Luminescent pyrenyl–GNA nucleosides: Synthesis, photophysics and confocal microscopy studies in cancer HeLa cells

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Supporting Information

Contents

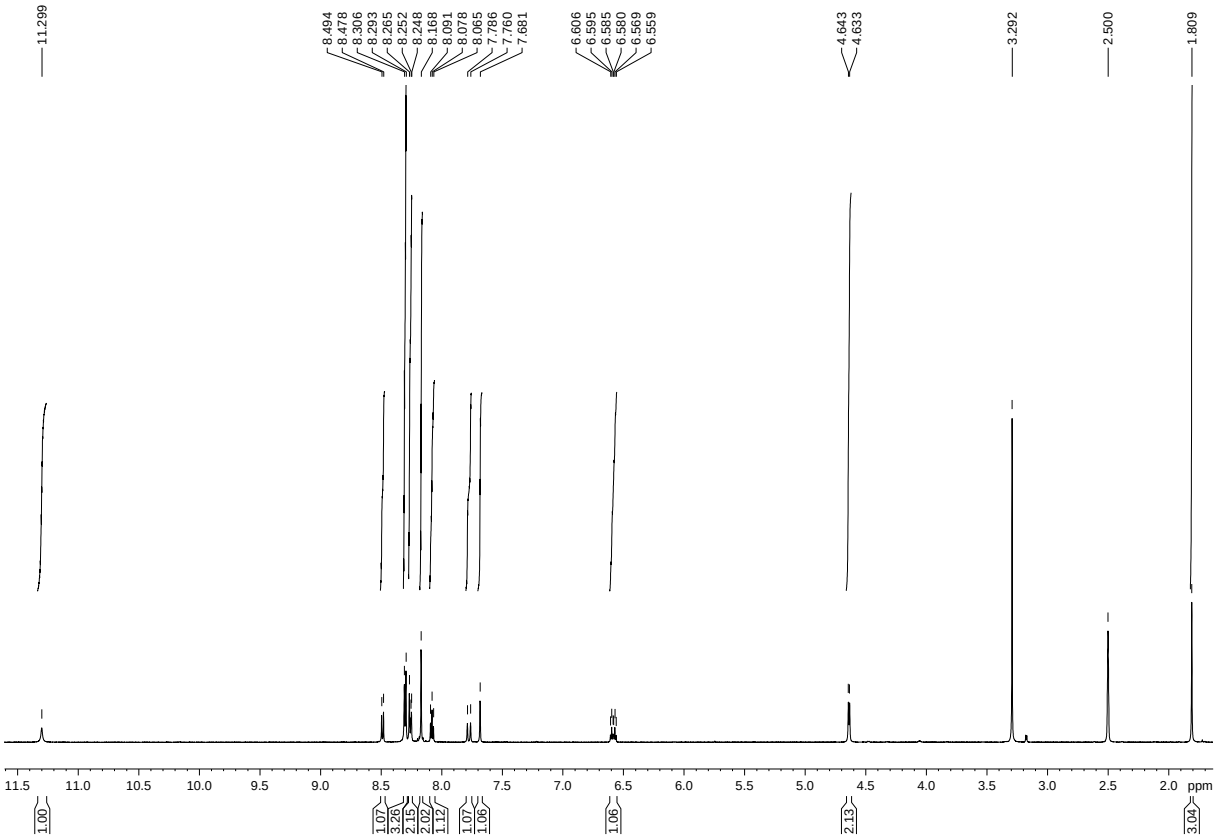

Figure S1 ^{1}H-NMR of compound **1** (600 MHz, DMSO-d_6)

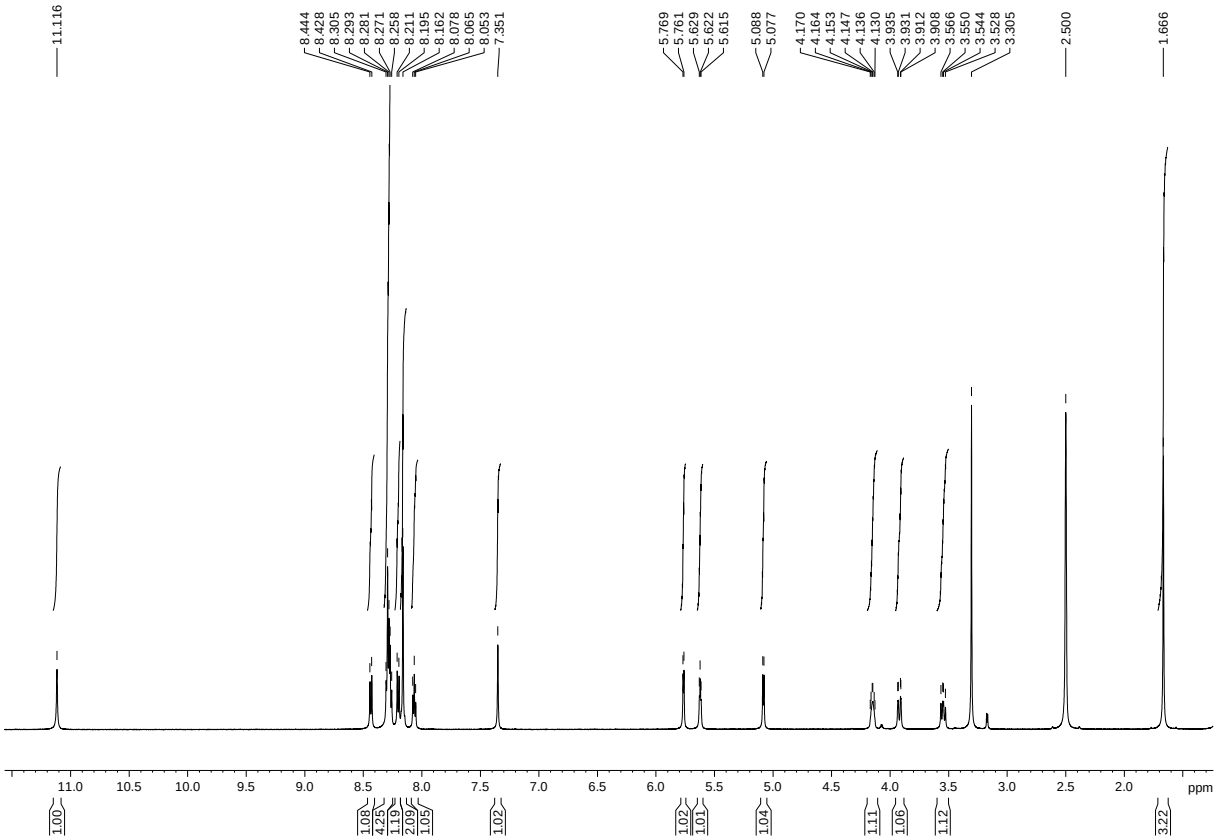

Figure S2 ^{1}H-NMR of compound (*R,S)*-**2** (600 MHz, DMSO-d_6)

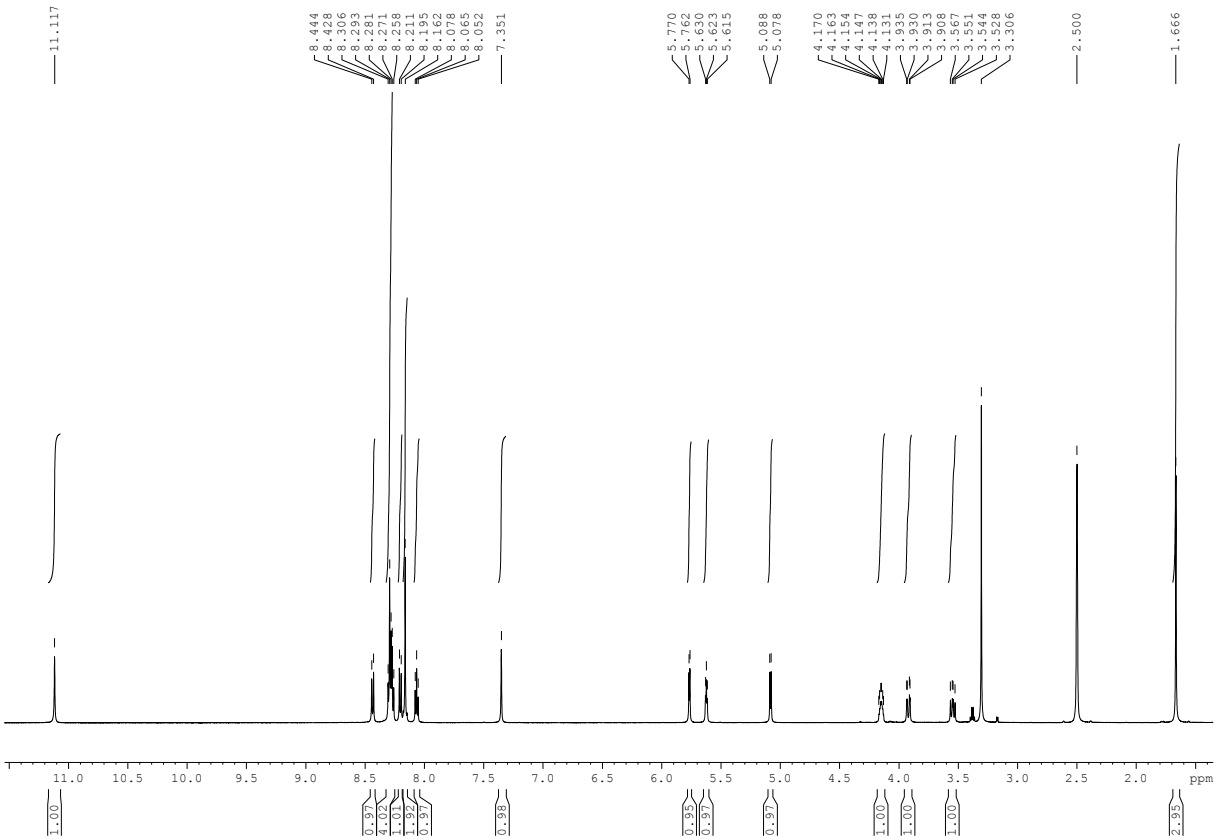

Figure S3 ^{1}H-NMR of compound (*S*,*R*)-**2** (600 MHz, DMSO-d_6)

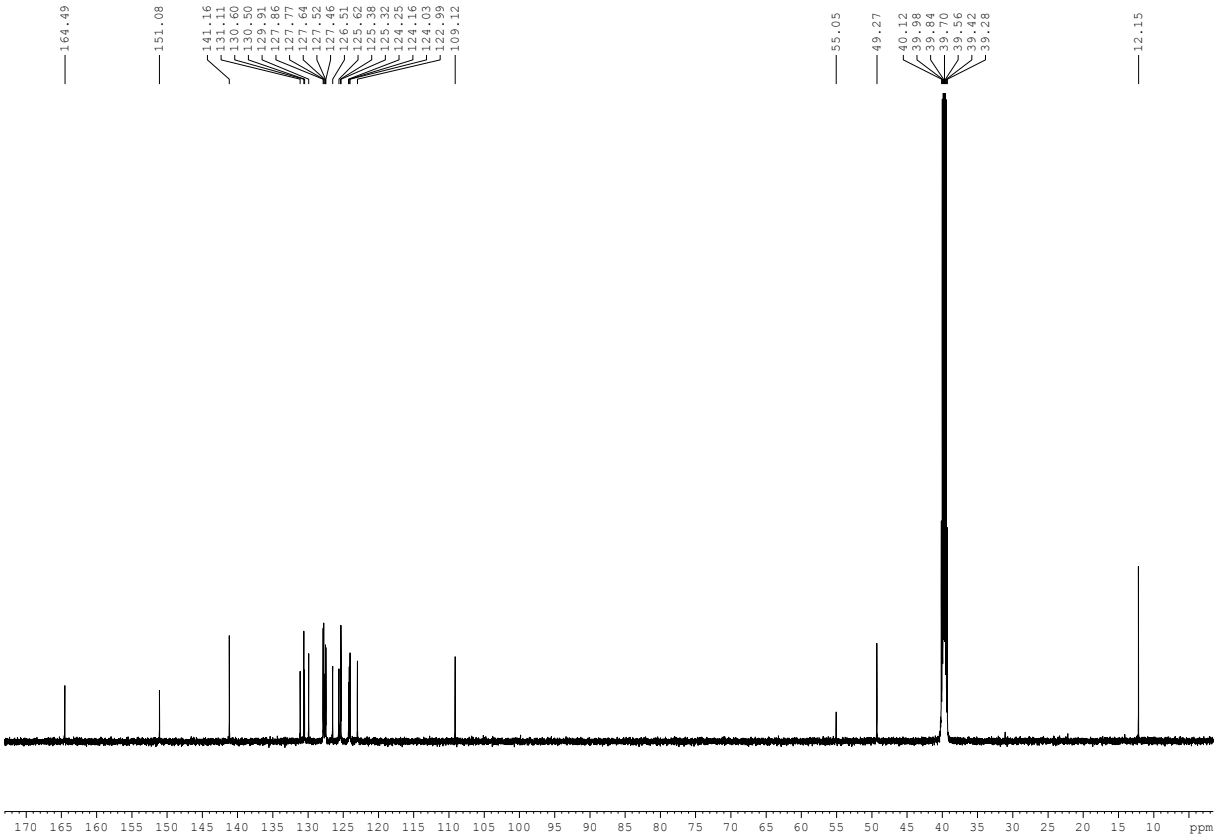

Figure S4 ^{13}C-NMR of compound **1** (150 MHz, DMSO-d_6)

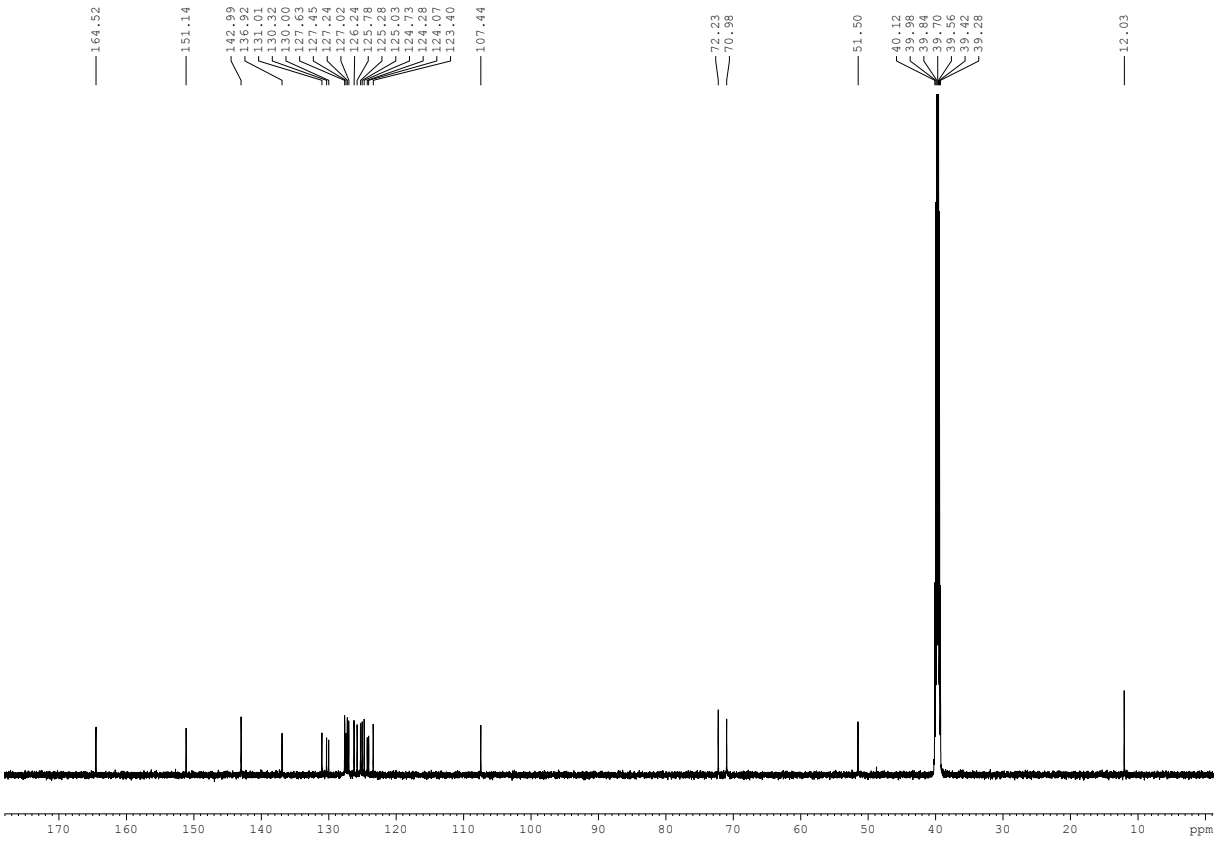

Figure S5 ^{13}C-NMR of compound (*R*,*S*)-**2** (150 MHz, DMSO-d_6)

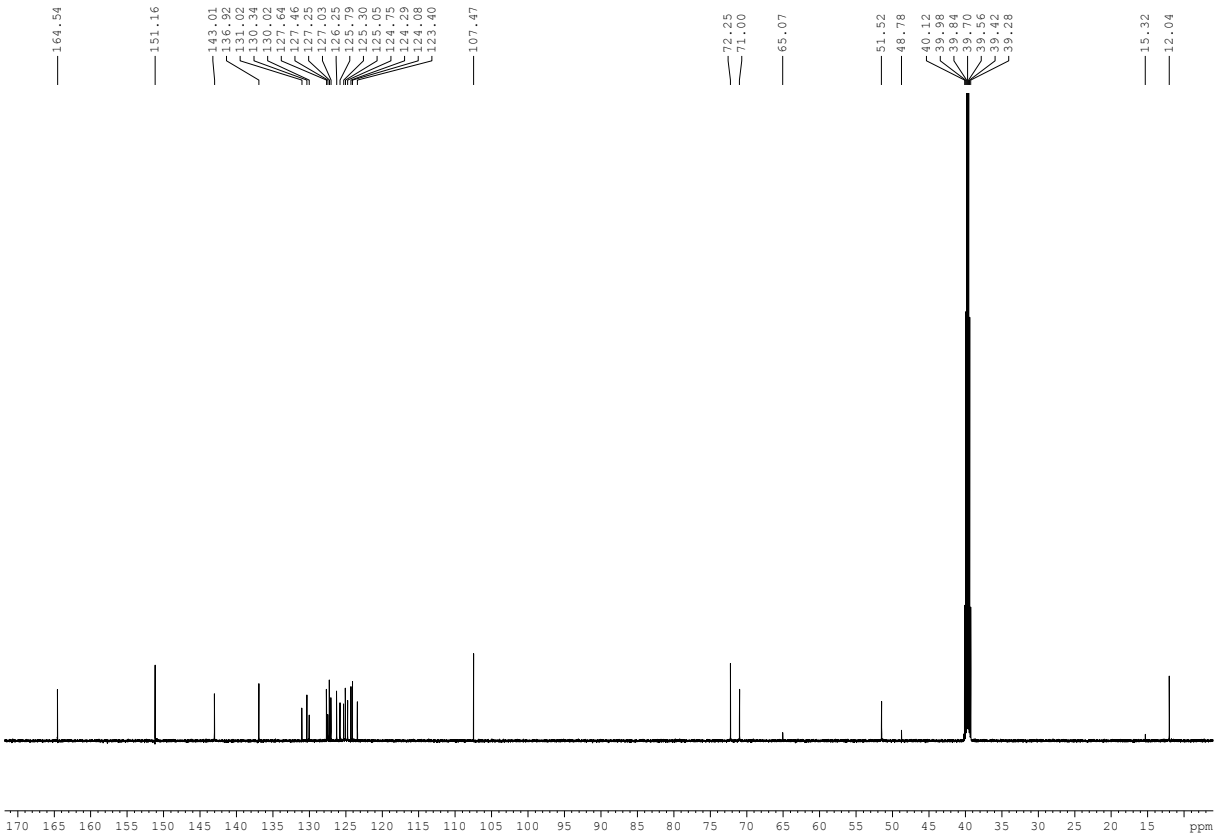

Figure S6 ^{13}C-NMR of compound (*S*,*R*)-**2** (150 MHz, DMSO-d_6)

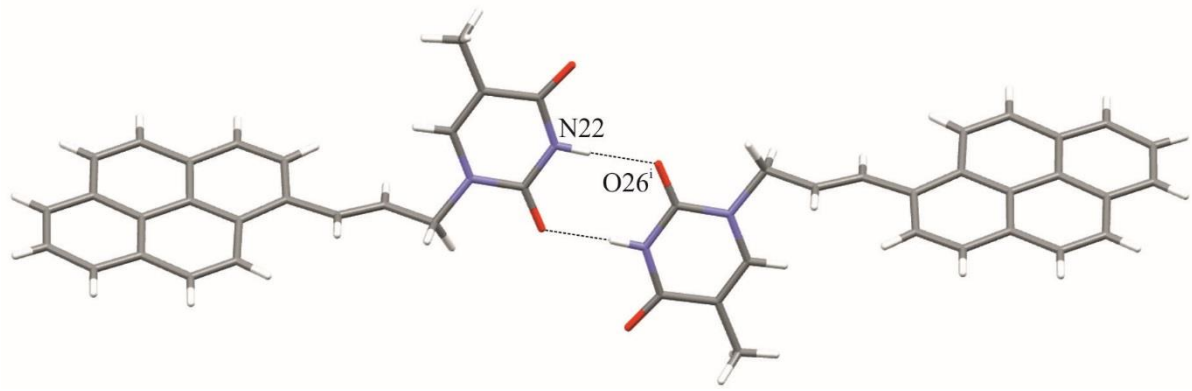

Figure S7 Dimeric structure observed in the crystal packing of compound **1**. The N−H···O hydrogen bonds are represented by dashed lines (N(22) --H(22) ..O(26) 0.84(2)Å, 2.04(2)Å 2.847(2)Å). Symmetry code: (i) −*x* + 3, *x* + 3, −*y* + 1, −*z* + 1.

TDDFT calculated electronic transitions

The predicted, conformationally averaged CD spectrum is dominated by the contribution of conformers A and B (Figures 6 and 7 in the manuscript) which account for > 90% of the population at 25 °C. The low-energy band in the experimental CD spectrum, peaking at 347 nm (-8.02603 mdeg), was assigned as the electronic transitions to excited singlet states $S_2 \leftarrow S_0$. For both conformers, we calculated that the electronic state has an excitation energy of ca. 3.56 eV, corresponding to the wavelength of 348 nm. On the basis of TDDFT calculation, the transition was assigned to an excitation from a π-HOMO (MO 105) to a π*-LUMO (MO 106) of the pyrene ring (Figure S8).

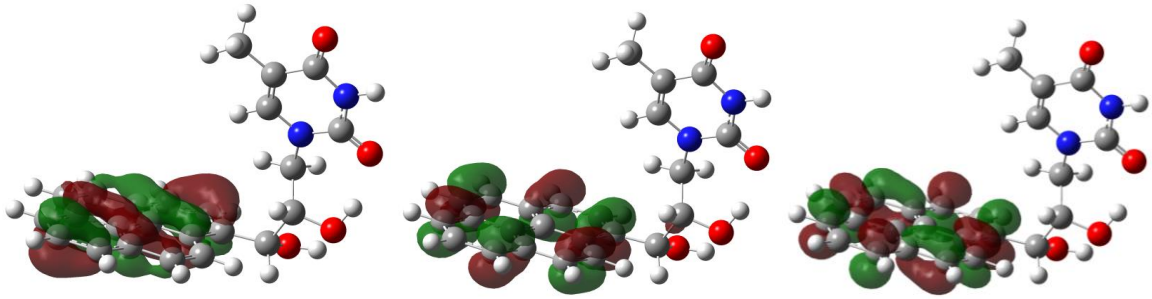

Figure S8 The representative frontier molecular orbitals of the most stable conformer (A) of (*R*,*S*)-2, calculated at the B3LYP/6-311+G(2d,2p)//B3LYP/6-311G(d,p) level. *Left*: HOMO-1 (MO 104); *Middle*: HOMO (MO 105); *Right*: LUMO (MO 106).

The higher-energy band (330 nm) observed experimentally was reproduced by TDDFT calculation (336 and 337 nm for conformers A and B, resp.) but the calculated oscillator strength (f = 0.0008) was too small to be observed in the predicted CD spectrum. The band corresponds to the vibronic transition $S_2 \leftarrow S_0$. The next experimental band (316 nm) also corresponds to the vibronic transition $S_2 \leftarrow S_0$, and is reproduced by our TDDFT calculation (323 and 331 nm for conformers A and B, resp.). The most intense band at 280 nm (24.553 mdeg) in the experimental CD spectrum was calculated as a transition at 277 nm and consists of HOMO-1 to LUMO excitation, *i.e.* corresponds to the $S_3 \leftarrow S_0$ transition.

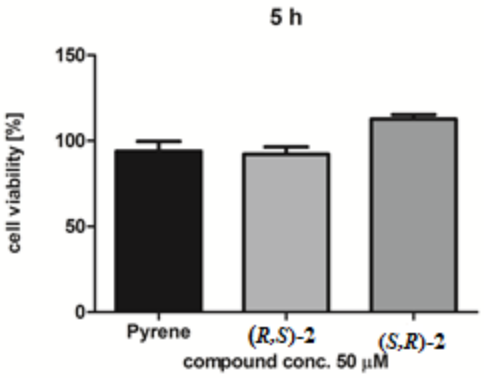

Figure S9 HeLa cells viability after 5 h incubation in presence of 50 µM of (*R*,*S*)-**2**, (*S*,*R*)-**2** and pyrene. The results represent mean ± SEM, N=3. No significant differences were observed (P>0.05).

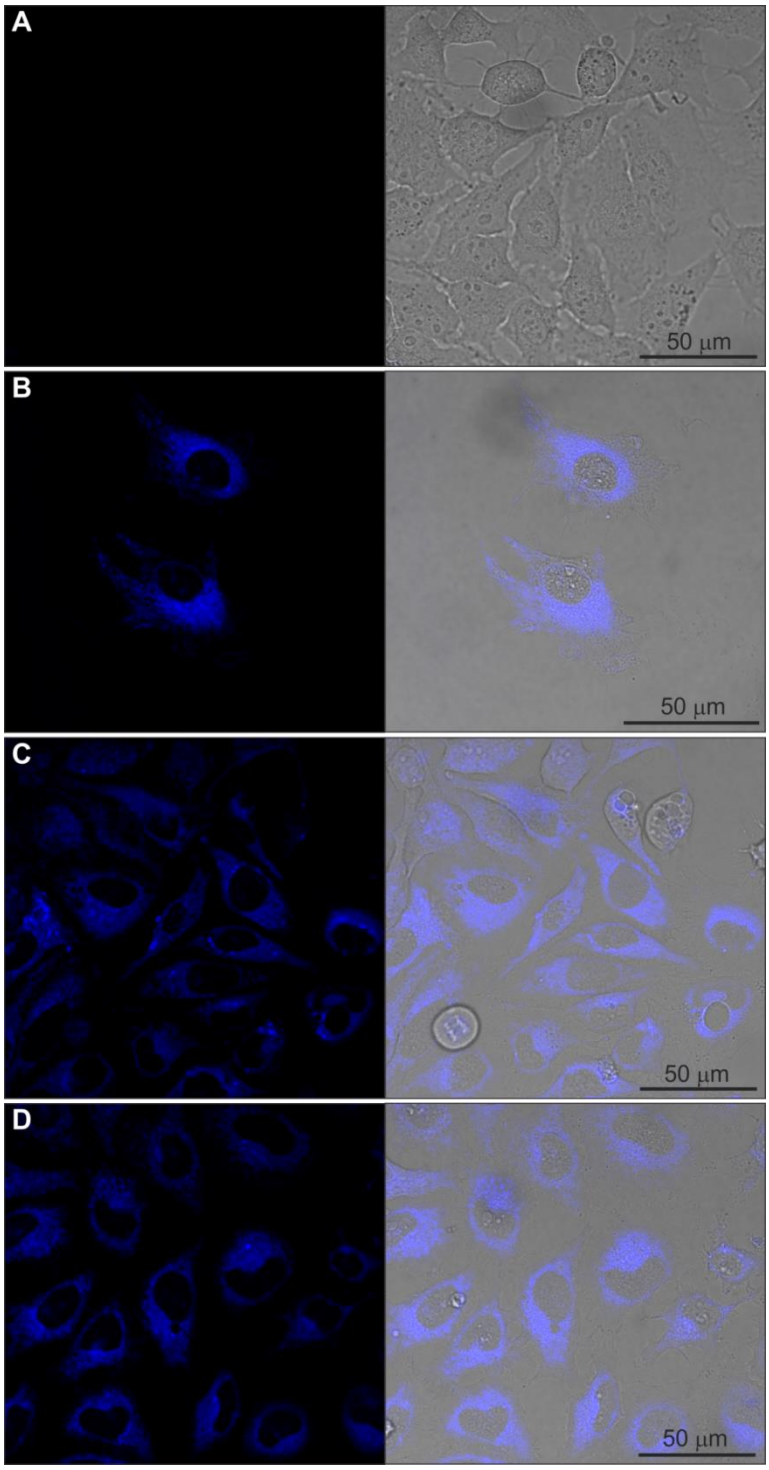

Figure S10 The images of untreated HeLa cells (A); after incubation with pyrene (B); derivative (*R*,*S*)-**2** (C) and derivative (*S*,*R*)-**2** (D). Fluorescence of compounds (blue colour), merged images of fluorescence and transmitted light (grey+blue). Scale bare – 50 μm.

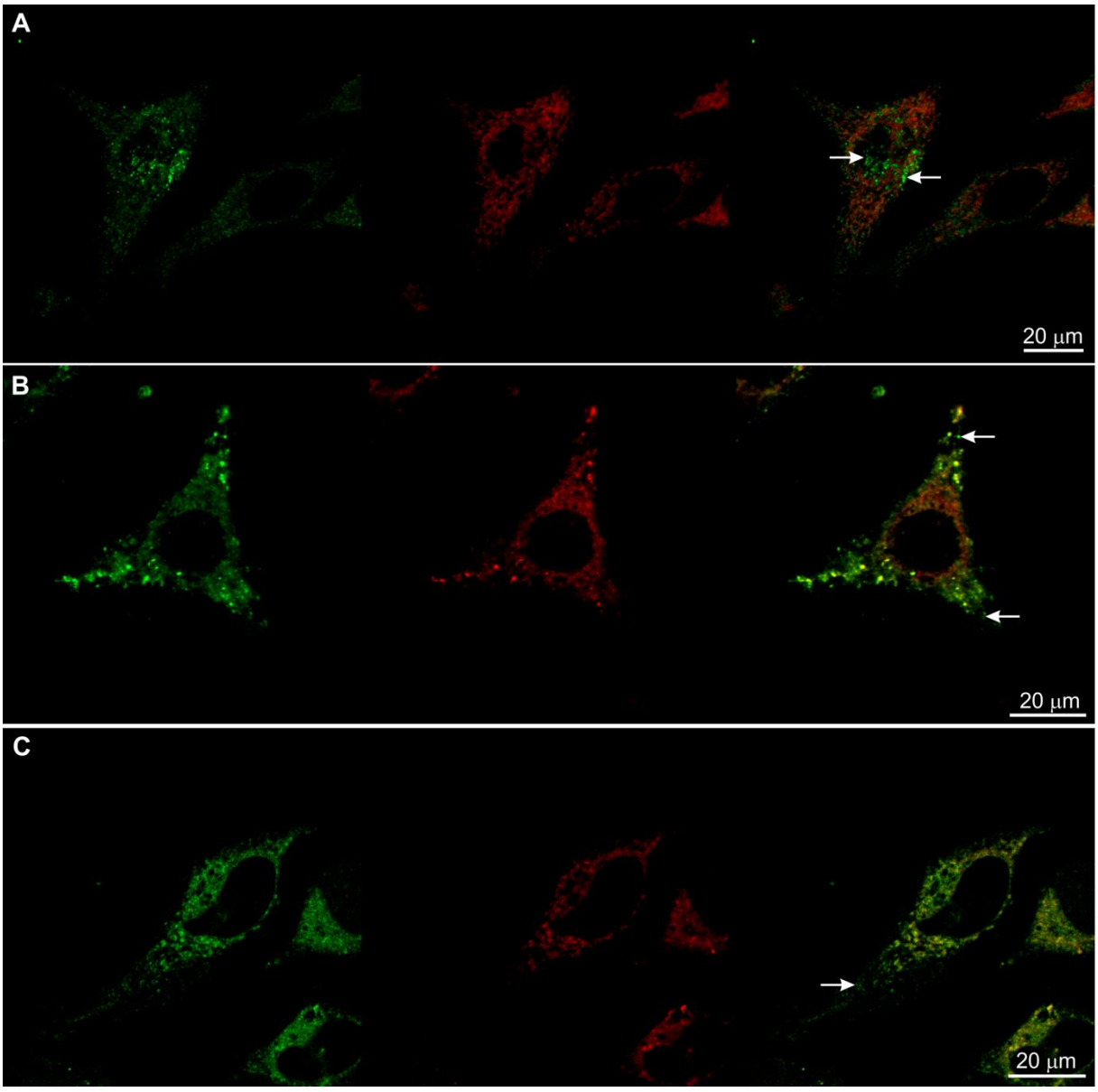

Figure S11 Co-localization of mitochondria-specific MitoTracker Red with pyrene (A); (*R*,*S*)-**2** (B); (*S*,*R*)-**2** (C) in HeLa cells. Compounds (green colour), mitochondria (red colour), merged images (yellow colour - colocalization). Arrows – compounds not cololocalized with mitochondria. Scale bare – 20 μm.

Table S1. Crystal data and structure refinement for **1**.

Identification code	**1**
Empirical formula	$C_{24}H_{18}N_2O_2$
Formula weight	366.40
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	7.4331(2)
b/Å	8.9471(3)
c/Å	26.8786(9)
α/°	90
β/°	94.896(3)
γ/°	90
Volume/Å^3	1781.03(9)
Z	4
ρ_{calc}g/cm^3	1.366
μ/mm^{-1}	0.701
F(000)	768.0
Crystal size/mm^3	0.19 × 0.11 × 0.08
Radiation	Cu$K\alpha$ (λ = 1.54184)
2Θ range for data collection/°	6.602 to 134.146
Index ranges	$-6 \leq h \leq 8$, $-10 \leq k \leq 10$, $-32 \leq l \leq 32$
Reflections collected	11956
Independent reflections	3178 [R_{int} = 0.0921, R_{sigma} = 0.0531]
Data/restraints/parameters	3178/1/258
Goodness-of-fit on F^2	1.073
Final R indexes [I>=2σ (I)]	R_1 = 0.0541, wR_2 = 0.1445
Final R indexes [all data]	R_1 = 0.0643, wR_2 = 0.1567
Largest diff. peak/hole / e Å^{-3}	0.29/-0.23

Table S2. Bond lengths for **1**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O(26)	C(21)	1.223(3)	C(4)	C(5)	1.439(3)
O(27)	C(23)	1.226(2)	C(4)	C(3)	1.349(3)
N(22)	C(23)	1.383(3)	C(23)	C(24)	1.457(3)
N(22)	C(21)	1.380(3)	C(1)	C(17)	1.474(3)
N(20)	C(21)	1.379(2)	C(1)	C(14)	1.403(3)
N(20)	C(25)	1.374(3)	C(5)	C(6)	1.390(3)
N(20)	C(19)	1.483(3)	C(13)	C(14)	1.379(3)
C(16)	C(15)	1.423(3)	C(17)	C(18)	1.332(3)
C(16)	C(5)	1.424(3)	C(24)	C(25)	1.338(3)
C(16)	C(9)	1.424(3)	C(24)	C(28)	1.498(3)
C(15)	C(12)	1.429(3)	C(9)	C(10)	1.442(3)
C(15)	C(2)	1.431(3)	C(9)	C(8)	1.391(3)
C(12)	C(13)	1.388(3)	C(6)	C(7)	1.390(3)
C(12)	C(11)	1.436(3)	C(11)	C(10)	1.344(3)
C(2)	C(1)	1.413(3)	C(19)	C(18)	1.479(3)
C(2)	C(3)	1.445(3)	C(7)	C(8)	1.387(3)

Table S3. Valence angles for **1**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(21)	N(22)	C(23)	127.65(16)	C(14)	C(1)	C(2)	118.69(18)
C(21)	N(20)	C(19)	117.77(17)	C(14)	C(1)	C(17)	119.95(18)
C(25)	N(20)	C(21)	120.85(17)	C(16)	C(5)	C(4)	117.64(18)
C(25)	N(20)	C(19)	121.27(17)	C(6)	C(5)	C(16)	119.86(18)
C(15)	C(16)	C(5)	120.41(17)	C(6)	C(5)	C(4)	122.50(19)
C(15)	C(16)	C(9)	120.51(19)	C(4)	C(3)	C(2)	121.76(18)
C(9)	C(16)	C(5)	119.05(18)	C(14)	C(13)	C(12)	120.95(19)
C(16)	C(15)	C(12)	119.43(18)	C(18)	C(17)	C(1)	126.1(2)
C(16)	C(15)	C(2)	120.65(18)	C(23)	C(24)	C(28)	118.74(18)
C(12)	C(15)	C(2)	119.84(18)	C(25)	C(24)	C(23)	117.78(19)
C(15)	C(12)	C(11)	118.48(19)	C(25)	C(24)	C(28)	123.47(18)
C(13)	C(12)	C(15)	118.93(18)	C(24)	C(25)	N(20)	124.59(18)
C(13)	C(12)	C(11)	122.6(2)	C(16)	C(9)	C(10)	118.50(19)
C(15)	C(2)	C(3)	117.21(17)	C(8)	C(9)	C(16)	119.2(2)
C(1)	C(2)	C(15)	119.41(18)	C(8)	C(9)	C(10)	122.29(19)
C(1)	C(2)	C(3)	123.35(17)	C(7)	C(6)	C(5)	120.4(2)
C(3)	C(4)	C(5)	122.11(19)	C(10)	C(11)	C(12)	122.1(2)
O(27)	C(23)	N(22)	120.69(18)	C(13)	C(14)	C(1)	122.02(19)
O(27)	C(23)	C(24)	124.8(2)	C(11)	C(10)	C(9)	120.89(19)
N(22)	C(23)	C(24)	114.51(17)	C(18)	C(19)	N(20)	112.11(18)
O(26)	C(21)	N(22)	122.77(18)	C(17)	C(18)	C(19)	123.2(2)
O(26)	C(21)	N(20)	122.72(19)	C(8)	C(7)	C(6)	120.3(2)
N(20)	C(21)	N(22)	114.50(18)	C(7)	C(8)	C(9)	121.1(2)
C(2)	C(1)	C(17)	121.32(18)				

Table S4 Torsion angles for **1**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(27)	C(23)	C(24)	C(25)	-176.3(2)	C(21)	N(22)	C(23)	C(24)	-4.3(3)
O(27)	C(23)	C(24)	C(28)	2.4(3)	C(21)	N(20)	C(25)	C(24)	-1.1(3)
N(22)	C(23)	C(24)	C(25)	3.4(3)	C(21)	N(20)	C(19)	C(18)	-144.76(19)
N(22)	C(23)	C(24)	C(28)	-177.88(18)	C(1)	C(2)	C(3)	C(4)	174.30(19)
N(20)	C(19)	C(18)	C(17)	-123.4(2)	C(1)	C(17)	C(18)	C(19)	-179.48(19)
C(16)	C(15)	C(12)	C(13)	176.32(18)	C(5)	C(16)	C(15)	C(12)	-178.15(17)
C(16)	C(15)	C(12)	C(11)	-1.8(3)	C(5)	C(16)	C(15)	C(2)	-1.4(3)
C(16)	C(15)	C(2)	C(1)	-173.49(17)	C(5)	C(16)	C(9)	C(10)	-179.65(17)
C(16)	C(15)	C(2)	C(3)	4.7(3)	C(5)	C(16)	C(9)	C(8)	1.0(3)
C(16)	C(5)	C(6)	C(7)	0.2(3)	C(5)	C(4)	C(3)	C(2)	-0.5(3)
C(16)	C(9)	C(10)	C(11)	-2.6(3)	C(5)	C(6)	C(7)	C(8)	1.3(3)
C(16)	C(9)	C(8)	C(7)	0.4(3)	C(3)	C(2)	C(1)	C(17)	-3.0(3)
C(15)	C(16)	C(5)	C(4)	-2.8(3)	C(3)	C(2)	C(1)	C(14)	179.35(18)
C(15)	C(16)	C(5)	C(6)	176.64(18)	C(3)	C(4)	C(5)	C(16)	3.8(3)
C(15)	C(16)	C(9)	C(10)	2.4(3)	C(3)	C(4)	C(5)	C(6)	-175.63(19)
C(15)	C(16)	C(9)	C(8)	-176.95(18)	C(13)	C(12)	C(11)	C(10)	-176.3(2)
C(15)	C(12)	C(13)	C(14)	-3.0(3)	C(17)	C(1)	C(14)	C(13)	-178.50(19)
C(15)	C(12)	C(11)	C(10)	1.7(3)	C(25)	N(20)	C(21)	O(26)	-179.3(2)
C(15)	C(2)	C(1)	C(17)	175.02(18)	C(25)	N(20)	C(21)	N(22)	0.5(3)
C(15)	C(2)	C(1)	C(14)	-2.6(3)	C(25)	N(20)	C(19)	C(18)	39.0(3)
C(15)	C(2)	C(3)	C(4)	-3.8(3)	C(9)	C(16)	C(15)	C(12)	-0.2(3)
C(12)	C(15)	C(2)	C(1)	3.2(3)	C(9)	C(16)	C(15)	C(2)	176.51(17)
C(12)	C(15)	C(2)	C(3)	-178.59(17)	C(9)	C(16)	C(5)	C(4)	179.20(17)
C(12)	C(13)	C(14)	C(1)	3.7(3)	C(9)	C(16)	C(5)	C(6)	-1.3(3)
C(12)	C(11)	C(10)	C(9)	0.5(3)	C(6)	C(7)	C(8)	C(9)	-1.6(4)
C(2)	C(15)	C(12)	C(13)	-0.5(3)	C(11)	C(12)	C(13)	C(14)	175.05(19)
C(2)	C(15)	C(12)	C(11)	-178.60(17)	C(14)	C(1)	C(17)	C(18)	-14.6(3)
C(2)	C(1)	C(17)	C(18)	167.8(2)	C(10)	C(9)	C(8)	C(7)	-178.9(2)
C(2)	C(1)	C(14)	C(13)	-0.8(3)	C(19)	N(20)	C(21)	O(26)	4.5(3)
C(4)	C(5)	C(6)	C(7)	179.66(19)	C(19)	N(20)	C(21)	N(22)	-175.78(18)
C(23)	N(22)	C(21)	O(26)	-177.9(2)	C(19)	N(20)	C(25)	C(24)	175.1(2)
C(23)	N(22)	C(21)	N(20)	2.4(3)	C(8)	C(9)	C(10)	C(11)	176.8(2)
C(23)	C(24)	C(25)	N(20)	-1.0(3)	C(28)	C(24)	C(25)	N(20)	-179.7(2)
C(21)	N(22)	C(23)	O(27)	175.43(19)					

Table S5. Gibbs free energies (G_{298})[a] and Boltzmann population (χ)[b] of the ten most stable conformers of the (*R*,*S*)-**2** , which span a range of 16 kJ/mol.

Conformer	G_{298} (Hartree)	ΔG_{298} (kJ/mol)	χ
A	-1337.35617172	0.0	0.59077
B	-1337.35571830	1.2	0.36547
C	-1337.35282057	8.8	0.01698
D	-1337.35224127	10.3	0.00919
E	-1337.35177466	11.5	0.00560
F	-1337.35172604	11.7	0.00532
G	-1337.35090196	13.8	0.00222
H	-1337.35068527	14.6	0.00176
I	-1337.35051127	14.9	0.00147
J	-1337.35029685	15.4	0.00117

[a] Gibbs free energy calculated at the B3LYP/6-311+G(2d,2p)//B3LYP/6-311G(d,p) level of theory. [b] Fractional populations of conformations were calculated from relative free energies, ΔG_{298}, using Boltzmann statistics.

Table S6. Gibbs free energies (G_{298})[a] and Boltzmann population (χ)[b] of the ten most stable conformers of the (*S*,*S*)-**2** , which span a range of 17 kJ/mol.

Conformer	G_{298} (Hartree)	ΔG_{298} (kJ/mol)	χ
a	-1337.35825981	0.0	0.95994
b	-1337.35391757	11.4	0.00965
c	-1337.35357423	12.3	0.00671
d	-1337.35352039	12.4	0.00634
e	-1337.35337937	12.8	0.00546
f	-1337.35310630	13.5	0.00409
g	-1337.35262466	14.8	0.00245
h	-1337.35257740	14.9	0.00233
i	-1337.35245534	15.2	0.00205
j	-1337.35172256	17.1	0.00094

[a] Gibbs free energy calculated at the B3LYP/6-311+G(2d,2p)//B3LYP/6-311G(d,p) level of theory. [b] Fractional populations of conformations were calculated from relative free energies, ΔG_{298}, using Boltzmann statistics.

Table S7. The PCC and MCC values for pyrene, (*R*,*S*)-**2** and (*S*,*R*)-**2** and MitoTracker® Deep Red FM in mitochondria of the HeLa cells. Means ± Standard Deviation (SD). Statistical significances of differences at $p \leq 0.05$.

Comp.	PCC	MCC
pyrene	0.414 ± 0.086	0.766 ± 0.035
(*R*,*S*)-**2**	0.539 ± 0.122	0.811 ± 0.053
(*S*,*R*)-**2**	0.571 ± 0.094	0.866 ± 0.015

B3LYP/6-311G(d,p) optimized coordinates

Conformer A (R,S)
C 5.13497500 2.34070900 -1.53735000
C 4.14599800 1.70821800 -2.28228800
C 3.28965200 0.77142400 -1.68567000
C 3.44015700 0.46962800 -0.30089000
C 4.46197700 1.12109200 0.45350600
C 5.29326300 2.05166000 -0.18558200
C 2.26714900 0.08875000 -2.42159700
C 2.57725000 -0.47922100 0.32623400
C 1.54640400 -1.12756200 -0.42485300
C 1.44092800 -0.81063100 -1.82567100
C 0.69494400 -2.05154800 0.22623300
C 0.90447200 -2.34259100 1.57633100
C 1.90987200 -1.72233600 2.30619500
C 2.75373600 -0.77868700 1.70979100
C 3.79263700 -0.11072100 2.44180700
C 4.60598900 0.79724000 1.84473500
H 5.38622100 1.29388500 2.41183600
H 3.91495100 -0.35091400 3.49277800
H 2.16607100 0.29934100 -3.48115900
H 5.78906300 3.06252300 -2.01329300
H 4.02945200 1.93399400 -3.33688200
H 6.06908500 2.54684100 0.38863300
H 0.69517600 -1.31247900 -2.42824500
H 0.26781300 -3.08100100 2.04506800
H 2.04903700 -1.97193800 3.35285800
C -0.44667000 -2.72531000 -0.50802000
C -1.65918700 -1.80034400 -0.78485000
H -1.33274000 -0.95251700 -1.40167300
C -2.27561300 -1.24493600 0.51228500
H -1.48796900 -1.02008600 1.22958800
H -2.93090900 -1.99617600 0.95398900
N -3.04265300 0.00455300 0.33163100
C -4.28225800 -0.06247100 -0.28095700
C -2.55210400 1.20630900 0.81446800
N -4.96813900 1.12911000 -0.31666400
C -3.21846400 2.37868400 0.75610800
H -1.56492300 1.14042300 1.25475000
C -4.54963800 2.39025400 0.15220800
O -4.73952600 -1.09621000 -0.75460200
O -5.26989200 3.36096600 0.03362100
C -2.67263600 3.67422500 1.27899800
H -2.61005600 4.41837100 0.48038600
H -3.33326200 4.09172200 2.04361300
H -1.67868600 3.54041600 1.70962600
O -2.56914000 -2.62561800 -1.50109500
H -3.46079700 -2.24782300 -1.40018000
H -5.87605400 1.09499500 -0.76316800
O -0.90142800 -3.84779600 0.23613800
H -1.69527500 -4.14384200 -0.23002900
H -0.09776100 -3.06311100 -1.49279700

Conformer B (R,S)

C 5.20946200 3.12596600 -0.19004900
C 3.82322700 3.19523300 -0.27670500
C 3.04559200 2.02896400 -0.25061800
C 3.68799100 0.76200800 -0.13398600
C 5.11179200 0.70234400 -0.04725900
C 5.84795900 1.89549100 -0.07667400
C 1.61587800 2.05806200 -0.34146400
C 2.91443900 -0.43754300 -0.10580500
C 1.48430900 -0.38178500 -0.18870300
C 0.87518200 0.91960000 -0.31167800
C 0.74641900 -1.58950400 -0.16402500
C 1.42635200 -2.80753300 -0.07056300
C 2.80874700 -2.86431000 0.01225800
C 3.57833400 -1.69434200 0.00111800
C 5.01069000 -1.72373800 0.08610700
C 5.74344600 -0.58123400 0.06464500
H 6.82571500 -0.62002800 0.12942200
H 5.49945300 -2.68895700 0.16710100
H 1.12484800 3.02069000 -0.43921900
H 5.79682600 4.03697100 -0.21217800
H 3.32982500 4.15709900 -0.36681200
H 6.92977100 1.84855100 -0.01102100
H -0.20140000 0.99566600 -0.37072200
H 0.84581100 -3.72042400 -0.09031700
H 3.30689900 -3.82571700 0.08001500
C -0.77337200 -1.62814800 -0.21296400
C -1.37420400 -1.54776000 1.22014900
H -0.98985000 -2.41683900 1.77354900
C -2.89851400 -1.66318800 1.24815500
H -3.22914100 -1.63905500 2.28782800
H -3.20313300 -2.61032200 0.80979900
N -3.60564000 -0.58830600 0.53283100
C -4.02258100 -0.82062300 -0.76785400
C -3.86906300 0.61495400 1.16729200
N -4.74846400 0.20831100 -1.32248200
C -4.56742400 1.62632900 0.60954400
H -3.44729200 0.68916700 2.16025400
C -5.07937800 1.45200000 -0.74778100
O -3.77207500 -1.85012000 -1.38418300
O -5.72758400 2.26529200 -1.37591100
C -4.84977000 2.92509000 1.30525400
H -4.44107300 3.76602100 0.73833400
H -5.92679700 3.09634000 1.38410600
H -4.41870800 2.93776100 2.30787700
O -1.05219200 -0.33490100 1.89225500
H -0.09351700 -0.23403900 1.90650800
H -5.06480700 0.05470700 -2.27173900
O -1.18730000 -2.84421100 -0.81561200
H -2.08249200 -2.69796700 -1.16427100
H -1.14207800 -0.77614800 -0.79370600

Conformer C (R,S)

C 6.63294500 -0.78346100 -0.95633600
C 5.68927300 -1.71615600 -0.54111900
C 4.41163600 -1.30771700 -0.13172700
C 4.08356300 0.07903000 -0.14400600
C 5.06238400 1.02878800 -0.56505900
C 6.32555600 0.57346300 -0.96798200
C 3.41732600 -2.23564100 0.31852300
C 2.78712700 0.51521300 0.26501200
C 1.79917500 -0.43513700 0.67510400
C 2.18011500 -1.82371100 0.70076700

C 0.51429900 0.02336500 1.05318900
C 0.26089500 1.39654100 1.07887100
C 1.22091000 2.32333500 0.69419800
C 2.48700300 1.90975700 0.26649000
C 3.49324900 2.84214600 -0.15701100
C 4.72034800 2.42301800 -0.55758400
H 5.46960100 3.13969500 -0.87687800
H 3.24850900 3.89910200 -0.14974400
H 3.67454900 -3.28895400 0.35806900
H 7.61611900 -1.11504400 -1.27059200
H 5.93543000 -2.77254100 -0.52864200
H 7.06807000 1.29592300 -1.28971300
H 1.47208800 -2.56213600 1.05327600
H -0.70382700 1.73167500 1.43518000
H 0.99264100 3.38347300 0.72834200
C -0.58927400 -0.94360300 1.43606300
C -1.16744600 -1.74976400 0.24845100
H -0.34883200 -2.32604700 -0.20227800
C -1.76571500 -0.91858500 -0.90920800
H -1.82569100 -1.55641500 -1.79189400
H -1.10644400 -0.08243600 -1.14238100
N -3.11993800 -0.38262800 -0.68775000
C -4.18747500 -1.24085600 -0.89763600
C -3.32498500 0.94780500 -0.37016900
N -5.42412100 -0.65021800 -0.78745900
C -4.54193800 1.52029500 -0.25614100
H -2.41687400 1.51267600 -0.21291700
C -5.72433500 0.69165900 -0.47878400
O -4.04495300 -2.42993200 -1.16008600
O -6.87916800 1.06373100 -0.41498800
C -4.75264800 2.96504900 0.08853000
H -5.32067900 3.47205300 -0.69615600
H -5.33475300 3.06306100 1.00889500
H -3.80096000 3.48257400 0.22203700
O -2.12327600 -2.61829100 0.84239000
H -2.73663300 -2.92618100 0.15438800
H -6.21492200 -1.26454500 -0.93528400
O -1.64254800 -0.23821100 2.08081600
H -2.34678600 -0.89013700 2.19300600
H -0.18454300 -1.69325700 2.13007500

Conformer D (R,S)

C -5.55682200 0.04863100 1.22157600
C -4.68416000 -0.98590700 1.53871900
C -3.43998800 -1.09327300 0.89992800
C -3.07269000 -0.12940900 -0.08326300
C -3.98083200 0.92290500 -0.40870600
C -5.21158400 0.99216700 0.25877300
C -2.52080700 -2.15440500 1.18330000
C -1.80901300 -0.21893400 -0.74186800
C -0.88689200 -1.25976600 -0.40574300
C -1.31219200 -2.23483100 0.56620200
C 0.37199400 -1.31040100 -1.05639200
C 0.64286600 -0.39579400 -2.07446500
C -0.25307700 0.61083500 -2.41152700
C -1.47718700 0.73629100 -1.74779700
C -2.41185200 1.78117400 -2.05715500
C -3.60388300 1.87472100 -1.41531800
H -4.29854400 2.67199300 -1.65762400
H -2.14052200 2.50192000 -2.82125500
H -2.81301000 -2.91229900 1.90273200
H -6.51466800 0.11902000 1.72457800
H -4.96062100 -1.72362200 2.28447900
H -5.89961400 1.79402300 0.01284600
H -0.66781300 -3.07160700 0.80204500
H 1.57354900 -0.47328500 -2.61912100
H -0.00420800 1.31013300 -3.20269400
C 1.38970600 -2.39212700 -0.69897000
C 1.96271400 -2.32724500 0.74546100
H 1.15864400 -2.10961100 1.45001100
C 3.12673700 -1.34343400 0.98833200
H 3.96648900 -1.61369500 0.35039900
H 3.44430900 -1.47359200 2.02388300
N 2.85415700 0.08291300 0.76834000
C 3.26283800 0.65267400 -0.42540400
C 2.25679500 0.84485600 1.75815200
N 3.05514500 2.00877600 -0.50801300
C 2.03273100 2.17151700 1.66266600
H 1.97432300 0.28542900 2.64168400
C 2.45452300 2.85813300 0.44167400
O 3.76797800 0.00725500 -1.33744500
O 2.32823000 4.04415600 0.21341900
C 1.37715700 2.98764200 2.73621700
H 2.03255100 3.80107100 3.05863100
H 0.46126500 3.45263400 2.36166100
H 1.12640300 2.37380300 3.60322600
O 2.45876600 -3.61471800 1.10196900
H 2.98590600 -3.91813100 0.35082200
H 3.34537300 2.44200800 -1.37541000
O 2.45446700 -2.54156100 -1.62546600
H 2.98007600 -1.72235500 -1.64534400
H 0.86696500 -3.35284800 -0.73401200

Conformer E (R,S)

C -5.90541400 2.60851900 -0.39056300
C -4.58642900 2.94191000 -0.10449100
C -3.60786200 1.94543200 0.02581100
C -3.97741900 0.57932700 -0.13786900
C -5.33375000 0.24769300 -0.43269000
C -6.27712000 1.27738000 -0.55321600
C -2.23850400 2.24685100 0.32035400
C -2.99649400 -0.44992900 -0.01109100
C -1.63746300 -0.12210500 0.28514100
C -1.30334600 1.26912500 0.44711400
C -0.67841200 -1.16216100 0.39760900
C -1.08513900 -2.48412100 0.20071500
C -2.40610300 -2.80602500 -0.08260800
C -3.38280200 -1.81125400 -0.19010800
C -4.75491200 -2.11517800 -0.48457100
C -5.68592900 -1.13426200 -0.59926700
H -6.71873400 -1.37973500 -0.82327800
H -5.03273900 -3.15551500 -0.61695300
H -1.95527600 3.28694600 0.44496000
H -6.64967900 3.39072500 -0.48876300
H -4.30160700 3.98123700 0.02005300
H -7.30788300 1.02451700 -0.77781600
H -0.28659400 1.53495400 0.69979900
H -0.35282400 -3.27886100 0.22566600

H -2.68568000 -3.84318200 -0.23349000
C 0.76437400 -0.81496300 0.73029000
C 1.75702800 -1.99172000 0.68273700
H 1.40937900 -2.76679900 1.38554300
C 3.14644800 -1.59236100 1.19557100
H 3.79841400 -2.46659700 1.16617800
H 3.05979400 -1.25409200 2.22578700
N 3.80813400 -0.52180400 0.42800700
C 4.50382500 -0.88199900 -0.71559200
C 3.79334600 0.78722100 0.88016000
N 5.19283400 0.15005900 -1.30903400
C 4.45699700 1.79843200 0.28029300
H 3.17832100 0.94360000 1.75767300
C 5.24536900 1.50189600 -0.91481400
O 4.51043600 -2.02383400 -1.15789800
O 5.89823900 2.30328900 -1.55325600
C 4.43284200 3.21591000 0.77077700
H 5.44372600 3.56341000 1.00073500
H 4.04048800 3.88627400 0.00115000
H 3.81672400 3.31334900 1.66645500
O 1.77957900 -2.50526700 -0.63636900
H 2.70089600 -2.63433700 -0.91348600
H 5.70561600 -0.09289600 -2.14728300
O 0.86390400 -0.17494300 2.02301000
H 0.13404800 -0.49106600 2.56597000
H 1.12077800 -0.07539200 0.00626000

Conformer F (R,S)

C -5.63431600 -2.69998600 0.47208000
C -4.57831500 -2.80617000 -0.42623500
C -3.65239100 -1.76295400 -0.56836100
C -3.79903300 -0.58436700 0.21869600
C -4.88620900 -0.48637200 1.13853800
C -5.78802700 -1.55457900 1.24624900
C -2.55303200 -1.83320900 -1.48370900
C -2.86560200 0.48843600 0.08955700
C -1.77231000 0.39395800 -0.83235000
C -1.66310500 -0.81450300 -1.60937600
C -0.86534900 1.47731000 -0.93754800
C -1.05561200 2.60926600 -0.13693300
C -2.11058700 2.70262000 0.75703600
C -3.03141900 1.65650300 0.89063200
C -4.13415000 1.72745300 1.80662600
C -5.01980300 0.70587500 1.92568600
H -5.84809000 0.77404000 2.62298700
H -4.24449800 2.62407000 2.40732600
H -2.43847500 -2.72839900 -2.08577900
H -6.34215800 -3.51515700 0.57048300
H -4.46140400 -3.70154600 -1.02724800
H -6.61364400 -1.47825500 1.94573400
H -0.85153000 -0.92644100 -2.31554900
H -0.35499400 3.42826200 -0.22390400
H -2.22809500 3.59414100 1.36381400
C 0.31891400 1.45875800 -1.88898400
C 1.69506600 1.18995700 -1.23152100
H 2.40504500 1.03603500 -2.05546800
C 1.70578400 -0.04525700 -0.33955900
H 1.26089600 -0.89101100 -0.85986800
H 1.13395000 0.15360800 0.56829600
N 3.06339300 -0.44817700 0.04179100
C 3.67304100 -1.45352600 -0.70604600
C 3.71890900 0.17696000 1.08584800
N 4.94443200 -1.77451600 -0.26920800
C 4.96581600 -0.14245700 1.49407400
H 3.15045000 0.97026400 1.55228200
C 5.67729700 -1.20486600 0.78746600
O 3.13855000 -2.00104400 -1.65231600
O 6.79963300 -1.60014800 1.04197800
C 5.66759400 0.53785200 2.63243800
H 5.93804100 -0.18256100 3.40947900
H 6.60088800 0.99738700 2.29525600
H 5.03892000 1.31174800 3.07703500
O 2.10642300 2.29432500 -0.43818300
H 2.05302700 3.07035300 -1.00973700
H 5.40904400 -2.50627600 -0.79120200
O 0.50877300 2.72958900 -2.53191400
H -0.34430700 3.03356800 -2.85825000
H 0.17614600 0.69304500 -2.65611900

Conformer G (R,S)

C 5.70047600 -2.51055300 0.66880300
C 4.64808400 -2.27050100 1.54498000
C 3.70122600 -1.27348100 1.26953900
C 3.82422000 -0.50210300 0.07771000
C 4.91027300 -0.75463300 -0.81333000
C 5.83203300 -1.76231500 -0.49677400
C 2.60814100 -0.98978700 2.15070600
C 2.86969200 0.51566600 -0.22238600
C 1.77614000 0.76715300 0.66471300
C 1.69626100 -0.02439900 1.86403500
C 0.84114500 1.77623900 0.33630700
C 1.01889500 2.52575500 -0.82818700
C 2.08083100 2.28673000 -1.68916700
C 3.01654300 1.28309200 -1.41534700
C 4.11991400 1.00802700 -2.29149400
C 5.02261200 0.03536500 -2.00656300
H 5.85025100 -0.16179400 -2.67972900
H 4.21649700 1.60012100 -3.19547700
H 2.52032100 -1.56628700 3.06567100
H 6.42382600 -3.28577800 0.89504600
H 4.55019500 -2.85587700 2.45301400
H 6.65608500 -1.95454900 -1.17561800
H 0.89441300 0.15666300 2.56815000
H 0.31352200 3.31680000 -1.04371700
H 2.19277700 2.88579300 -2.58668300
C -0.35453400 2.06241700 1.22468900
C -1.50743600 1.03021900 1.10106600
H -1.16970900 0.04315400 1.42852700
C -2.04934400 0.91360700 -0.32268400
H -1.25891900 0.56365400 -0.98310600
H -2.38994900 1.89096400 -0.66510100
N -3.17158400 -0.02382500 -0.42164000
C -2.87125800 -1.37167400 -0.60963800
C -4.47456400 0.41055500 -0.27842000
N -3.98809000 -2.18286900 -0.69640300
C -5.55546500 -0.39569200 -0.35069600
H -4.57209000 1.47246400 -0.09586400
C -5.34222200 -1.82280500 -0.58104200

O -1.73418900 -1.79420800 -0.68885600
O -6.21517700 -2.66579300 -0.66932200
C -6.96770800 0.08994200 -0.20564600
H -7.55200700 -0.13957500 -1.10103600
H -7.46774100 -0.40987400 0.62864100
H -6.99943100 1.16799000 -0.03553100
O -2.59694600 1.49409400 1.92088800
H -2.47377600 1.17050500 2.81827300
H -3.79739700 -3.16580400 -0.84289500
O -0.87250300 3.35366800 0.92888900
H -1.70317700 3.41390900 1.41841800
H -0.02919100 2.04134300 2.27546800

Conformer H (R,S)

C -5.12189200 3.27983900 -0.02461200
C -3.74852900 3.27248600 -0.23982000
C -3.03485400 2.06550600 -0.27630800
C -3.73196900 0.83695300 -0.09044300
C -5.14242000 0.85576300 0.12789700
C -5.81326500 2.08613200 0.15722500
C -1.62177600 2.01580000 -0.50560100
C -3.02338700 -0.40266700 -0.12154700
C -1.60793900 -0.42164200 -0.33625700
C -0.94239600 0.83971600 -0.53878300
C -0.92922400 -1.66639800 -0.34322000
C -1.66552600 -2.84138300 -0.15874400
C -3.03960900 -2.82928300 0.04217800
C -3.74246900 -1.62082700 0.06984300
C -5.16167700 -1.57148400 0.28267900
C -5.83001000 -0.39095600 0.31111600
H -6.90247200 -0.36959300 0.47381500
H -5.69193400 -2.50766200 0.42214600
H -1.09386800 2.94971700 -0.66907500
H -5.65841000 4.22164300 0.00048200
H -3.21434600 4.20557300 -0.38397700
H -6.88513100 2.09835700 0.32387500
H 0.11387500 0.83073000 -0.76152500
H -1.14405700 -3.79238600 -0.18085100
H -3.57664700 -3.76225600 0.17506100
C 0.58186100 -1.80140300 -0.46814400
C 1.28522000 -1.44691900 0.87317800
H 1.12600800 -0.38037600 1.08395900
C 2.79815600 -1.74178600 0.88697000
H 3.02730000 -2.62918200 0.29819500
H 3.07054700 -1.94338300 1.92358800
N 3.65741700 -0.65155600 0.40503900
C 4.11913800 -0.68130200 -0.90000600
C 4.01958000 0.36942200 1.26759500
N 4.97001700 0.35051100 -1.22460100
C 4.84010500 1.38858500 0.93861300
H 3.58856300 0.28812900 2.25811500
C 5.39210100 1.42243500 -0.41561800
O 3.79919100 -1.54654000 -1.70628400
O 6.14488300 2.26844200 -0.85473300
C 5.22763800 2.48727600 1.88289100
H 6.31270900 2.52122300 2.01251300
H 4.93055100 3.46153600 1.48539200
H 4.76209000 2.35225800 2.86089800
O 0.77799000 -2.25400200 1.93174400
H -0.18522600 -2.21255600 1.90232100
H 5.31451500 0.34466600 -2.17652000
O 1.07045900 -1.01396500 -1.54305800
H 1.93873700 -1.36074900 -1.80714900
H 0.79383000 -2.86304900 -0.65217500

Conformer I (R,S)

C -6.89156100 -1.26116900 0.46745000
C -5.76588500 -2.05054400 0.25812700
C -4.50882300 -1.46450600 0.05368700
C -4.38948200 -0.04431100 0.06170500
C -5.55148800 0.75654100 0.27713400
C -6.78783400 0.12579400 0.47732500
C -3.32599800 -2.24278200 -0.16640200
C -3.11861300 0.57232200 -0.14516400
C -1.94903600 -0.22846700 -0.36017700
C -2.11424200 -1.66097700 -0.36142200
C -0.70512300 0.41375500 -0.57281100
C -0.64576000 1.81089000 -0.57226700
C -1.77360500 2.58739500 -0.35814900
C -3.02352700 1.99454000 -0.14025000
C -4.20834000 2.77416000 0.07929600
C -5.41478200 2.18495900 0.27935100
H -6.30157300 2.78810800 0.44320300
H -4.11750500 3.85529000 0.07985800
H -3.41459400 -3.32415300 -0.17549800
H -7.85670100 -1.72981400 0.62337700
H -5.85195300 -3.13188500 0.25070300
H -7.66998700 0.73579500 0.64022900
H -1.24817200 -2.29206000 -0.50185200
H 0.30701800 2.28264600 -0.77295700
H -1.69459100 3.66938400 -0.36761000
C 0.59107100 -0.35123700 -0.79639900
C 1.30968100 -0.64290200 0.55235200
H 1.60557900 0.32664000 0.97853200
C 2.56282700 -1.53358800 0.41392700
H 2.44890200 -2.24612600 -0.40213300
H 2.65487300 -2.09449300 1.34443900
N 3.82641700 -0.81448400 0.20257800
C 4.32022400 -0.67903300 -1.08367000
C 4.51643400 -0.30549800 1.28990500
N 5.54000400 -0.04662600 -1.15973200
C 5.70314200 0.33094500 1.20780000
H 4.02413200 -0.46324000 2.24191000
C 6.31002100 0.49491100 -0.11306100
O 3.72682600 -1.08247800 -2.07690600
O 7.37180700 1.03738400 -0.34436800
C 6.44317300 0.87484300 2.39332500
H 7.43559700 0.42268700 2.47064200
H 6.59853500 1.95229000 2.29119700
H 5.89927200 0.68662600 3.32081200
O 0.47965200 -1.36690400 1.45465400
H -0.35736100 -0.89639600 1.54398900
H 5.91414200 0.06212800 -2.09408900
O 1.43198400 0.43061800 -1.62979500
H 2.10903800 -0.14844700 -2.01636000
H 0.37340300 -1.31243100 -1.27664300

Conformer J (R,S)

C 6.55568100 -1.99032600 -0.41061500
C 5.43492900 -2.43104600 0.28476000
C 4.30246700 -1.61376100 0.40889200
C 4.30610500 -0.31870100 -0.18610100
C 5.46208000 0.12395000 -0.89740100
C 6.57114700 -0.72845600 -0.99561900
C 3.12897200 -2.03068700 1.11762400
C 3.16350900 0.52946900 -0.07022200
C 1.99989600 0.08764600 0.64065700
C 2.03792100 -1.22886800 1.22683000
C 0.88602500 0.95605000 0.74640500
C 0.94975400 2.22351900 0.16163200
C 2.06966500 2.65121400 -0.53441400
C 3.19144400 1.82377300 -0.66729300
C 4.36712000 2.24197000 -1.37639600
C 5.45059200 1.43185200 -1.48787300
H 6.33219500 1.76263600 -2.02675800
H 4.37101100 3.23019600 -1.82417900
H 3.12523300 -3.01516700 1.57392900
H 7.42370100 -2.63418600 -0.49699400
H 5.42798400 -3.41578400 0.73979900
H 7.44902900 -0.39044000 -1.53590400
H 1.16916400 -1.59751500 1.75299400
H 0.10651100 2.88931700 0.29123200
H 2.08700300 3.64282400 -0.97427100
C -0.39899400 0.56672200 1.47174300
C -1.38643400 -0.15251500 0.51738700
H -1.68295200 0.58427300 -0.24132000
C -2.64033000 -0.62877400 1.27019200
H -2.54085700 -1.69676700 1.46090700
H -2.73866700 -0.11072500 2.22323200
N -3.87851900 -0.41526500 0.51213400
C -4.34904900 0.88619600 0.45151000
C -4.51462200 -1.44495100 -0.15582100
N -5.51657100 1.03452600 -0.26085600
C -5.65140800 -1.29092900 -0.86761800
H -4.02336600 -2.40564400 -0.06616900
C -6.24534700 0.04318200 -0.94900100
O -3.77122000 1.82479300 0.98535000
O -7.26444500 0.33197700 -1.54369600
C -6.34385000 -2.41145800 -1.58521200
H -7.36661800 -2.53286800 -1.21827100
H -6.41933300 -2.19868100 -2.65499800
H -5.81066700 -3.35481700 -1.45379400
O -0.84024800 -1.30735200 -0.10621400
H -0.07076000 -1.04110800 -0.62327400
H -5.88284200 1.97687500 -0.31132400
O -1.02507900 1.70989500 2.03833200
H -1.90835100 1.84365400 1.65691300
H -0.15749900 -0.11583400 2.29484900

Conformer a (S,S)

C -4.93749600 3.30001500 0.09318200
C -3.54721800 3.29923100 0.08273000
C -2.83328900 2.09522500 -0.00382500
C -3.54583200 0.86318600 -0.08200300
C -4.97334200 0.87579000 -0.07356300
C -5.64386300 2.10378500 0.01589300
C -1.40143200 2.05218000 -0.02635400
C -2.83813400 -0.37338500 -0.16895600
C -1.40789100 -0.39147600 -0.17112600
C -0.72658100 0.87517700 -0.10481200
C -0.73367200 -1.63141300 -0.25182200
C -1.47341500 -2.80942600 -0.35090400
C -2.86120300 -2.79673700 -0.35392500
C -3.56967500 -1.59430600 -0.25595100
C -5.00451500 -1.55025100 -0.24732000
C -5.67531600 -0.37358900 -0.15865200
H -6.76009500 -0.35728400 -0.15195600
H -5.54624800 -2.48800000 -0.31351000
H -0.85651500 2.98967900 0.01476600
H -5.47529600 4.23901300 0.16077200
H -3.00089200 4.23471500 0.14052800
H -6.72867200 2.11212600 0.02333100
H 0.35527600 0.89950300 -0.13129900
H -0.94162500 -3.74590300 -0.44793300
H -3.40899300 -3.72992300 -0.43215600
C 0.78228400 -1.70711400 -0.20562800
H 1.19577200 -0.91236000 -0.83396900
C 1.32157700 -1.55170600 1.24114700
H 0.90920300 -0.64713300 1.69590000
C 2.86373000 -1.51734100 1.30924100
H 3.25724800 -2.45941200 0.93021000
H 3.15853000 -1.42828100 2.35530000
N 3.50908200 -0.43088100 0.55495000
C 3.91440300 -0.68158800 -0.74814500
C 3.74706900 0.79440100 1.15500000
N 4.56294500 0.37218900 -1.35202400
C 4.37386400 1.82710600 0.55367900
H 3.38716700 0.86710100 2.17424500
C 4.84365500 1.64612300 -0.82009800
O 3.71430100 -1.74361800 -1.32371600
O 5.42485300 2.47784500 -1.48691500
C 4.62882300 3.14914500 1.21434800
H 5.70014100 3.36480600 1.24690700
H 4.16480300 3.96092000 0.64773600
H 4.23750500 3.16549600 2.23317900
O 1.22210500 -2.97335200 -0.69397700
H 2.10742600 -2.82756600 -1.06509900
O 0.89776800 -2.63937100 2.04211100
H 0.98808400 -3.42475900 1.48383400
H 4.86557900 0.20788200 -2.30412900

Conformer b (S,S)

C 5.39052700 -2.46057900 -1.46946600
C 4.36036000 -1.88633000 -2.20619800
C 3.49690000 -0.95044600 -1.61951300
C 3.68110900 -0.58743200 -0.25359200
C 4.74394300 -1.18083700 0.49240900
C 5.58179600 -2.11313200 -0.13628200
C 2.43093200 -0.32850400 -2.34734700
C 2.81147800 0.36262300 0.36294100
C 1.73896800 0.95563000 -0.38023600
C 1.59947500 0.57246100 -1.76211100
C 0.88596800 1.88228900 0.26407000
C 1.12757400 2.22328900 1.59844100
C 2.16791500 1.65764300 2.31870600

C 3.02069300 0.71688000 1.72808500
C 4.09939700 0.10678200 2.45202000
C 4.92110100 -0.80006100 1.86459200
H 5.73206600 -1.25267600 2.42535600
H 4.24527500 0.39015900 3.48909700
H 2.30123000 -0.58638900 -3.39331300
H 6.05022000 -3.18241000 -1.93757500
H 4.21712700 -2.15776800 -3.24667000
H 6.38875400 -2.56315000 0.43215000
H 0.82002200 1.02385600 -2.36124400
H 0.49180300 2.96983700 2.05670600
H 2.33070900 1.94631700 3.35175700
C -0.31634400 2.51318600 -0.41221700
H -0.20935900 2.48514000 -1.50414600
C -1.64844600 1.79838500 -0.04675200
H -1.70377000 1.74721300 1.04703600
C -1.73896400 0.38617900 -0.62742200
H -0.91672500 -0.22396900 -0.25478800
H -1.66666800 0.42180800 -1.71578300
N -2.99661400 -0.30318800 -0.29653600
C -4.09834500 -0.05663000 -1.10162800
C -3.06894000 -1.17805800 0.77243400
N -5.21745700 -0.78226100 -0.76699800
C -4.17662200 -1.87168000 1.10879600
H -2.14810000 -1.27425000 1.33497700
C -5.37928800 -1.69406800 0.29506900
O -4.07543700 0.73616400 -2.03462800
O -6.44404500 -2.25089400 0.47111200
C -4.24730400 -2.82091000 2.26783200
H -5.01810300 -2.50844200 2.97753900
H -4.52193700 -3.82388600 1.93034500
H -3.29181900 -2.87760300 2.79255200
O -0.42656800 3.86422300 0.00990400
H -1.33321000 4.12290600 -0.20992200
O -2.72886800 2.62869100 -0.46431400
H -3.13944700 2.25087100 -1.25952600
H -6.03351900 -0.61497500 -1.34219300

Conformer c (S,S)

C -5.33784800 3.08707900 0.23780300
C -4.12314400 3.07371100 -0.43781900
C -3.35571900 1.90152400 -0.50738600
C -3.83264800 0.71612000 0.12363700
C -5.08214700 0.74032200 0.81315200
C -5.81378200 1.93500600 0.85667200
C -2.10196800 1.84618600 -1.19760200
C -3.06604200 -0.48648700 0.06592300
C -1.81098200 -0.51248000 -0.61954600
C -1.36789000 0.70340300 -1.25175000
C -1.07055200 -1.71923600 -0.65884000
C -1.59077100 -2.86006000 -0.04770600
C -2.80858200 -2.83965300 0.62097700
C -3.56374600 -1.66509100 0.69825100
C -4.82472000 -1.61083300 1.38319600
C -5.54877200 -0.46439500 1.43965300
H -6.49981100 -0.43947300 1.96110000
H -5.18963600 -2.51559500 1.85790600
H -1.73925600 2.74466000 -1.68539000
H -5.91925900 4.00102100 0.28266200
H -3.75689800 3.97385800 -0.91966000
H -6.76310400 1.95289000 1.38135900
H -0.42825600 0.72169900 -1.78842300
H -1.04328000 -3.78984900 -0.13125300
H -3.18628500 -3.74550500 1.08326900
C 0.29355600 -1.78852700 -1.34259300
H 0.22820100 -1.31155400 -2.32426400
C 1.37867100 -1.07118000 -0.49953300
H 1.02380500 -0.08744200 -0.18311800
C 2.67872200 -0.90001800 -1.28077800
H 2.46850900 -0.42187000 -2.23613100
H 3.12942200 -1.87456300 -1.46929700
N 3.65159400 -0.06315800 -0.57461500
C 3.56858700 1.31344300 -0.77087200
C 4.56900100 -0.61560500 0.29838100
N 4.51745000 2.03240800 -0.07054800
C 5.48047900 0.10132400 0.98981500
H 4.49755300 -1.69082500 0.39620100
C 5.49662500 1.55292900 0.81900200
O 2.73769900 1.83265600 -1.49372900
O 6.25822600 2.32409900 1.37072400
C 6.48003300 -0.50680500 1.92893000
H 7.50097200 -0.27201700 1.61543900
H 6.36286200 -0.10105600 2.93758200
H 6.36974100 -1.59199300 1.97474500
O 0.72706000 -3.11905300 -1.58693200
H 1.12839500 -3.41870000 -0.75918000
O 1.68871500 -1.88177900 0.64400300
H 0.97582700 -1.78525400 1.28557100
H 4.48543500 3.03537800 -0.20131500

Conformer d (S,S)

C -7.11210700 -0.46191700 -0.82899400
C -6.18820200 -1.49746200 -0.74849200
C -4.84623900 -1.23716300 -0.43339100
C -4.43419500 0.10537900 -0.19443600
C -5.39079200 1.16094100 -0.27655800
C -6.72036200 0.85300700 -0.59552700
C -3.86514500 -2.27624900 -0.33219500
C -3.07294200 0.39214600 0.12474700
C -2.11147200 -0.66130100 0.20209000
C -2.56827900 -2.00653400 -0.02813200
C -0.75875700 -0.34941800 0.49928400
C -0.40411300 0.98232700 0.73840000
C -1.34090000 2.00708400 0.67323000
C -2.67837400 1.74226500 0.36449100
C -3.66363100 2.78345600 0.27788500
C -4.95651900 2.50704900 -0.02877100
H -5.68902200 3.30485300 -0.09209800
H -3.34794100 3.80470000 0.46273300
H -4.18083100 -3.30111200 -0.49769300
H -8.14539100 -0.67973800 -1.07437900
H -6.49936600 -2.52084200 -0.92910200
H -7.44705900 1.65591100 -0.65909100
H -1.86771700 -2.82281200 0.08095900
H 0.62228700 1.25158900 0.95365800
H -1.02676400 3.02912900 0.85422900
C 0.26124300 -1.47118800 0.56628000
H 0.14803500 -2.12591800 -0.30372500

C 1.74940800 -1.07711800 0.63235400
H 1.90412100 -0.37716100 1.46417400
C 2.27034300 -0.44632100 -0.65719300
H 1.65650400 0.40012700 -0.95561900
H 2.25326200 -1.19513400 -1.45154700
N 3.64971600 0.03465500 -0.52044200
C 3.83130100 1.33295200 -0.05687800
C 4.72245000 -0.80002700 -0.77152600
N 5.15567200 1.71072100 0.03703400
C 6.01411700 -0.42387600 -0.65815600
H 4.44371500 -1.80456500 -1.06036800
C 6.30451400 0.94177300 -0.22763100
O 2.90718100 2.07190100 0.23735600
O 7.41265700 1.42281500 -0.08610200
C 7.17327800 -1.33330700 -0.94131400
H 7.80806100 -0.92025500 -1.73014200
H 7.80650100 -1.44272700 -0.05657100
H 6.83191200 -2.32330800 -1.24965100
O 0.00675100 -2.34562600 1.69361900
H -0.30069500 -1.79474500 2.42289700
O 2.51794000 -2.25486600 0.84693400
H 2.03321000 -2.76397000 1.51124300
H 5.31547500 2.65555200 0.36209800

Conformer e (S,S)

C 4.96471400 2.13021200 -1.88984000
C 4.00711000 1.33230600 -2.50569300
C 3.18323300 0.48689700 -1.74830500
C 3.33534000 0.45033400 -0.33206600
C 4.32485900 1.26994000 0.28961500
C 5.12415800 2.10058900 -0.50803300
C 2.19621400 -0.36166800 -2.34702200
C 2.50357200 -0.40064800 0.45786000
C 1.50421400 -1.21566300 -0.16461900
C 1.40202300 -1.17281100 -1.60089800
C 0.67341700 -2.02740400 0.64717600
C 0.88704600 -2.04484900 2.02867000
C 1.86245300 -1.26711200 2.63790900
C 2.67827100 -0.42586500 1.87423900
C 3.68634900 0.40422500 2.47127900
C 4.47053600 1.21488300 1.71662400
H 5.22747000 1.83720200 2.18234700
H 3.80828700 0.36832400 3.54879100
H 2.10106700 -0.35758100 -3.42794800
H 5.59320100 2.77819100 -2.49030500
H 3.88998800 1.35542700 -3.58387400
H 5.87480500 2.72371600 -0.03362700
H 0.70482300 -1.84179300 -2.08219400
H 0.27228400 -2.69470800 2.64328500
H 1.99999800 -1.31166900 3.71298900
C -0.48532100 -2.84742200 0.10944000
H -0.85811100 -3.47615700 0.93225600
C -1.68860400 -1.99005600 -0.36249900
H -1.33415800 -1.24697200 -1.08924400
C -2.36369900 -1.25094700 0.80541600
H -1.62007900 -0.96619000 1.54872700
H -3.08402700 -1.92266100 1.27819100
N -3.05808100 -0.00510600 0.42424100
C -4.22490800 -0.09801200 -0.31572200
C -2.57331900 1.22516700 0.83756200
N -4.85279000 1.10395100 -0.54571000
C -3.18134200 2.40425000 0.59011300
H -1.64141100 1.17598800 1.38690000
C -4.43801200 2.39322000 -0.15692700
O -4.67047100 -1.15992200 -0.73397500
O -5.10186700 3.36735900 -0.44859200
C -2.64195500 3.73010900 1.03827700
H -2.46297600 4.38462900 0.18098500
H -3.36335600 4.24453000 1.67881200
H -1.70638400 3.61207600 1.58783200
O -0.06617200 -3.68414300 -0.95974800
H -0.88357100 -4.00217700 -1.36890200
O -2.56637500 -2.91754100 -0.98516000
H -3.43345700 -2.48752700 -1.08428400
H -5.70731500 1.05137600 -1.08599200

Conformer f (S,S)

C -5.21417400 3.21583400 -0.01337700
C -3.82846900 3.28201800 -0.10400000
C -3.05796300 2.11119600 -0.15298200
C -3.70829400 0.84372300 -0.10942500
C -5.13174000 0.78731800 -0.01865400
C -5.86008800 1.98416600 0.02886700
C -1.62919400 2.13699000 -0.25469600
C -2.94229500 -0.35996000 -0.15705100
C -1.51489700 -0.30724500 -0.24208300
C -0.89805400 0.99232900 -0.29632500
C -0.78204400 -1.51679000 -0.28553900
C -1.46488500 -2.73610100 -0.25686500
C -2.85047500 -2.79012700 -0.17572800
C -3.61310200 -1.61849800 -0.11875700
C -5.04589000 -1.64371100 -0.02920300
C -5.77101800 -0.49754300 0.01976200
H -6.85318400 -0.53338200 0.08771300
H -5.54052500 -2.60892400 -0.00186100
H -1.13303400 3.10066200 -0.30515000
H -5.79593300 4.12994000 0.02350800
H -3.32967200 4.24471000 -0.13902800
H -6.94176900 1.94015100 0.09847000
H 0.17789500 1.06518300 -0.38522200
H -0.88443700 -3.64644700 -0.32602100
H -3.35261000 -3.75166800 -0.15999900
C 0.73895100 -1.54292600 -0.31030400
H 1.10076400 -0.72023500 -0.93933800
C 1.29977600 -1.31613400 1.12781600
H 1.05426100 -0.28499000 1.42680100
C 2.81718000 -1.51723700 1.22353400
H 3.07613900 -2.49309500 0.81874400
H 3.09578100 -1.50313800 2.27771500
N 3.61036800 -0.49229900 0.52835600
C 4.02568100 -0.72989200 -0.77348000
C 3.96499700 0.67252500 1.18867600
N 4.81026800 0.26816800 -1.30871900
C 4.72333100 1.65217300 0.65408700
H 3.58265000 0.74248700 2.19981100
C 5.21399100 1.47820400 -0.71293400
O 3.72758400 -1.73315400 -1.40734700
O 5.90545900 2.26693200 -1.32507900

C 5.10302500 2.90682700 1.38277000
H 6.19013900 2.99929400 1.45307400
H 4.74955100 3.78991800 0.84364400
H 4.68480300 2.92199900 2.39090900
O 1.17253900 -2.77885700 -0.84363100
H 2.07321500 -2.64031600 -1.17808400
O 0.78171000 -2.24054400 2.06844200
H -0.16568900 -2.33122800 1.91176000
H 5.12275700 0.11014900 -2.25862900

Conformer g (S,S)

C 5.43271000 -2.47943000 1.24394800
C 4.37518000 -2.00949000 2.01425600
C 3.49696900 -1.03942100 1.50983800
C 3.69632600 -0.53381200 0.19307200
C 4.78670500 -1.02112800 -0.58817300
C 5.63824900 -1.99181500 -0.04273500
C 2.40201200 -0.52399100 2.27549500
C 2.81109400 0.45129200 -0.34043800
C 1.71165500 0.93389600 0.43935900
C 1.55630400 0.41297900 1.77321200
C 0.84192200 1.90097900 -0.12528000
C 1.09739500 2.37391800 -1.41644200
C 2.16237400 1.91188600 -2.17521300
C 3.03183200 0.94377900 -1.66153500
C 4.13880200 0.43804200 -2.42273200
C 4.97553000 -0.50025600 -1.91202100
H 5.80607900 -0.87546800 -2.50056500
H 4.29064100 0.82385000 -3.42519100
H 2.25849500 -0.89622400 3.28455700
H 6.10142400 -3.23106700 1.64789800
H 4.21899000 -2.39221900 3.01714100
H 6.46478400 -2.36293300 -0.63925400
H 0.76394400 0.80571000 2.39244600
H 0.43804700 3.12632000 -1.83761500
H 2.32717000 2.30067000 -3.17416700
C -0.39353300 2.43871200 0.57271200
H -0.77192600 3.28604200 -0.01469100
C -1.56629400 1.44436800 0.71371900
H -1.21970700 0.55646900 1.25672900
C -2.11899200 1.00712200 -0.63950700
H -1.32698600 0.56563500 -1.24048100
H -2.52885800 1.87523900 -1.16301800
N -3.17623300 -0.00255200 -0.52297400
C -2.83987900 -1.33079200 -0.78775000
C -4.46256500 0.36027600 -0.16728400
N -3.90610600 -2.20421800 -0.67252200
C -5.49142600 -0.50756500 -0.06067000
H -4.58074500 1.41412800 0.04340300
C -5.23857700 -1.92154600 -0.32591100
O -1.72047100 -1.69132500 -1.09409800
O -6.06353600 -2.81442800 -0.26761100
C -6.88385600 -0.10177700 0.32387100
H -7.59872700 -0.37174600 -0.45848900
H -7.20402900 -0.62178400 1.23108000
H -6.94680200 0.97402500 0.49874200
O -0.15733100 2.88861400 1.91941500
H 0.56463000 3.52507300 1.90607000
O -2.62467300 2.07786300 1.42326500
H -2.22196400 2.49702200 2.19403000
H -3.68962500 -3.17451200 -0.86065800

Conformer h (S,S)

C 5.61316500 2.92122800 -0.24567200
C 4.38588500 2.99670100 0.40280700
C 3.54074200 1.87911800 0.46766600
C 3.95071200 0.65735400 -0.14039300
C 5.21096200 0.59177800 -0.80714800
C 6.02267000 1.73387700 -0.84480200
C 2.26702600 1.91837000 1.12153000
C 3.10526900 -0.49114200 -0.08575500
C 1.84436600 -0.42956600 0.58629900
C 1.46096100 0.82556800 1.17874000
C 1.03367700 -1.58860500 0.63542000
C 1.46498600 -2.75428200 0.00122800
C 2.68611100 -2.81761500 -0.65619300
C 3.52828400 -1.70221200 -0.71049600
C 4.80033300 -1.73785200 -1.37524500
C 5.60413200 -0.64520400 -1.42059000
H 6.56270400 -0.68804000 -1.92685500
H 5.10736900 -2.66616300 -1.84539300
H 1.94569700 2.85102000 1.57287100
H 6.25516800 3.79385100 -0.28694500
H 4.06943600 3.92548300 0.86520000
H 6.98071100 1.68316600 -1.35117900
H 0.50065100 0.92016000 1.66882000
H 0.83008400 -3.63065300 0.02904100
H 2.99348100 -3.73973800 -1.13775500
C -0.30768600 -1.57468900 1.34918800
H -0.23255000 -0.95186200 2.24739700
C -1.45690700 -1.02389100 0.47711400
H -1.12942400 -0.09555300 0.00666800
C -2.69965600 -0.72901500 1.33300700
H -2.42667800 -0.12983000 2.20111400
H -3.14527800 -1.66319100 1.67826100
N -3.71252500 0.02665100 0.59245200
C -3.62392200 1.41639700 0.63154200
C -4.66715200 -0.61442700 -0.17233000
N -4.60657100 2.05631700 -0.09824900
C -5.61266400 0.02414800 -0.89451100
H -4.59711600 -1.69378400 -0.15761400
C -5.62520000 1.48509400 -0.88282700
O -2.76343600 2.01131000 1.25494100
O -6.41522200 2.19366700 -1.47761500
C -6.65089100 -0.68146700 -1.71598000
H -7.65795600 -0.41018500 -1.38727500
H -6.57715300 -0.39132600 -2.76768400
H -6.54038400 -1.76537300 -1.64577700
O -0.74961900 -2.88695800 1.72642700
H -0.04901200 -3.31449300 2.22949400
O -1.76899800 -1.92226600 -0.57641300
H -1.75937400 -2.80566200 -0.18466800
H -4.56972000 3.06739300 -0.08147200

Conformer i (S,S)

C 5.80636600 2.77190200 -0.47095900
C 4.61240700 2.94770400 0.21923200

C 3.71030000 1.88462800 0.37107300
C 4.02715900 0.61412000 -0.19116600
C 5.25438000 0.44505700 -0.89994500
C 6.12550200 1.53612000 -1.02512100
C 2.47055200 2.02604600 1.07472200
C 3.12241000 -0.48040800 -0.04830700
C 1.89275900 -0.31402800 0.66446000
C 1.60744700 0.98571500 1.21468200
C 1.02047100 -1.42087700 0.79771100
C 1.36371400 -2.64236300 0.21063700
C 2.55484900 -2.80622300 -0.48410800
C 3.45351200 -1.74267200 -0.62593000
C 4.69500400 -1.88265300 -1.33330400
C 5.55481400 -0.84054500 -1.46352800
H 6.48929700 -0.96249700 -2.00093500
H 4.93289600 -2.84900400 -1.76522400
H 2.22557900 2.99336000 1.50040900
H 6.49330000 3.60354200 -0.57931800
H 4.36738100 3.91355900 0.64775300
H 7.05833600 1.40674900 -1.56347200
H 0.68122000 1.14952400 1.74974600
H 0.67865400 -3.47361500 0.32082100
H 2.79637600 -3.76809900 -0.92382000
C -0.31268200 -1.31486800 1.52465500
H -0.22821600 -0.58850900 2.34216300
C -1.43196000 -0.80265500 0.59113300
H -1.17665900 0.22737400 0.31231000
C -2.78085500 -0.79104100 1.30677900
H -2.68283100 -0.30937900 2.27796300
H -3.11679900 -1.81693700 1.45037300
N -3.80430600 -0.05956400 0.55391600
C -3.91153700 1.30970100 0.78070300
C -4.58389000 -0.69951400 -0.38945800
N -4.90114600 1.92039600 0.03393900
C -5.53650300 -0.08633500 -1.12482100
H -4.36252300 -1.75210000 -0.50613400
C -5.75278000 1.34458600 -0.92633100
O -3.20187900 1.91314700 1.56501700
O -6.57313800 2.02772400 -1.51054200
C -6.38497400 -0.79170100 -2.14159300
H -7.44618600 -0.70132000 -1.89340600
H -6.25757400 -0.34547100 -3.13181700
H -6.12941100 -1.85140100 -2.20173000
O -0.74637000 -2.56803100 2.05092400
H -0.07846100 -2.87554800 2.67236700
O -1.59913100 -1.60817500 -0.56812800
H -0.79379500 -1.55669300 -1.09424900
H -5.00707700 2.91513500 0.18575100

Conformer j (S,S)

C 6.73238700 -1.14268900 -0.62517900
C 5.65770700 -1.98612600 -0.36840200
C 4.38551700 -1.46245800 -0.09498600
C 4.19842000 -0.05023300 -0.08108600
C 5.30931000 0.80657100 -0.34481800
C 6.56214100 0.23823200 -0.61376200
C 3.25548100 -2.29714100 0.18207900
C 2.90993300 0.50246800 0.19230700
C 1.79296200 -0.35461300 0.45291200
C 2.02807000 -1.77667200 0.44512200
C 0.52405400 0.22887000 0.70824900
C 0.39980200 1.62155000 0.71152700
C 1.48223400 2.45336800 0.46254500
C 2.74778200 1.92048000 0.19856100
C 3.88395000 2.75718700 -0.06711000
C 5.10584000 2.22735300 -0.32685200
H 5.95453500 2.87279600 -0.52735400
H 3.74108300 3.83255500 -0.05694500
H 3.39790200 -3.37293600 0.18565500
H 7.70945400 -1.56290000 -0.83536300
H 5.79470100 -3.06222600 -0.37699500
H 7.40456900 0.89143500 -0.81495700
H 1.21060100 -2.43896300 0.68646000
H -0.57653600 2.05909500 0.87985000
H 1.34718200 3.52952600 0.46749800
C -0.73535700 -0.58597400 0.95797800
H -1.51571800 0.09212400 1.31776400
C -1.26531200 -1.31522000 -0.30650700
H -0.40202900 -1.68491000 -0.87573800
C -2.05197000 -0.40247500 -1.25808400
H -2.20881900 -0.93889600 -2.19631800
H -1.48667000 0.50361100 -1.46903100
N -3.37230700 0.00518400 -0.75487000
C -3.54872200 1.30916300 -0.30409300
C -4.43335800 -0.88484700 -0.80500300
N -4.84323400 1.59927500 0.07855100
C -5.69495000 -0.58497100 -0.42976500
H -4.16422200 -1.86988300 -1.15738600
C -5.97264700 0.76051700 0.06310200
O -2.64979700 2.13091500 -0.24522000
O -7.05309600 1.17626900 0.43635500
C -6.83254500 -1.56161000 -0.48944400
H -7.26758300 -1.71270700 0.50243600
H -7.63613800 -1.18452700 -1.12806100
H -6.50278800 -2.52780600 -0.87578500
O -0.55457400 -1.62854500 1.93670800
H -0.21646100 -1.23349200 2.74641400
O -2.10794400 -2.40066000 0.04608000
H -1.80202300 -2.71565900 0.90741100
H -4.99332700 2.54433500 0.40754300