

**Electronic Supplementary Information for:**

**Theoretical study on the mechanism of a ring-opening reaction of oxirane by active-site aspartic dyad of HIV-1 Protease**

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**Table 1S**

Total energies ( $E_0$ ),  $ZPE$ , thermal ( $G_{\text{gas}}$ ) and solvation ( $G_{\text{sol}}$ , aqueous solution) corrections to Gibbs free energies (in *a.u.*).

Structure	B3LYP			
	$E_0$	$ZPE$	$G_{\text{gas}}$	$G_{\text{sol}}$
<b>1A</b>	-3156.81447509	0.967092158	0.861897523	-0.1569086
<b>TSA</b>	-3156.80016454	0.963562334	0.867462992	-0.1529509
<b>2A</b>	-3156.85678871	0.970492901	0.869680532	-0.1514033

  

	$E_0$ (MPW1K)	$E_0$ (M05-2X)	$E_0$ (LMP2)
<b>1A</b>	-3157.00201461	-3156.41607400	-3147.59590035
<b>TSA</b>	-3156.98302742	-3156.40294722	-3147.57134124
<b>2A</b>	-3157.04917370	-3156.46741768	-3147.63631472

Gaussian inputs with Cartesian coordinates of the B3LYP optimized structures from the  
reaction path **1A** → **TSA** → **2A**:

# b3lyp/6-31+G(d,p) opt=(modredundant) freq=normal

Starting complex **1A**

```
-1 1
C      0.00000000  0.00000000  0.00000000
H      1.09390000  0.00000000  0.00000000
C     -0.49409634  1.43903824  0.00000000
O     -0.09502247  2.26170308 -0.82002307
N     -1.44536627  1.73243597  0.94587607
H     -1.62604852  1.06950761  1.68872297
C     -2.06212566  3.04824368  1.08470682
H     -1.73090504  3.63302912  0.22427313
C     -3.58921638  2.87605109  1.05801142
H     -3.88160133  2.40087659  0.11720396
H     -3.89169882  2.19233359  1.86105724
C     -4.40374508  4.14171084  1.23940714
O     -3.94126319  5.20911907  1.62711398
O     -5.67995999  3.94667079  0.95915706
C     -1.56973123  3.67367603  2.40501776
O     -1.78205515  3.10377167  3.48368103
N     -0.88744007  4.83111244  2.28864894
H     -0.87647318  5.30644478  1.39495426
C     -0.29288092  5.56585030  3.39511481
H      0.31421246  4.87860650  3.99302926
C      0.63101934  6.66921176  2.79815101
H      0.79371609  7.41447896  3.58344943
C      1.97199452  6.10713302  2.33038630
H      1.83575130  5.34021865  1.56091496
H      2.57996425  6.90832771  1.90094382
H      2.51620949  5.66547396  3.17247104
O     -0.03449256  7.28287819  1.68355860
H     -0.32445450  8.19691111  1.91001386
C     -1.28336365  6.16372931  4.41152253
O     -0.85007000  6.57089664  5.49009100
N     -2.59239412  6.19465544  4.05715684
H     -2.87335472  5.88425842  3.13044197
C     -3.62096444  6.63782873  4.97115896
H     -3.13533604  7.13771761  5.81417415
H     -4.28205001  7.36498428  4.48934891
C     -4.52403442  5.54153848  5.54262490
O     -5.52411279  5.87399462  6.19866615
N     -4.19038471  4.25287606  5.31426686
H     -3.33064805  4.03403544  4.81498171
C     -5.04478734  3.13922605  5.75160866
H     -6.07547686  3.50736951  5.69173622
C     -4.86786610  1.93268480  4.83653366
H     -3.82718350  1.59860434  4.82111956
H     -5.48075932  1.10274627  5.19677771
H     -5.18307954  2.18772697  3.82034038
C     -4.77547110  2.77020611  7.23411489
O     -4.27218423  1.69866481  7.57191480
N     -5.17202434  3.71833167  8.11918729
H     -5.50140465  4.60504747  7.74185154
C     -4.94756024  3.56562871  9.54568372
H     -3.88184802  3.62689572  9.79892715
C     -0.09191821  12.16174465  1.85001165
H     -0.37127277  12.47665247  2.85956231
C     -0.83878599  10.87804341  1.52643841
O     -0.67905218  9.86587145  2.23038393
N     -1.68443995  10.93426631  0.47781014
H     -1.67088990  11.75750139 -0.11130289
C     -2.55717252  9.84374670  0.02179772
H     -2.58749378  9.10794277  0.82756677
C     -3.96241289  10.41377932 -0.23711708
H     -4.26588830  11.01138383  0.62714632
H     -3.91368150  11.09099889 -1.09976634
C     -5.08680436  9.39506647 -0.52705850
O     -4.73951008  8.23978791 -0.96210781
O     -6.25364125  9.78557580 -0.33466490
C     -1.93117220  9.25036771 -1.25555527
O     -1.69999406  9.97175646 -2.22676062
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N	-1.63457598	7.92740759	-1.19849206
H	-1.91682789	7.42895388	-0.36639724
C	-1.10726912	7.16402522	-2.31839532
H	-0.85236405	7.89522382	-3.09062130
C	0.19651979	6.39244821	-1.90682588
H	-0.10240653	5.48607298	-1.35429096
C	1.03302315	5.97480703	-3.10906004
H	1.38221477	6.87054314	-3.63780373
H	1.90826072	5.41594880	-2.76106621
H	0.44864219	5.35781963	-3.79388074
O	1.03775500	7.20434826	-1.09561036
H	0.64697917	7.31403128	-0.20954657
C	-2.15834085	6.19553944	-2.91458779
O	-1.85701346	5.43173499	-3.83294620
N	-3.38377289	6.21311551	-2.32477475
H	-3.64278028	6.98852931	-1.70948064
C	-4.43730885	5.30698909	-2.75201160
H	-3.98339799	4.49359713	-3.31829462
H	-4.93394600	4.89317616	-1.86435512
C	-5.52986257	5.90476185	-3.65293917
O	-5.93398527	5.25656687	-4.63493353
N	-6.04225001	7.10455881	-3.30433260
H	-5.66992458	7.60277198	-2.48307172
C	-7.14617955	7.72190608	-4.05635267
H	-7.75624257	6.89362470	-4.43881745
C	-7.98941292	8.61608310	-3.15170571
H	-7.39115444	9.39082228	-2.66560242
H	-8.76876690	9.10723456	-3.74087451
H	-8.46234596	8.01227513	-2.36934414
C	-6.60560725	8.49098032	-5.29176845
O	-6.70811975	9.71178602	-5.42476445
N	-6.02003136	7.69389068	-6.22435483
H	-5.93020264	6.70236130	-6.00765802
C	-5.33442312	8.25113748	-7.37750470
H	-4.98857384	7.42945283	-8.00968587
H	-5.48415483	4.35842412	10.07187708
H	-5.31691335	2.59324925	9.88399558
H	-0.33100251	-0.47591563	-0.93002068
H	-0.36212332	-0.58679453	0.84933791
H	-6.00878161	8.89086491	-7.95649818
H	-4.47089538	8.85861714	-7.07931563
H	0.98131773	11.95377920	1.85111156
H	-0.30169727	12.97539746	1.15022304
H	-6.25068922	4.76300135	1.16349693
C	-7.30670734	7.17754795	0.85995396
C	-6.87128175	7.05313627	2.25236480
H	-6.55694026	7.29702299	0.08246317
H	-5.80531814	7.06189160	2.46602054
O	-7.31845991	5.87208921	1.53135359
H	-8.30205426	7.55711373	0.64466682
H	-7.53164203	7.34176511	3.06678112

1 F  
50 F  
52 F  
101 F

# b3lyp/6-31+G(d,p) opt=(modredundant,calcfc,noeigentest) freq=noraman

Transition state **TSA**

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-1 1
C      0.00000000  0.00000000  0.00000000
H      1.09400000  0.00000000  0.00000000
C     -0.61062833  1.39435500  0.00000000
O     -1.82686788  1.57098233  0.01584212
N      0.28709715  2.42530348  0.01402135
H      1.26117218  2.22118945 -0.15982166
C     -0.10132540  3.83456550 -0.00210626
H     -1.08298863  3.89778219  0.47202975
C      0.93667938  4.63156886  0.79666401
H      0.98888550  4.23715082  1.81650568
H      1.92862485  4.48758993  0.35211200
C      0.69227234  6.13819512  0.87241189
O     -0.22222565  6.67097601  0.21317175
O      1.51092830  6.75497785  1.65104230
C     -0.18279592  4.31436435 -1.46466210
O      0.82946286  4.35464196 -2.17520319
N     -1.41239625  4.65081693 -1.91407901
H     -2.17783305  4.68891063 -1.25500995
C     -1.67853901  5.08832012 -3.27427405
H     -1.14674907  4.41934163 -3.95920491
C     -3.19319463  4.98290921 -3.57182191
H     -3.36591415  5.51907717 -4.50977004
C     -3.66056000  3.53512173 -3.70300892
H     -3.47705642  2.96913632 -2.78424011
H     -4.73344943  3.50710501 -3.91192727
H     -3.13310261  3.03804627 -4.52448621
O     -3.93485868  5.62566647 -2.51397194
H     -4.36482012  6.44697353 -2.84715339
C     -1.13265211  6.48310224 -3.63870866
O     -1.17497842  6.84045560 -4.81698327
N     -0.59823441  7.22567541 -2.63771415
H     -0.62720925  6.89549360 -1.67243451
C      0.08672480  8.47119731 -2.90579684
H     -0.14981648  8.77890381 -3.92778078
H     -0.26342596  9.25840480 -2.23111817
C      1.61300090  8.43376752 -2.78010717
O      2.24325035  9.50080333 -2.86247350
N      2.21383444  7.23965398 -2.58790375
H      1.65662302  6.38772418 -2.57182087
C      3.66066581  7.12568757 -2.35113189
H      3.95292577  8.04089133 -1.82389096
C      3.97404318  5.90843325 -1.48935318
H      3.61357835  4.99010220 -1.95963351
H      5.05520811  5.81683868 -1.36188134
H      3.51076547  6.02300881 -0.50571143
C      4.44615694  7.09821304 -3.68730886
O      5.06081695  6.10659072 -4.08191855
N      4.41868289  8.27334569 -4.36516285
H      3.81606993  9.01027120 -4.00302935
C      5.04820688  8.41025661 -5.66574614
H      4.52475465  7.82861178 -6.43485920
C     -7.27747203  9.22663075 -3.63745309
H     -7.87269746  9.95489209 -3.08068464
C     -6.11681576  8.65980533 -2.83887189
O     -5.34427796  7.83401547 -3.35032636
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H     -6.73325048  9.68242789 -1.18964309
C     -4.95914068  8.69176030 -0.62470455
H     -4.15704151  8.23533240 -1.20846348
C     -4.41937468  9.91287099  0.14144547
H     -4.14106873  10.69135648 -0.57304696
H     -5.21889363  10.30098432  0.78605535
C     -3.21081363  9.59029431  1.03441025
O     -3.26599761  8.53431566  1.72964695
O     -2.25232675  10.41431429  1.01214805
C     -5.62440335  7.66289523  0.31519751
O     -6.60478623  7.98470219  0.98393202
N     -5.08442328  6.41829063  0.29156444
H     -4.31979593  6.24944098 -0.35030086
C     -5.59116512  5.30429226  1.07977940
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H	-6.61550694	5.55687474	1.36691958
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H	-4.57384783	3.63352025	0.12376863
C	-6.47282323	2.90073459	0.82185553
H	-7.51838107	3.22799102	0.84398427
H	-6.40532435	2.00504835	0.19715971
H	-6.15526690	2.66892201	1.83869227
O	-6.13699320	4.26263200	-1.08458223
H	-5.46515193	4.71874114	-1.62133295
C	-4.79112485	5.08715205	2.38639046
O	-5.16207666	4.26300652	3.22291371
N	-3.64319520	5.80967738	2.50991641
H	-3.50450163	6.62442155	1.91400261
C	-2.78595511	5.65559346	3.67043291
H	-2.89162965	4.64009771	4.05271204
H	-1.74557520	5.81088646	3.36055343
C	-3.05568310	6.58948970	4.85945194
O	-2.87895754	6.17379883	6.01661659
N	-3.44085050	7.85326088	4.58337483
H	-3.51890299	8.15575414	3.60892703
C	-3.62706560	8.86059367	5.63611972
H	-2.89375984	8.63274641	6.41926627
C	-3.38557161	10.26087379	5.08330300
H	-4.10432185	10.50431177	4.29709099
H	-3.50599012	11.00085625	5.87796116
H	-2.37351549	10.33562296	4.67572979
C	-5.03504636	8.73938957	6.27768323
O	-5.87669260	9.63651760	6.20973534
N	-5.24662566	7.56958295	6.93041987
H	-4.51388597	6.86414436	6.88159543
C	-6.54990894	7.22579565	7.47038930
H	-7.29644178	7.10629984	6.67607133
H	5.03977876	9.46469813	-5.95108771
H	6.08212221	8.05573823	-5.62410182
H	-0.35935375	-0.54224279	-0.87933843
H	-0.35700883	-0.53296030	0.88594382
H	-6.46339922	6.28603831	8.01998425
H	-6.90247870	8.00919249	8.14823623
H	-6.87964053	9.70131632	-4.53912982
H	-7.92142873	8.40082430	-3.95365029
H	1.35210235	7.97913842	1.80350100
C	-0.44995978	9.58368226	1.89972889
C	0.61046755	9.82474377	0.93865922
H	-0.97343422	8.64025942	1.88673394
H	0.57523837	9.25567344	0.01178431
O	1.25897043	9.13178435	2.02380453
H	-0.58145085	10.26203144	2.72780783
H	0.98142375	10.84059053	0.81243596

1 F  
50 F  
52 F  
101 F

# b3lyp/6-31+G(d,p) opt=(modredundant) freq

covalent intermediate **2A**

-1 1  
C 0.00000000 0.00000000 0.00000000  
H 1.09410000 0.00000000 0.00000000  
C -0.61029556 1.39624703 0.00000000  
O -1.82908774 1.56358163 -0.06420556  
N 0.28083716 2.42132373 0.08925068  
H 1.27444088 2.23258825 0.08147056  
C -0.09048789 3.83532639 0.15218779  
H -1.15188665 3.89327825 -0.10006309  
C 0.14611205 4.37146265 1.58259893  
H -0.32502319 3.68070240 2.28560648  
H 1.22613242 4.36864465 1.77991201  
C -0.37739184 5.78761320 1.86501230  
O -0.20301879 6.66790768 0.95565130  
O -0.92328974 5.98655788 2.97459454  
C 0.77710018 4.54122850 -0.90173222  
O 1.99512188 4.35267127 -0.92219245  
N 0.12518896 5.30439797 -1.82402594  
H -0.85783524 5.49997845 -1.67170345  
C 0.84393543 6.08303510 -2.82211924  
H 1.90614454 5.88219359 -2.63502863  
C 0.55382264 5.63734764 -4.27079570  
H 1.09218400 6.33081014 -4.92256281  
C 1.00214529 4.20501977 -4.53598334  
H 0.45920221 3.50003161 -3.89852458  
H 0.81627746 3.94070032 -5.58106974  
H 2.07125505 4.09107170 -4.33063166  
O -0.85770070 5.73469583 -4.58108179  
H -1.04044798 6.54234492 -5.10558004  
C 0.67314593 7.61103481 -2.64485354  
O 0.80368730 8.36586088 -3.61344765  
N 0.44272796 8.02571334 -1.37614573  
H 0.26976013 7.33461617 -0.63725210  
C 0.33246767 9.43886927 -1.04464082  
H 0.66925900 10.01637208 -1.90453543  
H -0.71717715 9.70413264 -0.84498631  
C 1.14968319 9.91421161 0.16771523  
O 1.75896823 10.99672002 0.09539805  
N 1.10602197 9.16803866 1.28914954  
H 0.60187020 8.26848693 1.29248510  
C 1.69303502 9.62800811 2.55790667  
H 1.58733299 10.71956397 2.56706043  
C 0.95106876 9.02010290 3.74334218  
H 1.02725253 7.93077422 3.74814476  
H 1.38782275 9.38619346 4.67612901  
H -0.10748835 9.29097217 3.71621881  
C 3.21125185 9.31997166 2.62012674  
O 3.70003647 8.51055469 3.40866160  
N 3.96114081 10.04355630 1.74856833  
H 3.46754937 10.62264394 1.07214198  
C 5.39153389 9.82718640 1.63142882  
H 5.62082127 8.82938914 1.23714930  
C -3.53676385 9.37881280 -7.13157506  
H -4.40954763 9.98441475 -6.87439079  
C -3.02415737 8.53433519 -5.97518889  
O -2.00253810 7.85175365 -6.08761201  
N -3.75270432 8.59801217 -4.82109172  
H -4.67044654 9.02129327 -4.86487396  
C -3.49141179 7.73206250 -3.67210143  
H -2.43936074 7.45625454 -3.71626931  
C -3.76640755 8.48203690 -2.36565762  
H -3.15100618 9.38677138 -2.31875665  
H -4.81374970 8.80011946 -2.31835783  
C -3.48193103 7.63234432 -1.13798029  
O -3.07854521 6.47712664 -1.18694095  
O -3.74016691 8.30361016 -0.01958031  
C -4.38625077 6.48054124 -3.79347945  
O -5.61788282 6.58487602 -3.72043169  
N -3.73052293 5.32326132 -3.99217573  
H -2.71410096 5.36765601 -4.01725130  
C -4.38449383 4.04460704 -4.25478817

H	-5.04686312	4.14657162	-5.12050012
C	-3.27856099	3.00036189	-4.59948627
H	-2.63871395	2.88365999	-3.71063398
C	-3.84532693	1.64304686	-4.99368434
H	-4.45631992	1.73922682	-5.89690362
H	-3.01501306	0.96476367	-5.20925744
H	-4.46540028	1.21808490	-4.20285214
O	-2.49754184	3.45846032	-5.70255894
H	-1.86836946	4.14556370	-5.41984352
C	-5.28821287	3.57988387	-3.09514172
O	-6.22415975	2.81166733	-3.30791189
N	-4.97211830	4.04638352	-1.85528935
H	-4.19587832	4.68968715	-1.74569582
C	-5.72948989	3.67130983	-0.67928287
H	-6.22335400	2.71616014	-0.87533464
H	-5.05329464	3.53000481	0.16838165
C	-6.81563453	4.65012533	-0.22186180
O	-7.40203552	4.43236961	0.84926306
N	-7.09359415	5.71624820	-1.00649371
H	-6.63903312	5.81023888	-1.91239682
C	-8.05378947	6.75209025	-0.59911651
H	-7.96977712	6.82920652	0.49093441
C	-7.70548004	8.08924440	-1.24340254
H	-7.71636997	8.01493267	-2.33351834
H	-8.44042355	8.84332378	-0.95261037
H	-6.71560573	8.41484343	-0.91028074
C	-9.51732509	6.34029112	-0.91235804
O	-10.20371385	6.91840857	-1.75629422
N	-9.97986810	5.31978551	-0.14840158
H	-9.31069005	4.84835828	0.45815471
C	-11.31546095	4.77851242	-0.33157493
H	-11.40941545	4.24032342	-1.28285520
H	5.80659670	10.58021046	0.95729797
H	5.87157149	9.91656728	2.61074871
H	-0.36051672	-0.54170991	-0.87881757
H	-0.35617156	-0.53368221	0.88609318
H	-11.53023048	4.09046053	0.48900991
H	-12.05280228	5.58628701	-0.32880740
H	-2.72882785	10.03391522	-7.46732682
H	-3.79216159	8.71331929	-7.96120679
H	-1.94692574	7.35612162	3.35204057
C	-3.50924809	7.65042423	1.27238743
C	-2.84741415	8.66426282	2.20371088
H	-2.86614419	6.78587487	1.12166990
H	-1.91977140	9.01992918	1.73033932
O	-2.60872186	8.08597829	3.46779524
H	-4.48487716	7.33646231	1.65301943
H	-3.50709742	9.52734825	2.35053037

1 F  
50 F  
52 F  
101 F

A Jaguar input with Cartesian coordinates of the **TSA** transition state optimized at the M05-2X/6-31+G(d,p) level.

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iguess=1
maxitg=300
basis=6-31g**+
ip11=2
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igeopt=2
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dftname=m05-2x
ip24=2
itrvec= -2
&
&zmat
C1      -2.1343999971#      1.0193000042#      6.6135999792#
H2      -3.0204694744      0.4169256783      6.8109005515
C3      -1.5919402695      0.8437310853      5.1964672011
O4      -0.5818466646      1.4272185916      4.8145527353
N5      -2.2812508128      -0.0213628150      4.4031272910
H6      -3.1719725652      -0.3673997202      4.7198225954
C7      -1.8969349954      -0.3479588820      3.0304230348
H8      -0.8122315039      -0.2657999781      2.9692437902
C9      -2.3544681538      -1.7735745603      2.7306739554
H10     -1.8981042235      -2.4680523324      3.4365115792
H11     -3.4402257937      -1.8357550177      2.8528661915
C12     -2.0423830261      -2.2306025494      1.3111508747
O13     -1.7213192429      -1.3801169808      0.4596461720
O14     -2.1628381227      -3.4863129664      1.1063454883
C15     -2.5595818620      0.6539328252      2.0746887571
O16     -3.7818606184      0.6510391671      1.9014867441
N17     -1.7375531719      1.5560328226      1.5017017109
H18     -0.7409971885      1.4479194262      1.6122276066
C19     -2.2241038647      2.6432777481      0.6765655452
H20     -3.1550990294      3.0043494661      1.1209929926
C21     -1.2149627060      3.7985118345      0.6796368706
H22     -1.5760511831      4.5268328990      -0.0470233784
C23     -1.0700131174      4.4230985880      2.0583151832
H24     -0.7076706160      3.6890693875      2.7808560264
H25     -0.3560936652      5.2459289128      2.0124468610
H26     -2.0299932996      4.8090276845      2.4074138401
O27     0.0769121840      3.3144532596      0.2586643955
H28     0.3522715737      3.7976960762      -0.5453520381
C29     -2.6421090330      2.2462390632      -0.7487616557
O30     -3.1271299917      3.1084412504      -1.4809494244
N31     -2.5128767160      0.9453626067      -1.0779900187
H32     -2.0326583310      0.3036396509      -0.4515523012
C33     -3.0801058619      0.4080048162      -2.2958354014
H34     -3.3693001728      1.2384908989      -2.9386079813
H35     -2.3438559140      -0.2037484075      -2.8213077033
C36     -4.3110826163      -0.4741633677      -2.0947994183
O37     -4.8019168805      -1.0513783445      -3.0769294807
N38     -4.8006236810      -0.6098422385      -0.8499575495
H39     -4.3684040259      -0.1055711243      -0.0815276048
C40     -5.8400118530      -1.5921946864      -0.5301743617
H41     -5.7074792993      -2.4173810027      -1.2347536341
C42     -5.6745339209      -2.0803394862      0.8991934249
H43     -5.6805767868      -1.2368421397      1.5899106795
H44     -6.5034946391      -2.7373993542      1.1573207240
H45     -4.7361066814      -2.6283378918      0.9897872611
C46     -7.2537270468      -1.0252124085      -0.7665402708
O47     -8.0692639831      -0.8631018059      0.1387582992
N48     -7.5305664513      -0.7629943010      -2.0612031942
H49     -6.7867043852      -0.8872139661      -2.7388495142
C50     -8.8233999812#      -0.2272999962#      -2.4426999948#
H51     -8.9874146888      0.7529088330      -1.9916266227
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H53     2.9721077557      4.8228450649      -4.7772559272
C54     1.7856336284      4.2608693900      -3.0128739386
O55     1.0420390044      4.6270182607      -2.0952201730
N56     2.1523716776      2.9682815601      -3.1838096455
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H59	0.8145118531	2.2090187425	-1.7989279263
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H61	0.5824285619	1.0042496231	-3.9966281080
H62	2.1613166061	0.2533750777	-3.7137672793
C63	0.6223623925	-0.4530629010	-2.4125920351
O64	0.8229805939	-0.4654121428	-1.1748640963
O65	-0.0641612555	-1.2920299239	-3.0697107965
C66	2.8083677261	1.4631945864	-1.3711494793
O67	3.8567813613	0.9634008940	-1.7893465150
N68	2.5789840736	1.7403419712	-0.0734963499
H69	1.6358457149	2.0158019402	0.1722534032
C70	3.5368602277	1.4780379776	0.9947126401
H71	4.5033866242	1.9023269503	0.7177565430
C72	3.0336381371	2.1938704614	2.2706877722
H73	2.0563784101	1.7713674607	2.5430791359
C74	3.9858967653	2.0624765069	3.4432764824
H75	4.9544529221	2.4881494668	3.1762239210
H76	3.5715008235	2.6218618405	4.2815890906
H77	4.1323186856	1.0228170841	3.7244445724
O78	2.8965946094	3.5906365508	2.0136651267
H79	2.1178122648	3.7398954925	1.4611062776
C80	3.7868272248	-0.0227801406	1.2267638863
O81	4.7665722572	-0.4062484446	1.8654886519
N82	2.8833507656	-0.8653241445	0.6816117491
H83	2.1351362438	-0.5226700459	0.0812075894
C84	3.1046187991	-2.2911366633	0.7177751208
H85	3.3854285261	-2.6066039459	1.7218684846
H86	2.1816138984	-2.7965122193	0.4350396370
C87	4.2189374612	-2.7973874370	-0.1946480468
O88	4.5749482416	-3.9800141898	-0.0983981506
N89	4.7719264585	-1.9206961072	-1.0488423821
H90	4.4464071080	-0.9592547529	-1.0639555511
C91	5.9636446798	-2.2344696713	-1.8398839875
H92	5.8768453472	-3.2785934410	-2.1473059043
C93	6.0482977828	-1.3084761684	-3.0403016486
H94	6.1194267529	-0.2724159989	-2.7117165569
H95	6.9375386375	-1.5435364695	-3.6241029915
H96	5.1590702472	-1.4271837071	-3.6602646612
C97	7.2048093759	-2.0930643527	-0.9320817486
O98	8.0260615171	-1.1886034279	-1.0567528148
N99	7.2768849370	-3.0496905628	0.0214217082
H100	6.4783721807	-3.6687885652	0.1056100013
C101	8.1583999932#	-2.8908999984#	1.1619999978#
H102	7.8748931885	-2.0187373019	1.7553175315
H103	-8.8562535658	-0.1382578887	-3.5265465691
H104	-9.6197264590	-0.8916616967	-2.1055148189
H105	-2.3655873021	2.0735036198	6.7626362531
H106	-1.3419818103	0.7445729389	7.3084421257
H107	8.0937088584	-3.7861635356	1.7771250724
H108	9.1848773496	-2.7586964731	0.8218933448
H109	1.4435111082	5.7081390766	-4.5392550232
H110	2.8288337061	6.0618146307	-3.5022183293
H111	-1.8238899350	-3.9142146171	-0.1237939270
C112	-0.5923289577	-2.9468213881	-1.8754313991
C113	-2.0043464965	-3.2183979688	-2.0606217385
H114	-0.3017811411	-2.3499366862	-1.0276102204
H115	-2.6939391134	-2.5158939157	-1.6040654300
O116	-1.5640383065	-4.2453385373	-1.1431754198
H117	0.1260004854	-3.5111421428	-2.4427509406
H118	-2.3403349401	-3.6271156365	-3.0063537817

&