

Supporting Information

Theoretical Free Energy Profile and Benchmarking of Functionals for Amino-Thiourea Organocatalyzed Nitro-Michael Addition Reaction

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Table S1: Thermodynamic properties calculated for the reaction of the acetylacetone with the β -nitro-styrene catalyzed by the Takemoto's catalyst.^a

	PBE ^b	DLPNO- CCSD(T) ^c	$\Delta\Delta G_{\text{solv}}^{\text{d}}$	$\Delta G_{\text{vrt}}^{\text{e}}$	$\Delta G_{\text{g}}^{\text{f}}$	$\Delta G_{\text{sol}}^{\text{g}}$
Cata	2.87	3.11	-0.40	-0.04	3.07	2.67
TSHR	-3.88	-3.75	1.29	12.33	8.57	9.86
Cat-nitro	-7.59	-4.11	2.74	10.29	6.18	8.92
Cat-acet	-5.46	-10.07	1.92	12.11	2.04	3.96
Cat-R	-13.23	-20.61	6.08	25.82	5.22	11.30
TS1S-cat	-3.29	-7.48	5.61	26.50	19.02	24.63
TS1R-cat	0.35	-2.18	4.59	26.96	24.78	29.37
TS2S-cat	-8.33	-10.98	6.02	27.91	16.93	22.95
TS2R-cat	-5.09	-5.53	5.63	28.21	22.68	28.31
TS3S-cat	-4.46	-8.75	5.56	26.84	18.09	23.65
TS3R-cat	-3.75	-7.73	5.42	26.70	18.96	24.38
Cat-PZ1S	-13.41	-29.13	4.75	28.27	-0.86	3.89
Cat-PZ2S	-15.93	-30.38	5.64	28.30	-2.08	3.56
Cat-P1S	-14.48	-28.64	6.55	29.47	0.83	7.38
TSHP	-0.01	-13.70	6.62	26.63	12.93	19.55
P	-2.44	-20.43	1.66	12.16	-8.27	-6.61

a – Units in kcal mol⁻¹, standard state at 1 mol L⁻¹. Free reactants taken as reference (catalyst in the Catb isomeric form). Geometries obtained by PBE calculations. b – PBE calculations with the def2-SVP (ma-def2-SVP for N and O) basis set. c – DLPNO-CCSD(T) calculations with the def2-TZVPP (ma-def2-TZVPP for N and O) basis set. d – solvent effect (toluene) calculated by the SMD method using X3LYP/6-31+G(d) electronic density. e – Vibrational, rotational and translational contributions to the free energy obtained from PBE calculations. f – gas-phase free energy. g – Solution phase (toluene) free energy obtained by SMD computations.

Table S2: Thermodynamic properties calculated for the reaction of the acetylacetone with the β -nitro-styrene catalyzed by the Takemoto's catalyst.^a

	X3LYP^b	DLPNO- CCSD(T)^c	$\Delta\Delta G_{\text{solv}}^{\text{d}}$	$\Delta G_{\text{vrt}}^{\text{e}}$	$\Delta G_{\text{g}}^{\text{f}}$	$\Delta G_{\text{sol}}^{\text{g}}$
TS2S-cat	-2.93	-9.07	5.61	28.09	19.02	24.63
TS3R-cat	0.15	-6.70	5.19	27.39	20.70	25.89

a – Units in kcal mol⁻¹, standard state at 1 mol L⁻¹. Free reactants taken as reference (catalyst in the Catb isomeric form). Geometries obtained by X3LYP calculations b – X3LYP calculations with the def2-SVP (ma-def2-SVP for N and O) basis set. c – DLPNO-CCSD(T) calculations with the def2-TZVPP (ma-def2-TZVPP for N and O) basis set. d – solvent effect (toluene) calculated by the SMD method, using X3LYP/6-31+G(d) electronic density. e – Vibrational, rotational and translational contributions to the free energy obtained from X3LYP calculations. f – gas-phase free energy. g – Solution phase (toluene) free energy obtained by SMD computations.

Coordinates of the optimized structures, obtained with the PBE functional and the def2-SVP basis set (ma-def2-SVP basis set for O and N)

Acetacet

H	3.38668663253669	2.29786050420021	7.35334422045880
H	3.24901691732273	1.49978352897840	8.96633409277722
C	3.22384687097092	1.33239920141353	7.87444397627182
H	0.96938294520672	0.60987636783215	9.36654565468407
C	1.92823412322159	0.72770619100172	7.42883526362497
H	-2.36758098058535	0.07631612095967	8.34331653727852
C	0.87617868285737	0.41218801334832	8.29132743441745
H	4.06481307466473	0.66947842096998	7.58392993546772
O	1.82371945025640	0.49693903311514	6.13678659847454
C	-1.48329736393265	-0.52159870851270	8.64497235701486
C	-0.31966503520685	-0.16861282448378	7.75159493763882
H	0.84531108525658	0.07170673403540	6.03343212151330
H	-1.27242405503298	-0.34142032596943	9.71552611911912
O	-0.42423493093873	-0.39401620580336	6.50365874201778
H	-1.75417741659718	-1.58578605108526	8.49310200924100

cata

C	-0.16077221353846	0.93140798596462	2.78402240903728
S	-0.46564113937368	1.27958359253447	1.17393560716996
N	0.97424534955876	0.29212279973521	3.22041072513788
N	-1.01584538311497	1.21067517209384	3.84943317208988
C	-2.21007273843107	1.93969691193552	3.92786015452428
C	-2.63446900906914	2.87490812470571	2.95953261587762
C	-3.01225187997332	1.73655884488218	5.07540312734479
C	-4.20889351659334	2.44141369109845	5.24688533100523
C	-3.84445670241197	3.56301914412622	3.14119830026516
C	-4.64413034838269	3.35784847417616	4.27502380283523
H	-2.70159329772923	1.01178902449376	5.84352617866090
H	-2.01902894430573	3.04384918638762	2.06761713681444
C	-4.31361164919078	4.50788717662541	2.05446101208383
H	-5.58836558574498	3.90408934132421	4.39995825931648
C	-5.02024361047819	2.25606460778251	6.50962117756931
H	-0.79730162761478	0.69002284240678	4.70337168257757
F	-3.27662607012095	5.13834988405300	1.45510110726104
F	-4.99082896397435	3.84407326257845	1.08523468740479
F	-5.14659769493443	5.45940807184118	2.54178346852510
F	-4.72819819654453	1.08871924722128	7.13514184109561
F	-6.34911648838325	2.26257583502511	6.25352645484673
F	-4.78372270300040	3.25313408901069	7.39928587612435
C	2.07903591307133	-0.06755745180742	2.34080771976915
H	1.34957778604263	0.57829172093766	4.14469081555712
C	1.83600310428220	-1.34351191741583	1.51714693218751
C	3.33977779931142	-0.24055773350947	3.22207196990746
H	2.23212325010255	0.76847430095290	1.61640300858627
C	3.05221043449796	-1.65371787675026	0.63397198589158
H	0.92515167029361	-1.20174483409576	0.90260498528254
H	1.63998404046048	-2.18621226370574	2.21618999796634
C	4.34472712035868	-1.75433933572979	1.45615130204544
H	3.16212042563912	-0.85061359168843	-0.12905991430543
H	2.87990608759619	-2.59257345811645	0.06746494751688

C	4.56574440583018	-0.50517095902031	2.32406163366471
H	3.17256997298705	-1.15993233388966	3.82986952995842
N	3.44633233771885	0.84676883502122	4.20963895817233
H	5.21774649924462	-1.91823756704947	0.79024757834548
H	4.28768331469259	-2.64817535855341	2.11808987163330
H	5.47465485750234	-0.62538878623135	2.95001832470635
H	4.74496276249357	0.37399032238303	1.66744574017166
C	3.76137966059007	2.16451028601725	3.67003817721368
C	4.25252144811401	0.51514601493227	5.37479861403630
H	3.09147322606795	2.41017848967569	2.82332028091481
H	4.81754281849217	2.26154605316979	3.31379911691118
H	3.60417454548439	2.93149393259468	4.45601382712760
H	3.92172702763133	-0.45393511868550	5.79992525783741
H	4.11989435530412	1.29325064485192	6.15546732577097
H	5.34968754954207	0.44074067571003	5.16104788556349

catb

C	-1.61756602746319	0.52995093962036	3.07770629614450
S	-1.51384365879757	1.62395611331397	1.80691107286461
N	-0.65895444867665	-0.37581011295717	3.39522594459788
N	-2.77327608638999	0.50270035329443	3.85721375160733
C	-2.98667880303333	0.01614322596174	5.15467216337397
C	-4.31861020525390	-0.26162255919920	5.54929901582949
C	-1.94721249423987	-0.15530231494280	6.09732305836989
C	-2.24837565695261	-0.63236162473202	7.38565841558750
C	-4.59806097324179	-0.71412121831036	6.84115383195999
C	-3.56314837545947	-0.91703984461762	7.77341350666138
H	-0.90354361236632	0.10577807025980	5.84337327128242
H	-5.14164624479925	-0.12039322262585	4.83344208172417
C	-6.02064660769326	-1.03632288653199	7.24759238679833
H	-3.78112284366744	-1.27763344498346	8.78699900501171
C	-1.10439998251407	-0.81919817667204	8.35904959946937
H	-3.53833867519397	1.02487503252860	3.42376153254079
F	-6.92292930788168	-0.59453567349985	6.34056818569106
F	-6.20081957614323	-2.37290934498393	7.38178903938013
F	-6.32799433780188	-0.47400883239764	8.44086846933293
F	-0.37464358860963	0.31925258634430	8.49075681255506
F	-0.24869221049215	-1.78584123709316	7.93058859963921
F	-1.52697903239509	-1.17366447542651	9.59127304797535
C	0.69159216723533	-0.38227634595211	2.85293937402125
H	-0.84794923249973	-1.03352811519983	4.15581870351011
C	0.87378457242906	-1.44170809356632	1.75027553683313
C	1.72771028967458	-0.57052882125085	3.98709664016096
H	0.82367351860378	0.61430427859914	2.37693939520939
C	2.29631743592010	-1.40912837919539	1.17767476251029
H	0.12267422140615	-1.25322235903580	0.95634629992962
H	0.65525038333946	-2.44933254269024	2.17229598709799
C	3.34892692979749	-1.55361556678002	2.28318340017274
H	2.45056278712589	-0.44182551759579	0.64957288633091
H	2.41919947418499	-2.20400351519868	0.41254771897900
C	3.15184983114141	-0.50338818298722	3.38447063407306
H	1.59439739984082	-1.60692490520967	4.38306975591836
N	1.46123319354069	0.31269771176601	5.13417267189785
H	4.37227611241685	-1.47813943572467	1.85906425895965
H	3.27463425394505	-2.57043688881090	2.73148012260409

H	3.90399280031036	-0.64314174722884	4.18850093855490
H	3.32509781138182	0.51248466182037	2.96439541369350
C	1.51289391375406	1.74414960511876	4.86264486970478
C	2.21557089541067	-0.05053823385611	6.32543944138720
H	0.83834471479921	2.01696275048346	4.02726919324259
H	2.53854863558549	2.12588131248303	4.62335416929243
H	1.16422486194958	2.29416554757035	5.76093595187649
H	2.09193067124205	-1.13171094900893	6.53779475137789
H	1.82128551855676	0.50391124356167	7.19940033308841
H	3.31236958797441	0.16644113553896	6.25264770117633
cata-acet			
C	0.70638606230759	0.71811199323807	-1.23257774388337
S	1.38210382233883	2.15539269115698	-1.80667716786720
N	1.23932525755127	-0.50652186774586	-1.51040441628086
N	-0.40730909592120	0.62156359215767	-0.41416600374620
C	-1.30662644936537	1.57414583653697	0.08031923157482
C	-1.42630594533720	2.90036113666515	-0.39120613765740
C	-2.16430207754528	1.14181646461774	1.11820527344072
C	-3.10389994368742	2.01319392884120	1.68168147313411
C	-2.37799916832424	3.75688837705865	0.18230588457073
C	-3.21976042638166	3.33445728703209	1.22344857140571
H	-2.07574123752355	0.11034407295422	1.49313895865400
H	-0.75347191020313	3.25174905891279	-1.18476431075978
C	-2.53404621671980	5.15302817608881	-0.38191652473194
H	-3.94397817632898	4.02353733222630	1.67652186783379
C	-4.00584681285105	1.49205560664433	2.77687941547725
H	-0.54785962786571	-0.30704007246952	0.00792015668395
F	-1.35700712280192	5.65877991050633	-0.81584225058857
F	-3.38479567502179	5.16309691612134	-1.44036090999734
F	-3.03659766640795	6.01425016432722	0.53730252820977
F	-4.95421449864117	0.65509642879719	2.28418606657990
F	-4.64740470967502	2.48773418930576	3.42907722020403
F	-3.30658135896379	0.78223685680598	3.70285920272245
C	2.45747629729506	-0.71405375086363	-2.26363974507254
H	0.85284832997035	-1.37673355137012	-1.06840462241494
C	2.18684825734075	-1.12906856082479	-3.72493025069540
C	3.32483716289409	-1.78069260730152	-1.56290468742419
H	2.99012145470499	0.26329177960792	-2.29078040636165
C	3.49172047965179	-1.36908057026393	-4.49075732850172
H	1.58657144939423	-0.32572467143714	-4.19804060608306
H	1.56251153547525	-2.04936586013433	-3.72909230882724
C	4.37083127989281	-2.40118903753902	-3.77423013012908
H	4.04794410081248	-0.40966097843787	-4.58189784451478
H	3.27376258295577	-1.70069047266013	-5.52691576623451
C	4.64399293417134	-1.99594515585409	-2.31569476858152
H	2.75253432238729	-2.73236465391100	-1.54864468846593
N	3.49995793951694	-1.45361396487001	-0.08929000662671
H	5.33459761268905	-2.53831621930672	-4.30631498108292
H	5.25325216930243	-2.77939772581902	-1.81952654924116
H	5.24463027079488	-1.06072117957021	-2.30538798272352
C	4.11755033013202	-0.12514871181277	0.18888965351581
C	4.18298365882875	-2.54388442265031	0.65685292098951
H	3.50463176244783	0.67357081993446	-0.26943770873786
H	5.15090192693732	-0.08773853784620	-0.20384014237778

H	4.12221025189673	0.02276861252973	1.28315646963404
H	3.68875363690834	-3.50264009535356	0.41488473317135
H	4.06358061158867	-2.34358522403339	1.73703623633587
H	5.25701978160042	-2.59047083463952	0.39668957327053
H	3.86305199788293	-3.39100717995618	-3.78484142869565
H	-0.67446791107446	-5.21664807402417	0.23796951557564
H	-2.04496903729882	-4.29988597840654	0.96414855768600
C	-1.22924682693859	-4.25535326470674	0.21784019359478
H	-1.29527520394853	-2.50765336025971	2.23950717774769
C	-0.24535352121466	-3.11811936719051	0.45018208881450
H	0.33223721514867	0.38928743547963	3.36052352522576
C	-0.41114427823113	-2.30701510347818	1.61675350270222
H	-1.66477566675548	-4.16771845974278	-0.79829730929949
O	0.67300641153621	-2.96134389695308	-0.41269353728620
C	0.20339303176043	-0.70683339796191	3.47105361664580
C	0.53316390600154	-1.38485742903635	2.15026278625860
H	2.50871487710507	-1.40140752317504	0.41451865480642
H	0.92768642472826	-1.03808862534701	4.24428046676125
O	1.65682160210787	-1.07126694434484	1.63361450351576
H	-0.82228018303054	-0.91372133624805	3.82840823814806
cat-r			
C	0.49011912613517	-0.11798273745704	-0.46138654089436
S	0.92141990413775	1.29417965215239	-1.28649594591977
N	1.14064430636875	-1.31679712290933	-0.64719764237589
N	-0.51657962219577	-0.23710148338866	0.47335454718549
C	-1.23968861206000	0.71240993569244	1.20276474177714
C	-1.26634717359425	2.10065235918392	0.94365017317298
C	-1.98960368110951	0.21202745657850	2.29610588405312
C	-2.71534156002111	1.07866387336219	3.12057103672616
C	-2.01760885053195	2.95022943861790	1.77086118730172
C	-2.74083308432305	2.46044180501206	2.86766412450667
H	-1.98623072927995	-0.86893252915259	2.50471112896038
H	-0.68840638269580	2.49746787022447	0.09898319605572
C	-2.09251780487868	4.42150692886289	1.42219243951629
H	-3.31103148414916	3.14045803966721	3.51379889091440
C	-3.39532268638893	0.53109639520636	4.35118420243668
H	-0.70459122603569	-1.22394861712695	0.75738138314936
F	-0.92302476115891	4.88495666209694	0.92578194748003
F	-3.04387361999393	4.65391668904632	0.48128207759062
F	-2.40955950260314	5.18074545853005	2.50054682583664
F	-3.77383777854672	-0.76084997830321	4.20001706528892
F	-4.49105897057328	1.24482069398667	4.69383217681387
F	-2.55483889274167	0.56458444141656	5.43242342581858
C	2.04145478268206	-1.58158397641033	-1.74950339935058
H	0.79565466590184	-2.13260214664762	-0.07788052736637
C	1.44132888704009	-2.54934501911266	-2.79044194311249
C	3.37888252319984	-2.15978900656517	-1.23779444148896
H	2.21667860651814	-0.59895610096070	-2.24481178393693
C	2.42157517902442	-2.81129691485540	-3.94152063129088
H	0.49561129880364	-2.11067892367678	-3.16746832736729
H	1.17278711563757	-3.50555565513406	-2.28847658445858
C	3.77366230361741	-3.32018731659841	-3.42491983685893
H	2.57748845977162	-1.86842904856319	-4.51156207184221
H	1.98498240537358	-3.53854554131923	-4.65759348840891

C	4.37502732884022	-2.36160696037337	-2.38188223991950
H	3.16035166124755	-3.13017458749868	-0.74323618986918
N	3.91212619579353	-1.31518054018586	-0.08592966797664
H	4.48798309231833	-3.45458352895549	-4.26301969388481
H	5.33445251814469	-2.76965094292443	-2.00311719937576
H	4.60428075317946	-1.38942670296283	-2.87106956763468
C	4.34413958928105	0.06688027576547	-0.45692946660729
C	4.94202924761451	-2.03708016334222	0.71870040826122
H	3.50715413289013	0.58766967810025	-0.96409816639724
H	5.23848595307813	0.01275350976066	-1.10363256622042
H	4.58186981759636	0.60763973266390	0.47591161802763
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H	5.18017873489297	-1.42202327677270	1.60477951151764
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H	3.63979294194189	-4.32297198148004	-2.96238721286850
H	3.34134650494620	-6.19689668451891	2.00799888465180
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C	2.72680988067030	-6.21095573187800	1.08386524182209
H	0.08061561577041	-6.25904013095470	0.90016980204891
C	1.81669164665331	-4.98316811649546	1.05982401910364
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C	-2.06044318742706	-4.67070654987471	0.91724753347012
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H	3.09280604489801	-1.19342532834756	0.56292259530266
H	-2.54874042539936	-4.31635591622686	1.84968077729830
O	-0.39573060616634	-2.96211111278955	0.92092064462646
H	-2.18075586524976	-5.76858518484455	0.84967955262760
C	0.36902581116487	-1.56260365593457	4.44244207735695
C	1.27452739832922	-1.49765261841153	3.42915901821922
C	-0.36298663878108	-2.74318042510980	4.87819645643765
H	0.16763507377879	-0.62127603580960	4.98145053030176
N	1.94759647094764	-0.25086163462324	3.15934136863346
H	1.56817651983437	-2.30420718221548	2.73886075808449
O	1.71755415472954	0.75404036839396	3.83346517926055
O	2.78555574344906	-0.26314864862843	2.22390037449672
C	-1.34862965810464	-2.59811188331903	5.88933566576593
C	-0.12736012314407	-4.03452596503558	4.33720691648628
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C	-2.07321152910219	-3.70565565068989	6.34476263269872
C	-1.82735582355076	-4.97745498513851	5.80100942810208
H	-1.55225936802876	-1.59893715516170	6.30085217893797
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C	0.51800760649027	-4.38515350256734	0.14367107797826
C	-0.55781776385618	-3.56379804149090	0.15273715996082
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C	0.13831103161694	-5.58114063825626	2.34441019099289
C	0.56169886158363	-6.51401176743702	3.29523450712335
C	2.52180112949359	-7.01960089871185	1.94432242431066
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H	-0.04257212673318	-6.68362820979276	4.19928878803279
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H	2.08256638693897	-7.96813268383553	3.85350453459625
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N	1.16750100125786	-0.54551951485860	-1.40911253940964
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C	-1.56125627815005	1.52354884139851	-0.15527072849193
C	-1.34962901217568	2.92075787239235	-0.11217372346053
C	-2.80734934044407	1.01161265824424	0.27665724656854
C	-3.80627225031425	1.86776933624594	0.75737190456743
C	-2.36774537452347	3.76273846204063	0.35902779486673
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H	-2.98011600435406	-0.07475641203016	0.22813087598685
H	-0.38847748655036	3.32842463463366	-0.44936876354758
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C	-5.11166624528370	1.25983510736470	1.21517011458231
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F	-5.74751599234997	0.62008965199685	0.20245049454882
F	-5.96493798115173	2.18316226549833	1.71191523141382
F	-4.91108386376141	0.32978535203548	2.19266371838447
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C	3.41914165356861	-1.64410367628128	-1.37081151607239
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C	3.43428018507250	-1.47203399213530	-4.35274660377696
H	1.42175013482530	-0.66677628588269	-4.05051464958886
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H	3.22312625537253	-1.92592395452387	-5.34311741300808
C	4.72468501247023	-1.73692845929208	-2.18469001664188
H	2.99104601356962	-2.66952747575177	-1.28668159711655
N	3.61569834774712	-1.21370525118484	0.06649659721517
H	5.43181116374812	-2.34599457398754	-4.14978279785396
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H	4.41871198519943	-3.10934004879937	0.59135177908327
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H	-3.34433028009298	-3.47466554969204	0.94442468474327
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C	-2.86132812162852	-2.91554461798670	1.76973306305404
H	-0.70626190648661	-2.88299580534646	3.34063706049534
C	-1.46533921678840	-2.48583937423472	1.34044547115080
H	2.39975081151145	-1.32381331698100	3.39672797293899
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C	0.93143736517566	-2.27181487697021	2.12536766495032
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H	2.70485228145867	-3.05842616569220	3.09217484843742
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C	-1.39775447541184	2.22433368933675	-0.86185851606564
C	-1.11110659029332	3.59282811731998	-0.66343081278846
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C	-3.68349474527391	2.62612334331202	-0.08971284004536
C	-2.11491946424786	4.45589909827371	-0.19744748995299
C	-3.40620659993082	3.99067212101895	0.09342679632139
H	-2.93598694757436	0.68740465835492	-0.70972008957259
H	-0.10671147952570	3.97136294320845	-0.88573119189284
C	-1.80990917404636	5.93104838925560	-0.06086992561990
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C	-5.04199514255779	2.08199903487150	0.28875336935473
H	-0.80407922675110	0.28943662951716	-1.15039367606886
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F	-5.38043335165022	0.99914532203094	-0.45126359942830
F	-6.01751449442702	3.00974409152880	0.12778624946010
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C	2.56865067665816	0.03581448560852	-2.92041643313266
H	0.92978074260079	-0.66636328652935	-1.76507481590682
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C	3.71031127664011	-0.76987265560803	-2.25662880824361
H	2.93219428316278	1.06174011620244	-3.15412529641353
C	3.35185905237092	-0.76572483411881	-5.21011521715813
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H	5.72857066192872	-1.45300770301575	-2.74898843177769
H	5.31323120220668	0.15480091608328	-3.40915631448884
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H	5.20610301134760	-1.94827030624626	-0.38888760230376
H	5.32123603440394	-0.59175574218745	0.78243344647671
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H	4.61128968261853	-5.34340711410081	1.36593017461554
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C	0.77932141473858	-1.10238742890650	2.83277809556175
C	1.81321595202826	-1.64252231633619	1.86726972978195
H	3.29476661977616	-0.50742678557065	-0.21932674425563
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O	2.40454944982375	-0.82802354670349	1.12643063839880
H	0.66254192795428	-1.71923658494794	3.74341360334695
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C	0.67650828597712	-6.43303969841548	1.12646142769282
C	-0.58300694264125	-5.19602007954381	2.79326282443177
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H	-0.97944391240614	-4.24673023967979	3.18645301488647
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H	-3.93578369682709	3.87167093537562	1.52815262545428
C	-4.36967992481316	1.17317046890087	1.94117393020744
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F	-2.75066217371223	5.68649541307254	-1.03658388597413
F	-2.65376491178795	5.94082451303189	1.12694208573814
F	-5.02804849408414	0.20091771701918	1.26387246877879
F	-5.29053093401722	2.05406814266821	2.39283807579315
F	-3.81624457256235	0.57523884162929	3.03478380292739
C	2.54472180332437	-0.52663242541812	-2.65780968813257
H	0.69102518951925	-1.23307119941094	-1.91490505096696
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C	3.33191259236461	-1.74192033373222	-2.12679996068380
H	3.11275610497038	0.41202169843835	-2.46848094659808
C	3.67791604819865	-0.81655241462746	-4.92014924760802
H	1.80420275407578	0.24970874706988	-4.52777695451698
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H	4.27840626002933	0.11290393760821	-4.80054333646217
H	3.50305647342848	-0.93683632315937	-6.00914722071947
C	4.67590658804020	-1.89425606655059	-2.85131875694322
H	2.71764508770606	-2.65342381823490	-2.29404010998734
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H	5.21772141649644	-2.78739452900753	-2.47853694909758
H	5.31658684721583	-1.01135216958841	-2.63707351656291
C	4.14529841675701	-0.47283867967616	-0.07155004721493
C	4.10238640400154	-2.94512897274481	-0.05902586529079
H	3.56558844235145	0.42383134161109	-0.36394668780578
H	5.18124420801988	-0.41034650620964	-0.45123204983990
H	4.14936622106730	-0.55593915973743	1.02956177370999
H	3.71775277996955	-3.81252495600044	-0.62455210950337
H	3.77379519346318	-3.05868036182857	0.99195909403236
H	5.20252265124193	-2.88871619382377	-0.14746874054715
H	3.92552291688327	-2.95232186857661	-4.59590548824141
H	1.93092269059741	-3.87727980973220	5.43004264295516
H	0.65570720847914	-4.97290984546526	4.84045283615978
C	1.66746876564153	-4.58086253719558	4.61143104246036
H	-0.05676172719662	-2.72905723459983	3.92505965331927
C	1.69502018805600	-3.84536519733944	3.27710077561426
H	0.16879207359188	0.38418234082974	1.93736627472241
C	0.63451514998304	-2.85039602349544	3.07418832911547
H	2.39707427447918	-5.41105337064271	4.60080899664645

O	2.58684555613940	-4.09203591925555	2.44763953800891
C	0.06253148961658	-0.40937710501072	2.69948653770695
C	0.82575287041635	-1.65374913320849	2.27418937283204
H	2.51887690264757	-1.67499997621613	-0.16845786863437
H	0.46845502354189	-0.03371772838225	3.66245431340684
O	1.59342342857920	-1.60179056121237	1.28418485803247
H	-1.01427702730412	-0.61576109403581	2.86809867055158
C	-0.75337882978226	-4.02967849309815	1.69041824594027
C	-0.14458611422524	-4.03681587149046	0.42929738100320
C	-0.93476050520315	-5.25620109912855	2.49089777663301
H	-1.52017788997380	-3.25316830125898	1.83266559580311
N	-0.33007036781848	-2.99345995394057	-0.45532926342205
H	0.54551165358528	-4.80383615633260	0.06464808462025
O	-1.12751990356223	-2.04524563765712	-0.18332237903465
O	0.30261466464077	-3.00662595303488	-1.56143010214691
C	-1.92839511425415	-5.27490542941602	3.49929940733392
C	-0.17224600575085	-6.43050738007107	2.28058971296627
C	-0.39994913733305	-7.57822355783904	3.05082544274999
C	-2.15608056772397	-6.42399928452272	4.26789030736054
C	-1.39139476736906	-7.58177514807165	4.04659548220928
H	-2.53325814422850	-4.37040552088234	3.67308448079085
H	0.61411119285587	-6.44482119814753	1.51199689293421
H	0.20277432831796	-8.48165785616552	2.87122633198946
H	-2.93948653718836	-6.41812911723306	5.04159973509310
H	-1.56983559132025	-8.48695285211136	4.64694932900199
TS2R-cat			
C	0.57988860644013	-0.08405329529649	-0.49368350147919
S	0.97280739741408	1.43990116966019	-1.12191136650400
N	1.24769758498631	-1.22559683949519	-0.85613987528951
N	-0.43652852267225	-0.33854875473919	0.39807908207301
C	-1.27925525137376	0.51946412672678	1.11507301820949
C	-1.03809338961982	1.89337112195826	1.33816847827044
C	-2.43358443989372	-0.06978286417666	1.68703741870955
C	-3.31254606629915	0.69240048148779	2.46499509909490
C	-1.94407783834173	2.64510196855644	2.10254988080199
C	-3.08472325783270	2.06264741550676	2.67624104334498
H	-2.63574600940187	-1.13560964069671	1.50522967423853
H	-0.14628295438313	2.36179840360064	0.90472453131696
C	-1.71057005311462	4.13107418245413	2.26913560529916
H	-3.77959063786771	2.66345428945924	3.27854727035449
C	-4.47910938413633	0.01938458633073	3.14749832436315
H	-0.66461020412493	-1.34807244881300	0.53001910377796
F	-0.39664047392786	4.44953555003426	2.20847166988759
F	-2.33885463191236	4.84123552694377	1.29807581109590
F	-2.18635853078029	4.58265726454010	3.45678095823292
F	-4.83884186460817	-1.13670089797372	2.53958876116924
F	-5.57029445350681	0.81561649404606	3.19826472061612
F	-4.17015266443271	-0.29971133526788	4.44198807618050
C	2.18921580337846	-1.28852973396360	-1.95546680084695
H	0.96460228139793	-2.14250163053587	-0.45103708033135
C	1.58112774163276	-2.01525869274835	-3.17526595350509
C	3.51417331226688	-1.97291564118281	-1.54844343889861
H	2.38175631578903	-0.23073583299298	-2.24634663655482
C	2.55505087482260	-2.06874729465288	-4.35600706125939

H	0.64883321248031	-1.48215323348677	-3.45093026131645
H	1.28592480410052	-3.04276830704084	-2.86987883684541
C	3.88282387913151	-2.71061952141282	-3.94050145358053
H	2.74475092458108	-1.03711985840767	-4.72655378778282
H	2.10320296355769	-2.62623521759340	-5.20226211081832
C	4.49776000000577	-1.99416779906355	-2.72714156646953
H	3.27461163250146	-3.01541516413241	-1.24471487650165
N	4.11614260410071	-1.36234464055311	-0.28623735747622
H	4.60763790411842	-2.70285868624422	-4.78121778206008
H	5.44079041632595	-2.50089297802398	-2.44002482322214
H	4.76398242044720	-0.95285175334146	-3.01378073507698
C	4.33329804119615	0.11328039049242	-0.32683217528488
C	5.35420312903470	-2.07347757741618	0.15246156351665
H	3.37379070271073	0.63604484489223	-0.51864531022561
H	5.07219226072170	0.36367662632758	-1.11099968431116
H	4.72206652798535	0.42379950706341	0.66026350326536
H	5.18952682053921	-3.16438790200576	0.07733082066251
H	5.53235496461186	-1.82132042142260	1.21443750296480
H	6.21266278122425	-1.77431302281251	-0.47557528316929
H	3.71353293873429	-3.77943873331169	-3.68160319477144
H	2.84881762689571	-5.11494626908837	2.40067855977714
H	2.01353395378814	-6.50366435097904	1.66448514778140
C	2.38901575893703	-5.48141034954094	1.45637490692545
H	0.14000940972100	-5.28258625328769	2.73946164333968
C	1.26113221620189	-4.54587784054868	1.05223432219086
H	-2.62829273824630	-5.51285184946276	1.52660601282686
C	0.16094360053570	-4.44828376993666	2.02002483810376
H	3.15995144116092	-5.52530703942851	0.66457514179283
O	1.32609316448070	-3.93496881299211	-0.03207341141447
C	-2.37646983404569	-4.65641104714258	2.18915233503927
C	-1.15694640459083	-3.94889063890293	1.62669764549687
H	3.42141505561790	-1.53045433979807	0.53420991169477
H	-3.24354812388643	-3.96905206975229	2.20612857999406
O	-1.31502967392974	-2.97505464041002	0.86107221768893
H	-2.19484307394205	-5.06331869077372	3.20257157170383
C	0.75929032169661	-2.94328748868161	3.48724139030372
C	2.14882178529245	-2.97497948648740	3.73740677065877
C	-0.18759014046610	-3.26332178628481	4.58278928260082
H	0.44387708073151	-2.14606559833281	2.79579054622102
N	3.03499464891039	-2.33232819715314	2.89908119569845
H	2.62621775783707	-3.46482465736300	4.59329337029844
O	2.56899604313897	-1.71434512324392	1.87090129237945
O	4.26849854519051	-2.35035921629883	3.14240489057278
C	-1.37794599651827	-2.51020186095845	4.70854837193336
C	0.05764659060901	-4.29410888182729	5.52098377964315
C	-0.85845682974278	-4.56068279056065	6.54749714902226
C	-2.29252667563946	-2.77331971500636	5.73892579157836
C	-2.03706321038732	-3.80143668802869	6.66044768323821
H	-1.58434846433093	-1.69838577795844	3.99375514257729
H	0.97107731987459	-4.90358003120765	5.43866182846394
H	-0.65290735645938	-5.36928007397412	7.26606157845026
H	-3.20865378570896	-2.16916689520510	5.80905787130563
H	-2.75607023073300	-4.01329300065991	7.46680167824802

TS2S-cat

C	0.62487688647139	-0.07491242444270	-0.60715474532782
S	0.92201545481366	1.43983670102537	-1.30614084162368
N	1.35352170958182	-1.19205407588293	-0.92321322757908
N	-0.36501782753488	-0.35116204387972	0.30849715203086
C	-1.20231801639264	0.47422985974975	1.06766992018310
C	-1.11418889852180	1.88198465872400	1.15050863082713
C	-2.18719839047854	-0.18949816617811	1.84060489251022
C	-3.04066902378290	0.53069895827249	2.68369139854626
C	-1.99389441053773	2.58712288070425	1.98702540007731
C	-2.95942714697711	1.93077462651498	2.76561093116836
H	-2.27261860891433	-1.28454372310298	1.76474477724230
H	-0.35579562095741	2.40864904718472	0.55746840637506
C	-1.92712695057071	4.09886936798941	2.00708883727363
H	-3.63144579377619	2.49724414782134	3.42341421597644
C	-3.99420518257122	-0.22426208929278	3.57700389078633
H	-0.51440661651754	-1.36315059110528	0.49609519462338
F	-0.66623167392075	4.55361794806208	1.81783209202362
F	-2.69644963283647	4.64137034126701	1.02945016057227
F	-2.37135073477034	4.60547122448910	3.18483384135000
F	-4.42511753638856	-1.38064360025582	3.01592760225463
F	-5.08378715143259	0.50583998918453	3.90285754283656
F	-3.38800194033818	-0.56964310599454	4.75586608851426
C	2.32777564182790	-1.25454089002530	-1.99506124137681
H	1.10345453827245	-2.10914615026452	-0.49624267617254
C	1.81555994945966	-2.13504196598110	-3.15587551643064
C	3.69923882540818	-1.78021455313073	-1.50150453112744
H	2.43456295903309	-0.21087069683431	-2.36772601753995
C	2.82310811441994	-2.22848464040754	-4.30496807246753
H	0.85421421890095	-1.70549905142751	-3.50294664017508
H	1.58970409460187	-3.14736726235668	-2.75702983568424
C	4.17793923721719	-2.73479075801198	-3.80078259742109
H	2.95339823094919	-1.22592406472482	-4.77007577781119
H	2.43178977759732	-2.89318869090830	-5.10305751161586
C	4.70824010537642	-1.85618244726367	-2.65774416033969
H	3.53675964008834	-2.79598226386346	-1.08019652466915
N	4.23122622080617	-0.97761693375523	-0.31777749787616
H	4.92266125997829	-2.76225968421872	-4.62343564283538
H	5.67648980509766	-2.25858616357061	-2.29853396522090
H	4.90954636227544	-0.83495743922016	-3.05015387032656
C	4.35396152533453	0.49159488642165	-0.54270354479326
C	5.49437845310408	-1.54527880630345	0.23596929372043
H	3.36438148795047	0.91924443610525	-0.80789528743326
H	5.09105365174924	0.69337350150709	-1.34267079595735
H	4.69947036169791	0.95095696854697	0.40172712961195
H	5.36896411939590	-2.63301225899042	0.37889693096097
H	5.66714325795535	-1.08748284733376	1.22674291580154
H	6.34470189577947	-1.32299604833080	-0.43420191662047
H	4.07132821603384	-3.78092522971527	-3.43792827896873
H	2.59656720282164	-6.29559199515194	1.61387705701252
H	1.75729258377348	-6.90847511402573	0.16310676995070
C	2.26761539235087	-6.01995965746355	0.59175535128616
H	0.11860861724412	-5.89441695881059	2.07664877543386
C	1.31441627176660	-4.83434512344932	0.61919579187082
H	-2.70812552958627	-5.47528507007787	1.10087781160254

C	0.22342802321237	-4.91006725060850	1.59264532130817
H	3.15357425496525	-5.78383235593992	-0.02476811215182
O	1.47879510544074	-3.88987864307045	-0.17787924668766
C	-2.30240100935789	-4.82896772778008	1.90993985288735
C	-1.02450864962961	-4.17268655747668	1.41518318639816
H	3.53046908213451	-1.08858358693069	0.51594398406768
H	-3.05948013642215	-4.05733447972234	2.14482253365384
O	-1.08046495802364	-3.04130435859045	0.89145329247952
H	-2.12981388995354	-5.47177820890305	2.79503983213356
C	1.04462919800547	-3.86473790494142	3.33611604896656
C	1.38161790066919	-2.55667930588191	2.94142470432376
C	-0.00729679219630	-4.12816691249882	4.34525722706794
H	1.89296993010200	-4.56726168643989	3.34991177116262
N	2.57581029071824	-2.30749603039643	2.30300267494982
H	0.74085250871153	-1.67488217424221	3.04154474387953
O	3.43098413518849	-3.20867564271445	2.11097327486610
O	2.79426942782985	-1.09972624188455	1.90752168217249
C	-0.00147591651383	-5.36460600635236	5.03489925827866
C	-1.02208812513944	-3.19285946219354	4.65859397097659
C	-1.99771795330198	-3.48819637292531	5.62092864292232
C	-0.97454794990507	-5.65917036686830	5.99924076961731
C	-1.97922994007034	-4.72134512913396	6.29384844507811
H	0.78642572749960	-6.10107631497960	4.80814844689172
H	-1.06083504842359	-2.22004472169712	4.14815324767217
H	-2.77772300619941	-2.74327666441995	5.83596084795925
H	-0.94776691540638	-6.62508571084745	6.52651064784447
H	-2.74599467626236	-4.95021714037836	7.05002486625242

TS3R-cat

C	-4.92209807032201	-2.59777377882408	-1.42788698048522
C	-4.01446572724289	-2.86269668980159	-0.37338226678138
C	-4.30021102004739	-3.94187240848576	0.49815687656965
C	-5.44765456251217	-4.72683108785341	0.32610007491612
C	-6.34007116823472	-4.44850371292374	-0.72329953960056
C	-6.07072720742203	-3.38211826732286	-1.59832437276623
C	-2.77978166509434	-2.08077935582658	-0.16170636404903
C	-2.20505944599054	-1.28840712805484	-1.16534246420055
N	-0.89419722959305	-0.86926328157316	-1.09094790986694
O	-0.47010896705737	-0.03926287944838	-1.96823602607440
O	-0.11131683020634	-1.30652391989591	-0.19889517900618
C	-3.52582999182246	-0.62730476119248	1.42401131755194
C	-2.23358336853494	-0.10511693807037	1.84134241442418
O	-1.68697628931079	0.87839738236249	1.29472015305021
C	-4.47399985571735	0.14302888929240	0.61441999432758
O	-4.12746087590599	0.96405209266827	-0.25439275652248
N	-1.21333369165494	2.57771316275562	-2.05522209917483
C	-2.50531536011459	2.31730806305386	-2.75720966825465
C	-1.41868113142992	3.32001503924072	-0.73544304963223
C	-0.09025900007172	3.42341201197806	0.04773858402742
C	-0.34553042921390	4.07582539158246	1.42143380697454
C	-1.00953563262057	5.44969785381823	1.27566454291279
C	-2.30392454454562	5.35355331246400	0.46004763425843
C	-2.06043486897729	4.70158882604192	-0.91154202817979
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C	1.84989366164863	1.86679094740704	-0.15572285614045

N	2.16513031145478	0.53286193842529	-0.00802766626772
C	3.39955333476770	-0.12428789392718	-0.07504886761437
S	2.89901043786477	3.06133807031583	-0.73403678289420
C	-0.18754371670594	3.15727421191431	-2.97215632138179
H	0.63291879078755	4.06427095011097	-0.50410875579354
H	-0.98790033664185	3.39820964278158	2.02420570164639
H	0.62851346285486	4.15693039315432	1.94448614767468
H	-1.21504489304993	5.88316036192772	2.27642570607821
H	-0.30595855875744	6.14905210879850	0.77153241664051
H	-3.05152985030711	4.74922468679372	1.01890322406169
H	-2.75508389822831	6.35714085859469	0.31619603076318
H	-1.39383411348973	5.35733943633215	-1.51452295822192
H	-3.02187647819525	4.61857606134593	-1.45735226610560
H	-2.10781577228379	2.65015345476897	-0.17563115286487
H	1.34837326559941	-0.11272905421821	-0.02703027578832
H	-0.02140789289561	1.41894447733385	0.68499324529493
H	-0.08759486249694	2.48103668523008	-3.84053305826154
H	-0.51315347667403	4.15613236792034	-3.31538664494426
H	0.78911586127272	3.22480994657712	-2.45411275417486
H	-2.31076847719213	1.59837957041158	-3.57362855672765
H	-3.21856883312274	1.88464052710512	-2.02951218093785
H	-2.89974936921097	3.25895701793822	-3.17980379582315
H	-3.97338845337999	-1.37482063543263	2.09793547318586
H	-0.85076038386618	1.60560751326008	-1.80158881993461
H	-2.06812622215514	-2.50915062786225	0.55998925180981
H	-2.74620075485890	-0.87702544918878	-2.02144950520659
H	-3.59990211804839	-4.16501554067317	1.31901154273520
H	-5.64385450757169	-5.56543812868544	1.01166933587390
H	-7.24221908069705	-5.06385587371737	-0.86073985291950
H	-6.76322789870508	-3.16117067000327	-2.42515348530238
H	-4.73115178972639	-1.76558604658625	-2.12054854610839
C	3.37083931180983	-1.51184035354990	-0.34371146004909
C	4.55853691825426	-2.25514742721753	-0.37488186128974
C	5.79842789287749	-1.63634923696670	-0.15423098110400
C	5.82334807205971	-0.25719443546661	0.11254359223384
C	4.64462238045553	0.49994486046539	0.16303647034678
H	2.40581409866801	-2.00396026707494	-0.53498057926822
C	4.48832583931255	-3.75042257821131	-0.58313824407298
H	6.72846662387810	-2.21961170340134	-0.18512140979924
C	7.15901794071087	0.42482836705861	0.30988738286265
H	4.68409656645126	1.57324570285862	0.38235225723433
F	3.46291760161476	-4.10066293746913	-1.39775080093152
F	5.62805874823411	-4.24113690329343	-1.12631794077966
F	4.29716704085479	-4.40491228045772	0.59234734419809
F	7.04041841167108	1.60927269204036	0.95285937176003
F	8.00975945495588	-0.34845780581959	1.03163282650098
F	7.76877177273640	0.67272348908609	-0.87762922719277
C	-5.95015056311628	-0.12079221463529	0.87695527145658
C	-1.50403980267062	-0.82242042576020	2.96841025143251
H	-0.63633415038662	-1.36407790908419	2.53750215006658
H	-2.13679846101297	-1.54393826180177	3.51901054879232
H	-1.09683508929971	-0.07358066941524	3.67614450632825
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H	-6.23102313041159	0.28456013304006	1.87251707764605

H	-6.16881190943140	-1.20795436925295	0.90137846650220
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C	-2.26830943961812	3.22989718133004	-3.35945005951270
C	-1.66161194522430	3.43452023282870	-0.93141666980574
C	-0.58617879691711	3.14032849967732	0.14049445743744
C	-1.10792062369984	3.56409168283077	1.53088019585865
C	-1.51340323741958	5.04056494957760	1.56284763387233
C	-2.55055842319899	5.34282566071529	0.47703544132009
C	-2.04759131672769	4.92146847838087	-0.91322443313504
N	-0.16200288146867	1.75352647437773	0.13019970136880
C	1.15760221423292	1.36773464015702	0.17832337727229
N	1.29254381341304	0.02315799482050	0.42782013751715
C	2.38300981790124	-0.84753089546963	0.32113591016375
S	2.43058066883079	2.46487148907362	-0.02299502483563
C	0.11245695296697	3.39162064861769	-2.77017064200680
H	0.33173659372304	3.73509974403257	-0.07169455186250
H	-1.97266242970208	2.91930245717375	1.80309644274630
H	-0.30524325560701	3.35580497616264	2.26662048878448
H	-1.90992108344925	5.31039296232931	2.56372048571615
H	-0.61355369505128	5.67414867773731	1.40103552290064
H	-3.49313899652830	4.79641707469064	0.70336009887182
H	-2.81034811782180	6.42116928307201	0.46299292239415
H	-1.16483046287084	5.54239693651114	-1.18548533905195
H	-2.83413498047417	5.12946308364503	-1.66633919404020
H	-2.55244441909953	2.81049735396034	-0.69611879717117
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H	-0.91165682301310	1.05812565595688	0.32998672620916
H	0.33159463365871	2.88379237948998	-3.72662318605358
H	0.11607974241305	4.48912949290829	-2.91113605998504
H	0.88224920592264	3.09607337981498	-2.03068840090577
H	-2.03256604182631	2.61012726664429	-4.24342821368186
H	-3.26419780566393	2.93948890739321	-2.97773703125856
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C	2.16541123999265	-2.17208394970872	0.77169905020298
C	3.16938457963120	-3.14162342476590	0.65714972200605
C	4.42093118274271	-2.81927785988780	0.10923489828545
C	4.63767618064989	-1.50211924295996	-0.32656940207218
C	3.64219691949996	-0.51838453915869	-0.22934538231889
H	1.18960629557785	-2.42863980651729	1.21034059098198
C	2.89168543560253	-4.53249582162746	1.17472538205720
H	5.21074916096967	-3.57674424122829	0.02367469680254
C	5.95287544662937	-1.14776770930224	-0.98581161066214
H	3.82771887910808	0.50873609685441	-0.56829414687697
F	1.64475088850880	-4.96259240776985	0.80660387642623
F	3.77813806157027	-5.44194256772125	0.71129036869976
F	2.92576089561578	-4.58834975351045	2.52813890882710
F	6.29995050655791	0.14094036147663	-0.76761001789910
F	6.96732567460910	-1.92787650068363	-0.53407749612387
F	5.89388307900298	-1.32141040951590	-2.33172252327234
H	-0.17896983768029	-6.53399061037187	-0.90588488183117
H	-0.04001762002914	-4.07337340533287	-0.96627227490637
C	-1.02888452806139	-5.96007511867341	-1.30546507677020

O	0.50386487574698	0.13758722490291	-2.74063240134384
H	0.24696303763327	-2.14093898850252	-1.88339786221900
C	-0.94964985582752	-4.56164202103506	-1.34313657934448
C	-0.72334117877960	-1.66522695216729	-2.05976138618949
C	-2.18147347557960	-6.61804508973766	-1.76701163901200
H	-2.24167587019412	-7.71713927685176	-1.73824547685361
N	-0.61787187518003	-0.36956623108340	-2.50682448060588
C	-2.02441514693727	-3.78798287810490	-1.84007021884970
C	-1.97378651916592	-2.30386970721798	-1.90193125919762
O	-0.94265861684768	-1.51805651036023	1.19885293333783
C	-3.25722604373334	-5.86374492685551	-2.26516302698334
O	-1.69049778313152	0.33159488909414	-2.67588566046345
H	-1.19103877993609	-4.02579657530323	1.80379267777168
C	-3.17960183241983	-4.46428832950634	-2.29739245480817
C	-1.95308256951099	-2.19779521441975	0.92941962382308
H	-2.80073574056164	-1.83352493747717	-2.45561470184671
C	-2.16406006793741	-3.52230619491568	1.64243789328678
H	-4.16308464651084	-6.36911929021431	-2.63424497866382
H	-2.85315422433030	-4.19926741985324	1.10383533767385
C	-2.94484769347689	-1.78182617737501	-0.06012102589545
O	-2.71649852747785	0.59559391629454	0.26027914355963
H	-4.02644864636759	-3.87899306797140	-2.69106770675382
C	-3.35224660714481	-0.37508412761530	-0.19220481646529
H	-2.59934779585617	-3.31299748251369	2.64354446866537
H	-3.77642776367947	-2.48938621840367	-0.20253564985277
C	-4.65201729436205	-0.12430113929810	-0.94411027156289
H	-4.43416271875730	-0.15590612866281	-2.03447516142691
H	-5.03948278679047	0.88265472973277	-0.69983241295769
H	-5.42809547478654	-0.88605652730707	-0.73287942451543

Cat-PZ2S

C	0.58720341945945	-0.11207936543178	-0.61772651997910
S	0.87022870580427	1.41655529335504	-1.28473867914660
N	1.30171841508012	-1.22332005124343	-0.97966208003714
N	-0.39303710250917	-0.39966258605074	0.30874614618837
C	-1.21501824808116	0.43532136216146	1.07744288793559
C	-0.98495622607642	1.81210150705912	1.29668900446463
C	-2.32067750979993	-0.17741171120832	1.71416137903565
C	-3.15965422216225	0.56251848646261	2.55747503997131
C	-1.85311406683848	2.54152068993864	2.12274563648925
C	-2.94272224539472	1.93358300355889	2.76610240886457
H	-2.52282227731101	-1.24392873872353	1.53842393927431
H	-0.12802995814447	2.29861281813563	0.81534600141979
C	-1.63359019783736	4.02993671264043	2.28622498298221
H	-3.60618300817042	2.51536607535863	3.41962800652450
C	-4.25645613552401	-0.15207464217746	3.30884244409712
H	-0.54610837868534	-1.40548457319645	0.49951003272297
F	-0.32724430395924	4.36593731551373	2.17841552241119
F	-2.30585768032130	4.73438728560878	1.34067679466597
F	-2.07166030126697	4.47160854276077	3.49186034820820
F	-4.77886983494266	-1.18175499003431	2.60040753954191
F	-5.27169507903040	0.67326423875117	3.64665405070618
F	-3.78004859587409	-0.68589424218444	4.47536385138519
C	2.30662754640796	-1.25079126632004	-2.02594529176934
H	1.01948086640361	-2.14798826107258	-0.60865434692862

C	1.82043387865683	-2.09121190461367	-3.22659416904883
C	3.67015662018424	-1.78289780880495	-1.51188159523834
H	2.41640310869483	-0.19532204305466	-2.36125430304054
C	2.85216385259660	-2.14747303944466	-4.35611562530952
H	0.86666954411366	-1.64936323930086	-3.57995070995144
H	1.58630006868060	-3.11784512637593	-2.87095050150919
C	4.19322430368482	-2.67461679846048	-3.83738558675297
H	2.99616815021753	-1.12927890426661	-4.78106733008018
H	2.47643106097932	-2.78164383851567	-5.18584415276004
C	4.69767966452465	-1.83286048919355	-2.65679137515858
H	3.50876412380459	-2.81067113539242	-1.11980094241638
N	4.17904842900534	-1.01316331252093	-0.30613776009952
H	4.95655062067319	-2.67961007387083	-4.64360721423687
H	5.65831133371613	-2.24528098979947	-2.28925775420822
H	4.90858518945751	-0.80087232351036	-3.01431012189043
C	4.32100422139798	0.45385179619091	-0.49903576209340
C	5.42382431924972	-1.60279889880255	0.25535054698285
H	3.34488749684115	0.89874961301191	-0.78039899231796
H	5.08296365221674	0.67703686140335	-1.27153711932462
H	4.64041333683762	0.89348207397734	0.46427389852475
H	5.26727375455760	-2.68591186444857	0.40635917384221
H	5.60137287891593	-1.14250330327619	1.24493861711251
H	6.29176269172444	-1.40862390553115	-0.40320199696926
H	4.07479428750906	-3.73182387455070	-3.51104054538740
H	2.63578470587269	-6.15700415607883	1.50674167319329
H	1.67818603955213	-6.90439397318222	0.18777309715472
C	2.20453938323864	-5.97708289665847	0.50343375137657
H	0.15455080647877	-5.86248055025309	2.07419077053033
C	1.21550957041186	-4.83368594001227	0.52253175428128
H	-2.07694130705152	-6.16345274957652	0.81331402141890
C	0.25073495769157	-4.81239228409452	1.72914805041885
H	3.01365018503419	-5.76567136560619	-0.21806663166208
O	1.08289634096483	-4.07301156665781	-0.43592347356065
C	-2.27595774150698	-5.26563678116372	1.43609159290520
C	-1.12391514313326	-4.29582936033775	1.33410165788617
H	3.44331504279695	-1.14063240894917	0.57918380447860
H	-3.21955540165776	-4.78873548468994	1.11538388854585
O	-1.28944963598374	-3.13975877516027	0.94756385961168
H	-2.36940467498324	-5.62096793965911	2.48381124711669
C	0.83442258954342	-4.02008611058405	3.00354470745925
C	1.22909415028206	-2.61476709293803	2.72122007129270
C	-0.12855788147876	-4.16915560268185	4.17555660618255
H	1.76566606689542	-4.58163456238616	3.24118130044472
N	2.35701647353444	-2.39993010407167	2.04399576784203
H	0.69745187622574	-1.72370428421939	3.06897387834299
O	3.06050071140835	-3.37582091349094	1.59372140486825
O	2.76161116243278	-1.17056661181227	1.81678048847049
C	0.03170121390659	-5.24896892070849	5.06993199077163
C	-1.21055763801608	-3.28589715982101	4.38265583505373
C	-2.10659014553700	-3.48065089937823	5.44634168477907
C	-0.86103896830263	-5.44606125606170	6.13540036351902
C	-1.93578546812893	-4.56222549595762	6.32541310606775
H	0.87819560278822	-5.94171426182489	4.93150167223318
H	-1.36500227110365	-2.42998269314378	3.70924440900968

H	-2.94065591178328	-2.77574426343733	5.57915191336403
H	-0.71150677094371	-6.29198054240695	6.82443548915560
H	-2.63591808891425	-4.71258336750699	7.16172246975116
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C	0.700479	0.814644	-1.887989
S	1.437946	2.300608	-2.202899
N	1.205270	-0.370250	-2.366200
N	-0.409306	0.622163	-1.090752
C	-1.238993	1.564445	-0.470753
C	-1.473102	2.869930	-0.956534
C	-1.904661	1.146418	0.704368
C	-2.748690	2.022710	1.397575
C	-2.339384	3.726888	-0.259488
C	-2.974855	3.325754	0.926587
H	-1.748860	0.122982	1.073066
H	-0.967160	3.211377	-1.867583
C	-2.641610	5.088035	-0.846703
H	-3.634850	4.014621	1.469765
C	-3.334001	1.573617	2.714223
H	-0.513520	-0.341046	-0.689037
F	-1.551712	5.645845	-1.422122
F	-3.597883	5.005022	-1.808899
F	-3.098577	5.954932	0.090480
F	-3.652763	0.251679	2.706879
F	-4.450033	2.261054	3.045842
F	-2.444740	1.745251	3.734495
C	2.518942	-0.477393	-2.974372
H	0.749161	-1.251994	-2.050835
C	2.479398	-0.537460	-4.513884
C	3.319729	-1.687170	-2.434997
H	3.050867	0.467212	-2.712022
C	3.896041	-0.542049	-5.099569
H	1.906675	0.342985	-4.867762
H	1.918918	-1.444089	-4.834106
C	4.745484	-1.676439	-4.513296
H	4.383230	0.434610	-4.879656
H	3.855045	-0.624583	-6.205211
C	4.753814	-1.653541	-2.975244
H	2.828352	-2.623038	-2.784978
N	3.219498	-1.794124	-0.919533
H	5.787872	-1.623314	-4.889224
H	5.334667	-2.518097	-2.593584
H	5.264913	-0.732757	-2.618240
C	3.554919	-0.551151	-0.167984
C	3.932921	-2.974632	-0.350435
H	2.972495	0.302350	-0.558003
H	4.636258	-0.338046	-0.270431
H	3.295767	-0.712466	0.893824
H	3.693879	-3.865332	-0.959006
H	3.566416	-3.135423	0.682343
H	5.024778	-2.800309	-0.342601
H	4.342226	-2.655631	-4.855575
H	1.852628	-3.814931	5.774807
H	1.078875	-5.346338	5.296477

C	1.905251	-4.648184	5.042497
H	-0.183952	-3.307422	4.297545
C	1.705992	-4.135934	3.632687
H	0.093504	0.209341	3.242802
C	0.450578	-3.298077	3.387420
H	2.874945	-5.170681	5.132698
O	2.504863	-4.372052	2.733643
C	-0.131245	-0.791382	3.651684
C	0.815326	-1.825263	3.087572
H	2.158606	-2.064293	-0.795162
H	-0.029363	-0.763252	4.758386
O	1.819943	-1.528757	2.454079
H	-1.187408	-1.053857	3.436883
C	-0.459562	-3.901158	2.219280
C	0.213337	-3.884727	0.889999
C	-0.992177	-5.270010	2.631015
H	-1.323116	-3.208478	2.147982
N	0.117112	-2.817022	0.108340
H	0.854362	-4.686198	0.513378
O	-0.598867	-1.792276	0.403698
O	0.805677	-2.784340	-1.026340
C	-2.270796	-5.362654	3.220422
C	-0.242736	-6.455508	2.468501
C	-0.759344	-7.692688	2.885650
C	-2.788541	-6.598300	3.638107
C	-2.032407	-7.769371	3.472639
H	-2.873819	-4.448788	3.346876
H	0.756702	-6.417560	2.010963
H	-0.161199	-8.606251	2.745581
H	-3.791563	-6.645891	4.088456
H	-2.436005	-8.740678	3.796399

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C	0.63093231986939	-0.16647060622661	-0.25797750387319
S	1.45372450197897	1.27962040888660	0.03316038593482
N	1.14805049542158	-1.17026800070715	-1.03728390660790
N	-0.59236085635178	-0.52663167791255	0.27104476044408
C	-1.54759337367856	0.16209195443216	1.02674868401620
C	-1.52132390620816	1.54499632433341	1.31213491268658
C	-2.62368761302485	-0.61635177043933	1.51890482342714
C	-3.62637959740516	-0.03217685156948	2.30190861088794
C	-2.54830004807088	2.11496691947347	2.08090057861708
C	-3.60184251022244	1.34164990117406	2.59187191418942
H	-2.67199869222078	-1.69057406248040	1.28250918422221
H	-0.68740311994224	2.15521517797161	0.94242298589072
C	-2.54450303523753	3.61208146342292	2.31010848749558
H	-4.39118032196523	1.80012643851353	3.20171522192930
C	-4.69957390242461	-0.91481198962937	2.89745182551746
H	-0.79401409932645	-1.54152581640447	0.16836435229110
F	-1.28841036539545	4.10476090171713	2.40767768983672
F	-3.15194661639158	4.26530425054173	1.28794252570281
F	-3.20672135432490	3.94696560012984	3.44469927573885
F	-5.05500191076540	-1.91775588987558	2.06304753072883
F	-5.81465416789972	-0.22024247499291	3.21308378278507
F	-4.26023096944245	-1.50258150426592	4.05103849192665

C	2.40103529465217	-1.12076523257086	-1.76563906476070
H	0.51953635642119	-1.95919986496944	-1.24850925990840
C	2.13195730065020	-0.98946986056497	-3.28103093771642
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