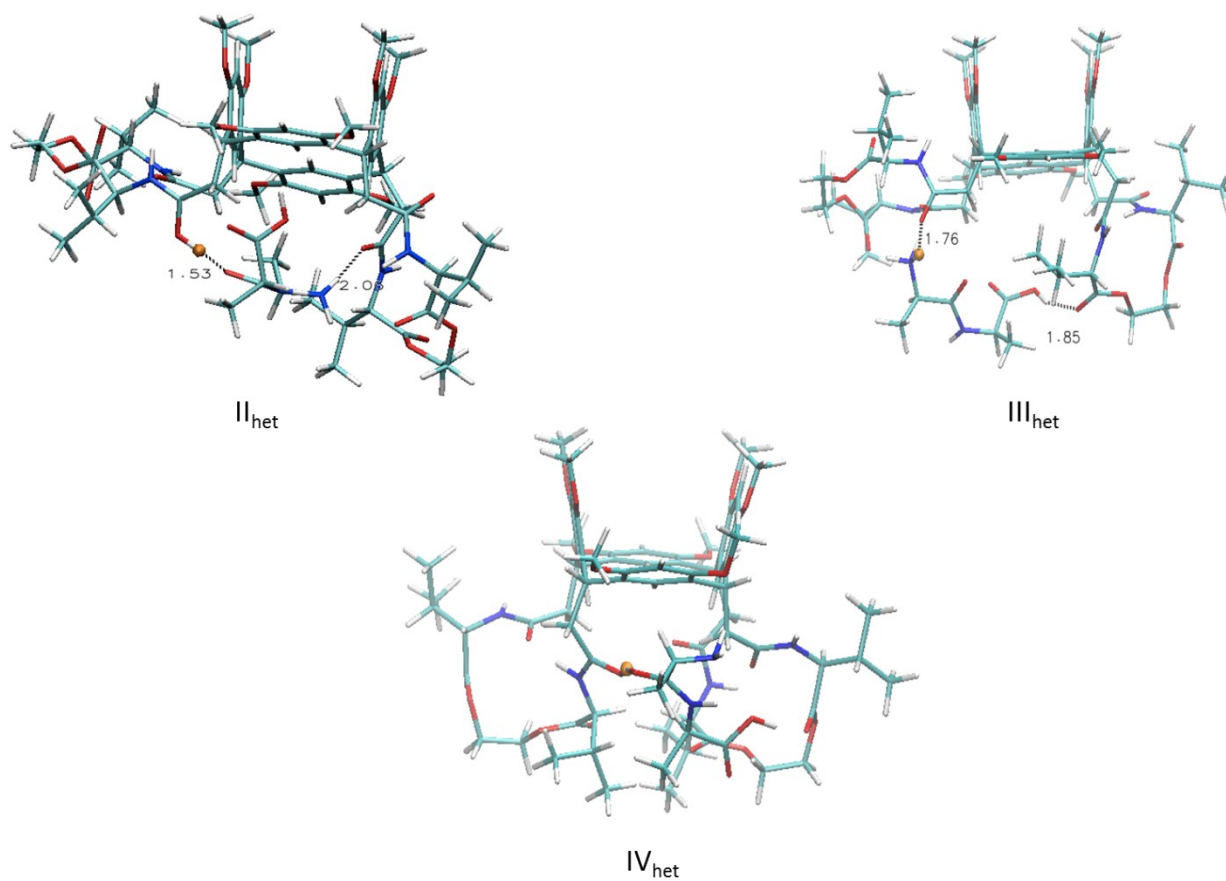
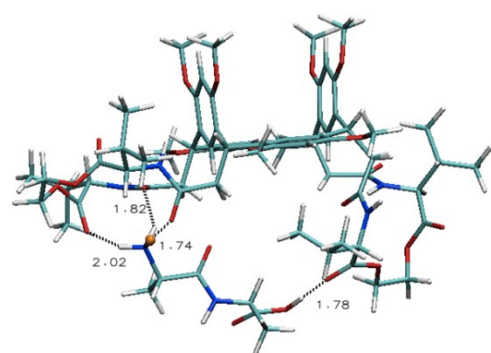
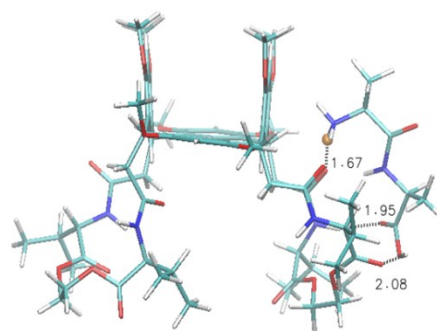


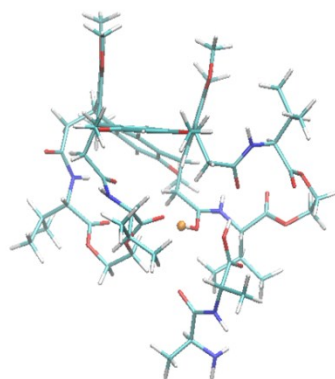
Figure S2 . B3LYP/6-31G*-calculated structures of the II_{het} - IV_{het} isomers of Table 2 of the main text.



II_{hom}



III_{hom}



IV_{hom}

Figure S3 . B3LYP/6-31G*-calculated structures of the **II_{hom}-IV_{hom}** isomers of Table 2 of the main text.

Table S1. Cartesian Coordinates for the B3LYP/6-31G*-calculated structures of Figure 3 of main text and Figures S2 and S3.

Cartesian Coordinates

I^L

180

E= -4367.77265400 Hartrees

G= -4366.398663 Hartrees

C	-3.265122	2.142479	3.646182
C	-2.895250	0.798217	3.774344
C	-2.832074	-0.042239	2.648975
C	-3.124181	0.524102	1.404530
C	-3.512422	1.853736	1.232074
C	-3.581679	2.657985	2.383716
O	-2.592007	0.219673	4.981753
C	-2.511252	-1.520247	2.833087
C	-3.915927	2.445920	-0.113380
O	-3.983726	3.954388	2.187405
C	-2.699322	0.998522	6.156120
C	-4.147023	4.796219	3.310998
C	0.861448	-3.154166	3.699215
C	-0.510754	-2.880804	3.650539
C	-1.011659	-1.811803	2.888262
C	-0.087419	-1.066618	2.155087
C	1.282343	-1.328534	2.142987
C	1.753305	-2.382093	2.942255
O	-1.448105	-3.642973	4.311054
C	2.219437	-0.538440	1.234988
O	3.104896	-2.601726	2.930253
C	-1.002334	-4.629935	5.223433
C	3.613905	-3.756187	3.570198
C	2.286720	3.041086	2.578219
C	2.410327	1.653804	2.491933
C	1.992590	0.970157	1.326849
C	1.460315	1.737979	0.289978
C	1.368126	3.142629	0.317891
C	1.780389	3.774784	1.498194
O	2.946366	0.877566	3.478028
C	0.941751	3.966146	-0.892143
O	1.762717	5.153149	1.605442
C	3.393637	1.503715	4.667409
C	0.564446	5.685924	2.172209
C	-2.424497	5.528537	-1.859989
C	-3.340554	4.603051	-1.344241
C	-2.903120	3.469446	-0.637581
C	-1.523878	3.293140	-0.493874
C	-0.571811	4.179754	-1.007472
C	-1.052246	5.312906	-1.693754
O	-4.696746	4.732476	-1.501074

O	-0.097491	6.166381	-2.182195
C	-5.204323	5.883372	-2.149610
C	-0.503650	7.321652	-2.893002
C	-5.312600	0.424666	-1.006389
O	-5.854233	0.224652	0.074326
C	-4.170013	1.413998	-1.236181
C	-2.462618	-2.786053	0.550953
O	-2.302427	-1.996219	-0.383464
C	-3.253273	-2.459987	1.814970
N	-5.682107	-0.263227	-2.141712
N	-1.920905	-4.035295	0.519816
C	2.997700	3.543822	-2.485104
O	3.457573	4.274521	-3.360824
C	1.488116	3.419197	-2.252493
C	2.866433	-2.385455	-0.431707
O	2.381889	-3.486215	-0.162472
C	2.139909	-1.059844	-0.232972
N	3.812878	2.775489	-1.698781
N	4.121019	-2.246790	-0.953516
H	2.614956	3.589348	3.453611
H	1.126955	1.226469	-0.606714
H	-3.070577	-0.126950	0.539967
H	-3.321000	2.776841	4.520543
H	-2.773688	6.402210	-2.392175
H	-1.180147	2.426787	0.063435
H	-0.459962	-0.238304	1.560952
H	1.231488	-3.974019	4.299795
H	-2.911500	-1.797769	3.811692
H	-4.855740	2.982866	0.046029
H	-2.004804	1.850744	6.145282
H	-3.721879	1.374321	6.305204
H	-2.436371	0.335002	6.983744
H	-3.197989	4.956303	3.842329
H	-4.888207	4.395037	4.016831
H	-4.503004	5.752793	2.921688
H	3.239660	-0.710559	1.588678
H	-0.450382	-5.435389	4.718108
H	-1.902491	-5.047152	5.680762
H	-0.364575	-4.198127	6.006682
H	3.450362	-3.727022	4.657267
H	3.167085	-4.672323	3.161533
H	4.688220	-3.760597	3.373886
H	1.384246	4.957974	-0.759364
H	2.573225	2.020856	5.183483
H	3.771595	0.700586	5.303131
H	4.201698	2.220522	4.468496
H	0.413004	5.315676	3.195928
H	0.690657	6.771559	2.194318
H	-0.312915	5.428970	1.566622
H	-4.913539	6.805168	-1.627001

H	-4.870833	5.942803	-3.195237
H	-6.292021	5.786029	-2.126270
H	-1.104576	7.994195	-2.264662
H	0.416833	7.829948	-3.187168
H	-1.077121	7.062837	-3.793739
H	-2.029593	-4.623443	1.331933
H	-3.262096	0.825871	-1.429371
H	-4.370711	1.966588	-2.162769
H	-4.198904	-1.994996	1.518136
H	-3.491183	-3.391822	2.338472
H	-5.124196	-0.143351	-2.979923
H	4.506013	-1.315974	-1.064166
H	1.175338	2.376837	-2.392395
H	1.036597	4.004304	-3.054817
H	2.592589	-0.318799	-0.898237
H	1.096095	-1.197268	-0.534002
H	3.430290	2.221619	-0.943054
C	5.017901	-3.380138	-1.135776
C	5.255809	2.794622	-1.857174
C	4.662194	-4.235589	-2.396978
C	4.799789	-3.460589	-3.713881
C	5.455051	-5.549678	-2.422358
C	5.902373	4.080993	-1.234387
C	7.323069	4.351703	-1.747860
C	5.833391	4.090018	0.298207
C	5.802061	1.505160	-1.255406
O	7.089296	1.299285	-1.602913
C	6.462627	-2.897810	-1.165528
O	6.566742	-1.684351	-1.776435
C	7.850423	-1.039233	-1.786393
C	7.811357	0.229365	-0.952080
O	5.172637	0.765786	-0.521486
O	7.407429	-3.519535	-0.734253
H	6.491592	3.327709	0.737238
H	4.815708	3.910328	0.659111
H	6.157130	5.062579	0.685777
H	8.829070	0.612712	-0.833824
H	7.370880	0.034026	0.028632
H	5.260933	4.883032	-1.616876
H	7.655944	5.341836	-1.415115
H	7.357963	4.339443	-2.844251
H	8.043840	3.614817	-1.378452
H	8.084419	-0.807284	-2.829704
H	8.600400	-1.725944	-1.384252
H	5.482257	2.805852	-2.929473
H	4.929488	-4.039217	-0.265870
H	3.602590	-4.477289	-2.251933
H	4.257716	-2.509979	-3.677476
H	4.385967	-4.050137	-4.539823
H	5.849054	-3.246512	-3.953338

H	6.530394	-5.375620	-2.549444
H	5.116380	-6.177294	-3.254772
H	5.318403	-6.118647	-1.495170
H	-0.449724	-5.783375	1.958787
O	-0.885215	-3.921544	-2.863844
H	1.320995	-5.780501	-1.404447
H	-5.151209	-5.706723	-2.721146
C	0.186868	-6.054905	1.108212
C	0.425583	-6.410485	-1.362568
C	-0.518079	-5.916120	-0.254224
H	1.073674	-5.412996	1.136947
H	0.738750	-7.440126	-1.153136
C	-0.967179	-4.446592	-0.502421
C	-1.538025	-4.288093	-1.911693
O	-5.143667	-2.214068	-4.032796
H	-3.136834	-3.621094	-3.751711
C	-4.899046	-4.769561	-3.222287
O	-2.826504	-4.700814	-2.004910
H	0.502005	-7.094485	1.259835
C	-3.396317	-4.587023	-3.318748
H	-5.318585	-4.765773	-4.233490
H	-0.043405	-6.394942	-2.351067
O	-5.556220	-3.756816	-2.428049
C	-5.615040	-2.519834	-2.953320
H	-9.743580	-0.759516	-1.591905
H	-7.801955	0.117055	-3.865437
H	-2.984583	-5.371659	-3.967176
C	-8.672900	-0.740391	-1.353864
C	-6.364395	-1.550184	-2.046893
C	-8.127993	-0.928704	-3.820383
H	-8.351321	0.304875	-1.303441
C	-7.879060	-1.508211	-2.420575
H	-9.198580	-0.956107	-4.055907
H	-7.593382	-1.480693	-4.600077
H	-8.532082	-1.171399	-0.357123
H	-8.217601	-2.555392	-2.409128
H	-6.282043	-1.893208	-1.012454
H	-0.077828	-3.806507	-0.471211
H	-1.425727	-6.538771	-0.258125

[I^L·H]⁺
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E= -4368.19265934 Hartrees

G= -4366.802686 Hartrees

C	5.209036	1.889867	-1.446290
C	4.226587	2.521748	-2.215610
C	2.874916	2.513659	-1.819230
C	2.562326	1.867068	-0.621526
C	3.510636	1.207782	0.165025
C	4.843656	1.206550	-0.281539

O	4.501354	3.142403	-3.407483
C	1.813678	3.090174	-2.758483
C	3.118413	0.395953	1.400337
O	5.737261	0.478140	0.464139
C	5.848938	3.210397	-3.851485
C	7.093636	0.408913	0.038458
C	-0.725962	5.407232	-1.062736
C	0.460216	4.917467	-1.627322
C	0.544275	3.585827	-2.074361
C	-0.584882	2.781397	-1.897741
C	-1.779374	3.219156	-1.314711
C	-1.836735	4.568569	-0.914252
O	1.575705	5.685988	-1.796362
C	-2.986231	2.300604	-1.104781
O	-3.026073	4.999259	-0.388242
C	1.541692	7.051075	-1.413056
C	-3.117643	6.334506	0.085110
C	-4.999181	1.720123	2.121058
C	-4.670942	2.114760	0.816977
C	-3.346306	2.084400	0.364551
C	-2.367178	1.676283	1.275700
C	-2.656396	1.223224	2.558843
C	-4.002567	1.249189	2.980657
O	-5.692292	2.460373	-0.052470
C	-1.578704	0.602855	3.448614
O	-4.247924	0.760373	4.235854
C	-6.275422	3.745643	0.177387
C	-5.574267	0.819650	4.741897
C	1.488326	2.856034	3.838415
C	2.422373	2.218642	3.013568
C	2.070518	1.072849	2.271240
C	0.768219	0.595603	2.413558
C	-0.187908	1.185600	3.245633
C	0.189283	2.342614	3.950448
O	3.714310	2.637456	2.882063
O	-0.770973	2.902881	4.746117
C	4.144482	3.786453	3.593893
C	-0.433856	4.024492	5.547114
C	2.498201	-2.122317	1.947669
O	1.371169	-2.558190	2.207606
C	2.731846	-1.032387	0.905434
C	1.475885	0.616075	-3.582080
O	0.516468	0.113204	-2.990199
C	1.559377	2.097492	-3.949766
N	3.588293	-2.650495	2.584869
N	2.536428	-0.143295	-3.990665
C	-1.880279	-1.626643	2.057247
O	-1.582297	-1.047621	0.950114
C	-1.607311	-0.960495	3.385340
C	-3.751110	-0.159397	-1.411776

O	-3.493593	-1.072197	-0.577918
C	-2.745234	0.907977	-1.783152
N	-2.400589	-2.844085	2.069627
N	-4.951356	-0.140427	-1.998838
H	-6.040956	1.741549	2.419649
H	-1.332317	1.667586	0.950179
H	1.527936	1.864423	-0.291807
H	6.238429	1.891434	-1.774944
H	1.772581	3.736469	4.398165
H	0.493249	-0.300344	1.876344
H	-0.501694	1.762784	-2.254365
H	-0.784437	6.440087	-0.749402
H	2.264458	3.968176	-3.228962
H	4.020583	0.319876	2.012422
H	6.482446	3.747504	-3.133263
H	6.265550	2.209626	-4.026054
H	5.825296	3.762968	-4.793034
H	7.585478	-0.284828	0.721240
H	7.578587	1.392630	0.091120
H	7.169609	0.019286	-0.984544
H	-3.859485	2.758353	-1.581397
H	1.357020	7.163338	-0.336517
H	0.778677	7.609548	-1.972109
H	2.528059	7.452593	-1.652074
H	-2.970019	7.061844	-0.724398
H	-4.127549	6.444832	0.485229
H	-2.390873	6.528105	0.884258
H	-1.860505	0.831425	4.480160
H	-5.546412	4.538632	-0.022580
H	-7.116881	3.833117	-0.515377
H	-6.645939	3.840035	1.206708
H	-5.944803	1.852258	4.773087
H	-6.261686	0.206304	4.144005
H	-5.525917	0.422088	5.757506
H	3.577501	4.678910	3.297381
H	4.058296	3.645628	4.679814
H	5.195168	3.924528	3.330481
H	-0.140346	4.885274	4.932314
H	-1.337347	4.274587	6.106413
H	0.375155	3.789825	6.251519
H	3.381899	0.319489	-4.301266
H	3.525305	-1.368030	0.231013
H	1.819390	-0.977072	0.305665
H	2.371502	2.240704	-4.669678
H	0.624927	2.367117	-4.453669
H	3.349573	-3.433368	3.181965
H	-5.138542	0.588050	-2.673292
H	-0.644043	-1.361141	3.730490
H	-2.369649	-1.321899	4.086307
H	-1.771195	0.512260	-1.493710

H	-2.723676	1.024342	-2.873264
H	-2.722763	-3.226716	2.952664
C	-6.014175	-1.088122	-1.684166
C	-2.460142	-3.766346	0.927604
C	-7.358947	-0.693631	-2.361283
C	-7.942449	0.590477	-1.753601
C	-7.257715	-0.602679	-3.894274
C	-1.250608	-4.756616	0.962515
C	-1.127159	-5.531307	-0.358390
C	-1.287232	-5.703119	2.171541
C	-3.825237	-4.446470	0.987162
O	-4.195012	-4.870318	-0.230425
C	-5.608499	-2.507675	-2.101430
O	-6.344936	-3.398814	-1.392049
C	-6.123889	-4.801955	-1.634858
C	-5.517818	-5.428995	-0.393259
O	-4.464341	-4.579883	2.009097
O	-4.805310	-2.788624	-2.957172
H	-1.307847	-5.160057	3.123038
H	-0.386612	-6.325526	2.178618
H	-2.154675	-6.373236	2.143548
H	-5.418640	-6.511601	-0.523414
H	-6.108804	-5.222911	0.501289
H	-0.370761	-4.107461	1.065225
H	-0.199832	-6.114332	-0.355383
H	-1.098341	-4.856437	-1.221962
H	-1.959878	-6.227630	-0.504674
H	-5.471151	-4.920340	-2.502317
H	-7.101494	-5.250789	-1.837338
H	-2.410893	-3.187558	0.006870
H	-6.158313	-1.096725	-0.599200
H	-8.040246	-1.518483	-2.117819
H	-8.923130	0.799684	-2.195346
H	-7.298953	1.459118	-1.932313
H	-8.068209	0.498453	-0.669485
H	-8.257281	-0.478216	-4.324087
H	-6.806208	-1.496971	-4.334700
H	-6.666689	0.263829	-4.220598
H	3.080147	-1.402509	-6.417219
O	5.056990	-1.056001	-3.391865
H	0.196111	-2.589571	-4.227625
H	6.316201	-4.738518	-0.582070
C	3.227287	-2.387849	-5.958571
C	0.844943	-2.464642	-5.100649
C	2.329977	-2.554555	-4.722459
H	2.979423	-3.143926	-6.712010
H	0.611676	-1.493257	-5.550927
C	2.679229	-1.534176	-3.591111
C	4.107623	-1.757339	-3.107700
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C	30.82376235896261	39.27400645010613	24.08670095777170
C	32.81128549069052	40.76314101544029	23.34382654388108
H	32.07834861189212	42.18423031874705	25.62773754904562
C	31.51748125721200	40.67773857495193	24.16529639414389
H	33.61805291863219	40.16597763528957	23.78145532635751
H	33.15332339235749	41.80374835400507	23.29781196172570
H	32.47870854779972	40.53680315372862	26.13113128032096
H	30.78508392487349	41.34137461806659	23.68956554487049
H	30.78896200015616	38.98336899600569	23.03334500979038
H	30.80777028715151	33.17020478473216	21.48582350245131
H	33.49592604079276	34.48342881506414	20.87359968004234
H	31.35598601841555	33.10519310099111	25.36627181677975
N	37.11894217391659	31.25241867956149	27.23118544263580
H	38.05005983193875	31.49655401862708	27.56178132977148
H	36.55758441473593	31.04201436186601	28.05468593047663
H	31.09254969658453	30.08570032569648	24.98113477981499
C	36.53227412543701	32.36798369733639	26.47719937726749
H	36.10322866062800	33.15250758760482	27.12036031811781
C	37.59388407174065	33.01329217715900	25.57575945952740
H	38.05049886481318	32.26124474742535	24.92236551767835
H	37.14025514550178	33.79043322858266	24.95402097560376
H	38.38474998298525	33.47379164544025	26.17981486103429
C	35.36558680800368	31.87356250042173	25.60512665506824
O	34.51072919130929	32.65231079450068	25.16710714463509
N	35.38456251307204	30.55276714628426	25.32667731275686
H	36.08574569775111	30.01037128908013	25.82320814574820
C	34.32454461128462	29.90737432234782	24.57556107007063
H	34.19601234784776	30.42829585147116	23.62238021669177
C	34.67453181058958	28.43541050129611	24.31841989481702
H	34.77998539865604	27.89174673697296	25.26423339881855
H	33.88311233911242	27.95582769725241	23.73512303438254
H	35.61346559309985	28.35910270329648	23.75978773748569
C	32.99073362546402	29.99652091072456	25.33292875148722
O	31.96168957333030	30.06593140930627	24.49249492622088
O	32.90709328975355	29.95964539106036	26.54739546311054