# Imine-based Chiroptical Sensing for Analysis of Chiral Amines: From Method Design to Synthetic Application

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## Supporting Information

## Materials and Methods

All reagents and solvents were purchased from commercial sources and used as received. The aldehyde sensor **HCA** was obtained from Matrix Scientific. All amines and ketone starting materials were purchased from either Sigma Aldrich, Alfa Aesar, or Acros Organics. Enzymes were purchased from Codexis, and PLP cofactor was obtained from Sigma Aldrich. Acetonitrile from Fisher Scientific was sparged with $N_2$ gas for at least 30 minutes prior to use. Circular dichroism measurements were performed at 25°C on a Jasco J-810 spectropolarimeter, using a Starna 0.1 cm jacketed cell. HPLC-CD measurements were acquired on an Agilent 1100 HPLC instrument, equipped with a Jasco CD 1595 HPLC-CD detector.

## Experimental

*a) Stock Solutions*

The host stock solution was made by dissolving **HCA** (123.11 mg, 0.1 mmol) to 100 mL in acetonitrile. Stock solutions of the guest were made by dissolving the guest [(*R*)-**MBA** (6.44 μL, 0.05 mmol), (*S*)-**MBA** (6.44 μL, 0.05 mmol), (*R*)-**CEA** (7.36

μL, 0.05 mmol), (*S*)-**CEA** (7.36 μL, 0.05 mmol), (*R*)-**CMA** (7.08 μL, 0.05 mmol), (*S*)-**CMA** (7.08 μL, 0.05 mmol), (*R*)-**PPA** (7.20 μL, 0.05 mmol), (*S*)-**PPA** (7.20 μL, 0.05 mmol), (*R*)-**AMH** (7.52 μL, 0.05 mmol), (*S*)-**AMH** (7.52 μL, 0.05 mmol), (*R*)-**MPP** (8.04 μL, 0.05 mmol), (*S*)-**MPP** (8.04 μL, 0.05 mmol), (*R*)-**2-AP** (3.98 μL, 0.05 mmol), (*S*)-**2-AP** (3.98 μL, 0.05 mmol), (*R*)-**2-PG** (6.86 mg, 0.05 mmol), (*S*)-**2-PG** (6.86 mg, 0.05 mmol), (*R*)-**β-MBA** (7.28 μL, 0.05 mmol), (*S*)-**β-MBA** (7.28 μL, 0.05 mmol), and (*S*)-**MPA (**4.46 mg, 0.05 mmol)] to 5 mL in acetonitrile. Each point of the binding and *ee* titration was a separate solution, containing **HCA** (2 mM) and indicated amount of guest (0-8 mM) diluted to 1 mL. The titrations were done this way because of the prohibitive nature of the small cuvette size and the inability to stir its contents.

*b) Samples tested using Iron(II) complex*

Every sample tested contained **HCA** (2 mM) and (*R*)-**MBA** (2 mM) in acetonitrile. To this complex the indicated additives were introduced with the amines. The IBA (isobutylamine), TEA (triethylamine), and $Pd(OAc)_2$ were at a concentration of 0.5 mM, while (R)-1,1-binaphthyl-2,2-diamine (BDA) was at 2.5 mM. The last sample contained 8.3% water by volume.

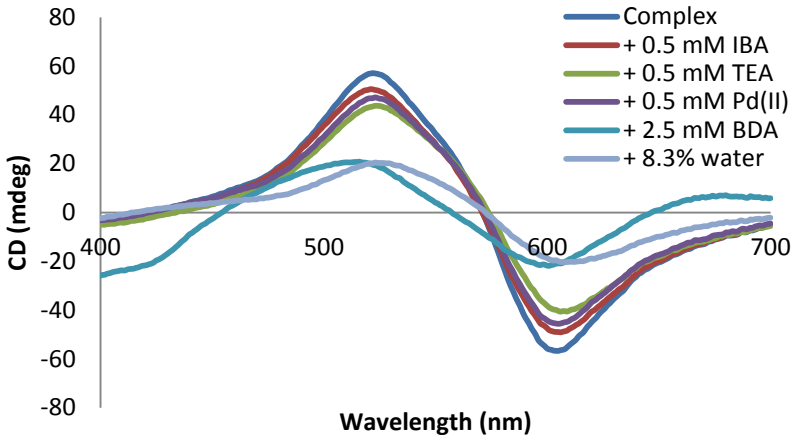


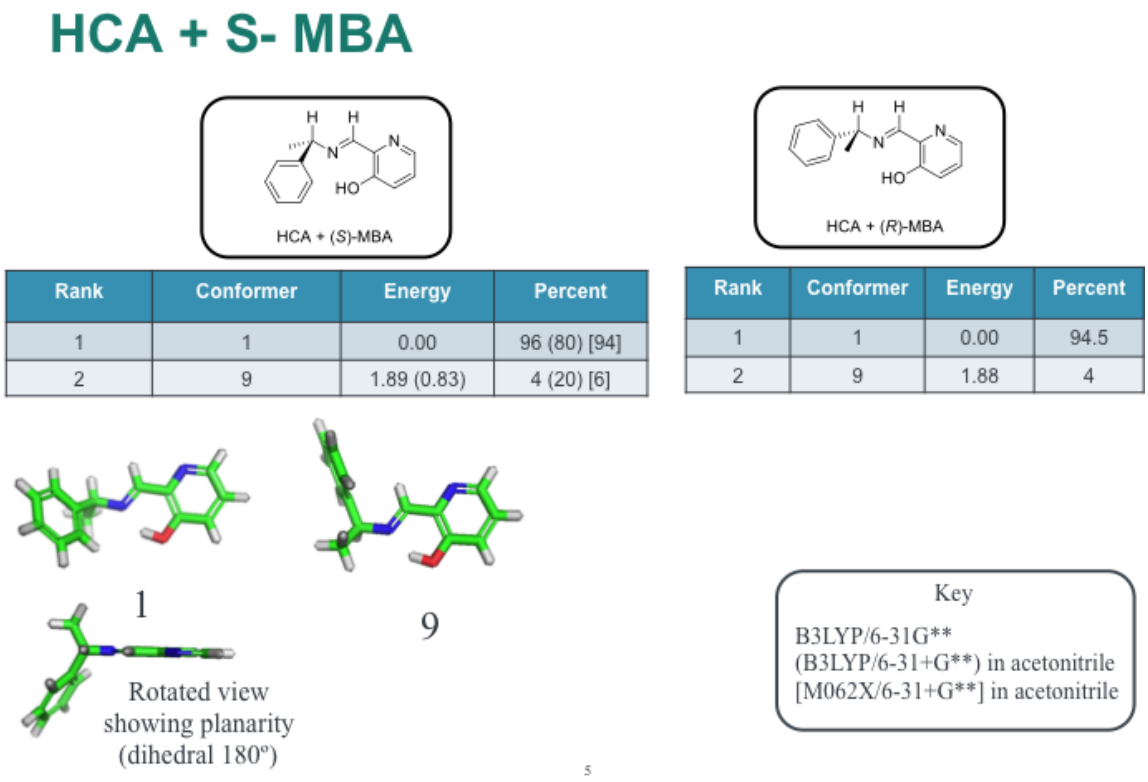

**Figure S1.** CD signals obtained for **HCA** (2 mM) and (*R*)-**MBA** (2 mM) with the indicated additive at the noted concentration. Samples were made in acetonitrile, with the CD signal recorded at 25°C.

*c) Computational method for CD Calculations*

Quantum chemical calculations were performed using Gaussian09.[1] Structures of the parent isomer of all structures were used for calculations in addition to tautomers when possible and both cis/trans forms of the imine [all parent isomers modeled with absolute configuration of (*R*) and (*S*)]. Conformational space was exhaustively sampled using three conformer generators (rules based and random displacement) followed by molecular mechanics minimization using MMFF94. The representative conformer sets (140 initial conformers per molecule) were minimized with higher level calculations to provide Boltzmann distributions for each structure at 298.15 K. Density functional theory (DFT) with the B3LYP functional[2] and the 6-31G** basis set[3-5] was used to identify the lowest energy conformers. All stationary points were confirmed with frequency calculations. To calculate ECD spectra, B3LYP geometries were used as input for M062X[6] calculations using the 6-31++G**[7,8] either *in vacuo* or in implicit solvent using Cramer and Truhlar's SMD continuum solvation methodology (solvent = acetonitrile). [9]

Only conformers which contributed more than 1.0% to the total *in vacuo* conformer distribution were sent for implicit solvation minimization or ECD. Time-dependent (TD-DFT) methodology[10] was employed using the keywords: TD=full,singlet,NStates=20 and integral=unltrafinegrid. Spectra were displayed using SpecDis.[11,12] We have used a $\sigma$ = 0.3 eV for band broadening. Final weighting of the conformer specific ECD spectra was done using the Boltzmann percentages calculated using M062X/6-31+G** energies. At that level of theory (*in vacuo* or implicit acetonitrile), neither the cis-imines, nor tautomers contribute to an appreciable level, and for this reason will not be included in the analysis.

***In vacuo* and implicit acetonitrile Boltzmann Populations and 3D Conformations:**




| Rank | Conformer | Energy | Percent |
|---|---|---|---|
| 1 | 1 | 0.00 | 96 (80) [94] |
| 2 | 9 | 1.89 (0.83) | 4 (20) [6] |

| Rank | Conformer | Energy | Percent |
|---|---|---|---|
| 1 | 1 | 0.00 | 94.5 |
| 2 | 9 | 1.88 | 4 |

**Figure S2:** Energies calculated at the M062X/6-31+G** level (*in vacuo* and acetonitrile) and reported in relative **Δ**G in kcal/mol.

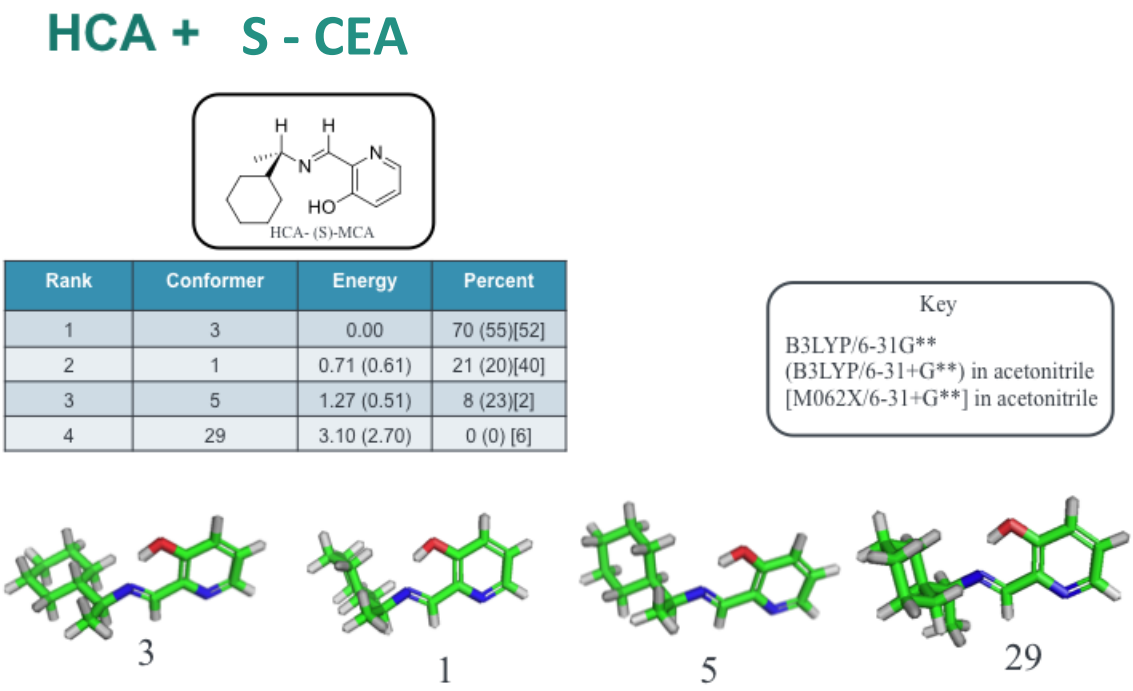
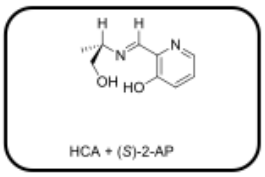
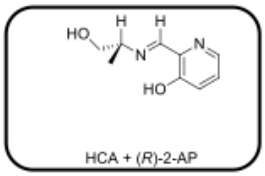



**Figure S3:** Energies calculated at the M062X/6-31+G** level (*in vacuo* and acetonitrile) and reported in relative **Δ**G in kcal/mol.

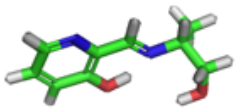
# HCA + S-2-AP



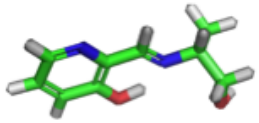

| Rank | Conformer | Energy | Percent |
|---|---|---|---|
| 1 | 1 | 0.0 | 95 (80)[62] |
| 2 | 37 | 1.73 (0.79) | 5 (20)[38] |




| Rank | Conformer | Energy | Percent |
|---|---|---|---|
| 1 | 1 | 0.0 | 96 |
| 2 | 37 | 1.84 | 4 |



1



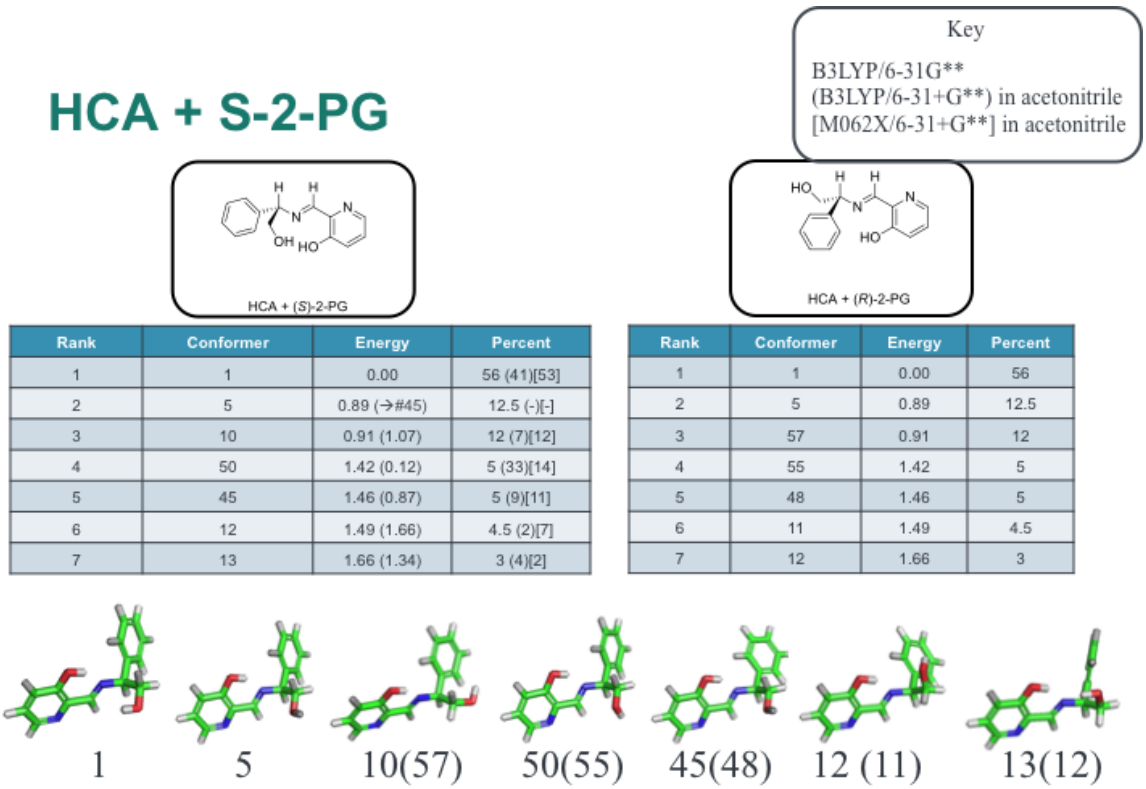
37

Key

B3LYP/6-31G**
(B3LYP/6-31+G**) in acetonitrile
[M062X/6-31+G**] in acetonitrile

The conformational modeling for this imine is analogous to what was seen for the other imines, and is in accordance with the model outlined in the paper (Figure 3C). The calculated CD signal for this imine, however, incorrectly predicts the sign of the signal (opposite of that observed).

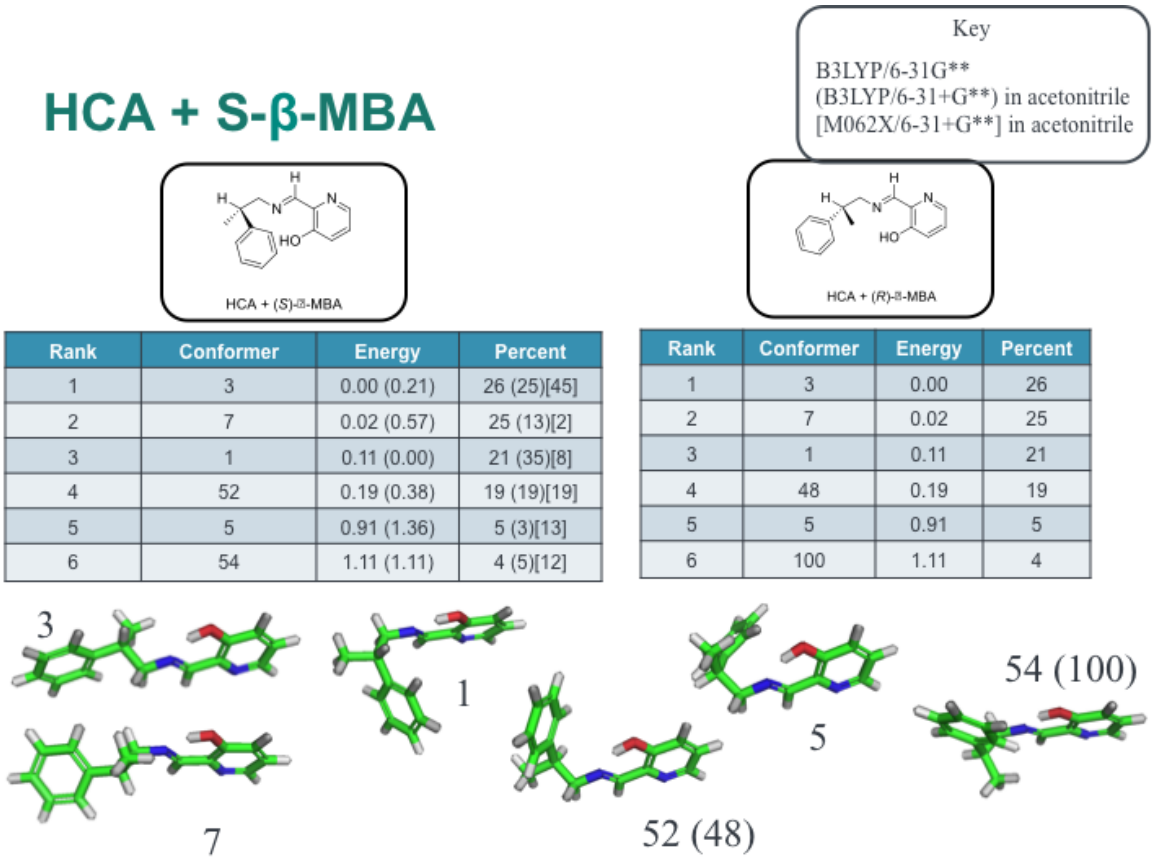
**Figure S4**: Energies calculated at the M062X/6-31+G** level (*in vacuo* and acetonitrile) and reported in relative **Δ**G in kcal/mol.




| Rank | Conformer | Energy | Percent |
|---|---|---|---|
| 1 | 1 | 0.00 | 56 (41)[53] |
| 2 | 5 | 0.89 (→#45) | 12.5 (-)[-] |
| 3 | 10 | 0.91 (1.07) | 12 (7)[12] |
| 4 | 50 | 1.42 (0.12) | 5 (33)[14] |
| 5 | 45 | 1.46 (0.87) | 5 (9)[11] |
| 6 | 12 | 1.49 (1.66) | 4.5 (2)[7] |
| 7 | 13 | 1.66 (1.34) | 3 (4)[2] |

| Rank | Conformer | Energy | Percent |
|---|---|---|---|
| 1 | 1 | 0.00 | 56 |
| 2 | 5 | 0.89 | 12.5 |
| 3 | 57 | 0.91 | 12 |
| 4 | 55 | 1.42 | 5 |
| 5 | 48 | 1.46 | 5 |
| 6 | 11 | 1.49 | 4.5 |
| 7 | 12 | 1.66 | 3 |

**Figure S5**: Energies calculated at the M062X/6-31+G** level (*in vacuo* and acetonitrile) and reported in relative **Δ**G in kcal/mol.

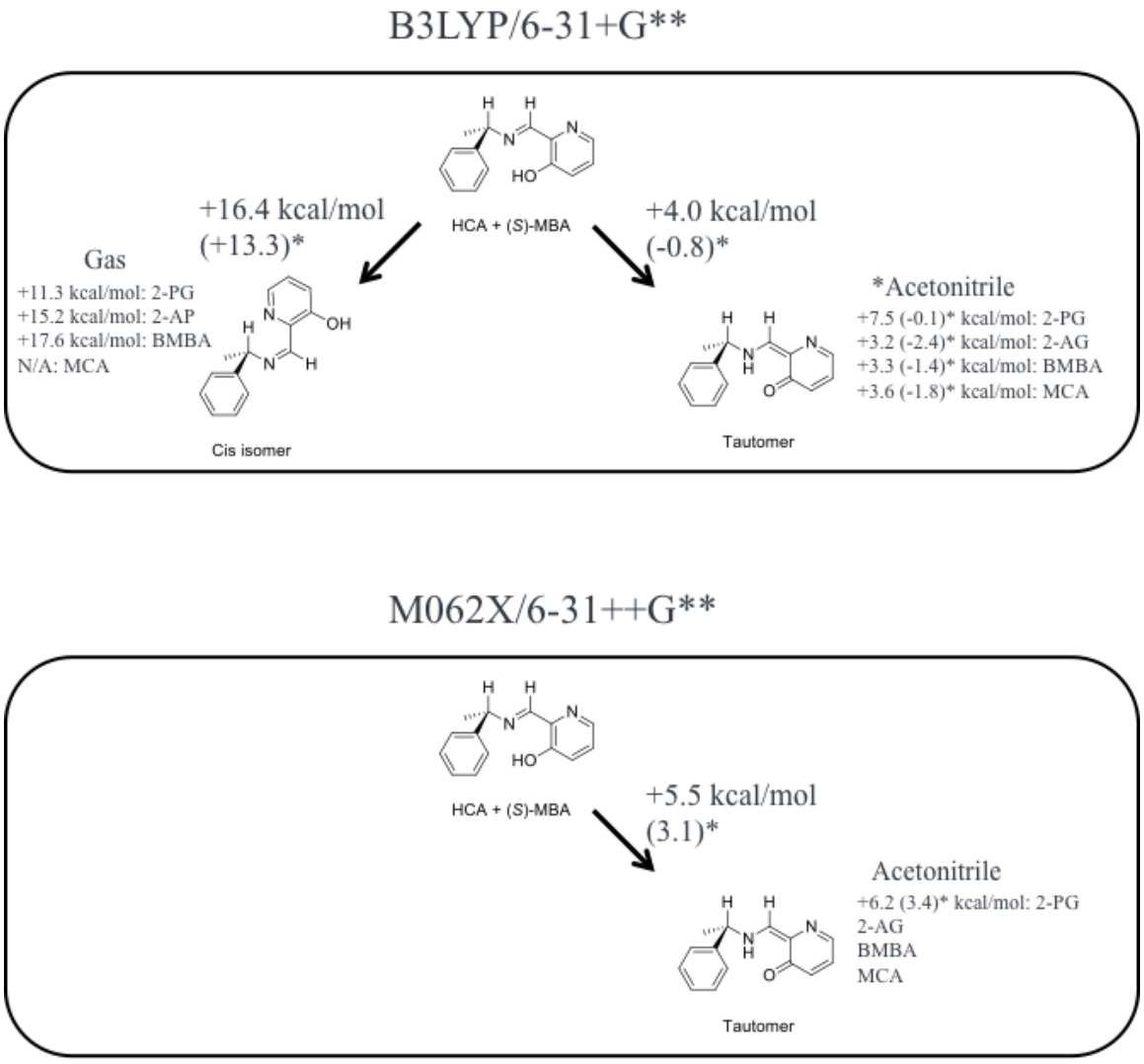



| Rank | Conformer | Energy | Percent |
|---|---|---|---|
| 1 | 3 | 0.00 (0.21) | 26 (25)[45] |
| 2 | 7 | 0.02 (0.57) | 25 (13)[2] |
| 3 | 1 | 0.11 (0.00) | 21 (35)[8] |
| 4 | 52 | 0.19 (0.38) | 19 (19)[19] |
| 5 | 5 | 0.91 (1.36) | 5 (3)[13] |
| 6 | 54 | 1.11 (1.11) | 4 (5)[12] |

| Rank | Conformer | Energy | Percent |
|---|---|---|---|
| 1 | 3 | 0.00 | 26 |
| 2 | 7 | 0.02 | 25 |
| 3 | 1 | 0.11 | 21 |
| 4 | 48 | 0.19 | 19 |
| 5 | 5 | 0.91 | 5 |
| 6 | 100 | 1.11 | 4 |

**Figure S6:** Energies calculated at the M062X/6-31+G** level (*in vacuo* and acetonitrile) and reported in relative **Δ**G in kcal/mol.

**Relative energies of tautomers and cis/trans imines:**




**Scheme S1**: Energies calculated at the B3LYP/6-31+G** or M062X/6-31+G** level (*in vacuo* and acetonitrile) and reported in relative **Δ**G in kcal/mol.

## Minima coordinates (xyz) for *in vacuo* structures (minimization of implicit acetonitrile did not alter coordinates considerably):

### Molecule HCA_S_MBA

***Conformer 1***

31
1 1 gaus C1 2.27438 -0.42185 -0.29393
2 1 gaus C2 2.56976 0.73760 0.46988
3 1 gaus C3 3.85343 1.29059 0.35067
4 1 gaus C4 4.76368 0.68263 -0.50037
5 1 gaus C5 4.38033 -0.46325 -1.21445
6 1 gaus N6 3.16961 -1.00348 -1.11559
7 1 gaus C7 0.95806 -1.05353 -0.22269
8 1 gaus N8 0.02038 -0.58710 0.51922
9 1 gaus H9 0.83455 -1.94831 -0.84621
10 1 gaus O10 1.67270 1.30398 1.28689
11 1 gaus C11 -1.27327 -1.27110 0.55087
12 1 gaus H12 -1.23803 -2.16016 -0.09865
13 1 gaus C13 -2.37445 -0.35415 0.03012
14 1 gaus C14 -1.55506 -1.73415 1.99097
15 1 gaus C15 -2.49401 0.96819 0.47806
16 1 gaus C16 -3.52829 1.78210 0.01793
17 1 gaus C17 -4.46152 1.28581 -0.89485
18 1 gaus C18 -4.34989 -0.02852 -1.34755
19 1 gaus C19 -3.31025 -0.83987 -0.88934
20 1 gaus H20 -1.58654 -0.87734 2.67014
21 1 gaus H21 -2.51947 -2.24772 2.04067
22 1 gaus H22 -0.77340 -2.41869 2.33442
23 1 gaus H23 4.09996 2.17719 0.92546
24 1 gaus H24 5.76538 1.08519 -0.61630
25 1 gaus H25 5.07971 -0.95553 -1.88623
26 1 gaus H26 -1.76779 1.36554 1.18043
27 1 gaus H27 -3.60442 2.80650 0.37109
28 1 gaus H28 -5.26635 1.92090 -1.25316
29 1 gaus H29 -5.06695 -0.42273 -2.06194
30 1 gaus H30 -3.22485 -1.86161 -1.25147
31 1 gaus H31 0.83924 0.75595 1.21925

***Conformer 9***

31
1 1 gaus C1 -1.92472 -0.40182 -0.08116
2 1 gaus C2 -2.91758 0.61299 -0.05198
3 1 gaus C3 -4.26023 0.21414 0.03005
4 1 gaus C4 -4.55075 -1.14075 0.07790
5 1 gaus C5 -3.50101 -2.07156 0.04371
6 1 gaus N6 -2.22247 -1.71497 -0.03324
7 1 gaus C7 -0.50292 -0.06674 -0.16804
8 1 gaus N8 -0.11087 1.15520 -0.21846
9 1 gaus H9 0.17688 -0.92359 -0.18440
10 1 gaus O10 -2.61003 1.91459 -0.10043
11 1 gaus C11 1.31026 1.52755 -0.33280
12 1 gaus H12 1.42353 1.90288 -1.35964
13 1 gaus C13 2.31704 0.40014 -0.14693
14 1 gaus C14 1.56574 2.71445 0.61069
15 1 gaus C15 2.53758 -0.18614 1.10866
16 1 gaus C16 3.46970 -1.21125 1.26355
17 1 gaus C17 4.20057 -1.66843 0.16469
18 1 gaus C18 3.98827 -1.09721 -1.08956
19 1 gaus C19 3.05043 -0.07408 -1.24101
20 1 gaus H20 1.43495 2.42364 1.65704
21 1 gaus H21 2.58472 3.09036 0.48382
22 1 gaus H22 0.86190 3.52343 0.39587
23 1 gaus H23 -5.03421 0.97421 0.05323
24 1 gaus H24 -5.57916 -1.48343 0.14120
25 1 gaus H25 -3.70730 -3.13884 0.08033
26 1 gaus H26 1.97453 0.15767 1.97178
27 1 gaus H27 3.62661 -1.65311 2.24329
28 1 gaus H28 4.92834 -2.46520 0.28666
29 1 gaus H29 4.55003 -1.44669 -1.95094
30 1 gaus H30 2.88859 0.36623 -2.22200
31 1 gaus H31 -1.61013 1.96633 -0.15765

## Molecule HCA_S_2AP

***Conformer 1***

25
1 1 gaus C1 1.26425 -0.52848 -0.04600
2 1 gaus C2 1.54710 0.83972 0.20380
3 1 gaus C3 2.88934 1.24640 0.18377
4 1 gaus C4 3.86689 0.29848 -0.07671
5 1 gaus C5 3.49097 -1.03415 -0.30871
6 1 gaus N6 2.22544 -1.43996 -0.29354
7 1 gaus C7 -0.11038 -1.02376 -0.04547
8 1 gaus N8 -1.11412 -0.24610 0.14851
9 1 gaus H9 -0.21999 -2.10175 -0.22040
10 1 gaus O10 0.58247 1.73468 0.45721
11 1 gaus C11 -2.46983 -0.79157 0.12930
12 1 gaus H12 -2.43987 -1.87571 -0.07190
13 1 gaus C13 -3.24137 -0.12587 -1.02844
14 1 gaus C14 -3.14479 -0.53585 1.48102
15 1 gaus O15 -3.36276 1.27724 -0.88067
16 1 gaus H16 -3.24472 0.53826 1.65334
17 1 gaus H17 -4.14533 -0.97973 1.49225
18 1 gaus H18 -2.56329 -0.97331 2.29713
19 1 gaus H19 -4.26128 -0.52342 -1.05340
20 1 gaus H20 -2.75480 -0.39080 -1.98012
21 1 gaus H21 3.12709 2.28798 0.37259
22 1 gaus H22 4.91550 0.57891 -0.10013
23 1 gaus H23 4.24301 -1.79282 -0.51241
24 1 gaus H24 -0.28114 1.23230 0.44369
25 1 gaus H25 -2.46527 1.63761 -0.87315

***Conformer 37***

25
1 1 gaus C1 1.28808 -0.52500 -0.09024
2 1 gaus C2 1.53808 0.84563 0.18902
3 1 gaus C3 2.87587 1.26956 0.22356
4 1 gaus C4 3.87709 0.34041 -0.01317
5 1 gaus C5 3.53058 -0.99293 -0.28183
6 1 gaus N6 2.27107 -1.41680 -0.32096
7 1 gaus C7 -0.07977 -1.03575 -0.14825
8 1 gaus N8 -1.08619 -0.27182 0.07168
9 1 gaus H9 -0.17773 -2.10227 -0.39231
10 1 gaus O10 0.55726 1.72619 0.41286
11 1 gaus C11 -2.43863 -0.80964 -0.00178
12 1 gaus H12 -2.41748 -1.84023 -0.39593
13 1 gaus C13 -3.26026 0.02690 -0.99052
14 1 gaus C14 -3.06799 -0.81800 1.39768
15 1 gaus O15 -3.40713 1.33969 -0.47228
16 1 gaus H16 -3.11321 0.19663 1.79795
17 1 gaus H17 -4.08547 -1.21996 1.35374
18 1 gaus H18 -2.47971 -1.44013 2.07787
19 1 gaus H19 -4.23713 -0.46513 -1.12915
20 1 gaus H20 -2.74543 0.03185 -1.96307
21 1 gaus H21 3.09065 2.31193 0.43482
22 1 gaus H22 4.92155 0.63665 0.00715
23 1 gaus H23 4.30098 -1.73695 -0.47121
24 1 gaus H24 -0.30946 1.22637 0.34380
25 1 gaus H25 -3.82105 1.88732 -1.15017

## Molecule HCA_2-PG

***Conformer 1***

32
1 1 gaus C1 -2.33516 0.07232 0.49746
2 1 gaus C2 -2.61380 -0.67133 -0.67888
3 1 gaus C3 -3.90607 -1.19542 -0.83237
4 1 gaus C4 -4.84051 -0.96266 0.16465
5 1 gaus C5 -4.47250 -0.21321 1.29364
6 1 gaus N6 -3.25447 0.29168 1.45827
7 1 gaus C7 -1.01114 0.64395 0.73183
8 1 gaus N8 -0.04818 0.49731 -0.10751

***Conformer 5***

32
1 1 gaus C1 -2.37250 0.14019 0.44176
2 1 gaus C2 -2.58623 -0.85921 -0.54341
3 1 gaus C3 -3.87308 -1.40605 -0.65435
4 1 gaus C4 -4.86627 -0.94836 0.19825
5 1 gaus C5 -4.55984 0.04331 1.14272
6 1 gaus N6 -3.34727 0.57506 1.26352
7 1 gaus C7 -1.05824 0.75663 0.61562
8 1 gaus N8 -0.04827 0.40740 -0.09552

9 1 gaus H9 -0.89850 1.19530 1.67335
10 1 gaus O10 -1.69304 -0.87946 -1.62926
11 1 gaus C11 1.24711 1.10581 0.18380
12 1 gaus H12 1.21112 1.62409 1.15402
13 1 gaus C13 1.52733 2.17943 -0.89389
14 1 gaus C14 2.35891 0.06949 0.21531
15 1 gaus C15 2.43667 -0.95408 -0.73854
16 1 gaus C16 3.49554 -1.86183 -0.71932
17 1 gaus C17 4.49421 -1.75800 0.25049
18 1 gaus C18 4.42567 -0.74182 1.20399
19 1 gaus C19 3.36393 0.16320 1.18553
20 1 gaus O20 0.56659 3.21691 -0.88438
21 1 gaus H21 1.59622 1.68747 -1.87597
22 1 gaus H22 2.49474 2.64401 -0.68336
23 1 gaus H23 -4.13955 -1.76792 -1.72391
24 1 gaus H24 -5.84949 -1.35408 0.07801
25 1 gaus H25 -5.19129 -0.01912 2.08626
26 1 gaus H26 1.65912 -1.05028 -1.48956
27 1 gaus H27 3.53862 -2.65289 -1.46239
28 1 gaus H28 5.31695 -2.46670 0.26526
29 1 gaus H29 5.19442 -0.65578 1.96643
30 1 gaus H30 3.31257 0.94902 1.93517
31 1 gaus H31 -0.85469 -0.43585 -1.31670
32 1 gaus H32 -0.28116 2.82517 -1.13503

9 1 gaus H9 -1.00080 1.52803 1.39193
10 1 gaus O10 -1.60836 -1.28377 -1.35409
11 1 gaus C11 1.22495 1.08984 0.10621
12 1 gaus H12 1.19392 1.69259 1.02680
13 1 gaus C13 1.45176 2.07664 -1.05205
14 1 gaus C14 2.37625 0.10029 0.20231
15 1 gaus C15 2.49991 -0.96360 -0.70095
16 1 gaus C16 3.58454 -1.83707 -0.62376
17 1 gaus C17 4.56268 -1.65893 0.35631
18 1 gaus C18 4.44784 -0.60300 1.26073
19 1 gaus C19 3.36042 0.26825 1.18313
20 1 gaus O20 0.46599 3.09210 -0.95389
21 1 gaus H21 1.38681 1.52821 -2.00321
22 1 gaus H22 2.46948 2.48614 -0.96463
23 1 gaus H23 -4.05745 -2.17129 -1.40113
24 1 gaus H24 -5.87311 -1.35069 0.13983
25 1 gaus H25 -5.32429 0.41565 1.82085
26 1 gaus H26 1.73877 -1.11737 -1.45944
27 1 gaus H27 3.66362 -2.66000 -1.32829
28 1 gaus H28 5.40531 -2.34139 0.41731
29 1 gaus H29 5.20002 -0.45970 2.03110
30 1 gaus H30 3.27218 1.08537 1.89492
31 1 gaus H31 -0.78748 -0.77221 -1.09876
32 1 gaus H32 0.46756 3.59916 -1.77471

***Conformer 10***

32
1 1 gaus C1 2.47706 0.25789 -0.45596
2 1 gaus C2 2.78713 -0.48988 0.71023
3 1 gaus C3 4.10430 -0.94739 0.86388
4 1 gaus C4 5.03134 -0.64847 -0.12250
5 1 gaus C5 4.63157 0.10073 -1.24066
6 1 gaus N6 3.38939 0.54321 -1.40580
7 1 gaus C7 1.12529 0.75957 -0.68874
8 1 gaus N8 0.16948 0.53733 0.14012
9 1 gaus H9 0.98783 1.32877 -1.61673
10 1 gaus O10 1.87242 -0.76210 1.65033
11 1 gaus C11 -1.15499 1.07415 -0.13225
12 1 gaus H12 -1.15823 1.65274 -1.06894
13 1 gaus C13 -1.51047 2.06038 1.01594
14 1 gaus C14 -2.20111 -0.02778 -0.23913
15 1 gaus C15 -3.37356 0.21100 -0.97199
16 1 gaus C16 -4.38192 -0.75240 -1.03970

***Conformer 50***

32
1 1 gaus C1 -2.38860 0.15802 0.41799
2 1 gaus C2 -2.57721 -0.93461 -0.46784
3 1 gaus C3 -3.86435 -1.48326 -0.56682
4 1 gaus C4 -4.88151 -0.93646 0.20049
5 1 gaus C5 -4.59850 0.14377 1.05061
6 1 gaus N6 -3.38620 0.67850 1.15894
7 1 gaus C7 -1.07732 0.78354 0.57292
8 1 gaus N8 -0.04488 0.36867 -0.06694
9 1 gaus H9 -1.04325 1.62258 1.27839
10 1 gaus O10 -1.57686 -1.44621 -1.19615
11 1 gaus C11 1.21601 1.07618 0.09739
12 1 gaus H12 1.18787 1.69849 1.00845
13 1 gaus C13 1.41115 2.03828 -1.10283
14 1 gaus C14 2.38749 0.11431 0.20577
15 1 gaus C15 3.36692 0.30815 1.18639
16 1 gaus C16 4.47439 -0.53728 1.26756

17 1 gaus C17 -4.22992 -1.97177 -0.37941
18 1 gaus C18 -3.06354 -2.22065 0.34613
19 1 gaus C19 -2.05796 -1.25653 0.41930
20 1 gaus O20 -2.76059 2.69090 0.82757
21 1 gaus H21 -0.76085 2.85709 1.03746
22 1 gaus H22 -1.45546 1.51872 1.97209
23 1 gaus H23 4.36263 -1.52129 1.74765
24 1 gaus H24 6.05913 -0.98733 -0.03525
25 1 gaus H25 5.34437 0.34698 -2.02419
26 1 gaus H26 -3.48994 1.15317 -1.50068
27 1 gaus H27 -5.28030 -0.55157 -1.61624
28 1 gaus H28 -5.01006 -2.72510 -0.43561
29 1 gaus H29 -2.93298 -3.17084 0.85601
30 1 gaus H30 -1.14935 -1.46476 0.97369
31 1 gaus H31 1.02095 -0.33196 1.35094
32 1 gaus H32 -3.44381 2.00819 0.88544

17 1 gaus C17 4.61492 -1.59222 0.36582
18 1 gaus C18 3.64250 -1.79529 -0.61532
19 1 gaus C19 2.53804 -0.94782 -0.69594
20 1 gaus O20 0.39757 3.02208 -1.18932
21 1 gaus H21 1.36356 1.46312 -2.03190
22 1 gaus H22 2.41494 2.48162 -1.03215
23 1 gaus H23 -4.03007 -2.31875 -1.23888
24 1 gaus H24 -5.88934 -1.33703 0.14802
25 1 gaus H25 -5.38218 0.58646 1.66112
26 1 gaus H26 3.25881 1.12377 1.89745
27 1 gaus H27 5.22204 -0.37459 2.03847
28 1 gaus H28 5.47333 -2.25441 0.42922
29 1 gaus H29 3.74231 -2.61701 -1.31853
30 1 gaus H30 1.78308 -1.11927 -1.45696
31 1 gaus H31 -0.76054 -0.91618 -0.97198
32 1 gaus H32 0.52775 3.65204 -0.46825

***Conformer 45***

32
1 1 gaus C1 2.36455 0.13306 -0.46973
2 1 gaus C2 2.61116 -0.73682 0.62481
3 1 gaus C3 3.90350 -1.26319 0.76552
4 1 gaus C4 4.86992 -0.91187 -0.16470
5 1 gaus C5 4.53242 -0.04269 -1.21367
6 1 gaus N6 3.31418 0.46781 -1.36449
7 1 gaus C7 1.04069 0.71520 -0.68234
8 1 gaus N8 0.05237 0.43553 0.08662
9 1 gaus H9 0.95549 1.39471 -1.53820
10 1 gaus O10 1.65907 -1.05779 1.51145
11 1 gaus C11 -1.23593 1.06836 -0.14885
12 1 gaus H12 -1.21648 1.63727 -1.09208
13 1 gaus C13 -1.49240 2.09053 0.97306
14 1 gaus C14 -2.36920 0.05068 -0.21068
15 1 gaus C15 -3.56503 0.40361 -0.85093
16 1 gaus C16 -4.64147 -0.48132 -0.89355
17 1 gaus C17 -4.53544 -1.73953 -0.29793
18 1 gaus C18 -3.34659 -2.10255 0.33467
19 1 gaus C19 -2.27028 -1.21437 0.37940
20 1 gaus O20 -0.52769 3.12294 0.84641
21 1 gaus H21 -1.42225 1.57244 1.94078
22 1 gaus H22 -2.51736 2.47651 0.86843
23 1 gaus H23 4.11299 -1.92998 1.59545
24 1 gaus H24 5.88012 -1.30208 -0.08606

***Conformer 12***

32
1 1 gaus C1 2.38927 -0.14213 -0.57257
2 1 gaus C2 2.68900 0.03773 0.80449
3 1 gaus C3 3.98576 -0.28147 1.23622
4 1 gaus C4 4.90119 -0.75158 0.30762
5 1 gaus C5 4.51235 -0.89245 -1.03401
6 1 gaus N6 3.29078 -0.59554 -1.46544
7 1 gaus C7 1.06079 0.16800 -1.09388
8 1 gaus N8 0.12260 0.57852 -0.32119
9 1 gaus H9 0.92967 0.02636 -2.17474
10 1 gaus O10 1.79131 0.49707 1.68399
11 1 gaus C11 -1.18501 0.90135 -0.86826
12 1 gaus H12 -1.16572 0.87182 -1.97063
13 1 gaus C13 -1.55154 2.35227 -0.45788
14 1 gaus C14 -2.24962 -0.07316 -0.37801
15 1 gaus C15 -2.18540 -0.65109 0.89805
16 1 gaus C16 -3.20817 -1.48985 1.34681
17 1 gaus C17 -4.30734 -1.75999 0.53162
18 1 gaus C18 -4.37789 -1.19020 -0.74111
19 1 gaus C19 -3.35647 -0.35393 -1.19033
20 1 gaus O20 -1.65126 2.53272 0.93849
21 1 gaus H21 -2.48204 2.62926 -0.97806
22 1 gaus H22 -0.76000 3.02696 -0.79808
23 1 gaus H23 4.23738 -0.15155 2.28360
24 1 gaus H24 5.91210 -1.00791 0.60979

25 1 gaus H25 5.27612 0.24632 -1.95274
26 1 gaus H26 -3.65100 1.37833 -1.32587
27 1 gaus H27 -5.55874 -0.19128 -1.39786
28 1 gaus H28 -5.37039 -2.43313 -0.33344
29 1 gaus H29 -3.25150 -3.08271 0.79312
30 1 gaus H30 -1.34391 -1.51214 0.85754
31 1 gaus H31 0.83460 -0.56506 1.22910
32 1 gaus H32 -0.53989 3.65151 1.65347

25 1 gaus H25 5.21657 -1.25727 -1.77817
26 1 gaus H26 -1.31955 -0.46666 1.52478
27 1 gaus H27 -3.14071 -1.93584 2.33491
28 1 gaus H28 -5.09985 -2.41483 0.88138
29 1 gaus H29 -5.22498 -1.40155 -1.38725
30 1 gaus H30 -3.41523 0.08132 -2.18514
31 1 gaus H31 0.95227 0.68861 1.17237
32 1 gaus H32 -2.35542 1.95116 1.25933

***Conformer 13***

32
1 1 gaus C1 2.34047 -0.24549 -0.47038
2 1 gaus C2 2.58975 0.07327 0.89005
3 1 gaus C3 3.87251 -0.17932 1.39812
4 1 gaus C4 4.82654 -0.72482 0.55319
5 1 gaus C5 4.48560 -1.01111 -0.77849
6 1 gaus N6 3.27667 -0.77969 -1.27939
7 1 gaus C7 1.03096 -0.00602 -1.07123
8 1 gaus N8 0.06929 0.53307 -0.41109
9 1 gaus H9 0.93086 -0.31986 -2.11795
10 1 gaus O10 1.64884 0.59684 1.68782
11 1 gaus C11 -1.22532 0.75246 -1.06330
12 1 gaus H12 -1.17070 0.43600 -2.11731
13 1 gaus C13 -1.49532 2.27597 -1.07348
14 1 gaus C14 -2.30002 -0.08493 -0.38100
15 1 gaus C15 -2.83521 0.26198 0.86821
16 1 gaus C16 -3.80689 -0.54125 1.46509
17 1 gaus C17 -4.25419 -1.70141 0.83019
18 1 gaus C18 -3.72554 -2.05513 -0.41126
19 1 gaus C19 -2.75422 -1.25126 -1.00897
20 1 gaus O20 -1.35888 2.89184 0.19504
21 1 gaus H21 -2.52137 2.45946 -1.40450
22 1 gaus H22 -0.81424 2.73559 -1.80717
23 1 gaus H23 4.08367 0.05692 2.43576
24 1 gaus H24 5.82923 -0.93282 0.91383
25 1 gaus H25 5.21913 -1.44168 -1.45610
26 1 gaus H26 -2.50092 1.17133 1.35407
27 1 gaus H27 -4.21678 -0.25805 2.43040
28 1 gaus H28 -5.01035 -2.32424 1.29926
29 1 gaus H29 -4.06771 -2.95430 -0.91547
30 1 gaus H30 -2.34482 -1.53316 -1.97623
31 1 gaus H31 0.81451 0.65863 1.14347
32 1 gaus H32 -0.46661 2.68532 0.50788

## Molecule HCA_BMBA

***Conformer 3***

34
1 1 gaus C1 -2.97266 -0.45551 -0.23929
2 1 gaus C2 -3.41886 0.88295 -0.07996
3 1 gaus C3 -4.79531 1.09807 0.08662
4 1 gaus C4 -5.64509 0.00265 0.08853
5 1 gaus C5 -5.11051 -1.28478 -0.07592
6 1 gaus N6 -3.81036 -1.51085 -0.23618
7 1 gaus C7 -1.55443 -0.75762 -0.41996
8 1 gaus N8 -0.66171 0.16531 -0.43657
9 1 gaus H9 -1.31292 -1.82129 -0.54272
10 1 gaus O10 -2.57761 1.92399 -0.08438
11 1 gaus C11 0.73497 -0.18993 -0.62473
12 1 gaus C12 1.62053 0.34549 0.52775
13 1 gaus H13 1.43459 1.42528 0.58562
14 1 gaus C14 3.09253 0.14927 0.19412
15 1 gaus C15 1.22927 -0.27202 1.88024
16 1 gaus C16 3.66525 -1.13004 0.13059
17 1 gaus C17 5.01162 -1.29797 -0.19256
18 1 gaus C18 5.81463 -0.18730 -0.45789
19 1 gaus C19 5.25936 1.09079 -0.39816
20 1 gaus C20 3.91091 1.25347 -0.07659
21 1 gaus H21 1.35662 -1.36014 1.87756
22 1 gaus H22 1.84978 0.13360 2.68445
23 1 gaus H23 0.18248 -0.05891 2.11446
24 1 gaus H24 1.07590 0.26707 -1.56191
25 1 gaus H25 0.86245 -1.27969 -0.72371
26 1 gaus H26 -5.15795 2.11327 0.20942
27 1 gaus H27 -6.71537 0.13429 0.21541
28 1 gaus H28 -5.76023 -2.15693 -0.07743
29 1 gaus H29 3.05697 -2.00627 0.33845
30 1 gaus H30 5.43441 -2.29777 -0.23558
31 1 gaus H31 6.86352 -0.31785 -0.70739
32 1 gaus H32 5.87446 1.96295 -0.60081
33 1 gaus H33 3.48610 2.25341 -0.03170
34 1 gaus H34 -1.65865 1.55066 -0.21659

***Conformer 7***

34
1 1 gaus C1 2.93079 -0.56094 -0.21731
2 1 gaus C2 3.46084 0.73655 0.01079
3 1 gaus C3 4.84040 0.84862 0.24052
4 1 gaus C4 5.61196 -0.30325 0.23349
5 1 gaus C5 4.99768 -1.54319 -0.00247
6 1 gaus N6 3.69296 -1.67195 -0.22230
7 1 gaus C7 1.50324 -0.75296 -0.46239
8 1 gaus N8 0.68228 0.23457 -0.47674
9 1 gaus H9 1.18932 -1.79078 -0.63434
10 1 gaus O10 2.69280 1.83287 0.00996
11 1 gaus C11 -0.73020 -0.01585 -0.70882
12 1 gaus C12 -1.59718 0.38682 0.51192
13 1 gaus H13 -1.25375 -0.22638 1.35514
14 1 gaus C14 -3.05442 0.03245 0.25172
15 1 gaus C15 -1.40709 1.86407 0.89636
16 1 gaus C16 -3.80429 0.69851 -0.72951
17 1 gaus C17 -5.13570 0.35899 -0.96818
18 1 gaus C18 -5.74602 -0.65513 -0.22787
19 1 gaus C19 -5.01308 -1.32615 0.75089
20 1 gaus C20 -3.68004 -0.98427 0.98435
21 1 gaus H21 -1.68718 2.53156 0.07425
22 1 gaus H22 -2.02952 2.11851 1.75909
23 1 gaus H23 -0.36423 2.06865 1.15188
24 1 gaus H24 -0.91546 -1.07303 -0.95177
25 1 gaus H25 -1.04035 0.58115 -1.57613
26 1 gaus H26 5.26646 1.83078 0.41678
27 1 gaus H27 6.68246 -0.25192 0.40759
28 1 gaus H28 5.58569 -2.45803 -0.01256
29 1 gaus H29 -3.34813 1.49435 -1.31237
30 1 gaus H30 -5.69782 0.88854 -1.73223
31 1 gaus H31 -6.78344 -0.91831 -0.41212
32 1 gaus H32 -5.47729 -2.11593 1.33470
33 1 gaus H33 -3.11604 -1.51214 1.74961
34 1 gaus H34 1.75882 1.52611 -0.18481

***Conformer 1***

34
1 1 gaus C1 -2.17284 -0.17970 -0.56972

***Conformer 52***

34
1 1 gaus C1 2.61383 0.52829 -0.08925

2 1 gaus C2 -2.70163 -0.48150 0.71304
3 1 gaus C3 -3.94668 0.06829 1.05342
4 1 gaus C4 -4.59509 0.87200 0.12818
5 1 gaus C5 -3.99341 1.11271 -1.11676
6 1 gaus N6 -2.81456 0.60232 -1.45924
7 1 gaus C7 -0.87939 -0.71296 -0.99176
8 1 gaus N8 -0.18563 -1.48124 -0.23236
9 1 gaus H9 -0.55104 -0.41303 -1.99472
10 1 gaus O10 -2.05538 -1.26134 1.58831
11 1 gaus C11 1.09991 -1.97351 -0.69368
12 1 gaus C12 2.25140 -1.52226 0.23753
13 1 gaus H13 1.96152 -1.81502 1.25428
14 1 gaus C14 2.42754 -0.01024 0.22935
15 1 gaus C15 3.54708 -2.27158 -0.12022
16 1 gaus C16 2.08919 0.74989 1.35558
17 1 gaus C17 2.23942 2.13765 1.36084
18 1 gaus C18 2.73047 2.79245 0.23165
19 1 gaus C19 3.06802 2.04879 -0.90066
20 1 gaus C20 2.91745 0.66229 -0.90011
21 1 gaus H21 3.86442 -2.06553 -1.14784
22 1 gaus H22 4.36250 -1.97273 0.54419
23 1 gaus H23 3.40935 -3.35403 -0.02607
24 1 gaus H24 1.30692 -1.65617 -1.72793
25 1 gaus H25 1.06179 -3.07070 -0.68544
26 1 gaus H26 -4.36870 -0.14931 2.02903
27 1 gaus H27 -5.55986 1.31313 0.35978
28 1 gaus H28 -4.48591 1.73966 -1.85652
29 1 gaus H29 1.70055 0.24802 2.23798
30 1 gaus H30 1.97062 2.70534 2.24711
31 1 gaus H31 2.84814 3.87209 0.23196
32 1 gaus H32 3.45002 2.54886 -1.78623
33 1 gaus H33 3.18760 0.10034 -1.79045
34 1 gaus H34 -1.20209 -1.54190 1.14538

2 1 gaus C2 2.45116 -0.87752 -0.20778
3 1 gaus C3 3.59544 -1.68000 -0.07849
4 1 gaus C4 4.81667 -1.06775 0.15679
5 1 gaus C5 4.87772 0.33079 0.25995
6 1 gaus N6 3.80730 1.10999 0.14085
7 1 gaus C7 1.46944 1.42836 -0.21119
8 1 gaus N8 0.28538 0.98810 -0.43762
9 1 gaus H9 1.69755 2.49642 -0.09646
10 1 gaus O10 1.26299 -1.44852 -0.43283
11 1 gaus C11 -0.81768 1.92678 -0.53432
12 1 gaus C12 -1.93396 1.60320 0.48680
13 1 gaus H13 -1.46402 1.60981 1.47846
14 1 gaus C14 -2.53016 0.21875 0.27211
15 1 gaus C15 -3.00356 2.71026 0.46553
16 1 gaus C16 -2.35644 -0.78592 1.23177
17 1 gaus C17 -2.90411 -2.05743 1.05246
18 1 gaus C18 -3.63780 -2.34698 -0.09734
19 1 gaus C19 -3.81696 -1.35646 -1.06492
20 1 gaus C20 -3.26809 -0.08798 -0.88079
21 1 gaus H21 -3.48073 2.79110 -0.51687
22 1 gaus H22 -3.78803 2.50312 1.19863
23 1 gaus H23 -2.56357 3.68476 0.70299
24 1 gaus H24 -1.23429 1.86107 -1.54823
25 1 gaus H25 -0.47533 2.96332 -0.38491
26 1 gaus H26 3.49411 -2.75674 -0.16581
27 1 gaus H27 5.72055 -1.66023 0.26154
28 1 gaus H28 5.82578 0.83061 0.44504
29 1 gaus H29 -1.78332 -0.56963 2.12980
30 1 gaus H30 -2.75386 -2.82052 1.81072
31 1 gaus H31 -4.06459 -3.33526 -0.24082
32 1 gaus H32 -4.38509 -1.57187 -1.96550
33 1 gaus H33 -3.41906 0.66949 -1.64576
34 1 gaus H34 0.58820 -0.71230 -0.49084

***Conformer 5***

34
1 1 gaus C1 -2.19190 0.01878 0.64034
2 1 gaus C2 -2.61925 -0.42900 -0.63740
3 1 gaus C3 -3.81542 0.09522 -1.14887
4 1 gaus C4 -4.51873 1.01472 -0.38544
5 1 gaus C5 -4.01810 1.39538 0.86929
6 1 gaus N6 -2.88482 0.91371 1.37065
7 1 gaus C7 -0.94608 -0.47139 1.22579

***Conformer 54***

34
1 1 gaus C1 2.61884 -0.43198 -0.23421
2 1 gaus C2 2.42466 0.97128 -0.14092
3 1 gaus C3 3.55046 1.77249 0.10141
4 1 gaus C4 4.78720 1.16030 0.23629
5 1 gaus C5 4.88056 -0.23578 0.12668
6 1 gaus N6 3.82686 -1.01353 -0.10209
7 1 gaus C7 1.49202 -1.32939 -0.47948

8 1 gaus N8 -0.22022 -1.34591 0.62809
9 1 gaus H9 -0.67861 -0.03869 2.19791
10 1 gaus O10 -1.91795 -1.31867 -1.35309
11 1 gaus C11 1.02317 -1.78283 1.23595
12 1 gaus C12 2.24508 -1.62083 0.29186
13 1 gaus H13 3.09181 -2.02174 0.86459
14 1 gaus C14 2.55944 -0.15998 -0.00001
15 1 gaus C15 2.10554 -2.47694 -0.97836
16 1 gaus C16 3.63039 0.46788 0.65017
17 1 gaus C17 3.93585 1.80856 0.41227
18 1 gaus C18 3.16975 2.54968 -0.48732
19 1 gaus C19 2.09920 1.93887 -1.14235
20 1 gaus C20 1.79676 0.59840 -0.90163
21 1 gaus H21 1.26057 -2.16152 -1.59584
22 1 gaus H22 3.00998 -2.40669 -1.58944
23 1 gaus H23 1.95071 -3.52973 -0.71826
24 1 gaus H24 0.92233 -2.85114 1.47135
25 1 gaus H25 1.21503 -1.24886 2.17897
26 1 gaus H26 -4.15929 -0.23185 -2.12459
27 1 gaus H27 -5.44894 1.43931 -0.75064
28 1 gaus H28 -4.55471 2.11515 1.48311
29 1 gaus H29 4.23679 -0.10354 1.34939
30 1 gaus H30 4.77371 2.27076 0.92664
31 1 gaus H31 3.40483 3.59279 -0.67777
32 1 gaus H32 1.49523 2.50724 -1.84398
33 1 gaus H33 0.95654 0.14294 -1.41566
34 1 gaus H34 -1.13124 -1.57884 -0.78795

8 1 gaus N8 0.29499 -0.88744 -0.62058
9 1 gaus H9 1.74380 -2.39667 -0.53445
10 1 gaus O10 1.21941 1.53934 -0.27526
11 1 gaus C11 -0.78892 -1.82404 -0.85574
12 1 gaus C12 -1.91342 -1.72947 0.21178
13 1 gaus H13 -2.61555 -2.52896 -0.05900
14 1 gaus C14 -2.68857 -0.42052 0.13095
15 1 gaus C15 -1.38096 -2.04052 1.61936
16 1 gaus C16 -2.19018 0.78157 0.65540
17 1 gaus C17 -2.91840 1.96681 0.54603
18 1 gaus C18 -4.16306 1.97475 -0.08515
19 1 gaus C19 -4.67331 0.78669 -0.60830
20 1 gaus C20 -3.94063 -0.39575 -0.49890
21 1 gaus H21 -0.63882 -1.30631 1.94468
22 1 gaus H22 -2.19515 -2.04206 2.34949
23 1 gaus H23 -0.90213 -3.02588 1.64172
24 1 gaus H24 -0.41440 -2.86015 -0.88678
25 1 gaus H25 -1.22499 -1.59577 -1.83613
26 1 gaus H26 3.42485 2.84762 0.17592
27 1 gaus H27 5.67844 1.75140 0.42387
28 1 gaus H28 5.84125 -0.73525 0.22860
29 1 gaus H29 -1.22201 0.80061 1.14429
30 1 gaus H30 -2.50919 2.88600 0.95529
31 1 gaus H31 -4.72988 2.89760 -0.16686
32 1 gaus H32 -5.64286 0.77748 -1.09836
33 1 gaus H33 -4.34894 -1.31781 -0.90668
34 1 gaus H34 0.56960 0.80168 -0.46606

## Molecule HCA_CEA

***Conformer 3***

37
1 1 gaus C1 -2.45675 0.10936 -0.46876
2 1 gaus C2 -2.80176 -0.13106 0.88746
3 1 gaus C3 -4.10065 -0.58498 1.16148
4 1 gaus C4 -4.97693 -0.77512 0.10386
5 1 gaus C5 -4.54485 -0.51010 -1.20475
6 1 gaus N6 -3.31881 -0.07956 -1.48659
7 1 gaus C7 -1.12184 0.58392 -0.83063
8 1 gaus N8 -0.21697 0.79900 0.05377
9 1 gaus H9 -0.95460 0.74074 -1.90418
10 1 gaus O10 -1.93713 0.05981 1.89149

***Conformer 1***

37
1 1 gaus C1 -2.31601 0.23627 -0.41307
2 1 gaus C2 -2.48949 -0.38090 0.85397
3 1 gaus C3 -3.71404 -1.01576 1.11015
4 1 gaus C4 -4.68743 -1.00815 0.12264
5 1 gaus C5 -4.42470 -0.36935 -1.09909
6 1 gaus N6 -3.27112 0.23691 -1.36301
7 1 gaus C7 -1.06373 0.91024 -0.75219
8 1 gaus N8 -0.08246 0.96789 0.07329
9 1 gaus H9 -1.02571 1.35703 -1.75427
10 1 gaus O10 -1.53334 -0.37082 1.79106

11 1 gaus C11 1.09645 1.29642 -0.35456
12 1 gaus H12 1.15439 1.32504 -1.45696
13 1 gaus C13 2.19441 0.33185 0.16237
14 1 gaus C14 1.24009 2.72929 0.18160
15 1 gaus C15 3.61564 0.82256 -0.18099
16 1 gaus C16 4.70014 -0.15390 0.30271
17 1 gaus C17 4.47541 -1.57280 -0.23519
18 1 gaus C18 3.06767 -2.07298 0.11308
19 1 gaus C19 1.98463 -1.09889 -0.37317
20 1 gaus H20 1.23883 2.73490 1.27660
21 1 gaus H21 2.16524 3.19379 -0.16761
22 1 gaus H22 0.40367 3.34573 -0.16000
23 1 gaus H23 -4.38506 -0.77505 2.19117
24 1 gaus H24 -5.98916 -1.12558 0.28143
25 1 gaus H25 -5.21658 -0.65267 -2.04815
26 1 gaus H26 3.79917 1.80914 0.25691
27 1 gaus H27 4.69426 -0.17990 1.40169
28 1 gaus H28 5.23496 -2.25598 0.16323
29 1 gaus H29 2.98465 -2.18983 1.20298
30 1 gaus H30 0.99551 -1.46477 -0.08042
31 1 gaus H31 -1.08452 0.38382 1.47902
32 1 gaus H32 1.99371 -1.06944 -1.47370
33 1 gaus H33 2.09970 0.30090 1.25916
34 1 gaus H34 3.69871 0.94378 -1.27167
35 1 gaus H35 5.68932 0.21600 0.00741
36 1 gaus H36 4.59945 -1.57038 -1.32763
37 1 gaus H37 2.89591 -3.06626 -0.31840

11 1 gaus C11 1.14911 1.65473 -0.30796
12 1 gaus H12 1.05658 2.02143 -1.34491
13 1 gaus C13 2.35505 0.67793 -0.28187
14 1 gaus C14 1.33893 2.87134 0.60985
15 1 gaus C15 2.22779 -0.40543 -1.36992
16 1 gaus C16 3.45128 -1.33340 -1.40791
17 1 gaus C17 3.71577 -1.96982 -0.03601
18 1 gaus C18 3.84296 -0.89785 1.05541
19 1 gaus C19 2.61473 0.02631 1.09087
20 1 gaus H20 1.35209 2.57773 1.66288
21 1 gaus H21 2.28009 3.38147 0.38035
22 1 gaus H22 0.52049 3.58421 0.47293
23 1 gaus H23 -3.86764 -1.49449 2.07165
24 1 gaus H24 -5.64619 -1.49005 0.28854
25 1 gaus H25 -5.17526 -0.35137 -1.88597
26 1 gaus H26 2.08264 0.06661 -2.35060
27 1 gaus H27 4.33505 -0.75585 -1.71485
28 1 gaus H28 4.62054 -2.58846 -0.07058
29 1 gaus H29 4.74370 -0.29608 0.86674
30 1 gaus H30 2.75409 0.79313 1.86124
31 1 gaus H31 -0.76105 0.13780 1.40491
32 1 gaus H32 1.73218 -0.55666 1.38419
33 1 gaus H33 3.23384 1.29390 -0.53025
34 1 gaus H34 1.32710 -1.00282 -1.17502
35 1 gaus H35 3.30901 -2.11007 -2.16881
36 1 gaus H36 2.88509 -2.64407 0.21588
37 1 gaus H37 3.98381 -1.36747 2.03620

***Conformer 5***

37
1 1 gaus C1 2.53081 -0.44478 -0.27955
2 1 gaus C2 2.78428 0.74865 0.44721
3 1 gaus C3 4.06397 1.31505 0.34903
4 1 gaus C4 5.01115 0.68667 -0.44517
5 1 gaus C5 4.66785 -0.49207 -1.12505
6 1 gaus N6 3.46121 -1.04522 -1.04657
7 1 gaus C7 1.21810 -1.08671 -0.22919
8 1 gaus N8 0.25537 -0.60018 0.46606
9 1 gaus H9 1.11931 -2.00409 -0.82431
10 1 gaus O10 1.85161 1.33332 1.20925
11 1 gaus C11 -1.04470 -1.26847 0.47448
12 1 gaus H12 -0.98463 -2.19169 -0.12745
13 1 gaus C13 -2.09541 -0.35278 -0.21218

***Conformer 29***

37
1 1 gaus C1 -2.32002 0.40475 0.07808
2 1 gaus C2 -2.42191 -0.90782 -0.45436
3 1 gaus C3 -3.62247 -1.60487 -0.25222
4 1 gaus C4 -4.64326 -0.98313 0.45096
5 1 gaus C5 -4.45064 0.31873 0.93790
6 1 gaus N6 -3.32086 0.99689 0.75781
7 1 gaus C7 -1.09849 1.19299 -0.09110
8 1 gaus N8 -0.08249 0.71747 -0.71560
9 1 gaus H9 -1.13600 2.19357 0.34956
10 1 gaus O10 -1.42038 -1.48053 -1.13309
11 1 gaus C11 1.16023 1.46982 -0.90134
12 1 gaus H12 1.30490 1.50446 -1.99176
13 1 gaus C13 2.35816 0.64492 -0.34667

| | |
|---|---|
| 14 1 gaus C14 -1.37754 -1.66166 1.92088 | 14 1 gaus C14 1.14996 2.91844 -0.39779 |
| 15 1 gaus C15 -2.31523 1.00127 0.48893 | 15 1 gaus C15 2.29621 0.40573 1.17390 |
| 16 1 gaus C16 -3.30116 1.88249 -0.29505 | 16 1 gaus C16 3.52617 -0.36730 1.67861 |
| 17 1 gaus C17 -4.63805 1.16561 -0.53208 | 17 1 gaus C17 3.71752 -1.69031 0.92378 |
| 18 1 gaus C18 -4.42929 -0.19492 -1.21333 | 18 1 gaus C18 3.77261 -1.46011 -0.59306 |
| 19 1 gaus C19 -3.44110 -1.07195 -0.42783 | 19 1 gaus C19 2.53611 -0.69428 -1.08793 |
| 20 1 gaus H20 -1.40417 -0.78540 2.57426 | 20 1 gaus H20 1.00880 2.98959 0.68486 |
| 21 1 gaus H21 -2.34455 -2.16869 1.97947 | 21 1 gaus H21 2.10507 3.39396 -0.63915 |
| 22 1 gaus H22 -0.61489 -2.34355 2.30821 | 22 1 gaus H22 0.35886 3.50144 -0.87987 |
| 23 1 gaus H23 4.27898 2.22730 0.89571 | 23 1 gaus H23 -3.72130 -2.60932 -0.65052 |
| 24 1 gaus H24 6.01104 1.09860 -0.54272 | 24 1 gaus H24 -5.58524 -1.49448 0.62479 |
| 25 1 gaus H25 5.39659 -1.00052 -1.75216 | 25 1 gaus H25 -5.23913 0.82437 1.49065 |
| 26 1 gaus H26 -1.35943 1.52194 0.60890 | 26 1 gaus H26 1.38747 -0.16454 1.40768 |
| 27 1 gaus H27 -2.85588 2.14664 -1.26470 | 27 1 gaus H27 3.43350 -0.55224 2.75546 |
| 28 1 gaus H28 -5.30610 1.79313 -1.13405 | 28 1 gaus H28 2.88047 -2.36364 1.15626 |
| 29 1 gaus H29 -4.04169 -0.03585 -2.22951 | 29 1 gaus H29 3.85652 -2.41714 -1.12141 |
| 30 1 gaus H30 -3.28089 -2.02289 -0.95231 | 30 1 gaus H30 2.60893 -0.51565 -2.16857 |
| 31 1 gaus H31 1.03066 0.76205 1.14272 | 31 1 gaus H31 -0.67993 -0.80190 -1.16290 |
| 32 1 gaus H32 -3.88639 -1.32210 0.54481 | 32 1 gaus H32 1.64478 -1.31471 -0.93167 |
| 33 1 gaus H33 -1.68192 -0.13667 -1.20964 | 33 1 gaus H33 3.25172 1.25436 -0.55361 |
| 34 1 gaus H34 -2.71384 0.83393 1.49898 | 34 1 gaus H34 2.21681 1.35701 1.71268 |
| 35 1 gaus H35 -3.46486 2.82653 0.23798 | 35 1 gaus H35 4.42254 0.25565 1.54682 |
| 36 1 gaus H36 -5.14120 1.01156 0.43329 | 36 1 gaus H36 4.62850 -2.19508 1.26695 |
| 37 1 gaus H37 -5.38705 -0.71719 -1.32450 | 37 1 gaus H37 4.67820 -0.88738 -0.83951 |

**Calculation of CD Spectra:**

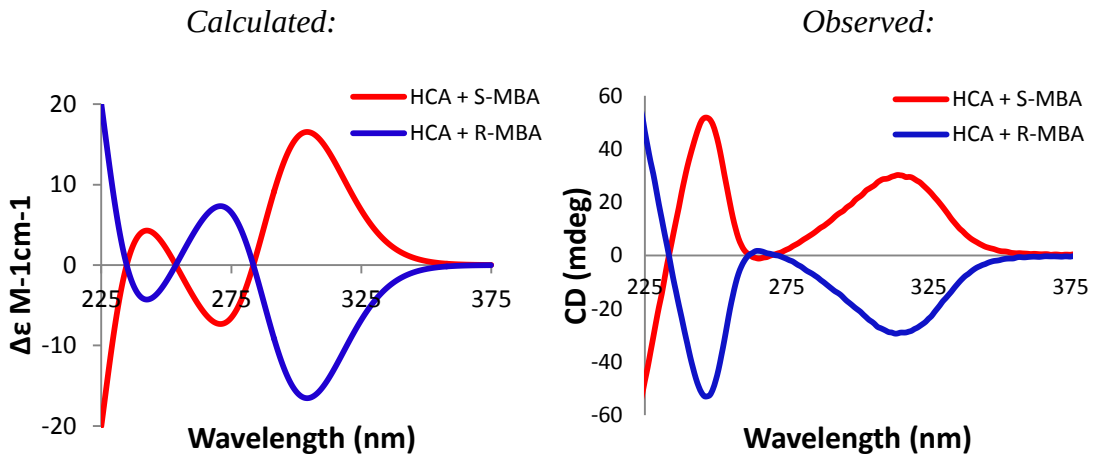



**Figure S7**: Calculated (left) and observed (right) CD spectra for the imine complexes formed between **HCA** (2 mM) and each enantiomer of **MBA** (2 mM).

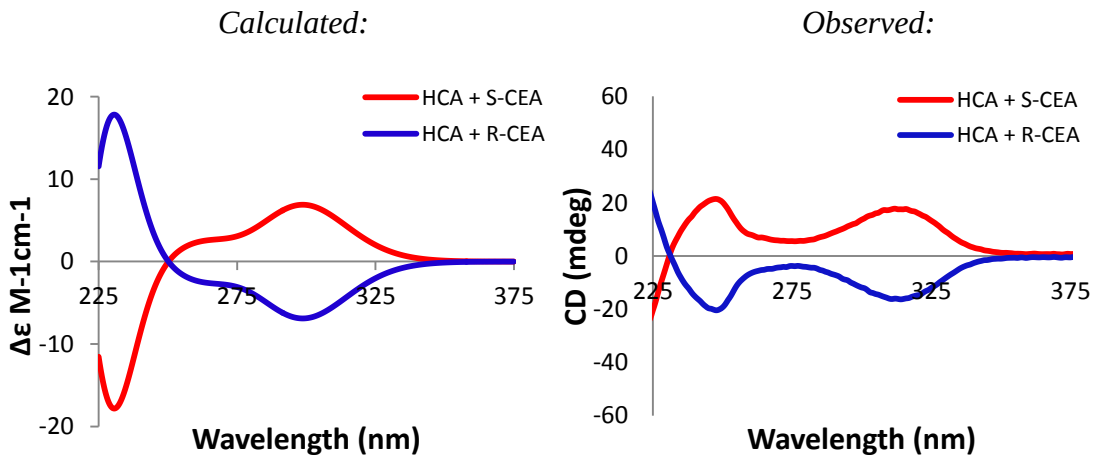



**Figure S8**: Calculated (left) and observed (right) CD spectra for the imine complexes formed between **HCA** (2 mM) and each enantiomer of **CEA** (2 mM).

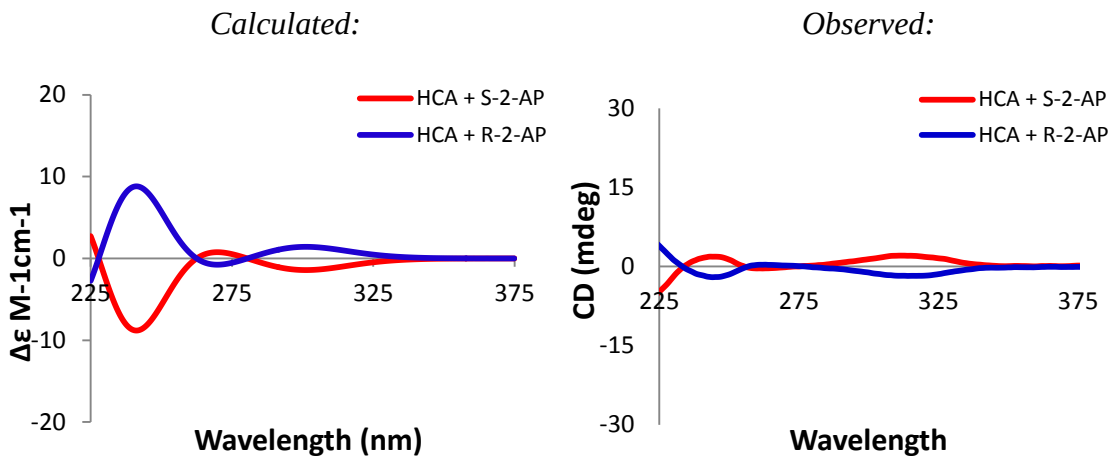



**Figure S9**: Calculated (left) and observed (right) CD spectra for the imine complexes formed between **HCA** (2 mM) and each enantiomer of **2-AP** (2 mM).

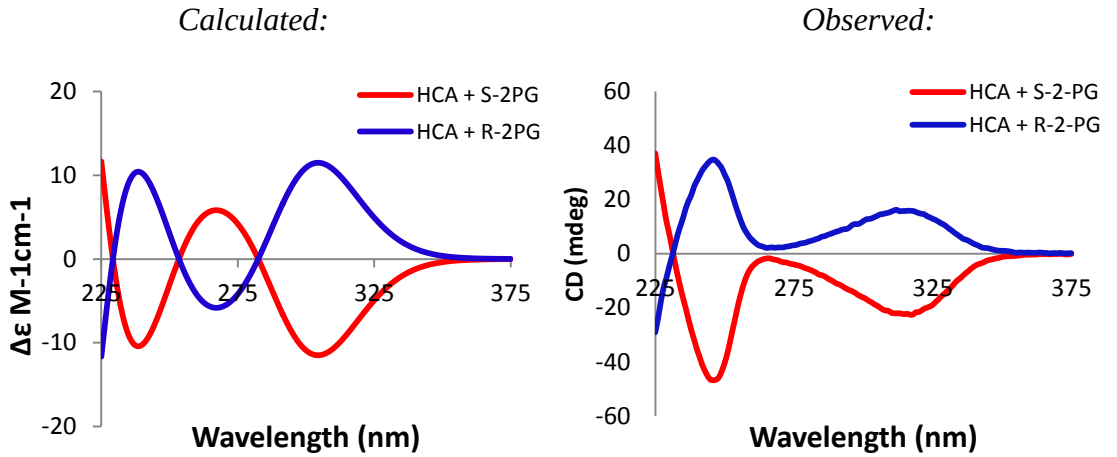



**Figure S10**: Calculated (left) and observed (right) CD spectra for the imine complexes formed between **HCA** (2 mM) and each enantiomer of **2-PG** (2 mM).

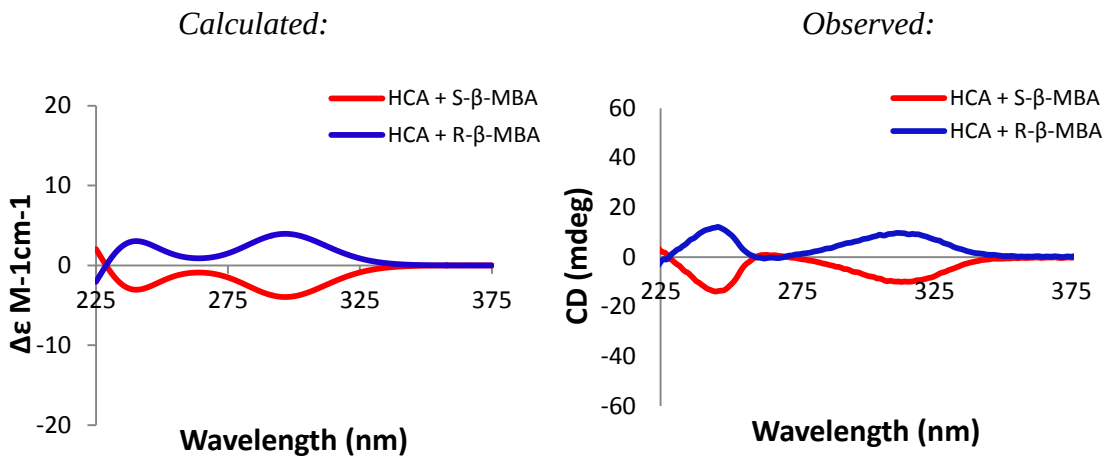



**Figure S11**: Calculated (left) and observed (right) CD spectra for the imine complexes formed between **HCA** (2 mM) and each enantiomer of **β-MBA** (2 mM).

*d) Unknown ee Calculations: Stand-Alone CD Spectrophotometer*

**MBA:**

Eight test solutions of 1 mL were independently made for the **MBA** guest (2 mM total amine content per vial) with **HCA** (2 mM) in acetonitrile. These solutions were transferred to the 0.1 cm jacketed CD cell, which was maintained at 25°C by a water circulation bath, and the CD spectrum recorded. Two standards were also created, representing either pure (*R*)-**MBA** or (*S*)-**MBA** (2 mM) with **HCA** (2 mM). These standards were used to create a 2-point calibration curve,[13] which is pictured below. The best-fit trendline of this plot was used to relate the measured CD signal at 317 nm of the unknown guest to the *ee* of the sample. The results of this analysis, along with the errors, are also shown below in **Figure S12** and **Table S1**.

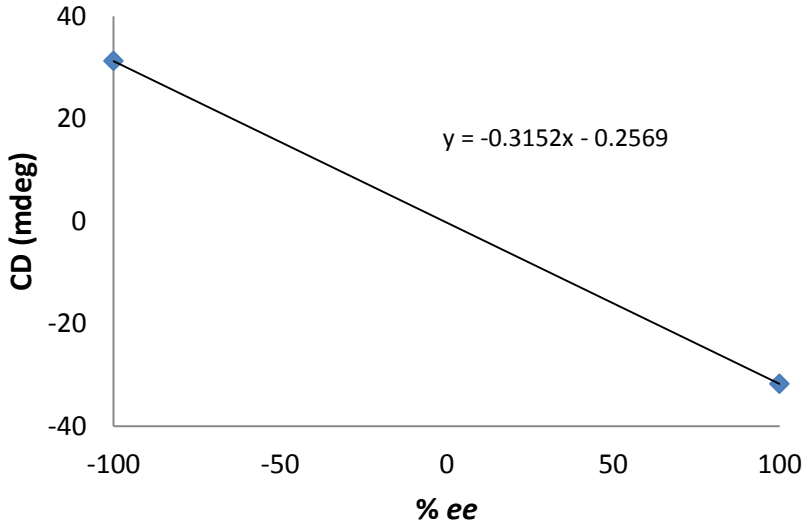



**Figure S12.** Calibration curve for **MBA** (2 mM) and **HCA** (2 mM) in acetonitrile at 25°C, measured by the stand alone CD spectrophotometer.

| **Unknown** | **$CD_{317nm}$** | **% *ee* $_{calc}$** | **% *ee* $_{actual}$** | **% Error** |
|---|---|---|---|---|
| 1 | -28.0 | 90.7 | 90.0 | 0.7 |
| 2 | 11.1 | -35.2 | -40.0 | 4.8 |
| 3 | -5.3 | 17.3 | 20.0 | 2.7 |
| 4 | 23.2 | -74.3 | -75.0 | 0.7 |
| 5 | 4.1 | -13.0 | -10.0 | 3.0 |
| 6 | 26.2 | -83.9 | -85.0 | 1.1 |
| 7 | -9.9 | 32.2 | 35.0 | 2.8 |
| 8 | -0.02 | 0.4 | 0.0 | 0.4 |

**Table S1**. Results of the stand alone CD spectrophotometer analysis of the eight unknown samples of **MBA**. The average error was determined to be 2.0%.

**MPP:**

Eight test solutions of 1 mL were independently made for the **MPP** guest (2 mM total amine content per vial) with **HCA** (2 mM) in acetonitrile. These solutions were transferred to the 0.1 cm jacketed CD cell, which was maintained at 25°C by a water circulation bath, and the CD spectrum recorded. Two standards were also created, representing either pure (*R*)-**MPP** or (*S*)-**MPP** (2 mM) with **HCA** (2 mM). These standards were used to create a 2-point calibration curve,[13] which is pictured below. The best-fit trendline of this plot was used to relate the measured CD signal at 317 nm of the unknown guest to the *ee* of the sample. The results of this analysis, along with the errors, are also shown below in **Figure S13** and **Table S2**.

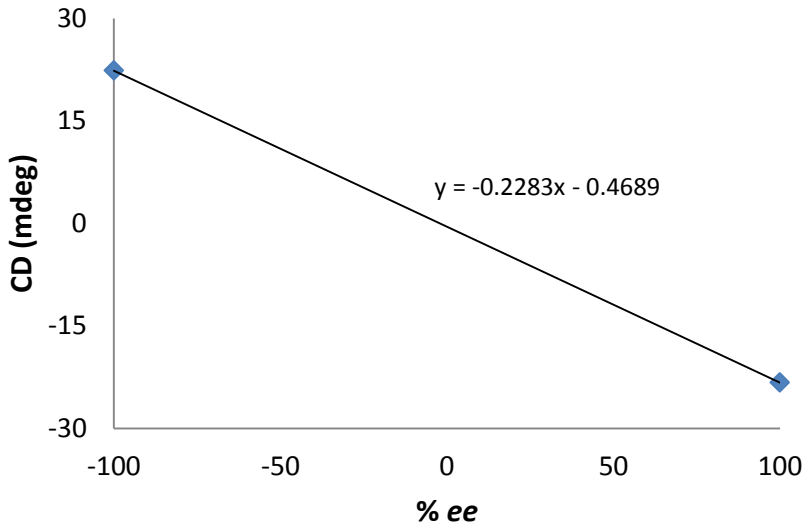



**Figure S13.** Calibration curve for **MPP** (2 mM) and **HCA** (2 mM) in acetonitrile at 25°C, measured by the stand alone CD spectrophotometer.

| Unknown | $CD_{317nm}$ (mdeg) | % *ee* $_{calc}$ | % *ee* $_{actual}$ | % Error |
|---|---|---|---|---|
| 1 | -18.5 | 79.0 | 80.0 | 1.0 |
| 2 | -8.9 | 37.0 | 38.5 | 1.5 |
| 3 | 20.4 | -91.5 | -90.0 | 1.5 |
| 4 | 1.34 | -7.9 | 0.0 | 7.9 |
| 5 | -5.4 | 21.6 | 25.0 | 3.4 |
| 6 | -3.4 | 12.7 | 15.0 | 2.3 |
| 7 | 12.4 | -56.6 | -50.0 | 6.6 |
| 8 | 10.9 | -50.0 | -45.1 | 5.0 |

**Table S2.** Results of the stand alone CD spectrophotometer analysis of the eight unknown samples of **MPP**. The average error was determined to be 3.6%.

**AMH:**

Eight test solutions of 1 mL were independently made for the **AMH** guest (2 mM total amine content per vial) with **HCA** (2 mM) in acetonitrile. These solutions were transferred to the 0.1 cm jacketed CD cell, which was maintained at 25°C by a water circulation bath, and the CD spectrum recorded. Two standards were also created, representing either pure (*R*)-**AMH** or (*S*)-**AMH** (2 mM) with **HCA** (2 mM). These standards were used to create a 2-point calibration curve,[13] which is pictured below. The best-fit trendline of this plot was used to relate the measured CD signal at 317 nm of the unknown guest to the *ee* of the sample. The results of this analysis, along with the errors, are also shown below in **Figure S14** and **Table S3**.

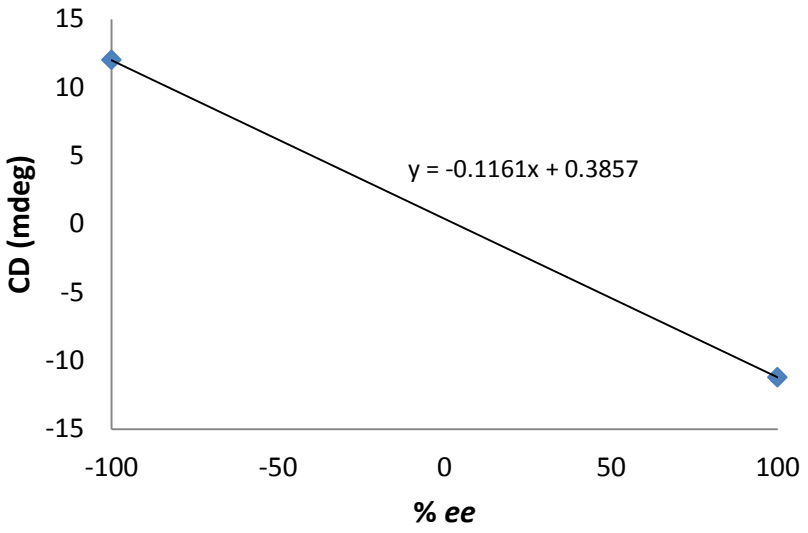



**Figure S14.** Calibration curve for **AMH** (2 mM) and **HCA** (2 mM) in acetonitrile at 25°C, measured by the stand alone CD spectrophotometer.

| **Unknown** | **$CD_{317nm}$ (mdeg)** | **% *ee* $_{calc}$** | **% *ee* $_{actual}$** | **% Error** |
|---|---|---|---|---|
| 1 | -11.9 | 106.2 | 100.0 | 6.2 |
| 2 | 0.7 | -2.5 | 0.0 | 2.5 |
| 3 | -4.9 | 45.2 | 45.0 | 0.2 |
| 4 | -8.1 | 73.1 | 70.0 | 3.1 |
| 5 | 6.9 | -56.4 | -60.0 | 3.6 |
| 6 | 5.1 | -40.2 | -35.0 | 5.2 |
| 7 | -9.0 | 80.8 | 80.0 | 0.8 |
| 8 | -1.0 | 12.0 | 10.0 | 2.0 |

**Table S3.** Results of the stand alone CD spectrophotometer analysis of the eight unknown samples of **AMH**. The average error was determined to be 2.9%.

*e)* *Unknown ee Calculations: HPLC-CD Detector*

**MBA:**

The same eight test samples prepared for the stand alone spectrophotometer were used for the HPLC-CD detector, independently comprised of **MBA** guest (2 mM total amine content per vial) with **HCA** (2 mM) in acetonitrile. A 5 uL sample was injected onto the HPLC column, and the UV and CD were measured at 317 nm. The same two pure (*R*)-**MBA** and (*S*)-**MBA** (2 mM) enantiomeric standards were used. From these standards a 2-point calibration curve was created,[13] which is pictured below. The best-fit trendline of this plot was used to relate the measured CD signal at 317 nm of the unknown guest to the *ee* of the sample. The results of this analysis, along with the errors, are also shown below in **Figure S15** and **Table S4**.

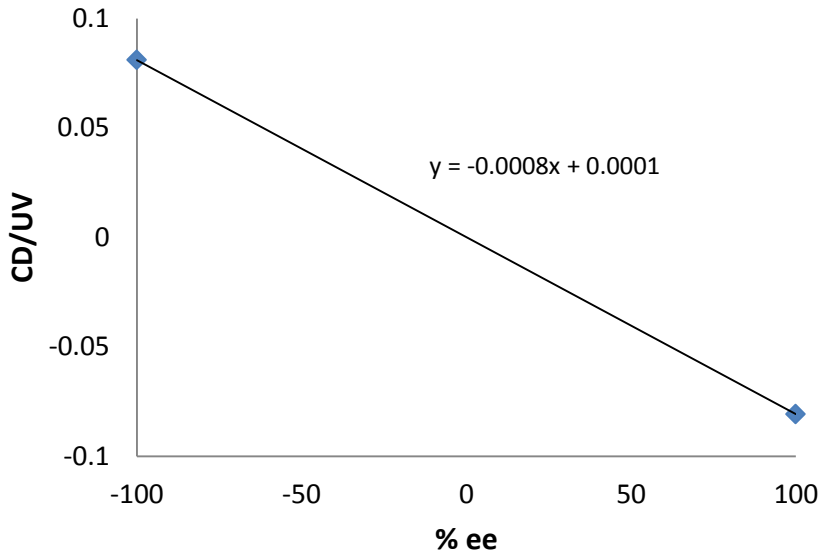



**Figure S15**. Calibration curve for **MBA** (2 mM) and **HCA** (2 mM) in acetonitrile at 25°C,with the CD and UV signals measured at 317 using the HPLC-CD.

| Unknown | $CD_{317nm}/UV_{317nm}$ | % *ee* $_{calc}$ | % *ee* $_{actual}$ | % Error |
|---|---|---|---|---|
| 1 | -0.074 | 91.3 | 90.0 | 1.3 |
| 2 | 0.032 | -40.5 | -40.0 | 0.5 |
| 3 | -0.017 | 20.5 | 20.0 | 0.5 |
| 4 | 0.060 | -75.9 | -75.0 | 0.9 |
| 5 | 0.007 | -9.8 | -10.0 | 0.2 |
| 6 | 0.069 | -86.8 | -85.0 | 1.8 |
| 7 | -0.031 | 37.7 | 35.0 | 2.7 |
| 8 | -0.001 | 1.2 | 0.0 | 1.2 |

**Table S4.** Results of the HPLC-CD analysis of the eight unknown samples of **MBA**. The average error was determined to be 1.1%

**MPP:**

The same eight unknown samples prepared for the stand alone spectrophotometer were used for the HPLC-CD detector, independently comprised of **MPP** guest (2 mM total amine content per vial) with **HCA** (2 mM) in acetonitrile. A 5 uL sample was injected onto the HPLC column, and the UV and CD were measured at 317 nm. The same two pure (*R*)-**MPP** and (*S*)-**MPP** (2 mM) enantiomeric standards were used. From these standards a 2-point calibration curve was created,[13] which is pictured below. The best-fit trendline of this plot was used to relate the measured CD signal at 317 nm of the unknown guest to the *ee* of the sample. The results of this analysis, along with the errors, are also shown in **Figure S16** and **Table S5**.

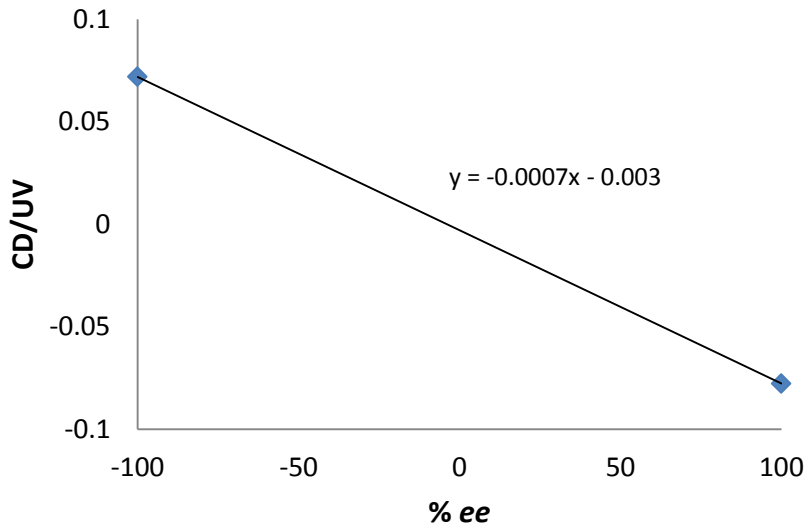



**Figure S16**. Calibration curve for **MPP** (2 mM) and **HCA** (2 mM) in acetonitrile at 25°C,with the CD and UV signals measured at 317 using the HPLC-CD.

| **Unknown** | **$CD_{317nm}/UV_{317nm}$** | **% *ee* $_{calc}$** | **% *ee* $_{actual}$** | **% Error** |
|---|---|---|---|---|
| 1 | -0.062 | 84.3 | 80.0 | 4.3 |
| 2 | -0.030 | 38.5 | 38.5 | 0.0 |
| 3 | 0.065 | -96.9 | -90.0 | 6.9 |
| 4 | -0.0006 | -3.4 | 0.0 | 3.4 |
| 5 | -0.019 | 23.2 | 25.0 | 1.8 |
| 6 | -0.012 | 12.6 | 15.0 | 2.4 |
| 7 | 0.036 | -55.0 | -50.0 | 5.0 |
| 8 | 0.033 | -51.5 | -45.0 | 6.5 |

**Table S5.** Results of the HPLC-CD analysis of the eight unknown samples of **MPP**. The average error was determined to be 3.8%

**AMH:**

The same eight unknown samples prepared for the stand alone spectrophotometer were used for the HPLC-CD detector, independently comprised of **AMH** guest (2 mM total amine content per vial) with **HCA** (2 mM) in acetonitrile. A 5 uL sample was injected onto the HPLC column, and the UV and CD were measured at 317 nm. The same two pure (*R*)-**AMH** and (*S*)-A**MH** (2 mM) enantiomeric standards were used. From these standards a 2-point calibration curve was created,[13] which is pictured below. The best-fit trendline of this plot was used to relate the measured CD signal at 317 nm of the unknown guest to the *ee* of the sample. The results of this analysis, along with the errors, are also shown below in **Figure S17** and **Table S6**.

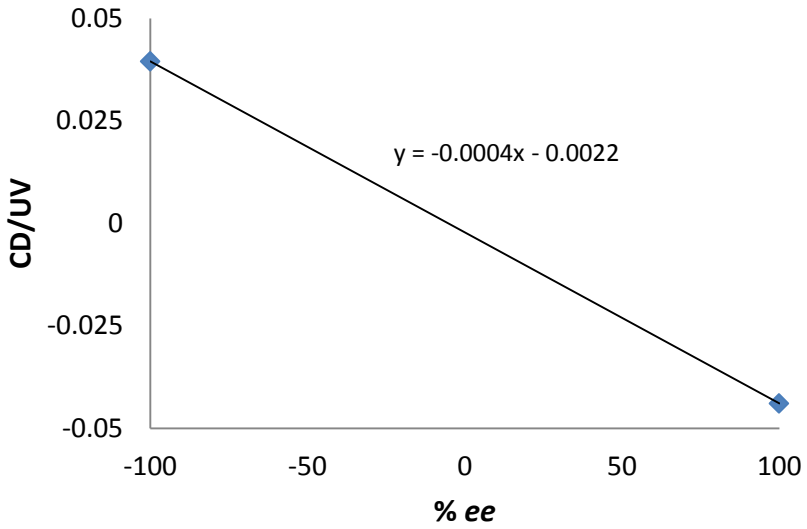



**Figure S17**. Calibration curve for **AMH** (2 mM) and **HCA** (2 mM) in acetonitrile at 25°C,with the CD and UV signals measured at 317 using the HPLC-CD.

| Unknown | $CD_{317nm}/UV_{317nm}$ | % *ee* calc | % *ee* actual | % Error |
|---|---|---|---|---|
| 1 | -0.044 | 103.2 | 100.0 | 3.2 |
| 2 | -0.0007 | -3.8 | 0.0 | 3.8 |
| 3 | -0.019 | 43.1 | 45.0 | 1.9 |
| 4 | -0.031 | 70.9 | 70.0 | 0.9 |
| 5 | 0.023 | -64.2 | -60.0 | 4.2 |
| 6 | 0.013 | -39.0 | -35.0 | 4.0 |
| 7 | -0.035 | 81.5 | 80.0 | 1.5 |
| 8 | -0.005 | 6.6 | 10.0 | 3.4 |

**Table S6.** Results of the HPLC-CD analysis of the eight unknown samples of **AMH**. The average error was determined to be 2.9%

*f) Synthetic Samples Reaction and Workup*

A stock solution was made by dissolving pyridoxal-5'-phosphate (PLP) (25 mg, 0.098 mmol) in 20 mL 0.2 M borate buffer at pH 10.5 that contained 1 M isopropylamine. A portion of this stock solution (600 uL) was added to each reaction vial, which contained a premeasured amount of transaminase (5 mg). The stock solution for the starting material ketone was made by dissolving the ketone (20 mg) in pure DMSO (1.6 mL). After the enzyme had dissolved, a portion of the ketone stock solution (150 uL) was added to the enzyme vial. The reaction vials were capped, and shaken with a constant temperature of 45°C at 350 rpm. After 24 hours the vials were removed from the heating incubator. They sat at room temperature for 10 minutes,

until the insoluble enzyme had settled to the bottom. The top 500 uL of the solution was removed by pipet, and transferred to a deep well 2 mL Adam block 96 well plate. A 1 mL portion of DCM was added to the plate, and the wells were covered and agitated to mix. The amine guest was partitioned to the organic layer, and this layer was removed by pipet (0.75 mL) and transferred to the next row of wells. The solvent was evaporated from the wells by blowing $N_2$ gas over the top, and redisolved in acetonitrile (350 uL). This was split into two 175 uL portions. To the first was added **HCA** (4 mM) at diluted to 1 mL, the **HCA** at a higher concentration to account for the excess isopropylamine present in solution. The second portion was used to determine yield and *ee* for each product. The LCAP at 210 nm was determined using an Agilent 1100 HPLC (Column: Waters X-Bridge C18 (150x4.6mm, 3.5 um), Gradient elution: A=2 mM NH4HCO2 pH 10.5 in water, B=2 mM NH4HCO2 pH 10.5 in 90% MeCN/10% water; 5-95% B (0-3 min), 95% (3-5 min), 5 min post time; 1.5 mL/min, room temperature. 1 uL sample injection).

g) Synthetic **MBA** *ee* Determination

The calibration curve for synthetic **MBA** was found by plotting the g-factor (area of the CD at 317 divided by area of the UV at 317) against *ee* for pure enantiomers of **MBA**. One equivalent of guest (2 mM) was used relative to **HCA** (200 uL, 2 mM). From these standards a 2-point calibration curve was created,[13] which is pictured below. The best-fit trendline of this plot was used to relate the measured CD signal at 317 nm of the unknown guest to the *ee* of the sample. The *ee* values for the unknown

synthetic samples were found by imputing the g-factor for each sample as the y-value in the trendline. The results are found in **Figure S18** and **Table S7**.

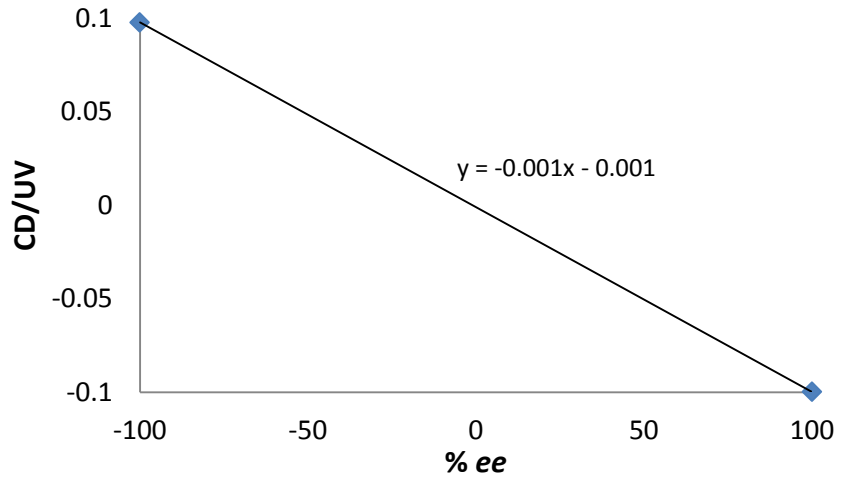



**Figure S18**. Calibration curve for synthetic **MBA** (2 mM) and **HCA** (4 mM) in acetonitrile at 25°C,with the CD and UV signals measured at 317 using the HPLC-CD.

| **Enzyme** | **LCAP$_{210\ nm}$ (HPLC)** | **% *ee* (Calc)** | **% *ee* (SFC)[14]** | **% Error** |
|---|---|---|---|---|
| TA PIG5 | 8.4% | -98.0 | -100 | 2.0 |
| ATA-234 | 32.7% | -96.9 | -100 | 3.1 |
| ATA-412 | 41.1% | 99.2 | 100 | 0.8 |
| ATA-303 | 28.2% | 100.5 | 100 | 0.5 |
| ATA-014 | 74.7% | 99.0 | 100 | 1.0 |
| CDX-010 | 91.7% | 95.5 | 100 | 4.5 |
| CDX-017 | 52.8% | 97.3 | 100 | 2.6 |

**Table S7.** Results of the HPLC-CD analysis of the synthetic samples of **AMH**. The average error was determined to be 1.8%

h) Synthetic **CMA** *ee* Determination

The calibration curve for synthetic **CMA** was found by plotting the g-factor (area of the CD at 317 divided by area of the UV at 317) against *ee* for pure enantiomers of **CMA**. One equivalent of guest (2 mM) was used relative to **HCA** (200 uL, 2 mM). From these standards a 2-point calibration curve was created,[13] which is pictured below. The best-fit trendline of this plot was used to relate the measured CD signal at 317 nm of the unknown guest to the *ee* of the sample. The *ee* values for the unknown synthetic samples were found by imputing the g-factor for each sample as the y-value in the trendline. The results are found in **Figure S19** and **Table S8**.

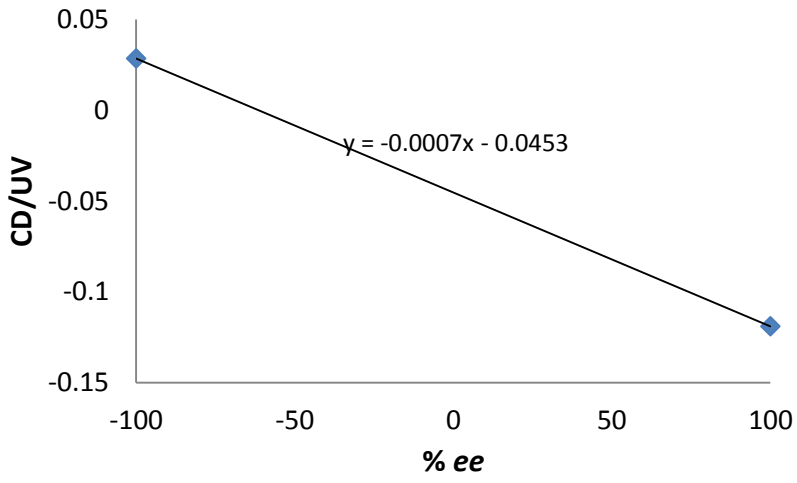



**Figure S19.** Calibration curve for synthetic **CMA** (2 mM) and **HCA** (4 mM) in acetonitrile at 25°C,with the CD and UV signals measured at 317 using the HPLC-CD.

| **Enzyme** | **LCAP$_{210\ nm}$ (HPLC)** | **% *ee* (Calc)** | **% *ee* (SFC)**[15] | **% Error** |
|---|---|---|---|---|
| TA PIG5 | 30.8% | -104.1 | -97.9 | 6.2 |
| ATA-234 | 77.2% | -97.6 | -97.7 | 0.1 |
| ATA-412 | 89.3% | 96.1 | 100 | 3.9 |
| ATA-303 | 55.1% | 97.9 | 100 | 2.1 |
| ATA-014 | 93.5% | 90.5 | 100 | 9.5 |
| CDX-010 | 94.6% | 92.5 | 100 | 7.5 |
| CDX-017 | 94.4% | 91.4 | 99.8 | 8.4 |

**Table S8.** Results of the HPLC-CD analysis of the synthetic samples of **CMA**. The average error was determined to be 4.7%

i) Synthetic **MPP** *ee* Determination

The calibration curve for synthetic **MPP** was found by plotting the g-factor (area of the CD at 317 divided by area of the UV at 317) against *ee* for pure enantiomers of **MPP**. One equivalent of guest (2 mM) was used relative to **HCA** (200 uL, 2 mM). From these standards a 2-point calibration curve was created,[13] which is pictured below. The best-fit trendline of this plot was used to relate the measured CD signal at 317 nm of the unknown guest to the *ee* of the sample. The *ee* values for the unknown synthetic samples were found by imputing the g-factor for each sample as

the y-value in the trendline. The results of this analysis can be found in **Figure S20** and **Table S9**.

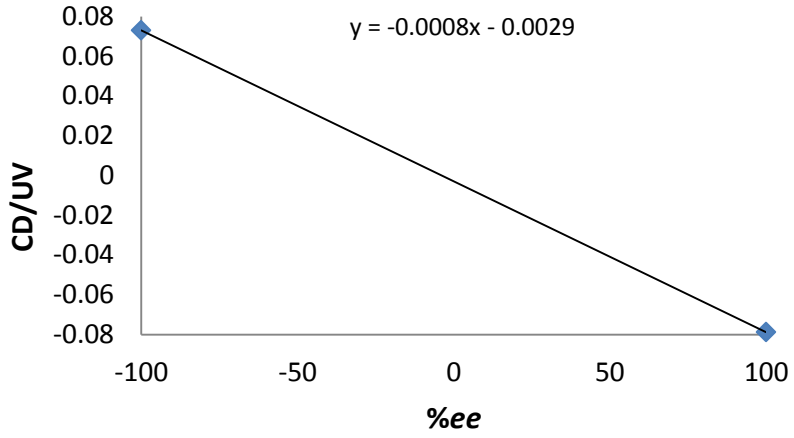



**Figure S20.** Calibration curve for synthetic **MPP** (2 mM) and **HCA** (4 mM) in acetonitrile at 25°C,with the CD and UV signals measured at 317 using the HPLC-CD.

| **Enzyme** | **LCAP$_{210\ nm}$ (HPLC)** | **% *ee* (Calc)** | **% *ee* (SFC)**[16] | **% Error** |
|---|---|---|---|---|
| TA PIG5 | 16.8% | -96.3 | -93.9 | 2.4 |
| ATA-234 | 81.3% | -96.0 | -96.0 | 0.0 |
| ATA-412 | 92.3% | 92.7 | 95.7 | 2.9 |
| ATA-303 | 71.9% | 71.4 | 75.6 | 4.2 |
| ATA-014 | 96.5% | 48.1 | 49.8 | 1.7 |
| CDX-010 | 99.5% | 54.7 | 59.4 | 4.6 |
| CDX-017 | 99.5% | 69.9 | 72.6 | 2.7 |

**Table S9.** Results of the HPLC-CD analysis of the synthetic samples of **MPP**. The average error was determined to be 2.3%.

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13) The use of 2-point calibration curves for these analyses can be justified because of the agreement found for MBA in the main text, as well as occassional spot checking to determine accuracy for the other analytes. The focus of this work is rapid *ee* determination, so more data points and repetitions would slow down the process.
14) MBA *ee* determined using chiral SFC : IC-3 column (150x4.6mm, 3um); Isocratic mobile phase (6% MeOH with 25 mM IBA/94% CO2); 3mL/min, 175 bar, 40°C; 11 min method, no post.

15) CMA *ee* determined using chiral SFC : OZ-3 column (150x4.6mm, 3um); Isocratic mobile phase (6% MeOH with 25 mM IBA/94% CO2); 3mL/min, 200 bar, 40°C; 9 min method, no post.
16) MPP *ee* determined using chiral SFC : AD-3 column (150x4.6mm, 3um); Isocratic mobile phase (6% IPA with 25 mM IBA/94% CO2); 3mL/min, 200 bar, 40°C; 10 min method, no post.