Supporting Information

Predictive Chirality Sensing via Schiff Base Formation

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1. Structure Optimization and Optical Properties

DFT Calculations.

The Molecular Mechanics conformational search was performed using the Macromodel software[Error! Bookmark not defined.] and the MMFF force field by retaining all the conformations within the 10 kcal/mol range. Redundant conformations were then removed by the same software. Ground state optimizations were then optimized by DFT with the Gaussian 16 rev A.03 series of programs, using B3LYP/6-31G(d) and PCM-B3LYP/6-311++G(2d,p) and standard convergence parameters. The analysis of the vibrational frequencies for all the optimized structures showed the absence of imaginary frequencies. If not differently stated, the energy values presented in the results and discussion section derive from the ZPE-corrected enthalpy. This avoids artifacts that might result from the use of empirical scaling factors for frequencies,[1] and from the idealization of low-frequency vibrators as harmonic oscillators.[2] The latter factor is particularly important in the present case because more than 20% of the frequencies are below 500 cm^{-1}, and more than 10% are below 200 cm^{-1}.[3] The ECD spectra were calculated with TD-DFT using CAM-B3LYP and the 6-311++G(2d,p) basis set. For each conformation 25 discrete transitions were calculated (lowest calculated wavelength < 200 nm). The ECD spectra were generated by convolution of Gaussian shaped lines (0.25 eV line width) by the Gaussview Software[4]. The simulated spectra resulting from the Boltzmann averaged sum of the conformations were red-shifted and vertically scaled to get the best match with the experimental spectra.

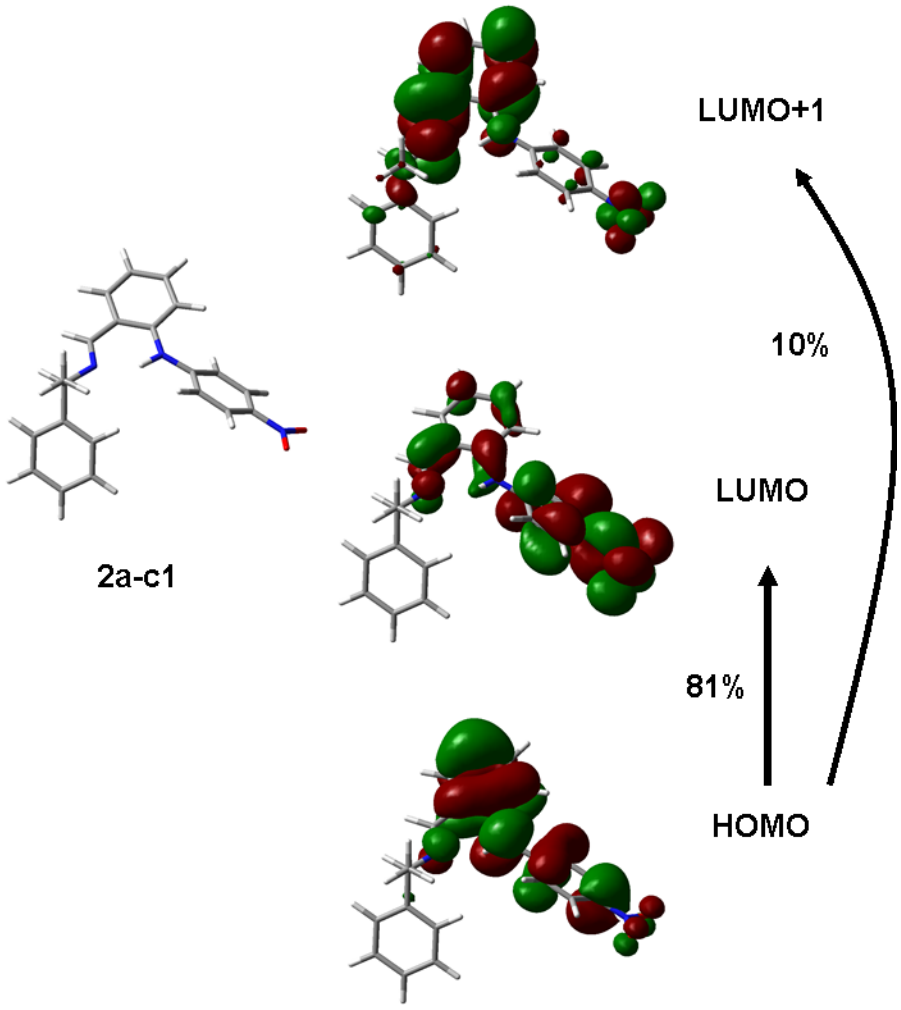


Figure S1. MOs involved in the UV/CD transition at 343 nm of **2a**.

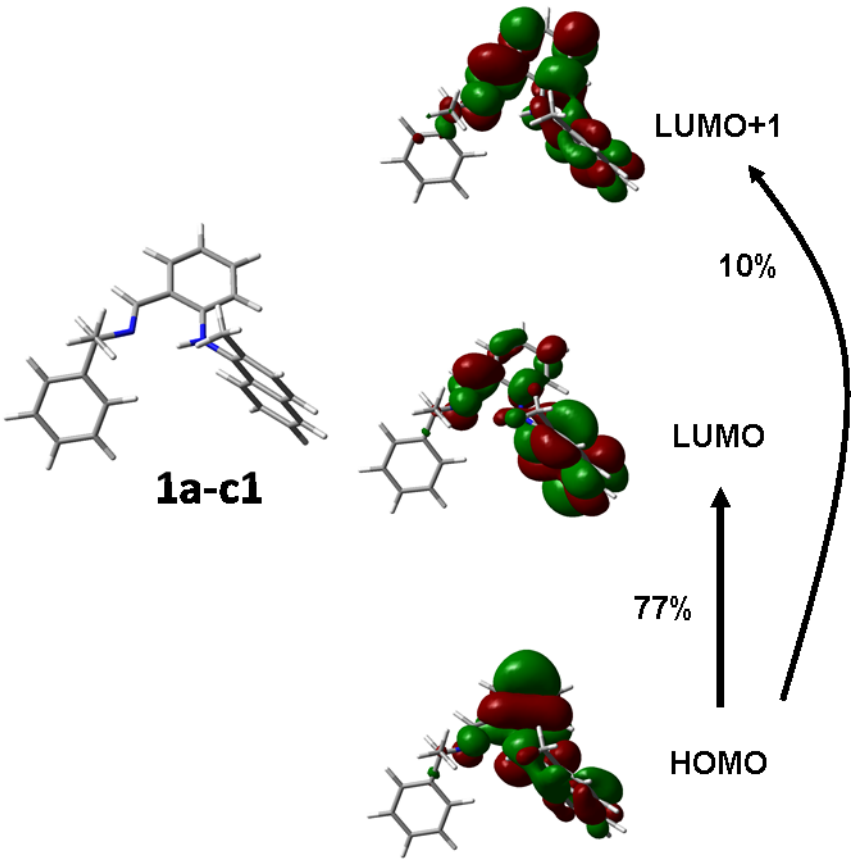


Figure S2. MOs involved in the UV/CD transition at 376 nm of **1a**.

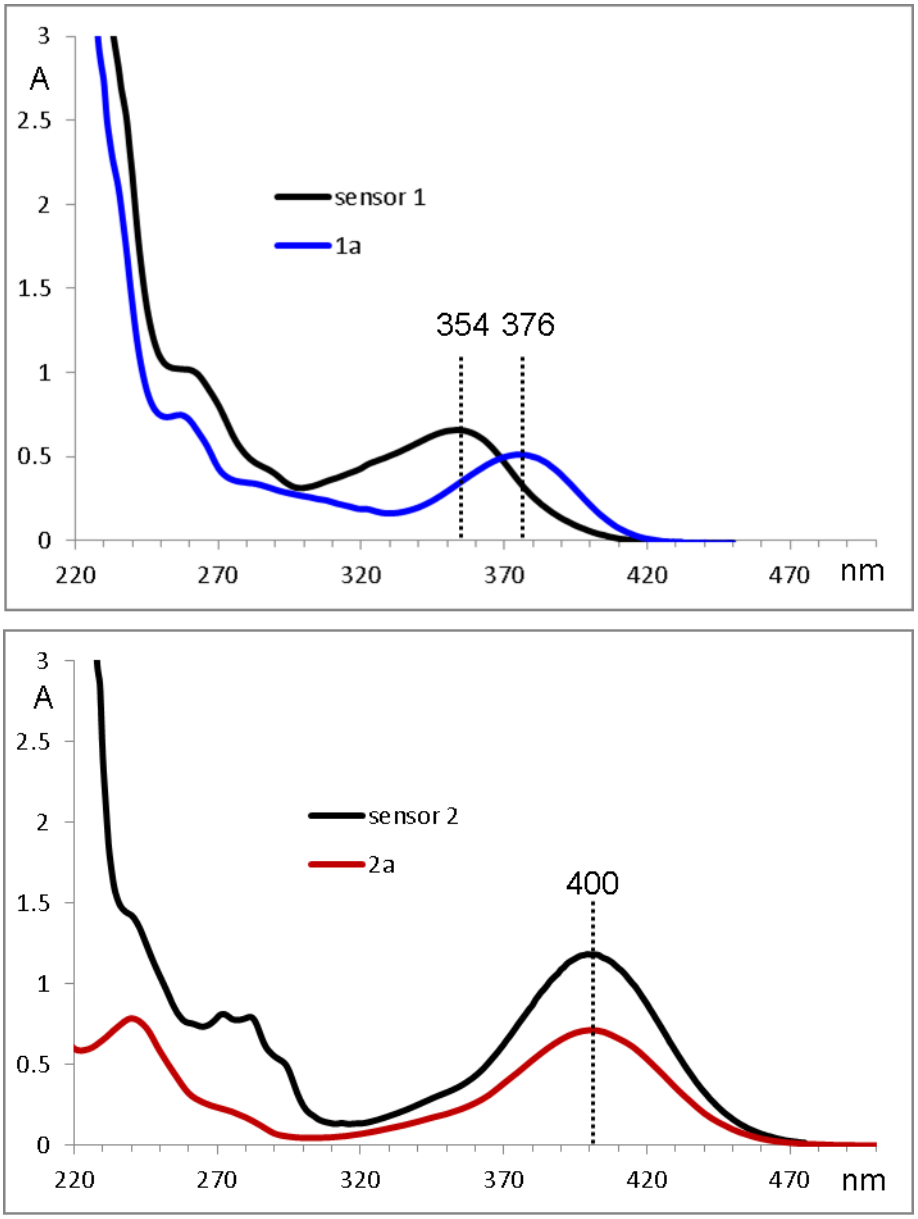


Figure S3 Top: UV spectrum of **1** (black) and of the imine formed from **1** (68 μM) and (*R*)-1-phenylethan-1-amine (**1a**, blue) in acetonitrile (local λ_{max}=376 nm). Bottom: UV spectrum of **2** (black) and of the imine formed from **2** (60 μM) and (*R*)-1-phenylethan-1-amine (**2a**, red) in acetonitrile (local λ_{max}=400 nm).

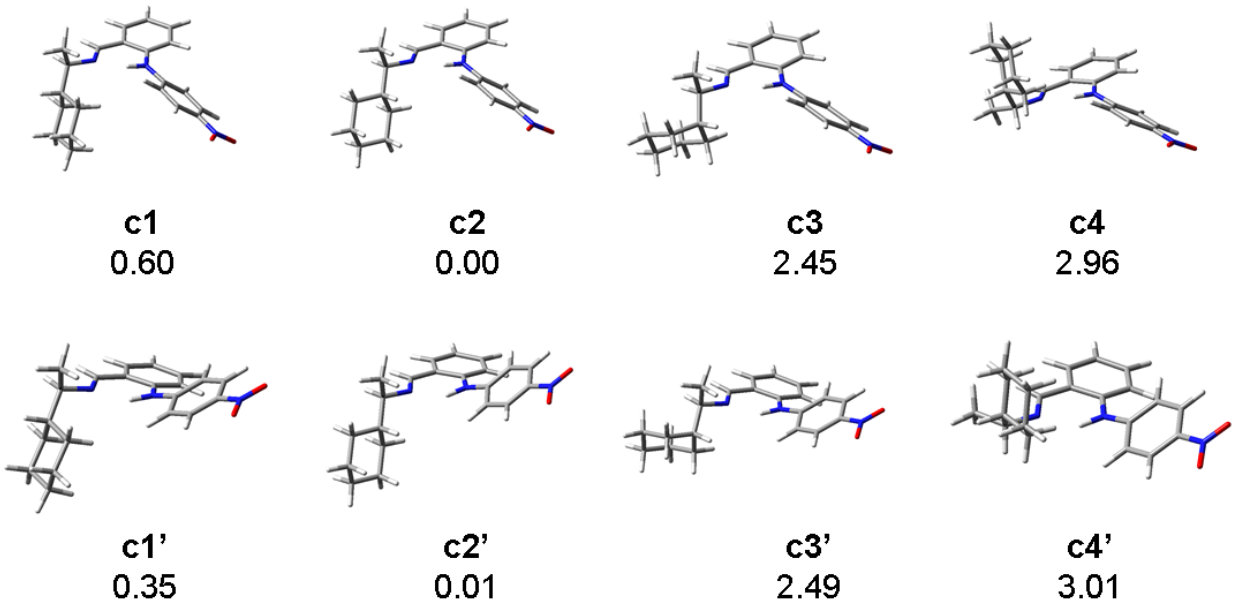


Figure S4. Geometries and relative energies of the most stable conformations of **2b**, optimized at the PCM-B3LYP/6-311++G(2d,p) level (energies in kcal/mol).

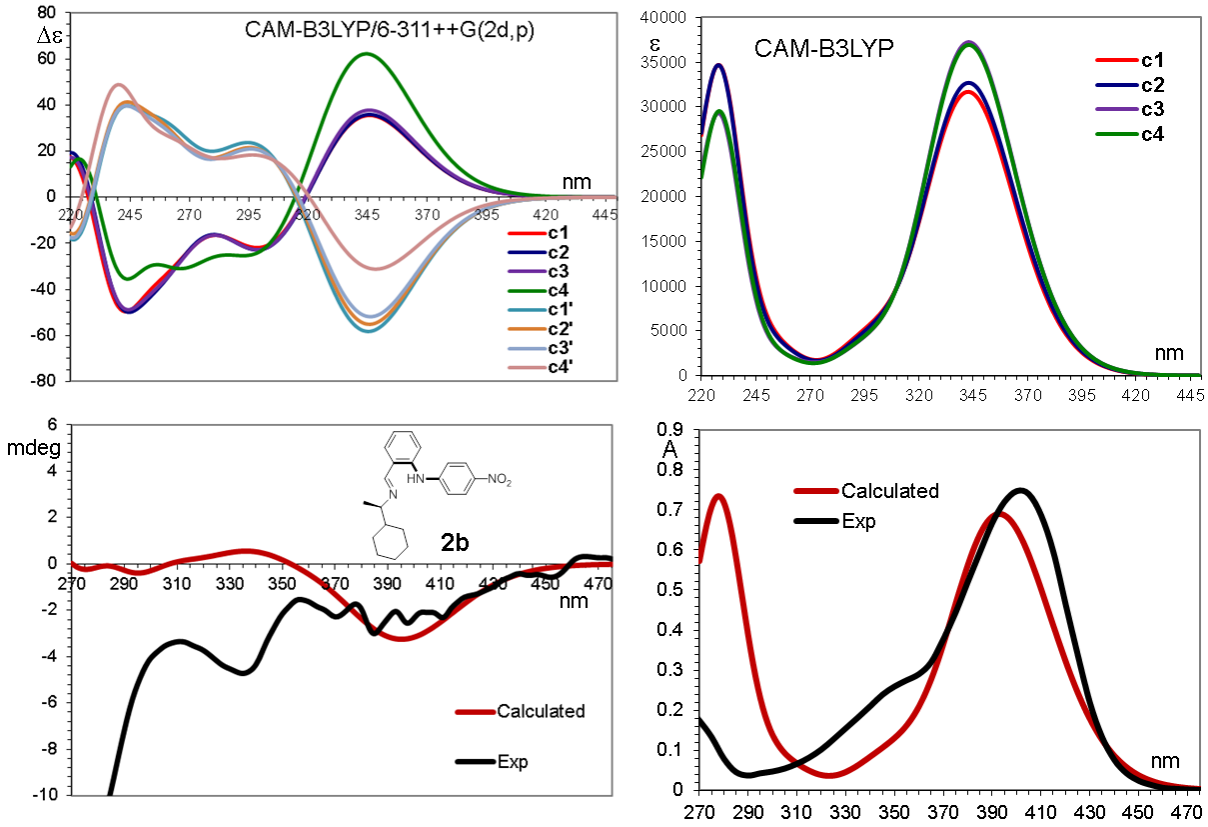


Figure S5. Top left: ECD simulations for the eight conformations of compound **2b**, obtained at the TD-DFT CAM-B3LYP/6-311++G(2d,p) level. Bottom Left: Simulated and experimental ECD spectra obtained using the conformational ratio derived from the energies reported in Figure S2. Top right: calculated UV spectra for conformations **c1**-**c4**. Bottom Right: simulated and experimental UV spectra. The simulated UV and ECD spectra were red-shifted by 50 nm.

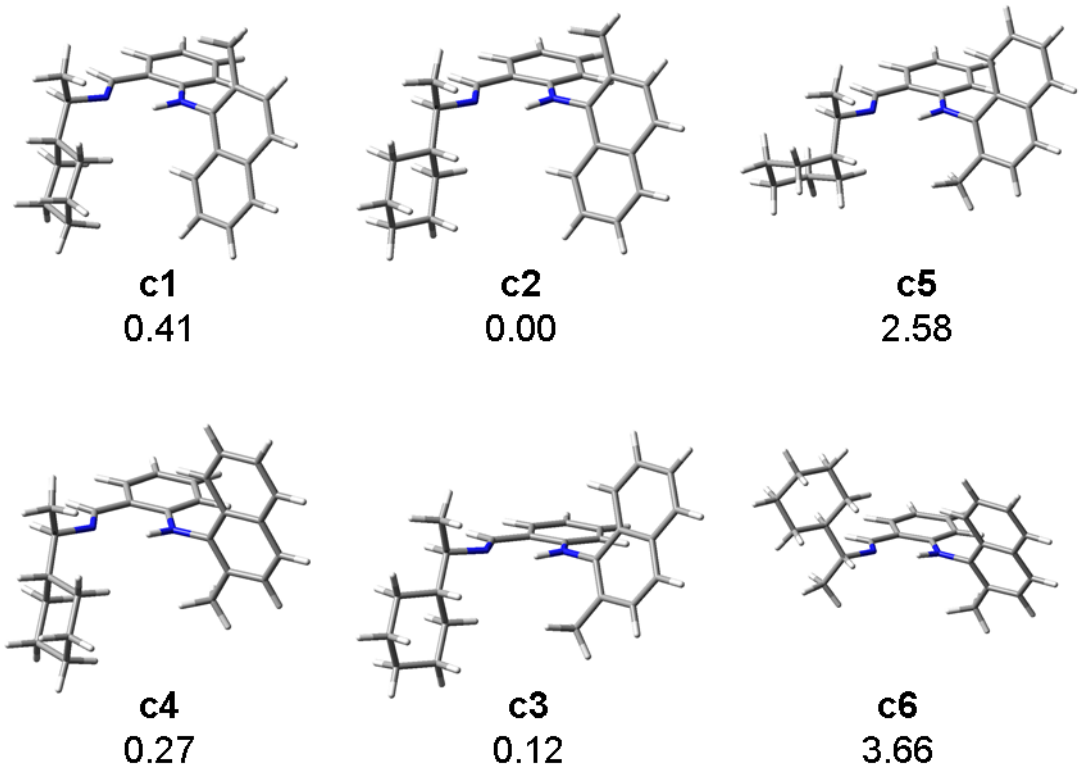


Figure S6. Geometries and relative energies of the best six conformations of **1b**, optimized at the PCM-B3LYP/6-311++G(2d,p) level (the conformations derived from the naphthyl rotation in conformations **c5** and **c6** are not shown; relative energies in kcal/mol).

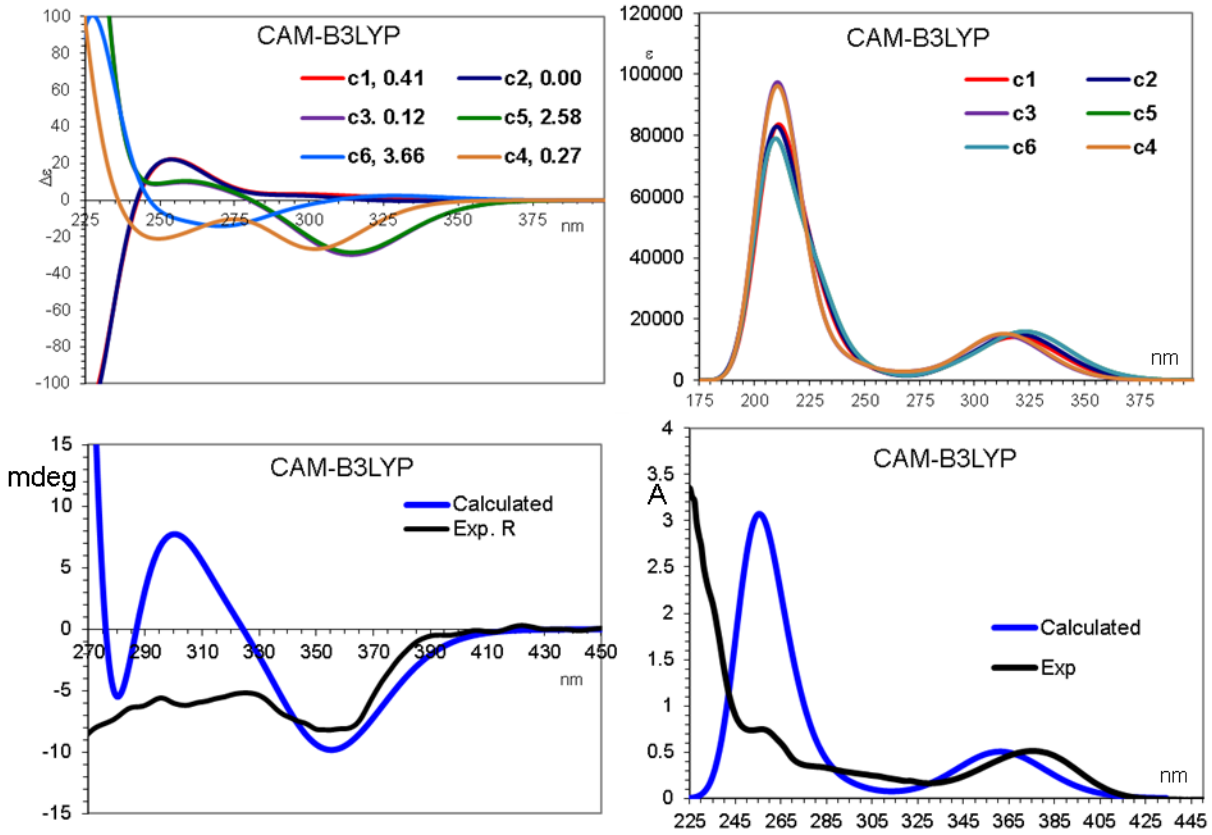
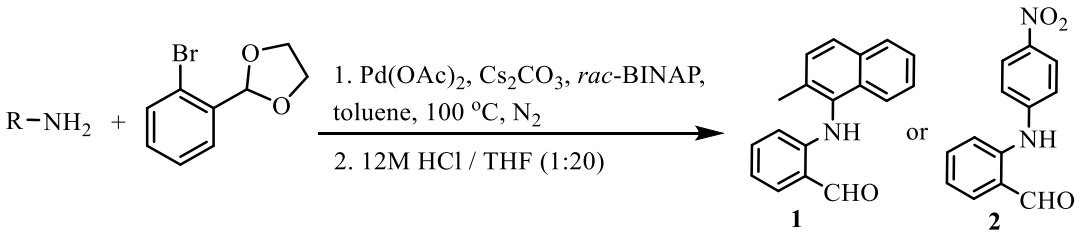


Figure S7. Top: ECD and UV simulations for the six conformations of compound **1b**, obtained at the TD-DFT CAM-B3LYP/6-311++G(2d,p) level. Bottom: Simulated (blue) ECD spectra obtained using the conformational ratio derived from the energies reported in Figure S4 and experimental results (black). The simulated spectra have been red-shifted by 45 nm.

2. Synthetic Procedures and Compound Characterization

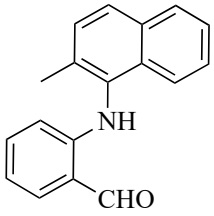
All reagents and solvents were commercially available and used without further purification. NMR spectra were obtained at 400 MHz (^{1}H NMR) and 100 MHz (^{13}C NMR) using CD_3CN or $CDCl_3$ as solvent. NMR signals are reported in ppm using the solvent peak as reference.



1 **2**

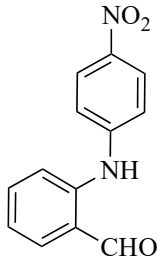
2-(2-Bromophenyl)-1,3-dioxolane (636 mg, 2.78 mmol for the synthesis of **1** and 400 mg, 1.75 mmol for the synthesis of **2**),[5] Cs_2CO_3 (1.15 eq), $Pd(OAc)_2$ (4 mol%), *rac*-BINAP (7.5 mol%) and 1.1 equivalents of either 2-methylnaphthalen-1-amine (for synthesis of **1**) or 4-nitroaniline (for the synthesis of **2**) were dissolved in toluene (12 mL for the case of **1** and 8 mL for the case of **2**) under nitrogen atmosphere. The reaction mixture was heated to 100 °C for 16 and 14 hours for **1** and **2**, respectively. After cooling, toluene was removed *in vacuo* and the mixture was diluted with water and extracted with EtOAc (3x). The organic layers were combined and dried over Na_2SO_4. The crude product was then purified by silica column chromatography with hexanes/EtOAc gradients (3-15% EtOAc for **1**, and 5-15% EtOAc for **2**). Deprotection was carried out using 12M HCl in THF (1:20 v/v) at room temperature followed by extraction with ethyl acetate. The organic layers were combined and dried over Na_2SO_4. Solvent removal under vacuum gave the pure sensors.

2-((2-Methylnaphthalen-1-yl)amino)benzaldehyde[6]



Compound **1** was obtained in 49% yield (358.4 mg, 1.37 mmol) over two steps. ^{1}H NMR (400 MHz, in $CDCl_3$) δ 10.05 (s, 1H), 9.90 (s, 1H), 7.92-7.83 (m, 2H), 7.77 (d, J = 8.4 Hz, 1H), 7.62 (dd, J = 7.7, 1.7 Hz, 1H), 7.51 – 7.38 (m, 3H), 7.19 (dd, J = 8.7, 7.1 Hz, 1H), 6.82 – 6.71 (m, 1H), 6.15 (d, J = 8.5 Hz, 1H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.7, 150.3, 136.4, 135.9, 133.8, 133.4, 132.7, 131.7, 129.2, 128.2, 127.3, 126.8, 125.6, 123.3, 118.7, 116.3, 113.2, 18.5.

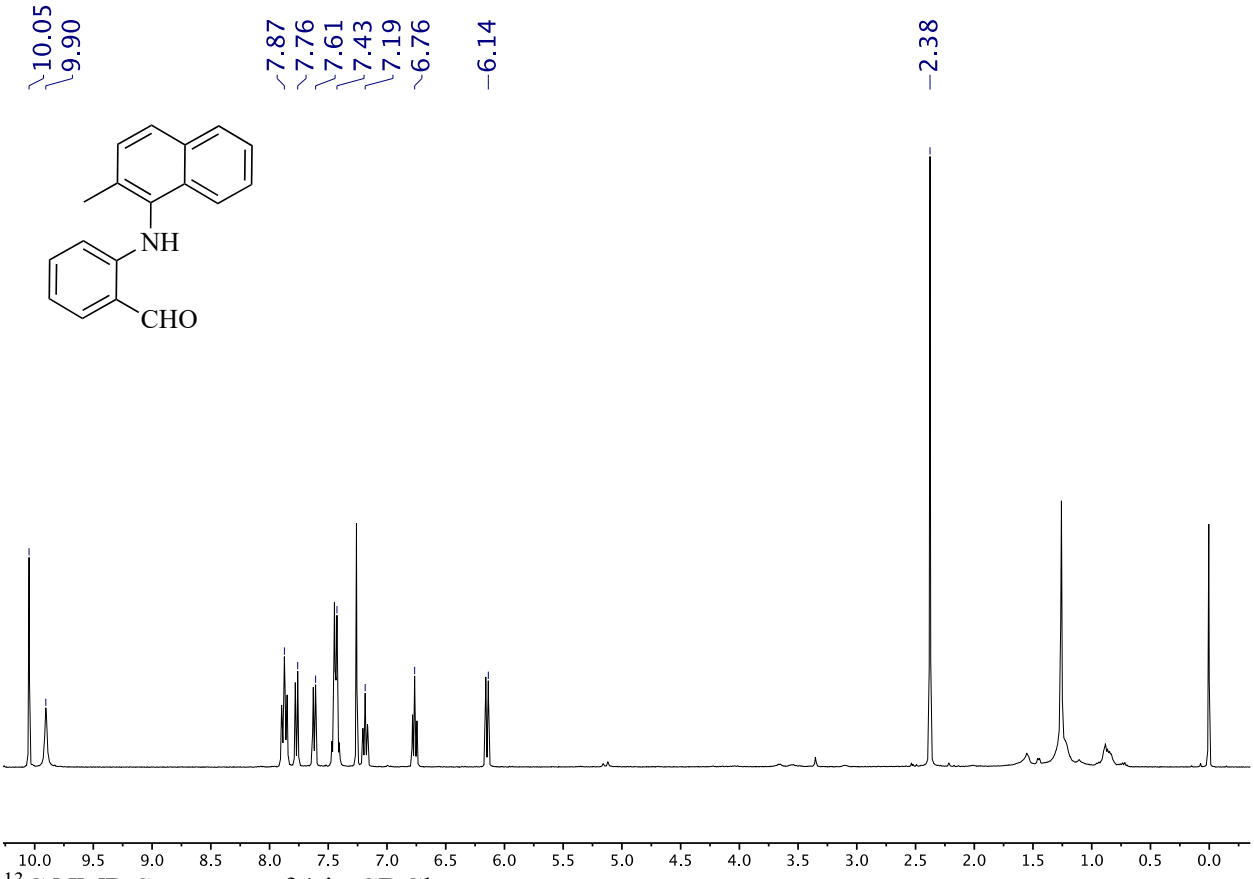
2-((4-Nitrophenyl)amino)benzaldehyde[7]



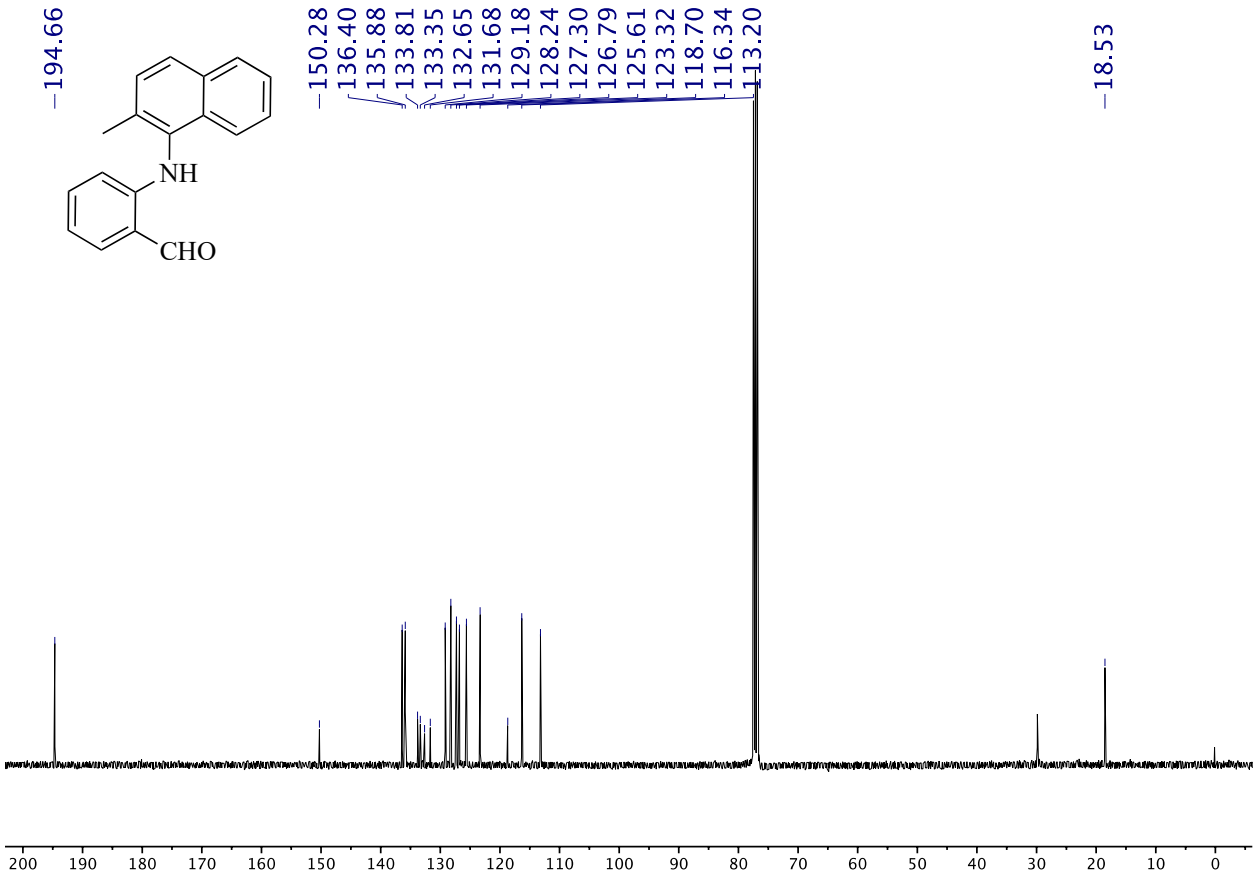
Compound **2** was obtained in 49% yield (210.3 mg, 0.87 mmol) over two steps. ^{1}H NMR (400 MHz, CD_3CN) δ 10.11(br, 1H), 9.96 (s, 1H), 8.18 (d, 9.38 Hz, 2H), 7.80 (d, *J* = 7.45, 1H), 7.57 (d, 4.07 Hz, 2H), 7.38 (d, *J* = 9.22 Hz, 2H), 7.20 – 7.07 (m, 1H). ^{13}C NMR (100 MHz, CD_3CN) δ 196.0, 148.3, 137.6, 136.5, 126.5, 123.3, 121.8, 119.4, 118.3, 116.8.

2. NMR Spectra

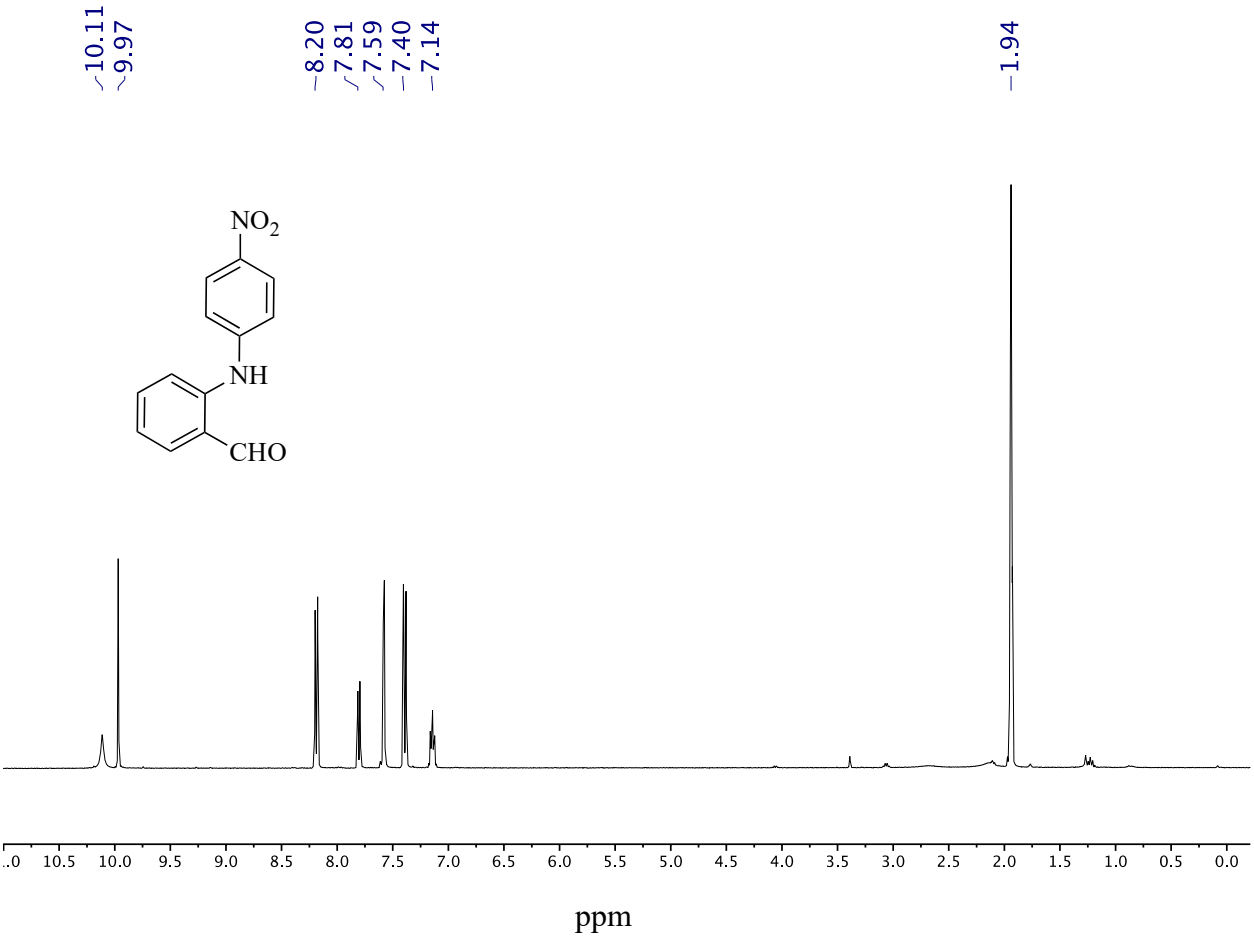
^{1}H NMR Spectrum of **1** in $CDCl_3$



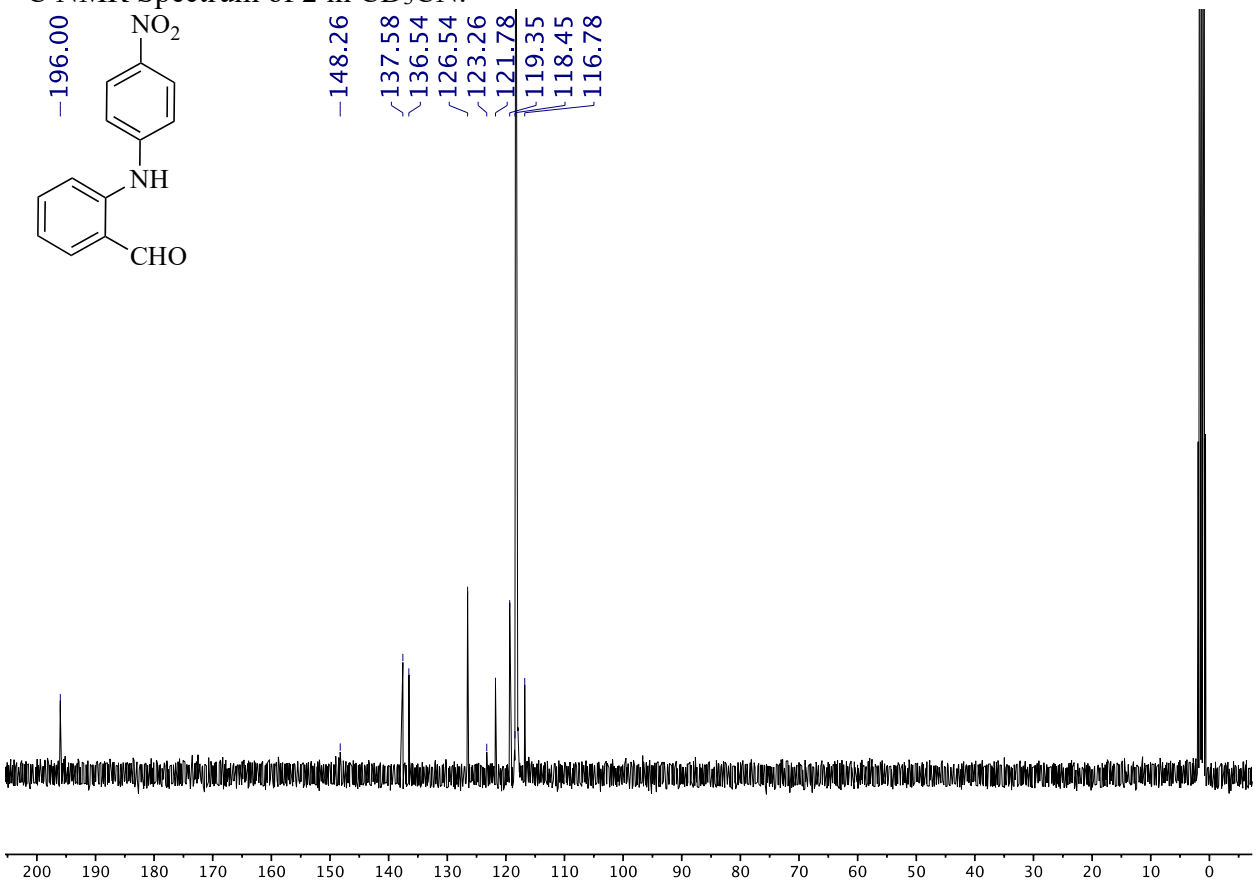
^{13}C NMR Spectrum of **1** in $CDCl_3$


194.66
150.28
136.40
135.88
133.81
133.35
132.65
131.68
129.18
128.24
127.30
126.79
125.61
123.32
118.70
116.34
113.20
18.53
NH
CHO
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

^{1}H NMR Spectrum of **2** in CD_3CN.



^{13}C NMR Spectrum of **2** in CD_3CN.



3. Chiroptical Sensing

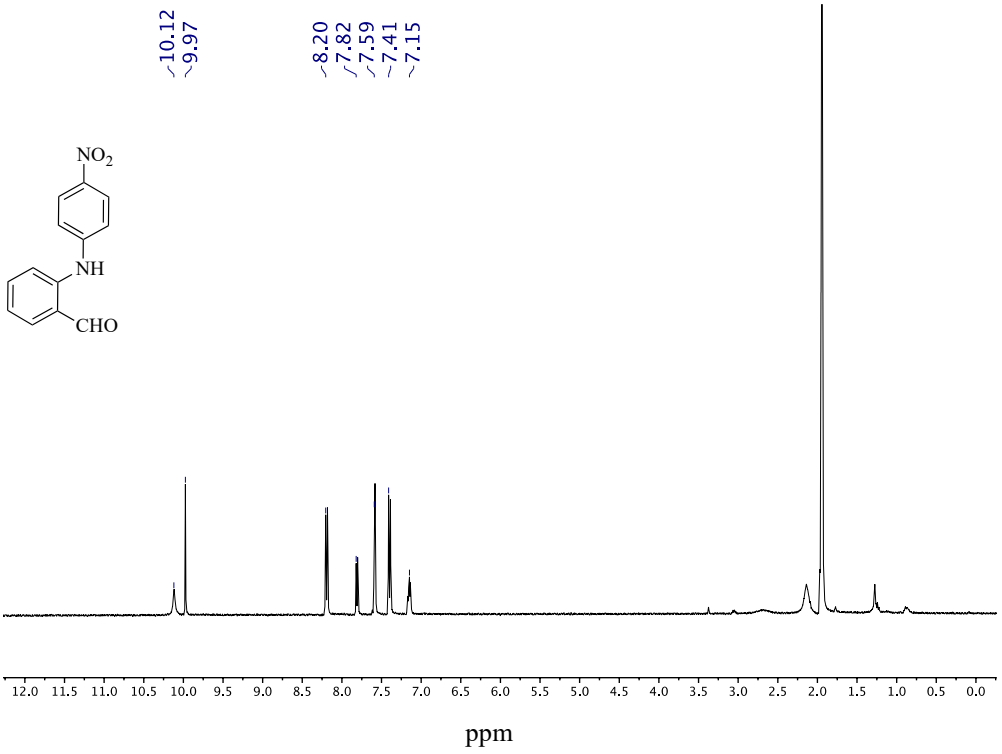
All CD measurements were taken at submillimolar sensor concentrations with chiral analytes used in stoichiometric amounts in acetonitrile as the bulk sensing solvent. All CD spectra were collected with a standard sensitivity of 100 mdeg, a data pitch of 1.0 nm, a band width of 1 nm, a scanning speed of 500 nm min^{-1} and a response of 1 s using a quartz cuvette (10 mm path length). UV-vis spectra were taken using 0.5 s integration time and scanning intervals of 1 nm using a quartz cuvette (10 mm path length). CD scans were corrected using a binomial smoothing function. The chiral substrates surveyed do not produce a CD profile above 250 nm at the experimental conditions in the absence of the sensor.

3.1. Chiroptical sensing with 1

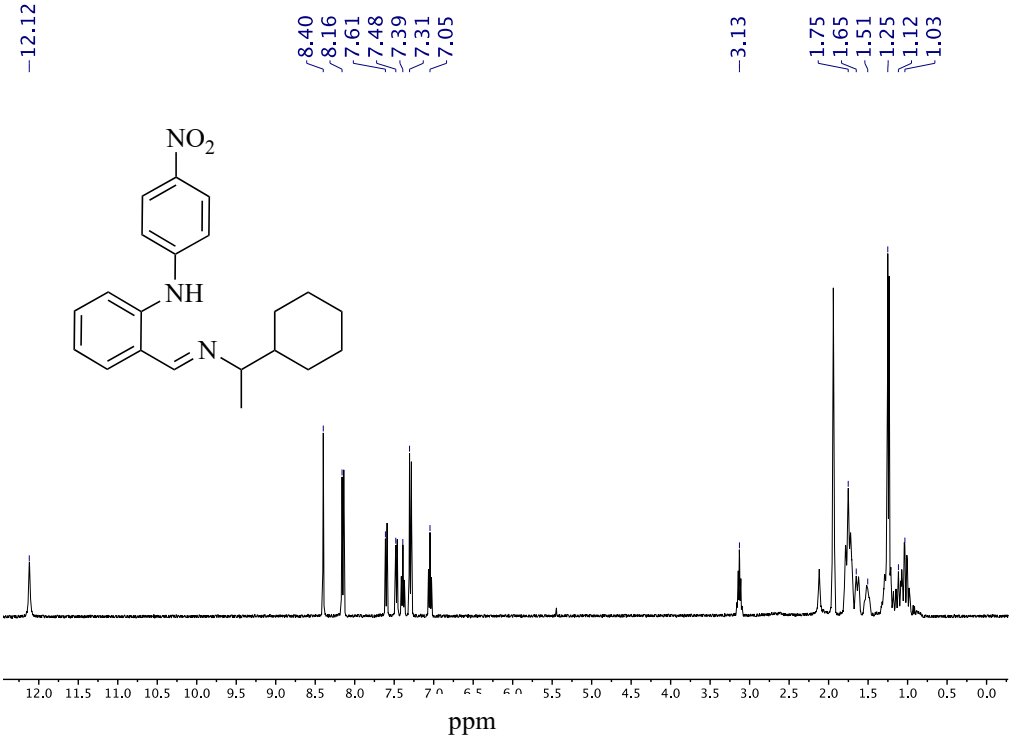
A solution of **1** (27 mM for sensing of chiral amines and 23 mM for sensing of chiral amino alcohols) was prepared in anhydrous dichloromethane and 250 µL amounts were distributed into vials containing 750 µL of anhydrous dichloromethane to generate reaction concentrations of 6.8 mM (6.4 mM for sensing of chiral amino alcohols). Molecular sieves (4A) were added to each vial followed by equimolar amounts of the chiral substrate. The vials were sealed and placed on a shaker apparatus for 12 hours. CD and UV measurements were then taken by dispensing 20-180 µL aliquots of the imine condensation reactions into 2 mL of anhydrous acetonitrile to afford the desired sensing concentrations mentioned below.

As an example, the condensation conversion of the sensor **2** with amine **b** was monitored by NMR spectroscopy.

^{1}H NMR Spectrum of **2** in CD_3CN.

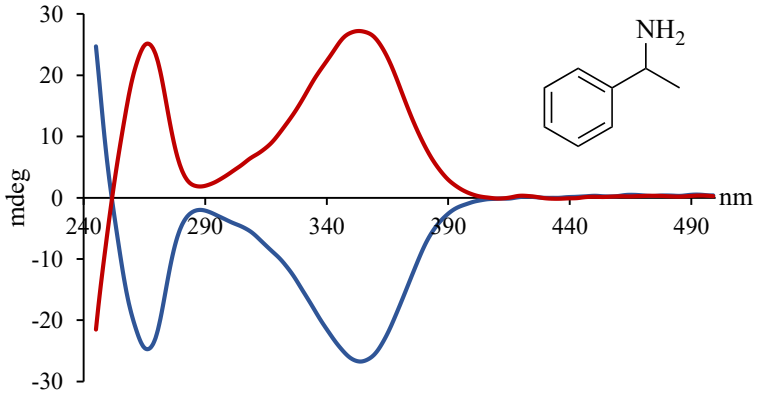


^{1}H NMR Spectrum of **2b** in CD_3CN.

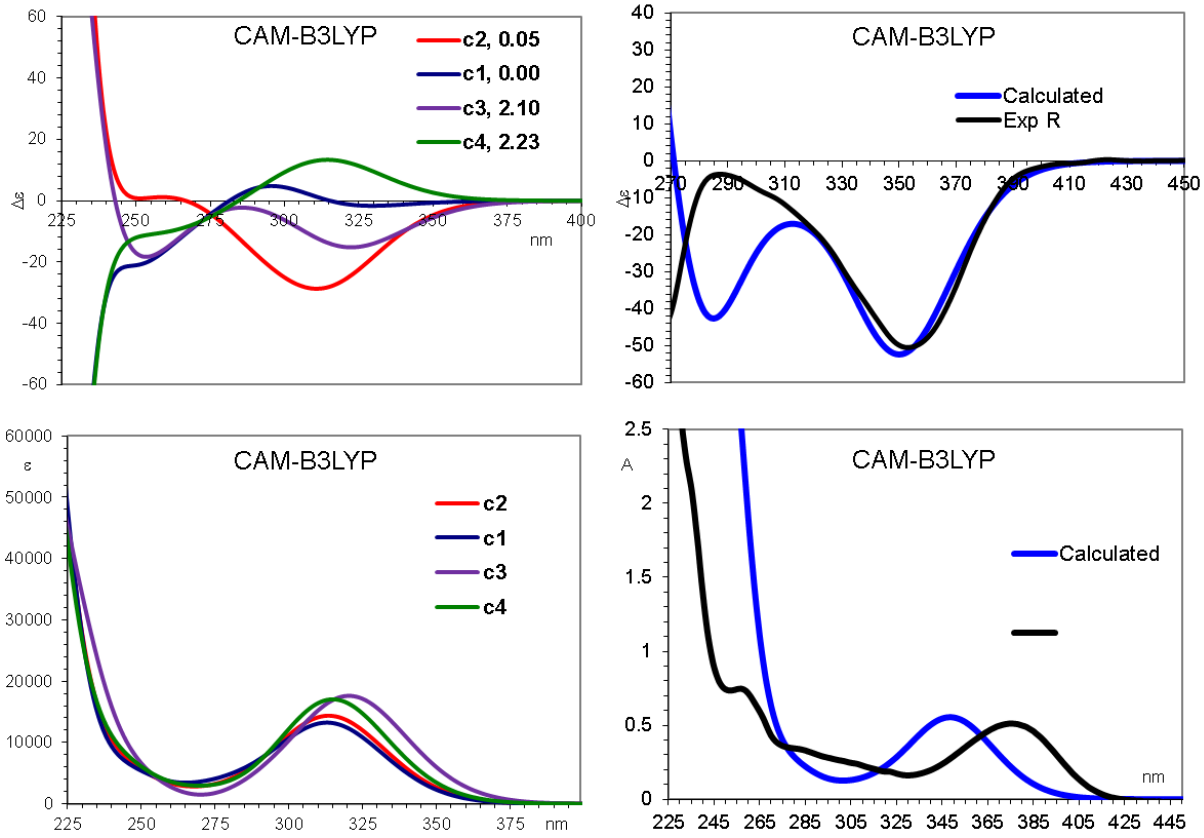


Complete condensation of **2** and analyte **b** to **2b** in d^3-ACN is evident from the disappearance of the aldehyde peak (9.97 ppm for **2**) while the signature CH imine proton of **2b** is observed as a sharp singlet at 8.40 ppm. The biarylamine NH proton in **2b** is also significantly shifted downfield to 12.12 ppm which is consistent with the expected intramolecular hydrogen bonding.

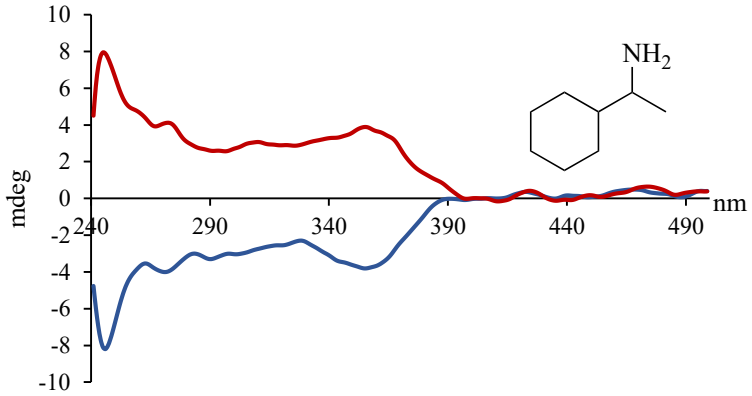
CD spectra of the imine formed from **1** with (*R*)-1-phenylethan-1-amine (blue) and (*S*)-1-phenylethan-1-amine (red) at 68 μM.



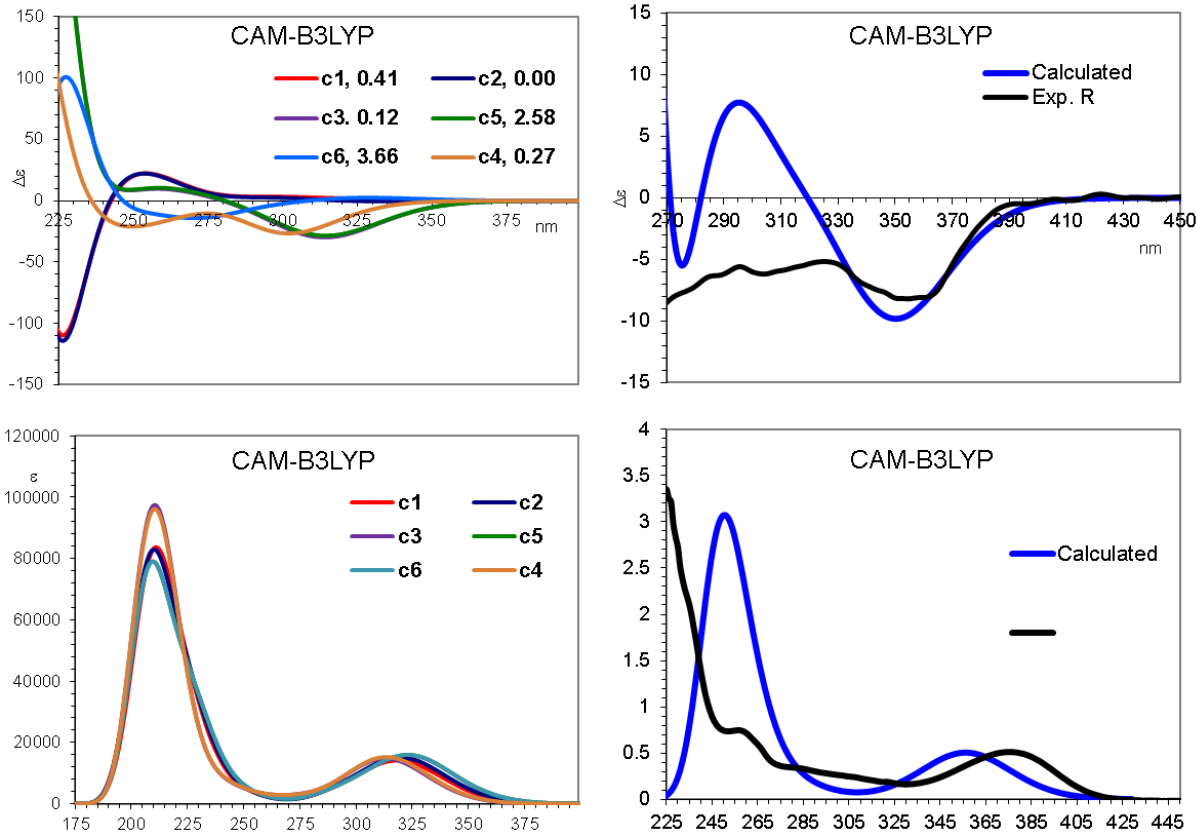
UV and ECD simulation of the four conformations of **1a**, and Boltzmann–averaged spectra
(relative energies are reported in the legend in kcal/mol),
TD-DFT CAM-B3LYP/6-311++G(2d,p) level
(calculated UV and ECD spectra were red-shifted by 35 nm)



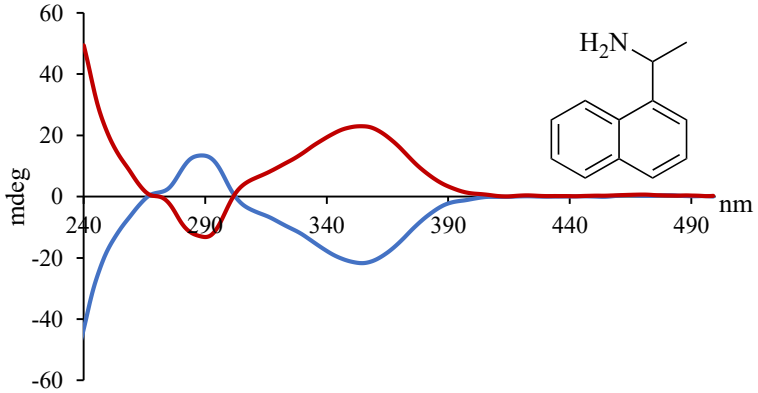
CD spectra of the imine formed from **1** with (*R*)-1-cyclohexylethan-1-amine (blue) and (*S*)-1-cyclohexylethan-1-amine (red) at 68 μM.



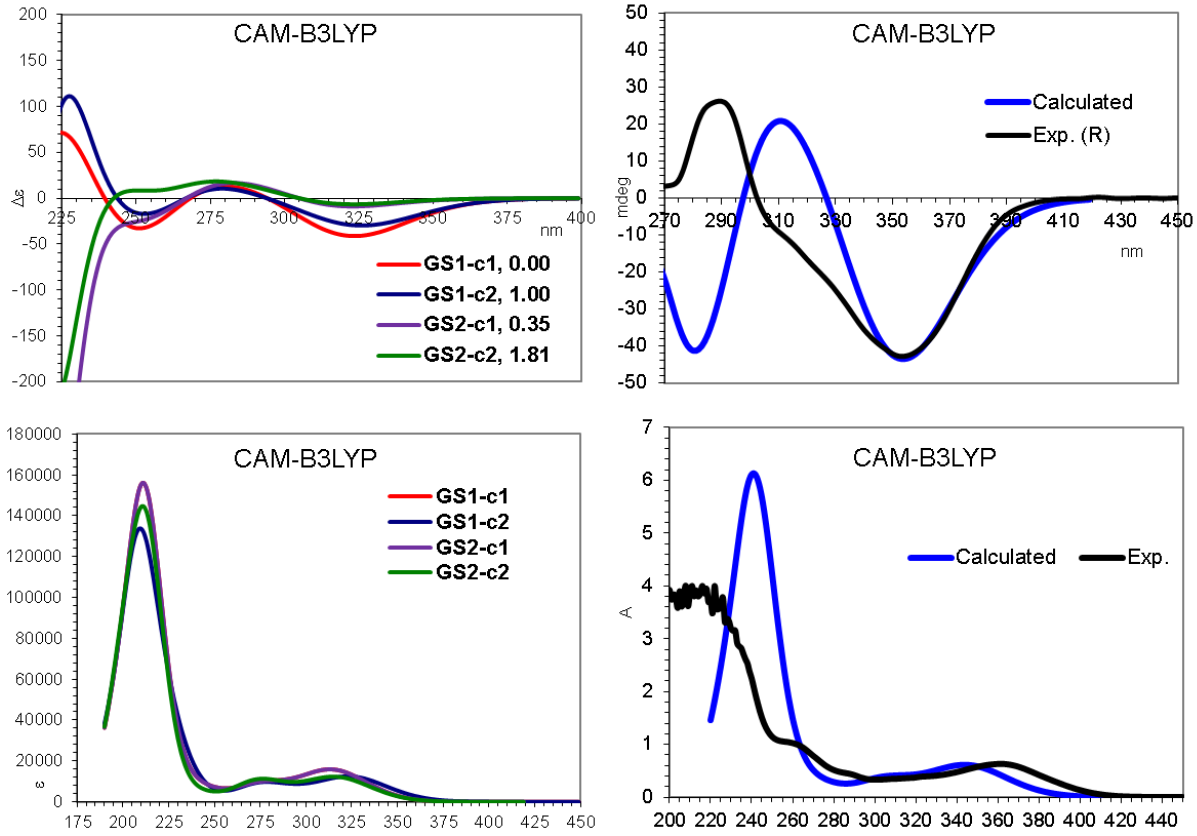
UV and ECD simulation of the four conformations of **1b**, and Boltzmann–averaged spectra
(relative energies are reported in the legend in kcal/mol),
TD-DFT CAM-B3LYP/6-311++G(2d,p) level
(UV and ECD spectra were red-shifted by 40 nm)



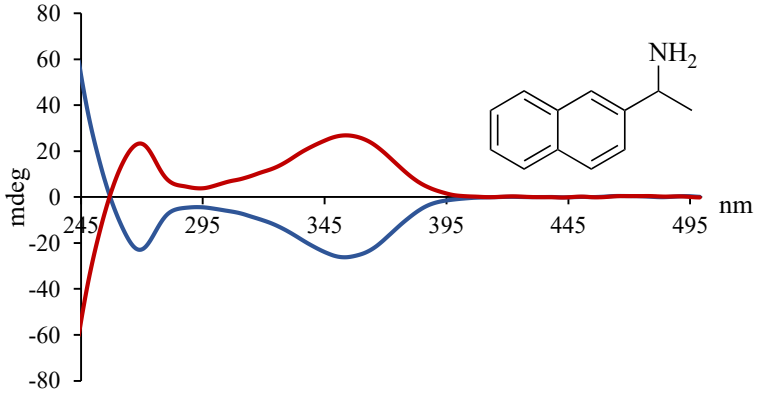
CD spectra of the imine formed from **1** with (*R*)-1-(naphthalen-1-yl)ethan-1-amine (blue) and (*S*)-1-(naphthalen-1-yl)ethan-1-amine (red) at 68 μM.



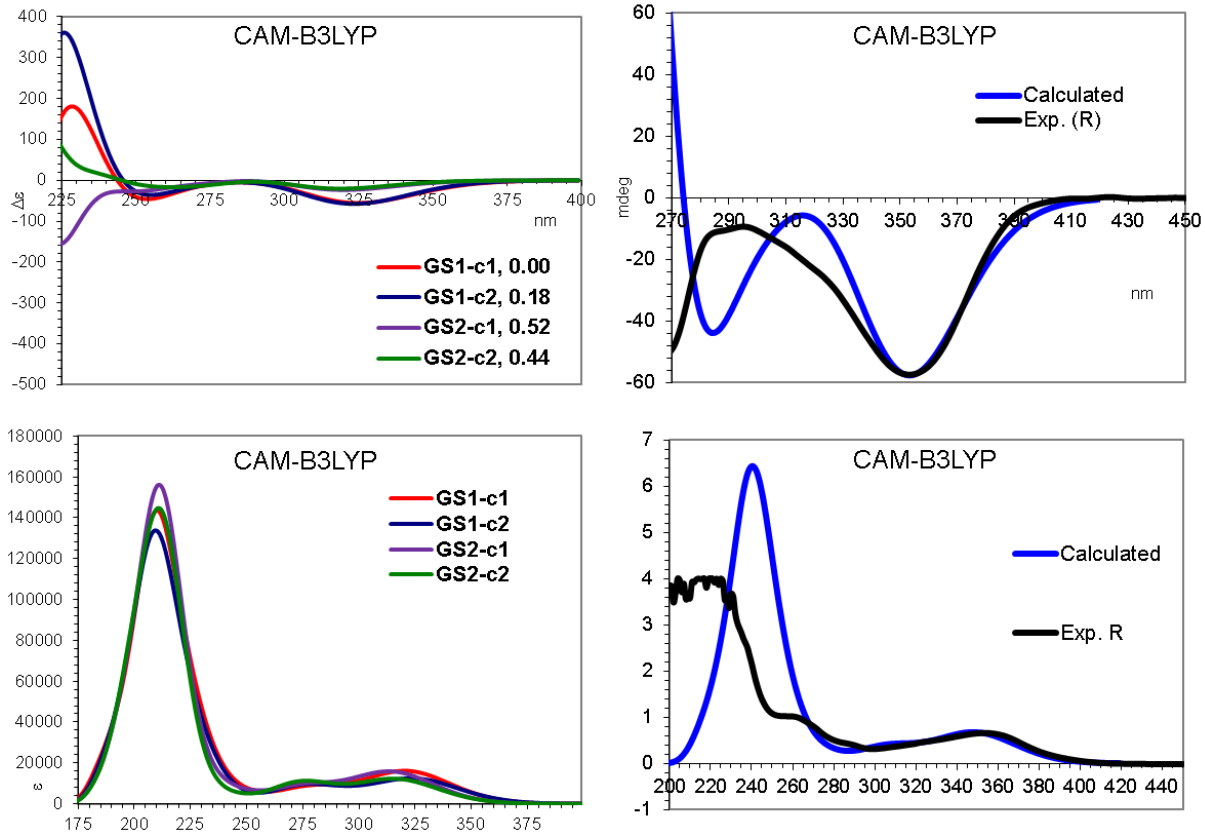
UV and ECD simulation of the four conformations of **1c**, and Boltzmann–averaged spectra
(relative energies are reported in the legend in kcal/mol),
TD-DFT CAM-B3LYP/6-311++G(2d,p) level
(calculated UV and ECD spectra were red-shifted by 30nm)



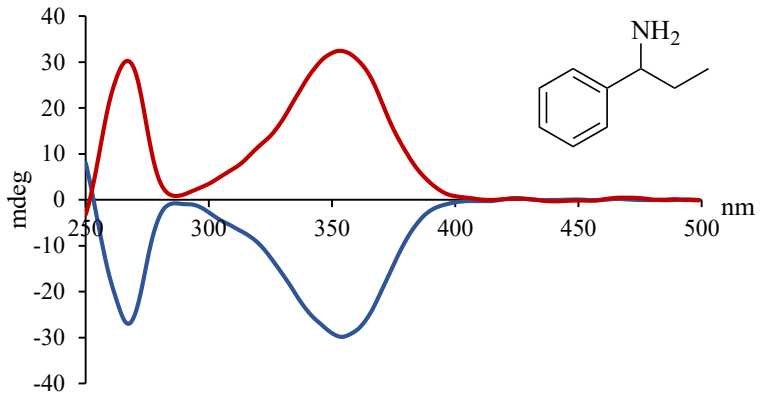
CD spectra of the imine formed from **1** with (*R*)-1-(naphthalen-2-yl)ethan-1-amine (blue) and (*S*)-1-(naphthalen-2-yl)ethan-1-amine (red) at 68 μM.



UV and ECD simulation of the four conformations of **1d**, and Boltzmann–averaged spectra
(relative energies are reported in the legend in kcal/mol),
TD-DFT CAM-B3LYP/6-311++G(2d,p) level
(calculated UV and ECD spectra were red-shifted by 30nm)

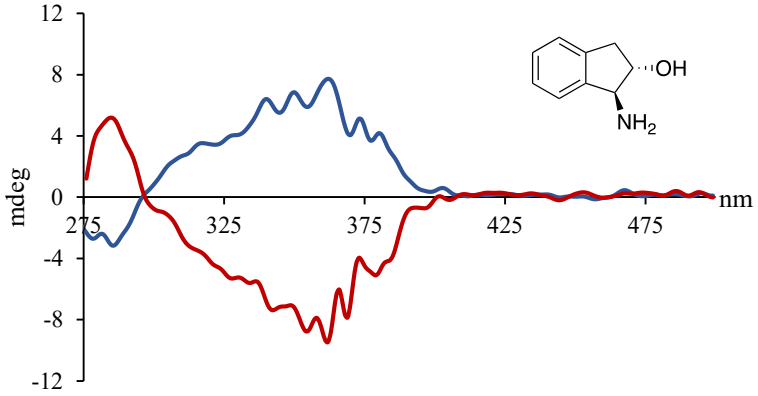


CD spectra of the imine formed from **1** with (*R*)-1-phenylpropan-1-amine (blue) and (*S*)-1-phenylpropan-1-amine (red) at 136 μM.

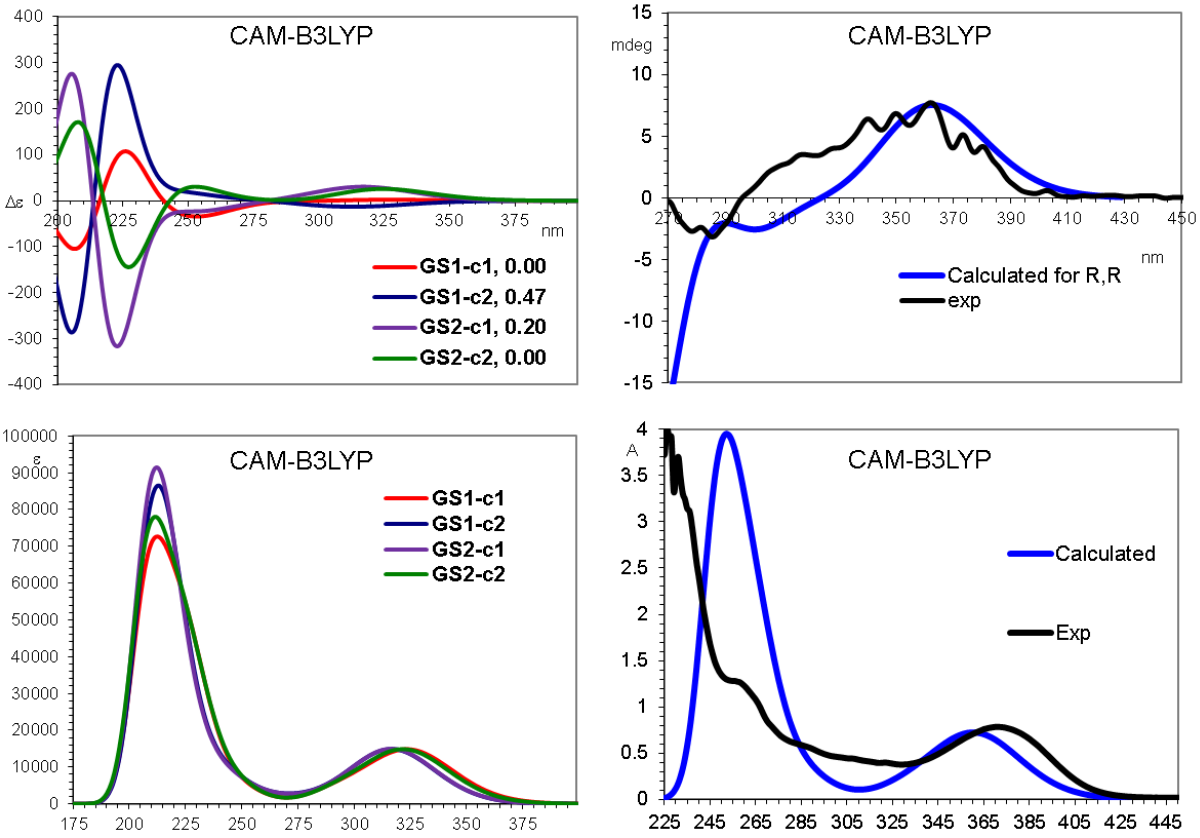


Because of the similarity to **1a**, we did not calculate the spectra for **1e**.

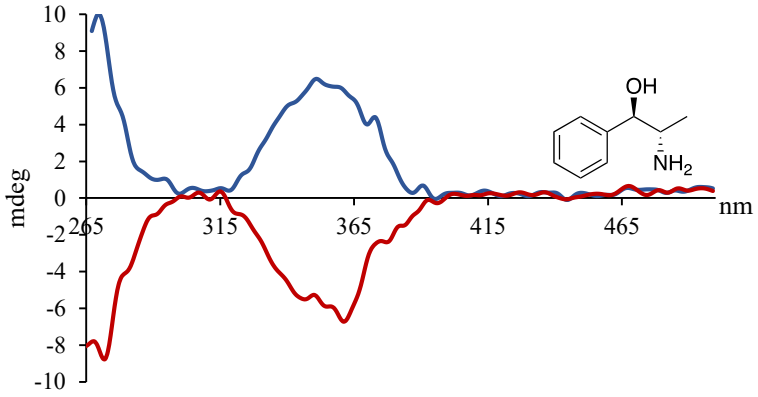
CD spectra of the imine formed from **1** with (1*R*,2*R*)-1-amino-2,3-dihydro-1*H*-inden-2-ol (blue) and (1*S*,2*S*)-1-amino-2,3-dihydro-1*H*-inden-2-ol (red) at 512 μM.



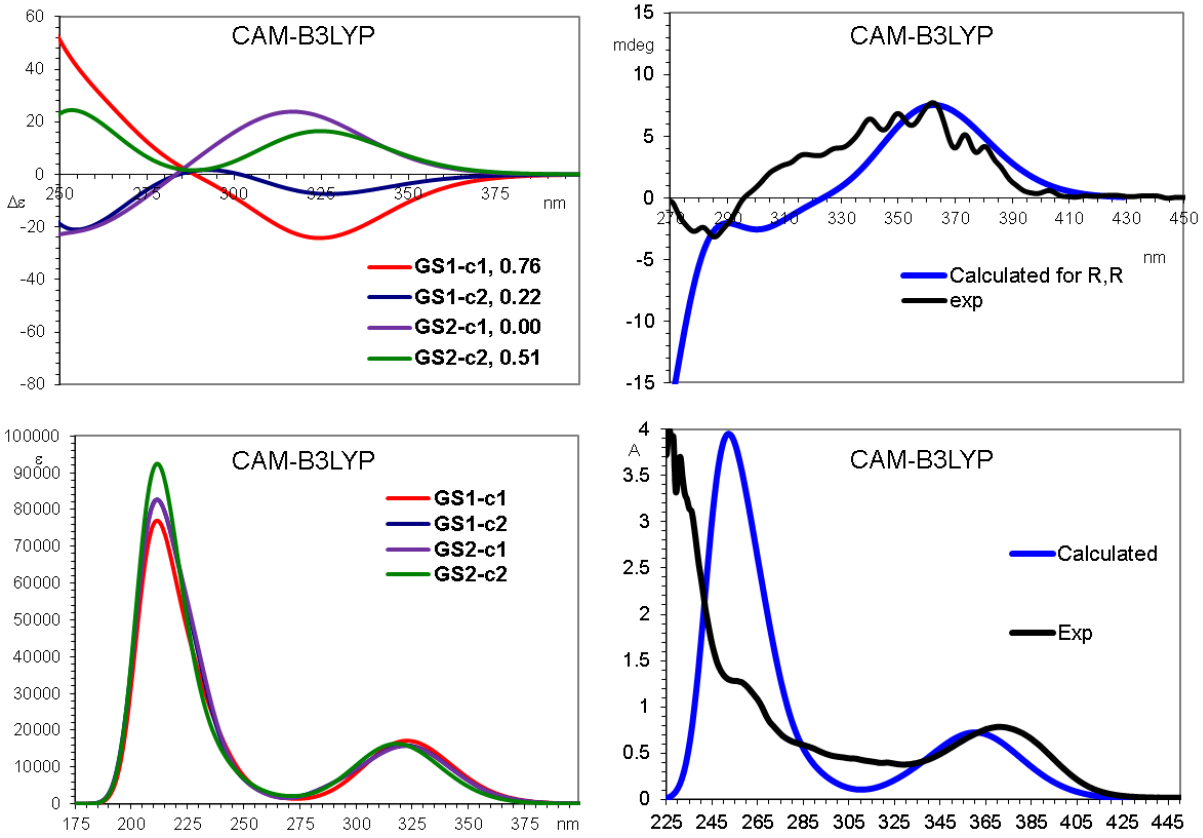
UV and ECD simulation of the four conformations of **1g**, and Boltzmann–averaged spectra
(relative energies are reported in the legend in kcal/mol),
TD-DFT CAM-B3LYP/6-311++G(2d,p) level
(UV and ECD spectra were red-shifted by 35 nm)



CD spectra of the imine formed from **1** with (1*R*,2*S*)-2-amino-1-phenylpropan-1-ol (blue) and (1*S*,2*R*)-2-amino-1-phenylpropan-1-ol (red) at 512 μM.



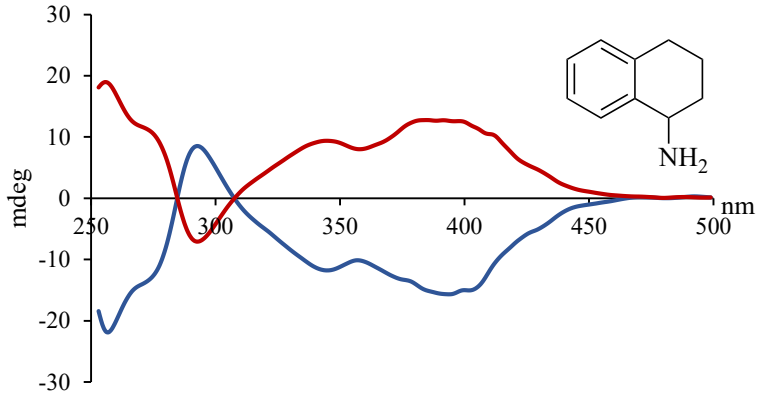
UV and ECD simulation of the four conformations of **1h**, and Boltzmann–averaged spectra
(relative energies are reported in the legend in kcal/mol),
TD-DFT CAM-B3LYP/6-311++G(2d,p) level
(UV and ECD spectra were red-shifted by 40 nm)



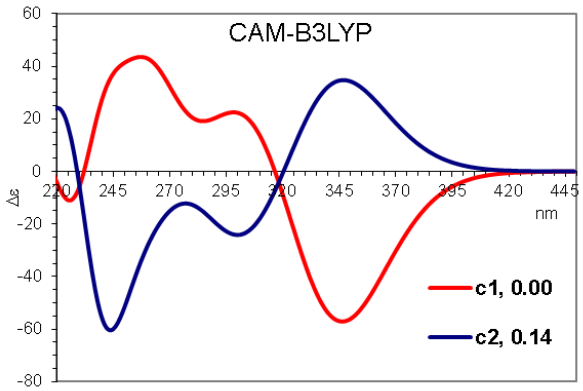
3.2. Chiroptical sensing with 2

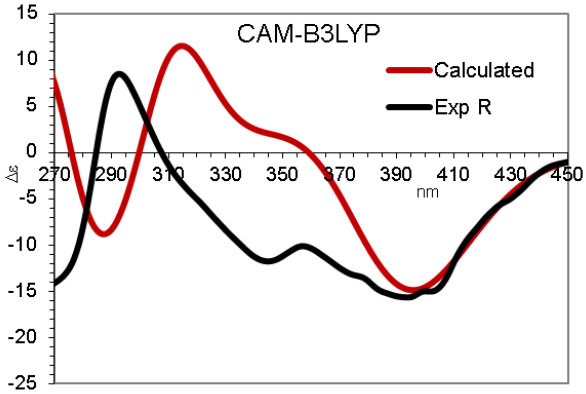
A solution of **2** (19 mM) was prepared in anhydrous acetonitrile and 250 µL amounts were distributed into vials containing 750 µL of anhydrous acetonitrile to generate reaction concentrations of 4.8 mM. Molecular sieves (4A) were added to each vial followed by equimolar amounts of the chiral substrate. The vials were sealed and placed on a shaker apparatus for 14 hours. CD and UV measurements were then taken by dispensing 20-180 µL aliquots of the imine condensation reactions into 2 mL of anhydrous acetonitrile to afford the desired sensing concentrations mentioned below.

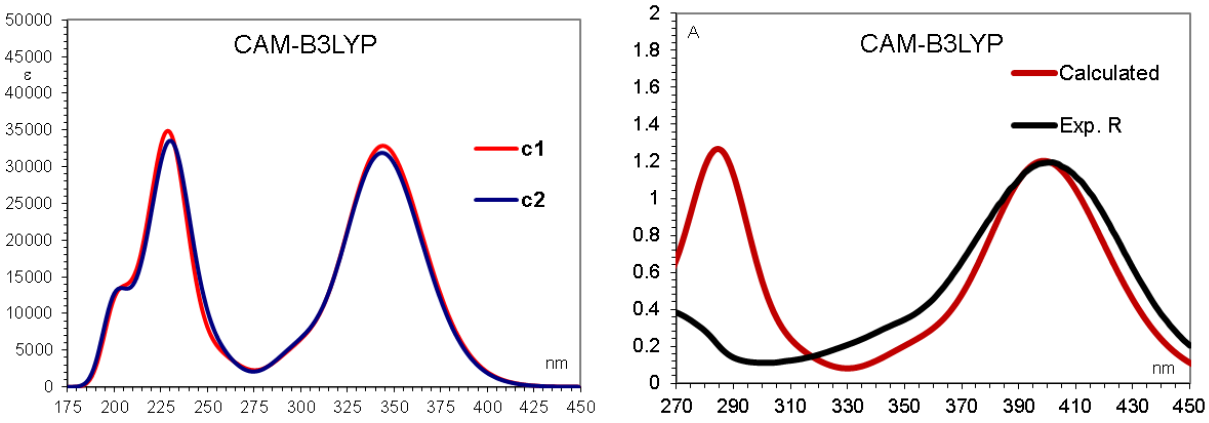
CD spectra of the imine formed from **2** with (*R*)-1,2,3,4-tetrahydronaphthalen-1-amine (blue) and (*S*)-1,2,3,4-tetrahydronaphthalen-1-amine (red) at 120 µM.



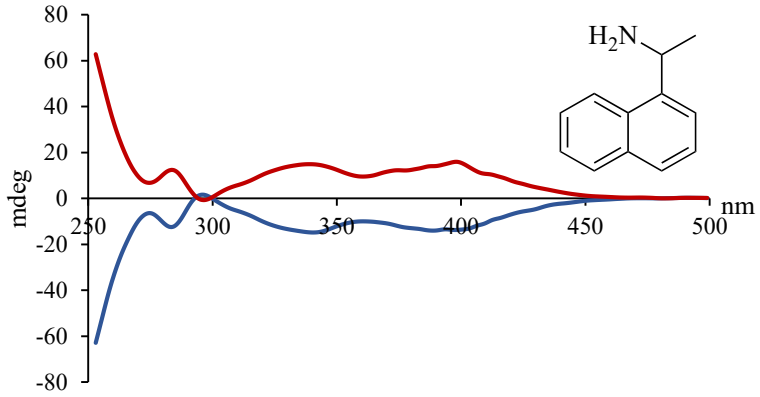
UV and ECD simulation of the four conformations of **2f**, and Boltzmann–averaged spectra
(relative energies are reported in the legend in kcal/mol),
TD-DFT CAM-B3LYP/6-311++G(2d,p) level
(simulated UV and ECD spectra were red-shifted by 55 nm)



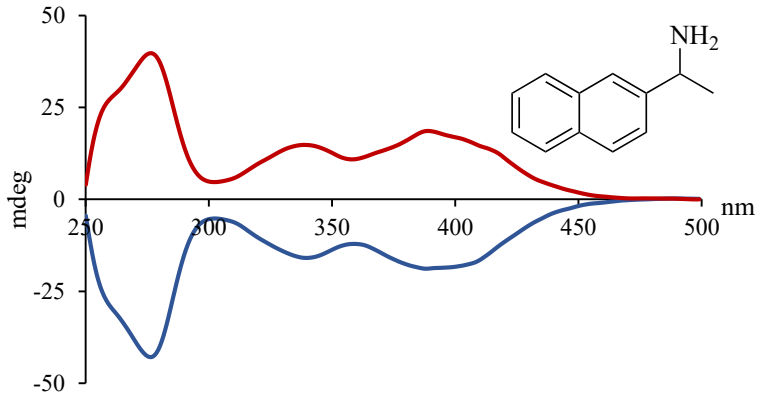




CD spectra of the imine formed from **2** with (*R*)-1-(naphthalen-1-yl)ethan-1-amine (blue) and (*S*)-1-(naphthalen-1-yl)ethan-1-amine (red) at 120 μM.

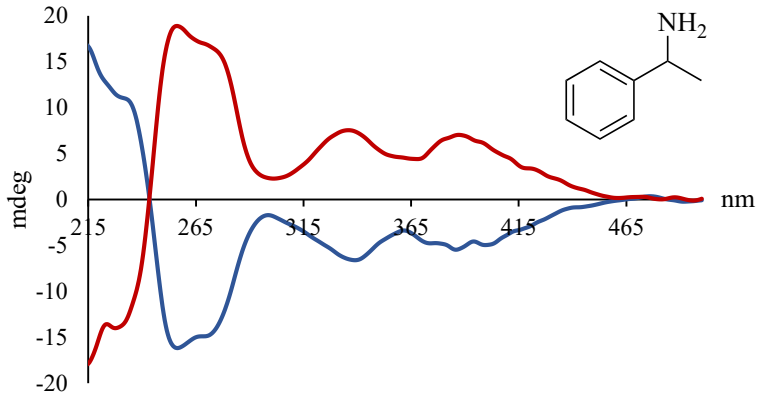


CD spectra of the imine formed from **2** with (*R*)-1-(naphthalen-2-yl)ethan-1-amine (blue) and (*S*)-1-(naphthalen-2-yl)ethan-1-amine (red) at 96 μM.

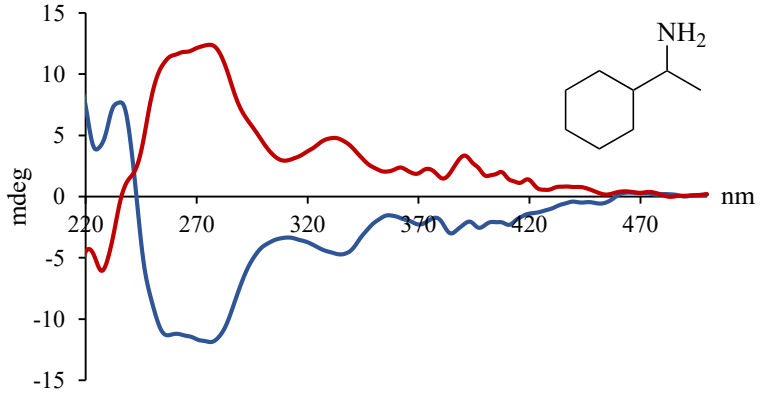


A solution of **2** (24 mM) was prepared in anhydrous acetonitrile and 500 µL amounts were distributed into vials containing 500 µL of anhydrous acetonitrile to generate reaction concentrations of 12 mM. Molecular sieves (4A) were added to each vial followed by equimolar amounts of the chiral substrate. The vials were sealed and placed on a shaker apparatus for 14 hours. CD and UV measurements were then taken by dispensing 20-180 µL aliquots of the imine condensation reactions into 2 mL of anhydrous acetonitrile to afford the desired sensing concentrations mentioned below.

CD spectra of the imine formed from **2** with (*R*)-1-phenylethan-1-amine (blue) and (*S*)-1-phenylethan-1-amine (red) at 60 µM.



CD spectra of the imine formed from **2** with (*R*)-1-cyclohexylethan-1-amine (blue) and (*S*)-1-cyclohexylethan-1-amine (red) at 90 µM.

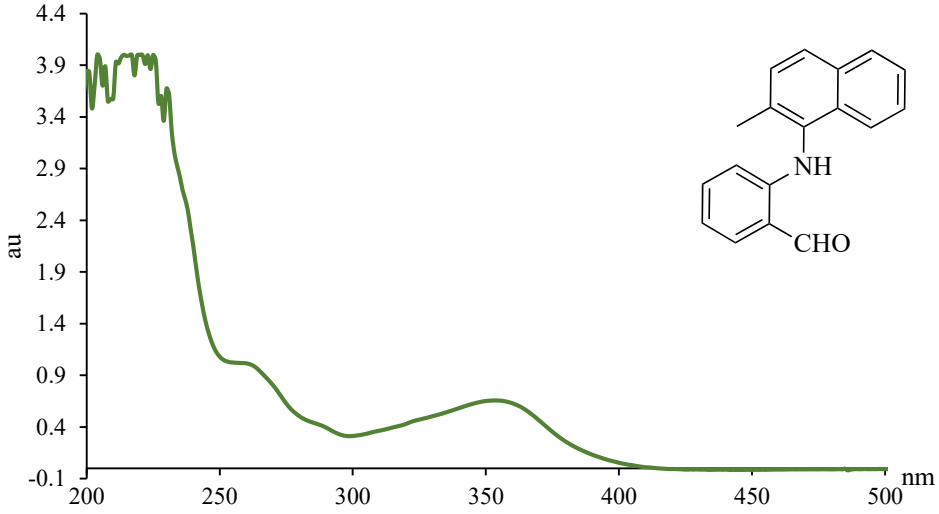


4. UV Analysis

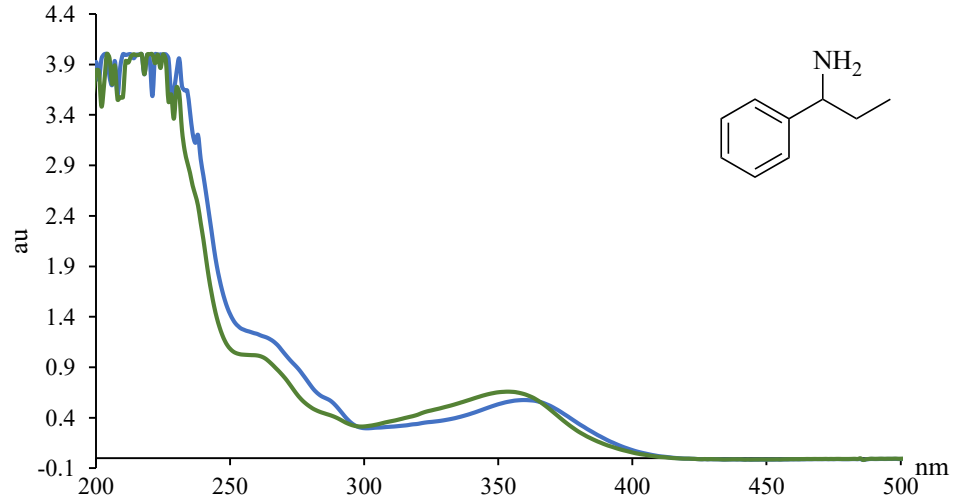
4.1 UV Spectra of the Imines Formed with 1

All solutions prepared according to SI protocol in **3** described above.

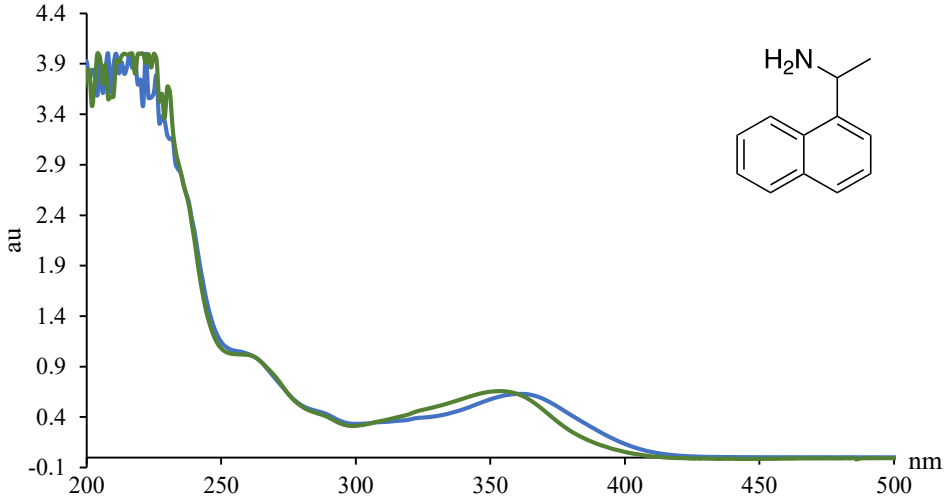
UV spectrum of **1** (68 μM) in acetonitrile (local λ_{max}=353 nm).



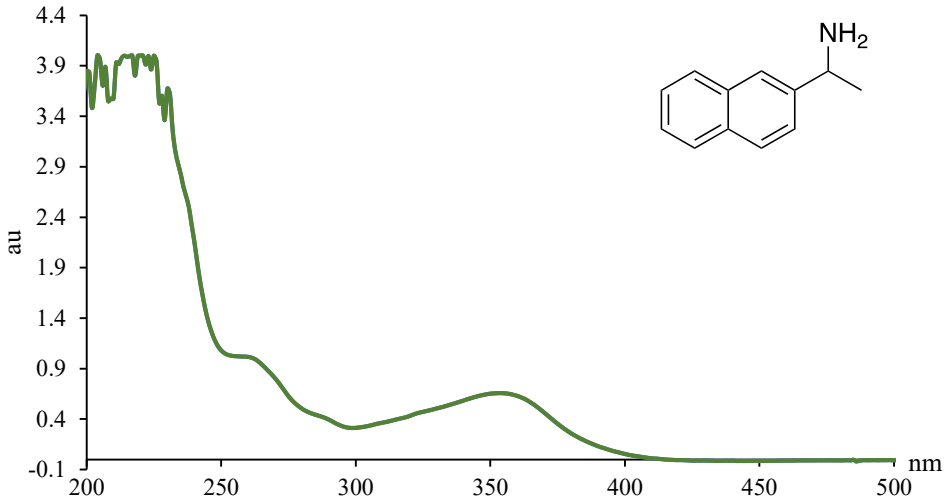
UV spectrum of **1** (green) and the imine formed from **1** (68 μM) and (*R*)-1-phenylpropan-1-amine (blue) in acetonitrile (local λ_{max}=360 nm).



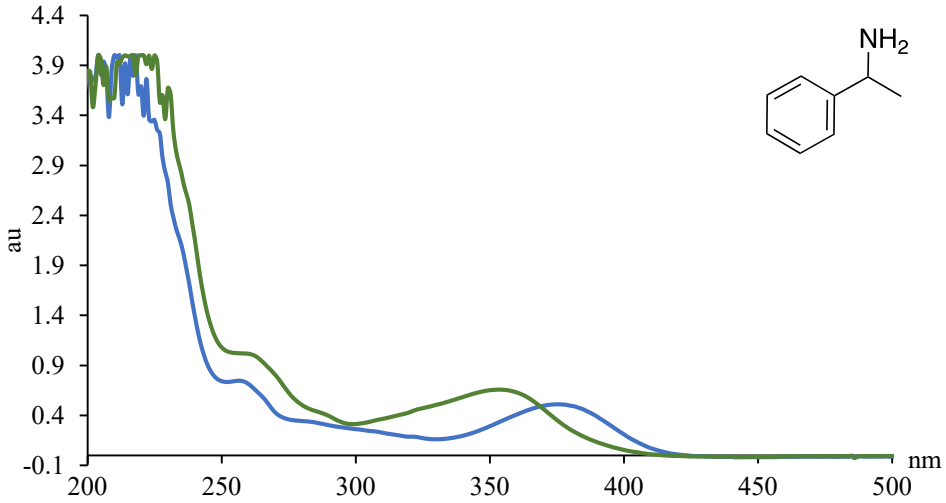
UV spectrum of **1** (green) and the imine formed from **1** (68 μM) and (*R*)-1-(naphthalen-1-yl)ethan-1-amine (blue) in acetonitrile (local λ_{max}=361 nm).



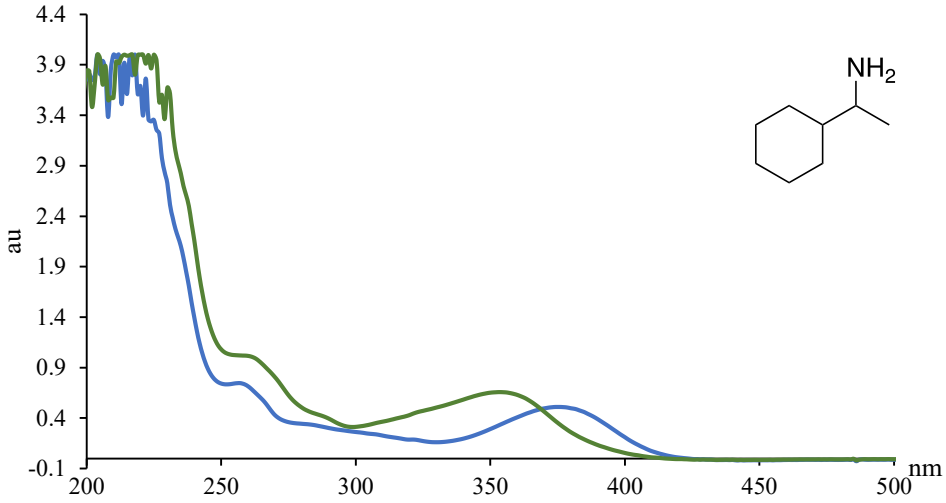
UV spectrum of **1** (green) and the imine formed from **1** (68 μM) and (*R*)-1-(naphthalen-2-yl)ethan-1-amine (blue) in acetonitrile (local λ_{max}=354 nm).



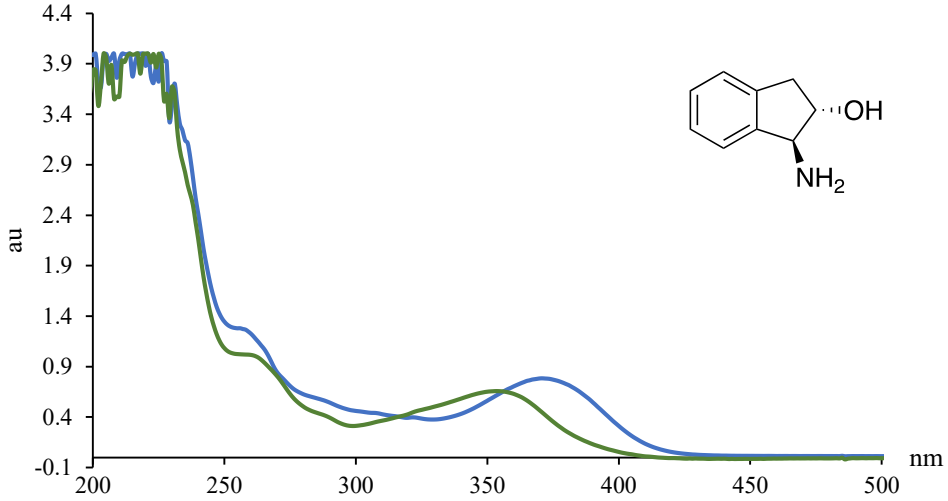
UV spectrum of **1** (green) and the imine formed from **1** (68 μM) and (*R*)-1-phenylethan-1-amine (blue) in acetonitrile (local λ_{max}=376 nm).



UV spectrum of **1** (green) and the imine formed from **1** (68 μM) and (*R*)-1-cyclohexylethan-1-amine (blue) in acetonitrile (local λ_{max}=376 nm).

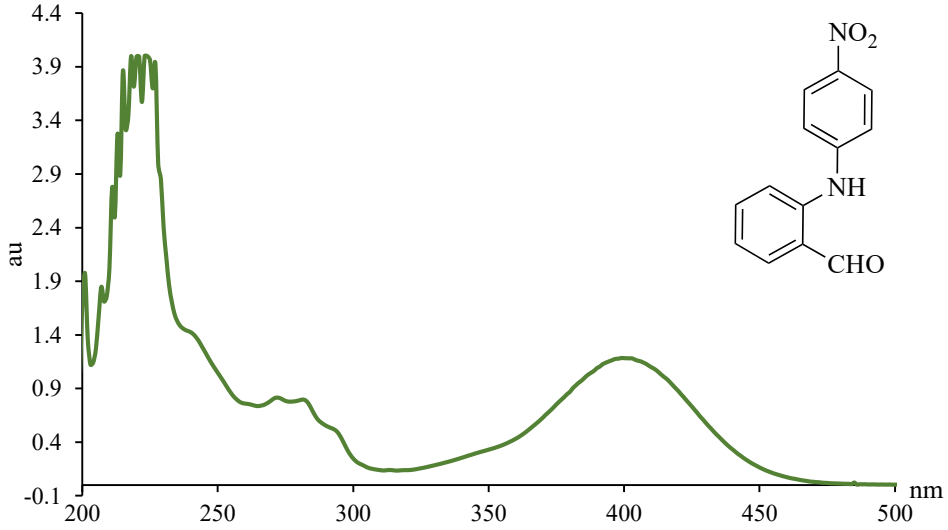


UV spectrum of **1** (68 μM) (green) and the imine formed from **1** (64 μM) and (1*R*,2*R*)-1-amino-2,3-dihydro-1*H*-inden-2-ol (blue) in acetonitrile (local λ_{max}=371 nm).

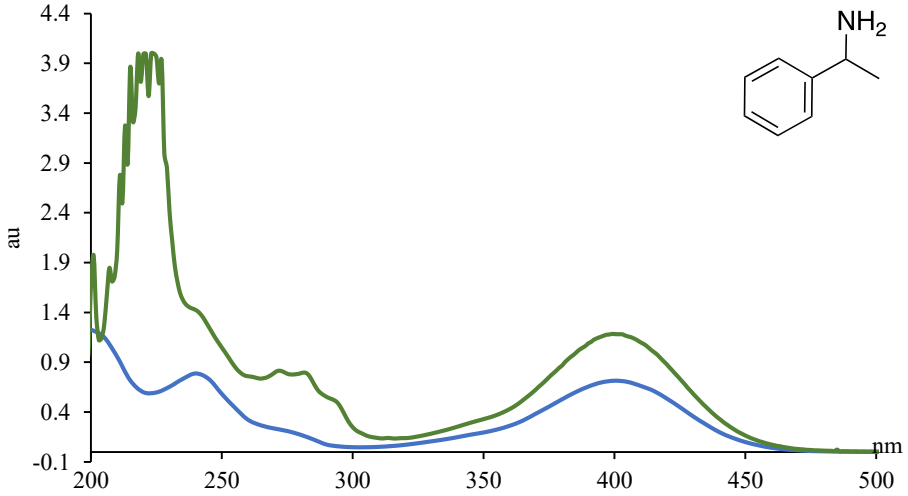


4.2 UV Spectra of the Imines Formed with 2

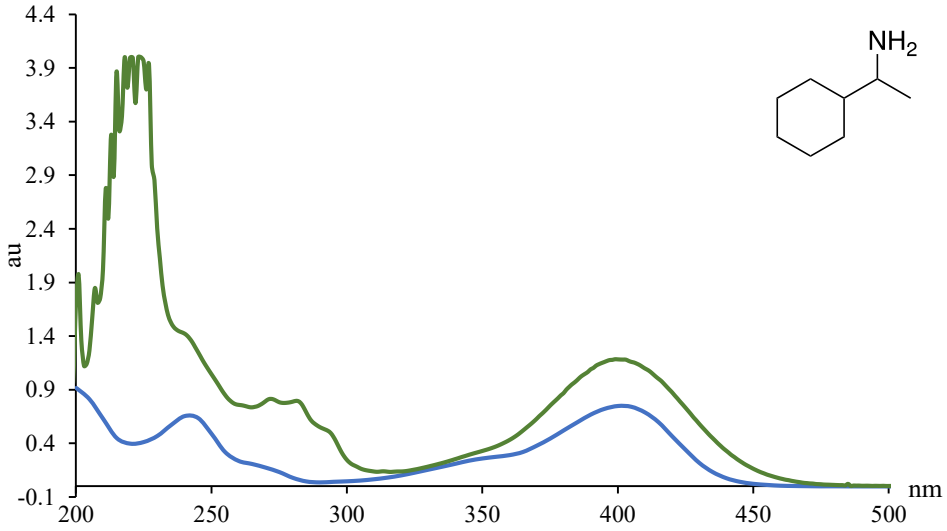
UV spectrum of **2** (48 μM) in acetonitrile (local λ_{max}=391 nm).



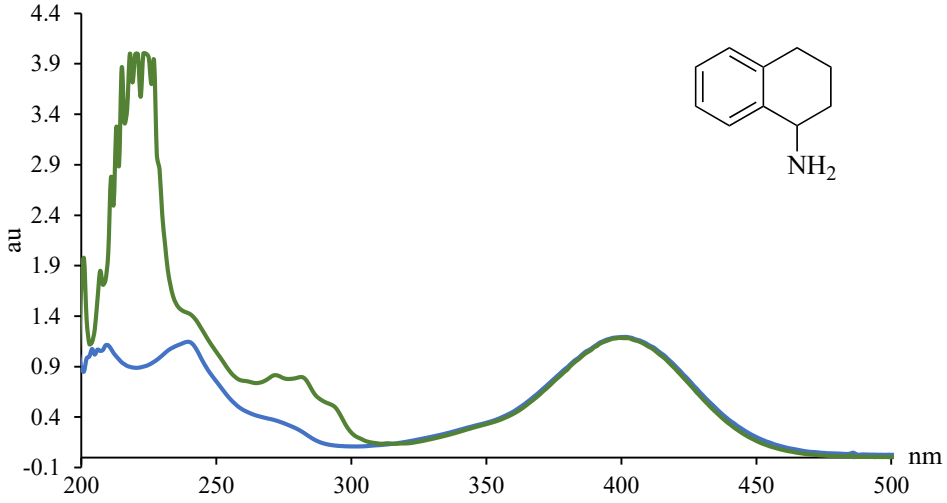
UV spectrum of **2** (48 µM) (green) and of the imine formed from **2** (60 µM) and (*S*)-1-phenylethan-1-amine (blue) in acetonitrile (local λ_{max}=400 nm).



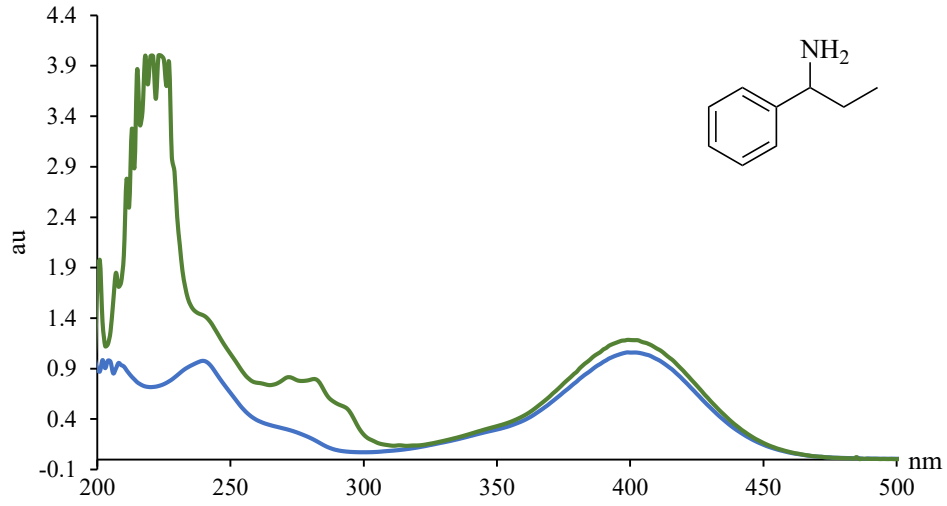
UV spectrum of **2** (48 µM) (green) and of the imine formed from **2** (60 µM) and (*S*)-1-cyclohexylethan-1-amine in acetonitrile (local λ_{max}=400 nm).



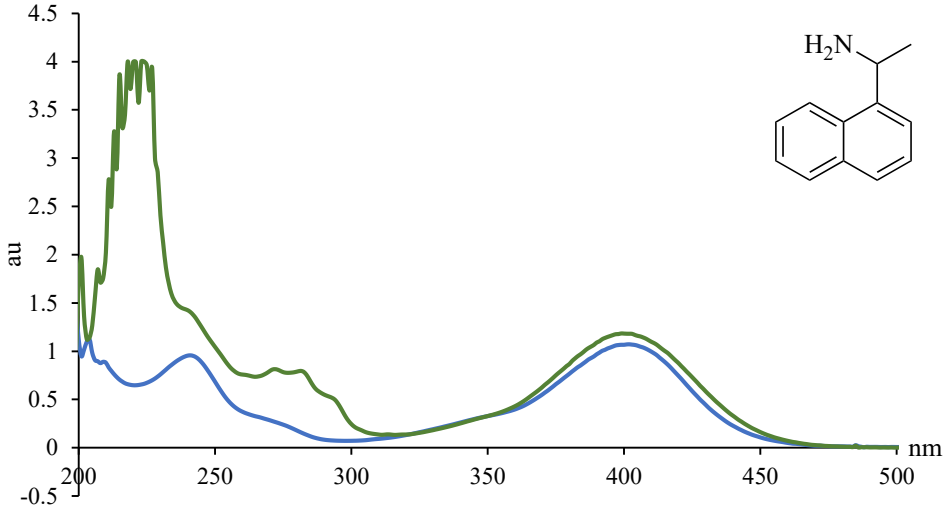
UV spectrum of **2** (48 μM) (green) and of the imine formed from **2** (48 μM) and (*R*)-1,2,3,4-tetrahydronaphthalen-1-amine (blue) in acetonitrile (local λ_{max}=402 nm).



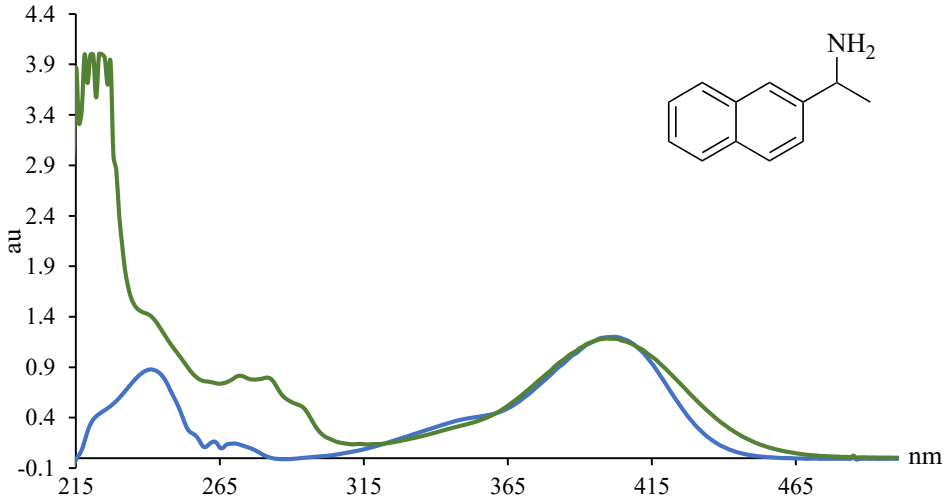
UV spectrum of **2** (48 μM) (green) and of the imine formed from **2** (48 μM) and (*S*)-1-phenylpropan-1-amine (blue) in acetonitrile (local λ_{max}=399 nm).



UV spectrum of **2** (48 µM) (green) and of the imine formed from **2** (48 µM) and (*R*)-1-(naphthalen-1-yl)ethan-1-amine (blue) in acetonitrile (local λ_{max}=402 nm).



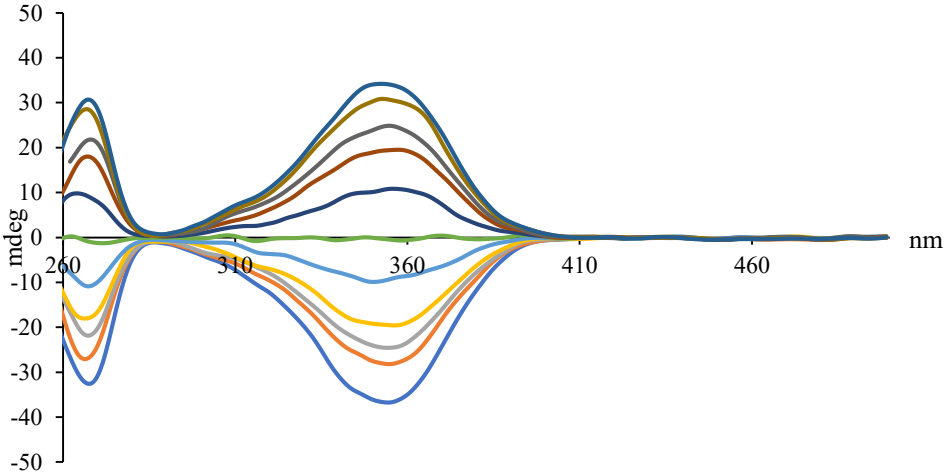
UV spectrum of **2** (48 µM) (green) and of imine formed from **2** (48 µM) and (*R*)-1-(naphthalen-2-yl)ethan-1-amine in acetonitrile (local λ_{max}=402 nm).



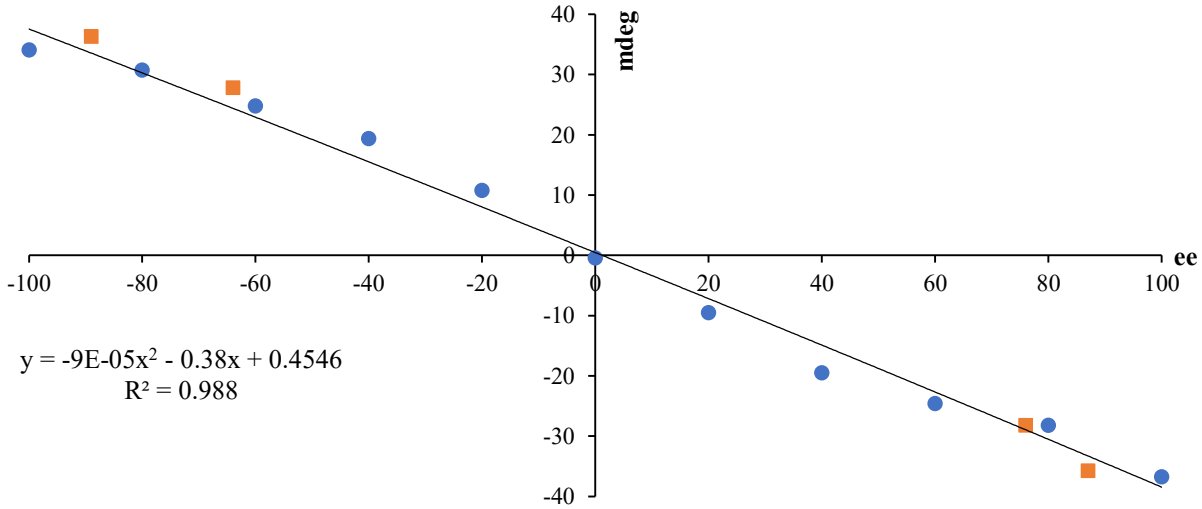
5. Quantitative Ee Determination

A solution of **1** (19.6 mM) was prepared in anhydrous dichloromethane and 250 µL amounts were distributed into vials containing 750 µL of anhydrous dichloromethane to generate reaction concentrations of 4.9 mM. Molecular sieves (4Å) were added to each vial followed by equimolar amounts of 1-phenylpropan-1-amine with varied *ee* values (100, 80, 60, 40, 20, 0, -20, -40, -60, -80, -100 *%ee*). The vials were sealed and placed on a shaker apparatus for 12 hours. CD and UV measurements were then taken by dispensing 100 µL aliquots of the imine condensation reactions into 2 mL of anhydrous acetonitrile to afford an ee calibration curve. A second set of imine condensation reactions were prepared following the same procedure described using random ee mixtures of the same amine (87, 76, -64, -89 %ee).

Calibration curve of the chiroptical responses of **1** with varied enantiomeric compositions of 1-phenylpropan-1-amine.



Correlation of the chiroptical responses of **1** (blue) at 354 nm to the ee's of the scalemic samples and random ee compositions of 1-phenylpropan-1-amine (orange) for enantiomeric determination using calibration curve fitting.

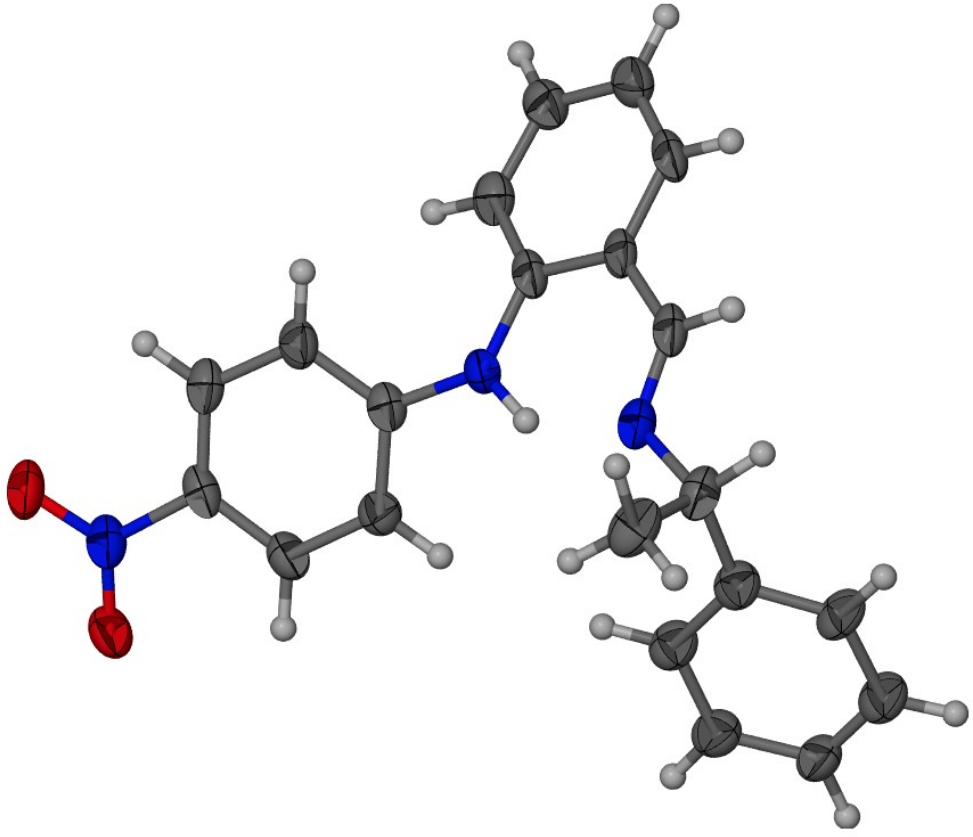


Comparison of *ee* values of the randomly prepared enantiomeric mixtures of 1-phenylpropan-1-amine with the CD sensing results.

Sample composition		**Chiroptical sensing results**	
Absolute configuration	**Actual ee**	**Absolute configuration**	**Ee values**
S	87	*S*	93
S	76	*S*	74
R	64	*R*	73
R	89	*R*	97

6. Crystallographic Analysis

A single crystal of the imine formed from **2** and (*S*)-1-phenylethan-1-amine was obtained by slow evaporation of a solution in methanol. Single crystal X-ray analysis was performed at 100 K using a Bruker Apex DUO equipped with an APEXII CCD detector with a multi-layer mirror monochromated Cu-Kα IμS radiation (λ = 1.54178 Å). Data were integrated and corrected using the SAINT v8.37A and SADABS v2016/2 software within APEX 3. The structures were solved by direct methods and refined with full-matrix least-square analysis using SHELX-2018-1 software. Non-hydrogen atoms were refined with anisotropic displacement parameters. Crystal data: $C_{21}H_{19}N_3O_2$, M = 345.39, yellow column, 0.212 x 0.118 x 0.056 mm^3, orthorhombic, space group $P2_12_12_1$ a = 7.6371(4), b = 14.5261(8), c = 16.1757(8) Å, V =1794.49(16) Å^3, Z = 4.



7. Computational Data

Compound 1a, conformation c1

C	-0.15001300	3.93357100	-0.62510100
C	-0.28703900	2.58803200	-0.23474700
C	0.79735700	1.68474600	-0.47152800
C	1.95518700	2.18104400	-1.11025000
C	2.04892800	3.51535800	-1.47952800
C	0.99860100	4.41122500	-1.23746400
N	0.69065600	0.37227100	-0.07520100
C	1.61133200	-0.66644600	-0.39752000
C	2.81063900	-0.80969100	0.37164000
C	3.71624100	-1.87379300	0.05338700
C	3.38165200	-2.76619400	-0.99713800
C	2.21114400	-2.61320600	-1.70091300
C	1.30537100	-1.55601000	-1.42054400
C	3.13448700	0.06017300	1.44856900
C	4.30135800	-0.10423000	2.16095500
C	5.20401900	-1.14591300	1.83601600
C	4.91334500	-2.01127500	0.80661800
C	0.03899800	-1.40814600	-2.23127500
C	-1.55176800	2.18793900	0.37020200
N	-1.84291500	1.00450800	0.77592900
C	-3.16622900	0.77828700	1.35651900
C	-3.00984500	0.45458400	2.85368600
C	-3.88048300	-0.34170800	0.60857900
C	-3.28972600	-1.60532000	0.46340000
C	-3.95667300	-2.63070600	-0.20617100
C	-5.22859400	-2.41048100	-0.74152900
C	-5.82500900	-1.15765400	-0.60287300
C	-5.15195700	-0.13198500	0.06565800
H	-2.29122300	3.00094500	0.45889300
H	-0.98407600	4.60719000	-0.43777200
H	2.77727700	1.50245600	-1.30895000
H	2.95619100	3.86366500	-1.96709500
H	1.07955300	5.45399900	-1.52786600
H	-0.23665400	0.11967200	0.27514700
H	4.06545500	-3.57715900	-1.23674100
H	1.96845700	-3.30602800	-2.50306300
H	2.44003900	0.85322400	1.70286800
H	4.53178500	0.56883600	2.98258700
H	6.12218900	-1.26192400	2.40558300
H	5.59601800	-2.81970700	0.55479200
H	0.03306400	-2.10617100	-3.07407100
H	-0.85917900	-1.60331800	-1.63182600
H	-0.06419600	-0.39200700	-2.62756100
H	-3.78151400	1.69029500	1.26785600
H	-3.98768000	0.26006500	3.30714800
H	-2.38120000	-0.43044000	2.99464600
H	-2.53923300	1.29413300	3.37686400
H	-2.30068800	-1.78492100	0.87614900
H	-3.48406500	-3.60429100	-0.30877700
H	-5.74829100	-3.20978900	-1.26313600
H	-6.81284700	-0.97392100	-1.01756600
H	-5.62130200	0.84453200	0.16492200

Compound 1a, conformation c2

C	-0.15035700	3.93358300	-0.62491800
C	-0.28725800	2.58800100	-0.23465400
C	0.79717300	1.68480800	-0.47160700
C	1.95491500	2.18122800	-1.11039400
C	2.04853800	3.51557600	-1.47957100
C	0.99817100	4.41135800	-1.23733900
N	0.69057300	0.37227200	-0.07545700
C	1.61142500	-0.66632100	-0.39776100
C	2.81057700	-0.80960100	0.37163900
C	3.71629500	-1.87360300	0.05343100
C	3.38198600	-2.76587000	-0.99730400
C	2.21163200	-2.61284800	-1.70131700
C	1.30572400	-1.55574200	-1.42097400
C	3.13415100	0.06013600	1.44876100
C	4.30087200	-0.10431300	2.16137300
C	5.20365500	-1.14591700	1.83648600
C	4.91324600	-2.01114200	0.80690400
C	0.03948500	-1.40791300	-2.23190800
C	-1.55190200	2.18778100	0.37039800
N	-1.84284200	1.00433800	0.77623500
C	-3.16614900	0.77794800	1.35685300
C	-3.00963400	0.45397600	2.85393100
C	-3.88036100	-0.34192700	0.60871600
C	-5.15181400	-0.13213800	0.06577100
C	-5.82481600	-1.15770600	-0.60296400
C	-5.22837200	-2.41049900	-0.74180800
C	-3.95646300	-2.63078400	-0.20644800
C	-3.28956500	-1.60549900	0.46332700
H	-2.29146800	3.00069000	0.45904600
H	-0.98445200	4.60712700	-0.43745600
H	2.77703100	1.50270600	-1.30921600
H	2.95573700	3.86398900	-1.96718100
H	1.07903900	5.45416000	-1.52766200
H	-0.23658600	0.11960200	0.27523500
H	4.06590000	-3.57675300	-1.23687100
H	1.96914800	-3.30555500	-2.50362800
H	2.43960300	0.85311800	1.70300100
H	4.53111300	0.56863900	2.98315100
H	6.12170000	-1.26194800	2.40624800
H	5.59600400	-2.81950900	0.55509800
H	0.03405800	-2.10539000	-3.07516200
H	-0.85872800	-1.60390800	-1.63277300
H	-0.06410100	-0.39156100	-2.62752800
H	-3.78145600	1.68995400	1.26837700
H	-3.98741600	0.25929800	3.30744300
H	-2.38091600	-0.43103100	2.99467900
H	-2.53904000	1.29345600	3.37723300
H	-5.62118300	0.84435400	0.16517900
H	-6.81264000	-0.97391900	-1.01766500
H	-5.74803100	-3.20972800	-1.26357300
H	-3.48382500	-3.60433800	-0.30920600
H	-2.30052700	-1.78515000	0.87605600

Compound 1a, conformation c3

C	-0.25120000	3.82030200	-1.08075600
C	-0.36593300	2.56073600	-0.46249500
C	0.82187700	1.80571100	-0.20387900
C	2.06529300	2.36938200	-0.56467200
C	2.13387700	3.61492300	-1.17281500
C	0.97534200	4.35568100	-1.44291200
N	0.72611500	0.56486000	0.38394400
C	1.81641800	-0.25721500	0.78428500
C	2.56373600	-0.97767100	-0.20396300
C	3.64265400	-1.81982800	0.22081600
C	3.91539200	-1.93888700	1.60784600
C	3.15971000	-1.25731900	2.53098100
C	2.10079800	-0.39720100	2.13778500
C	2.26714900	-0.90318200	-1.59258100
C	3.01393400	-1.60497100	-2.51255600
C	4.09424600	-2.41885200	-2.09432800
C	4.39626200	-2.52462500	-0.75623700
C	1.30486000	0.34631300	3.18444900
C	-1.70426700	2.10795600	-0.10301400
N	-1.98223600	1.00151100	0.48637000
C	-3.37835200	0.71074600	0.79341800
C	-3.52082200	0.52997900	2.31734400
C	-3.86604500	-0.53129600	0.05120400
C	-5.22405800	-0.64839300	-0.27174400
C	-5.71441500	-1.79062300	-0.90531300
C	-4.84789800	-2.83543000	-1.23106900
C	-3.49172100	-2.72513500	-0.92001900
C	-3.00402900	-1.58242900	-0.28367900
H	-2.51109100	2.80924300	-0.37257500
H	-1.16436500	4.38084100	-1.27126300
H	2.97378300	1.81486600	-0.35816400
H	3.10835500	4.01757600	-1.43801500
H	1.03654600	5.32867200	-1.92016200
H	-0.21277300	0.33932600	0.72073900
H	4.73075600	-2.58171400	1.93099800
H	3.37856400	-1.36014300	3.59108600
H	1.43494100	-0.28907200	-1.91778200
H	2.76988100	-1.53746100	-3.56942300
H	4.67717600	-2.96398200	-2.83181900
H	5.21692600	-3.15604000	-0.42337100
H	1.80644100	0.30652200	4.15633900
H	1.16585800	1.39712900	2.90984800
H	0.30227700	-0.08253800	3.31480000
H	-4.01950200	1.55676800	0.48880300
H	-4.56040900	0.31174100	2.58336100
H	-2.89656900	-0.30214700	2.65967900
H	-3.20647700	1.43927900	2.84158000
H	-5.90474400	0.16502400	-0.02712200
H	-6.77118600	-1.86047500	-1.15045000
H	-5.22547700	-3.72472400	-1.72881600
H	-2.80718500	-3.52962300	-1.17683300
H	-1.94572200	-1.49569500	-0.06020000

Compound 1a, conformation c4

C	-1.36560100	-2.86881300	-1.20608700
C	-0.85936500	-1.68163200	-0.64493300
C	0.54419200	-1.58498900	-0.38220000
C	1.36770800	-2.67597600	-0.73688700
C	0.82817100	-3.82723200	-1.29406900
C	-0.54825900	-3.94236000	-1.52795600
N	1.05086900	-0.44042900	0.18691100
C	2.40791500	-0.18921100	0.51500500
C	3.10122700	0.83819800	-0.20790400
C	4.45340200	1.15065000	0.14687700
C	5.07424100	0.41629200	1.18979400
C	4.38315500	-0.56264600	1.86139000
C	3.03132500	-0.87391100	1.55471200
C	2.49592400	1.55961200	-1.27257100
C	3.18449800	2.55062800	-1.93742600
C	4.51507800	2.86886200	-1.57581700
C	5.13388100	2.17901600	-0.55825000
C	2.30035400	-1.90518600	2.37806300
C	-1.81063000	-0.60515600	-0.38530000
N	-1.49087200	0.55349100	0.06893600
C	-2.49716200	1.61043500	0.26764200
C	-2.15097700	2.35333500	1.56955500
C	-3.96022900	1.18396300	0.22242600
C	-4.51468500	0.36582100	1.21909300
C	-5.85877800	-0.00274700	1.17639000
C	-6.67687500	0.44132200	0.13438200
C	-6.13819200	1.25076400	-0.86548400
C	-4.79002500	1.61318100	-0.82032200
H	-2.85314200	-0.85686300	-0.61915600
H	-2.43579100	-2.92754900	-1.39458900
H	2.43869700	-2.59475600	-0.58465200
H	1.49321000	-4.64632800	-1.55690100
H	-0.96502600	-4.84670000	-1.96011600
H	0.36814200	0.31985400	0.26373800
H	6.10304200	0.64598100	1.45671600
H	4.86629300	-1.10553300	2.67036600
H	1.47998700	1.31273200	-1.56251900
H	2.70503000	3.08910000	-2.75067200
H	5.04682500	3.65336200	-2.10757300
H	6.15870200	2.41126200	-0.27744400
H	2.79969400	-2.05691600	3.34023100
H	1.26706100	-1.59626500	2.56535100
H	2.25064000	-2.87715000	1.87058100
H	-2.33840300	2.32046300	-0.55746100
H	-2.80894700	3.21772900	1.70679500
H	-2.26056200	1.69691700	2.43932400
H	-1.11301000	2.69940900	1.53691600
H	-3.88847700	0.01060600	2.03363700
H	-6.26917700	-0.63602000	1.95874500
H	-7.72515800	0.15649000	0.10306200
H	-6.76463600	1.60090600	-1.68180900
H	-4.37672700	2.24452400	-1.60422600

Compound 1b, conformation c1

C	0.26890200	3.99761600	-1.20843000
C	0.09687200	2.78857700	-0.50932000
C	1.19572000	1.87593500	-0.42444900
C	2.40010000	2.21650300	-1.07854200
C	2.52653300	3.41774700	-1.76242200
C	1.46386600	4.32840200	-1.83010000
N	1.04914500	0.69858700	0.26909500
C	2.04547400	-0.29382300	0.46597300
C	3.13298800	-0.05770800	1.30177200
C	4.08186500	-1.09736100	1.49485200
C	3.93528200	-2.33243300	0.91162800
C	2.82341800	-2.60771400	0.07472100
C	1.86705900	-1.56889300	-0.16611400
C	-1.21126300	2.53137900	0.08259700
N	-1.55176700	1.45719500	0.69895300
C	-2.89871500	1.36950200	1.25614900
C	-2.80015400	1.37950600	2.78994900
C	-3.65425000	0.12996900	0.70757200
C	-3.88673100	0.23910700	-0.81173400
C	-4.70019400	-0.94317100	-1.36026500
C	-4.04648200	-2.28651000	-1.00538700
C	-3.81327500	-2.40561600	0.50740500
C	-2.99793300	-1.22136100	1.05291100
H	-1.93655400	3.35343000	-0.03751300
C	2.63509600	-3.87653700	-0.53568400
C	1.55701400	-4.11419500	-1.35763400
C	0.62246600	-3.08249400	-1.61257300
C	0.77453400	-1.84125100	-1.03385400
C	3.30962700	1.25457100	2.02490500
H	-0.57535500	4.68253700	-1.25902700
H	3.22572200	1.51316700	-1.05429500
H	3.46778000	3.64558400	-2.25672400
H	1.57010200	5.26787000	-2.36331700
H	0.09426700	0.51984900	0.59304900
H	4.93172800	-0.90561400	2.14559500
H	4.66709100	-3.11639700	1.09140800
H	-3.48518000	2.25678500	0.95215300
H	-3.79086300	1.25350500	3.24233100
H	-2.14859300	0.57827500	3.15160200
H	-2.38240600	2.33051200	3.13738900
H	-4.64354300	0.15110700	1.19403200
H	-2.91318200	0.27710500	-1.32024700
H	-4.39510100	1.18571700	-1.04326100
H	-4.81435200	-0.84854700	-2.44791400
H	-5.71540000	-0.91328300	-0.93680400
H	-3.08049600	-2.36781600	-1.52611000
H	-4.66575300	-3.11911600	-1.36347900
H	-3.30215000	-3.34833700	0.74080500
H	-4.78640900	-2.44329900	1.02000400
H	-2.88351500	-1.32616400	2.13858100
H	-1.98633500	-1.25219200	0.62705600
H	3.36395700	-4.66003600	-0.34105000
H	1.42482900	-5.08930500	-1.81863300
H	-0.21729400	-3.26956000	-2.27676500

H	0.06469300	-1.04871200	-1.24581500
H	3.98048000	1.13725500	2.88176400
H	3.73407500	2.02835600	1.37218900
H	2.34920700	1.63838000	2.38310900

Compound 1b, conformation c2

C	0.34607000	3.91271800	-1.18694200
C	0.20958300	2.69117500	-0.50203800
C	1.33968400	1.81768700	-0.41188900
C	2.53741500	2.20716100	-1.05071000
C	2.62835600	3.41873700	-1.72197500
C	1.53518900	4.29222600	-1.79181600
N	1.22888500	0.62977700	0.27137400
C	2.25936200	-0.32332900	0.48046200
C	3.33979100	-0.03849500	1.31077700
C	4.32835000	-1.03936700	1.50978500
C	4.22696900	-2.28492700	0.93983300
C	3.12096700	-2.61197000	0.11375600
C	2.12389400	-1.61345000	-0.13282600
C	-1.09659900	2.37908700	0.06771900
N	-1.40491400	1.28010000	0.65588000
C	-2.75296300	1.12168800	1.19660300
C	-2.63960700	1.07666100	2.72926800
C	-3.40638300	-0.14852000	0.59310400
C	-4.81069400	-0.42310700	1.16941200
C	-5.46599000	-1.66435500	0.54083900
C	-5.52157200	-1.57068300	-0.98964900
C	-4.12593900	-1.30971600	-1.57162600
C	-3.47626500	-0.06675400	-0.94530400
H	-1.84917500	3.17664800	-0.04731600
C	2.97737800	-3.89462700	-0.47938800
C	1.90235600	-4.18443700	-1.28847500
C	0.92511300	-3.19384200	-1.54580600
C	1.03400800	-1.94028200	-0.98460300
C	3.46871400	1.28392000	2.02546500
H	-0.52176200	4.56725400	-1.24095100
H	3.38676100	1.53279400	-1.02589600
H	3.56571800	3.68389100	-2.20491500
H	1.61368100	5.24031300	-2.31448800
H	0.27478500	0.40625200	0.56868300
H	5.17279600	-0.80850700	2.15490700
H	4.98942900	-3.03821700	1.12328500
H	-3.37720200	1.99192700	0.91827400
H	-3.62446500	1.05423800	3.20508200
H	-2.07695300	0.19219500	3.04959000
H	-2.10901300	1.96287100	3.09275600
H	-2.75588500	-0.99730500	0.85805200
H	-5.45079900	0.45469800	0.98803200
H	-4.76290800	-0.55465900	2.25628200
H	-6.47402100	-1.80059500	0.95334800
H	-4.88995200	-2.55708200	0.82632400
H	-6.19440400	-0.74953400	-1.27910000
H	-5.94897000	-2.48887400	-1.41278500
H	-4.18098900	-1.19350900	-2.66173300

H	-3.48655300	-2.18520200	-1.38364500
H	-2.47105400	0.07849800	-1.35568300
H	-4.05940400	0.82485400	-1.22668100
H	3.73777800	-4.64665800	-0.28130000
H	1.80433700	-5.16972400	-1.73625300
H	0.08541000	-3.42300700	-2.19662200
H	0.28831600	-1.18108500	-1.19605300
H	2.49329100	1.64076500	2.37071100
H	4.13303500	1.19212000	2.89056100
H	3.87725700	2.06632000	1.37288600

Compound 1b, conformation c3

C	0.07651500	3.83049600	-0.51976000
C	-0.05260500	2.47350000	-0.16930000
C	1.02107500	1.57600000	-0.46895500
C	2.15871200	2.09039100	-1.12908000
C	2.24395300	3.43528500	-1.46066100
C	1.20517800	4.32505400	-1.15589100
N	0.92140000	0.25090800	-0.11260900
C	1.87255300	-0.76673500	-0.40132300
C	1.57194000	-1.72403200	-1.36354600
C	2.50725400	-2.76222300	-1.61508100
C	3.70304100	-2.83402800	-0.94229300
C	4.03206400	-1.87593600	0.05072100
C	3.09642300	-0.83031000	0.34221400
C	-1.29475000	2.05873000	0.47362200
N	-1.59428900	0.85489900	0.80490700
C	-2.87310500	0.60290700	1.46496800
C	-2.57682900	0.17498400	2.91168900
C	-3.66937800	-0.45906500	0.66345800
C	-5.01415200	-0.81739200	1.32898700
C	-5.81433500	-1.84464000	0.51075700
C	-6.03633200	-1.37911200	-0.93432400
C	-4.70158500	-1.03323600	-1.60767900
C	-3.90616900	-0.00397100	-0.79083500
H	-2.00620500	2.87919800	0.66495600
C	5.25281000	-1.93440400	0.77573800
C	5.53747300	-1.01314800	1.75712600
C	4.60348700	0.00655800	2.06104300
C	3.41398000	0.09610400	1.37292300
C	0.27529700	-1.67446100	-2.13668000
H	-0.74799700	4.49975700	-0.28146300
H	2.97136800	1.41699800	-1.37749300
H	3.13515900	3.79623000	-1.96823500
H	1.27959300	5.37638800	-1.41562200
H	0.00098800	-0.01545300	0.24711400
H	2.26702100	-3.50537100	-2.37165100
H	4.41057000	-3.63034500	-1.16093300
H	-3.47487500	1.53118300	1.49182000
H	-3.49603500	0.05649500	3.49303400
H	-2.02761900	-0.77344000	2.92947600
H	-1.95845300	0.93041700	3.40752800
H	-3.04861600	-1.36930300	0.63688200
H	-5.61315700	0.09988200	1.44247400
H	-4.85247300	-1.21068900	2.33897800

H	-6.77593800	-2.04206400	1.00185700
H	-5.26829500	-2.79973600	0.50169000
H	-6.68332100	-0.48909300	-0.93366000
H	-6.56705900	-2.15090100	-1.50656400
H	-4.87178300	-0.65340700	-2.62333300
H	-4.10307300	-1.95034300	-1.71526200
H	-2.94580100	0.19971300	-1.27638700
H	-4.45799700	0.94966400	-0.77809100
H	5.95816300	-2.72871300	0.54217000
H	6.47371700	-1.06947700	2.30591200
H	4.82675900	0.72226300	2.84784600
H	2.69798300	0.87304800	1.61588600
H	0.30924100	-2.34834200	-2.99842700
H	-0.57941000	-1.97654200	-1.51679300
H	0.06269100	-0.66255800	-2.49682700

Compound 1b, conformation c4

C	0.24520623	3.96017365	-1.27725120
C	0.08638771	2.77187026	-0.54047706
C	1.18251116	1.85551380	-0.46054167
C	2.37010633	2.17090482	-1.15660317
C	2.48372626	3.35210184	-1.87669234
C	1.42423369	4.26673439	-1.94038520
N	1.04914500	0.69858700	0.26909500
C	2.04547400	-0.29382300	0.46597300
C	1.96075337	-1.52719368	-0.17325789
C	3.00339263	-2.47123151	0.02729578
C	4.10260864	-2.18651044	0.80040491
C	4.22589100	-0.92813510	1.44362141
C	3.17484027	0.03246589	1.28770092
C	-1.20621325	2.53870952	0.09399324
N	-1.53503728	1.48391205	0.74896347
C	-2.86653307	1.41945951	1.34511041
C	-2.72565738	1.47112282	2.87476453
C	-3.64319349	0.16972038	0.85199518
C	-3.91693192	0.23833261	-0.66280146
C	-4.75120562	-0.95383485	-1.15586709
C	-4.09478272	-2.29068403	-0.78199457
C	-3.82054884	-2.36944394	0.72654911
C	-2.98447027	-1.17539453	1.21648576
H	-1.93035841	3.36136021	-0.02889254
C	5.35352548	-0.59645086	2.24136654
C	5.44232350	0.62503361	2.86940677
C	4.39516024	1.56712127	2.73265608
C	3.28892767	1.27774535	1.96373761
C	0.81273993	-1.87014763	-1.09012570
H	-0.59663711	4.64835731	-1.32361667
H	3.19250178	1.46369659	-1.13554664
H	3.41212672	3.56074270	-2.40274526
H	1.52049095	5.19052606	-2.50212364
H	0.10266992	0.53441412	0.62394376
H	2.92962507	-3.43477972	-0.47133602
H	4.89526183	-2.92094932	0.92191732

H	-3.45664731	2.30144216	1.03286423
H	-3.70413957	1.36341188	3.35746632
H	-2.06844570	0.67636593	3.24045569
H	-2.29366328	2.42888176	3.18414985
H	-4.61857338	0.21002032	1.36463617
H	-2.95759786	0.25662982	-1.19868423
H	-4.42668197	1.18115864	-0.90641850
H	-4.89483604	-0.88853427	-2.24217839
H	-5.75418143	-0.90637204	-0.70570874
H	-3.14395110	-2.39193565	-1.32656725
H	-4.72791328	-3.12920705	-1.09977444
H	-3.30797347	-3.30834701	0.97185448
H	-4.77935377	-2.38731617	1.26649467
H	-2.84068621	-1.25092609	2.30109428
H	-1.98517186	-1.22384484	0.76406030
H	6.14867384	-1.33087151	2.34793499
H	6.31032120	0.86607082	3.47711849
H	4.46155165	2.52324274	3.24526264
H	2.48123331	1.99663866	1.87574891
H	1.08509776	-2.69068181	-1.76136261
H	-0.08020906	-2.17858326	-0.53115605
H	0.52121748	-1.00589813	-1.69519883

Compound 1b, conformation c5

C	-0.38120500	3.62687700	-0.18044400
C	-0.33131700	2.23271900	0.00622300
C	0.86770200	1.53072300	-0.33701300
C	1.94501400	2.26948200	-0.87398500
C	1.85271800	3.64348800	-1.04559600
C	0.68911900	4.34190100	-0.69636500
N	0.94203900	0.17135900	-0.13939000
C	2.03770200	-0.66650000	-0.48713600
C	1.91063500	-1.53822000	-1.56262300
C	2.99170200	-2.40329700	-1.87686600
C	4.16031300	-2.38873300	-1.15445000
C	4.31413800	-1.51600200	-0.04678300
C	3.23016400	-0.64840400	0.30817300
C	-1.52503100	1.58007900	0.53276100
N	-1.66547400	0.31563400	0.70724500
C	-2.91891200	-0.18305000	1.27073100
C	-2.61922200	-0.71278200	2.68294500
C	-3.49503900	-1.27804800	0.32925500
C	-4.79828900	-1.92750400	0.84977300
C	-6.01840600	-0.99487900	0.75829900
C	-6.22115200	-0.48001300	-0.67516300
C	-4.94469900	0.17820200	-1.22148800
C	-3.73187800	-0.76105500	-1.10853800
H	-2.34956400	2.26891100	0.78167500
C	5.50362500	-1.49121000	0.73030900
C	5.61926000	-0.65977100	1.82033700
C	4.54001800	0.18089000	2.18506800
C	3.37573200	0.18668200	1.44964400
C	0.64920300	-1.57608400	-2.39259800
H	-1.29942800	4.14532500	0.08901100

H	2.85246500	1.74666500	-1.15461700
H	2.70219100	4.17963400	-1.46164700
H	0.62471900	5.41713600	-0.83059500
H	0.05540900	-0.25835100	0.13768500
H	2.88653400	-3.07985000	-2.72160700
H	4.98074200	-3.05061300	-1.42152500
H	-3.64239300	0.64518200	1.36201400
H	-3.53291300	-1.01972500	3.20094300
H	-1.93932500	-1.57138800	2.63776100
H	-2.13757400	0.06649300	3.28269500
H	-2.72237100	-2.05929500	0.28119700
H	-4.67465000	-2.29482400	1.87472000
H	-4.99538900	-2.81677300	0.23346900
H	-5.89090000	-0.14062000	1.43853800
H	-6.91596100	-1.52630800	1.10020200
H	-7.06221500	0.22432100	-0.71330400
H	-6.49315900	-1.32669300	-1.32329800
H	-4.75090600	1.10889900	-0.66922900
H	-5.08852300	0.47095800	-2.26951900
H	-3.90238800	-1.63107800	-1.75937200
H	-2.82922500	-0.26582400	-1.48225900
H	6.32216400	-2.14956500	0.44824900
H	6.53341300	-0.65118500	2.40783000
H	4.63095800	0.82412800	3.05634300
H	2.54880700	0.82532700	1.73883500
H	-0.17927800	-2.05306000	-1.85231200
H	0.31430700	-0.56782100	-2.65762300
H	0.80712700	-2.14189100	-3.31605300

Compound 1b, conformation c6

C	0.46677200	3.50706800	-1.28766800
C	0.26587800	2.34089000	-0.52584800
C	-1.04250800	1.76155700	-0.47935000
C	-2.06946000	2.36900900	-1.23544900
C	-1.82680100	3.51514800	-1.97953000
C	-0.55595600	4.10488500	-2.00877800
N	-1.25904700	0.63479900	0.27657700
C	-2.49799300	-0.03032500	0.46478300
C	-3.52850900	0.56611500	1.18640300
C	-4.73860300	-0.15542000	1.36925900
C	-4.90381600	-1.43180800	0.88962300
C	-3.85882300	-2.07520900	0.17790500
C	-2.63748500	-1.36230000	-0.05061200
C	1.42021400	1.77804600	0.16623000
N	1.40834900	0.68028200	0.83544200
C	2.64938500	0.22440300	1.49411700
C	3.10809500	1.24392300	2.55176000
C	3.74926900	-0.16008500	0.46761400
C	5.04062700	-0.65914800	1.14867300
C	6.11407700	-1.07656200	0.12959500
C	5.58883200	-2.12344000	-0.86181700
C	4.31016100	-1.62973500	-1.55189200
C	3.23890600	-1.22184700	-0.52956400
H	2.33766100	2.37745900	0.06239000
C	-3.99047900	-3.39948700	-0.31866100

C	-2.96740200	-3.99869400	-1.01758000
C	-1.76598000	-3.29021200	-1.25650800
C	-1.60575000	-2.00473000	-0.78741100
C	-3.38141100	1.93500700	1.80353900
H	1.46604700	3.93804800	-1.30710300
H	-3.05372800	1.91294700	-1.24195900
H	-2.64069700	3.95316000	-2.55218800
H	-0.37363200	5.00394300	-2.58903300
H	-0.40178800	0.22394800	0.66232100
H	-5.54162900	0.31863700	1.92875100
H	-5.83485500	-1.96754700	1.05872100
H	2.37249700	-0.69639200	2.02519600
H	3.87673200	0.82172200	3.20587200
H	3.51798800	2.15108400	2.09166900
H	2.25810200	1.53703200	3.17664900
H	4.00491700	0.74781600	-0.10341100
H	4.79513500	-1.52010800	1.79012200
H	5.45200200	0.11387000	1.80773500
H	6.99788300	-1.45771400	0.65727200
H	6.44469300	-0.18713000	-0.42738000
H	5.37169500	-3.05738900	-0.32221100
H	6.35911500	-2.36401900	-1.60578600
H	3.91267000	-2.40427100	-2.22035000
H	4.55272000	-0.76540200	-2.18814500
H	2.34658100	-0.85165700	-1.04554900
H	2.92346000	-2.11167800	0.03713100
H	-4.92039700	-3.93301400	-0.13530800
H	-3.08087400	-5.01247500	-1.39216500
H	-0.96573900	-3.76311500	-1.81964900
H	-0.68627800	-1.46305200	-0.98291600
H	-2.37217900	2.08042100	2.20141500
H	-3.55033400	2.73662400	1.07295500
H	-4.10031900	2.07039900	2.61781800

Compound 1c, conformation GS1-c1

C	2.19517300	0.44301000	-1.14921700
H	2.77129100	1.32751200	-1.46754900
C	2.04346100	-0.50266300	-2.35897300
H	1.42846600	-1.36452000	-2.08104400
H	1.55529300	0.01834000	-3.19008100
H	3.01683600	-0.87016500	-2.69758200
N	0.85996100	0.86204300	-0.73218000
C	0.58251300	2.11591500	-0.74942100
H	1.34685100	2.84849600	-1.05668100
C	-0.70755800	2.69859100	-0.40205800
C	-0.84281300	4.09449800	-0.52200800
C	-1.83539200	1.92736300	0.02326900
C	-2.03634700	4.74662900	-0.25195900
H	0.02574500	4.66590800	-0.84348400
C	-3.05086200	2.60190100	0.27071600
C	-3.14272400	3.98046300	0.13814200
H	-2.11382000	5.82477200	-0.35045100
H	-3.92417700	2.02204900	0.54924000
H	-4.09551900	4.46576300	0.33498500
N	-1.71427800	0.56413200	0.16278500
H	-0.83520800	0.18672200	-0.20024200
C	-2.73865800	-0.33599200	0.55831100
C	-3.21129200	-0.34620300	1.86744000
C	-3.22607100	-1.27796600	-0.40803700
C	-4.21586300	-1.28668900	2.22104600
C	-4.21583400	-2.23451700	-0.01106500
C	-2.76589900	-1.29779500	-1.75279300
C	-4.70141800	-2.20406800	1.32160200
C	-4.68619400	-3.17900800	-0.96190300
H	-2.03387600	-0.56213900	-2.06920000
C	-3.24411300	-2.22675800	-2.65094800
H	-5.45788900	-2.92436000	1.62379000
C	-4.21027800	-3.18099000	-2.25330000
H	-5.43390200	-3.90379600	-0.64798400
H	-2.88105000	-2.22390900	-3.67526700
H	-4.57821200	-3.90913500	-2.97109600
H	-4.58526300	-1.28614600	3.24380000
C	-2.66521700	0.58721400	2.91953100
H	-1.58632100	0.72724400	2.79994000
H	-3.12008400	1.58452300	2.86103100
H	-2.85737200	0.19333700	3.92253400
C	2.95084500	-0.23947000	-0.00706800
C	4.38270000	-0.35218000	-0.04934000
C	2.26563400	-0.77960600	1.06309300
C	5.18256000	0.18152500	-1.10039700
C	5.05830500	-1.03079400	1.02225400
C	2.93555600	-1.44849300	2.11387000
H	1.18688000	-0.67732000	1.10211400
C	6.55454900	0.05396200	-1.09751800
H	4.70948100	0.70257500	-1.92569600
C	6.47421400	-1.14544000	0.99324000
C	4.30283500	-1.57416200	2.09486700
H	2.35724500	-1.86017000	2.93677200
C	7.21151500	-0.61819700	-0.04144500

H	7.13664000	0.47404900	-1.91353700
H	6.96740500	-1.66281400	1.81310200
H	4.82694700	-2.08653800	2.89821300
H	8.29387000	-0.71397100	-0.04943800

Compound 1c, conformation GS1-c2

C	-2.52432800	1.49403900	1.35016900
H	-2.96946000	2.50275700	1.38547800
C	-2.54614000	0.95479400	2.79510100
H	-2.11990100	-0.04858100	2.86698700
H	-1.97159100	1.61999200	3.44908000
H	-3.57798300	0.91315900	3.16002500
N	-1.14321600	1.59628400	0.87244200
C	-0.66185200	2.77204800	0.68266200
H	-1.28406300	3.66202900	0.87498800
C	0.69277800	3.07045100	0.23332900
C	1.08398800	4.42206100	0.20379800
C	1.63666700	2.06801400	-0.15646500
C	2.36131000	4.81351300	-0.16833500
H	0.35118600	5.17228300	0.49454200
C	2.94036800	2.47912800	-0.51081700
C	3.28886700	3.82257800	-0.51630800
H	2.63814100	5.86296000	-0.18088700
H	3.67671100	1.72359000	-0.76315300
H	4.30288300	4.10220100	-0.79146400
N	1.25945500	0.74692400	-0.16239200
H	0.33291900	0.57538900	0.23431900
C	2.05248600	-0.36154700	-0.55694900
C	2.42970400	-0.53851200	-1.88501900
C	2.39390700	-1.33482600	0.44057800
C	3.19811000	-1.68372500	-2.22702200
C	3.13857000	-2.49673600	0.05652600
C	2.02118500	-1.18944400	1.80501500
C	3.53946500	-2.63528000	-1.29730400
C	3.45745000	-3.47063300	1.04018000
H	1.48318500	-0.29764700	2.10940900
C	2.34647900	-2.15348600	2.73460600
H	4.11218700	-3.51173300	-1.59095100
C	3.06728900	-3.30897500	2.35027700
H	4.01909400	-4.35111500	0.73634100
H	2.05446300	-2.02248800	3.77318600
H	3.31726200	-4.06201400	3.09274500
H	3.49549600	-1.81294900	-3.26496100
C	2.01339900	0.42572300	-2.96795100
H	0.99021300	0.77902600	-2.80634600
H	2.65456000	1.31616300	-2.99632100
H	2.06524600	-0.05299600	-3.95084500
C	-3.39434100	0.67612400	0.39395600
C	-3.10067400	-0.67736000	0.00829100
C	-4.53932400	1.27636500	-0.09507200
C	-1.94421200	-1.39011300	0.43722800
C	-4.01697700	-1.36158800	-0.86329900
C	-5.43889000	0.60031900	-0.95104300
H	-4.76020600	2.30284700	0.18883400

C	-1.70773400	-2.68752500	0.03891700
H	-1.22684600	-0.89767100	1.08006200
C	-3.74338100	-2.70047800	-1.25386900
C	-5.18254000	-0.69501900	-1.32641900
H	-6.32775900	1.11354400	-1.30791100
C	-2.61592600	-3.35438200	-0.81507900
H	-0.81133000	-3.19758900	0.38068400
H	-4.44906400	-3.20024100	-1.91371600
H	-5.86401700	-1.22906700	-1.98447400
H	-2.41921400	-4.37746600	-1.12410700

Compound 1c, conformation GS2-c1

C	-2.43698700	1.02470300	0.80878600
H	-3.00881000	1.90527300	0.47174000
C	-2.54284400	0.93292600	2.34535300
H	-1.94516300	0.09038800	2.70815200
H	-2.16531300	1.85128600	2.80837200
H	-3.57867800	0.77904800	2.66228000
N	-1.03001200	1.19990600	0.46132400
C	-0.69024600	2.25139500	-0.19282700
H	-1.45305900	2.98992400	-0.48981600
C	0.66856200	2.59138200	-0.59636600
C	0.85639700	3.80318900	-1.28796000
C	1.80721600	1.77269600	-0.31214600
C	2.10933800	4.23191000	-1.69842700
H	-0.02033700	4.41304400	-1.49701800
C	3.07874500	2.22827500	-0.72353000
C	3.21999400	3.42983800	-1.40335600
H	2.22720700	5.16978300	-2.23198700
H	3.95116000	1.62482600	-0.49957800
H	4.21429200	3.74894200	-1.70600600
N	1.63959700	0.57532200	0.34675600
H	0.69602500	0.43676000	0.71643600
C	2.68415700	-0.28504700	0.78855200
C	3.36363400	-1.11909300	-0.15802900
C	2.98814700	-0.34695800	2.14349500
C	3.04271100	-1.12258600	-1.54318500
C	4.39656400	-1.99669200	0.30729700
C	4.00018000	-1.24249300	2.57899300
C	3.72320000	-1.93434600	-2.42324200
H	2.24473900	-0.47922600	-1.89657600
C	5.08245200	-2.81589600	-0.62957000
C	4.69168500	-2.03432400	1.69429500
C	4.75831400	-2.78544300	-1.96633600
H	3.46148900	-1.92536500	-3.47800400
H	5.86843300	-3.47419200	-0.26650100
H	5.47201700	-2.70353200	2.04883600
H	5.28901000	-3.41802400	-2.67277000
H	4.23506600	-1.28419500	3.63982200
C	2.26203800	0.51697500	3.14763900
H	2.19976200	1.55699500	2.81050800
H	1.23155800	0.17421800	3.31013800
H	2.77000800	0.49845400	4.11679000
C	-3.02646100	-0.21911800	0.13976500
C	-4.44941100	-0.36535700	0.00395900

C	-2.20047700	-1.22732500	-0.31644900
C	-5.38498000	0.62255300	0.42587700
C	-4.97087200	-1.56318300	-0.59483900
C	-2.71945200	-2.40473700	-0.90373600
H	-1.12627500	-1.10579200	-0.23237400
C	-6.74228800	0.44190200	0.27179100
H	-5.02970700	1.54208100	0.87827900
C	-6.37610300	-1.71787100	-0.73700200
C	-4.07569200	-2.57228800	-1.03859100
H	-2.03348300	-3.17385700	-1.24860700
C	-7.24772800	-0.74151300	-0.31367000
H	-7.43003700	1.21586000	0.60222700
H	-6.75169100	-2.63163800	-1.19203100
H	-4.48411000	-3.47409500	-1.48864100
H	-8.31995300	-0.87440300	-0.42948100

Compound 1c, conformation GS2-c2

C	-2.81569800	1.65416800	0.89705000
H	-3.26191400	2.62004800	0.60595600
C	-3.00869100	1.52062300	2.42038400
H	-2.60383000	0.58127500	2.80499400
H	-2.50529000	2.34748800	2.93328100
H	-4.07557100	1.55624500	2.66540500
N	-1.38609900	1.67185000	0.57421700
C	-0.92469200	2.71452300	-0.01835100
H	-1.59952100	3.55046700	-0.26706100
C	0.46289600	2.93047200	-0.40907100
C	0.78367500	4.16392900	-1.00745500
C	1.50398600	1.97092100	-0.20260000
C	2.07606500	4.48265200	-1.39513600
H	-0.02001900	4.88168400	-1.16013900
C	2.81816000	2.31295200	-0.59107700
C	3.09123800	3.54151900	-1.17520900
H	2.29671400	5.44075400	-1.85509000
H	3.61710100	1.59832900	-0.42723600
H	4.11416500	3.77106300	-1.46343100
N	1.20557100	0.75418600	0.36124300
H	0.23856200	0.66766800	0.67995200
C	2.14597900	-0.25904000	0.70358400
C	2.67510100	-1.10974200	-0.32042600
C	2.49801300	-0.43874000	2.03600100
C	2.30303700	-0.98239900	-1.68654600
C	3.60559100	-2.13699600	0.04366500
C	3.40562100	-1.47829800	2.37095500
C	2.83951100	-1.81447200	-2.64360400
H	1.57966700	-0.22316900	-1.96185400
C	4.14326300	-2.97447600	-0.97060900
C	3.95079900	-2.29584300	1.41039100
C	3.77340100	-2.81706300	-2.28642800
H	2.54050500	-1.70481800	-3.68262400
H	4.85231700	-3.74801900	-0.68447900
H	4.65366900	-3.07770500	1.68843000
H	4.19027600	-3.46455100	-3.05315300

H	3.67925900	-1.61304200	3.41465000
C	1.93447300	0.44989500	3.12007800
H	2.00185200	1.50767300	2.84546600
H	0.87366000	0.23973900	3.30951300
H	2.47137000	0.30292100	4.06234600
C	-3.57067600	0.58529600	0.10267300
C	-3.23686100	-0.81264300	0.12308400
C	-4.65344600	1.00139500	-0.64939100
C	-2.13508700	-1.35217800	0.84651000
C	-4.05083400	-1.72917000	-0.62851400
C	-5.45181200	0.09779000	-1.38756800
H	-4.90509000	2.05925500	-0.67308800
C	-1.85742600	-2.70131500	0.83606800
H	-1.49408700	-0.68218800	1.40375000
C	-3.73657400	-3.11514200	-0.61705100
C	-5.15662900	-1.24277500	-1.37529800
H	-6.29465300	0.47293000	-1.96179400
C	-2.66565800	-3.59670200	0.09859000
H	-1.00469700	-3.07933800	1.39351700
H	-4.36444500	-3.79184700	-1.19230100
H	-5.76068000	-1.95115000	-1.93737200
H	-2.43597800	-4.65878700	0.09592600

Compound 1d, conformation GS1-c1

C	-1.81772900	1.04062900	1.87606900
H	-2.29425000	2.01000800	2.10170600
C	-1.51610400	0.33361900	3.21015500
H	-1.02906700	-0.63131100	3.03566200
H	-0.84808600	0.94835900	3.82347700
H	-2.44263300	0.15739200	3.76673700
N	-0.56179300	1.25082400	1.15637300
C	-0.20128200	2.45703400	0.90085400
H	-0.83360000	3.30256800	1.21764900
C	1.02568700	2.84425000	0.21558800
C	1.29247100	4.22032100	0.08857900
C	1.97103700	1.90448600	-0.30521000
C	2.44875100	4.69624400	-0.51101500
H	0.56051800	4.92117900	0.48531400
C	3.15512700	2.40299700	-0.89144000
C	3.38230000	3.76849800	-0.99191500
H	2.63035000	5.76291100	-0.59684000
H	3.89938000	1.69893000	-1.24781200
H	4.30648800	4.11616400	-1.44703100
N	1.71396600	0.55795200	-0.20691100
H	0.89239000	0.33169200	0.35947300
C	2.53528300	-0.49786700	-0.68075800
C	2.70336400	-0.71650900	-2.04515400
C	3.13143200	-1.37651500	0.28445100
C	3.51307000	-1.80605100	-2.46485400
C	3.91523800	-2.48527000	-0.17193400
C	2.97614600	-1.18708800	1.68467500
C	4.09699900	-2.66622900	-1.56727600
C	4.49092900	-3.36530300	0.78285600
H	2.40325400	-0.33647300	2.03890200
C	3.54893100	-2.05908900	2.58465100
H	4.69768400	-3.50253000	-1.91684900
C	4.31061000	-3.16249100	2.13218600
H	5.08029600	-4.20646800	0.42499800
H	3.42054300	-1.89564000	3.65138700
H	4.75636900	-3.84332800	2.85232900
H	3.64599400	-1.96799100	-3.53191300
C	2.02414100	0.14558400	-3.08037100
H	1.01426000	0.42126000	-2.76091000
H	2.56652100	1.08367000	-3.25555100
H	1.95563800	-0.38196600	-4.03695600
C	-2.78659800	0.23473700	1.02027900
C	-4.07527000	0.67838500	0.81255800
C	-2.38327200	-1.00096800	0.44142500
C	-5.00996800	-0.06944700	0.04623000
C	-3.25927700	-1.74868300	-0.30855600
H	-1.36495100	-1.34739300	0.59017900
C	-4.59443100	-1.31325500	-0.52890600
H	-2.93681000	-2.69010700	-0.74770800
C	-5.52584000	-2.06131400	-1.29675800
C	-7.22193000	-0.37322600	-0.92076700
C	-6.81051000	-1.60371200	-1.48899300
H	-7.51418600	-2.18549700	-2.07831000

H	-4.39859900	1.62519100	1.24197100
H	-8.23791600	-0.02147000	-1.07916100
H	-5.20619100	-3.00543900	-1.73207100
C	-6.34147700	0.37527600	-0.17166300
H	-6.65557700	1.32061100	0.26519200

Compound 1d, conformation GS1-c2

C	-1.82761500	1.75975300	1.73355100
H	-2.16916700	2.80791900	1.81402600
C	-1.54457600	1.24128800	3.15817100
H	-1.17973900	0.20997700	3.11624800
H	-0.78379100	1.86131800	3.64494400
H	-2.45369900	1.26127400	3.76808800
N	-0.59273200	1.69272000	0.96334500
C	-0.10039300	2.78453900	0.49973300
H	-0.61609900	3.74300700	0.67483100
C	1.13933700	2.89397500	-0.25859200
C	1.55463700	4.18318600	-0.64163800
C	1.95613600	1.77127100	-0.60531100
C	2.73591600	4.40318300	-1.33358700
H	0.91945800	5.02505200	-0.37320100
C	3.16815700	2.01285700	-1.28815600
C	3.54295000	3.30081300	-1.64470700
H	3.03292300	5.40749600	-1.61859700
H	3.81735100	1.17415700	-1.51526100
H	4.48440700	3.44910800	-2.16790800
N	1.55394300	0.50273300	-0.25630000
H	0.74665800	0.48133800	0.37206800
C	2.25700200	-0.70379200	-0.51347700
C	2.36484200	-1.20342800	-1.80809700
C	2.79505500	-1.42761300	0.60248900
C	3.05237000	-2.43050800	-2.00902200
C	3.45456500	-2.67779800	0.36957900
C	2.70248600	-0.94907700	1.93775900
C	3.57609700	-3.14979400	-0.96277900
C	3.97217300	-3.40384000	1.47515500
H	2.22559900	0.00792500	2.12181200
C	3.21676700	-1.67764200	2.98801300
H	4.08234100	-4.09505700	-1.14323800
C	3.85427100	-2.91975200	2.75809800
H	4.46633000	-4.35427000	1.28697600
H	3.13765100	-1.29334200	4.00147300
H	4.25436400	-3.48517000	3.59536800
H	3.13834600	-2.81303100	-3.02330800
C	1.74749500	-0.49696800	-2.98971400
H	0.78240200	-0.05425500	-2.72399600
H	2.37914800	0.32300200	-3.35526400
H	1.59560100	-1.19375300	-3.82009300
C	-2.94907600	0.95898200	1.07665600
C	-2.71915400	0.01273800	0.10102500
C	-4.28561000	1.18839000	1.50848000
C	-3.78242600	-0.73841900	-0.46988500
C	-5.33763400	0.48119800	0.97741100
H	-4.47408700	1.94353800	2.26893800

C	-3.55824300	-1.71808200	-1.47448000
C	-5.12275300	-0.50398100	-0.02374900
H	-6.35341700	0.67346900	1.31561100
C	-4.60627800	-2.43213200	-2.01126600
C	-6.18232600	-1.25544800	-0.59765700
C	-5.93164400	-2.19887400	-1.56903400
H	-6.75047200	-2.76853400	-2.00031700
H	-1.70743800	-0.16124900	-0.25232500
H	-2.53983900	-1.89600300	-1.81220600
H	-4.41982200	-3.17918600	-2.77822700
H	-7.19865900	-1.07304600	-0.25557200

Compound 1d, conformation GS2-c1

C	-2.06990800	1.89658000	1.19158400
H	-2.53279200	2.82297800	0.81034900
C	-1.99926800	1.99360000	2.72654300
H	-1.54426400	1.09184200	3.14977100
H	-1.39447800	2.85652700	3.02630700
H	-3.00357600	2.10303400	3.14919600
N	-0.71374400	1.75455600	0.66293100
C	-0.28950400	2.63964100	-0.16573300
H	-0.94278400	3.47617200	-0.46356200
C	1.03368500	2.66239400	-0.77687700
C	1.33217200	3.73468200	-1.63895700
C	2.03707200	1.67217300	-0.53088000
C	2.56852300	3.86665600	-2.25228500
H	0.55735000	4.47798200	-1.81658200
C	3.29655000	1.82660200	-1.15089700
C	3.54957600	2.89982500	-1.99328900
H	2.77291100	4.70237800	-2.91409800
H	4.07024300	1.09157800	-0.95935600
H	4.53029200	2.98627900	-2.45462100
N	1.75624800	0.60822300	0.29409600
H	0.85386600	0.67912900	0.77012700
C	2.67769000	-0.39537400	0.70586500
C	3.04129400	-1.44209700	-0.20265500
C	3.16671100	-0.37617200	2.00690700
C	2.51934500	-1.52415100	-1.52263200
C	3.95389000	-2.45581500	0.23701400
C	4.05110600	-1.40619200	2.42255600
C	2.89851500	-2.54203600	-2.36909500
H	1.80779100	-0.77478100	-1.85069600
C	4.32829700	-3.48799800	-0.66506700
C	4.44334100	-2.40782700	1.56757300
C	3.81700700	-3.53118300	-1.94163600
H	2.48612200	-2.59015900	-3.37341800
H	5.02589200	-4.24918500	-0.32312500
H	5.13223000	-3.17928500	1.90345500
H	4.10963700	-4.32659600	-2.62175700
H	4.43242700	-1.38394300	3.44060000
C	2.77291200	0.71650100	2.97284100
H	2.86144400	1.70690400	2.51419600
H	1.73071400	0.61302000	3.30261600
H	3.40376100	0.69233100	3.86678000

C	-2.93925400	0.72716400	0.74601300
C	-4.19044700	0.94883100	0.21075900
C	-2.48555500	-0.61234600	0.90117200
C	-5.03889400	-0.12308700	-0.17783500
C	-3.27763200	-1.67339100	0.53249300
H	-1.49309600	-0.79049200	1.30360900
C	-6.33135500	0.09236700	-0.72686400
C	-4.57377000	-1.46743300	-0.01342600
H	-2.91619600	-2.69227700	0.65221200
C	-5.41866600	-2.54023200	-0.40341000
C	-7.12782700	-0.96911600	-1.09483300
C	-6.66736700	-2.29868200	-0.93162600
H	-7.30478100	-3.12812600	-1.22599800
H	-4.55050300	1.96767200	0.07744700
H	-6.68314000	1.11404500	-0.85192800
H	-5.06127600	-3.55976700	-0.27753200
H	-8.11475000	-0.79001600	-1.51310400

Compound 1d, conformation GS2-c2

C	2.10343300	-2.49136100	0.78953700
H	2.44684200	-3.40521400	0.27068200
C	2.11062800	-2.77411200	2.30539300
H	1.75736900	-1.89390600	2.85243800
H	1.45201300	-3.61775500	2.53874400
H	3.12065900	-3.01320300	2.65388400
N	0.74338500	-2.16440200	0.38529500
C	0.16047800	-2.91373700	-0.47929000
H	0.68681900	-3.78504300	-0.90274100
C	-1.19429500	-2.72067200	-0.98066200
C	-1.68947600	-3.66452600	-1.90033000
C	-2.03550500	-1.63302100	-0.58385700
C	-2.96755100	-3.57750000	-2.43057300
H	-1.03595400	-4.48404400	-2.19296800
C	-3.33791200	-1.56189200	-1.12469000
C	-3.78735700	-2.51424800	-2.02842500
H	-3.32549300	-4.31778900	-3.13911200
H	-3.98875000	-0.74914300	-0.82200000
H	-4.79606800	-2.42827300	-2.42487900
N	-1.56271700	-0.69127100	0.30134900
H	-0.66348900	-0.93366400	0.72458800
C	-2.31186700	0.39289400	0.84078500
C	-2.53877800	1.56108200	0.04284800
C	-2.75988000	0.32585100	2.15458700
C	-2.05254900	1.68437600	-1.28762900
C	-3.27008300	2.65584300	0.60865300
C	-3.46451500	1.43351700	2.69580300
C	-2.29407000	2.82262300	-2.02446700
H	-1.48098600	0.86710800	-1.71315500
C	-3.50631600	3.81242500	-0.18233700
C	-3.72222500	2.55816900	1.94973500
C	-3.03299000	3.89636600	-1.47152200
H	-1.91227300	2.89958500	-3.03907000
H	-4.06661900	4.63558200	0.25515800
H	-4.27368800	3.39002900	2.38145500

H	-3.21864000	4.78697500	-2.06581000
H	-3.81473200	1.37430900	3.72345900
C	-2.50619400	-0.89633200	3.00523500
H	-2.74534400	-1.81774300	2.46416800
H	-1.45294300	-0.96984200	3.30674700
H	-3.10759700	-0.86669200	3.91907400
C	3.07632000	-1.36733800	0.43931700
C	2.65681200	-0.10387200	0.08144000
C	4.47290600	-1.63474700	0.50017700
C	3.58525500	0.93072500	-0.21534800
C	5.39827400	-0.65818500	0.21884700
H	4.81021500	-2.63402400	0.76792700
C	3.16379700	2.23680200	-0.58406300
C	4.98813100	0.65315100	-0.14404300
H	6.46180400	-0.88169900	0.26544700
C	5.91212200	1.68952000	-0.44218400
C	4.08419900	3.22154700	-0.86645700
C	5.47185900	2.94589200	-0.79482600
H	6.18832800	3.73140400	-1.02002500
H	6.97687100	1.47380300	-0.38691300
H	3.74814900	4.21648000	-1.14621100
H	1.59508300	0.11137500	0.01165300
H	2.09785200	2.44564900	-0.63898800

Compound 1g, conformation GS1-c1

C	0.99870100	2.33674000	-0.54433500
H	1.72689200	3.11842100	-0.81165100
C	-0.38590200	2.65810900	-0.86232500
C	-0.63326200	3.86986600	-1.53458800
C	-1.48900000	1.80113600	-0.54906300
C	-1.90874500	4.25390100	-1.91972600
H	0.21644900	4.51192500	-1.75803200
C	-2.77895900	2.19431900	-0.96899400
C	-2.97880400	3.39468100	-1.63635000
H	-2.07254900	5.19382200	-2.43728300
H	-3.61589100	1.53105300	-0.77873700
H	-3.98566500	3.66243900	-1.94737900
N	-1.26788400	0.62518300	0.12806900
H	-0.27825500	0.38838600	0.24176900
C	-2.25291000	-0.30549800	0.54789600
C	-3.17457000	0.02452000	1.53804200
C	-2.23138600	-1.62035200	-0.02730700
C	-4.12602200	-0.95279700	1.93591600
C	-3.18447600	-2.59255300	0.41833400
C	-1.29646100	-1.99824200	-1.02885300
C	-4.13517800	-2.21833700	1.40264400
C	-3.15402400	-3.89831200	-0.13967800
H	-0.58090600	-1.26437500	-1.38412800
C	-1.29309300	-3.27409100	-1.54885800
H	-4.86474400	-2.95194800	1.73730000
C	-2.22781500	-4.23665800	-1.09983000
H	-3.88018500	-4.62918300	0.20894900
H	-0.56870300	-3.54316900	-2.31290200
H	-2.21431200	-5.23962500	-1.51791800
H	-4.84786300	-0.68594900	2.70427500
C	-3.16758900	1.37041200	2.21988900
H	-2.14496000	1.73135000	2.36773700
H	-3.68881800	2.13511300	1.62963200
H	-3.66110000	1.31046800	3.19517900
N	1.39665900	1.23794700	-0.00798800
C	2.81408200	1.07346200	0.24760900
C	3.39698400	-0.20918500	-0.31844100
C	3.12846000	0.93549000	1.75689900
H	3.38584400	1.94377400	-0.12589100
C	3.12908700	-0.81984600	-1.53989600
C	4.32794400	-0.75950600	0.57324300
C	4.43216400	0.09927400	1.81375800
O	3.21602900	2.22739200	2.33644200
H	2.30704000	0.35873200	2.20802000
C	3.80672500	-1.99828700	-1.86778200
H	2.39929700	-0.39153800	-2.22213900
C	5.00190600	-1.93404800	0.24592200
H	4.53188100	-0.47727300	2.74147900
H	5.29117600	0.78310300	1.75734600
H	3.21130900	2.12458200	3.29997700
C	4.73637500	-2.55048600	-0.98121000
H	3.60637100	-2.49125300	-2.81552800
H	5.71987500	-2.37233200	0.93535000
H	5.25276100	-3.46983800	-1.24500900

Compound 1g, conformation GS1-c2

C	1.26850700	2.12576300	-0.62003600
H	1.99209100	2.84543500	-1.03302800
C	-0.11340300	2.58611800	-0.61443400
C	-0.36310300	3.89525700	-1.06859700
C	-1.21223300	1.78843800	-0.16103900
C	-1.63671700	4.44283500	-1.07787500
H	0.48364700	4.48598900	-1.41240800
C	-2.50171300	2.36465000	-0.16210500
C	-2.70330100	3.66140000	-0.61307900
H	-1.80255700	5.45547500	-1.43186100
H	-3.33980000	1.77851700	0.19762500
H	-3.70999400	4.07196700	-0.59960200
N	-0.99000500	0.49665600	0.25778300
H	0.00042900	0.25008800	0.33679900
C	-1.96337200	-0.38676000	0.80053700
C	-1.91659000	-0.69712300	2.15497600
C	-2.93537600	-0.99493500	-0.05984700
C	-2.86364600	-1.61336700	2.68304600
C	-3.89411100	-1.89764700	0.50557100
C	-2.97645400	-0.75221700	-1.46020500
C	-3.82969300	-2.18753000	1.89265000
C	-4.86898800	-2.49135000	-0.34089900
H	-2.23636600	-0.09224100	-1.89834500
C	-3.93033400	-1.35026900	-2.25322800
H	-4.55409900	-2.87601600	2.32124300
C	-4.89240600	-2.22299200	-1.69004200
H	-5.59565500	-3.16990800	0.10013000
H	-3.94313100	-1.15460000	-3.32220100
H	-5.64178400	-2.68485700	-2.32723100
H	-2.82336700	-1.84782800	3.74408600
C	-0.87922300	-0.07886200	3.06221800
H	0.11543600	-0.51410100	2.89603000
H	-0.78619500	0.99820400	2.88887500
H	-1.13568700	-0.23991500	4.11400300
N	1.66924200	0.98546200	-0.18054000
C	3.09012000	0.70069700	-0.22138400
C	3.42902000	-0.69868800	-0.69931400
C	3.74087000	0.72851100	1.18318900
H	3.62433100	1.44960500	-0.83568900
C	2.82532600	-1.44279700	-1.70828200
C	4.51167500	-1.21403100	0.02716800
C	4.96777700	-0.21069300	1.06338100
O	4.03777000	2.07045300	1.53361400
H	3.01586700	0.29146400	1.88693600
C	3.32143900	-2.71883700	-1.99321000
H	1.97425300	-1.04301800	-2.25304900
C	5.00509800	-2.48532900	-0.25746900
H	5.25646900	-0.66464000	2.01927800
H	5.82560400	0.37663500	0.70572000
H	4.24769000	2.09503700	2.47929600
C	4.40435600	-3.23471900	-1.27449900
H	2.85801400	-3.31666800	-2.77364400
H	5.83953600	-2.89618600	0.30633800
H	4.77729000	-4.23002900	-1.50205700

Compound 1g, conformation GS2-c1

C	1.16903500	2.22903200	-0.20877300
H	1.85992000	3.08622600	-0.18867700
C	-0.18953800	2.54937100	-0.62522800
C	-0.45923000	3.88157400	-0.99258100
C	-1.24291900	1.58246200	-0.70117400
C	-1.70882800	4.28628200	-1.43600400
H	0.35210700	4.60363000	-0.92479100
C	-2.50593600	2.00572700	-1.17098500
C	-2.72819700	3.32853200	-1.52625400
H	-1.89135300	5.31993600	-1.71256100
H	-3.30666200	1.27950200	-1.25332500
H	-3.71353200	3.61836500	-1.88304300
N	-1.00223900	0.28215200	-0.32216300
H	-0.01689400	0.08328800	-0.12787500
C	-1.91336000	-0.80526700	-0.41919100
C	-1.68265600	-1.79778700	-1.36534800
C	-3.01128000	-0.90295100	0.49703500
C	-2.56835300	-2.90535000	-1.42786700
C	-3.90313100	-2.02009500	0.39403600
C	-3.24233600	0.05699900	1.52032100
C	-3.65073900	-3.01187100	-0.58813900
C	-5.00192600	-2.11343400	1.29039400
H	-2.55482500	0.88910200	1.62175700
C	-4.31288900	-0.06800500	2.37749100
H	-4.32423900	-3.86230400	-0.66341400
C	-5.20802500	-1.15855700	2.25915000
H	-5.67619500	-2.96194100	1.19867800
H	-4.47084000	0.67464700	3.15512300
H	-6.05104600	-1.24218100	2.93977500
H	-2.38421000	-3.67554800	-2.17299300
C	-0.51415500	-1.71042000	-2.31875400
H	-0.45535700	-0.72188000	-2.78704200
H	0.44394800	-1.87652100	-1.80897600
H	-0.60066100	-2.46184100	-3.10977400
N	1.58539800	1.05468200	0.10919500
C	2.96812900	0.90191900	0.51505500
C	3.68124200	-0.25699200	-0.15697800
C	3.10467400	0.54146600	2.01482500
H	3.53382800	1.83894100	0.35468400
C	3.58948400	-0.68449600	-1.47846900
C	4.52659300	-0.90654900	0.75319400
C	4.43643900	-0.24576700	2.11071500
O	3.04981500	1.72973100	2.78763400
H	2.26775100	-0.12747800	2.26522700
C	4.35896500	-1.77810800	-1.88871800
H	2.92439500	-0.18113000	-2.17525900
C	5.29249600	-1.99588200	0.34337200
H	4.45703400	-0.95423800	2.94772700
H	5.25701200	0.46941900	2.26483800
H	2.90447000	1.48024800	3.71255400
C	5.20464900	-2.42776500	-0.98419200
H	4.29646700	-2.12806900	-2.91583700
H	5.94497200	-2.51069400	1.04489200
H	5.79403400	-3.27958400	-1.31355800

Compound 1g, conformation GS2-c2

C	-1.10010500	2.29677800	-0.38745500
H	-1.84603500	3.08172300	-0.58693400
C	0.27095400	2.77334700	-0.26848300
C	0.50231800	4.14640600	-0.47509800
C	1.38183100	1.91960600	0.02561000
C	1.77337800	4.69769700	-0.41918100
H	-0.35434300	4.78080800	-0.69376900
C	2.67291300	2.49150400	0.05750900
C	2.85823300	3.84993900	-0.15811400
H	1.92501300	5.75987200	-0.58331900
H	3.52680400	1.84667200	0.23573900
H	3.86703200	4.25452000	-0.12881100
N	1.17045300	0.58057600	0.25282800
H	0.21179600	0.27081100	0.06824300
C	2.16265700	-0.38868200	0.55515800
C	2.80979500	-0.38749000	1.78728500
C	2.43338800	-1.40821700	-0.41697700
C	3.77267000	-1.39813600	2.05171200
C	3.38722900	-2.43131100	-0.10810600
C	1.79196500	-1.43972900	-1.68508400
C	4.05263500	-2.39044800	1.14413000
C	3.64352100	-3.44986900	-1.06440900
H	1.08632200	-0.65419800	-1.93477900
C	2.06533100	-2.44083100	-2.59127900
H	4.78206000	-3.16185400	1.37930600
C	2.99604100	-3.46005800	-2.27882800
H	4.36577800	-4.22467700	-0.81740700
H	1.56761200	-2.44566100	-3.55749400
H	3.20163100	-4.24468800	-3.00201700
H	4.27862000	-1.38909500	3.01424200
C	2.49251700	0.63388200	2.85134600
H	3.00322100	1.58849100	2.67020200
H	1.42021600	0.85172400	2.87873100
H	2.80112800	0.27345200	3.83771000
N	-1.46498300	1.06751700	-0.28830500
C	-2.86882600	0.75353100	-0.46649800
C	-3.44099000	-0.15443200	0.60674800
C	-3.13372100	-0.06272200	-1.75471100
H	-3.47273700	1.67746400	-0.54037300
C	-3.18669100	-0.15064000	1.97472700
C	-4.34145300	-1.06935100	0.04349300
C	-4.42648800	-0.86212500	-1.45237200
O	-3.21530800	0.82240800	-2.86028400
H	-2.29326800	-0.76325600	-1.87444000
C	-3.85065900	-1.07590900	2.78622800
H	-2.47363500	0.55044300	2.40031800
C	-5.00215400	-1.99088800	0.85274100
H	-4.49691300	-1.79615200	-2.02306200
H	-5.29382200	-0.24370000	-1.72456200
H	-3.18953600	0.29260500	-3.67128300
C	-4.75270100	-1.98763700	2.22913300
H	-3.65963700	-1.09131700	3.85607500
H	-5.69625600	-2.70965400	0.42320500
H	-5.25840700	-2.70552100	2.86974400

Compound 1h, conformation GS1-c1

C	0.79096900	2.32032100	0.13297400
H	1.48506800	3.15414400	-0.06785400
C	-0.62355300	2.67546300	0.10371500
C	-0.95171200	4.03576300	-0.04383900
C	-1.67802500	1.71648200	0.25019600
C	-2.26373600	4.48437100	-0.02409200
H	-0.13693900	4.74751600	-0.16284900
C	-3.00699900	2.19238600	0.29473900
C	-3.28719500	3.54488900	0.15836300
H	-2.49123500	5.53975600	-0.13697700
H	-3.81488400	1.48509100	0.44105800
H	-4.32297400	3.87304100	0.19856400
N	-1.36714700	0.37698400	0.34260400
H	-0.36796000	0.20310800	0.49149300
C	-2.26117400	-0.70377500	0.54814500
C	-2.11028400	-1.48045600	1.69426400
C	-3.23584200	-1.04904400	-0.44664800
C	-2.97869800	-2.58333200	1.89627000
C	-4.11759200	-2.15225200	-0.19935500
C	-3.34298200	-0.36594600	-1.68974100
C	-3.96643200	-2.90122400	0.99520300
C	-5.09853300	-2.48659900	-1.17211600
H	-2.65313600	0.44132100	-1.90642000
C	-4.29517100	-0.72602200	-2.61721900
H	-4.63334600	-3.73986600	1.18024300
C	-5.19273700	-1.78847900	-2.35358300
H	-5.76951700	-3.31767700	-0.96669000
H	-4.35482800	-0.19366000	-3.56287200
H	-5.94468000	-2.05730400	-3.09067700
H	-2.86128400	-3.17516200	2.80095400
C	-1.03505000	-1.16920400	2.70859500
H	-0.03322200	-1.38459900	2.31334500
H	-1.04202900	-0.10997100	2.98923300
H	-1.17110900	-1.76674100	3.61538200
N	1.23538000	1.14572900	0.39339900
C	2.96457300	-0.43370900	-0.26215100
O	2.40146600	-1.46140200	0.55074400
H	2.43881000	-0.39428200	-1.22914800
H	2.49051700	-2.29724100	0.06678100
C	4.44727200	-0.65131800	-0.53346300
C	5.23822900	-1.42562800	0.32379500
C	5.04544600	-0.06615200	-1.65757600
C	6.59893300	-1.60500400	0.06608500
H	4.77608500	-1.88989000	1.18957700
C	6.40516400	-0.23953900	-1.91418300
H	4.43886300	0.52456300	-2.34166000
C	7.18715800	-1.01104900	-1.05124400
H	7.19934700	-2.21063900	0.74016300
H	6.85242400	0.21933000	-2.79214700
H	8.24568100	-1.15228500	-1.25262800
C	2.67236300	0.91733300	0.44066000
H	3.20989800	1.69730400	-0.12576400
C	3.15473100	0.94568900	1.89768800
H	2.96818100	1.93373700	2.33103000

H	2.62013500	0.19984300	2.49088300
H	4.22805900	0.73899300	1.95611600

Compound 1h, conformation GS1-c2

C	0.60686300	2.40920400	-0.02303300
H	1.35033900	3.20768000	-0.18796000
C	-0.76230100	2.76020800	-0.37912800
C	-0.99155800	4.04156800	-0.91333100
C	-1.86312900	1.85240000	-0.25063400
C	-2.24687000	4.45192300	-1.33623900
H	-0.14306600	4.71789900	-0.99876100
C	-3.12919500	2.27492300	-0.71440700
C	-3.31189700	3.54633000	-1.23991500
H	-2.39775200	5.44658000	-1.74383200
H	-3.96053000	1.57966300	-0.67191800
H	-4.30097600	3.83448900	-1.58770700
N	-1.66082800	0.60539500	0.29172200
H	-0.67477400	0.37517900	0.45698400
C	-2.64152700	-0.40317800	0.47304500
C	-3.66683000	-0.24715300	1.40184400
C	-2.51033700	-1.61893200	-0.27897100
C	-4.61383100	-1.29534900	1.55398700
C	-3.46631300	-2.66743200	-0.08244900
C	-1.46342500	-1.82406900	-1.21844300
C	-4.52325300	-2.46638800	0.84236800
C	-3.33266600	-3.87385100	-0.82022700
H	-0.73810400	-1.03367900	-1.37731600
C	-1.36338000	-3.00649400	-1.91865200
H	-5.25411900	-3.25813200	0.98874200
C	-2.30410700	-4.04438600	-1.71852500
H	-4.06297700	-4.66390500	-0.66051200
H	-0.55845100	-3.14273700	-2.63648900
H	-2.21375400	-4.97187800	-2.27767900
H	-5.41654100	-1.16348400	2.27575400
C	-3.77664900	0.98152900	2.27058300
H	-2.78671800	1.34194300	2.56699500
H	-4.27252400	1.81217200	1.75182100
H	-4.35392100	0.76333500	3.17474700
N	0.96718800	1.26461000	0.43127500
C	2.83308000	-0.18662300	-0.15906800
O	2.10359300	-1.32678500	0.28098100
H	2.55098100	0.06259200	-1.19497700
H	2.33621000	-2.06775100	-0.30005100
C	4.34029400	-0.40103400	-0.11831800
C	4.91571700	-1.35421500	0.73062700
C	5.17933400	0.36501700	-0.93861700
C	6.30027800	-1.53281600	0.76261000
H	4.26842400	-1.95616600	1.36105200
C	6.56273000	0.19238400	-0.90437400
H	4.74422000	1.09822500	-1.61535200
C	7.12800600	-0.75916200	-0.05206400

H	6.73179400	-2.27826600	1.42574400
H	7.19875200	0.79336600	-1.54915400
H	8.20537600	-0.89947900	-0.02818900
C	2.37250000	1.01600900	0.71064800
H	2.99098200	1.87864600	0.40473900
C	2.55850500	0.77257700	2.21314800
H	2.23747900	1.65596600	2.77453600
H	1.95732700	-0.08111700	2.53585500
H	3.60881100	0.57516700	2.44931300

Compound 1h, conformation GS2-c1

C	0.85580200	2.09465400	0.35337400
H	1.59414500	2.90039500	0.50610900
C	-0.47067200	2.54827100	-0.04669500
C	-0.66181900	3.93156400	-0.22261600
C	-1.56144200	1.65661700	-0.30697100
C	-1.86814500	4.46065600	-0.65516200
H	0.17753700	4.59311500	-0.01634800
C	-2.77656600	2.20901100	-0.77023700
C	-2.92131600	3.57912400	-0.93509200
H	-1.99081500	5.53167200	-0.78243800
H	-3.60274900	1.54548400	-0.99827800
H	-3.87225900	3.96764100	-1.29145200
N	-1.39769500	0.30563700	-0.10483300
H	-0.42906500	0.03519400	0.09483000
C	-2.32285200	-0.71934100	-0.44074800
C	-2.00640000	-1.59446400	-1.47485200
C	-3.51991700	-0.89138100	0.32801600
C	-2.90858000	-2.64515500	-1.78378700
C	-4.42462100	-1.94580600	-0.02459600
C	-3.83789500	-0.07131200	1.44559000
C	-4.08705600	-2.81099900	-1.09635200
C	-5.62164900	-2.10961100	0.72387800
H	-3.14145400	0.70594000	1.73904800
C	-5.00202700	-0.26398300	2.15542200
H	-4.77058200	-3.61442000	-1.36058500
C	-5.90988300	-1.28642100	1.78772600
H	-6.30473100	-2.90779400	0.44210900
H	-5.22447300	0.37056500	3.00927700
H	-6.82731600	-1.42397000	2.35375100
H	-2.65789900	-3.32137500	-2.59764700
C	-0.72793100	-1.43554100	-2.26431600
H	-0.63272300	-0.41938500	-2.66464600
H	0.16073900	-1.61411700	-1.64526100
H	-0.70197700	-2.13723800	-3.10417600
N	1.19172100	0.86578600	0.50955800
C	3.18040700	-0.32480900	-0.26075800
O	2.48171200	-1.56845200	-0.27867300
H	2.99438200	0.21995200	-1.20000800
H	2.86731500	-2.10566300	-0.98874200
C	4.68413600	-0.50750900	-0.10820800
C	5.22118300	-1.64872600	0.50039200
C	5.55961100	0.48021900	-0.57903200

C	6.60284200	-1.79566700	0.63958200
H	4.54814000	-2.42112700	0.86004000
C	6.93944400	0.33836900	-0.43579600
H	5.15644600	1.36492900	-1.06835000
C	7.46580700	-0.80247800	0.17474600
H	7.00426500	-2.68815600	1.11273200
H	7.60412700	1.11313900	-0.80899400
H	8.54104400	-0.91774900	0.28190200
C	2.56379100	0.54511600	0.87003900
H	3.17759900	1.46227300	0.92091100
C	2.58339800	-0.14790600	2.23749000
H	2.16129900	0.51875500	2.99626600
H	1.98506900	-1.06194900	2.20822200
H	3.60615400	-0.40342100	2.53181300

Compound 1h, conformation GS2-c2

C	-0.77828900	2.12014800	-0.78363700
H	-1.55286400	2.84733400	-1.08145300
C	0.55879100	2.67869800	-0.62673200
C	0.74199700	4.03693900	-0.94531500
C	1.68357900	1.90987000	-0.18557000
C	1.98137000	4.65393000	-0.86507300
H	-0.12625600	4.60582600	-1.27264600
C	2.94368300	2.54680800	-0.13157700
C	3.08316300	3.88737600	-0.46242600
H	2.09649200	5.70327800	-1.11776500
H	3.81206000	1.96418400	0.15663800
H	4.06969800	4.34175400	-0.41184300
N	1.51793000	0.58897500	0.15651400
H	0.58832000	0.21105500	-0.05451500
C	2.52965500	-0.29012000	0.62349600
C	3.09846900	-0.12190800	1.88274500
C	2.90454400	-1.39571700	-0.21068700
C	4.09002600	-1.04477800	2.31135200
C	3.88634800	-2.32537500	0.26231700
C	2.33892100	-1.60318300	-1.49797100
C	4.47266700	-2.11235300	1.53651300
C	4.24789300	-3.42715800	-0.55799200
H	1.60691500	-0.89408800	-1.86968900
C	2.71231100	-2.68213700	-2.26897900
H	5.22317600	-2.81260200	1.89557900
C	3.67325100	-3.60679100	-1.79561400
H	4.99146100	-4.12910500	-0.18722700
H	2.26880300	-2.82295100	-3.25110100
H	3.95838800	-4.45407600	-2.41351700
H	4.53493100	-0.90413900	3.29369100
C	2.66831200	0.98834700	2.80944100
H	3.15335800	1.94176700	2.56311800
H	1.58916600	1.15882800	2.74335900
H	2.92084700	0.74530700	3.84650600
N	-1.07637300	0.88353900	-0.61331200
C	-2.94444900	-0.24307300	0.48455800
O	-2.20357200	-1.45031200	0.62157800
H	-2.69996300	0.44343700	1.31118100

H	-2.45558500	-1.85296100	1.46728500
C	-4.45004100	-0.47552200	0.49108000
C	-4.99513300	-1.71498900	0.13496400
C	-5.31798200	0.56266400	0.85529500
C	-6.37796100	-1.90968600	0.13696200
H	-4.32553400	-2.52489500	-0.13793900
C	-6.69944600	0.37232400	0.85300300
H	-4.90718900	1.52661300	1.15018300
C	-7.23425300	-0.86703800	0.49318000
H	-6.78570000	-2.87848300	-0.14028700
H	-7.35808700	1.18768700	1.14084200
H	-8.31027400	-1.01925000	0.49640100
C	-2.45320000	0.45521600	-0.81268300
H	-3.11221400	1.32757100	-0.96884900
C	-2.53086600	-0.45614200	-2.04383000
H	-2.20821200	0.09397300	-2.93379800
H	-1.87884400	-1.32348000	-1.91430400
H	-3.55538700	-0.80578100	-2.20580200

Compound 2a, conformation c1

C	-1.70045700	4.00093000	-0.46499000
C	-1.31501800	2.71041900	-0.06264900
C	0.07678700	2.40791200	0.04343500
C	1.00790300	3.43331300	-0.20992600
C	0.58789900	4.69876300	-0.60419800
C	-0.77142800	4.99267700	-0.74867200
N	0.44858800	1.13684400	0.45569800
C	1.64909300	0.45869300	0.30331000
C	2.61887700	0.77171300	-0.67374900
C	3.77683400	0.01518800	-0.78374600
C	3.98040800	-1.06873700	0.07115200
C	3.02697900	-1.41452400	1.03236900
C	1.87578100	-0.65442500	1.14557000
C	-2.38527700	1.76007500	0.24449900
N	-2.21471900	0.57579700	0.70410000
C	-3.39611800	-0.24436900	0.97551900
C	-3.40348000	-0.62521100	2.46681900
C	-3.40726700	-1.47942100	0.08120200
C	-4.58212600	-1.85085200	-0.58167600
C	-4.62448800	-2.99980300	-1.37422100
C	-3.48458100	-3.79040200	-1.51948200
C	-2.30473200	-3.42484500	-0.86706400
C	-2.26714200	-2.27977000	-0.07218800
H	-3.40100200	2.14489300	0.06111000
N	5.19979300	-1.85787400	-0.04687900
O	5.33572000	-2.82540900	0.70733500
O	6.02901900	-1.51632300	-0.89475300
H	-2.76347200	4.21598100	-0.54887600
H	2.06396000	3.24439300	-0.06056000
H	1.33360600	5.46757000	-0.78808800
H	-1.09564100	5.98018200	-1.06125000
H	-0.34375100	0.58615900	0.80350500
H	2.44598300	1.57991600	-1.37316700
H	4.52138800	0.24160500	-1.53723100
H	3.20854600	-2.26303100	1.68054800
H	1.13757300	-0.89987300	1.90411400
H	-4.31157100	0.33362800	0.76368100
H	-3.42881000	0.27338700	3.09304500
H	-4.27996200	-1.23961400	2.69718800
H	-2.50603900	-1.19837100	2.72158100
H	-5.47345500	-1.23549600	-0.47780300
H	-5.54652800	-3.27166100	-1.88141700
H	-3.51255400	-4.68260300	-2.13915600
H	-1.41020200	-4.03187700	-0.97931400
H	-1.34230900	-1.99863100	0.42310900

Compound 2a, conformation c2

C	1.39411300	4.06210900	0.07224300
C	1.08208400	2.70083600	-0.08763700
C	-0.21790400	2.24231200	0.28657200

C	-1.11829900	3.16626300	0.85116400
C	-0.77234900	4.50511400	0.99510300
C	0.48388800	4.97062200	0.59473000
N	-0.51290300	0.89549400	0.13890500
C	-1.73704500	0.24405200	0.09580700
C	-1.74297300	-1.14412500	0.36370500
C	-2.91348100	-1.87999700	0.29870400
C	-4.10727900	-1.23408200	-0.03324600
C	-4.12927700	0.13189200	-0.31749000
C	-2.95360500	0.86652300	-0.25877900
C	2.13644400	1.83270000	-0.61392900
N	2.04900100	0.56143100	-0.75341300
C	3.20196200	-0.16073800	-1.29585400
C	2.82331900	-0.75049700	-2.66609300
C	3.65086400	-1.23695800	-0.31440200
C	4.96823800	-1.25794000	0.15463800
C	5.39842000	-2.25052200	1.03829300
C	4.50953000	-3.23479500	1.46932200
C	3.18989200	-3.22104400	1.01028400
C	2.76563700	-2.23090800	0.12540700
H	3.06435400	2.35995300	-0.88716400
N	-5.34549300	-2.00035000	-0.09307100
O	-5.28631100	-3.21090500	0.14018500
O	-6.38487900	-1.39727900	-0.37440400
H	2.38554200	4.39897500	-0.22257200
H	-2.08007900	2.82265300	1.21175800
H	-1.49065500	5.18968900	1.43825700
H	0.74901500	6.01734600	0.70452100
H	0.31337600	0.32900300	-0.08115100
H	-0.81221100	-1.62947400	0.64413700
H	-2.92482700	-2.94193800	0.51133900
H	-5.06544700	0.59875400	-0.59853000
H	-2.97001200	1.91506200	-0.52852500
H	4.04479600	0.53519300	-1.44441900
H	3.66794800	-1.30716100	-3.08525200
H	1.97215000	-1.43261600	-2.57500400
H	2.54768800	0.04864600	-3.36269900
H	5.66580200	-0.49037500	-0.17381100
H	6.42651700	-2.25048000	1.39076300
H	4.84003500	-4.00693500	2.15876500
H	2.49066800	-3.98410700	1.34232200
H	1.73755400	-2.22765700	-0.22718600

Compound 2a, conformation c3

C	1.71885500	3.07502300	-0.08236900
C	1.10484300	1.81473000	0.01932600
C	-0.30557800	1.75135700	0.23602400
C	-1.01536100	2.95688200	0.39648800
C	-0.37144100	4.18506300	0.29357300
C	1.00124500	4.25752300	0.03897100
N	-0.90347900	0.50378400	0.34327600
C	-2.22799600	0.12666900	0.18326200
C	-3.19044400	0.88263600	-0.52146100

C	-4.48782300	0.41246600	-0.66567000
C	-4.84299100	-0.82119100	-0.11867800
C	-3.90452900	-1.60116600	0.56266100
C	-2.61271800	-1.12782900	0.71109900
C	1.97708500	0.64153100	-0.08737100
N	1.58915500	-0.56731200	0.09178800
C	2.51273100	-1.70817800	-0.04643400
C	2.21709300	-2.69486500	1.09573200
C	3.99575300	-1.37630500	-0.16358600
C	4.73055300	-0.89895400	0.93284800
C	6.08910200	-0.60847500	0.81081500
C	6.73966500	-0.79035400	-0.41205200
C	6.02047800	-1.25922400	-1.51134900
C	4.65936700	-1.54514600	-1.38506800
H	3.02229300	0.87609000	-0.32342100
N	-6.20763500	-1.30798300	-0.26929600
O	-7.01552900	-0.58887300	-0.86421300
O	-6.48154700	-2.41397400	0.20573700
H	2.79201400	3.10909200	-0.25665300
H	-2.07041200	2.92703100	0.63979000
H	-0.94961800	5.09561000	0.42659200
H	1.50006500	5.21770200	-0.04681500
H	-0.21622000	-0.25574600	0.42121600
H	-2.91137600	1.81747700	-0.99083300
H	-5.22945100	0.98153600	-1.21297200
H	-4.20512600	-2.55761300	0.97244300
H	-1.87926700	-1.71739500	1.25411200
H	2.21293500	-2.20229000	-0.98188300
H	2.45214400	-2.25559600	2.07080800
H	1.15550500	-2.96227300	1.09353900
H	2.81028400	-3.60727000	0.97805100
H	4.23749300	-0.75099900	1.89027000
H	6.64147000	-0.24233900	1.67228700
H	7.79911100	-0.56763000	-0.50563200
H	6.51643200	-1.40406600	-2.46746000
H	4.10471300	-1.91114200	-2.24657100

Compound 2a, conformation c4

C	1.74848800	3.11482400	0.00724000
C	1.13261600	1.86448100	-0.17436800
C	-0.28865500	1.80960500	-0.30537000
C	-1.01076900	3.01840400	-0.30386500
C	-0.36488800	4.23701300	-0.12629800
C	1.02125300	4.29711500	0.04489600
N	-0.88881500	0.57262100	-0.49295200
C	-2.19799200	0.16893100	-0.28097600
C	-3.11336000	0.84541200	0.55505300
C	-4.39596300	0.35019300	0.74133100
C	-4.78258600	-0.83028900	0.10549500
C	-3.88965400	-1.53278500	-0.70843900
C	-2.61284200	-1.03418400	-0.89821900
C	2.01306400	0.69422000	-0.23750700
N	1.61650600	-0.49576400	-0.50304000
C	2.55711200	-1.62768700	-0.59067300

C	1.91084500	-2.83295700	0.11321500
C	3.98276300	-1.36941600	-0.11771500
C	4.28649600	-1.20371200	1.24254800
C	5.59784200	-0.97690000	1.65951600
C	6.63206200	-0.91191500	0.72257900
C	6.34383400	-1.06998700	-0.63296700
C	5.02849800	-1.29286400	-1.04589300
H	3.07096700	0.91433000	-0.04883900
N	-6.13173400	-1.34338000	0.30137000
O	-6.89983400	-0.69225200	1.01539300
O	-6.43317300	-2.40231500	-0.25692800
H	2.83059100	3.14185700	0.11455000
H	-2.07930500	3.00217100	-0.48059900
H	-0.95289600	5.15093000	-0.13462100
H	1.52207200	5.24927400	0.18878100
H	-0.20577200	-0.16956600	-0.68792000
H	-2.80688100	1.73507600	1.09050700
H	-5.10092800	0.85752900	1.38865300
H	-4.21370600	-2.44941800	-1.18576300
H	-1.91591300	-1.56211100	-1.54316800
H	2.60682500	-1.87056200	-1.66199600
H	1.79282100	-2.64949400	1.18614500
H	0.91769800	-3.02362400	-0.30584700
H	2.52668700	-3.72860300	-0.01647700
H	3.49204000	-1.25072100	1.98299000
H	5.81316900	-0.85369400	2.71768200
H	7.65424100	-0.73923600	1.04834400
H	7.14064300	-1.02119000	-1.37042300
H	4.81102000	-1.41574700	-2.10486800

Compound 2b, conformation c1

C	2.07429600	3.88367500	0.44646000
C	1.58098400	2.63471000	0.03180100
C	0.16819500	2.44944000	-0.06778700
C	-0.67297800	3.54604000	0.20153400
C	-0.14722600	4.76794900	0.60670800
C	1.23236300	4.94604600	0.74675100
N	-0.30944700	1.21638900	-0.48798800
C	-1.56152200	0.63935300	-0.33664900
C	-1.87993800	-0.44896700	-1.18201600
C	-3.09101100	-1.10964900	-1.07207400
C	-4.01329400	-0.68841900	-0.11032500
C	-3.71946200	0.37080000	0.74917500
C	-2.50207100	1.02794100	0.64222000
C	2.56657900	1.60219300	-0.29560300
N	2.29401900	0.44490600	-0.77430500
C	3.39158600	-0.46966600	-1.07911400
C	3.43384400	-0.69862500	-2.59776900
C	3.25986500	-1.78736700	-0.26917000
C	3.42687100	-1.54024600	1.24260100
C	3.38247500	-2.84704400	2.04958000
C	2.09575600	-3.63624300	1.76800100
C	1.91795200	-3.88648700	0.26370300
C	1.96361800	-2.57641300	-0.54066000
H	3.61261200	1.89645100	-0.11259300
N	-5.29481600	-1.37206700	0.00372700
O	-5.51239100	-2.32024600	-0.75603000
O	-6.09236300	-0.96653800	0.85401000
H	3.15201100	4.00867100	0.52553400
H	-1.74174400	3.44786100	0.05582100
H	-0.82556200	5.59404500	0.80271700
H	1.63922100	5.89957700	1.06814500
H	0.43239600	0.60889300	-0.85455700
H	-1.16216700	-0.75656300	-1.93719500
H	-3.34208800	-1.93831500	-1.72269900
H	-4.44274200	0.65617600	1.50337400
H	-2.26288300	1.81602300	1.34496500
H	4.35100100	-0.00840300	-0.78082800
H	2.47789800	-1.07844100	-2.97098800
H	3.64631100	0.24047000	-3.11967700
H	4.21782200	-1.41974400	-2.85566500
H	4.10507300	-2.41529000	-0.59549800
H	2.62351300	-0.87434900	1.58774100
H	4.37265600	-1.01304500	1.43139800
H	3.47036200	-2.62894600	3.12156800
H	4.25240100	-3.46665200	1.78517800
H	1.23271900	-3.06738100	2.14425400
H	2.10473100	-4.58808000	2.31409100
H	2.71749900	-4.55536200	-0.08856300
H	0.97104100	-4.40742800	0.07345300
H	1.86618600	-2.79997500	-1.61012900
H	1.10017800	-1.95463300	-0.26794100

Compound 2b, conformation c2

C	-1.02549600	4.21684900	-0.45921400
C	-0.79634500	2.89161100	-0.05131000
C	0.54977500	2.42704800	0.06046800
C	1.59589400	3.33596800	-0.18892900
C	1.32952800	4.64150100	-0.58673600
C	0.01501200	5.09231500	-0.73961200
N	0.76782100	1.11963100	0.47105600
C	1.88140900	0.30636600	0.32313400
C	1.96848200	-0.83089600	1.15918600
C	3.02477800	-1.71845800	1.05196300
C	4.02177700	-1.48097000	0.10185100
C	3.95313000	-0.37696500	-0.74873000
C	2.88997600	0.50848800	-0.64426900
C	-1.97191100	2.07408200	0.25636900
N	-1.93915200	0.88670700	0.73726700
C	-3.19799800	0.20345800	1.03131200
C	-3.30504800	0.06165100	2.55832300
C	-3.23577400	-1.15457600	0.28418800
C	-4.52556200	-1.94917200	0.57632400
C	-4.57626400	-3.27987900	-0.19283100
C	-4.40046000	-3.07556700	-1.70326000
C	-3.11257600	-2.29700600	-2.00251600
C	-3.06495300	-0.96614900	-1.23704500
H	-2.93618800	2.56744100	0.05481300
N	5.14235900	-2.40533300	-0.00955400
O	6.01289300	-2.15958200	-0.84938600
O	5.15935900	-3.38455500	0.74179400
H	-2.05558300	4.55496300	-0.54849600
H	2.62173100	3.02505400	-0.03349200
H	2.16136600	5.31716500	-0.76706200
H	-0.18956100	6.11032400	-1.05562900
H	-0.08346600	0.66814500	0.82495300
H	1.19624700	-0.99594700	1.90531500
H	3.09956100	-2.58629900	1.69563300
H	4.72597000	-0.23480500	-1.49430900
H	2.81925300	1.33467900	-1.34038400
H	-4.04842100	0.81437400	0.67574200
H	-4.26861400	-0.36326600	2.85336800
H	-2.50756500	-0.58382600	2.94414800
H	-3.20734100	1.04153400	3.03715000
H	-2.38034400	-1.74482500	0.65018600
H	-5.39552400	-1.33540800	0.29449800
H	-4.62067400	-2.15087300	1.64928800
H	-5.52355000	-3.79260700	0.01742200
H	-3.77716700	-3.93903700	0.17742000
H	-5.26259900	-2.51665100	-2.09698100
H	-4.39268200	-4.04343000	-2.22040900
H	-2.24470200	-2.90947000	-1.71651000
H	-3.01870500	-2.11058000	-3.07990700
H	-2.12153200	-0.44955000	-1.44408700
H	-3.86936900	-0.30923800	-1.60529400

Compound 2b, conformation c3

C	1.28777200	3.91329000	0.17839100
C	0.92306500	2.59192900	-0.13177400
C	-0.46383800	2.25705800	-0.20141900
C	-1.41133500	3.28128500	-0.01151600
C	-1.01168000	4.57862400	0.28965600
C	0.34296100	4.90583000	0.40158900
N	-0.81577800	0.95216800	-0.51528100
C	-2.00260300	0.26682800	-0.30213800
C	-2.97274300	0.63693600	0.65475800
C	-4.11711600	-0.12798700	0.82954500
C	-4.30668900	-1.27705300	0.06096200
C	-3.35126800	-1.67991000	-0.87602900
C	-2.21354900	-0.91236300	-1.05366600
C	2.00761000	1.64171400	-0.38790800
N	1.85123600	0.43213400	-0.78157600
C	3.03369200	-0.39046200	-1.03806600
C	3.12004500	-0.62041700	-2.55591000
C	2.90939100	-1.71596700	-0.23517400
C	4.09142100	-2.68794600	-0.45756600
C	5.39298200	-2.22426600	0.21906400
C	5.18494800	-1.97877200	1.72151600
C	4.02081000	-1.00894100	1.97672200
C	2.73158000	-1.47966800	1.28248500
H	3.01857700	2.05062800	-0.23012800
N	-5.51207000	-2.07430600	0.24571700
O	-6.34226200	-1.68376100	1.07142700
O	-5.63667200	-3.09753800	-0.43334000
H	2.34738300	4.15250100	0.23663700
H	-2.46491800	3.06397900	-0.13765700
H	-1.77003200	5.34497200	0.42605600
H	0.65155000	5.91819800	0.64227600
H	-0.01819100	0.39369900	-0.84051700
H	-2.81073500	1.49912700	1.28922900
H	-4.86174200	0.14327900	1.56800500
H	-3.52059300	-2.57938400	-1.45509800
H	-1.47169300	-1.20648100	-1.79083600
H	3.93862800	0.15400100	-0.72055000
H	4.03414700	-1.15601200	-2.82800500
H	2.25988700	-1.20068400	-2.90938500
H	3.12146800	0.33819400	-3.08514000
H	1.99547400	-2.20127000	-0.60748200
H	4.25944100	-2.86886200	-1.52520100
H	3.80533300	-3.65958300	-0.02990300
H	5.75635700	-1.30118300	-0.25518700
H	6.17720900	-2.97605900	0.06323200
H	6.10773200	-1.59856000	2.17813100
H	4.96552400	-2.93836600	2.21298600
H	3.84247300	-0.90672900	3.05474100
H	4.29728400	-0.00690500	1.61776100
H	2.41592500	-2.42909700	1.73813900
H	1.91853100	-0.76744200	1.46004700

Compound 2b, conformation c4

C	1.53027700	3.90270700	-0.07611400
C	1.12805600	2.57425800	0.14383000
C	-0.15818800	2.15959800	-0.31714500
C	-0.94716100	3.08394900	-1.02822400
C	-0.51116200	4.38829300	-1.23387500
C	0.72768400	4.81571700	-0.74739900
N	-0.55197300	0.84641600	-0.09728500
C	-1.82254500	0.29281300	-0.04504300
C	-1.92259300	-1.11441600	-0.14505500
C	-3.14792500	-1.75232400	-0.06433700
C	-4.30470700	-0.98896300	0.11559300
C	-4.23509900	0.39954500	0.23528600
C	-3.00508400	1.03704100	0.16050600
C	2.07989100	1.69407600	0.83034500
N	1.92746700	0.42911600	0.96738400
C	2.92115000	-0.40294600	1.65178600
C	4.06456300	0.33642800	2.36217400
C	3.43955000	-1.50747900	0.68359900
C	2.32235500	-2.47175800	0.23992700
C	2.86348500	-3.60566800	-0.64510900
C	3.61491300	-3.05404100	-1.86542000
C	4.72492700	-2.08221000	-1.44018300
C	4.18215400	-0.95347600	-0.54775500
H	2.96437300	2.21493600	1.21785700
N	-5.59900100	-1.65284500	0.19091100
O	-5.62191700	-2.88415100	0.10527000
O	-6.60227900	-0.94863400	0.33707700
H	2.50741500	4.21001500	0.29037700
H	-1.89121800	2.76384800	-1.45224800
H	-1.14376100	5.07387300	-1.79137500
H	1.06319600	5.83618400	-0.90306100
H	0.22317400	0.25315700	0.22237300
H	-1.01877500	-1.69716100	-0.29910000
H	-3.22916900	-2.82916000	-0.14761500
H	-5.14537900	0.96239700	0.40262400
H	-2.95598300	2.10928400	0.30189500
H	2.34995700	-0.93329800	2.42894100
H	3.67969700	1.05410800	3.09545700
H	4.68338800	-0.38801800	2.90184000
H	4.71900200	0.87716300	1.67039400
H	4.16122500	-2.09640600	1.27213600
H	1.56454900	-1.90732800	-0.32052300
H	1.81747100	-2.88854100	1.12223000
H	2.04052100	-4.25713400	-0.96566400
H	3.54534800	-4.23414800	-0.05307400
H	2.90446400	-2.52733500	-2.51968100
H	4.03509500	-3.87629500	-2.45836800
H	5.49984800	-2.63701900	-0.89043500
H	5.21664200	-1.65523200	-2.32352800
H	5.00928200	-0.30126800	-0.24040800
H	3.49051300	-0.32999700	-1.13121800

Compound 2b, conformation c1'

C	-1.40035300	3.96526400	0.14785600
C	-1.02777700	2.62077000	0.26921100

C	0.22913800	2.20751300	-0.25187500
C	1.02109300	3.14850200	-0.92373000
C	0.61715500	4.47142300	-1.03309100
C	-0.59124200	4.89522500	-0.48508600
N	0.58401200	0.86750900	-0.13075100
C	1.82268700	0.27092600	-0.11283400
C	1.86287100	-1.13887900	-0.22200200
C	3.05491400	-1.82291900	-0.18602500
C	4.25023600	-1.11323200	-0.03689800
C	4.23724200	0.27545200	0.09541900
C	3.04106600	0.96148100	0.05920400
C	-1.98737900	1.71849300	0.91241400
N	-1.87103100	0.45061200	0.97190400
C	-2.91569800	-0.32090700	1.64327000
C	-2.31009100	-1.00867700	2.87176100
C	-3.59600800	-1.31502300	0.66956000
C	-4.39775600	-0.58471500	-0.41995600
C	-5.15186000	-1.56138500	-1.33054100
C	-4.20659200	-2.59529400	-1.95168200
C	-3.39646500	-3.32391400	-0.87425400
C	-2.64417000	-2.34163300	0.03387300
H	-2.86380600	2.21892500	1.34424200
N	5.50264400	-1.82193800	-0.00658600
O	5.48754300	-3.05575300	-0.09389200
O	6.54976500	-1.17329500	0.10666200
H	-2.35528000	4.27263200	0.55939100
H	1.94213900	2.83928300	-1.39540800
H	1.25070800	5.17322600	-1.56208600
H	-0.90174900	5.92897400	-0.56543200
H	-0.20947700	0.28158500	0.15751400
H	0.93578600	-1.68429900	-0.34630200
H	3.07572800	-2.89877800	-0.28019400
H	5.16596400	0.80762800	0.24168900
H	3.04992100	2.03051500	0.20375600
H	-3.70284100	0.36383100	1.99406200
H	-1.47088900	-1.65010600	2.59823500
H	-1.94633600	-0.26405800	3.58277800
H	-3.06378600	-1.62020700	3.37323600
H	-4.31565200	-1.86987800	1.28682400
H	-3.71392500	0.01850000	-1.02811200
H	-5.10169000	0.11372400	0.04503700
H	-5.67907900	-1.00968000	-2.11473100
H	-5.91981900	-2.08132200	-0.74485500
H	-3.51821000	-2.08756500	-2.63841100
H	-4.77264000	-3.31435200	-2.55160200
H	-4.07468000	-3.93255100	-0.26361600
H	-2.68833100	-4.01774400	-1.33738000
H	-2.10700600	-2.89694000	0.80704600
H	-1.88896500	-1.81307500	-0.55737700

Compound 2b, conformation c2’

C	-1.01480900	4.21598600	-0.49601500
C	-0.77997600	2.90161400	-0.07360200
C	0.56342100	2.45637200	0.06893100
C	1.60220200	3.36918200	-0.15934400

C	1.33289100	4.66672700	-0.57056700
C	0.02161700	5.09785000	-0.75705200
N	0.78092400	1.15182700	0.49969100
C	1.86772500	0.32509900	0.34105200
C	1.89584400	-0.85821800	1.11590900
C	2.92836600	-1.75897500	1.00379600
C	3.96941600	-1.50243400	0.10638500
C	3.95472000	-0.35434100	-0.68597000
C	2.91849300	0.54922400	-0.57348300
C	-1.95528500	2.07713600	0.22227000
N	-1.91858500	0.90664100	0.72484300
C	-3.17711800	0.21624500	1.00860500
C	-3.30762900	0.09269700	2.53173500
C	-3.19724800	-1.14760800	0.27893800
C	-4.47878700	-1.94734300	0.57534100
C	-4.51651600	-3.28527300	-0.17504700
C	-4.33559700	-3.10180200	-1.68427200
C	-3.05828300	-2.31437100	-1.98918500
C	-3.02522800	-0.97691700	-1.24078300
H	-2.91583800	2.55571100	-0.00757100
N	5.05857300	-2.43624600	-0.00970900
O	5.97920400	-2.18053200	-0.79530700
O	5.03496900	-3.46290200	0.67990000
H	-2.04242000	4.54207700	-0.61177300
H	2.62623100	3.07640000	0.01916600
H	2.15851400	5.34861300	-0.73533500
H	-0.18633400	6.10851200	-1.08388100
H	-0.07908700	0.71057100	0.84870100
H	1.09218300	-1.04777100	1.81663600
H	2.94631100	-2.65476700	1.60713500
H	4.74957900	-0.18546100	-1.39787000
H	2.90505100	1.40934100	-1.22448600
H	-4.01975700	0.81727800	0.63258300
H	-4.27514400	-0.32323600	2.81301300
H	-2.52236200	-0.55058500	2.93700600
H	-3.21704700	1.07578300	2.99773100
H	-2.34152300	-1.72462200	0.65540400
H	-5.34953400	-1.34553000	0.28408100
H	-4.57389000	-2.13610000	1.64664100
H	-5.45946300	-3.79862200	0.03597700
H	-3.71765900	-3.93264400	0.20677600
H	-5.19946000	-2.56052800	-2.08937200
H	-4.31268000	-4.07451500	-2.18484600
H	-2.18721700	-2.91296100	-1.69576200
H	-2.96641800	-2.13926400	-3.06539500
H	-2.08878700	-0.45706600	-1.45436200
H	-3.83232000	-0.33381300	-1.61657800

Compound 2b, conformation c3’

C	-1.21083500	3.76539100	0.40547000
C	-0.82445200	2.42075800	0.34321500
C	0.48861800	2.10397000	-0.10272400
C	1.32594500	3.14679200	-0.52225300
C	0.90791400	4.46801700	-0.45310600
C	-0.35961600	4.79068700	0.02578600

N	0.85457800	0.76373400	-0.16911500
C	2.09510200	0.17165000	-0.14814200
C	3.28560700	0.81886400	0.24497000
C	4.48303300	0.13423700	0.26251700
C	4.52435700	-1.21013000	-0.10762800
C	3.35469500	-1.88071100	-0.47787000
C	2.16148300	-1.19800500	-0.49581700
C	-1.82829400	1.42143900	0.72027700
N	-1.68256200	0.16052500	0.60530000
C	-2.77368900	-0.72085400	1.02619600
C	-2.31267100	-1.46685100	2.28473100
C	-3.12833000	-1.67714900	-0.14254900
C	-4.22893400	-2.70042800	0.20778600
C	-5.62778300	-2.07647900	0.31108200
C	-5.99863000	-1.32102100	-0.97071400
C	-4.92822900	-0.28801300	-1.34240400
C	-3.53397600	-0.92487400	-1.42744000
H	-2.76527500	1.84247400	1.10671200
N	5.77903300	-1.91555400	-0.09678400
O	6.80555700	-1.29742500	0.21013400
O	5.78621500	-3.11619000	-0.39424200
H	-2.21012800	3.99649100	0.75717000
H	2.29697000	2.92439600	-0.93914700
H	1.57832300	5.25029400	-0.78830300
H	-0.68167600	5.82231500	0.08497200
H	0.04856600	0.13572700	-0.05823400
H	3.26880600	1.84589600	0.57466100
H	5.38942100	0.63055700	0.57749200
H	3.39709700	-2.92380300	-0.75527200
H	1.25447500	-1.71031200	-0.79181100
H	-3.64987300	-0.11321300	1.28901300
H	-3.11988000	-2.06540300	2.70756400
H	-1.47302000	-2.12887000	2.05770800
H	-1.98969100	-0.75515300	3.04691800
H	-2.20837300	-2.23364100	-0.35695000
H	-3.98480200	-3.24008800	1.12504500
H	-4.24359000	-3.45269700	-0.58937100
H	-5.67089500	-1.38995700	1.16406100
H	-6.36412900	-2.86037400	0.51232900
H	-6.97259600	-0.83540600	-0.85750400
H	-6.10113600	-2.04112000	-1.79197500
H	-5.17482800	0.18192100	-2.29929600
H	-4.92820300	0.51667300	-0.59857400
H	-3.52890000	-1.64452700	-2.25421300
H	-2.78607200	-0.16794400	-1.67423700

Compound 2b, conformation c4’

C	1.50203600	3.90477900	-0.01327600
C	1.09656900	2.57756900	0.17336600
C	-0.17116000	2.17304700	-0.32687200
C	-0.93938000	3.09925600	-1.04501400
C	-0.50190200	4.40439700	-1.22036200
C	0.71712400	4.82301100	-0.69277700
N	-0.56245200	0.85040900	-0.13772600
C	-1.81762500	0.29474000	-0.07099200

C	-1.90286700	-1.11731500	-0.09752300
C	-3.11459000	-1.76057900	-0.00951900
C	-4.28600500	-1.00656300	0.11037300
C	-4.22859200	0.38649800	0.16131600
C	-3.01271800	1.03160400	0.07281100
C	2.03617300	1.68510600	0.86408500
N	1.88912700	0.42273900	0.95805000
C	2.87339100	-0.42105500	1.64482600
C	3.99113300	0.30951800	2.39426400
C	3.42006600	-1.50110100	0.67085200
C	2.32886500	-2.47576400	0.20059300
C	2.90261900	-3.59175800	-0.68109200
C	3.66953200	-3.02120400	-1.87912600
C	4.75150800	-2.03468800	-1.42722600
C	4.17504600	-0.92444700	-0.53782000
H	2.90416300	2.19929100	1.28513800
N	-5.55872700	-1.67240400	0.19490800
O	-5.58277700	-2.90925700	0.18180700
O	-6.58437300	-0.98572400	0.27854400
H	2.46418800	4.20839900	0.38411600
H	-1.86855200	2.78997000	-1.50067500
H	-1.11739400	5.09515300	-1.78408300
H	1.05435900	5.84320000	-0.82352600
H	0.22055500	0.26038900	0.17337100
H	-0.99463000	-1.69793300	-0.19905000
H	-3.16932100	-2.83895200	-0.04067300
H	-5.13872600	0.95508600	0.28586800
H	-2.98737100	2.10706100	0.15391300
H	2.28788500	-0.96988400	2.39284000
H	3.58602700	1.00279900	3.13499000
H	4.59980300	-0.42369900	2.92653700
H	4.65330100	0.87089400	1.73238300
H	4.13814300	-2.08278600	1.26358800
H	1.57359100	-1.92423000	-0.36871300
H	1.81867400	-2.90670000	1.06839800
H	2.09734600	-4.24842600	-1.02398800
H	3.57928600	-4.21387200	-0.08255300
H	2.96625900	-2.50507200	-2.54414300
H	4.11606300	-3.83082600	-2.46432300
H	5.52401100	-2.57812100	-0.86950400
H	5.24841300	-1.59330700	-2.29645400
H	4.98227500	-0.26460900	-0.20845800
H	3.48786400	-0.30950300	-1.12975500

Compound 2f, conformation c1

C	0.49551400	4.37655100	-0.10697900
C	0.38938700	2.97506800	-0.13339900
C	-0.86282700	2.36989400	0.19660300
C	-1.92651300	3.20542100	0.58971700
C	-1.78202400	4.58807400	0.60612100
C	-0.57292200	5.19010200	0.24412100
N	-0.95532300	0.98682400	0.17856400
C	-2.06684900	0.15873800	0.11705400
C	-1.88983400	-1.18876500	0.50767700
C	-2.93352600	-2.09507800	0.44003000
C	-4.18144400	-1.66576800	-0.02007600
C	-4.38013100	-0.34690700	-0.42970500
C	-3.33098400	0.55923800	-0.36743100
C	1.59485600	2.22055700	-0.47761800
H	2.46328900	2.84199800	-0.74928100
N	-5.28780300	-2.61193900	-0.08406300
O	-5.07153400	-3.77671900	0.26227400
O	-6.38032500	-2.19747400	-0.48180300
H	1.45269400	4.82313700	-0.36733300
H	-2.85853500	2.76368400	0.91994000
H	-2.62304000	5.20127100	0.91870600
H	-0.46569600	6.27009900	0.25315900
H	-0.04183300	0.52851700	0.08042300
H	-0.91927200	-1.50614700	0.87870100
H	-2.80512000	-3.12607300	0.74596800
H	-5.35079200	-0.05114500	-0.80877600
H	-3.48016600	1.56690200	-0.73419700
N	1.69028400	0.94153800	-0.46399600
C	2.95564300	0.32626300	-0.85373400
C	3.44647600	-0.63242700	0.23400500
C	2.77491100	-0.37708600	-2.21024100
H	3.72352700	1.11189500	-0.98441400
C	3.33503400	-0.25596900	1.58033700
C	4.04996700	-1.86232300	-0.08766400
C	4.00639100	-1.21979600	-2.54990900
H	1.88357600	-1.01666300	-2.16106300
H	2.58342200	0.37999900	-2.97969200
C	3.80666300	-1.07529600	2.60231100
H	2.86503900	0.69192700	1.82642400
C	4.52489900	-2.67559800	0.95146800
C	4.17501300	-2.34408200	-1.52279900
H	3.91483100	-1.64120900	-3.55776000
H	4.90017500	-0.58021900	-2.55471600
C	4.40727400	-2.29532300	2.28525300
H	3.70753500	-0.76358600	3.63865300
H	4.99356300	-3.62544600	0.70144900
H	5.14007900	-2.84810900	-1.65897700
H	3.40751100	-3.11132500	-1.70708700
H	4.78414000	-2.94385700	3.07172500

Compound 2f, conformation c2

C	0.60816000	4.40822200	0.49392400
C	0.49951800	3.04218100	0.18062000
C	-0.79423800	2.49245200	-0.07658400
C	-1.90381400	3.35992600	-0.06505400
C	-1.75576500	4.70764700	0.24274300
C	-0.49915800	5.24404000	0.54011600
N	-0.89407800	1.14397800	-0.38496100
C	-1.98289000	0.28635100	-0.31829900
C	-1.89596200	-0.92657200	-1.03969200
C	-2.91943300	-1.85710800	-0.99994300
C	-4.05719600	-1.58771700	-0.23443800
C	-4.16198700	-0.40849600	0.50380400
C	-3.13196500	0.52064200	0.46785900
C	1.74133100	2.27075900	0.11818800
H	2.64262200	2.82656200	0.42298500
N	-5.14416800	-2.55734600	-0.19728300
O	-5.01003200	-3.59953800	-0.84481600
O	-6.13944300	-2.28400200	0.47973400
H	1.59822300	4.81041200	0.69741200
H	-2.88121400	2.97961400	-0.33533300
H	-2.63369400	5.34813700	0.23794600
H	-0.38820700	6.29523100	0.78644200
H	0.01713400	0.70972600	-0.57150700
H	-1.01220300	-1.11936400	-1.64120900
H	-2.86004900	-2.78418700	-1.55669300
H	-5.04311300	-0.24099200	1.11117600
H	-3.20037300	1.40953300	1.08207600
N	1.83064000	1.05182700	-0.27070400
C	3.15016800	0.42896000	-0.32712000
C	3.16851000	-0.87560400	0.47358400
C	3.53976700	0.21286200	-1.79973900
H	3.89868300	1.11040500	0.11925300
C	2.51895100	-0.92695400	1.71525200
C	3.86387400	-2.00971300	0.01465700
C	4.81166700	-0.63189100	-1.90368300
H	2.71072200	-0.29136800	-2.31426100
H	3.66772800	1.18990600	-2.28038800
C	2.54699200	-2.07680600	2.49945900
H	1.97737600	-0.05260700	2.06457200
C	3.88834400	-3.15950900	0.81710700
C	4.56208600	-2.03203700	-1.33418200
H	5.13937900	-0.70246400	-2.94746300
H	5.62470500	-0.14205400	-1.34968100
C	3.23820400	-3.20247300	2.04706800
H	2.03321300	-2.09454000	3.45683900
H	4.42835300	-4.03523100	0.46229900
H	5.50484900	-2.58731000	-1.25165200
H	3.94176800	-2.59907900	-2.04516900
H	3.27216200	-4.10618400	2.64977400

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