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Supporting Information

Absolute Configuration of Remisporine B

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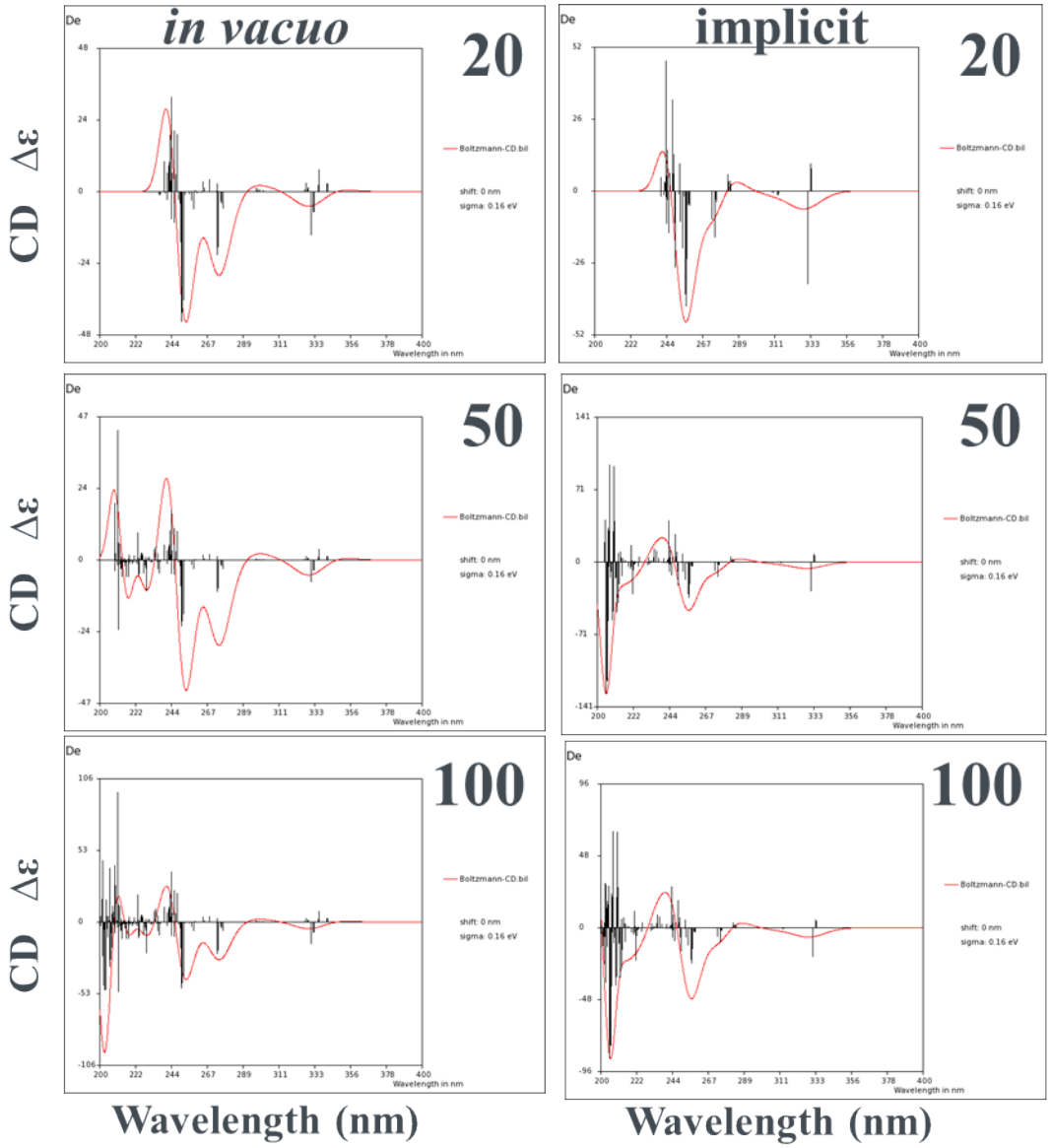
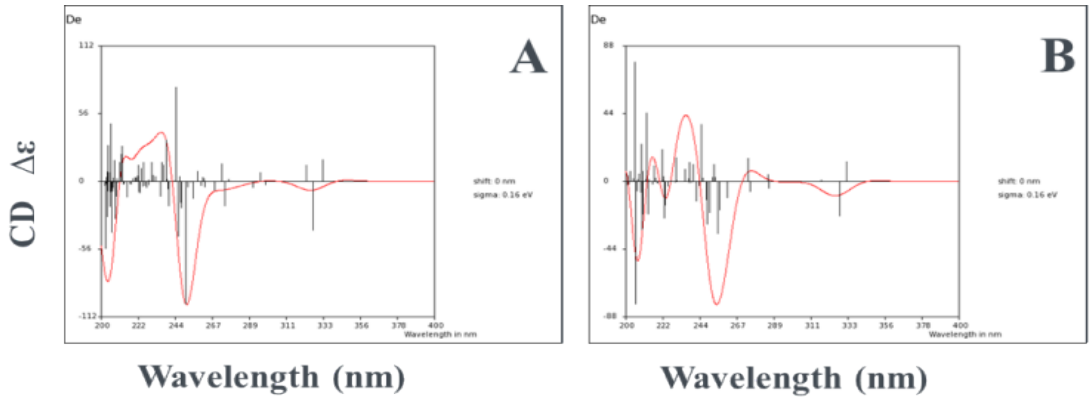
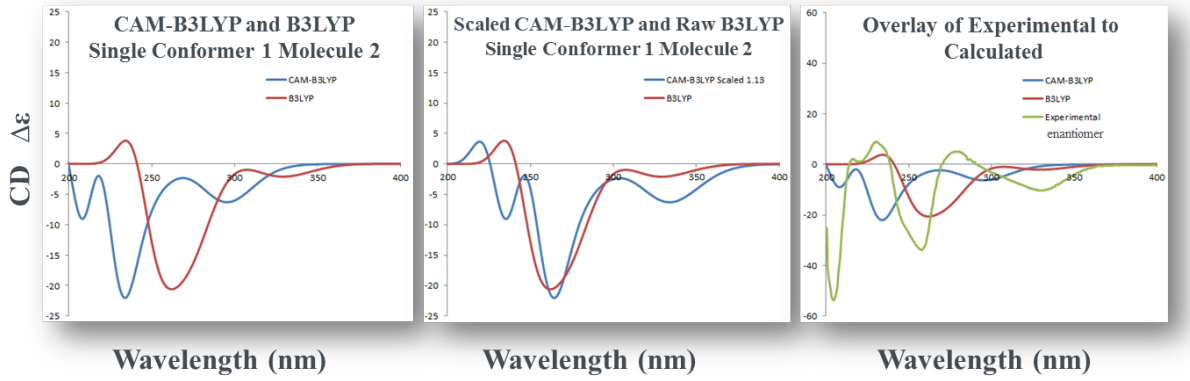


S1: Calculated ECD (σ=0.16) for the Boltzmann weighted *in vacuo* and implicit methanol **2** (NSTATES=20,50,100).



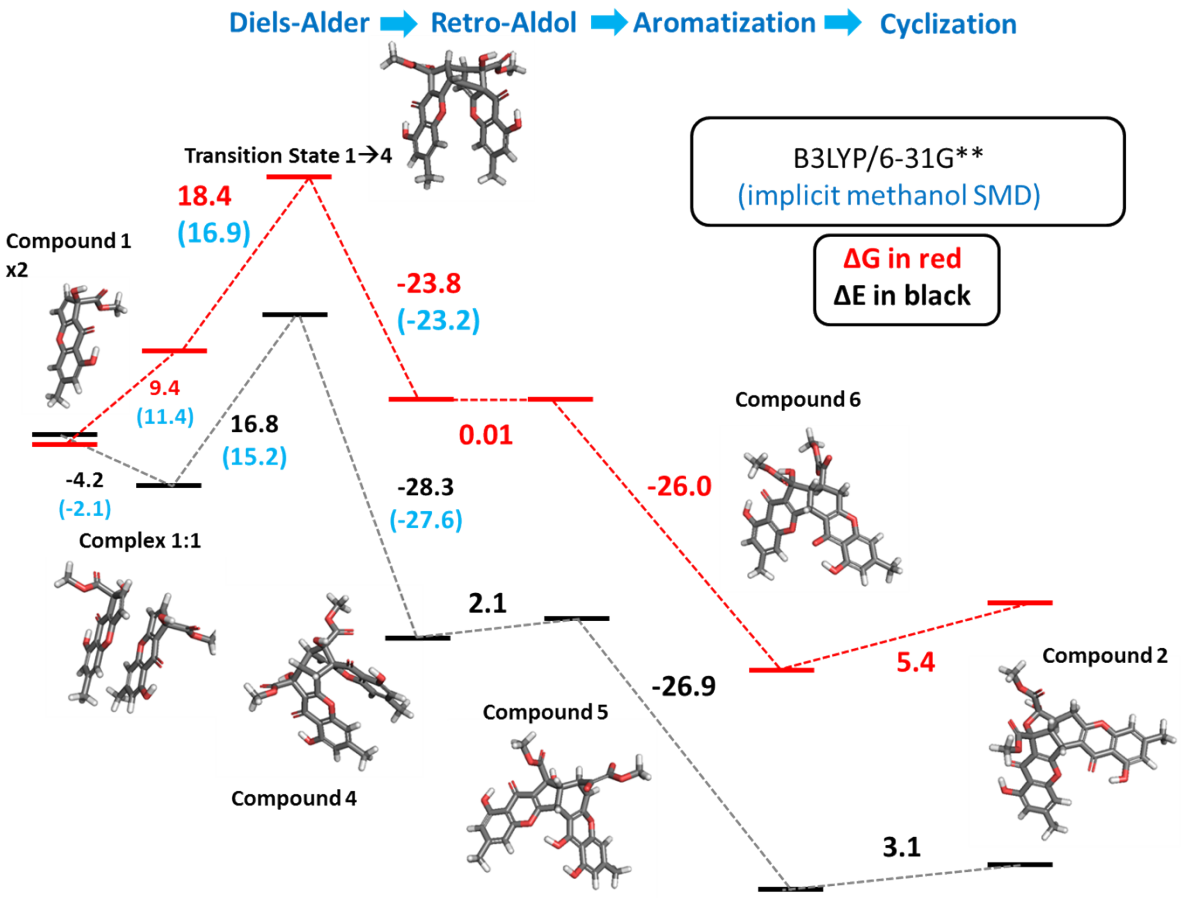
S2: Comparison of the calculated ECD (NSTATES=100, σ=0.16) for 2 (SSRRR) as a complex with 9 explicit methanol molecules *in vacuo* (A), and as the explicit complex in implicit methanol (B).



The CAM-B3LYP and B3LYP calculated ECD for a single conformer of Molecule 2 using NSTATES=20 are equivalent once the CAM wavelength axis is scaled by 1.3. The unscaled B3LYP ECD is in better agreement with the peak positioning of the experimental enantiomer whereas CAM-B3LYP needs scaling to align optimally.

S3: Comparison of the calculated ECD (NSTATES=20, σ=0.3) for Molecule 2 conformer 1 using CAM-B3LYP and B3LYP. The experimental curve shown is for the enantiomer of the original publication spectrum.

S4: B3LYP/6-31G** in vacuo and selected implicit methanol energetics (ΔG, 298K, kcal/mol)



S5: M062X/6-31+G** in vacuo energetics (ΔG, 298K, kcal/mol)

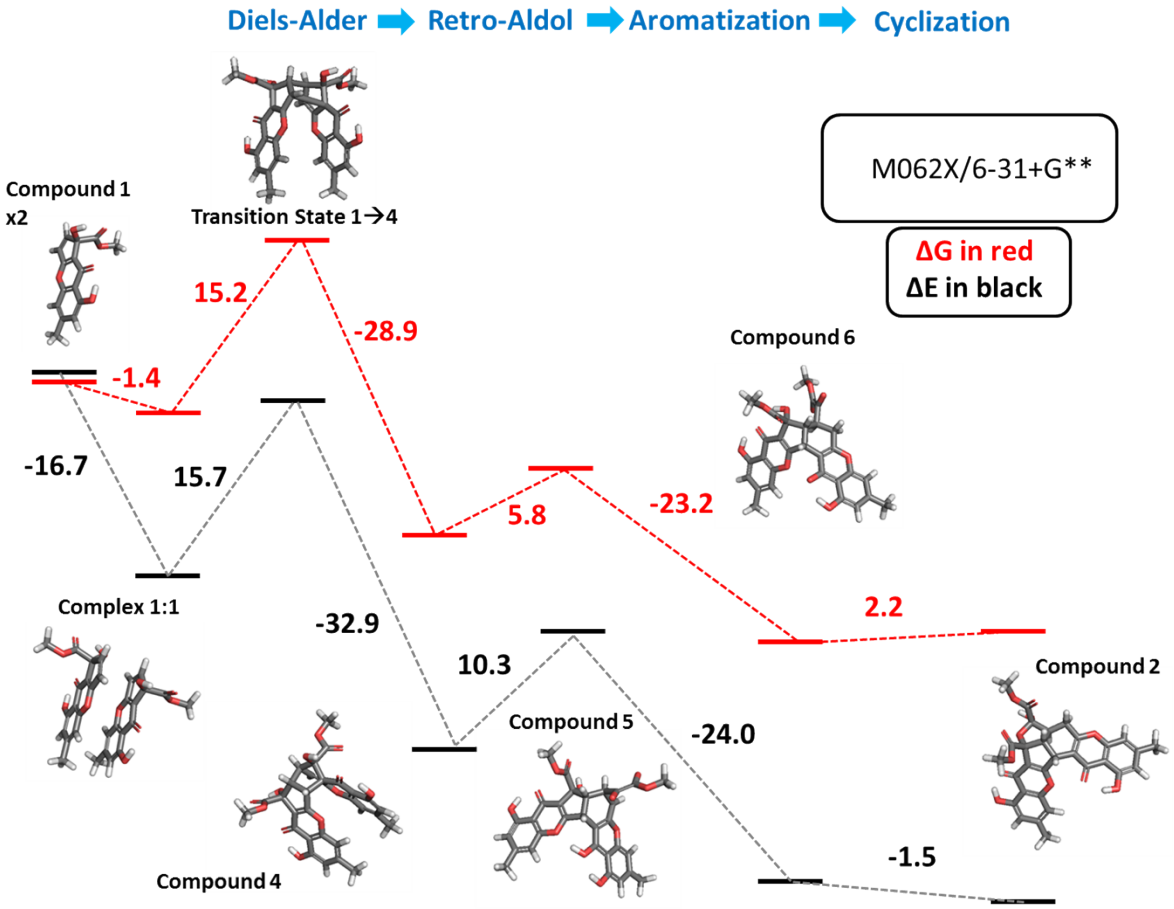


Table comparing other DFT functionals for the treatment of the first step in the proposed reaction scheme

	Formation of vdW complex	Formation of vdW complex	Diels Alder barrier from vdW complex	Diels Alder barrier from vdW complex
Method	**ΔE**	**ΔG**	**ΔE**	**ΔG**
M062X/6-31+G**	-16.7	-1.4	15.7	15.2
B3LYP/6-31G**	-4.2	9.4	16.8	18.4
B3LYP/6-31G** implicit methanol	-2.1	11.4	15.2	16.9
B3LYP-D2/6-31G**	-21.9	-6.2	10.2	12.5
B3LYP-D3/6-31G**	-24.2	-8.2	18.4	19.7
CAM-B3LYP/6-31G**	-6.9	6.2	TS did not converge	TS did not converge

Note: transition state for CAM-B3LYP did not converge

Table of B3LYP and M062X energies

	UM062X/6-31+G**	UM062X/6-31+G**	B3LYP/6-31G**	B3LYP/6-31G**
	E	G	E	G
Structure				
1	-1029.806754	-1029.607858	-1030.176794	-1029.982885
4	-2059.667507	-2059.239815	-2060.378382	-2059.960437
5	-2059.651036	-2059.230597	-2060.375082	-2059.960423
6	-2059.68929	-2059.267588	-2060.418027	-2060.001797
2	-2059.69165	-2059.264117	-2060.41314	-2059.993194
TS	-2059.615067	-2059.19375	-2060.333353	-2059.92136
vdW complex	-2059.640076	-2059.218	-2060.360244	-2059.950763

Coordinates for Minima

Molecule 2 Conformer 1: -2060.413070
B3LYP/6-31G**
8 2.6486 -1.62912 -0.728508
8 0.046434 2.10333 0.183073
8 1.77371 -2.58598 -2.65511
8 -3.26486 -1.84391 -0.761265
8 3.02525 -4.49109 -1.2581
8 4.05765 1.33139 -0.39458
8 1.35342 -4.42783 0.26477
8 -2.50387 1.31526 1.70575
8 4.37047 3.82056 -1.08139
8 -5.04599 1.88172 1.6935
6 0.654323 -1.436 0.575394
6 0.358409 -1.90599 -0.850973
6 2.11158 -0.917835 0.397686
6 -0.26149 -0.253503 0.911616
6 1.67334 -2.54662 -1.27344
6 1.8726 0.554432 0.138151
6 -1.00985 -2.56126 -0.930857
6 0.572406 0.886323 0.357318
6 -1.67707 -0.487047 0.406092
6 -1.99705 -1.55909 -0.378016
6 2.83827 1.55919 -0.253825
6 1.96696 -3.92785 -0.653876
6 -2.74002 0.371547 0.918976
6 2.25244 2.8836 -0.458353
6 0.88168 3.11985 -0.244089
6 -4.0866 0.050929 0.476658
6 -4.31463 -1.05307 -0.357827
6 3.0571 3.98171 -0.873059
6 0.29887 4.36668 -0.429848
6 -5.20771 0.826796 0.884641
6 -5.58354 -1.40389 -0.802802
6 1.10359 5.43376 -0.847851
6 2.47344 5.23564 -1.06358
6 3.50479 -5.71714 -0.669815
6 -6.67664 -0.624393 -0.403848
6 -6.48334 0.480325 0.436783
6 0.492781 6.79367 -1.08656
6 -8.06339 -0.958698 -0.898027
1 0.570843 -2.26552 1.27925
1 0.321161 -1.01931 -1.49502
1 -0.330506 -0.090242 1.99554
1 4.34475 -6.0297 -1.28843

1 3.82852 -5.53071 0.356063
1 2.71748 -6.47373 -0.672707
1 -0.467178 6.89747 -0.574434
1 1.1556 7.59261 -0.741298
1 0.317527 6.95755 -2.15675
1 -8.13814 -2.00441 -1.2074
1 -8.81562 -0.772884 -0.126068
1 -8.32561 -0.338122 -1.7635
1 -1.05117 -3.48975 -0.34903
1 -1.29127 -2.80264 -1.96104
1 -0.761263 4.49112 -0.240852
1 -5.70576 -2.26936 -1.4441
1 3.11081 6.05515 -1.37931
1 -7.32366 1.08566 0.760382
1 2.61075 -3.0244 -2.87178
1 4.57489 2.86769 -0.876511
1 -4.07417 1.93012 1.90146
6 3.00373 -1.23102 1.6078
8 2.81776 -0.323091 2.58566
8 3.71913 -2.1999 1.6997
6 3.56912 -0.555932 3.79168
1 3.29841 0.254971 4.46678
1 4.64016 -0.538682 3.57895
1 3.30719 -1.52414 4.22489

Molecule 2 Conformer 3: -2060.412349
B3LYP/6-31G**
8 2.76488 -1.37579 -0.639283
8 -0.155618 2.14423 0.265589
8 1.9595 -2.26384 -2.63482
8 -3.12614 -2.02615 -0.760846
8 3.26083 -4.22065 -1.41537
8 3.90235 1.69694 -0.332893
8 1.71639 -4.25583 0.235659
8 -2.64251 1.135 1.77282
8 4.01213 4.20567 -1.01009
8 -5.22153 1.49794 1.74283
6 0.736094 -1.33666 0.622954
6 0.490198 -1.79424 -0.815723
6 2.14624 -0.701962 0.470649
6 -0.272478 -0.235948 0.973374
6 1.85254 -2.315 -1.25393
6 1.78774 0.747671 0.204581
6 -0.819865 -2.55576 -0.924751
6 0.466897 0.973165 0.432051
6 -1.66182 -0.573959 0.453854
6 -1.88867 -1.64927 -0.357209

6 2.66917 1.82678 -0.185233
6 2.23554 -3.70713 -0.712781
6 -2.79498 0.188908 0.969409
6 1.97868 3.10114 -0.381293
6 0.594451 3.22682 -0.158583
6 -4.10761 -0.228892 0.505303
6 -4.23885 -1.32906 -0.353717
6 2.69127 4.26117 -0.794119
6 -0.086101 4.42406 -0.334263
6 -5.29105 0.449181 0.91318
6 -5.47157 -1.76838 -0.822947
6 0.629284 5.55387 -0.751519
6 2.0088 5.46605 -0.975605
6 3.77977 -5.47883 -0.94142
6 -6.62646 -1.08593 -0.422514
6 -6.53003 0.013479 0.442179
6 -0.091362 6.86015 -0.983058
6 -7.97927 -1.52019 -0.933089
1 0.71157 -2.18197 1.31242
1 0.383117 -0.897752 -1.43773
1 -0.351797 -0.094384 2.05906
1 4.59215 -5.73544 -1.61969
1 4.14882 -5.37108 0.080563
1 3.00007 -6.24302 -0.963837
1 -1.00485 6.92464 -0.385962
1 0.544293 7.71458 -0.734441
1 -0.378336 6.96257 -2.03679
1 -7.93606 -2.50871 -1.39688
1 -8.71529 -1.55229 -0.123812
1 -8.35542 -0.814985 -1.68368
1 -0.792998 -3.49896 -0.365684
1 -1.07389 -2.79269 -1.96308
1 -1.1515 4.46324 -0.137881
1 -5.51821 -2.62596 -1.48434
1 2.57756 6.33504 -1.28989
1 -7.4189 0.545378 0.765355
1 2.81644 -2.64672 -2.87606
1 4.29239 3.27169 -0.807674
1 -4.25886 1.62001 1.96276
6 2.98195 -0.843113 1.74725
8 3.98086 -1.72791 1.63799
8 2.70577 -0.237944 2.76152
6 4.76717 -1.90075 2.83201
1 5.5422 -2.61972 2.56895
1 4.1477 -2.28094 3.64777
1 5.21038 -0.949961 3.13539

Molecule 2 Conformer 3: -2060.413140

B3LYP/6-31G**
8 2.53062 -1.82386 -0.862132
8 0.263564 2.07557 0.21486
8 1.54143 -2.53505 -2.84585
8 -3.38368 -1.55422 -0.818263
8 1.28953 -4.39531 0.149659
8 4.19051 0.984951 -0.423264
8 2.40766 -4.80788 -1.77309
8 -2.33727 1.4462 1.74041
8 4.7116 3.46018 -1.029
8 -4.82532 2.21889 1.78288
6 0.569582 -1.51554 0.473931
6 0.220991 -1.90349 -0.962462
6 2.06464 -1.1192 0.295233
6 -0.239246 -0.271979 0.862875
6 1.47216 -2.61086 -1.47127
6 1.94961 0.378214 0.096613
6 -1.19607 -2.44196 -1.05201
6 0.684656 0.812165 0.339746
6 -1.67522 -0.371262 0.369129
6 -2.09238 -1.38505 -0.445843
6 2.99606 1.31085 -0.266774
6 1.76057 -4.07048 -1.05898
6 -2.65924 0.552925 0.926137
6 2.52478 2.68678 -0.419246
6 1.18073 3.03186 -0.183932
6 -4.0328 0.357888 0.493467
6 -4.36058 -0.695045 -0.373263
6 3.4185 3.72567 -0.80284
6 0.706548 4.33001 -0.319666
6 -5.08208 1.20805 0.94305
6 -5.65909 -0.926678 -0.810826
6 1.5977 5.3383 -0.708017
6 2.94378 5.03119 -0.943696
6 1.75162 -5.65648 0.683097
6 -6.67995 -0.075236 -0.370171
6 -6.38685 0.981299 0.503235
6 1.10441 6.75289 -0.894794
6 -8.096 -0.278547 -0.852177
1 0.422265 -2.35353 1.15605
1 0.236261 -0.985763 -1.56289
1 -0.284772 -0.14237 1.95266
1 1.1822 -5.8126 1.59821
1 1.57219 -6.46143 -0.03121
1 2.81825 -5.58328 0.902551
1 0.171194 6.92719 -0.353045
1 1.84456 7.48042 -0.549113
1 0.915761 6.9605 -1.95509

1 -8.24683 -1.28811 -1.24269
1 -8.81692 -0.109144 -0.046995
1 -8.33593 0.427742 -1.65604
1 -1.31832 -3.38758 -0.508105
1 -1.50393 -2.6167 -2.08799
1 -0.337671 4.53841 -0.116462
1 -5.85927 -1.75612 -1.47947
1 3.64717 5.80367 -1.23693
1 -7.17093 1.64199 0.858257
1 2.17952 -3.2151 -3.1259
1 4.83498 2.48661 -0.860085
1 -3.8505 2.18298 1.9775
6 2.93459 -1.55462 1.48459
8 2.87872 -0.645543 2.47743
8 3.5289 -2.60447 1.55348
6 3.62892 -0.978951 3.65991
1 3.47402 -0.149569 4.34891
1 4.68831 -1.08576 3.41741
1 3.26655 -1.91436 4.09315

Molecule 2 Conformer 4: -2060.412247
B3LYP/6-31G**
2.65783 -1.58904 -0.790361
8 0.067152 2.13188 0.284499
8 1.73403 -2.28248 -2.81562
8 -3.26933 -1.7519 -0.815766
8 1.60607 -4.25048 0.12854
8 4.06829 1.36282 -0.363108
8 2.66061 -4.5725 -1.84364
8 -2.48182 1.28868 1.7883
8 4.38953 3.87807 -0.946674
8 -5.02224 1.86255 1.81924
6 0.659227 -1.42323 0.512786
6 0.352885 -1.8138 -0.931706
6 2.11688 -0.910794 0.353126
6 -0.247482 -0.252325 0.911367
6 1.65853 -2.413 -1.4444
6 1.88156 0.575732 0.147802
6 -1.01696 -2.46013 -1.04342
6 0.587438 0.906054 0.399486
6 -1.66794 -0.457019 0.405442
6 -1.99828 -1.48688 -0.428352
6 2.85101 1.59079 -0.205917
6 2.01911 -3.87219 -1.08849
6 -2.72599 0.381713 0.963045
6 2.27164 2.92656 -0.345582
6 0.905137 3.16185 -0.104892
6 -4.07653 0.085714 0.514668

6 -4.31417 -0.977606 -0.368569
6 3.07961 4.03742 -0.717017
6 0.329226 4.41957 -0.2255
6 -5.19219 0.846383 0.964396
6 -5.58685 -1.30326 -0.821421
6 1.13703 5.49979 -0.60216
6 2.50272 5.3028 -0.84251
6 2.03595 -5.56307 0.550708
6 -6.67457 -0.538747 -0.380501
6 -6.47188 0.525274 0.508773
6 0.532927 6.87329 -0.769544
6 -8.06542 -0.8439 -0.881929
1 0.571594 -2.27621 1.1867
1 0.300598 -0.88828 -1.51772
1 -0.300377 -0.139804 2.00195
1 1.5903 -5.71409 1.53279
1 1.68943 -6.3211 -0.154288
1 3.12548 -5.59694 0.610348
1 -0.411078 6.96456 -0.226243
1 1.21275 7.65222 -0.412158
1 0.328551 7.08085 -1.82695
1 -8.14579 -1.87265 -1.24253
1 -8.81228 -0.694314 -0.096989
1 -8.33073 -0.180111 -1.7137
1 -1.0692 -3.42131 -0.515643
1 -1.3024 -2.64089 -2.08478
1 -0.727546 4.54239 -0.017659
1 -5.71624 -2.13693 -1.50223
1 3.14271 6.13198 -1.12598
1 -7.30774 1.11864 0.864467
1 2.40485 -2.91832 -3.12002
1 4.59082 2.91659 -0.784038
1 -4.0491 1.89982 2.02307
6 2.95994 -1.16475 1.6077
8 3.95829 -2.03537 1.41954
8 2.69569 -0.638248 2.66877
6 4.78018 -2.27322 2.57767
1 5.54737 -2.97424 2.251
1 4.18636 -2.69794 3.3908
1 5.23247 -1.33996 2.91973

Coordinates of explicitly solvated remisporine B
B3LYP/6-31G**: -3102.069801
8 3.07647 -0.882961 0.209253
8 -0.951551 1.37481 0.767976
8 2.9423 -1.39587 -2.0602
8 -2.15218 -3.07982 -1.5111

8 2.93638 -3.87056 0.473575
8 3.05835 2.26586 1.07621
8 4.504 -3.40541 -1.08271
8 -3.20479 -0.471519 1.42756
8 2.53498 4.67098 0.381071
8 -5.71693 -0.387656 0.35336
6 0.938202 -1.69455 0.907746
6 1.13362 -1.88653 -0.595771
6 2.0658 -0.664329 1.195
6 -0.424048 -1.02297 1.14077
6 2.65071 -1.8477 -0.798417
6 1.31274 0.643454 1.02725
6 0.187437 -2.94656 -1.13677
6 -0.027933 0.427677 0.956579
6 -1.49731 -1.59606 0.231368
6 -1.20334 -2.49734 -0.750539
6 1.84973 1.97515 0.9194
6 3.47474 -3.12538 -0.513761
6 -2.88017 -1.21033 0.473911
6 0.845797 2.98922 0.610775
6 -0.525671 2.67405 0.564494
6 -3.86397 -1.7357 -0.463277
6 -3.46894 -2.70412 -1.40395
6 1.22246 4.33364 0.362356
6 -1.50703 3.62383 0.318001
6 -5.23634 -1.35658 -0.453115
6 -4.36317 -3.33332 -2.26256
6 -1.1114 4.9467 0.075893
6 0.248823 5.29142 0.088034
6 3.70879 -5.02202 0.867771
6 -5.71346 -2.97946 -2.20577
6 -6.13798 -1.99063 -1.30663
6 -2.15747 5.99657 -0.209048
6 -6.71598 -3.63266 -3.12544
1 1.05568 -2.62924 1.45767
1 0.815972 -0.962418 -1.0912
1 -0.756364 -1.14325 2.18022
1 3.13425 -5.50489 1.65703
1 3.84544 -5.69699 0.02062
1 4.68767 -4.71094 1.23798
1 -2.66503 5.79473 -1.16084
1 -2.9314 5.99914 0.565504
1 -1.71991 6.99644 -0.259367
1 -6.26933 -4.45504 -3.68913
1 -7.56815 -4.02485 -2.56103
1 -7.11463 -2.90788 -3.84446
1 0.392772 -3.9456 -0.731688
1 0.227977 -3.00502 -2.22783

1 -2.55129 3.32329 0.335935
1 -3.99576 -4.07634 -2.96094
1 0.563729 6.31259 -0.099008
1 -7.17889 -1.68365 -1.26218
1 3.92772 -1.23422 -2.20951
1 3.00712 3.8609 0.741054
1 -5.00503 0.115866 0.812025
6 2.6264 -0.80181 2.61376
8 3.87723 -1.24054 2.66054
8 1.93123 -0.549162 3.58504
6 4.4651 -1.37373 3.97717
1 3.84158 -1.99247 4.62344
1 4.58295 -0.385419 4.42756
1 5.43897 -1.82982 3.8078
6 2.46434 0.199769 -4.9559
1 2.14111 -0.782588 -5.32635
1 2.1715 0.958236 -5.68613
1 3.55498 0.19404 -4.85823
8 1.8437 0.531089 -3.71357
1 2.2487 -0.043241 -3.03075
6 3.30257 3.76754 -3.14746
1 3.92873 3.64931 -4.03561
1 2.6723 2.87521 -3.04919
1 2.66745 4.64986 -3.29187
8 4.18586 3.94194 -2.03692
1 3.66198 4.22786 -1.26992
6 -5.87384 2.80237 1.61548
1 -5.67805 3.80693 2.01846
1 -6.43486 2.91575 0.683421
1 -6.50744 2.26418 2.3337
8 -4.67581 2.10302 1.31826
1 -4.18724 1.95992 2.15809
6 6.12672 1.60618 -0.295646
1 6.65996 2.46872 0.125483
1 5.20328 1.44761 0.269611
1 6.76263 0.725147 -0.1792
8 5.89585 1.78007 -1.69287
1 5.28988 2.54616 -1.81479
6 0.882553 -2.86248 5.97649
1 1.01881 -3.64393 6.72945
1 -0.080883 -2.36946 6.17384
1 0.817291 -3.35063 4.99131
8 1.9805 -1.97542 6.07839
1 1.89147 -1.31775 5.36858
6 6.44926 -1.30777 -2.96923
1 7.1743 -1.07658 -2.18023
1 6.19915 -2.36802 -2.90268
1 6.91872 -1.10632 -3.94021

8 5.24692 -0.5623 -2.81513
1 5.45114 0.339072 -2.44796
6 -1.50624 0.81706 -2.9269
1 -0.964407 1.75889 -3.08085
1 -2.25427 0.717954 -3.72884
1 -2.04136 0.897263 -1.9738
8 -0.631793 -0.29698 -2.88286
1 0.183392 -0.048902 -3.36723
6 -8.49828 1.15608 -1.23432
1 -8.35966 2.14253 -0.766375
1 -7.72492 1.03593 -2.00687
1 -9.47344 1.15789 -1.73052
8 -8.50272 0.103154 -0.293611
1 -7.61931 0.055604 0.10979
6 -2.15912 1.86862 4.13115
1 -1.52534 1.13772 4.64992
1 -1.54249 2.40759 3.39926
1 -2.51998 2.58878 4.86981
8 -3.29805 1.25514 3.54244
1 -3.01323 0.537625 2.94637

Compound 1
M062X/6-31+G**
8 0.8362 1.9261 0.1113
8 -2.7759 -0.1401 1.5292
8 -3.827 -1.3258 -0.0663
8 -0.3632 -1.9219 -0.7642
8 2.1409 -2.6657 -0.5365
6 -2.6392 1.939 -0.4938
6 -2.3662 0.4608 -0.756
6 -1.5153 2.589 -0.1645
6 -0.8702 0.3772 -0.5331
6 -0.4226 1.6084 -0.187
6 -3.0839 -0.4379 0.2716
6 0.0074 -0.7572 -0.5451
6 1.4022 -0.4034 -0.2497
6 1.7713 0.9144 0.0659
6 2.4225 -1.388 -0.2557
6 3.0803 1.2745 0.356
6 -3.3636 -0.9921 2.5219
6 4.07 0.2917 0.3357
6 3.7365 -1.0318 0.0314
6 5.5018 0.6443 0.6457
8 -2.8009 0.1147 -2.0373
1 -3.0585 -2.0259 2.3495
1 -2.9886 -0.6287 3.4761

1 -4.4521 -0.9214 2.4787
1 5.847 0.1039 1.5322
1 6.1552 0.3649 -0.186
1 5.6182 1.7143 0.8294
1 -3.6314 2.3567 -0.6133
1 -1.3923 3.6384 0.0688
1 3.3067 2.3085 0.5919
1 4.4946 -1.8088 0.0141
1 1.17 -2.7389 -0.6933
1 -3.1349 -0.7956 -1.9967

Compound 2
M062X/6-31+G**
8 2.6506 -1.5169 -0.8285
8 -0.0338 2.0748 0.215
8 1.8057 -2.5947 -2.6788
8 -3.2068 -1.9431 -0.7371
8 3.2141 -4.3172 -1.1544
8 3.9805 1.466 -0.4194
8 1.4626 -4.3521 0.2581
8 -2.4926 1.2131 1.7179
8 4.1827 3.9974 -1.0836
8 -5.0644 1.7543 1.6877
6 0.7041 -1.4333 0.5425
6 0.3941 -1.9071 -0.8738
6 2.1324 -0.8614 0.3254
6 -0.2391 -0.2902 0.9074
6 1.723 -2.4963 -1.3052
6 1.84 0.6003 0.1093
6 -0.9441 -2.6124 -0.9248
6 0.5393 0.8832 0.3581
6 -1.6438 -0.5573 0.4089
6 -1.9486 -1.6342 -0.3662
6 2.7654 1.6471 -0.2693
6 2.0904 -3.8313 -0.6331
6 -2.7179 0.2805 0.932
6 2.123 2.9526 -0.4441
6 0.7499 3.123 -0.2073
6 -4.0614 -0.0633 0.4896
6 -4.2637 -1.173 -0.3371
6 2.8681 4.0882 -0.8506
6 0.111 4.3451 -0.3632
6 -5.1946 0.6897 0.8881
6 -5.5238 -1.5507 -0.782
6 0.861 5.4483 -0.7731
6 2.2325 5.3156 -1.0116
6 3.764 -5.4587 -0.4834
6 -6.6276 -0.7912 -0.3906

6 -6.4593 0.3204 0.4423
6 0.1928 6.7826 -0.9811
6 -8.005 -1.1515 -0.8834
1 0.6693 -2.2691 1.2457
1 0.316 -1.0197 -1.517
1 -0.3008 -0.1424 1.9944
1 4.677 -5.7033 -1.0218
1 3.9808 -5.1953 0.5535
1 3.0566 -6.2893 -0.5162
1 -0.7671 6.8313 -0.4627
1 0.8254 7.5976 -0.6205
1 0.0101 6.9523 -2.0473
1 -8.0478 -2.1897 -1.2194
1 -8.7521 -1.0083 -0.0989
1 -8.2837 -0.512 -1.7275
1 -0.9456 -3.5308 -0.3259
1 -1.2366 -2.8688 -1.9476
1 -0.9507 4.4177 -0.1552
1 -5.6257 -2.4221 -1.4194
1 2.8301 6.1669 -1.3222
1 -7.3113 0.9134 0.7592
1 2.6818 -2.9385 -2.9059
1 4.4616 3.0689 -0.9059
1 -4.1116 1.846 1.92
6 3.0567 -1.1892 1.4961
8 2.954 -0.2815 2.471
8 3.7258 -2.1892 1.5582
6 3.7463 -0.5426 3.6351
1 3.5444 0.2801 4.3179
1 4.8034 -0.5721 3.3649
1 3.4582 -1.4978 4.0789

Compound 3
M062X/6-31+G**
8 0.0497 -1.3713 -1.5122
8 4.8624 -1.206 -1.2765
8 3.439 -2.7813 -0.5358
8 1.7318 -2.2647 2.1756
8 -0.0984 -4.1557 2.4453
6 2.8533 0.7794 -0.7197
6 3.1068 -0.4827 0.1441
6 1.8815 0.201 -1.7402
6 1.6028 -0.7679 0.3473
6 1.1506 -0.7045 -1.0821
6 3.794 -1.6274 -0.6027
6 1.1879 -1.9886 1.1005

6 0.0706 -2.7197 0.5308
6 -0.4867 -2.3474 -0.7165
6 -0.5689 -3.7508 1.2613
6 -1.6279 -2.9538 -1.206
6 5.6109 -2.2294 -1.9429
6 -2.2559 -3.9592 -0.4575
6 -1.7273 -4.355 0.7675
6 -3.4991 -4.6109 -1.0024
8 3.8034 -0.2155 1.3312
1 4.9756 -2.7452 -2.6657
1 6.4299 -1.7157 -2.4419
1 5.9892 -2.9501 -1.2154
1 -3.2562 -5.2191 -1.8796
1 -3.9692 -5.2577 -0.259
1 -4.2239 -3.8546 -1.3184
1 3.7421 1.2566 -1.1294
1 1.732 0.5736 -2.743
1 -2.0242 -2.6287 -2.1622
1 -2.1948 -5.1344 1.3597
1 0.7058 -3.6386 2.6618
1 3.5988 -0.9275 1.9592
8 -1.2253 0.1977 0.9274
8 1.0597 3.9295 1.7643
8 1.4641 5.113 -0.1048
8 -1.6627 3.7043 -1.1701
8 -4.2151 3.1103 -1.4653
6 2.0714 1.6471 0.318
6 1.1205 2.7288 -0.2942
6 1.1752 0.59 1.0266
6 -0.2597 2.139 -0.0781
6 -0.1991 1.0026 0.64
6 1.2414 4.0646 0.4503
6 -1.53 2.6281 -0.5716
6 -2.6487 1.7175 -0.3002
6 -2.4591 0.5275 0.4197
6 -3.9563 1.9929 -0.7754
6 -3.483 -0.3773 0.6624
6 1.1305 5.1459 2.52
6 -4.7591 -0.0898 0.1788
6 -4.9894 1.0925 -0.5328
6 -5.8982 -1.0428 0.4338
8 1.421 2.9534 -1.6442
1 0.3699 5.8456 2.1688
1 0.9485 4.8602 3.5539
1 2.1177 5.5983 2.4086
1 -6.6086 -0.6083 1.1442
1 -6.4442 -1.2534 -0.4901
1 -5.5381 -1.987 0.8484

1 2.7789 2.0865 1.0224
1 1.3232 0.535 2.1086
1 -3.2653 -1.2891 1.2102
1 -5.9775 1.3307 -0.9142
1 -3.3809 3.6266 -1.5427
1 1.2413 3.8872 -1.8351

Compound 4
M062X/6-31+G**
6 2.0121 -0.0002 0.7099
6 1.084 0.4968 -0.2965
6 2.2083 -1.2991 0.9799
6 1.5026 -2.3609 0.1738
6 2.428 -2.6409 -0.9985
6 1.2108 1.7807 -0.7069
6 2.2123 2.6672 -0.1278
6 2.9206 2.1806 0.9863
8 2.7131 0.9176 1.4534
6 2.4828 3.9881 -0.5419
6 3.4178 4.7628 0.147
6 4.0919 4.2599 1.2553
6 3.8363 2.9527 1.6805
8 1.8825 4.5763 -1.6008
6 5.105 5.1009 1.9876
8 -0.5085 -1.8444 2.0419
8 -1.9105 0.9882 -1.0293
8 -2.2808 -3.6697 -0.4492
8 -1.5886 -4.218 1.6193
8 -3.909 -1.5533 1.4995
8 -5.9758 0.0801 1.3832
6 0.1368 -1.9281 -0.3412
6 -0.9892 -2.0582 0.743
6 0.0709 -0.4719 -0.8905
6 -1.9407 -0.9694 0.329
6 -1.3417 -0.1173 -0.5174
6 -1.652 -3.4376 0.6985
6 -3.306 -0.7635 0.7618
6 -3.9129 0.4573 0.2235
6 -3.2004 1.3024 -0.6427
6 -5.2338 0.835 0.5671
6 -3.7346 2.4712 -1.1571
6 -2.9807 -4.9195 -0.5208
6 -5.039 2.8289 -0.8005
6 -5.7778 2.0124 0.0568
6 -5.6537 4.0818 -1.3674
1 -0.1479 -2.5739 -1.177
1 0.1881 -0.4884 -1.982
8 0.4404 2.3435 -1.6842

6 3.7678 -3.2989 -0.6114
8 2.1878 -2.3522 -2.1458
8 3.9357 -3.8376 0.457
8 4.6654 -3.2244 -1.5825
6 5.9288 -3.8333 -1.2922
1 4.8931 5.1178 3.0606
1 6.1115 4.691 1.8565
1 5.106 6.1291 1.62
1 -3.4339 -4.9449 -1.5095
1 -3.7432 -4.9563 0.2596
1 -2.2821 -5.748 -0.3903
1 -6.1363 3.8657 -2.3264
1 -6.4129 4.486 -0.6946
1 -4.8965 4.8502 -1.5396
1 6.5494 -3.6474 -2.166
1 5.798 -4.9048 -1.1274
1 6.3653 -3.3816 -0.3991
1 1.4127 -3.2694 0.7811
1 2.9044 -1.595 1.755
1 3.595 5.7722 -0.2091
1 4.3422 2.5208 2.5375
1 -3.1377 3.0917 -1.8171
1 -6.7895 2.277 0.3462
1 1.2119 3.9845 -1.9714
1 -0.7728 -2.6041 2.585
1 -5.4461 -0.7046 1.6503
1 -0.4185 1.9039 -1.7658

Compound 5
M062X/6-31+G**
6 -1.8893 -1.7564 -0.1151
6 -1.6438 -0.6662 0.6463
6 -0.8575 -2.7696 -0.4902
6 0.5622 -2.2039 -0.3726
6 1.5413 -3.3591 -0.518
6 -2.7446 0.2053 1.042
6 -4.0495 -0.1512 0.5014
6 -4.1897 -1.2852 -0.3054
8 -3.1096 -2.0747 -0.5903
6 -5.2077 0.6189 0.7789
6 -6.4322 0.2418 0.2396
6 -6.5383 -0.8965 -0.5683
6 -5.4106 -1.6694 -0.8454
8 -5.137 1.7095 1.5511
6 -7.8839 -1.2915 -1.1189
8 3.0735 -1.4276 0.1494
8 -0.2005 1.8904 0.1889
8 3.9916 -0.4624 2.4443

8 1.9623 -0.6408 3.3944
8 3.8548 1.3897 -0.3006
8 3.941 3.8199 -1.3497
6 0.7737 -1.5114 0.9843
6 2.1453 -0.7751 0.9808
6 -0.2734 -0.383 1.1948
6 1.77 0.5943 0.47
6 0.4401 0.7945 0.5782
6 2.6738 -0.6403 2.4168
6 2.635 1.5742 -0.1313
6 1.9322 2.7867 -0.543
6 0.5419 2.9082 -0.3642
6 2.6191 3.8729 -1.1412
6 -0.1593 4.0443 -0.7413
6 4.5582 -0.2497 3.7427
6 0.5382 5.1057 -1.3196
6 1.9197 5.0137 -1.5193
6 -0.1895 6.3659 -1.7088
1 0.7189 -2.2512 1.7879
1 -0.37 -0.1757 2.2692
8 -2.5764 1.1699 1.8025
6 2.3936 -3.3607 -1.7945
8 1.599 -4.2665 0.2727
8 2.0617 -2.7575 -2.7882
8 3.4749 -4.1136 -1.6769
6 4.3044 -4.175 -2.8422
1 -8.3734 -0.4384 -1.5966
1 -7.7938 -2.0944 -1.8532
1 -8.5382 -1.6379 -0.3126
1 4.3437 -1.104 4.3872
1 5.6285 -0.1425 3.5803
1 4.1395 0.6548 4.1883
1 -0.0441 7.1369 -0.945
1 0.19 6.7607 -2.6545
1 -1.2624 6.1899 -1.8099
1 4.6297 -3.1713 -3.1234
1 5.1536 -4.7952 -2.5639
1 3.7519 -4.6209 -3.672
1 -1.0517 -3.1086 -1.5132
1 -0.9664 -3.6411 0.1695
1 0.7359 -1.4904 -1.1845
1 -7.3036 0.8487 0.4649
1 -5.4634 -2.5578 -1.4648
1 -1.2305 4.083 -0.5773
1 2.4726 5.8283 -1.9763
1 -4.2059 1.8068 1.8571
1 3.8074 -0.8112 -0.015
1 4.2714 2.9468 -1.0436

Compound Transition State
M062X/6-31+G**
8 -0.6153 0.9344 1.3924
8 2.6659 3.2878 1.7998
8 3.3326 4.176 -0.1497
8 0.2357 3.1234 -2.0119
8 -2.351 3.3387 -2.4036
6 2.857 0.6997 0.676
6 2.505 1.9161 -0.1965
6 1.7473 0.4457 1.5126
6 0.99 1.8126 -0.1839
6 0.6369 1.1021 0.9453
6 2.894 3.2514 0.4921
6 -0.0148 2.4405 -1.006
6 -1.3862 2.181 -0.5399
6 -1.6381 1.4742 0.6515
6 -2.5068 2.655 -1.2635
6 -2.9162 1.2497 1.1322
6 2.9356 4.5469 2.4327
6 -4.0077 1.7199 0.3978
6 -3.7998 2.41 -0.7973
6 -5.4015 1.489 0.9202
8 3.1374 1.903 -1.4384
1 2.2952 5.3216 2.0066
1 2.7143 4.3947 3.4868
1 3.982 4.8211 2.2878
1 -5.6327 2.2083 1.713
1 -6.1492 1.6052 0.1323
1 -5.4932 0.4856 1.3472
1 3.869 0.5737 1.0503
1 1.7418 -0.1594 2.4074
1 -3.0457 0.6815 2.0479
1 -4.6344 2.783 -1.3826
1 -1.3849 3.4463 -2.566
1 3.1711 2.8183 -1.7581
8 -0.6156 -0.9341 -1.3923
8 2.6648 -3.2883 -1.7998
8 3.3318 -4.1767 0.1495
8 0.2349 -3.1237 2.0117
8 -2.3518 -3.3385 2.4035
6 2.8568 -0.7003 -0.676
6 2.5045 -1.9166 0.1965
6 1.7471 -0.4459 -1.5125
6 0.9896 -1.8127 0.184
6 0.6366 -1.1021 -0.9452
6 2.8932 -3.252 -0.4922
6 -0.0154 -2.4406 1.006

6 -1.3867 -2.1808 0.5399
6 -1.6385 -1.4738 -0.6514
6 -2.5074 -2.6547 1.2635
6 -2.9166 -1.249 -1.1321
6 2.9342 -4.5475 -2.4327
6 -4.0082 -1.719 -0.3977
6 -3.8003 -2.4093 0.7972
6 -5.4019 -1.4877 -0.9201
8 3.137 -1.9037 1.4384
1 2.2937 -5.3221 -2.0067
1 2.7129 -4.3952 -3.4868
1 3.9806 -4.8218 -2.288
1 -5.6334 -2.2069 -1.7128
1 -6.1495 -1.6036 -0.1321
1 -5.4933 -0.4842 -1.3471
1 3.8688 -0.5746 -1.0504
1 1.7417 0.1591 -2.4073
1 -3.0459 -0.6805 -2.0477
1 -4.6351 -2.7822 1.3825
1 -1.3857 -3.4463 2.5658
1 3.1708 -2.819 1.7579

Compound vdW complex
M062X/6-31+G**
8 -0.8435 0.3333 -1.4897
8 -4.2084 -2.2844 -1.2507
8 -4.5129 -3.3686 0.6941
8 -3.473 -0.0071 1.6705
8 -3.51 2.6061 1.8142
6 -1.4277 -3.0859 -0.8858
6 -2.3151 -2.5073 0.2137
6 -0.8255 -2.1161 -1.5886
6 -2.0506 -1.0225 0.0735
6 -1.2337 -0.8409 -0.9969
6 -3.8069 -2.7767 -0.0867
6 -2.6465 0.0945 0.748
6 -2.2064 1.3905 0.2132
6 -1.3352 1.472 -0.8882
6 -2.675 2.6054 0.7675
6 -0.9255 2.6783 -1.4314
6 -5.6011 -2.4618 -1.5448
6 -1.3977 3.8653 -0.8659
6 -2.2667 3.8235 0.2263
6 -0.9741 5.1871 -1.4506
8 -2.0177 -3.0715 1.4599
1 -6.2054 -1.9659 -0.783

1 -5.7524 -2.005 -2.5203
1 -5.846 -3.5252 -1.57
1 -1.5351 5.3973 -2.3672
1 -1.1542 6.006 -0.75
1 0.0892 5.1719 -1.7078
1 -1.315 -4.1557 -1.0158
1 -0.1215 -2.2205 -2.4026
1 -0.2353 2.6791 -2.269
1 -2.6467 4.737 0.6736
1 -3.7173 1.6672 2.0372
1 -2.8639 -3.261 1.8974
8 0.8435 0.3334 1.4897
8 4.2082 -2.285 1.2506
8 4.5122 -3.3693 -0.6942
8 3.4731 -0.0075 -1.6704
8 3.5106 2.6056 -1.814
6 1.4273 -3.086 0.8859
6 2.3146 -2.5075 -0.2136
6 0.8252 -2.1161 1.5887
6 2.0505 -1.0227 -0.0735
6 1.2336 -0.8409 0.997
6 3.8064 -2.7772 0.0867
6 2.6465 0.0942 -0.7479
6 2.2066 1.3902 -0.2131
6 1.3354 1.472 0.8881
6 2.6755 2.6051 -0.7674
6 0.9257 2.6783 1.4312
6 5.6009 -2.4626 1.5446
6 1.3982 3.8652 0.8658
6 2.2674 3.8233 -0.2262
6 0.9746 5.1871 1.4504
8 2.0171 -3.0717 -1.4598
1 6.2051 -1.9669 0.7827
1 5.7524 -2.0058 2.52
1 5.8455 -3.5261 1.5698
1 1.5354 5.3972 2.3672
1 1.1551 6.0059 0.7498
1 -0.0888 5.172 1.7073
1 1.3144 -4.1558 1.016
1 0.1213 -2.2204 2.4028
1 0.2354 2.6792 2.2687
1 2.6476 4.7367 -0.6735
1 3.7179 1.6667 -2.0369
1 2.8632 -3.2616 -1.8974