

Exploring the noncovalent chemistry in the catalytic centers of Snake Venom Metalloproteinases: A computational perspective.

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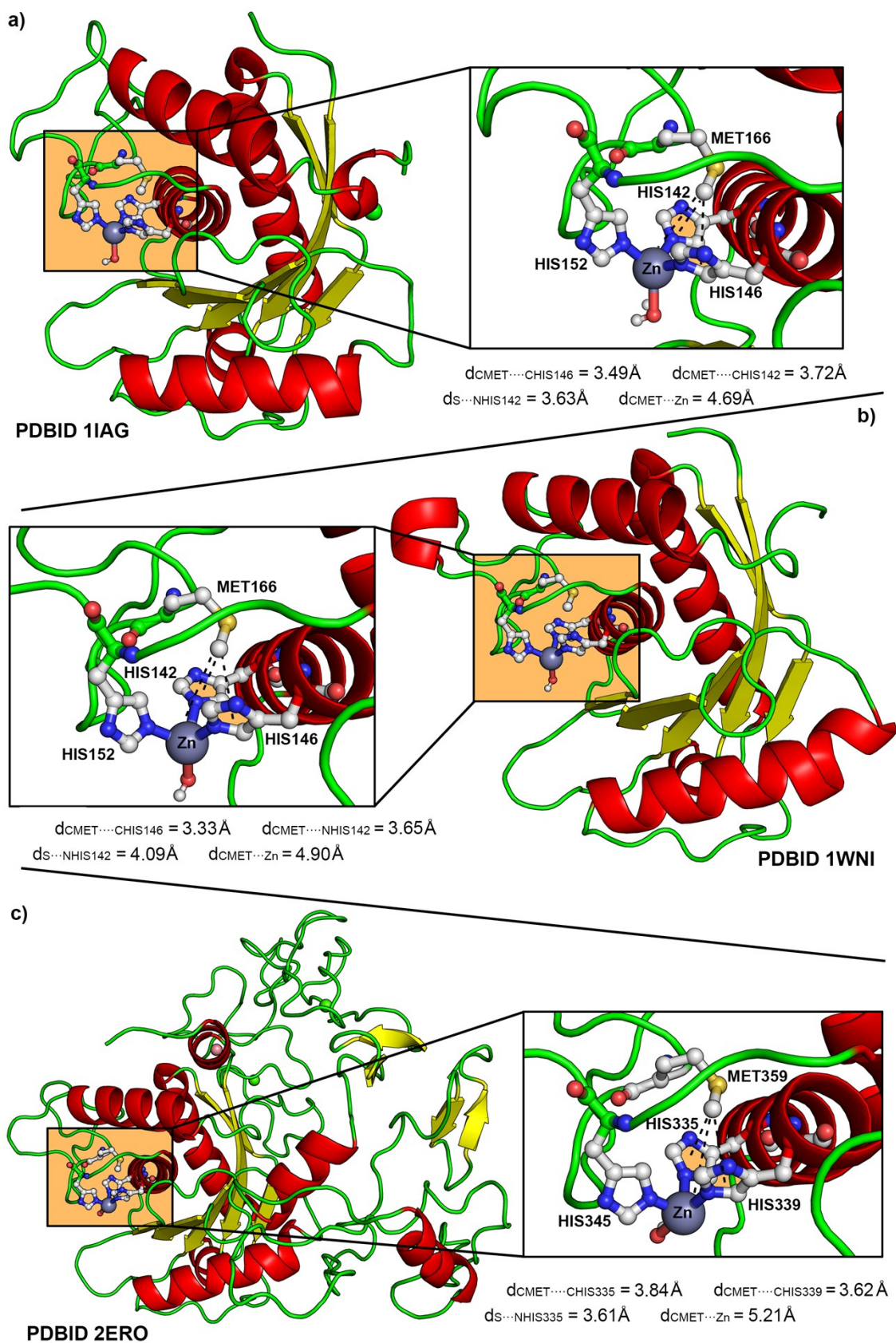


Figure S1. Partial views of the X-ray structures corresponding to PDBIDs (a) 1IAG, (b) 1WNI and (c) 2ERO. The NCIs involving the MET residue and the Zn(II) center are magnified inside the square parts of the figure with indication of the $\text{S}\cdots\text{HIS}$, $\text{C}_{\text{MET}}\cdots\text{HIS}$ and $\text{C}\cdots\text{Zn}$ distance values.

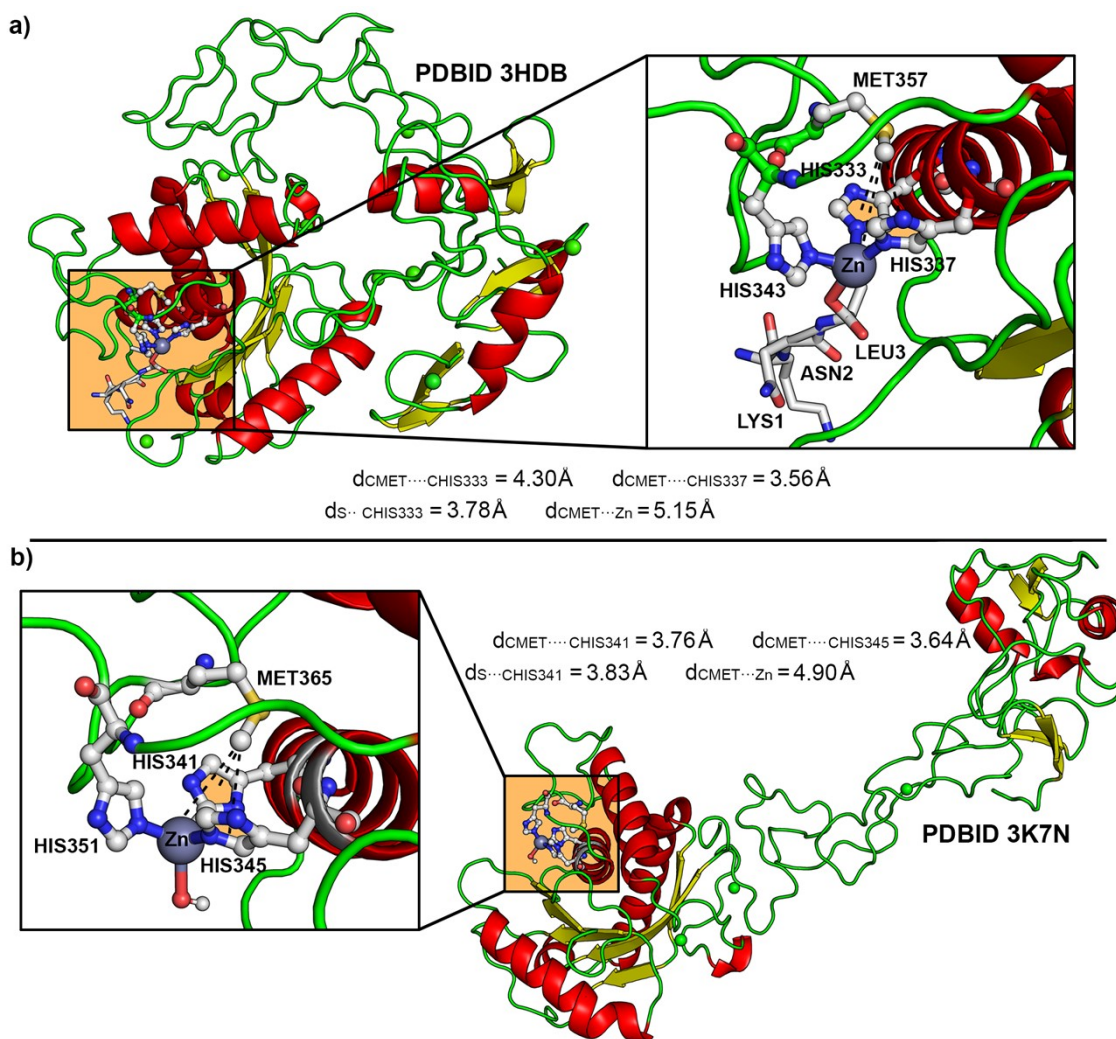


Figure S2. Partial views of the X-ray structures corresponding to PDBIDs (a) 3HDB and (b) 3K7N. The NCIs involving the MET residue and the Zn(II) center are magnified inside the square parts of the figure with indication of the $S \cdots HIS$, $C_{MET} \cdots HIS$ and $C \cdots Zn$ distance values.

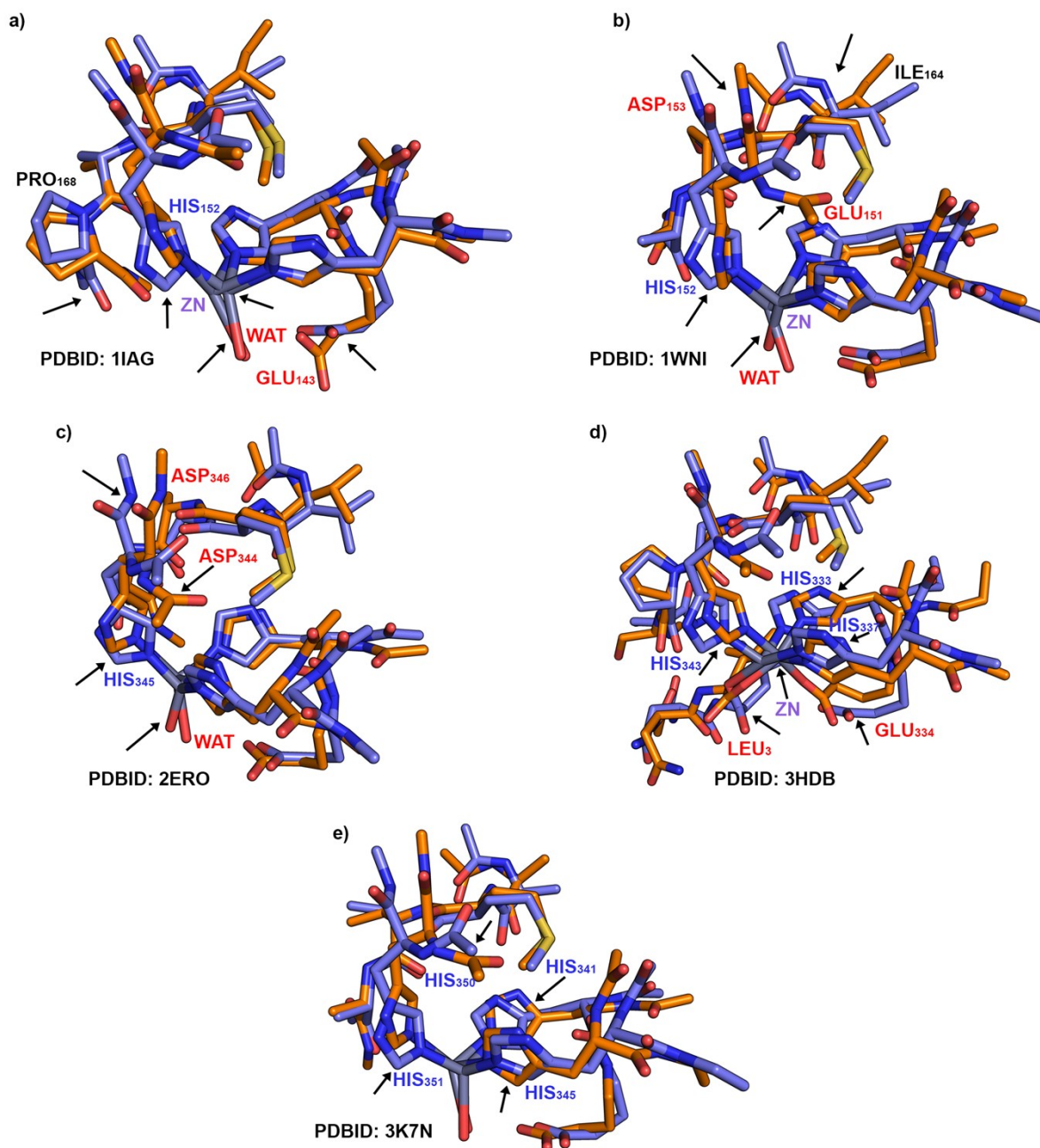


Figure S3. Structural superposition between the initial (colored in blue) and final (colored in orange) xTB geometries in 1IAG, 1WNI, 2ERO, 3HDB and 3K7N structures. The protein residues/groups that changed their position more noticeably during calculations were highlighted using black arrows.

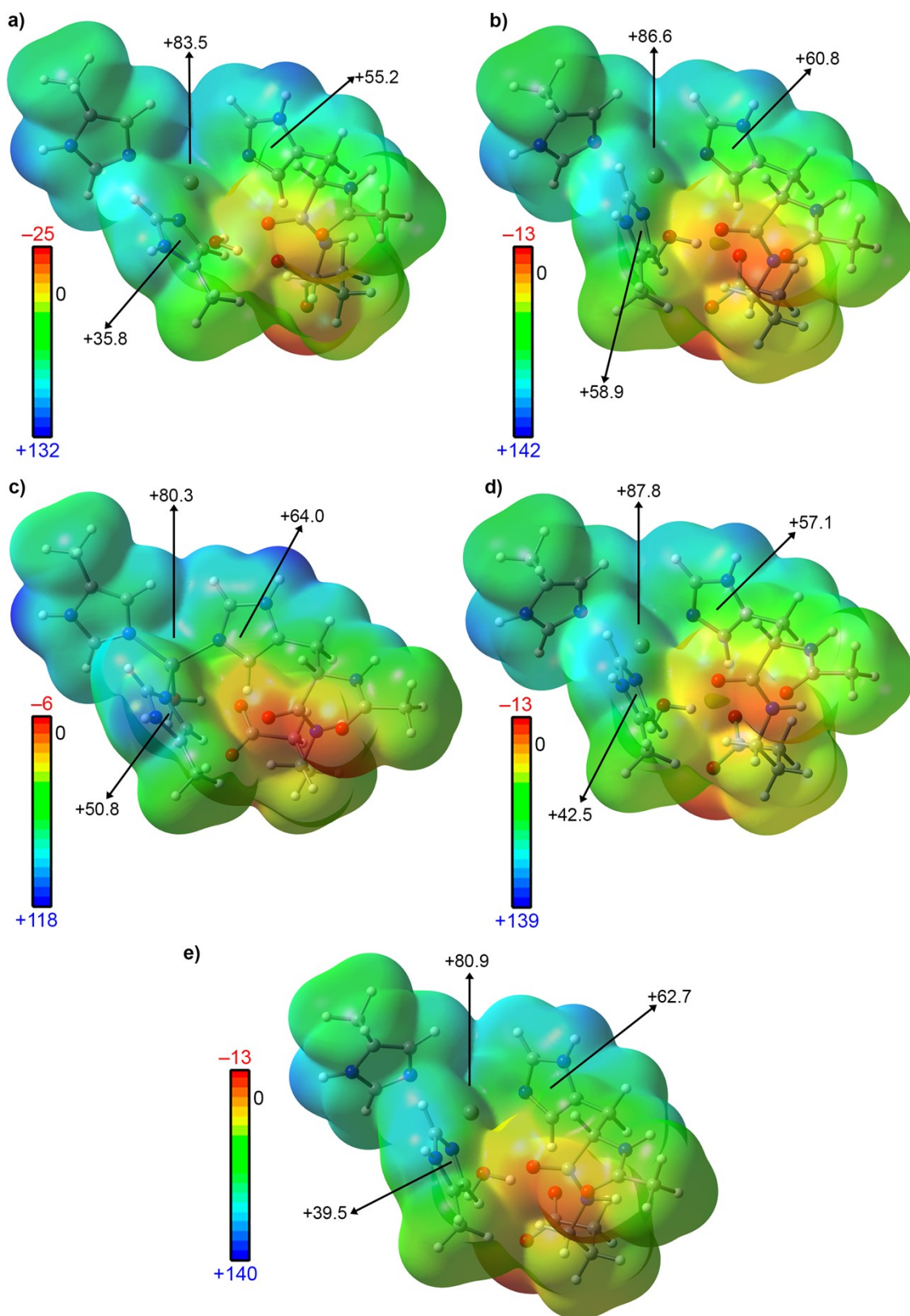


Figure S4. MEP values (in kcal·mol⁻¹) over the Zn-HIS pocket in (a) 1IAG, (b) 1WNI, (c) 2DW2, (d) 2ERO and (e) 3K7N structures. Energy values at concrete points of the surface are given in kcal·mol⁻¹ (0.001 a.u.).

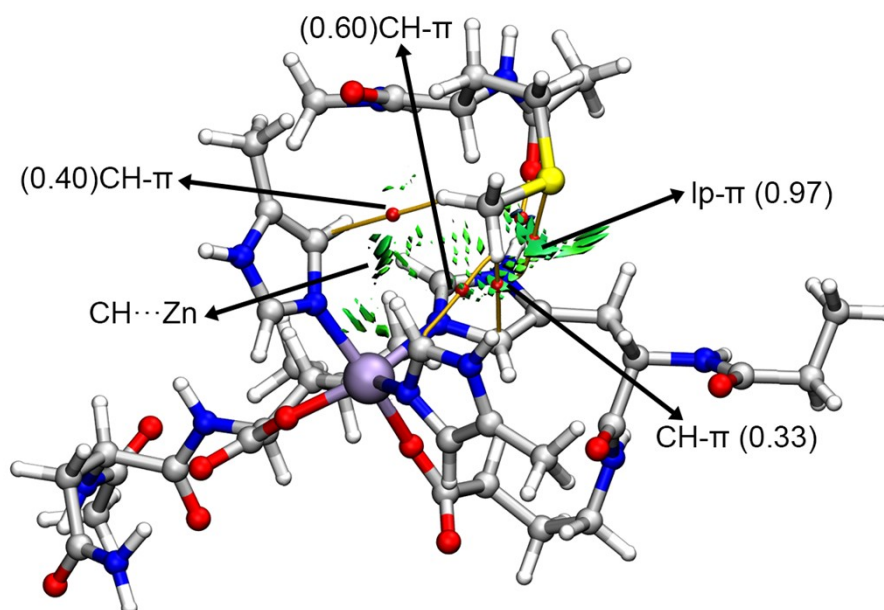


Figure S5. NCIplot analysis and QTAIM distribution of intermolecular bcps (in red spheres) and bond paths in PDBID-3HDB. The name of the NCIs involved in the MET \cdots Zn recognition is also indicated, including the values of the density at the bcps that characterize those interactions in a.u. (into parenthesis). NCIplot surfaces only include intermolecular contacts between MET residue and the Zn(II) centre. NCIplot colour range $-0.04 \text{ au} \leq (\text{sign}\lambda_2)\rho \leq +0.04 \text{ au}$. Isosurface value $\text{RDG} = 0.5$ and ρ cutoff 0.05 a.u.

Table S1. Values of the electron density (ρ), its laplacian ($\nabla^2\rho$), potential (V) and kinetic (G) energies in a.u. and the $-G/V$ ratio at the PBE0-D3/def2-TZVP level of theory characterizing the S $\text{lp}-\pi$ and $\text{CH}-\pi$ interactions present in structures 1IAG, 1WNI, 2ERO, 3HDB and 3K7N.

PDBID	Interaction	ρ	$\nabla^2\rho$	V	G	$-G/V$
1IAG	$\text{lp}-\pi$	0.87	2.86	-0.45	0.58	1.28
	$\text{CH}-\pi$	0.32	1.02	-0.14	0.20	1.43
	$\text{CH}-\pi$	0.69	2.40	-0.39	0.49	1.26
	$\text{CH}-\pi$	0.57	1.79	-0.30	0.37	1.23

1WNI	Lp- π	0.62	2.10	-0.29	0.41	1.41
	CH- π	0.40	1.31	-0.19	0.26	1.37
	CH- π	0.38	1.32	-0.18	0.26	1.44
2ERO	Lp- π	0.62	2.16	-0.30	0.42	1.40
	CH- π	0.66	2.38	-0.36	0.48	1.33
	CH- π	0.41	1.40	-0.20	0.28	1.40
3HDB	Lp- π	0.97	0.32	-0.54	0.66	1.22
	CH- π	0.40	1.23	-0.18	0.25	1.39
	CH- π	0.60	1.82	-0.30	0.38	1.27
	CH- π	0.33	2.04	-0.34	0.42	1.24
3K7N	Lp- π	0.91	3.03	-0.49	0.62	1.27
	CH- π	0.68	2.40	-0.38	0.49	1.29
	CH- π	0.53	1.72	-0.28	0.35	1.25

Cartesian coordinates of the cluster models

Cluster model of 1BUD

C	19.88165323990316	12.56577022091141	20.63082713849669
C	20.49399999999996	13.92800000000000	20.85300000000001
O	21.67328510120327	14.10442566508717	21.12107660205811
N	19.61853745228912	14.94565253072357	20.77255962209581
C	19.99999999999999	16.34300000000000	20.85200000000001
C	20.66700000000001	16.69099999999998	22.19500000000001
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C	18.68803791102681	17.12874683716031	20.66665826412706
C	18.86568140692057	18.59396888474927	20.55033949467018
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C	19.05914929550078	19.56918459549335	21.48562378565189
C	18.98444968632427	20.54154289559818	19.57723565090216
N	19.12932140255391	20.77159344869880	20.86048971196934
N	20.08461795813509	16.14706937160026	23.26630407829031
C	20.53067727111929	16.38000255318139	24.62344052930622
C	19.36270722127097	16.43531485445317	25.60321954982475
C	18.37122041753137	17.54399279756868	25.27340346762477
C	18.96419901452763	18.97471448512580	25.35803727520273
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O	18.26541780170870	19.86352591947580	24.80459936898852
C	24.92359024764945	16.04002334768190	21.49232925698876
C	25.55200000000001	16.97099999999999	22.49600000000003
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N	24.66801705527743	17.68395009839423	23.22706596061553
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C	26.22600000000005	18.32100000000002	25.04999999999997
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N	23.82374261034801	21.75098864983506	23.77079869395483
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N	22.04904435503785	21.59286713540665	22.48756953144371
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C	26.25625256983983	23.69744238496489	19.15897505524021

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H	15.43018787571156	24.17108761890975	16.01635387098497

Cluster model of 1IAG

C	17.27698722411968	12.80647860675251	24.52872850836408
C	17.14820905419300	11.44247253552434	23.90265669444955
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N	18.29779046778117	10.95146285637671	23.39467259509709
C	18.32683703515710	9.71141628789375	22.64170210956891
C	17.46448210671470	8.65804669574946	23.34365312958981
O	16.63206659441393	8.00746576925486	22.72780481300839
C	19.76193917551150	9.18110093257943	22.48617252160903
C	19.75801682646292	7.91687784449158	21.69444721166310
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C	19.40640173465118	6.63298015546020	22.02102631962107
C	19.92707196598776	6.61807889232644	19.94698123487338
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C	17.93289433453141	7.13765860511902	26.67304698241878
C	19.14725124490529	6.30263218966833	26.26342800794226
C	18.70610572841176	4.87762243039617	25.82492372434747
O	18.37952754937698	4.74016490739909	24.62327381129254
O	18.70411137056273	3.98609496511160	26.69338133464831
C	14.42001855010252	10.39744142751027	20.97902601758705
C	13.39667779333118	9.50291739627077	21.62824521796722
O	12.18551850829001	9.65185259680448	21.49485015699462
N	13.92947712197882	8.52388839785160	22.38011886962385
C	13.12136873535577	7.66210662604987	23.20504454254498
C	12.76710377014387	8.30911648411822	24.55454016262280
O	11.80519985223348	7.91708552826253	25.20494298140944
C	13.83149290344420	6.32918386340055	23.50529590049139
C	14.54911859709055	5.75678068869884	22.33327964797141
N	14.05210366791114	5.75059753188324	21.05719295887155
C	15.77344753703169	5.15078060689703	22.24711369917312
C	14.97585883207709	5.16529527033189	20.26742653119354
N	16.01976117915980	4.79076920989861	20.96111565453898
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C	13.50065670916746	5.37288232225881	16.24491751787162
O	14.08249426372678	5.88864855544020	17.18990063262303
N	14.11255388993900	5.10577557280453	15.07365696322556
C	15.44178490417651	5.57143295490816	14.75726168496652
C	15.40927168773792	6.24445822976895	13.37866480721582
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C	16.45806459524632	4.40647128719922	14.75993066871993
C	16.59062733371258	3.84395009935438	16.12896699883634
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C	21.19126860060146	11.71989736421421	17.00526384031209
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C	20.15327093576527	12.83344872158401	17.24513806885183
C	20.81723758031086	14.21741962974905	17.16516600906260
C	19.49127865412952	12.64395665159157	18.60954627763692
C	19.80835745993533	15.33790659307257	16.93460350788829
N	19.74095263606895	9.89634028955514	16.35701780589859
C	19.02163628241457	8.64950047311287	16.46368929675771
C	19.53154584468526	7.56924881410162	15.50143051665250
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C	17.51009292212639	8.83315579114450	16.31804192974025
C	16.91331662372369	9.76335914997123	17.36274634433481
S	17.41064519519089	9.36076931184514	19.07704508021972
C	16.69468941761468	7.71695666912748	19.29046682148933
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C	21.47418826444442	6.24101446583182	14.99102282673603
C	20.99684681594214	5.20984929477374	16.03894825546162
O	20.37396508375233	5.59440326417224	17.02412842170700
C	22.98637684088697	6.40990351540004	14.96504209942845
N	21.27911942120146	3.91879961945746	15.85122488711004
C	20.73294451353421	2.92283357038627	16.77512069794974
C	21.08848888897668	3.14551386112990	18.24510222360472
O	20.34850222453103	2.74005232565435	19.13373997497679
C	21.28120215643532	1.59343747336208	16.24665546007984
C	21.39983352750338	1.85157088755454	14.74703745605951
C	21.91090309777408	3.29005507751047	14.70052778458697
N	22.28633686682943	3.70734068298073	18.46993954816652
C	22.75383615854633	4.06612805639975	19.78816752086890
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H	16.34806990324296	13.06412629971772	25.02857125202364
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H	19.82462707223041	6.19130342554258	27.11164417572803

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Cluster model of lWNI

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C	17.03250590559319	49.51810836240438	5.64334473446375
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C	15.49673849774208	49.41568615706325	5.68079962784601
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C	14.36793309506292	46.63408114435470	3.66934420038911
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C	17.67999400273591	51.95215161977511	2.79897831521382
C	16.89881164871214	53.23618335499341	2.55153863441162
C	15.40378890684841	52.98555814100885	2.39759432176434
C	15.05214895991653	52.09296152853607	1.17791682525436
O	13.99087985851892	51.42963112436458	1.29134283368737
O	15.80446324436346	52.09715576222172	0.18923287457798
C	21.01671980937159	48.04723838978279	4.71712461806456
C	21.44199304233193	48.11455011713167	3.27426195977498
O	22.52478703738863	47.70379299949239	2.86836879366374
N	20.54253449649014	48.69125013700808	2.45401592953146
C	20.79986123828252	48.81725058980271	1.03680883557395
C	22.01285696142385	49.71936058199613	0.75458712634467
O	22.71614215132207	49.54529916147040	-0.23031451548347
C	19.59638581832073	49.41180729454665	0.30013377955293
C	18.35368427424798	48.59391555220524	0.41547540405410

N	18.33536297869610	47.26953222270537	0.74364471113649
C	17.04584133381483	48.92703540304987	0.17397253432433
C	17.05696220509017	46.86243300669356	0.70139626481451
N	16.25375533660770	47.83544107332133	0.34961547550352
N	22.16036056479210	50.73175490351793	1.61464576471041
C	23.24189862197005	51.68672807258901	1.54714253612225
C	20.63446576230130	44.55693769650781	-1.04787113309364
C	19.68936229560668	44.19298690724937	0.06837659591868
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N	18.87052905668815	43.15958358903318	-0.20845776943345
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O	19.68956920607912	40.77635963428475	0.65931854303167
C	16.64885296282934	42.17924493586261	0.23995320329271
C	15.90565929621479	43.38164109070786	-0.22503215771048
N	16.08453961378501	43.94502146681226	-1.46127713458092
C	14.96075419266808	44.15692213904818	0.39186589720171
C	15.26380361881680	45.01019603432504	-1.54406614624354
N	14.57135917646849	45.16050678032980	-0.44256603312186
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O	15.92915264091893	41.99810004611463	3.55031563419626
C	17.77516287847373	43.15121339479815	5.32322508603219
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C	13.34292160882185	41.33501910842193	4.25101498826172
C	12.78723509859704	42.46452391829993	3.35487211852422
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C	10.96954489043142	42.58963739272033	0.29381185196601
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H	17.49761789748429	51.24697527674317	1.98369919671012
H	20.20194188587266	47.33799254991259	4.82761742569755
H	21.85563798302545	47.73084008474422	5.32909465763530
H	23.78597379379348	51.50496369617240	0.62236855832978
H	20.07290234168231	44.92154745077516	-1.90486304539240
H	19.52248022138083	39.11706078775619	2.36929839513375
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H	11.71743651246821	42.12704502465327	6.28022871864113
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H	11.96534974606573	42.59032786631150	-0.13908159973483
H	10.33899908518434	43.27693987342696	-0.26201931976899
H	11.54077008584225	44.00977771159582	1.81092752880265
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H	20.65775686569754	49.01959874798443	5.04556523132721

H	19.17696217066388	50.95149059578139	8.80421743566625
H	18.33650012447863	52.38689674290826	8.20172288667603
H	18.75484702987524	52.17269292547873	2.83635931669633
H	17.91666961153216	38.77621803177231	3.05630997496171
H	19.11121658744103	39.70263161667539	3.99503787628277
H	21.21318437859896	43.68754557981894	-1.34890319122187
H	21.31365347624877	45.33765590469136	-0.71438403886678
H	13.74007037207379	40.04688559360981	8.98002994558413
H	12.09429347280099	40.47478890793501	8.47875096722179
H	10.53928594856186	41.59329986270892	0.22383337835706
H	21.56365428294454	50.75745545803738	2.42888509855960
H	19.62111801602355	48.94744073137168	2.80111646412611
H	16.94345139266837	50.44814354831650	7.53198779913635
H	16.96158156943978	51.91155383787464	4.77722368149945
H	10.16323852122177	42.50976712613715	4.13153432526719
H	11.47911390597280	41.14150106101897	2.51749417784689
H	14.76655021341708	42.19525915230773	10.10392231114982
H	16.19567157761627	42.45396758809105	7.44542112190791
H	13.94239393912451	42.41041704001830	5.94280476249187
H	17.43961651672875	41.18317857938101	2.83836464496308
H	19.12696768752392	42.55420401104670	-0.97736557243567
H	14.91086425186473	46.64737924888825	5.69808291158306
H	16.71320326151144	43.61232620313623	-2.17556863405208
H	8.23728705540362	43.77900857404601	5.04323618406228
H	7.81614547294606	42.09265955347045	4.66924388795947

Cluster model of 2DW2

C	83.46072709397421	3.37260556819164	28.08165232687860
C	82.47756349922139	4.36788376032041	27.52195872132137
O	81.56081832228752	4.86042456818814	28.17096738767151
N	82.66829239193068	4.66655818625488	26.21479380341597
C	81.88878441367535	5.69450938783705	25.55058407379212
C	80.40735004297034	5.52523836148405	25.89937387496801
O	79.72234884226823	6.47135531720054	26.27692690607115
C	82.10998691871767	5.61525069253102	24.02983643550334
C	81.33723623490197	6.65022858309826	23.28538493026167
N	81.92474686753719	7.49678792292121	22.38459047380622

C	80.01377146372363	6.98545382408404	23.29309334340933
C	80.97458419967165	8.30435618788838	21.89425019039137
N	79.79555477568593	8.02049425489603	22.43089576483608
N	79.91702707391909	4.30004075128372	25.68009268860160
C	78.52255150616557	3.95956749767834	25.85049493514694
C	78.03094404665627	3.01302999458793	24.75668332149110
C	78.23954243079096	3.54816437477093	23.34284629113905
C	77.45839867266058	4.82997094589485	22.99915908758913
O	76.68620472325932	5.34172071621439	23.82128397220434
O	77.68464976795964	5.29364639721126	21.84243608875380
C	81.83561006480080	8.15361952974296	28.71642046866007
C	80.49831881615428	8.64942489743878	29.20058629690353
O	80.36651546817961	9.41718351120241	30.14946659066689
N	79.44697945994882	8.17960259590695	28.50258641542069
C	78.09138696575930	8.42899276860925	28.93390963763496
C	77.72455026384326	7.61452474191337	30.18744042163182
O	76.88226328871338	8.01626811270465	30.97970776405665
C	77.07263505853297	8.07397405157858	27.84085478726915
C	77.32898609511460	8.74695154387787	26.53991591878140
N	77.61317858657037	10.08115110357609	26.39771688516107
C	77.32529186201654	8.23542312461357	25.27585415002267
C	77.78266760644652	10.33461884331669	25.08503091491812
N	77.60845684179992	9.22401360431156	24.37552918258436
N	78.34495776411484	6.43431184809035	30.28566901792878
C	78.14920145142935	5.52094698441638	31.38706528697382
C	77.44904814803579	15.20948142515167	24.67688781668246
C	78.41861463341219	14.37787187254471	23.87134370762023
O	78.78430955911500	13.25795301928228	24.20853297073832
N	78.81992952348146	14.96175030044492	22.72587758380868
C	79.83972613493496	14.41416776747209	21.86856728343559
C	80.84397689490019	15.50970459478907	21.51367140782191
O	80.57048054390349	16.70365894830940	21.63663405685838
C	79.22915781455265	13.83699922484422	20.56297645118952
C	78.47338256952696	12.59517309219084	20.85252245159566
N	77.10372451077359	12.47759538082895	20.81366974468639
C	78.93908380445704	11.38929984095844	21.29184005678901
C	76.78873389656481	11.22516117435454	21.22300400494462
N	77.89591822597662	10.54248649565761	21.51856016990919

N	81.98903278074536	15.03071332548492	21.01038917557549
C	83.09241836478775	15.87808570028431	20.62207588993613
C	88.58203448066692	11.36060739550771	20.51222532613730
C	87.55266969593080	10.32816541431284	20.89507664529819
O	86.63739813713210	9.95468656371936	20.15680410384710
N	87.67623413781041	9.85996863326923	22.16369132711164
C	86.89524964121023	8.72990782598705	22.62859725613909
C	85.40545590637967	9.02530381501272	22.45176739707925
O	84.61846777935577	8.14236552954960	22.11558220355803
C	87.24088038944629	8.39012946764379	24.09427606083892
C	88.52646953187285	7.55445254927146	24.20225384156765
C	86.10711079955963	7.60451673315885	24.75579598468078
C	89.80135054878913	8.21579555835986	23.68868429937442
N	85.04032427256857	10.28843749662919	22.75043204833096
C	83.68186334517900	10.77073466829034	22.72511718173948
C	83.32215378103051	11.58297448020685	21.48513788855599
O	82.26856007174646	12.25310077634425	21.45464537297130
C	83.36508531069059	11.58966908275848	23.98387697210045
C	83.54953444630205	10.79992956077477	25.27027530390418
S	82.67763349982005	9.19668197694157	25.27674464663591
C	80.95328893078343	9.73581768251761	25.37095671803606
N	84.19518528158736	11.57831981700171	20.44123593607139
C	83.66204790109487	11.94986108919807	19.13940174223542
C	82.40137360121653	11.12345703806616	18.87012721312461
O	82.21651737867114	10.03266265243044	19.41834320677376
C	84.72317364041113	11.73281826631226	18.05988065939507
C	85.80785099597027	12.80681105201627	18.10640322147848
C	86.88862061180301	12.54761727764772	17.06410683576174
N	81.50087773803989	11.64424709920992	18.00586370014293
C	80.23172086478425	10.97220591511260	17.78082944248017
C	80.33269041646759	9.77096296565245	16.83255190496046
O	79.40762140890064	8.97752824532364	16.72994150063208
C	79.33491404860735	12.05254880117941	17.16554695014133
C	80.33366420000054	12.95299033953625	16.44232854442457
C	81.53902828241223	12.95846936278670	17.38189911402877
N	81.44288649059905	9.71773812609655	16.08465104712268
C	81.73469972834930	8.63819609581565	15.17012480806714
Zn	78.04224623609562	8.87442202181290	22.48305245773347

O	76.65501443943991	7.60503696660313	21.88646173657425
H	83.12693889858264	3.04947608030610	29.06313795986425
H	76.96470752712608	2.84892514679054	24.91860842019856
H	78.54353632881886	2.05246764193105	24.84877025007798
H	77.93487858701971	2.79552048181303	22.61151758088664
H	79.29163048014584	3.77374531806689	23.15429192664080
H	77.95433618265020	4.89082701398425	25.81505722855249
H	82.04899687691486	8.54878220042181	27.72682313851012
H	82.61206107156767	8.47088833021746	29.40560555811341
H	77.37652833437045	5.93703871956978	32.03097036253096
H	76.57953936532712	15.45886790919368	24.07398055141782
H	82.75904807700124	16.91319606937975	20.67712162926602
H	89.58374204377272	10.95264971457889	20.62942243661160
H	87.37610633841069	9.33337773251581	24.63471017119823
H	86.38789802471412	7.33057954391328	25.76904567977004
H	85.18539091945551	8.17879897085471	24.80281003332024
H	85.90851874936702	6.69786705157167	24.18962597017206
H	88.37418426448176	6.61439241139877	23.66805860193510
H	88.66869422165247	7.31220909295276	25.25719528575221
H	90.65475891682046	7.58533570834158	23.92785134790396
H	89.77873655168364	8.34031050072298	22.60894611676968
H	89.95908007827725	9.18103260160648	24.16623380613276
H	87.09363357839656	7.85103859039567	21.99709481390145
H	82.33532140830576	11.94013265271382	23.89496899982880
H	84.01260641802912	12.46947191355973	24.01673700217723
H	83.19484486735783	11.36980310671217	26.12870554258470
H	84.59559617956572	10.53842365075260	25.42263127350424
H	80.35835890791257	8.83644987382927	25.50391930107020
H	80.66800523815796	10.23860070068949	24.45068723514717
H	80.83162285867712	10.39696074718982	26.22438953214025
H	83.03732140114316	9.88123650136275	22.71468016326622
H	84.25286320798580	11.73345089074375	17.07497911460295
H	85.17441917988457	10.75061222397738	18.21511128653113
H	86.24721413127335	12.81230074896755	19.10400192022592
H	85.35851849118619	13.78638859005399	17.93079590895075
H	86.46802806350924	12.57528366606133	16.06167897577764
H	87.33202551346780	11.56609027365681	17.21815846482515
H	83.38159981319592	13.00819105403311	19.18960901852434

H	78.82419538254742	12.59926666764389	17.95613172091821
H	78.59298146630253	11.61507913295539	16.50171210116911
H	79.94530137644090	13.95382695502069	16.27488523993527
H	80.60428069573879	12.51368800186697	15.48285730168962
H	82.47726971763224	13.11708998897512	16.84870737255898
H	81.43506811494996	13.74099563310383	18.14321427403461
H	79.83386093955785	10.58605315154945	18.72592471655829
H	80.83851235727917	8.02684198827910	15.08160171377791
H	82.18929390987859	6.69112445816776	25.90257753993842
H	81.82543283808695	4.62096586259651	23.67497560890221
H	83.16983442202995	5.77297577487015	23.82112227086876
H	79.20840089891158	6.56019829604315	23.85210929373954
H	81.15897788351538	9.03724347131869	21.13265357435877
H	78.00463204760827	9.48335331961165	29.22556710459079
H	76.08056427934007	8.33576306957775	28.21906993342685
H	77.09671015283197	6.99787869484568	27.66378951337107
H	77.11466864879947	7.23143866606796	24.96360707041569
H	78.03718444084826	11.29573951698542	24.68314316346135
H	80.34529962444230	13.60007081895870	22.39604688744120
H	80.06181538193009	13.60144228256390	19.90124612790316
H	78.59274423649423	14.59100960404097	20.09962935003099
H	79.95926646821367	11.10002694326984	21.44883013118600
H	75.79476588719184	10.83699004267283	21.28695512486131
H	77.06660779346564	6.65165522241930	21.77821221545362
H	75.90793418240700	7.44477469935481	22.47643097183805
H	83.55136204646385	2.51245508782320	27.42407589142611
H	84.43620968191715	3.84412187307840	28.18006860921061
H	78.36892556919558	3.49349072036586	26.83097562935782
H	83.50659631559196	4.34796725890363	25.75238342060145
H	82.92474310957708	7.58439628078354	22.18834737004820
H	77.69756107029426	10.75061420741567	27.14517221923210
H	76.45068317291938	13.19309885358832	20.53819758815256
H	81.81507761402354	7.06812715150476	28.65177546092660
H	79.07266212318459	5.40559505227522	31.95530668465521
H	77.83059067301025	4.54874320119247	31.01174811580633
H	79.05029204248306	6.19342579056793	29.60362073098586
H	79.59285723616594	7.54491549390575	27.71996387709724
H	80.54536964504177	3.54834037063112	25.44110308243048

H	83.94380756467146	15.73724908110543	21.28938417519169
H	77.13304057477916	14.65352517796227	25.55493379935941
H	77.93052640863745	16.13292194904914	24.99125443579074
H	83.39864609606747	15.64888587070490	19.60070943095398
H	82.15425228209419	14.02465753294088	21.08716690083741
H	78.62335410518163	15.94167379253547	22.56324530872844
H	88.43550873039625	11.65465996710374	19.47780787540259
H	88.48797367454061	12.23756860241660	21.14979090318688
H	87.67125203539972	13.29926229290707	17.12889469640408
H	82.19603727308879	10.35228870392709	16.30313516720745
H	84.88173302318526	10.82797958303764	20.41489102068533
H	85.76604706770864	10.96137899384068	22.94555757834467
H	88.48351244019327	10.12385522400634	22.70594060628132
H	82.00130068499080	9.04289626364881	14.19425829925484
H	82.55293386910434	8.02223862645069	15.54627626504337

Cluster model of 2ERO

C	32.12038347924617	14.25953376393721	84.88579019973230
C	32.14376691183537	13.89656207693933	86.34849718826885
O	31.95279208256501	12.76316470168961	86.76742859773381
N	32.36612868741742	14.94254156112849	87.17435205713110
C	32.58892460700387	14.77520630941784	88.59825440060399
C	31.59291542099642	13.77367626657683	89.18775275394459
O	31.95900507809944	12.90438926587176	89.97025706259079
C	32.46236810258166	16.12834679493292	89.32121785951220
C	32.72576321055763	15.98596847100358	90.78024243820917
N	33.97415693644305	16.12201248057126	91.32465866177917
C	31.89571839261689	15.68978947587107	91.82763123780576
C	33.86095958657501	15.91538735130137	92.64489752004975
N	32.61694374866857	15.65457338241930	92.97913334888992
N	30.32012035621919	13.96607965425270	88.84194208020175
C	29.25124969254625	13.09469559285489	89.27912265283294
C	27.89769444544644	13.79234793898691	89.23428192433346
C	27.84028707795964	15.00727711028913	90.15206309617909
C	28.04950059271881	14.65792556781013	91.64900572736560
O	28.55143126438092	15.57622673474850	92.34465481500686
O	27.70645945023659	13.53830202787561	92.06353530891305

C	34.09523990924662	10.70942641300678	88.13356072189484
C	33.40285887069831	9.65353849682566	88.95285323366397
O	33.70799079570342	8.46524192228482	88.92432850732516
N	32.39016735904472	10.11356791880933	89.71261633033471
C	31.62648161372264	9.22106673723419	90.55540299018028
C	30.84983601321645	8.18135268427773	89.73028344209537
O	30.59805107288231	7.07354160594173	90.18222720073584
C	30.61617766173923	9.98842077533955	91.41257198082927
C	31.23896805029182	11.01187847696683	92.30140880676821
N	32.54768022775117	10.99652235306408	92.68751912073699
C	30.68273768009508	12.08849173233046	92.94208168249033
C	32.73658026368032	12.03752893922265	93.51260732036467
N	31.62803987574769	12.71104693548603	93.69624675716736
N	30.41723013723367	8.62649633064438	88.54640336446936
C	29.69970531119923	7.80616947696500	87.59841886377458
C	34.60403190255214	7.94180714623010	94.23227325287563
C	35.26741982464479	9.26267094174893	93.93714730272470
O	35.09950220585792	9.87323397043260	92.88604516456478
N	36.00056764461981	9.75725193792126	94.95336844745219
C	36.87303698378816	10.90119756279156	94.80179954387543
C	38.31656015807889	10.39914536192855	94.59804022592527
O	38.60075485857506	9.22062486089366	94.78038856163064
C	36.80053853063157	11.82386756364175	96.03419973414881
C	35.43535462493811	12.37727174087449	96.24314193642586
N	34.47988522310406	11.77663212510149	97.01920212827778
C	34.84932324057852	13.51888947477156	95.76669776922662
C	33.38320656106481	12.55776411419424	96.98959682739770
N	33.57744481333106	13.62002681284239	96.24676895965455
N	39.18233454616084	11.34058079195540	94.22838354166338
C	40.58785565753144	11.07693632281995	94.01684558597236
C	41.14675221204249	19.22953636396366	91.32534930690666
C	39.84229569659322	18.56764533193908	90.96756522210147
O	38.89218842116942	18.48497387046084	91.73872407730315
N	39.80925155656364	18.01819657086951	89.73860599350958
C	38.58296445017404	17.50105283914526	89.15730611430128
C	37.80435167136025	16.69612093115638	90.19963253027333
O	36.60687697161330	16.85514529278979	90.36724907746839
C	38.86966853398678	16.62857840081732	87.91804661138049

C	37.55454096325786	16.10233133559350	87.34384442369738
C	39.61406490314693	17.42057228276408	86.84184359455304
N	38.52727879773528	15.75270904893236	90.83321348425487
C	37.94604083564549	14.81577315998507	91.76225964531289
C	38.37181506739477	15.02446735400429	93.21957204999400
O	38.35949922707198	14.09257809139031	94.01916682875950
C	38.18156994260660	13.36417051420942	91.33300510223404
C	37.56713946180842	13.02358242686733	89.98375250271475
S	35.83234076524177	13.57161673697879	89.80352552309036
C	35.03693587151300	12.75450818657785	91.20717935712004
N	38.77039716691969	16.25921273055366	93.54742851364661
C	38.71159528472666	16.66555867422506	94.93914584802599
C	37.23410826282001	16.57264124725332	95.36936778298640
O	36.37270422648497	16.22788955589001	94.57453328102015
C	39.27996605238155	18.06824757062093	95.09252988796828
N	36.97691109921967	16.80734429364113	96.66330062310666
C	35.59562095125416	16.88523950290045	97.10075140249806
C	34.87506340739452	18.01005443946878	96.33910917232622
O	35.44834890280635	19.06360240932948	96.09031249880917
N	33.60621862556579	17.74794549595680	96.02040523569606
C	32.76923816022061	18.67442872528848	95.29206062794934
Zn	31.69023322470520	14.68815128489455	94.89510192221486
H	31.75576242042972	13.41362417453053	84.31071598066495
H	31.45565103759628	16.52459938462205	89.17953379170633
H	33.18872000896073	16.82291429599940	88.89501136231382
H	30.83666388357858	15.52668371528653	91.83282464482775
H	34.67733631080158	15.99186876418596	93.33369440041733
H	33.59278285435556	14.36328289474056	88.77729772045507
H	27.14445766665853	13.07549013027486	89.56494771540046
H	27.66713478190137	14.09026849695863	88.20849647878379
H	26.85758044034018	15.48117269396796	90.08111663907852
H	28.59152692103592	15.75354039827708	89.88739303021042
H	29.47364879609587	12.78903197800947	90.30469828182726
H	34.62794668954798	11.39343466870150	88.78735089567800
H	34.79678050968047	10.23956308587928	87.45141463244319
H	29.46809608040222	6.86174672734112	88.08703907451670
H	33.86484269700509	8.06687062211669	95.02005899972377
H	40.77755212431117	10.02992700397911	94.24664776348280

H	41.34748122657009	20.05078630561419	90.64171702133089
H	39.48748270350767	15.77896334274007	88.22603196985705
H	37.75211849755012	15.44832748605589	86.49893423354943
H	36.93931692477279	16.93101371841983	87.00233325495088
H	36.98750378560978	15.54169907768540	88.08328992833384
H	39.66634436259836	16.82826603621127	85.93219899270615
H	40.63357008390361	17.65889339214739	87.13350472251044
H	39.08671196652451	18.34423304006227	86.61598371646292
H	37.92837828467664	18.33427193999536	88.86279587221802
H	37.75292191674004	12.71979401073425	92.10108428412533
H	39.25438448951145	13.16435090548586	91.28933434921262
H	37.59197181988163	11.94632059713998	89.81746352201080
H	38.08698394161593	13.52294038820107	89.16820138281209
H	35.33732300835280	11.71122791364389	91.24996372302040
H	36.86699422354821	15.02507857733371	91.75276834213494
H	39.23942673115877	18.39803291555698	96.12560844142830
H	40.31534343460178	18.07875885475822	94.76313888106887
H	38.70892219502885	18.76474321659562	94.48233157762205
H	39.28009164163270	15.93825100109753	95.53114282962127
H	35.57713790028783	17.10732086007143	98.16708372220137
H	35.10264992535888	15.92988104113471	96.91009062924263
H	33.34314516513621	19.58095966136329	95.10968906151054
H	32.30905924484976	8.64123770805702	91.19306402117185
H	30.06945210149784	9.25860091215523	92.01771847600125
H	29.88894199893335	10.48409358734333	90.76623294015734
H	29.67362631611588	12.44812837785612	92.88867886897521
H	33.68278948089373	12.27311385517283	93.95210023915271
H	36.54364672943422	11.44287545837514	93.91003210824923
H	37.48499448503949	12.65615621513440	95.87085373136983
H	37.12036137979982	11.26351260376939	96.91433742884769
H	35.26750546776491	14.26921954360274	95.12715140092092
H	32.47675943120782	12.34312656380366	97.51625838121846
H	33.28273513041333	10.36367707115644	92.39391597192132
H	34.58699872508650	10.91161845151870	97.52585403699960
H	34.83330848328301	16.35998512171473	90.83628627977528
H	32.20311281461093	11.11183079766678	89.77164071561901
H	30.72730951740812	9.53621839576309	88.23604950528076
H	33.36027564994278	11.28637408196188	87.57729360100430

H	28.77666931154065	8.30395022975747	87.30291731975541
H	30.31221724687698	7.61618390280907	86.71626965267413
H	35.28989913348148	13.26983405714461	92.13010927564676
H	33.96622872727589	12.82568371266645	91.03522107641778
H	32.63187897194351	15.83156049500074	86.77583547001598
H	30.09115133336730	14.65076966239000	88.13754484947317
H	31.48168100157254	15.12149329653289	84.71481944780290
H	29.22852677265287	12.19937179061012	88.64402916380448
H	36.27035945416978	9.11694838671823	95.68824711771893
H	38.87167755747294	12.30356310662210	94.12408088741356
H	41.18812892198050	11.71011014306218	94.66909108066903
H	40.85595765933358	11.27088044039631	92.97800897980140
H	35.34409711652822	7.21380464257831	94.55412453763570
H	34.10813126901989	7.57263797071292	93.33809230694834
H	38.62670188600435	17.01397163511297	92.87913382514260
H	37.68328920835397	17.23514178031985	97.24046500509088
H	33.21915641198117	16.81786244020840	96.15372187176480
H	39.51872283206907	15.68570339587857	90.65928228426056
H	40.56846842349529	18.20558141093337	89.10008294670178
O	29.19599726556785	14.77965443126446	94.78304012710394
H	28.73291477703378	13.94138863706307	94.85313559056328
H	28.95380811847350	15.13083011821842	93.88374975938939
H	33.12993844498382	14.49828345689740	84.55901447646438
H	41.08886219598805	19.61729778433504	92.33804718211800
H	41.96090280293496	18.51213879464371	91.25796206914669
H	32.46081083809375	18.23493852368241	94.34329822439938
H	31.88169714491144	18.91335049948518	95.87726686910602

Cluster model of 3HDB

C	6.98873649986198	35.18037835017601	45.66841833483598
C	5.77164504273979	36.07329769413590	45.74327200416212
O	5.56655478579346	36.98356032794128	44.94652368367926
C	6.61913166324259	33.83079151473935	45.04629286518763
N	4.90127328799330	35.75340391322876	46.71720329911000
C	3.69254073211001	36.51844560105481	46.96879215345862
C	4.09841247555131	37.85221222090707	47.63584853260144
O	4.17371548103699	38.86918925799088	46.96444553334223

C	2.66424396251449	35.68493133673456	47.73222526967886
C	1.40896954867503	36.46177929041180	47.94529158673050
N	0.28739833284134	35.92904646845166	48.51782402425538
C	1.08983691844250	37.75572057779700	47.64649891095433
C	-0.64705542495128	36.89011964632041	48.55106408984177
N	-0.19242222903488	38.01183534413769	48.03375068301115
N	4.46148314420242	37.78564525283434	48.92149632787648
C	4.82839107194795	38.96422389869093	49.68092488176369
C	4.05364578678950	39.08313243850932	50.99168240902672
C	2.54210189468132	39.08505226000916	50.79429331227732
C	1.99082444563407	40.25959735505371	49.94200694145795
O	2.67066584260619	41.27953356020395	49.77694511561823
O	0.83027576127300	40.05333181983065	49.49468106349119
C	2.70651659626247	36.54254169340319	43.14123802658356
C	2.62709275405196	38.04064751611754	43.02682269750544
O	1.75771249474487	38.61297117001561	42.36809543725151
N	3.57504131427975	38.71364673624010	43.69897765393068
C	3.78817860281812	40.12942280366953	43.52775071888389
C	5.22855452351522	40.48338902890237	43.12024387231047
O	5.44374970687917	41.52229906798234	42.50550738366820
C	3.45336846678320	40.95789774063474	44.78068437682460
C	2.05545383637043	40.77299608854828	45.26186013410201
N	1.01930175331620	40.30625578358240	44.50210083678427
C	1.52868480698497	40.98549055364818	46.50668624710413
C	-0.06368428572343	40.22648540982326	45.28845201828813
N	0.20953332878593	40.63711690011372	46.51282708379713
N	6.18485177824319	39.62796827323709	43.48377783325962
C	7.58433367166023	39.85373778315389	43.19908262638359
C	-3.76544460905192	40.24841303220532	42.05549028737499
C	-3.72955130440851	39.26308147793663	43.19762515320853
O	-2.71339894038272	38.98727394803741	43.81950370509998
N	-4.92750712894294	38.72156432221113	43.49512247321614
C	-5.10106053749857	37.65646479559022	44.45148385747927
C	-6.14884796218112	36.67825953132066	43.89810469264689
O	-6.84461925694471	36.98036179570202	42.93596773685161
C	-5.55255935200171	38.20241670940052	45.82877202708200
C	-4.46143483715249	39.02261739857073	46.41682025670087
N	-4.35202265624849	40.37827637772080	46.27216280318917

C	-3.32747324073052	38.63545295590029	47.07448863693545
C	-3.19026693887120	40.75552550275410	46.82960974570315
N	-2.54821944896737	39.72232831071538	47.32276999575114
N	-6.21456888981949	35.52270184224741	44.55553109355028
C	-7.15590759527238	34.47729330787628	44.22141984892910
C	-4.15093974607917	29.61652376909339	49.65563099020559
C	-3.02586729886895	30.59641274806688	49.45629455143841
O	-2.98892631530497	31.70277255158445	49.98394149258076
N	-2.06175661992453	30.18659088603342	48.60902183694702
C	-0.83018912081946	30.93772042904492	48.43727908851582
C	-1.15169323577834	32.41698479388011	48.22682625917643
O	-0.53334156742971	33.29264137687273	48.81046712156077
C	-0.00752018525333	30.38723446665628	47.25420853108100
C	0.55688617667990	28.99941549594443	47.59667513989609
C	1.12666179661946	31.35180135671613	46.90807682618831
C	0.95300088310653	28.20590956050402	46.35574488053916
N	-2.09713036560661	32.65779330943859	47.30217501450922
C	-2.49157653524394	33.97972339066072	46.87353143403634
C	-3.79312322011737	34.47270171318778	47.51863909776471
O	-4.54311213442830	35.24870089368144	46.93291084786798
C	-2.58546220730101	34.06387522073390	45.34735615332117
C	-1.23646156271175	33.92793784043862	44.65593794807624
S	0.02889279196928	35.08343876393364	45.29552622628858
C	-0.66412038720150	36.67643613971079	44.80318298094789
N	-4.05379491446040	34.01603741614672	48.74318333832473
C	-5.16688129330515	34.57569111938686	49.47753513157876
C	-4.96001223126352	36.08761896284609	49.63451467743614
O	-3.83641133896875	36.56811735843082	49.70689967976114
N	-6.06947088478427	36.83914864597484	49.68539626517996
C	-5.99153847520654	38.28874177780525	49.73480450304363
C	-5.81254635836361	38.85152742303981	51.14426803330764
O	-5.55189126109571	40.03954466821661	51.31564240223999
C	-7.35317730689874	38.74036113964434	49.19307270207434
C	-8.28424329551283	37.64677246135186	49.71107219116279
C	-7.44691500340950	36.37871801406411	49.54325172258519
N	-6.05082892259961	38.00135522996625	52.14194682192245
C	-5.97027223371902	38.31827439501956	53.54526383004696
C	-5.67125269701314	37.00773819260390	54.28256471163399

O	-5.89388299947643	35.93181725802170	53.72979299919425
C	-7.31338914146605	38.90046457991892	54.02829967910424
O	-7.19871995655450	39.25280710730447	55.38129294765849
N	-5.20272625794347	37.16591411240908	55.50972015831592
C	-4.86595098825252	36.06524477921366	56.38132186378663
C	-4.07554763392177	41.36433736629511	57.80821399997303
C	-4.23743059934548	41.05159034560263	56.34359243205898
O	-4.14692820471465	39.91951006966153	55.88134271988925
N	-4.55223743631433	42.11494796774883	55.57631375596137
C	-4.52148867153934	41.98485990781526	54.13717865848039
C	-3.12066494558382	41.56096539365630	53.66514384360587
O	-2.11197733197262	41.89582713426145	54.28009372042182
C	-4.84899128063064	43.32070551050172	53.46166935096107
C	-3.78629547671356	44.33284262569767	53.85805512938899
O	-3.76938605091725	44.82965575745909	54.98026243774753
N	-2.91708106466717	44.65552905312516	52.89621448427186
N	-3.13065621976063	40.82235727842610	52.55761204758004
C	-1.96315299391836	40.60692540847349	51.73171754988087
C	-2.06626656658529	41.61555423981334	50.53185111579145
O	-1.67215579000382	41.28596644086678	49.39549211622251
C	-1.79765035098630	39.14723466067068	51.33527026174373
C	-1.25714211072567	38.25730461069722	52.46279132989225
C	-2.32344756815614	37.92346923057871	53.50334281753310
C	-0.69573464742953	36.96130547882535	51.88229117268227
O	-2.56636576064547	42.72147878449884	50.80282216270724
Zn	-0.70306664419775	39.99010745944069	48.20342653540735
H	6.22163915079516	33.97519837855282	44.04477345406777
H	5.87243997461689	33.31581091959359	45.64398940750473
H	7.50458957206380	33.20511602310003	44.97788209933443
H	7.73618095520400	35.67643774724372	45.04904678712186
H	4.34715649694008	40.02289274507589	51.46127197408124
H	4.32558807051555	38.26329232309651	51.66110503088409
H	2.04250615031973	39.15895678606834	51.76361571726033
H	2.20336001247653	38.16475833609583	50.31539053852293
H	4.61501244259796	39.83362115230901	49.05579120812897
H	2.03280262025209	36.19687688651231	43.92343245906517
H	2.38340031607480	36.09934780698544	42.20346381952775
H	7.66991735404141	40.77830886979766	42.63120013226322

H	-4.55764331026241	40.97707448593238	42.20123003824129
H	-7.74817848172207	34.81171408678039	43.37167485655641
H	-3.78467053295677	28.74429633765160	50.19270699967425
H	-0.67347129020113	30.29613240386498	46.38993865617105
H	1.74464993160907	30.93413592697692	46.11949118044635
H	0.74853171563869	32.31353021457567	46.56945069511038
H	-0.17893563905682	28.41690715076369	48.15420427155220
H	1.42663491854198	29.12237147228583	48.24413948721669
H	1.33182063190837	27.22858881040345	46.64393491554219
H	0.09655181493557	28.06020146730997	45.70140626141827
H	1.73051131413517	28.71507834639463	45.79374413086233
H	-0.22632560770980	30.88569080937660	49.35421026592159
H	-3.03181872329220	35.02773067017274	45.09938886228522
H	-3.25227888227253	33.28309475427888	44.97574467507950
H	-1.33584199568531	34.10758159642618	43.58633991851127
H	-0.80586124519031	32.94137721378229	44.81538349925131
H	0.06401712365235	37.43513376075200	45.07210784886129
H	-0.83028471721543	36.69378532516349	43.73027442832512
H	-1.58473260194899	36.87818787097670	45.34140895628819
H	-1.70761316165082	34.66838255491821	47.21931181119564
H	-5.20636093056468	34.11570309142460	50.46511177705149
H	-6.09093640743943	34.37327422420985	48.93249443957217
H	-7.33333073521757	38.74356233193948	48.10502334534472
H	-7.61163360998438	39.73425700245510	49.54970652278124
H	-9.21479912146921	37.59631462412975	49.15280694333092
H	-8.51138665741213	37.81738559735231	50.76286649698579
H	-7.68629787191597	35.62294283685269	50.29280919392225
H	-7.59066886329070	35.95971261035431	48.54262612640357
H	-5.14556246356399	38.64437561505327	49.13755651964777
H	-8.09636500598817	38.14171219895875	53.88383613136801
H	-7.54426091687688	39.77697142331253	53.40594266632561
H	-8.03585462937069	39.62613383492526	55.68543136924905
H	-5.17522715310279	39.04204787191784	53.74389866617663
H	-5.08298121549349	35.13704334943494	55.85584231231133
H	-4.89584046289669	41.98735345525132	58.15115700602109
H	-5.82160539427137	43.67012337516245	53.80913789058217
H	-4.85760227174703	43.18213956314163	52.38214580684988
H	-2.12869508503952	45.23153360969615	53.14801671325050

H	-2.81731184711339	44.06235636589061	52.07616148542440
H	-5.25050172200320	41.22522787804215	53.83735649840950
H	-1.08916506247757	39.13141911673105	50.50622739802181
H	-2.75085840077098	38.75584493810108	50.97192026072696
H	-0.44497112393134	38.80276688019988	52.96039209156247
H	-1.91287522927934	37.25659561288539	54.25804267642251
H	-2.68415999049005	38.81583429906259	54.00753113151417
H	-3.16371463342300	37.42403486754940	53.02494008714833
H	-0.27847090103575	36.34204225057052	52.67215007723890
H	-1.48988674427624	36.40941502218823	51.38676676517422
H	0.08410060418154	37.18525078923996	51.16060912101432
H	-1.09140345544342	40.94042448719145	52.31258205722971
H	3.27376541614015	36.79891424506788	45.99580574929478

Cluster model of 3K7N

C	-23.84134209445437	-36.25047795971020	20.81460091675682
C	-23.60639068549136	-37.33659989115816	19.79776285790885
O	-22.63905508972707	-38.08795809073571	19.82014224123807
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C	-24.54003307430815	-38.47619725351050	17.84931795962300
C	-23.12027994392626	-38.69601528727439	17.32124408251664
O	-22.65171691447314	-39.82282127336623	17.22162415081303
C	-25.48885592908286	-38.17242077595038	16.67665327692809
C	-25.46348234199936	-39.28453339611539	15.68257681672719
N	-22.48585825574152	-37.58904737658690	16.93365153426858
C	-21.12925037616359	-37.58672469190180	16.43157700159067
C	-20.88301977223076	-36.43296193010084	15.46726979315267
C	-21.72979282649098	-36.53925392691872	14.20515644077810
C	-21.40630256457854	-37.78374059480534	13.33575434436626
O	-22.28081610315500	-38.07696947767307	12.48170232110927
O	-20.33699694740521	-38.39069940976774	13.51422763374750
C	-23.01846019892036	-41.31965492613398	20.65524815940632
C	-21.64338882176486	-41.79604370166556	20.26629270255546
O	-20.91455234346059	-42.43912323521496	21.01465375892726
N	-21.26758705937814	-41.44184790280853	19.02204797526197
C	-19.90038294340629	-41.60345040562476	18.58382951884277
C	-18.94723947164675	-40.71485270969477	19.40536563774082

O	-17.78247988901285	-41.03545423366086	19.60091841953717
C	-19.71910194999785	-41.21825238542238	17.11105810221251
C	-20.72431752455396	-41.80970525845892	16.18211322033803
N	-21.46306992034667	-42.92694122555852	16.44216664760403
C	-21.09606090090566	-41.41265243997728	14.92376380350927
C	-22.24427541384311	-43.15079935974603	15.37284431528059
N	-22.03950323122404	-42.26092462013422	14.43256818946975
N	-19.48722619540433	-39.56262282756226	19.81033953357534
C	-18.79788545721011	-38.57181262844917	20.61003393408183
C	-19.09502782740712	-37.17433004052109	20.08599201069440
C	-20.72104398742499	-46.66456595059613	17.76190718774694
C	-22.13240177330738	-46.21645084018787	17.47753962522939
O	-22.57278666708528	-45.13032380645728	17.83795378290693
N	-22.84770548832129	-47.07925171056210	16.72915230761685
C	-24.26830078148812	-46.93249856822799	16.50466516019140
C	-25.03294105263664	-47.85361783471919	17.47457156266480
O	-24.45085076682818	-48.71973617541161	18.11623345047612
C	-24.63702349800374	-47.27530276141805	15.04828576705995
C	-24.09838045437047	-46.27311438223728	14.09043165180574
N	-22.95712592325220	-46.44315854806081	13.35376796396118
C	-24.57756168728235	-45.04034388318669	13.73850461413013
C	-22.79626869319673	-45.34083077948127	12.59625716488964
N	-23.76203253394650	-44.47947567859664	12.80340877020147
N	-26.34394061895173	-47.61973243650834	17.52569478222782
C	-27.24976582901558	-48.38641789864649	18.35093799436914
C	-33.54067021101827	-43.33032078335045	16.22179961377145
C	-32.24392182006341	-42.60938130474226	16.47694291153273
O	-31.37485005149586	-42.45599143025111	15.62451811671943
N	-32.07838010131178	-42.17724816039211	17.74140590797299
C	-30.98067708628622	-41.30723824397963	18.12838539924013
C	-29.66735019176030	-41.73963872250454	17.47330411016257
O	-28.92703957210880	-40.92501764093713	16.94751751415538
C	-30.82079454673112	-41.30726256238840	19.64702803179219
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C	-28.12270479616373	-43.61355599097838	17.16089238162999
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O	-27.46066026619487	-45.51818662149527	15.84831893894662
C	-27.30063370381239	-44.20861928598568	18.30873139447889

C	-26.79128396489476	-43.16425724145653	19.28905887753609
S	-25.94907576216760	-41.75167081918031	18.48984558789767
C	-24.67947896822863	-42.57274358494526	17.49468293947658
N	-29.39334646730729	-44.50726685814143	15.28320333385022
C	-29.44981208417840	-45.15688550148395	13.98380258422972
C	-28.30896267699796	-44.57088122996394	13.13444720868563
O	-27.82523717565405	-43.48055542441688	13.40470086153399
C	-30.82668092173926	-44.91230534996242	13.36239737554354
C	-31.02324175987588	-45.60079521212714	12.01733797750543
N	-27.84317029133194	-45.36061745906427	12.15932548085787
C	-26.85135790970792	-44.87869638559794	11.21709217275202
C	-27.52605234808665	-43.99697431846956	10.15448536149412
O	-28.70750946876677	-44.13081384898408	9.86112687830338
C	-26.14744146096512	-46.05876380593690	10.55609967914465
N	-26.69833880332031	-43.12467198342386	9.57251317787779
C	-27.11307223805717	-42.19945397936753	8.54213687052592
Zn	-23.51654623450744	-41.97427303349051	12.64033093854631
O	-21.81742084358000	-40.50077915900239	11.52309627096273
H	-22.99741902115551	-36.20413575744649	21.49667053479214
H	-19.83082078619804	-36.46143027535520	15.17987719135940
H	-21.08023449367965	-35.48178431077095	15.96775189230286
H	-21.56300696767790	-35.66852374568393	13.56550626943981
H	-22.79651177047775	-36.58027868729987	14.43523158822129
H	-20.96510396801679	-38.53396540007296	15.91324138156536
H	-23.75731934424115	-41.65261867801006	19.93441991347388
H	-23.26862828730184	-41.68832843221162	21.64483319634653
H	-18.64901831739894	-36.43116335563883	20.73912861414373
H	-20.17161717984313	-37.02068090248896	20.05436414331137
H	-17.73172399946561	-38.80303216789842	20.56055776827369
H	-20.15333287672915	-46.70648752024785	16.83529712620550
H	-26.67840407693249	-49.17075768523530	18.84427743812575
H	-34.37343624514261	-42.64061882399528	16.33846254370777
H	-30.66760137019906	-42.31639599778445	20.02020423913098
H	-31.17120635016266	-40.28380389063550	17.77529796736402
H	-26.45329103362130	-44.73627479419793	17.86983260192207
H	-27.90437414796090	-44.93641669845582	18.85466897752366
H	-26.09111690839342	-43.61528110305905	19.99237854992600
H	-27.60690220863623	-42.69989381118557	19.84053209726905

H	-23.99084575343867	-41.79405610346031	17.17743177891444
H	-25.12946824744791	-43.02854920358324	16.61654502439145
H	-24.15315129255427	-43.31294024566313	18.09068312864428
H	-27.56070252812669	-42.77953923786043	16.71662687076129
H	-30.96619191177203	-43.83500297570206	13.25098353883666
H	-31.57259243107648	-45.27808724900467	14.07093296399593
H	-30.37680149596464	-45.17021816273024	11.25581880228445
H	-29.27047488617169	-46.22836064086209	14.12682305262126
H	-26.85061522626865	-46.62251941642227	9.94694816762968
H	-25.73045692548056	-46.70850755627992	11.32051362165099
H	-26.13860605159124	-44.26558479838793	11.77812791467355
H	-28.15278884384287	-42.41107394390995	8.29926633455285
H	-24.85101198646692	-39.41801377157959	18.32365226161196
H	-25.18268600981106	-37.24443621956926	16.18993601333140
H	-26.50444658357112	-38.06243762294702	17.05970967875205
H	-19.58767892814572	-42.64107978427420	18.75803393796131
H	-18.70982260027550	-41.51540606039499	16.81130763813470
H	-19.77707873992322	-40.13233136881495	17.01468823566207
H	-20.74429786621682	-40.56994645958858	14.36103012161441
H	-22.94131035836511	-43.96002885635892	15.31848930705560
H	-24.52516171447089	-45.89015196372370	16.71623764789545
H	-25.72392945308388	-47.27030172589205	14.96800359982178
H	-24.26364290188743	-48.27250488434846	14.81182381960261
H	-25.45799313526459	-44.54156261029939	14.08927557929761
H	-21.98971144991219	-45.19421437987445	11.90870791643644
H	-21.50690160321867	-43.45987393031399	17.30126067387329
H	-22.35370754555682	-47.25104605004405	13.37256084794963
H	-21.87106443537229	-40.86338686653069	18.44258119589464
H	-20.46755337392094	-39.38412844083022	19.63480235298095
H	-19.12646357092697	-38.66087627658037	21.65188421677477
H	-18.69051413935259	-37.04934775202792	19.08455102123883
H	-23.01521057989832	-40.23142437912036	20.65781921619318
H	-22.50172229578278	-48.02578826786726	16.64734193480205
H	-26.74342722723614	-46.88259954142178	16.95016573138974
H	-20.24374667035260	-45.96039909555568	18.43849751879501
H	-28.02899501108350	-48.83382095020345	17.73500316255000
H	-27.70743446400163	-47.74757281891011	19.10665431894343
H	-25.38058683483089	-36.84641312247123	18.90407580392865

H	-22.91196483901978	-36.68832542377038	17.09259088783711
H	-23.96240187333084	-35.28988812961493	20.32106601375115
H	-24.74318839660931	-36.46995925153263	21.38117848356480
H	-20.42866304641520	-37.52269885620159	17.27385867057716
H	-29.95926636342684	-43.66568692761197	15.37219460926928
H	-28.36636346559656	-46.17957238264407	11.88787033710896
H	-25.76014063588988	-43.01556761407358	9.93325773174259
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H	-30.83066830507534	-46.66832268921450	12.09795356125013
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H	-32.85229989847968	-42.23649327746897	18.38828320164311
H	-31.70638321047083	-40.88539800974219	20.11494721755881
H	-29.96356585386677	-40.69868113223257	19.92175358004573
H	-25.34268086513541	-45.70074669682349	9.92207440526084
H	-33.54500901754673	-43.71828965360864	15.20741144611244
H	-33.66383017534753	-44.14842089901246	16.92671811686275
H	-26.49583110036022	-42.32961899845261	7.65322117573315
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H	-20.72471679445660	-47.65063926254231	18.21897243217173
H	-20.90975423364319	-40.65125378295827	11.79902902834747
H	-22.02361183678167	-39.57637604642004	11.82863339665802
H	-23.62278669506166	-39.14738103745295	14.46198695367272
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Cluster model of 4Q11

N	-6.67614900687278	-5.25313734472086	7.07496578071551
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C	-10.45876374339739	-7.45021029439999	7.44231522543799
O	-10.59719520367672	-8.45100445741197	6.74767903065455
C	-11.43332904487530	-6.86704918336334	9.71194032203034
C	-12.74230758376336	-7.47278972369868	9.34822873332111
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C	-13.32097721865410	-7.67777314268239	8.12813376976802
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C	-10.10650622950951	-4.65579039627067	5.05517020194075
C	-9.91778385671737	-3.52167751785485	6.07010875283167
C	-11.17182192071643	-3.28622284708453	6.96412657280361
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C	-8.75212005975983	-11.20886157376161	9.03441000476720
C	-8.97567676647143	-11.87254635900590	7.70437957548078
O	-8.56092374910062	-12.99725051551042	7.43908269937566
N	-9.68900956785504	-11.14553333716847	6.81506904093706
C	-9.69023382100267	-11.52732843695727	5.42236816563212
C	-8.32542529765517	-11.26042349786735	4.75809922726012
O	-7.95178145513818	-11.92848816975900	3.80128939599830
C	-10.73974108920983	-10.76310541466491	4.60270549744612
C	-12.12316232889994	-10.82451189772735	5.14280571135241
N	-12.79218965177256	-11.96171545378357	5.50143532576269
C	-13.00020589828397	-9.80194736364536	5.36807841702286
C	-14.01005581977895	-11.60736631497799	5.93547575512559
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C	-16.06819312710290	-15.12843362149674	7.18213422818968
C	-16.09339776800537	-14.26577328563799	8.41882877590457
O	-15.10729890590699	-13.67662347020050	8.84538547324687
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C	-17.53184329445368	-13.51168883181900	10.25976874251303
C	-18.19815166709051	-14.52746429986062	11.20611043802943
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C	-18.45759889606330	-12.28794417727259	10.13242693880559
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C	-18.16869675901641	-9.73533992965824	7.60329220564975
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C	-14.08775428287774	-9.56175639917471	16.53267733898963
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C	-10.84961372400601	-9.34716166673234	14.67157560307552
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C	-10.44043984436407	-8.84962551282323	13.28620726140642
C	-8.57304233955027	-9.58551236082331	15.78714846966812
N	-13.55893799249115	-10.41984183693735	13.58489209005690
C	-14.36659252892546	-10.83734055542640	12.45332718945077
C	-15.85392146088294	-10.77641979117820	12.82864646946921
O	-16.56735750279888	-11.76805119576804	12.91177246425918
C	-13.92543051533070	-12.21135831841343	11.95402908496881
C	-12.44848786251308	-12.22110050927837	11.57535963943796
S	-12.00477666023768	-10.85166065732551	10.43924300441362
C	-12.46230617956548	-11.56705645771816	8.84354926089390
N	-16.29287480006823	-9.53896565045549	13.06498056986231
C	-17.63710491132240	-9.29271631489699	13.54264487096385
C	-18.61405408170934	-9.22856857972860	12.35719454024264
O	-18.26772617188202	-8.94832248233460	11.22079198774216
C	-17.68763781398621	-8.00353747503302	14.35702292068461
N	-19.88655007365027	-9.47867375403925	12.70549711952544
C	-20.97243920250611	-9.66191495455481	11.75407063870396
C	-20.90958975816961	-8.64597188489964	10.60848710207952
O	-20.98551688992690	-9.01722905160617	9.44249196450145
C	-22.31366113158672	-9.55611945224802	12.47575079345238
N	-20.85558147214828	-7.36878668010764	10.98276154409811
C	-20.83302816857967	-6.26433066503549	10.05093323287997
C	-19.96708522702115	-5.08090190558069	3.78509038524587
C	-18.51906350273164	-4.74773549916259	4.06316488784364
O	-17.95996774942453	-3.75183658327264	3.61954367536910
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C	-15.99098874766832	-6.97801274645648	5.48911809813905
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C	-16.23846697401149	-4.69837245644487	6.44911652661284
C	-16.50336634079209	-5.37840626023887	7.75532511028026
C	-17.49252322686743	-6.25892578259071	8.09546613524829
C	-15.71578938685909	-5.19027764892450	8.93488495092079
N	-17.38252628028010	-6.62327604407692	9.41128225350940
C	-16.30054664292331	-5.99107614076003	9.94745387962076
C	-14.58334231309441	-4.43214810292230	9.23444881356833
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C	-14.67343262953309	-5.25980465832408	11.50825780277247
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Zn	-15.47193567116939	-8.99916662095536	6.67595165429016
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H	-6.74569790645988	-4.25706112850305	7.23190627684820
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H	-8.11832915895016	-11.83823659307047	9.65136121217501
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H	-20.03377684390826	-6.04248967522507	3.28324407623398
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H	-16.50973870691228	-16.09916691839311	7.39133672072161
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H	-17.87612772447328	-15.43877787367360	14.18809418025077
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H	-10.51728916511058	-5.41639118397387	7.60907955234480
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H	-18.34771616334116	-6.50763818839342	5.11618712632453
H	-20.76826877591325	-7.14099284794845	11.96161077799772
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H	-21.66387755597575	-5.58892838708684	10.25418391206878
H	-19.89475304581669	-5.71371326003720	10.12516114440286
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Cartesian coordinates of the MET···Zn models

1BUD (includes GLU)

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C	20.00000000	16.34300000	20.85200000
C	20.66700000	16.69100000	22.19500000
O	21.64843531	17.41851115	22.25140265
C	18.68803791	17.12874684	20.66665826
C	18.86568141	18.59396888	20.55033949
N	18.82172152	19.23410680	19.34565266
C	19.05914930	19.56918460	21.48562379
C	18.98444969	20.54154290	19.57723565
N	19.12932140	20.77159345	20.86048971
N	20.08461796	16.14706937	23.26630408
C	20.53067727	16.38000255	24.62344053
C	19.36270722	16.43531485	25.60321955
C	18.37122042	17.54399280	25.27340347
C	18.96419901	18.97471449	25.35803728
O	20.03888013	19.16039971	25.94962244
O	18.26541780	19.86352592	24.80459937
C	24.01015487	19.47393802	24.79909612
C	23.33935158	20.47906762	23.93269759
N	23.82374261	21.75098865	23.77079869
C	22.23982662	20.40350881	23.12580562
C	23.01602274	22.38224079	22.89771741
N	22.04904436	21.59286714	22.48756953
C	21.88071956	25.26325608	17.77059739
C	21.37231416	25.10722728	19.15863954
N	20.58064455	26.04779880	19.76336206
C	21.51335141	24.10403012	20.07244273
C	20.27775987	25.58748812	20.99549393
N	20.82715542	24.41649299	21.20959673
C	18.95900000	16.84200000	15.00700000
C	19.28500000	18.08200000	15.85600000
O	18.57693642	18.31976438	16.82613296
N	20.31796470	18.85333132	15.49696020

C	20.74900000	19.98500000	16.29900000
C	20.08300000	21.30600000	15.94200000
O	20.57977510	22.38084775	16.26417304
C	22.27346737	20.09922167	16.30880157
C	22.94776620	18.88373427	16.93401852
S	22.21656135	18.36451142	18.53066934
C	22.61428608	19.77654094	19.58202600
N	18.93376144	21.22665370	15.26496259
C	18.13200000	22.40400000	15.00800000
Zn	19.91900000	22.36800000	22.18600000
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H	19.77302326	16.62412918	26.59628602
H	18.84504546	15.47328139	25.61821022
H	17.53520635	17.52212346	25.97754113
H	17.95641461	17.43389046	24.26927385
H	21.05947160	17.33594143	24.63850176
H	17.91682646	16.59246397	15.24493219
H	22.54770572	20.99006481	16.87500878
H	22.65014990	20.22548473	15.29181952
H	24.00204244	19.09399794	17.10958687
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H	20.42406850	19.77301123	17.32821112
H	18.72733100	23.11783624	14.43078345
H	20.72349586	16.59406115	20.06675406
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H	18.21133082	16.77777666	19.74878125
H	19.11313680	19.49513829	22.55291823
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H	24.42600054	19.97291107	25.67686434
H	23.27863956	18.73899256	25.13525652
H	21.58608831	19.57043546	22.96855703
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H	19.03372448	21.31003341	24.78016211
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H	19.31414312	15.50715591	23.14463452
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H	18.66889502	18.80726456	18.42961978
H	20.28592909	26.92574223	19.36428602
H	24.80503594	18.98587889	24.27482293
H	22.64782504	24.55478491	17.53710694
H	17.25329527	22.11834461	14.46838996
H	17.81923069	22.84853465	15.92966388
H	19.07309065	17.02912685	13.95968588
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1BUD

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C	19.05914930	19.56918460	21.48562379
C	18.98444969	20.54154290	19.57723565
N	19.12932140	20.77159345	20.86048971
C	24.01015487	19.47393802	24.79909612
C	23.33935158	20.47906762	23.93269759
N	23.82374261	21.75098865	23.77079869
C	22.23982662	20.40350881	23.12580562
C	23.01602274	22.38224079	22.89771741
N	22.04904436	21.59286714	22.48756953
C	21.88071956	25.26325608	17.77059739
C	21.37231416	25.10722728	19.15863954
N	20.58064455	26.04779880	19.76336206

C	21.51335141	24.10403012	20.07244273
C	20.27775987	25.58748812	20.99549393
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C	19.28500000	18.08200000	15.85600000
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C	20.08300000	21.30600000	15.94200000
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C	22.27346737	20.09922167	16.30880157
C	22.94776620	18.88373427	16.93401852
S	22.21656135	18.36451142	18.53066934
C	22.61428608	19.77654094	19.58202600
N	18.93376144	21.22665370	15.26496259
C	18.13200000	22.40400000	15.00800000
Zn	19.91900000	22.36800000	22.18600000
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H	22.55431728	19.42518366	20.60761753
H	20.42406850	19.77301123	17.32821112
H	18.72733100	23.11783624	14.43078345
H	18.03299056	16.91937220	21.51586770
H	18.21133082	16.77777666	19.74878125
H	19.11313680	19.49513829	22.55291823
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H	23.27863956	18.73899256	25.13525652
H	21.58608831	19.57043546	22.96855703
H	23.13630083	23.39881770	22.58602241
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H	19.59898589	16.04094180	15.31298009
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H	17.25329527	22.11834461	14.46838996
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H	22.64782504	24.55478491	17.53710694
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IIAG (includes GLU)

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N	18.29779047	10.95146286	23.39467260
C	18.32683704	9.71141629	22.64170211
C	17.46448211	8.65804670	23.34365313
O	16.63206659	8.00746577	22.72780481
C	19.76193918	9.18110093	22.48617252
C	19.75801683	7.91687784	21.69444721
N	20.08780362	7.88307289	20.36647574
C	19.40640173	6.63298016	22.02102632
C	19.92707197	6.61807889	19.94698123
N	19.52136909	5.84070976	20.92310688
N	17.73917884	8.48833891	24.63892606
C	17.06455778	7.52462969	25.48142559
C	17.93289433	7.13765861	26.67304698
C	19.14725124	6.30263219	26.26342801
C	18.70610573	4.87762243	25.82492372
O	18.37952755	4.74016491	24.62327381

O	18.70411137	3.98609497	26.69338133
C	13.83149290	6.32918386	23.50529590
C	14.54911860	5.75678069	22.33327965
N	14.05210367	5.75059753	21.05719296
C	15.77344754	5.15078061	22.24711370
C	14.97585883	5.16529527	20.26742653
N	16.01976118	4.79076921	20.96111565
C	16.45806460	4.40647129	14.75993067
C	16.59062733	3.84395010	16.12896700
N	15.81721099	2.82272571	16.61386679
C	17.39804294	4.21276913	17.17047008
C	16.18170873	2.61615649	17.89676015
N	17.13476110	3.43638612	18.25294199
C	21.19126860	11.71989736	17.00526384
C	20.59331537	10.34206178	17.29762925
O	20.84927515	9.73550186	18.32420270
N	19.74095264	9.89634029	16.35701781
C	19.02163628	8.64950047	16.46368930
C	19.53154584	7.56924881	15.50143052
O	18.76354496	6.82450241	14.90147394
C	17.51009292	8.83315579	16.31804193
C	16.91331662	9.76335915	17.36274634
S	17.41064520	9.36076931	19.07704508
C	16.69468942	7.71695667	19.29046682
N	20.86216657	7.50434873	15.36004487
C	21.47418826	6.24101447	14.99102283
Zn	18.30308907	3.73510304	20.52418573
O	18.31989794	2.62583857	22.93288290
H	16.34806990	13.06412630	25.02857125
H	17.32923077	6.55269163	27.37067863
H	18.26236055	8.04302058	27.19163111
H	19.82462707	6.19130343	27.11164418
H	19.67320838	6.77300462	25.43073591
H	16.85370280	6.64143638	24.87237963
H	22.02586109	11.84578591	17.70954164
H	17.05604980	7.84494763	16.40804719
H	17.27547147	9.22177173	15.32444015
H	15.82457657	9.73211471	17.32122620

H	17.24624995	10.78975530	17.22062454
H	16.66880144	7.52325209	20.35956174
H	15.68796680	7.70133492	18.88224195
H	17.31184861	6.96255571	18.80979384
H	19.23598430	8.26084569	17.46914001
H	21.08706624	5.94626147	14.00877402
H	17.89138599	9.86380426	21.64346999
H	20.19391834	8.99549710	23.47119398
H	20.36299205	9.92596325	21.96225734
H	19.08655281	6.22321682	22.95880389
H	20.12319525	6.28131315	18.95021908
H	13.08292215	5.62892285	23.88621535
H	14.56944710	6.48153017	24.29415659
H	16.48529404	4.95224905	23.02198341
H	14.85919771	5.05665061	19.20836471
H	17.42631533	4.79783502	14.45030956
H	16.12714147	3.64216931	14.05551217
H	18.15661554	4.96812360	17.20017053
H	15.74812004	1.87298559	18.53341382
H	19.09836339	2.11417403	23.16634221
H	17.47790092	13.54341522	23.75453764
H	18.09247095	12.81981169	25.24655988
H	18.40589550	9.09587546	25.09093930
H	19.11301643	11.54512196	23.34449131
H	21.44692645	8.13539533	15.89796906
H	19.58487059	10.45180756	15.52924231
H	18.29019367	3.37300415	23.57210020
H	16.11158477	7.94298433	25.83125960
H	13.17517950	6.15008484	20.76490138
H	20.37248518	8.66522143	19.78308709
H	15.10332492	2.32780975	16.10259718
H	13.33804400	7.25540115	23.29665816
H	15.75466672	5.21277645	14.75808338
H	21.14375999	5.52721488	15.71642430
H	22.53742171	6.35976188	14.97275554
H	21.55661584	11.74001867	15.99977066
H	20.47057512	12.49304863	17.17181122

1IAG

C	19.76193918	9.18110093	22.48617252
C	19.75801683	7.91687784	21.69444721
N	20.08780362	7.88307289	20.36647574
C	19.40640173	6.63298016	22.02102632
C	19.92707197	6.61807889	19.94698123
N	19.52136909	5.84070976	20.92310688
C	13.83149290	6.32918386	23.50529590
C	14.54911860	5.75678069	22.33327965
N	14.05210367	5.75059753	21.05719296
C	15.77344754	5.15078061	22.24711370
C	14.97585883	5.16529527	20.26742653
N	16.01976118	4.79076921	20.96111565
C	16.45806460	4.40647129	14.75993067
C	16.59062733	3.84395010	16.12896700
N	15.81721099	2.82272571	16.61386679
C	17.39804294	4.21276913	17.17047008
C	16.18170873	2.61615649	17.89676015
N	17.13476110	3.43638612	18.25294199
C	21.19126860	11.71989736	17.00526384
C	20.59331537	10.34206178	17.29762925
O	20.84927515	9.73550186	18.32420270
N	19.74095264	9.89634029	16.35701781
C	19.02163628	8.64950047	16.46368930
C	19.53154584	7.56924881	15.50143052
O	18.76354496	6.82450241	14.90147394
C	17.51009292	8.83315579	16.31804193
C	16.91331662	9.76335915	17.36274634
S	17.41064520	9.36076931	19.07704508
C	16.69468942	7.71695667	19.29046682
N	20.86216657	7.50434873	15.36004487
C	21.47418826	6.24101447	14.99102283
Zn	18.30308907	3.73510304	20.52418573
O	18.31989794	2.62583857	22.93288290
H	22.02586109	11.84578591	17.70954164
H	17.05604980	7.84494763	16.40804719
H	17.27547147	9.22177173	15.32444015

H	15.82457657	9.73211471	17.32122620
H	17.24624995	10.78975530	17.22062454
H	16.66880144	7.52325209	20.35956174
H	15.68796680	7.70133492	18.88224195
H	17.31184861	6.96255571	18.80979384
H	19.23598430	8.26084569	17.46914001
H	21.08706624	5.94626147	14.00877402
H	20.19391834	8.99549710	23.47119398
H	20.36299205	9.92596325	21.96225734
H	19.08655281	6.22321682	22.95880389
H	20.12319525	6.28131315	18.95021908
H	13.08292215	5.62892285	23.88621535
H	14.56944710	6.48153017	24.29415659
H	16.48529404	4.95224905	23.02198341
H	14.85919771	5.05665061	19.20836471
H	17.42631533	4.79783502	14.45030956
H	16.12714147	3.64216931	14.05551217
H	18.15661554	4.96812360	17.20017053
H	15.74812004	1.87298559	18.53341382
H	19.09836339	2.11417403	23.16634221
H	21.44692645	8.13539533	15.89796906
H	19.58487059	10.45180756	15.52924231
H	18.29019367	3.37300415	23.57210020
H	13.17517950	6.15008484	20.76490138
H	20.37248518	8.66522143	19.78308709
H	15.10332492	2.32780975	16.10259718
H	13.33804400	7.25540115	23.29665816
H	15.75466672	5.21277645	14.75808338
H	18.76342015	9.55008510	22.59438729
H	22.53742171	6.35976188	14.97275554
H	21.14375999	5.52721488	15.71642430
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1WNI (includes GLU)

C	19.10315681	51.65126719	7.97501566
C	18.75969344	50.89864026	6.71497855

O	19.53200427	50.76194713	5.77636452
N	17.50310299	50.40277313	6.69262986
C	17.03250591	49.51810836	5.64334473
C	17.48665733	50.01535453	4.26858952
O	17.94752104	49.24066082	3.43802598
C	15.49673850	49.41568616	5.68079963
C	14.99378766	48.49781689	4.62084966
N	14.79624519	47.15928396	4.82764025
C	14.67169506	48.72044131	3.30894593
C	14.36793310	46.63408114	3.66934420
N	14.28150949	47.55257703	2.73529425
N	17.28049014	51.31039621	4.03277304
C	17.67999400	51.95215162	2.79897832
C	16.89881165	53.23618335	2.55153863
C	15.40378891	52.98555814	2.39759432
C	15.05214896	52.09296153	1.17791683
O	13.99087986	51.42963112	1.29134283
O	15.80446324	52.09715576	0.18923287
C	19.59638582	49.41180729	0.30013378
C	18.35368427	48.59391555	0.41547540
N	18.33536298	47.26953222	0.74364471
C	17.04584133	48.92703540	0.17397253
C	17.05696221	46.86243301	0.70139626
N	16.25375534	47.83544107	0.34961548
C	16.64885296	42.17924494	0.23995320
C	15.90565930	43.38164109	-0.22503216
N	16.08453961	43.94502147	-1.46127713
C	14.96075419	44.15692214	0.39186590
C	15.26380362	45.01019603	-1.54406615
N	14.57135918	45.16050678	-0.44256603
C	14.94921705	44.00580154	9.02827092
C	15.19480720	44.23538399	7.53560115
O	14.81441366	45.24788892	6.97481752
N	15.89223741	43.26069516	6.92044148
C	16.26850350	43.33114027	5.52839282
C	15.48812291	42.36371261	4.63314806
O	15.92915264	41.99810005	3.55031563
C	17.77516288	43.15121339	5.32322509

C	18.60934845	44.25109533	5.96369331
S	17.99328579	45.93898166	5.61722052
C	18.00012397	45.96269524	3.81014676
N	14.32666090	41.92395927	5.13504946
C	13.34292161	41.33501911	4.25101499
Zn	13.94560149	47.44539495	0.40598698
O	13.69503683	49.69818602	-0.68890265
H	20.05999760	52.14858738	7.84737729
H	15.06279406	50.40491771	5.52677313
H	15.19312338	49.03519046	6.65762627
H	14.67369502	49.63569818	2.75132127
H	14.09980579	45.60523806	3.53967269
H	17.46462652	48.51497658	5.77331926
H	17.26943363	53.67704326	1.62480250
H	17.07596938	53.94149429	3.36727068
H	14.88067794	53.93320130	2.24371068
H	14.97662336	52.50718152	3.28077706
H	17.49761790	51.24697528	1.98369920
H	14.18179625	44.73552845	9.32190955
H	17.95960700	43.13295857	4.24827045
H	18.09035538	42.18892833	5.73226225
H	19.64008066	44.19739218	5.61303562
H	18.59910132	44.18235821	7.04987118
H	17.87080660	47.00080224	3.51591263
H	18.94778975	45.58476918	3.43625788
H	17.17132473	45.37473317	3.42498964
H	15.97536478	44.33608343	5.19324270
H	13.85187434	40.59706083	3.62228741
H	19.86953630	49.51507841	-0.75470191
H	19.39136604	50.41430610	0.68178573
H	19.11610483	46.67641946	1.00105477
H	16.64063215	49.88311390	-0.09485338
H	16.74970422	45.86458442	0.93402724
H	16.07638940	41.71235324	1.04040042
H	16.76767695	41.46838883	-0.58001267
H	14.53291682	44.05131064	1.36808565
H	15.18303817	45.64260026	-2.40373631
H	13.75357622	50.35061049	0.06029948

H	14.38415497	49.96531818	-1.30238399
H	19.17696217	50.95149060	8.80421744
H	18.33650012	52.38689674	8.20172289
H	18.75484703	52.17269293	2.83635932
H	16.94345139	50.44814355	7.53198780
H	16.96158157	51.91155384	4.77722368
H	16.19567158	42.45396759	7.44542112
H	13.94239394	42.41041704	5.94280476
H	14.91086425	46.64737925	5.69808291
H	16.71320326	43.61232620	-2.17556863
H	12.56281417	40.87652806	4.82208271
H	12.95812685	42.11716430	3.63046532
H	14.58753832	43.01331163	9.19871818
H	15.83982739	44.18754998	9.59278906
H	17.61593214	42.42379544	0.62706161
H	20.43737827	48.99632918	0.81492465

1WNI

C	15.49673850	49.41568616	5.68079963
C	14.99378766	48.49781689	4.62084966
N	14.79624519	47.15928396	4.82764025
C	14.67169506	48.72044131	3.30894593
C	14.36793310	46.63408114	3.66934420
N	14.28150949	47.55257703	2.73529425
C	19.59638582	49.41180729	0.30013378
C	18.35368427	48.59391555	0.41547540
N	18.33536298	47.26953222	0.74364471
C	17.04584133	48.92703540	0.17397253
C	17.05696221	46.86243301	0.70139626
N	16.25375534	47.83544107	0.34961548
C	16.64885296	42.17924494	0.23995320
C	15.90565930	43.38164109	-0.22503216
N	16.08453961	43.94502147	-1.46127713
C	14.96075419	44.15692214	0.39186590
C	15.26380362	45.01019603	-1.54406615
N	14.57135918	45.16050678	-0.44256603
C	14.94921705	44.00580154	9.02827092

C	15.19480720	44.23538399	7.53560115
O	14.81441366	45.24788892	6.97481752
N	15.89223741	43.26069516	6.92044148
C	16.26850350	43.33114027	5.52839282
C	15.48812291	42.36371261	4.63314806
O	15.92915264	41.99810005	3.55031563
C	17.77516288	43.15121339	5.32322509
C	18.60934845	44.25109533	5.96369331
S	17.99328579	45.93898166	5.61722052
C	18.00012397	45.96269524	3.81014676
N	14.32666090	41.92395927	5.13504946
C	13.34292161	41.33501911	4.25101499
Zn	13.94560149	47.44539495	0.40598698
O	13.69503683	49.69818602	-0.68890265
H	15.06279406	50.40491771	5.52677313
H	15.19312338	49.03519046	6.65762627
H	14.67369502	49.63569818	2.75132127
H	14.09980579	45.60523806	3.53967269
H	14.18179625	44.73552845	9.32190955
H	17.95960700	43.13295857	4.24827045
H	18.09035538	42.18892833	5.73226225
H	19.64008066	44.19739218	5.61303562
H	18.59910132	44.18235821	7.04987118
H	17.87080660	47.00080224	3.51591263
H	18.94778975	45.58476918	3.43625788
H	17.17132473	45.37473317	3.42498964
H	15.97536478	44.33608343	5.19324270
H	13.85187434	40.59706083	3.62228741
H	19.86953630	49.51507841	-0.75470191
H	19.39136604	50.41430610	0.68178573
H	19.11610483	46.67641946	1.00105477
H	16.64063215	49.88311390	-0.09485338
H	16.74970422	45.86458442	0.93402724
H	16.07638940	41.71235324	1.04040042
H	16.76767695	41.46838883	-0.58001267
H	14.53291682	44.05131064	1.36808565
H	15.18303817	45.64260026	-2.40373631
H	13.75357622	50.35061049	0.06029948

H	14.38415497	49.96531818	-1.30238399
H	16.19567158	42.45396759	7.44542112
H	13.94239394	42.41041704	5.94280476
H	14.91086425	46.64737925	5.69808291
H	16.71320326	43.61232620	-2.17556863
H	17.61593214	42.42379544	0.62706161
H	12.95812685	42.11716430	3.63046532
H	12.56281417	40.87652806	4.82208271
H	20.43737827	48.99632918	0.81492465
H	16.56405091	49.48686653	5.65476960
H	15.83982739	44.18754998	9.59278906
H	14.58753832	43.01331163	9.19871818

2DW2 (includes GLU)

C	83.46072709	3.37260557	28.08165233
C	82.47756350	4.36788376	27.52195872
O	81.56081832	4.86042457	28.17096739
N	82.66829239	4.66655819	26.21479380
C	81.88878441	5.69450939	25.55058407
C	80.40735004	5.52523836	25.89937387
O	79.72234884	6.47135532	26.27692691
C	82.10998692	5.61525069	24.02983644
C	81.33723623	6.65022858	23.28538493
N	81.92474687	7.49678792	22.38459047
C	80.01377146	6.98545382	23.29309334
C	80.97458420	8.30435619	21.89425019
N	79.79555478	8.02049425	22.43089576
N	79.91702707	4.30004075	25.68009269
C	78.52255151	3.95956750	25.85049494
C	78.03094405	3.01302999	24.75668332
C	78.23954243	3.54816437	23.34284629
C	77.45839867	4.82997095	22.99915909
O	76.68620472	5.34172072	23.82128397
O	77.68464977	5.29364640	21.84243609
C	77.07263506	8.07397405	27.84085479
C	77.32898610	8.74695154	26.53991592
N	77.61317859	10.08115110	26.39771689

C	77.32529186	8.23542312	25.27585415
C	77.78266761	10.33461884	25.08503091
N	77.60845684	9.22401360	24.37552918
C	79.22915781	13.83699922	20.56297645
C	78.47338257	12.59517309	20.85252245
N	77.10372451	12.47759538	20.81366974
C	78.93908380	11.38929984	21.29184006
C	76.78873390	11.22516117	21.22300400
N	77.89591823	10.54248650	21.51856017
C	86.89524964	8.72990783	22.62859726
C	85.40545591	9.02530382	22.45176740
O	84.61846778	8.14236553	22.11558220
N	85.04032427	10.28843750	22.75043205
C	83.68186335	10.77073467	22.72511718
C	83.32215378	11.58297448	21.48513789
O	82.26856007	12.25310078	21.45464537
C	83.36508531	11.58966908	23.98387697
C	83.54953445	10.79992956	25.27027530
S	82.67763350	9.19668198	25.27674465
C	80.95328893	9.73581768	25.37095672
N	84.19518528	11.57831982	20.44123594
C	83.66204790	11.94986109	19.13940174
Zn	78.04224624	8.87442202	22.48305246
O	76.65501444	7.60503697	21.88646174
H	83.12693890	3.04947608	29.06313796
H	76.96470753	2.84892515	24.91860842
H	78.54353633	2.05246764	24.84877025
H	77.93487859	2.79552048	22.61151758
H	79.29163048	3.77374532	23.15429193
H	77.95433618	4.89082701	25.81505723
H	87.09363358	7.85103859	21.99709481
H	82.33532141	11.94013265	23.89496900
H	84.01260642	12.46947191	24.01673700
H	83.19484487	11.36980311	26.12870554
H	84.59559618	10.53842365	25.42263127
H	80.35835891	8.83644987	25.50391930
H	80.66800524	10.23860070	24.45068724
H	80.83162286	10.39696075	26.22438953

H	83.03732140	9.88123650	22.71468016
H	83.38159981	13.00819105	19.18960902
H	82.18929391	6.69112446	25.90257754
H	81.82543284	4.62096586	23.67497561
H	83.16983442	5.77297577	23.82112227
H	79.20840090	6.56019830	23.85210929
H	81.15897788	9.03724347	21.13265357
H	76.08056428	8.33576307	28.21906993
H	77.09671015	6.99787869	27.66378951
H	77.11466865	7.23143867	24.96360707
H	78.03718444	11.29573952	24.68314316
H	80.06181538	13.60144228	19.90124613
H	78.59274424	14.59100960	20.09962935
H	79.95926647	11.10002694	21.44883013
H	75.79476589	10.83699004	21.28695512
H	77.06660779	6.65165522	21.77821222
H	75.90793418	7.44477470	22.47643097
H	83.55136205	2.51245509	27.42407589
H	84.43620968	3.84412187	28.18006861
H	78.36892557	3.49349072	26.83097563
H	83.50659632	4.34796726	25.75238342
H	82.92474311	7.58439628	22.18834737
H	77.69756107	10.75061421	27.14517222
H	76.45068317	13.19309885	20.53819759
H	80.54536965	3.54834037	25.44110308
H	84.88173302	10.82797958	20.41489102
H	85.76604707	10.96137899	22.94555758
H	77.78240777	8.32131847	28.60239496
H	79.64994825	14.23477126	21.46276132
H	87.47147852	9.56369348	22.28557864
H	87.13481433	8.49439957	23.64449323
H	84.40452924	11.79799384	18.38404898
H	82.78112437	11.37239332	18.95124032

2DW2

C	81.88878441	5.69450939	25.55058407
C	82.10998692	5.61525069	24.02983644

C	81.33723623	6.65022858	23.28538493
N	81.92474687	7.49678792	22.38459047
C	80.01377146	6.98545382	23.29309334
C	80.97458420	8.30435619	21.89425019
N	79.79555478	8.02049425	22.43089576
C	77.07263506	8.07397405	27.84085479
C	77.32898610	8.74695154	26.53991592
N	77.61317859	10.08115110	26.39771689
C	77.32529186	8.23542312	25.27585415
C	77.78266761	10.33461884	25.08503091
N	77.60845684	9.22401360	24.37552918
C	79.22915781	13.83699922	20.56297645
C	78.47338257	12.59517309	20.85252245
N	77.10372451	12.47759538	20.81366974
C	78.93908380	11.38929984	21.29184006
C	76.78873390	11.22516117	21.22300400
N	77.89591823	10.54248650	21.51856017
C	86.89524964	8.72990783	22.62859726
C	85.40545591	9.02530382	22.45176740
O	84.61846778	8.14236553	22.11558220
N	85.04032427	10.28843750	22.75043205
C	83.68186335	10.77073467	22.72511718
C	83.32215378	11.58297448	21.48513789
O	82.26856007	12.25310078	21.45464537
C	83.36508531	11.58966908	23.98387697
C	83.54953445	10.79992956	25.27027530
S	82.67763350	9.19668198	25.27674465
C	80.95328893	9.73581768	25.37095672
N	84.19518528	11.57831982	20.44123594
C	83.66204790	11.94986109	19.13940174
Zn	78.04224624	8.87442202	22.48305246
O	76.65501444	7.60503697	21.88646174
H	87.09363358	7.85103859	21.99709481
H	82.33532141	11.94013265	23.89496900
H	84.01260642	12.46947191	24.01673700
H	83.19484487	11.36980311	26.12870554
H	84.59559618	10.53842365	25.42263127
H	80.35835891	8.83644987	25.50391930

H	80.66800524	10.23860070	24.45068724
H	80.83162286	10.39696075	26.22438953
H	83.03732140	9.88123650	22.71468016
H	83.38159981	13.00819105	19.18960902
H	81.82543284	4.62096586	23.67497561
H	83.16983442	5.77297577	23.82112227
H	79.20840090	6.56019830	23.85210929
H	81.15897788	9.03724347	21.13265357
H	76.08056428	8.33576307	28.21906993
H	77.09671015	6.99787869	27.66378951
H	77.11466865	7.23143867	24.96360707
H	78.03718444	11.29573952	24.68314316
H	80.06181538	13.60144228	19.90124613
H	78.59274424	14.59100960	20.09962935
H	79.95926647	11.10002694	21.44883013
H	75.79476589	10.83699004	21.28695512
H	77.06660779	6.65165522	21.77821222
H	75.90793418	7.44477470	22.47643097
H	82.92474311	7.58439628	22.18834737
H	77.69756107	10.75061421	27.14517222
H	76.45068317	13.19309885	20.53819759
H	84.88173302	10.82797958	20.41489102
H	85.76604707	10.96137899	22.94555758
H	79.64994825	14.23477126	21.46276132
H	77.78240777	8.32131847	28.60239496
H	80.85364473	5.57623270	25.79429798
H	82.46359883	4.93649126	26.04037679
H	87.13481433	8.49439957	23.64449323
H	87.47147852	9.56369348	22.28557864
H	82.78112437	11.37239332	18.95124032
H	84.40452924	11.79799384	18.38404898

ZERO (includes GLU)

C	32.12038348	14.25953376	84.88579020
C	32.14376691	13.89656208	86.34849719
O	31.95279208	12.76316470	86.76742860
N	32.36612869	14.94254156	87.17435206

C	32.58892461	14.77520631	88.59825440
C	31.59291542	13.77367627	89.18775275
O	31.95900508	12.90438927	89.97025706
C	32.46236810	16.12834679	89.32121786
C	32.72576321	15.98596847	90.78024244
N	33.97415694	16.12201248	91.32465866
C	31.89571839	15.68978948	91.82763124
C	33.86095959	15.91538735	92.64489752
N	32.61694375	15.65457338	92.97913335
N	30.32012036	13.96607965	88.84194208
C	29.25124969	13.09469559	89.27912265
C	27.89769445	13.79234794	89.23428192
C	27.84028708	15.00727711	90.15206310
C	28.04950059	14.65792557	91.64900573
O	28.55143126	15.57622673	92.34465482
O	27.70645945	13.53830203	92.06353531
C	30.61617766	9.98842078	91.41257198
C	31.23896805	11.01187848	92.30140881
N	32.54768023	10.99652235	92.68751912
C	30.68273768	12.08849173	92.94208168
C	32.73658026	12.03752894	93.51260732
N	31.62803988	12.71104694	93.69624676
C	36.80053853	11.82386756	96.03419973
C	35.43535462	12.37727174	96.24314194
N	34.47988522	11.77663213	97.01920213
C	34.84932324	13.51888947	95.76669777
C	33.38320656	12.55776411	96.98959683
N	33.57744481	13.62002681	96.24676896
C	38.58296445	17.50105284	89.15730611
C	37.80435167	16.69612093	90.19963253
O	36.60687697	16.85514529	90.36724908
N	38.52727880	15.75270905	90.83321348
C	37.94604084	14.81577316	91.76225965
C	38.37181507	15.02446735	93.21957205
O	38.35949923	14.09257809	94.01916683
C	38.18156994	13.36417051	91.33300510
C	37.56713946	13.02358243	89.98375250
S	35.83234077	13.57161674	89.80352552

C	35.03693587	12.75450819	91.20717936
N	38.77039717	16.25921273	93.54742851
C	38.71159528	16.66555867	94.93914585
Zn	31.69023322	14.68815128	94.89510192
H	31.75576242	13.41362417	84.31071598
H	31.45565104	16.52459938	89.17953379
H	33.18872001	16.82291430	88.89501136
H	30.83666388	15.52668372	91.83282464
H	34.67733631	15.99186876	93.33369440
H	33.59278285	14.36328289	88.77729772
H	27.14445767	13.07549013	89.56494772
H	27.66713478	14.09026850	88.20849648
H	26.85758044	15.48117269	90.08111664
H	28.59152692	15.75354040	89.88739303
H	29.47364880	12.78903198	90.30469828
H	37.92837828	18.33427194	88.86279587
H	37.75292192	12.71979401	92.10108428
H	39.25438449	13.16435091	91.28933435
H	37.59197182	11.94632060	89.81746352
H	38.08698394	13.52294039	89.16820138
H	35.33732301	11.71122791	91.24996372
H	36.86699422	15.02507858	91.75276834
H	39.28009164	15.93825100	95.53114283
H	30.06945210	9.25860091	92.01771848
H	29.88894200	10.48409359	90.76623294
H	29.67362632	12.44812838	92.88867887
H	33.68278948	12.27311386	93.95210024
H	37.48499449	12.65615622	95.87085373
H	37.12036138	11.26351260	96.91433743
H	35.26750547	14.26921954	95.12715140
H	32.47675943	12.34312656	97.51625838
H	33.28273513	10.36367707	92.39391597
H	34.58699873	10.91161845	97.52585404
H	34.83330848	16.35998512	90.83628628
H	35.28989913	13.26983406	92.13010928
H	33.96622873	12.82568371	91.03522108
H	32.63187897	15.83156050	86.77583547
H	30.09115133	14.65076966	88.13754485

H	31.48168100	15.12149330	84.71481945
H	29.22852677	12.19937179	88.64402916
H	38.62670189	17.01397164	92.87913383
H	39.51872283	15.68570340	90.65928228
O	29.19599727	14.77965443	94.78304013
H	28.73291478	13.94138864	94.85313559
H	28.95380812	15.13083012	93.88374976
H	33.12993844	14.49828346	84.55901448
H	36.85087067	11.18330277	95.17860437
H	37.68613001	16.60106837	95.23774587
H	39.11137770	17.65218639	95.04703360
H	39.48645694	17.88206922	89.58559087
H	38.78185056	16.89581887	88.29763399
H	31.32221981	9.45216207	90.81354687

ZERO

C	32.46236810	16.12834679	89.32121786
C	32.72576321	15.98596847	90.78024244
N	33.97415694	16.12201248	91.32465866
C	31.89571839	15.68978948	91.82763124
C	33.86095959	15.91538735	92.64489752
N	32.61694375	15.65457338	92.97913335
C	30.61617766	9.98842078	91.41257198
C	31.23896805	11.01187848	92.30140881
N	32.54768023	10.99652235	92.68751912
C	30.68273768	12.08849173	92.94208168
C	32.73658026	12.03752894	93.51260732
N	31.62803988	12.71104694	93.69624676
C	36.80053853	11.82386756	96.03419973
C	35.43535462	12.37727174	96.24314194
N	34.47988522	11.77663213	97.01920213
C	34.84932324	13.51888947	95.76669777
C	33.38320656	12.55776411	96.98959683
N	33.57744481	13.62002681	96.24676896
C	38.58296445	17.50105284	89.15730611
C	37.80435167	16.69612093	90.19963253
O	36.60687697	16.85514529	90.36724908

N	38.52727880	15.75270905	90.83321348
C	37.94604084	14.81577316	91.76225965
C	38.37181507	15.02446735	93.21957205
O	38.35949923	14.09257809	94.01916683
C	38.18156994	13.36417051	91.33300510
C	37.56713946	13.02358243	89.98375250
S	35.83234077	13.57161674	89.80352552
C	35.03693587	12.75450819	91.20717936
N	38.77039717	16.25921273	93.54742851
C	38.71159528	16.66555867	94.93914585
Zn	31.69023322	14.68815128	94.89510192
H	31.45565104	16.52459938	89.17953379
H	33.18872001	16.82291430	88.89501136
H	30.83666388	15.52668372	91.83282464
H	34.67733631	15.99186876	93.33369440
H	37.92837828	18.33427194	88.86279587
H	37.75292192	12.71979401	92.10108428
H	39.25438449	13.16435091	91.28933435
H	37.59197182	11.94632060	89.81746352
H	38.08698394	13.52294039	89.16820138
H	35.33732301	11.71122791	91.24996372
H	36.86699422	15.02507858	91.75276834
H	39.28009164	15.93825100	95.53114283
H	30.06945210	9.25860091	92.01771848
H	29.88894200	10.48409359	90.76623294
H	29.67362632	12.44812838	92.88867887
H	33.68278948	12.27311386	93.95210024
H	37.48499449	12.65615622	95.87085373
H	37.12036138	11.26351260	96.91433743
H	35.26750547	14.26921954	95.12715140
H	32.47675943	12.34312656	97.51625838
H	33.28273513	10.36367707	92.39391597
H	34.58699873	10.91161845	97.52585404
H	34.83330848	16.35998512	90.83628628
H	35.28989913	13.26983406	92.13010928
H	33.96622873	12.82568371	91.03522108
H	38.62670189	17.01397164	92.87913383
H	39.51872283	15.68570340	90.65928228

O	29.19599727	14.77965443	94.78304013
H	28.73291478	13.94138864	94.85313559
H	28.95380812	15.13083012	93.88374976
H	38.78185056	16.89581887	88.29763399
H	39.48645694	17.88206922	89.58559087
H	39.11137770	17.65218639	95.04703360
H	37.68613001	16.60106837	95.23774587
H	36.85087067	11.18330277	95.17860437
H	31.32221981	9.45216207	90.81354687
H	32.55033580	15.18779733	88.81869584

3HDB (includes GLU)

C	6.98873650	35.18037835	45.66841833
C	5.77164504	36.07329769	45.74327200
O	5.56655479	36.98356033	44.94652368
C	6.61913166	33.83079151	45.04629287
N	4.90127329	35.75340391	46.71720330
C	3.69254073	36.51844560	46.96879215
C	4.09841248	37.85221222	47.63584853
O	4.17371548	38.86918926	46.96444553
C	2.66424396	35.68493134	47.73222527
C	1.40896955	36.46177929	47.94529159
N	0.28739833	35.92904647	48.51782402
C	1.08983692	37.75572058	47.64649891
C	-0.64705542	36.89011965	48.55106409
N	-0.19242223	38.01183534	48.03375068
N	4.46148314	37.78564525	48.92149633
C	4.82839107	38.96422390	49.68092488
C	4.05364579	39.08313244	50.99168241
C	2.54210189	39.08505226	50.79429331
C	1.99082445	40.25959736	49.94200694
O	2.67066584	41.27953356	49.77694512
O	0.83027576	40.05333182	49.49468106
C	3.45336847	40.95789774	44.78068438
C	2.05545384	40.77299609	45.26186013
N	1.01930175	40.30625578	44.50210084
C	1.52868481	40.98549055	46.50668625

C	-0.06368429	40.22648541	45.28845202
N	0.20953333	40.63711690	46.51282708
C	-5.55255935	38.20241671	45.82877203
C	-4.46143484	39.02261740	46.41682026
N	-4.35202266	40.37827638	46.27216280
C	-3.32747324	38.63545296	47.07448864
C	-3.19026694	40.75552550	46.82960975
N	-2.54821945	39.72232831	47.32277000
C	-0.83018912	30.93772043	48.43727909
C	-1.15169324	32.41698479	48.22682626
O	-0.53334157	33.29264138	48.81046712
N	-2.09713037	32.65779331	47.30217501
C	-2.49157654	33.97972339	46.87353143
C	-3.79312322	34.47270171	47.51863910
O	-4.54311213	35.24870089	46.93291085
C	-2.58546221	34.06387522	45.34735615
C	-1.23646156	33.92793784	44.65593795
S	0.02889279	35.08343876	45.29552623
C	-0.66412039	36.67643614	44.80318298
N	-4.05379491	34.01603742	48.74318334
C	-5.16688129	34.57569112	49.47753513
C	-4.07554763	41.36433737	57.80821400
C	-4.23743060	41.05159035	56.34359243
O	-4.14692820	39.91951007	55.88134272
N	-4.55223744	42.11494797	55.57631376
C	-4.52148867	41.98485991	54.13717866
C	-3.12066495	41.56096539	53.66514384
O	-2.11197733	41.89582713	54.28009372
C	-4.84899128	43.32070551	53.46166935
C	-3.78629548	44.33284263	53.85805513
O	-3.76938605	44.82965576	54.98026244
N	-2.91708106	44.65552905	52.89621448
N	-3.13065622	40.82235728	52.55761205
C	-1.96315299	40.60692541	51.73171755
C	-2.06626657	41.61555424	50.53185112
O	-1.67215579	41.28596644	49.39549212
C	-1.79765035	39.14723466	51.33527026
C	-1.25714211	38.25730461	52.46279133

C	-2.32344757	37.92346923	53.50334282
C	-0.69573465	36.96130548	51.88229117
O	-2.56636576	42.72147878	50.80282216
Zn	-0.70306664	39.99010746	48.20342654
H	6.22163915	33.97519838	44.04477345
H	5.87243997	33.31581092	45.64398941
H	7.50458957	33.20511602	44.97788210
H	7.73618096	35.67643775	45.04904679
H	4.34715650	40.02289275	51.46127197
H	4.32558807	38.26329232	51.66110503
H	2.04250615	39.15895679	51.76361572
H	2.20336001	38.16475834	50.31539054
H	4.61501244	39.83362115	49.05579121
H	-0.22632561	30.88569081	49.35421027
H	-3.03181872	35.02773067	45.09938886
H	-3.25227888	33.28309475	44.97574468
H	-1.33584200	34.10758160	43.58633992
H	-0.80586125	32.94137721	44.81538350
H	0.06401712	37.43513376	45.07210785
H	-0.83028472	36.69378533	43.73027443
H	-1.58473260	36.87818787	45.34140896
H	-1.70761316	34.66838255	47.21931181
H	-5.20636093	34.11570309	50.46511178
H	-6.09093641	34.37327422	48.93249444
H	-4.89584046	41.98735346	58.15115701
H	-5.82160539	43.67012338	53.80913789
H	-4.85760227	43.18213956	52.38214581
H	-2.12869509	45.23153361	53.14801671
H	-2.81731185	44.06235637	52.07616149
H	-5.25050172	41.22522788	53.83735650
H	-1.08916506	39.13141912	50.50622740
H	-2.75085840	38.75584494	50.97192026
H	-0.44497112	38.80276688	52.96039209
H	-1.91287523	37.25659561	54.25804268
H	-2.68415999	38.81583430	54.00753113
H	-3.16371463	37.42403487	53.02494009
H	-0.27847090	36.34204225	52.67215008
H	-1.48988674	36.40941502	51.38676677

H	0.08410060	37.18525079	51.16060912
H	-1.09140346	40.94042449	52.31258206
H	3.27376542	36.79891425	45.99580575
H	3.05861747	35.35428704	48.69664654
H	2.42933182	34.79442174	47.14191182
H	1.69160960	38.51977040	47.20135040
H	-1.62735199	36.76035152	48.96760897
H	3.63582769	42.00985954	44.54547503
H	4.12065471	40.67179142	45.59491361
H	2.01565479	41.35408604	47.38781772
H	-1.01676053	39.87158488	44.94597945
H	-5.74430203	37.35527397	46.48630011
H	-6.45932205	38.79310854	45.69701368
H	-3.04752864	37.65562874	47.39844478
H	-2.83948222	41.76526878	46.88224744
H	1.08753438	39.96239525	43.54374952
H	-5.02351556	40.98430963	45.82534256
H	0.14241323	34.95536310	48.79057768
H	5.15324890	35.04009959	47.38524914
H	4.34670323	36.93323148	49.44860629
H	5.90281183	38.93927044	49.89247612
H	7.40231521	35.03300869	46.66640294
H	-4.03928024	40.44191253	58.37940930
H	-4.37672509	43.05095281	55.92578273
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H	-2.59081795	31.87812461	46.89274388
H	-3.41265476	33.40294807	49.23466285
H	-3.14315559	41.90796182	57.94589828
H	-1.73728772	30.38448355	48.56377448
H	-0.25954111	30.55587336	47.61663686
H	-5.02259175	35.63024886	49.58702713
H	-5.24064167	37.82524617	44.87727334
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3HDB			
C	2.66424396	35.68493134	47.73222527
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N	-0.19242223	38.01183534	48.03375068
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C	-5.55255935	38.20241671	45.82877203
C	-4.46143484	39.02261740	46.41682026
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O	-0.53334157	33.29264138	48.81046712
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C	-3.79312322	34.47270171	47.51863910
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C	-2.58546221	34.06387522	45.34735615
C	-1.23646156	33.92793784	44.65593795
S	0.02889279	35.08343876	45.29552623
C	-0.66412039	36.67643614	44.80318298
N	-4.05379491	34.01603742	48.74318334
C	-5.16688129	34.57569112	49.47753513
C	-4.07554763	41.36433737	57.80821400
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C	-4.52148867	41.98485991	54.13717866
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O	-3.76938605	44.82965576	54.98026244
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N	-3.13065622	40.82235728	52.55761205
C	-1.96315299	40.60692541	51.73171755
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O	-1.67215579	41.28596644	49.39549212
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C	-1.25714211	38.25730461	52.46279133
C	-2.32344757	37.92346923	53.50334282
C	-0.69573465	36.96130548	51.88229117
O	-2.56636576	42.72147878	50.80282216
Zn	-0.70306664	39.99010746	48.20342654
H	-0.22632561	30.88569081	49.35421027
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H	-0.80586125	32.94137721	44.81538350
H	0.06401712	37.43513376	45.07210785
H	-0.83028472	36.69378533	43.73027443
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H	-1.70761316	34.66838255	47.21931181
H	-5.20636093	34.11570309	50.46511178
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H	-4.89584046	41.98735346	58.15115701
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H	-5.25050172	41.22522788	53.83735650
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H	-1.91287523	37.25659561	54.25804268
H	-2.68415999	38.81583430	54.00753113
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H	-0.27847090	36.34204225	52.67215008
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H	0.08410060	37.18525079	51.16060912

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H	3.05861747	35.35428704	48.69664654
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H	-1.62735199	36.76035152	48.96760897
H	3.63582769	42.00985954	44.54547503
H	4.12065471	40.67179142	45.59491361
H	2.01565479	41.35408604	47.38781772
H	-1.01676053	39.87158488	44.94597945
H	-5.74430203	37.35527397	46.48630011
H	-6.45932205	38.79310854	45.69701368
H	-3.04752864	37.65562874	47.39844478
H	-2.83948222	41.76526878	46.88224744
H	1.08753438	39.96239525	43.54374952
H	-5.02351556	40.98430963	45.82534256
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H	-4.37672509	43.05095281	55.92578273
H	-4.02163494	40.64709607	52.09857224
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H	-5.02259175	35.63024886	49.58702713
H	-1.73728772	30.38448355	48.56377448
H	-0.25954111	30.55587336	47.61663686
H	3.38429215	36.26858622	47.19764358
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3K7N (includes GLU)

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C	-23.12027994	-38.69601529	17.32124408
O	-22.65171691	-39.82282127	17.22162415

C	-25.48885593	-38.17242078	16.67665328
C	-25.46348234	-39.28453340	15.68257682
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C	-21.12925038	-37.58672469	16.43157700
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C	-21.40630256	-37.78374059	13.33575434
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O	-20.33699695	-38.39069941	13.51422763
C	-19.71910195	-41.21825239	17.11105810
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C	-21.09606090	-41.41265244	14.92376380
C	-22.24427541	-43.15079936	15.37284432
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C	-24.09838045	-46.27311438	14.09043165
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C	-24.57756169	-45.04034388	13.73850461
C	-22.79626869	-45.34083078	12.59625716
N	-23.76203253	-44.47947568	12.80340877
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O	-28.92703957	-40.92501764	16.94751751
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C	-24.67947897	-42.57274358	17.49468294
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H	-21.08023449	-35.48178431	15.96775189
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H	-31.17120635	-40.28380389	17.77529797
H	-26.45329103	-44.73627479	17.86983260
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H	-26.09111691	-43.61528110	19.99237855
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H	-25.12946825	-43.02854920	16.61654502
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H	-24.85101199	-39.41801377	18.32365226
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H	-26.50444658	-38.06243762	17.05970968
H	-18.70982260	-41.51540606	16.81130764
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H	-25.38058683	-36.84641312	18.90407580
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H	-20.42866305	-37.52269886	17.27385867
H	-29.95926636	-43.66568693	15.37219461
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H	-20.90975423	-40.65125378	11.79902903
H	-22.02361184	-39.57637605	11.82863340
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N	-24.93786925	-40.76773178	14.10515824
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H	-26.68279432	-41.93816799	14.33394107
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H	-24.38099018	-47.03726672	16.05956505
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N	-22.03950323	-42.26092462	14.43256819
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C	-24.57756169	-45.04034388	13.73850461
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N	-23.76203253	-44.47947568	12.80340877
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C	-28.29331700	-44.63411264	16.03093299
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C	-27.30063370	-44.20861929	18.30873139
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S	-25.94907576	-41.75167082	18.48984559

C	-24.67947897	-42.57274358	17.49468294
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O	-21.81742084	-40.50077916	11.52309627
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H	-26.45329103	-44.73627479	17.86983260
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H	-23.99084575	-41.79405610	17.17743178
H	-25.12946825	-43.02854920	16.61654502
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H	-29.27047489	-46.22836064	14.12682305
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H	-20.74429787	-40.56994646	14.36103012
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H	-28.65626398	-44.74927467	13.39301090
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C	-10.45876374	-7.45021029	7.44231523
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C	-11.43332904	-6.86704918	9.71194032
C	-12.74230758	-7.47278972	9.34822873
N	-13.61695011	-7.99146362	10.25847651
C	-13.32097722	-7.67777314	8.12813377
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N	-10.40745349	-6.20564605	6.96090697
C	-10.84714556	-5.86943061	5.62368440
C	-10.10650623	-4.65579040	5.05517020
C	-9.91778386	-3.52167752	6.07010875
C	-11.17182192	-3.28622285	6.96412657
O	-12.08256415	-2.56536730	6.52598358
O	-11.14366316	-3.84947912	8.08803059
C	-10.73974109	-10.76310541	4.60270550
C	-12.12316233	-10.82451190	5.14280571
N	-12.79218965	-11.96171545	5.50143533
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C	-14.01005582	-11.60736631	5.93547576
N	-14.16919823	-10.29969651	5.86371896
C	-18.45759890	-12.28794418	10.13242694
C	-17.99688602	-11.31137848	9.10480011

N	-18.86671593	-10.47015761	8.46984522
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C	-14.36659253	-10.83734056	12.45332719
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O	-16.56735750	-11.76805120	12.91177246
C	-13.92543052	-12.21135832	11.95402908
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