

Electronic Supplementary Information for:

**Theoretical study on an intriguing excited-state proton transfer
process induced by weakened intramolecular hydrogen bonds**

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Table S1. Calculated S₀- and S₁-stated salient geometrical parameters, such as bond lengths (Å) and bond angles (°), of Anti and Syn in ACN, DCM, and CYH solvents.

		Anti		Syn	
		S ₀	S ₁	S ₀	S ₁
ACN	N ₁ -H ₂	1.02	1.01	1.02	1.01
		8	6	8	6
	H ₂ ···O ₃	1.78	2.26	1.78	2.50
		3	5	5	6
	δ(N ₁ -H ₂ ···O ₃)	139.	96.0	139.	83.1
		6		5	
	N ₄ -H ₅	1.02	1.03	1.02	1.02
		8	0	8	8
	H ₅ ···O ₆	1.78	1.76	1.78	1.78
		4	4	4	5
	δ(N ₄ -H ₅ ···O ₆)	139.	140.	139.	139.
		5	1	5	4
DCM	N ₁ -H ₂	1.02	1.01	1.02	1.01
		9	6	9	6
	H ₂ ···O ₃	1.77	2.44	1.77	2.40
		6	8	7	4
	δ(N ₁ -H ₂ ···O ₃)	139.	86.6	139.	88.6
		9		7	
	N ₄ -H ₅	1.02	1.02	1.02	1.02
		9	9	9	9
	H ₅ ···O ₆	1.77	1.78	1.77	1.77
		8	1	7	2
	δ(N ₄ -H ₅ ···O ₆)	139.	139.	139.	139.
		7	6	8	9
CYH	N ₁ -H ₂	1.03	1.01	1.03	1.01
		0	7	0	6
	H ₂ ···O ₃	1.76	2.25	1.76	2.27
		4	9	8	8
	δ(N ₁ -H ₂ ···O ₃)	140.	96.4	140.	95.4
		3		0	
	N ₄ -H ₅	1.03	1.03	1.03	1.03
		0	0	0	0
	H ₅ ···O ₆	1.76	1.76	1.76	1.76
		7	5	8	3
	δ(N ₄ -H ₅ ···O ₆)	140.	140.	140.	140.
		0	1	1	2

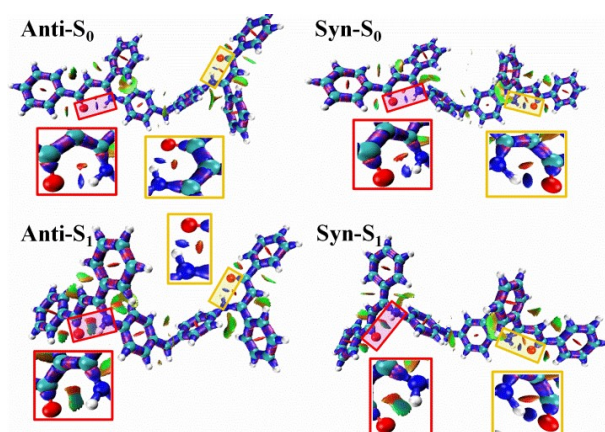


Fig. S1. IRI isosurfaces of Anti and Syn in S_0 and S_1 states obtained from DCM solvent. (Red box: IHB $N_1-H_2 \cdots O_3$, Yellow box: IHB $N_4-H_5 \cdots O_6$)

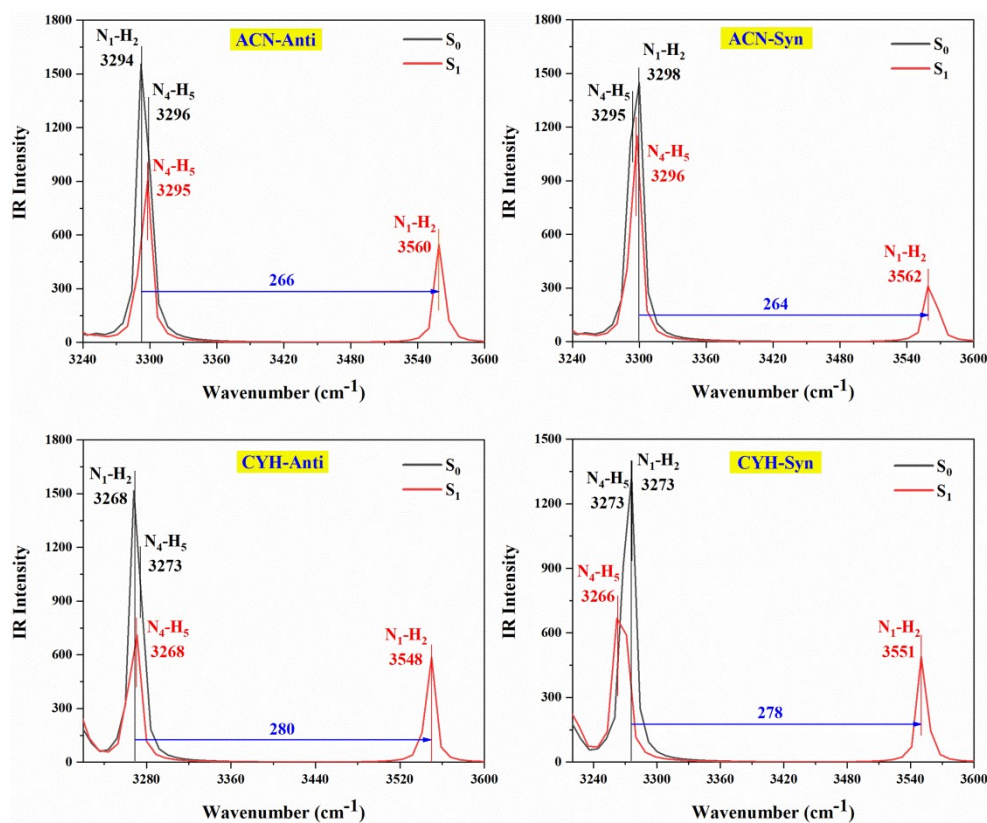


Fig. S2. Simulated S₀- and S₁-stated IR vibrational spectra of optimized Anti and Syn structures at the region of N₁-H₂ and N₄-H₅ stretching bands in ACN and CYH solvents.

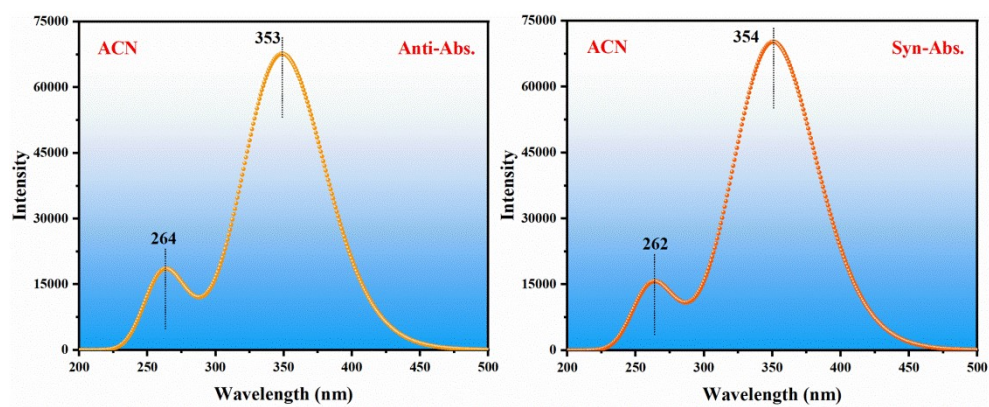


Fig. S3(a). Simulated absorption spectra for Anti and Syn in ACN based on the TD-DFT/M06-2X/def2-TZVP theoretical level.

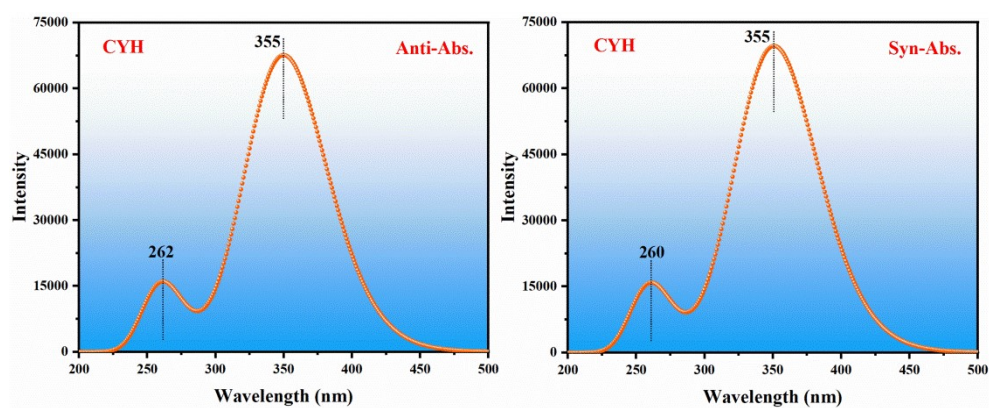


Fig. S3(b). Simulated absorption spectra of Anti and Syn in CYH based on the TD-DFT/M06-2X/def2-TZVP theoretical level.

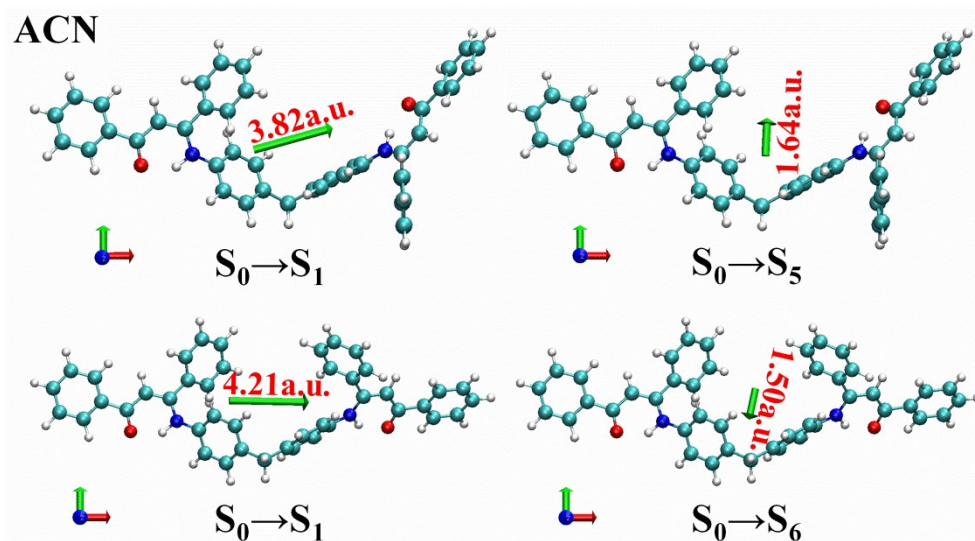


Fig. S4(a). Calculated dipole moments of Anti and Syn in ACN solvent.

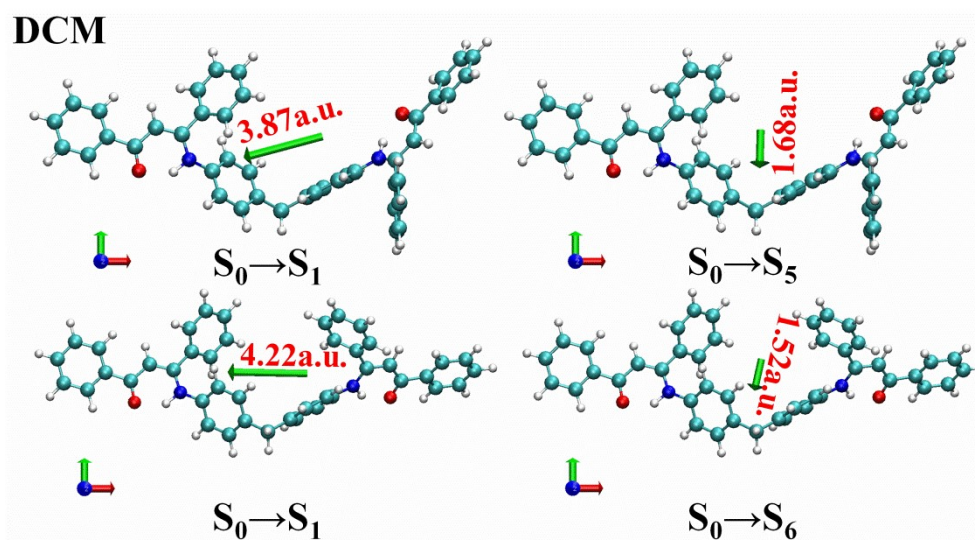


Fig. S4(b). Calculated dipole moments of Anti and Syn in DCM solvent.

CYH

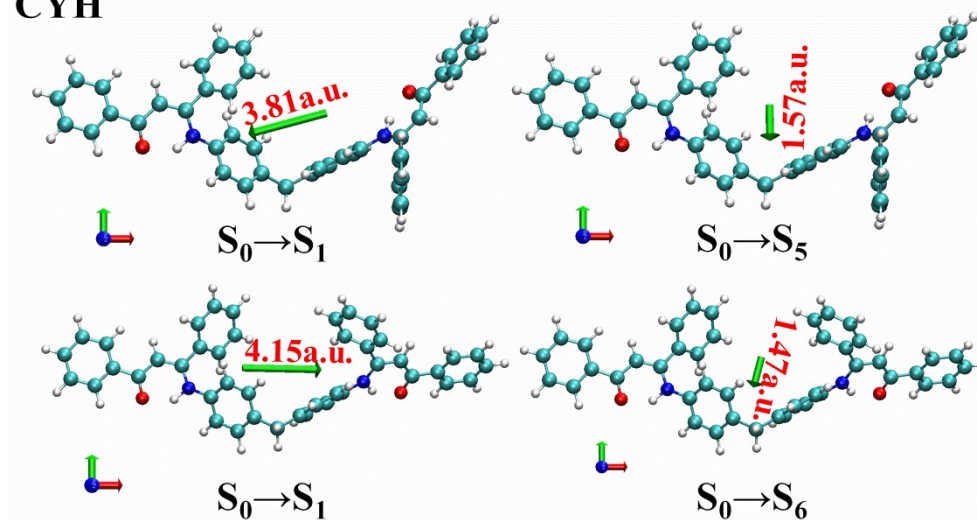


Fig. S4(c). Calculated dipole moments of Anti and Syn in CYH solvent.

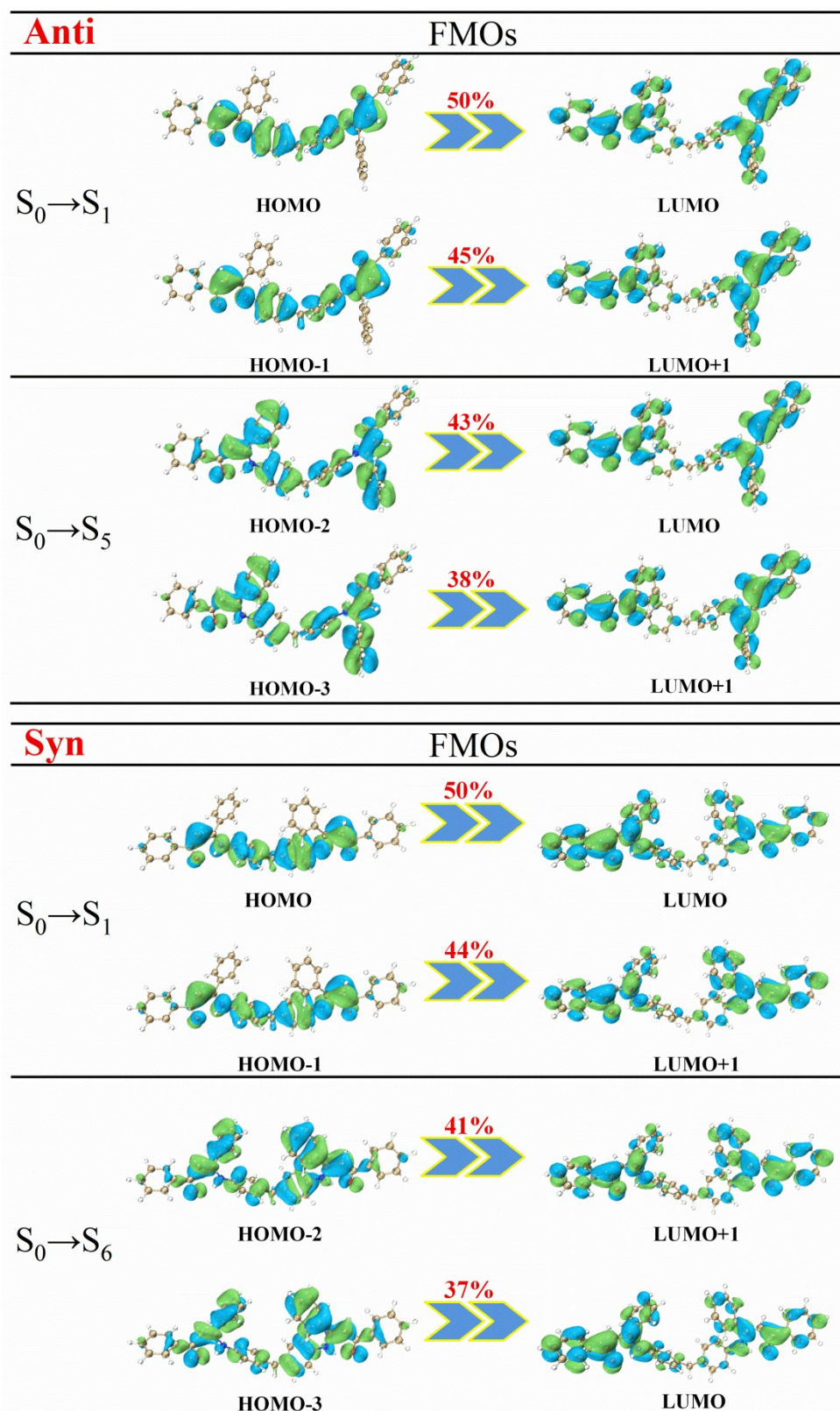


Fig. S5(a). Related FMOs of Anti and Syn in ACN solvent.

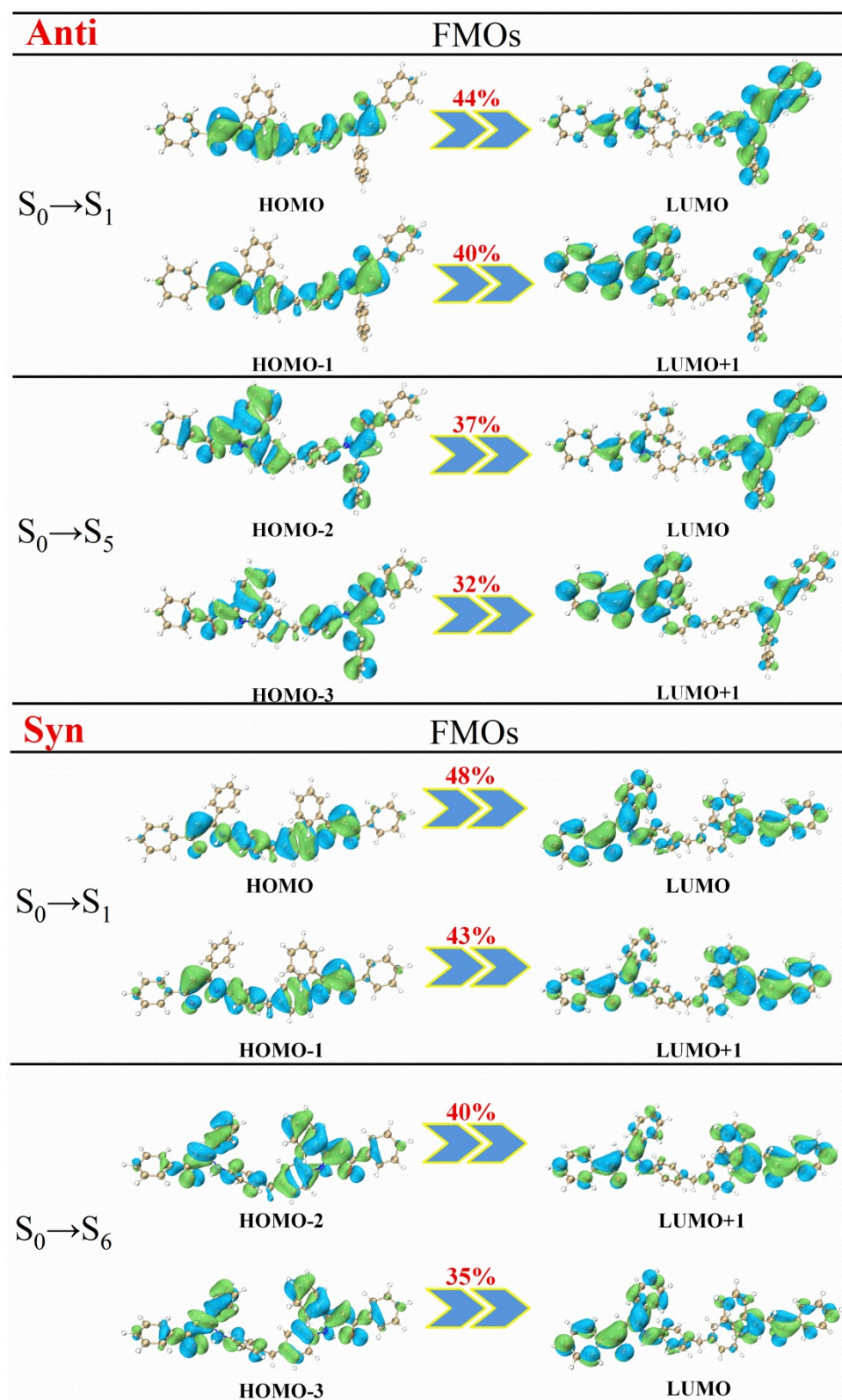


Fig. S5(b). Related FMOs of Anti and Syn in CYH solvent.

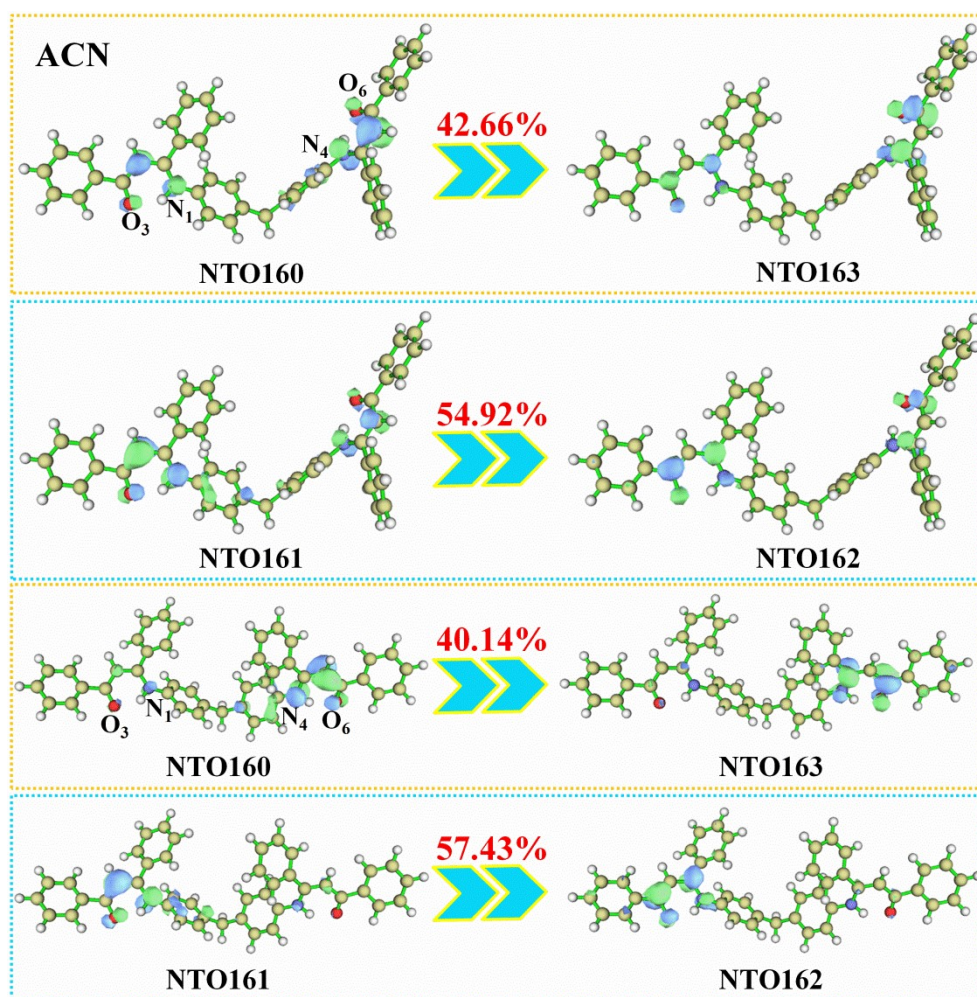


Fig. S6(a). Related NTO orbitals in ACN solvent.

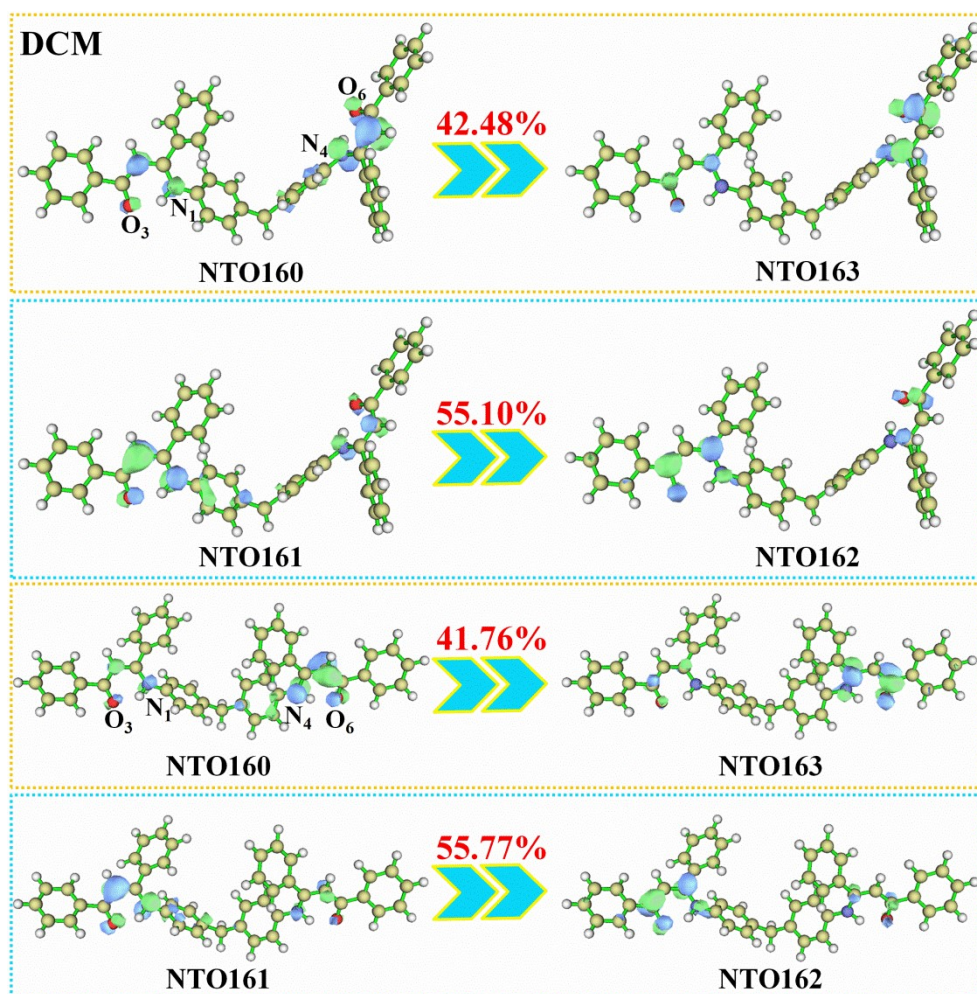


Fig. S6(b). Related NTO orbitals in DCM solvent.

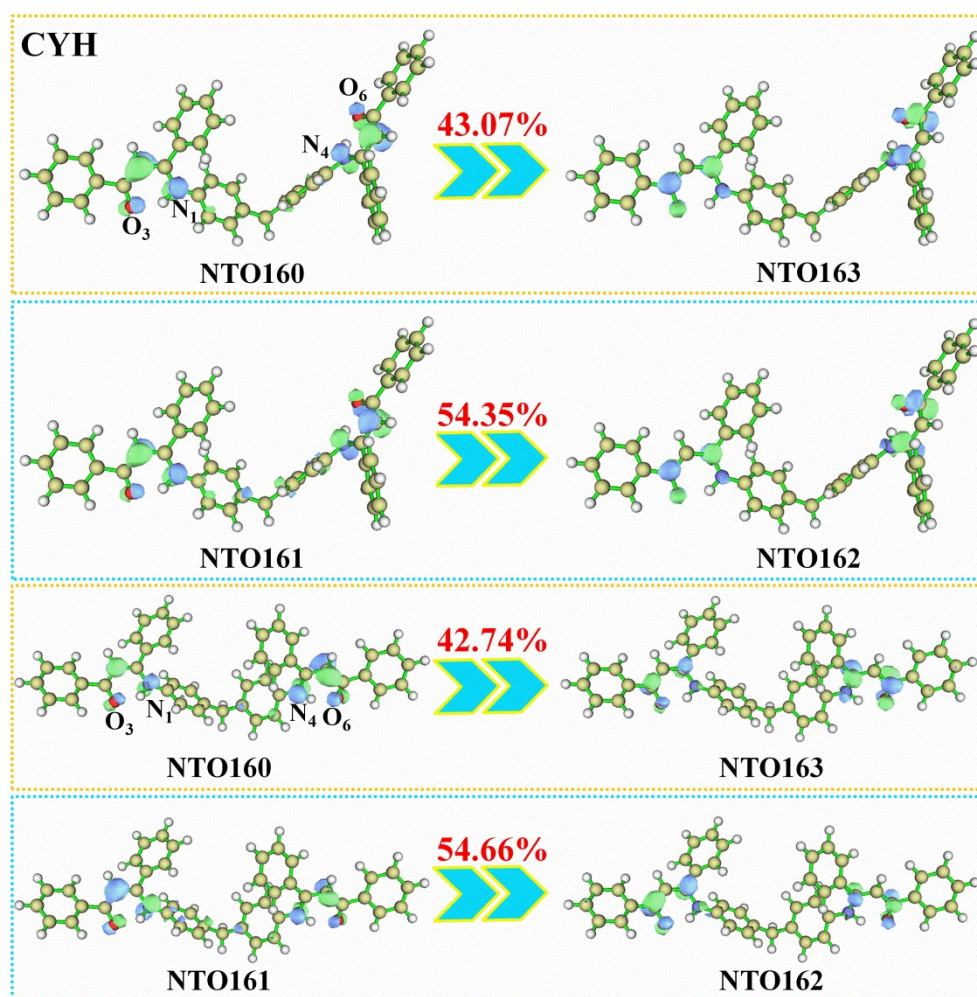


Fig. S6(c). Related NTO orbitals in CYH solvent.

Table S2. Calculated NBO charges (a.u.) of proton donor N₁ and N₄ atoms and proton acceptor O₃ and O₆ atoms for Anti and Syn in ACN, DCM, and CYH solvents.

			N ₁	O ₃	N ₄	O ₆
ACN	Anti	S ₀	-0.584	-0.668	-0.584	-0.668
		S ₁	-0.401	-0.694	-0.584	-0.665
	Syn	S ₀	-0.584	-0.668	-0.584	-0.668
		S ₁	-0.400	-0.693	-0.585	-0.665
DCM	Anti	S ₀	-0.584	-0.664	-0.584	-0.664
		S ₁	-0.403	-0.693	-0.585	-0.660
	Syn	S ₀	-0.585	-0.659	-0.585	-0.659
		S ₁	-0.406	-0.692	-0.587	-0.655
CYH	Anti	S ₀	-0.585	-0.649	-0.586	-0.649
		S ₁	-0.416	-0.692	-0.589	-0.644
	Syn	S ₀	-0.587	-0.649	-0.586	-0.649
		S ₁	-0.416	-0.691	-0.589	-0.645

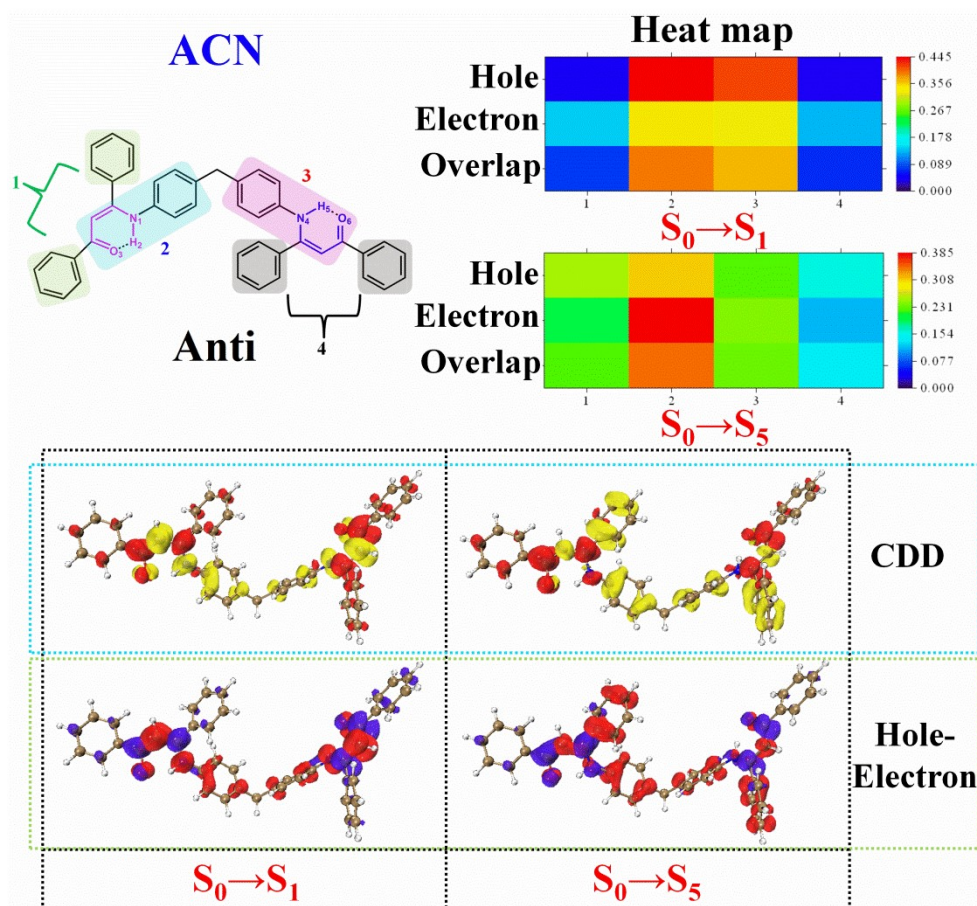


Fig. S7(a). Calculated hole-electron distribution, charge density difference (CDD) maps, and heat maps concerning fragment contribution to hole/electron of Anti in ACN solvent. In CDD maps, the regions with increasing electron density from the ground state to the excited state are shown in red, whereas the regions with decreasing density are shown in yellow. In hole-electron distribution maps, red refers to the hole, whereas violet represents the electron.

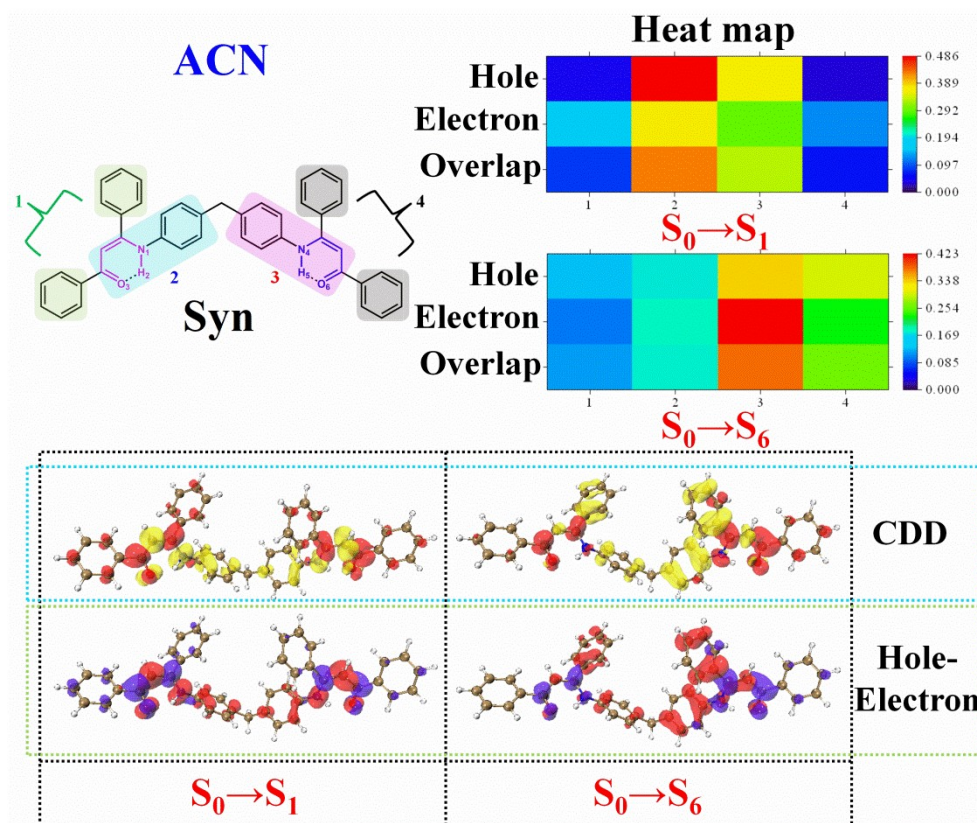


Fig. S7(b). Calculated hole-electron distribution, charge density difference (CDD) maps, and heat maps concerning fragment contribution to hole/electron of Syn in ACN solvent. In CDD maps, the regions with increasing electron density from the ground state to the excited state are shown in red, whereas the regions with decreasing density are shown in yellow. In hole-electron distribution maps, red refers to the hole, whereas violet represents the electron.

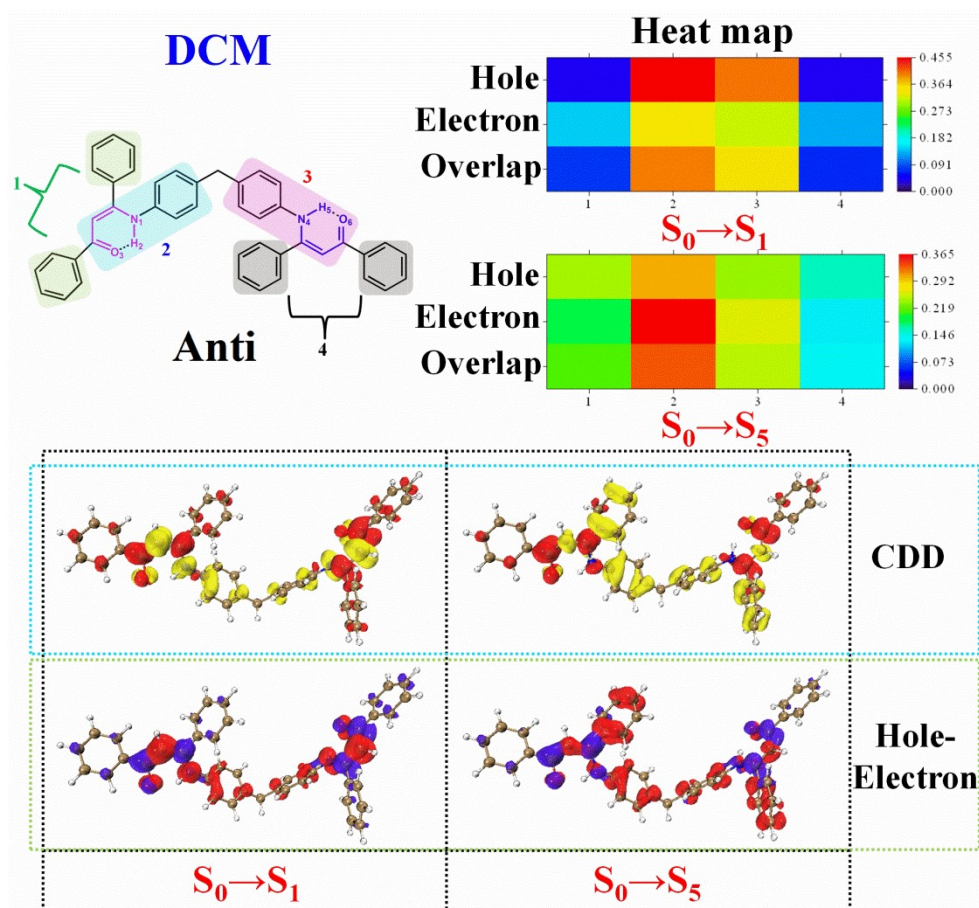


Fig. S7(c). Calculated hole-electron distribution, charge density difference (CDD) maps, and heat maps concerning fragment contribution to hole/electron of Anti in DCM solvent. In CDD maps, the regions with increasing electron density from the ground state to the excited state are shown in red, whereas the regions with decreasing density are shown in yellow. In hole-electron distribution maps, red refers to the hole, whereas violet represents the electron.

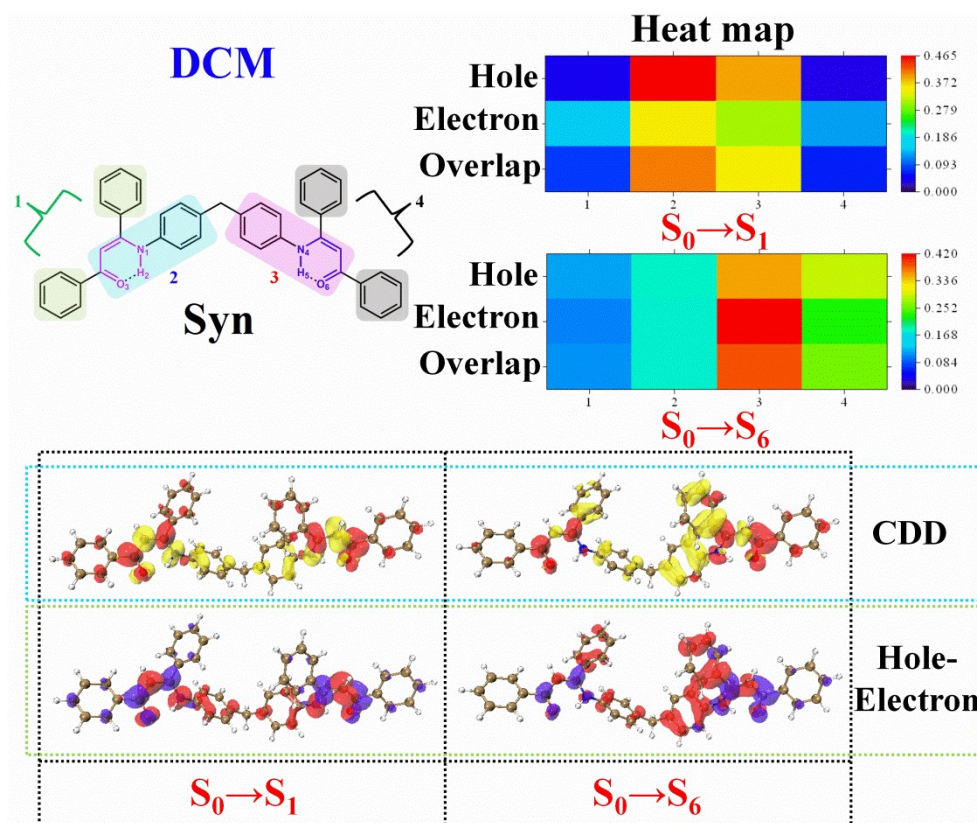


Fig. S7(d). Calculated hole-electron distribution, charge density difference (CDD) maps, and heat maps concerning fragment contribution to hole/electron of Syn in DCM solvent. In CDD maps, the regions with increasing electron density from the ground state to the excited state are shown in red, whereas the regions with decreasing density are shown in yellow. In hole-electron distribution maps, red refers to the hole, whereas violet represents the electron.

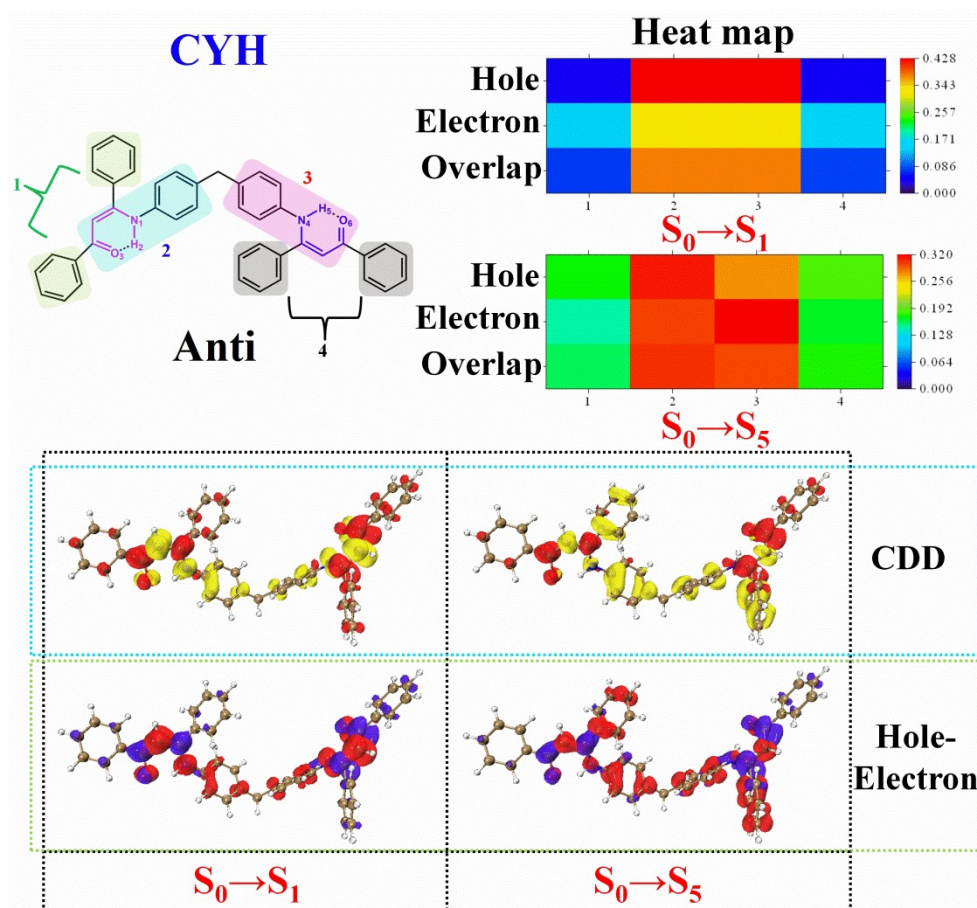


Fig. S7(e). Calculated hole-electron distribution, charge density difference (CDD) maps, and heat maps concerning fragment contribution to hole/electron of Anti in CYH solvent. In CDD maps, the regions with increasing electron density from the ground state to the excited state are shown in red, whereas the regions with decreasing density are shown in yellow. In hole-electron distribution maps, red refers to the hole, whereas violet represents the electron.

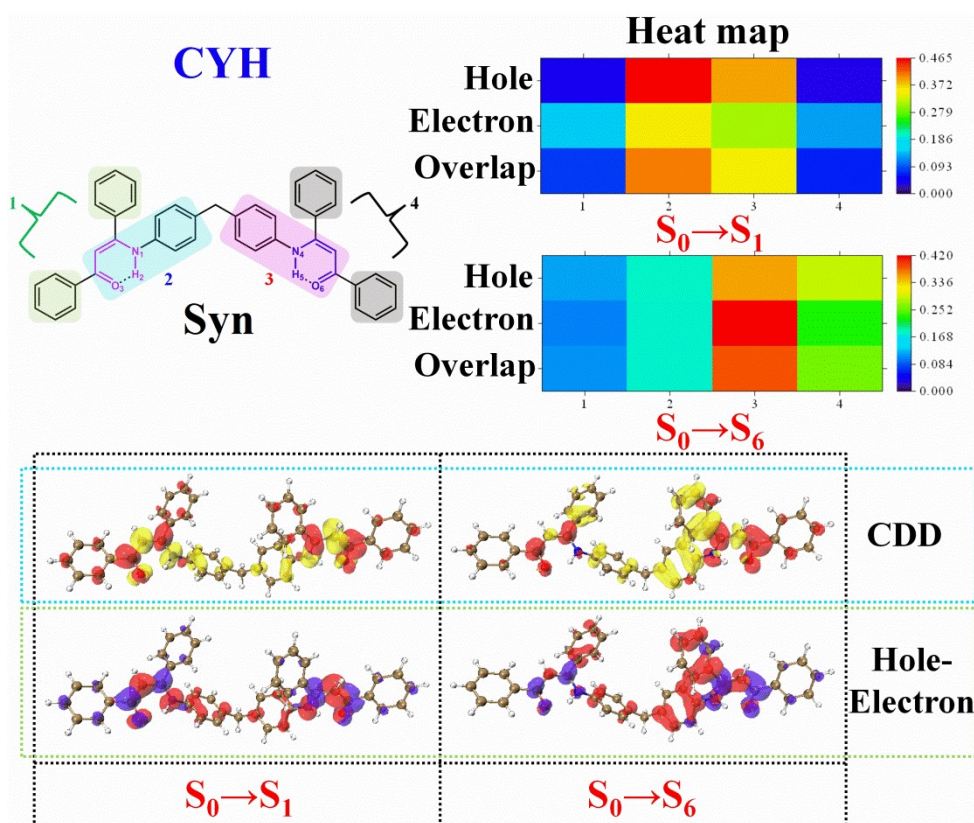


Fig. S7(f). Calculated hole-electron distribution, charge density difference (CDD) maps, and heat maps concerning fragment contribution to hole/electron of Syn in CYH solvent. In CDD maps, the regions with increasing electron density from the ground state to the excited state are shown in red, whereas the regions with decreasing density are shown in yellow. In hole-electron distribution maps, red refers to the hole, whereas violet represents the electron.

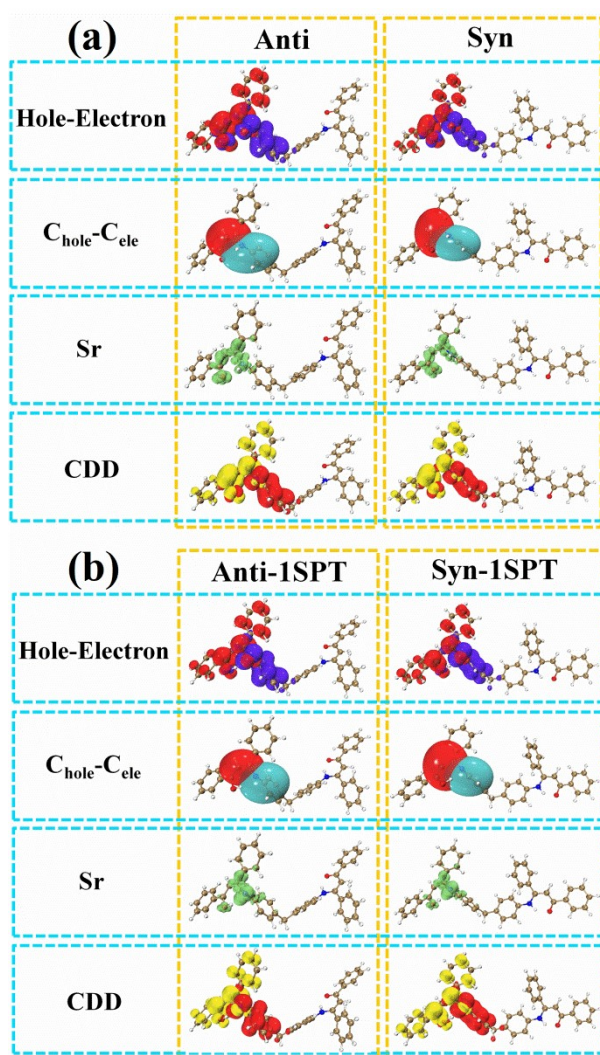


Fig. S8(a). Calculated hole-electron distribution (red: hole, violet: electron), graphical hole-electron overlap index (Sr), CDD maps (red: regions with increasing charge density, yellow: regions with decreasing charge density), and $C_{\text{hole}}-C_{\text{ele}}$ functions diagrams (red: C_{hole} , cyan: C_{ele}) for Anti and Syn (a) as well as Anti-1SPT and Syn-1SPT (b) in ACN.

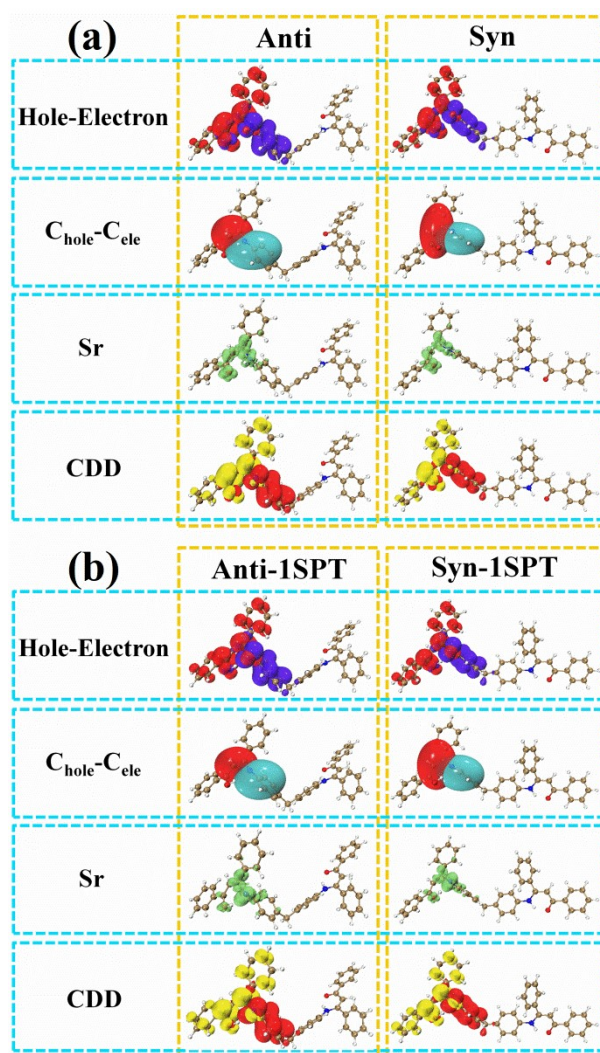


Fig. S8(b). Calculated hole-electron distribution (red: hole, violet: electron), graphical hole-electron overlap index (Sr), CDD maps (red: regions with increasing charge density, yellow: regions with decreasing charge density), and $C_{\text{hole}}-C_{\text{ele}}$ functions diagrams (red: C_{hole} , cyan: C_{ele}) for Anti and Syn (a) as well as Anti-1SPT and Syn-1SPT (b) in CYH.

Table S3. The significant index associated with the fluorescence properties of the four molecules in ACN, DCM, and CYH solvents.

			D ^a	S _r ^b	T ^c	HDI ^d	EDI ^e
ACN	Anti	S ₁ →S ₀	2.673	0.302	1.028	11.30	8.78
	Anti-1SPT	S ₁ →S ₀	2.786	0.291	1.178	11.99	9.03
	Syn	S ₁ →S ₀	2.657	0.301	0.915	11.37	8.92
	Syn-1SPT	S ₁ →S ₀	2.770	0.295	1.071	11.97	8.99
DCM	Anti	S ₁ →S ₀	2.717	0.297	1.083	11.17	8.88
	Anti-1SPT	S ₁ →S ₀	2.798	0.294	1.198	11.82	8.99
	Syn	S ₁ →S ₀	2.752	0.293	1.142	11.37	8.82
	Syn-1SPT	S ₁ →S ₀	2.813	0.294	1.137	11.85	8.94
CYH	Anti	S ₁ →S ₀	2.848	0.284	1.248	10.94	8.69
	Anti-1SPT	S ₁ →S ₀	2.879	0.292	1.331	11.44	8.92
	Syn	S ₁ →S ₀	2.841	0.284	1.278	11.04	8.79
	Syn-1SPT	S ₁ →S ₀	2.865	0.292	1.233	11.66	8.88

^a D represents the distance between the electron centroid and the hole centroid. (Å)

^b S_r denotes the overlap degree between holes and electrons.

^c t index refers to the degree of separation between holes and electrons. (Å)

^d HDI is the hole delocalization index.

^e EDI is the electron delocalization index.

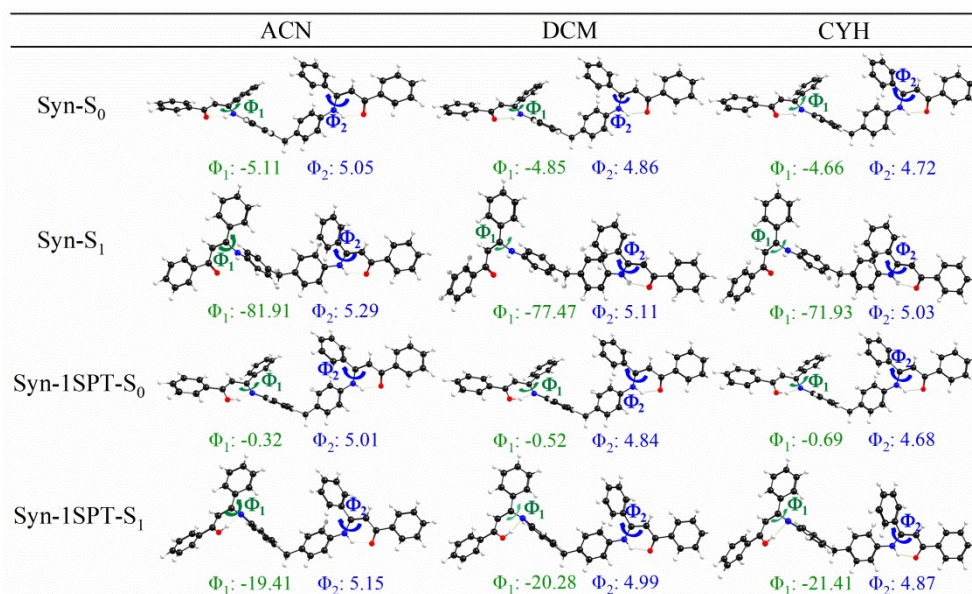


Fig. S9. S₀- and S₁-stated geometries of Syn and Syn-1SPT optimized in various solvent conditions.

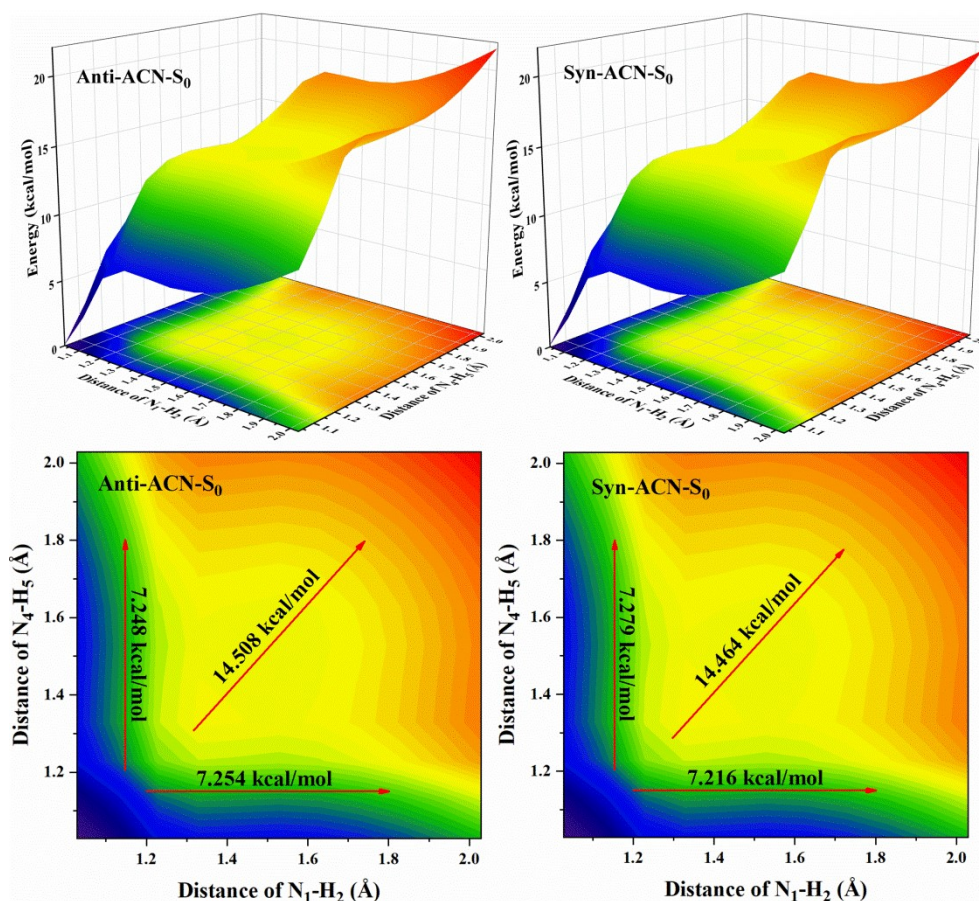


Fig. S10(a). Calculated S_0 -stated potential energy surfaces (PESs) for Anti and Syn as functions of N_1 - H_2 and N_4 - H_5 bond lengths in step of 0.1 Å based on DFT/B3LYP/6-31G(d,p) theoretical level in ACN solvent. Herein, the energy of S_0 -stated Anti and Syn structures is designated as zero-point energy.

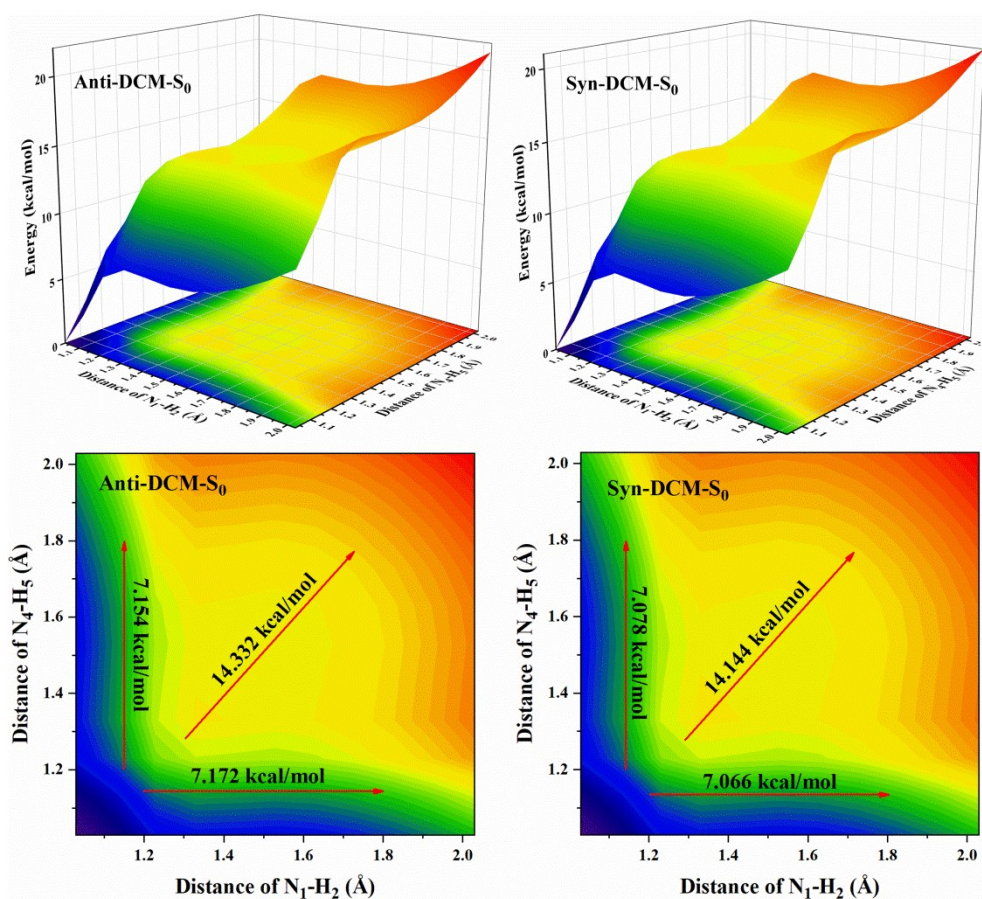


Fig. S10(b). Calculated S_0 -stated potential energy surfaces (PESs) for Anti and Syn as functions of N_1-H_2 and N_4-H_5 bond lengths in step of 0.1 Å based on DFT/B3LYP/6-31G(d,p) theoretical level in DCM solvent. Herein, the energy of S_0 -stated Anti and Syn structures is designated as zero-point energy.

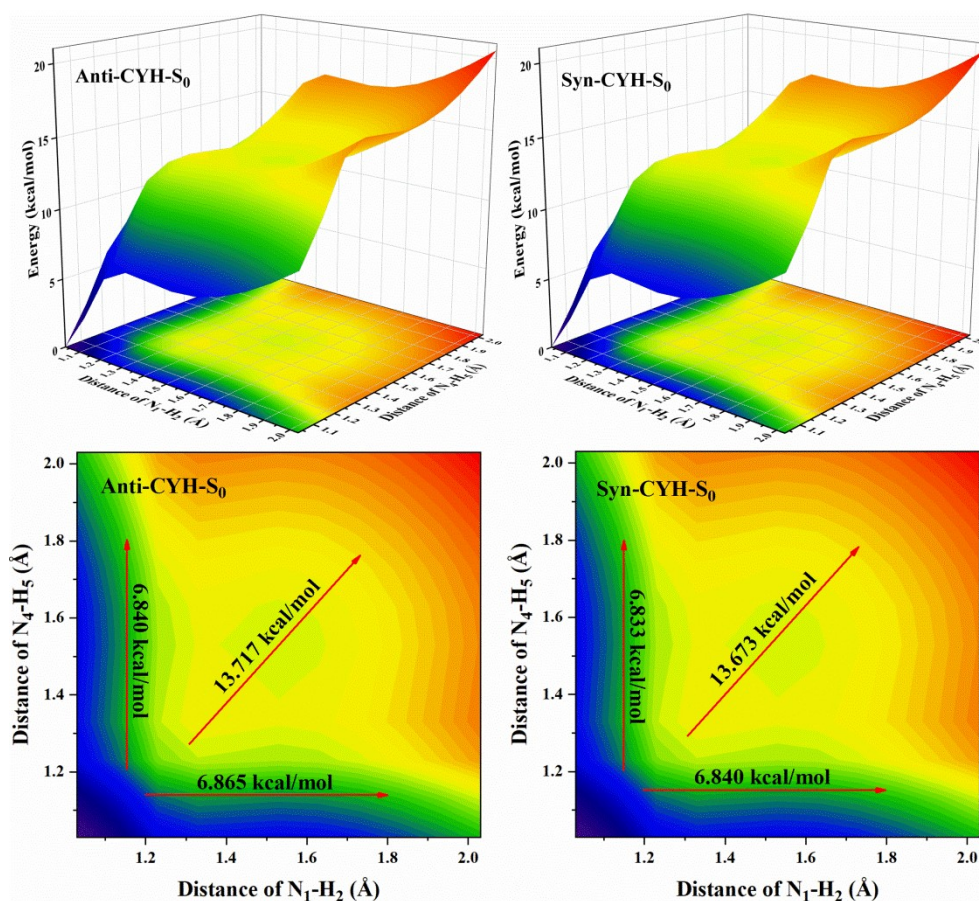


Fig. S10(c). Calculated S₀-stated potential energy surfaces (PESs) for Anti and Syn as functions of N₁-H₂ and N₄-H₅ bond lengths in step of 0.1 Å based on DFT/B3LYP/6-31G(d,p) theoretical level in CYH solvent. Herein, the energy of S₀-stated Anti and Syn structures is designated as zero-point energy.

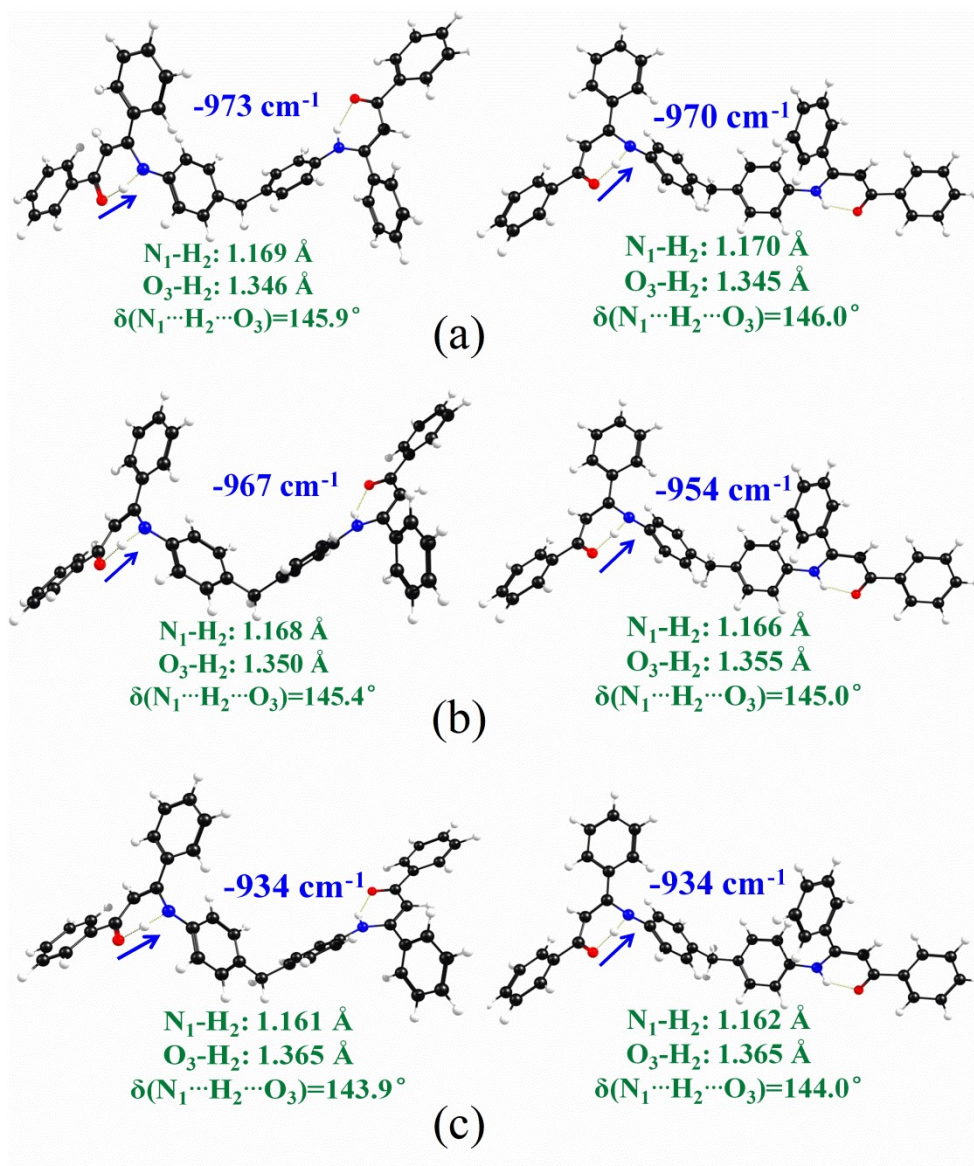


Fig. S11(a). The S₁-stated TS1 structures for Anti and Syn in ACN (a), DCM (b), and CYH (c) solvents. TS1 has separated Anti/Syn and Anti-1SPT/Syn-1SPT configurations in the excited state. Herein, the significant intramolecular hydrogen bond parameters and imaginary frequencies of the corresponding TS1 structures are all exhibited.

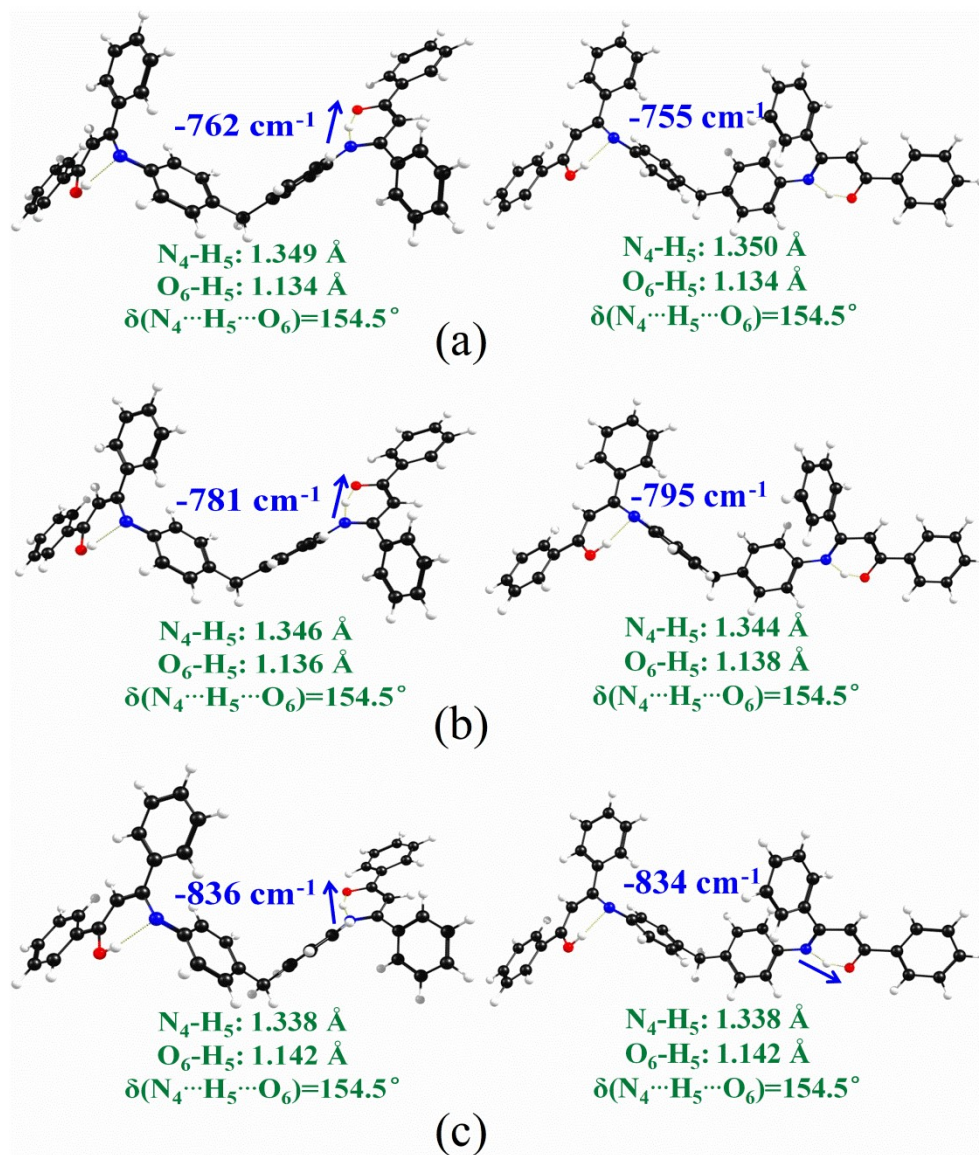


Fig. S11(b). The S_1 -stated TS2 structures for Anti and Syn in ACN (a), DCM (b), and CYH (c) solvents. TS2 has separated Anti-1SPT/Syn-1SPT and Anti-DPT/Syn-DPT configurations in the excited state. Herein, the significant intramolecular hydrogen bond parameters and imaginary frequencies of the corresponding TS2 structures are all exhibited.

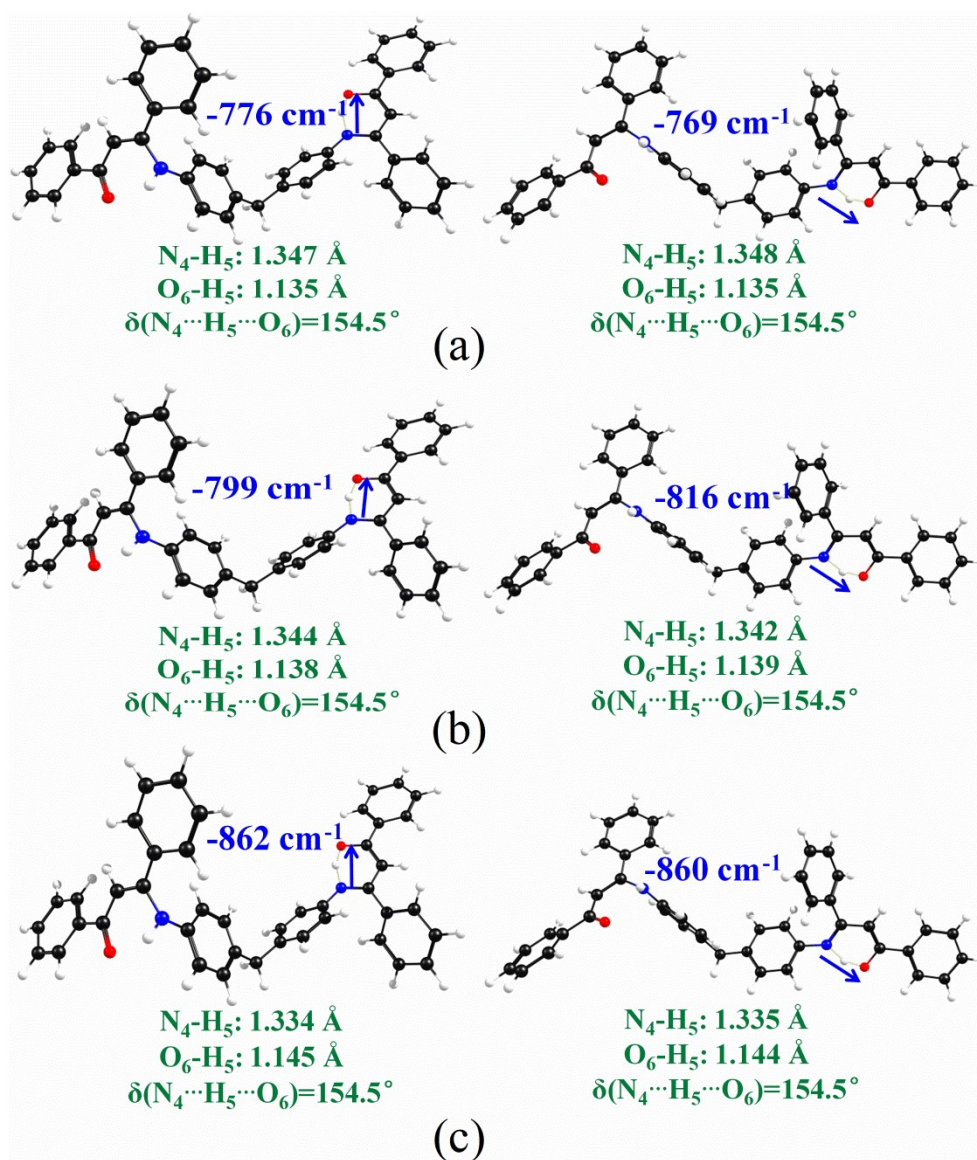


Fig. S11(c). The S_1 -stated TS3 structures for Anti and Syn in ACN (a), DCM (b), and CYH (c) solvents. TS3 has separated Anti/Syn and Anti-2SPT/Syn-2SPT configurations in the excited state. Herein, the significant intramolecular hydrogen bond parameters and imaginary frequencies of the corresponding TS3 structures are all exhibited.

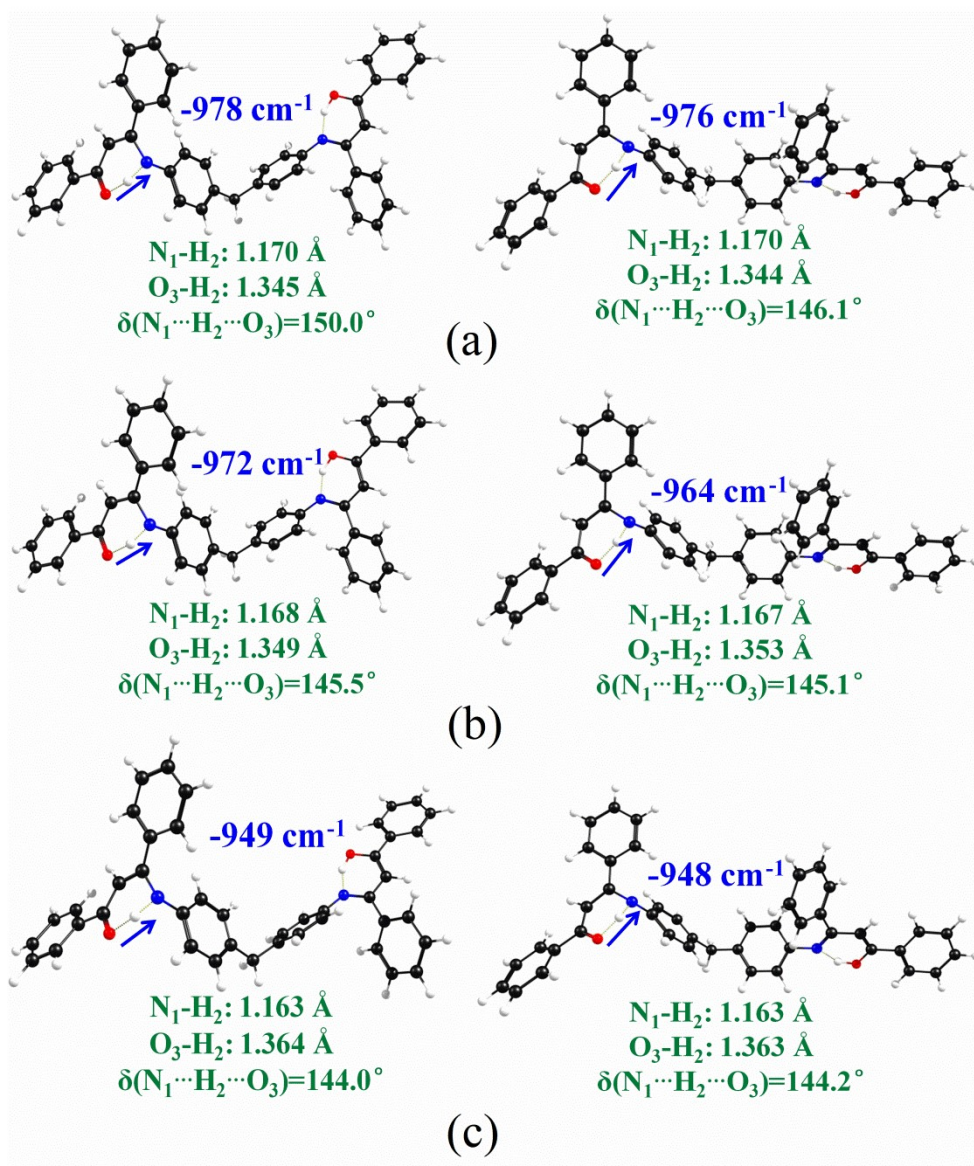


Fig. S11(c). The S_1 -stated TS4 structures for Anti and Syn in ACN (a), DCM (b), and CYH (c) solvents. TS4 has separated Anti-2SPT/Syn-2SPT and Anti-DPT/Syn-DPT configurations in the excited state. Herein, the significant intramolecular hydrogen bond parameters and imaginary frequencies of the corresponding TS4 structures are all exhibited.

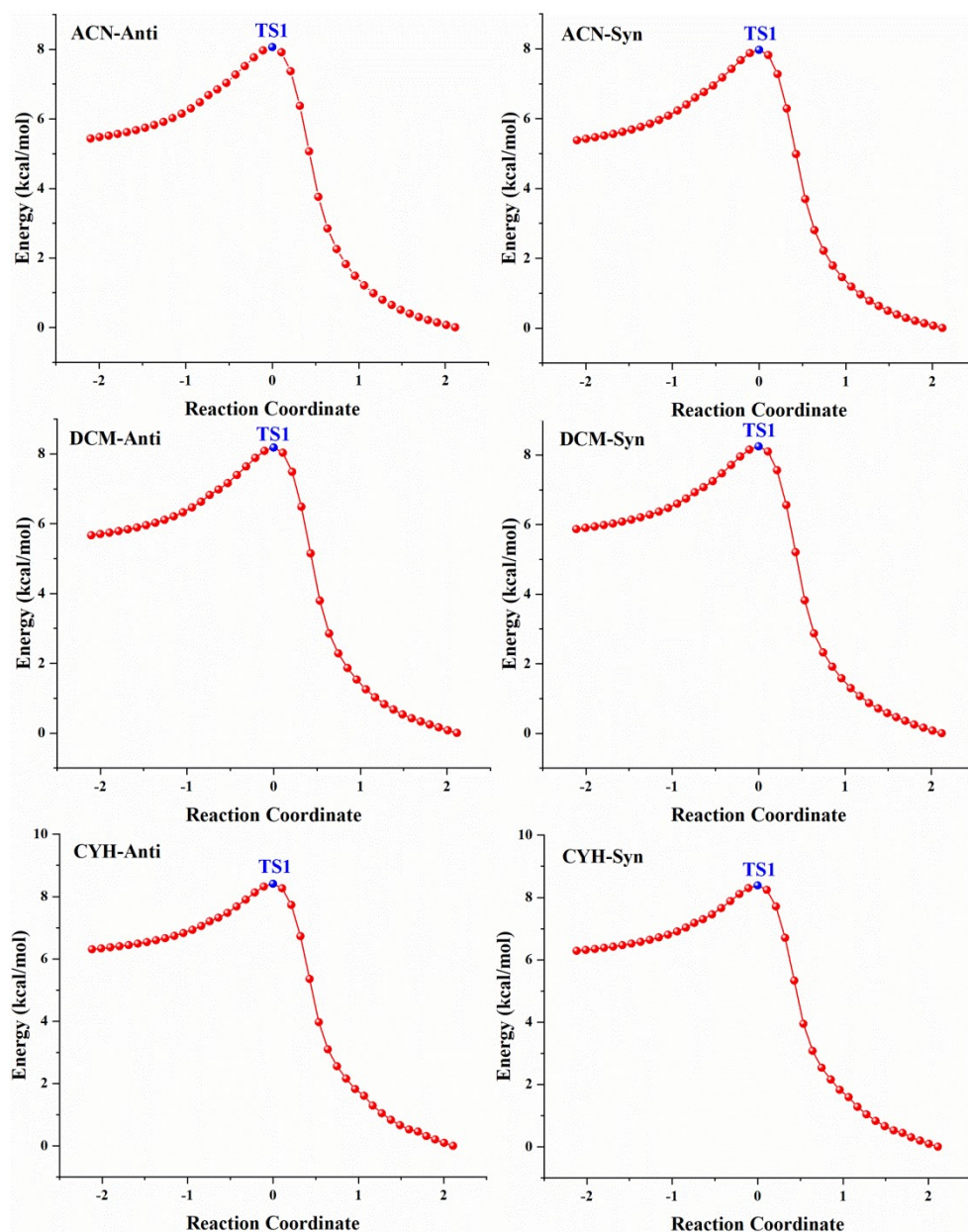


Fig. S12(a). The energy profile along the S₁-stated IRC for the proton-transferred channel (Anti/Syn → Anti-1SPT/Syn-1SPT) under various solvent conditions based on the identical theoretical level used in geometric optimization.

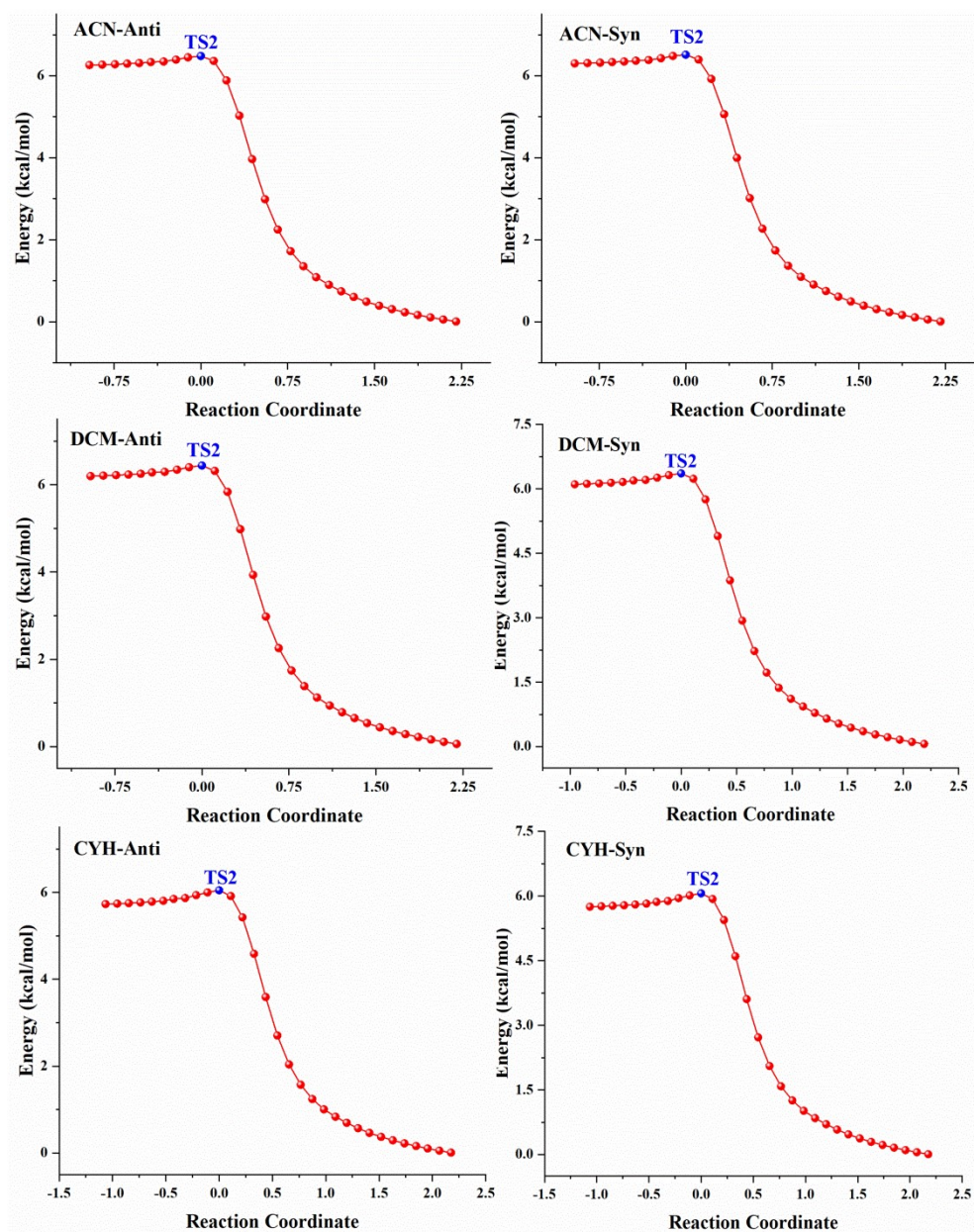


Fig. S12(b). The energy profile along the S_1 -stated IRC for the proton-transferred channel (Anti-1SPT/Syn-1SPT $\rightarrow$ Anti-DPT/Syn-DPT) under various solvent conditions based on the identical theoretical level used in geometric optimization.

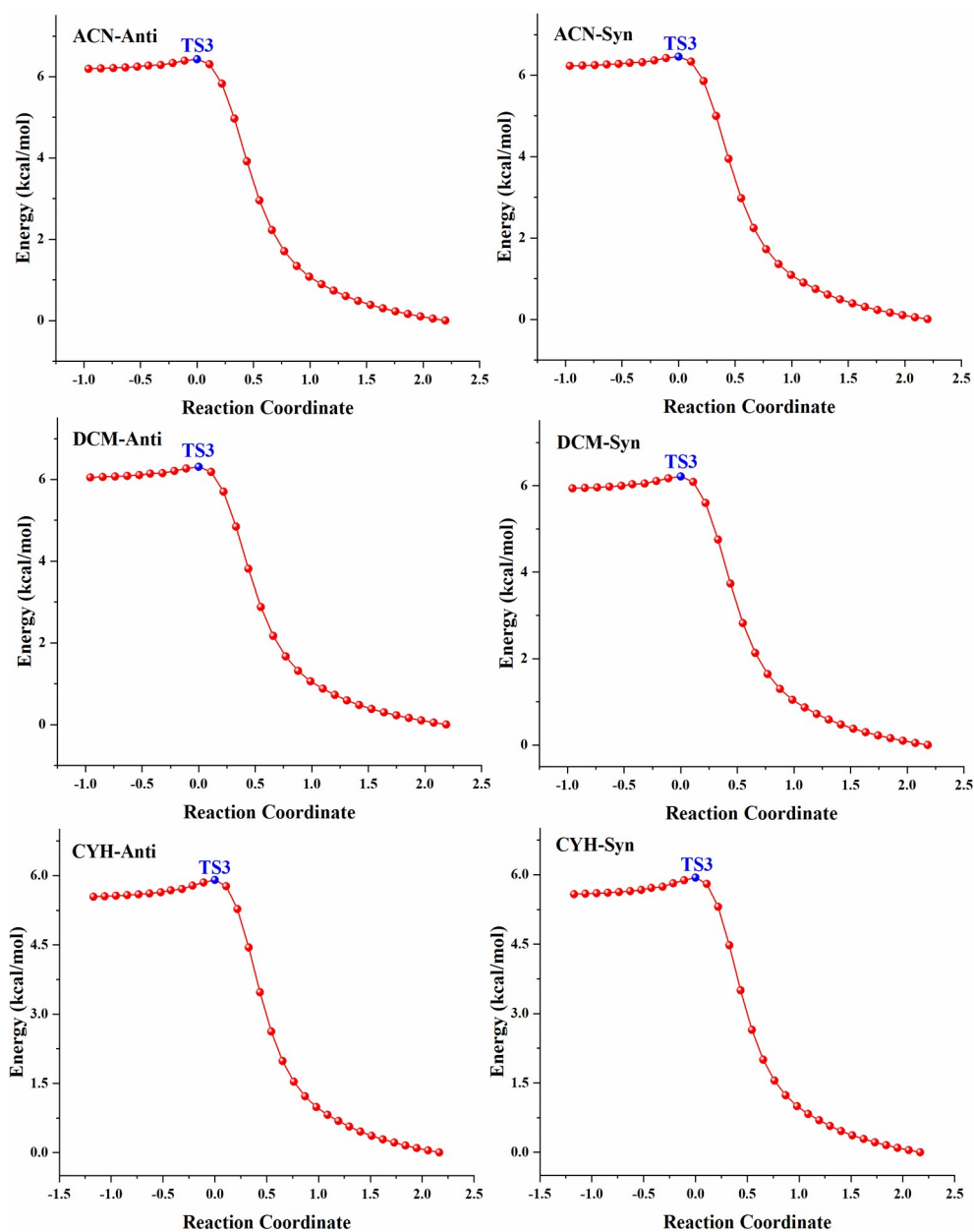


Fig. S12(c). The energy profile along the S_1 -stated IRC for the proton-transferred channel (Anti/Syn $\rightarrow$ Anti-2SPT/Syn-2SPT) under various solvent conditions based on the identical theoretical level used in geometric optimization.

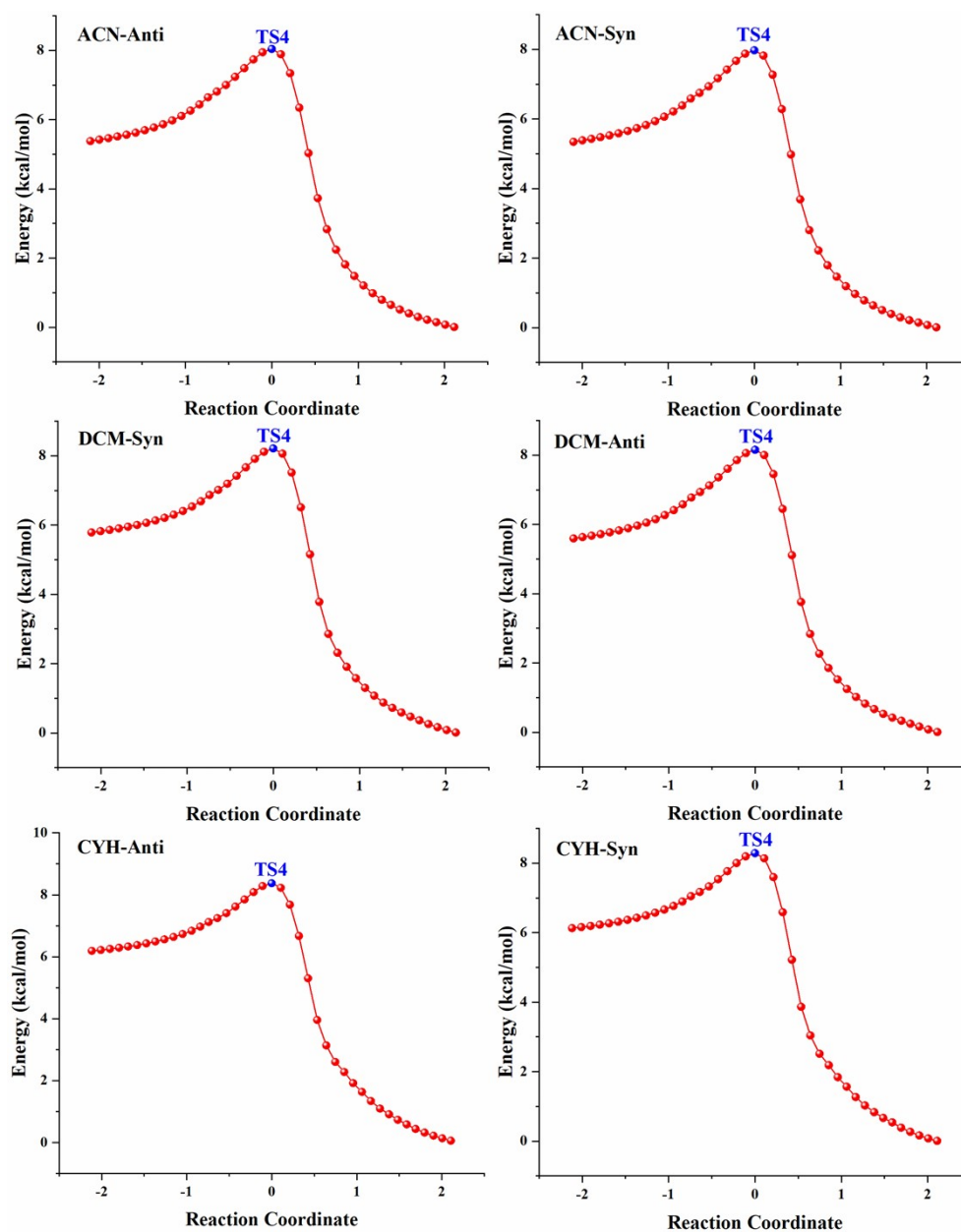


Fig. S12(d). The energy profile along the S_1 -stated IRC for the proton-transferred channel (Anti-2SPT/Syn-2SPT $\rightarrow$ Anti-DPT/Syn-DPT) under various solvent conditions based on the identical theoretical level used in geometric optimization.

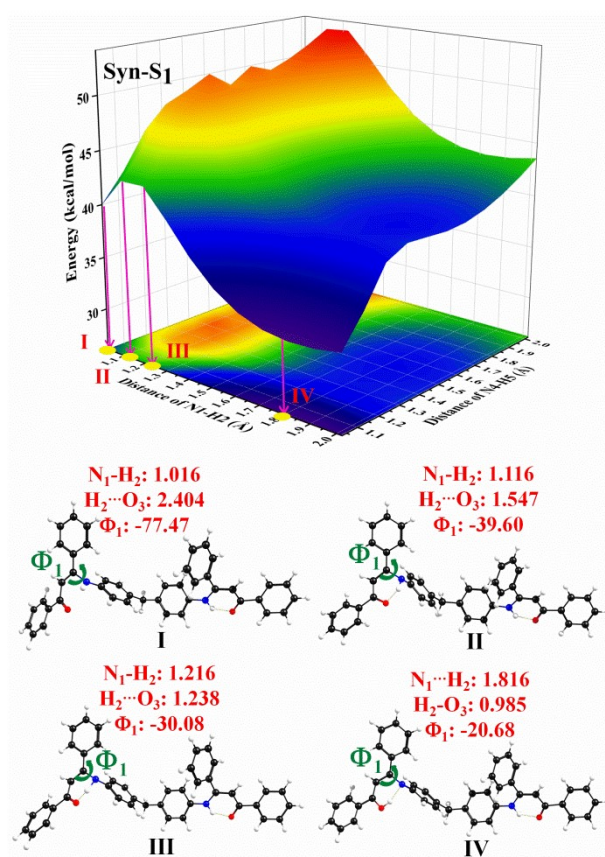


Fig. S13. Constructed S₁-stated PES for Syn with four representative points in DCM solvent. Herein, the energy of the S₁-stated Syn structure is designated as zero-point energy.

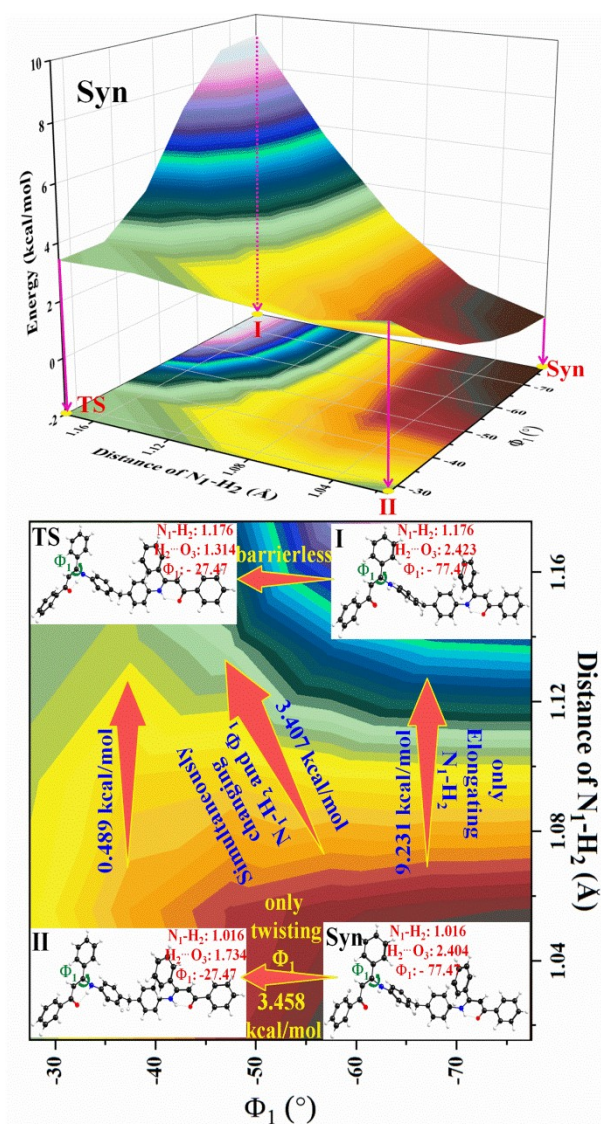


Fig. S14. Calculated PES as functions of N₁-H₂ bond length and Φ₁ dihedral angle of Syn in DCM solvent and the corresponding projection plane. Herein, the energy of the S₁-stated Syn structure is designated as zero-point energy.

Molecular Structures:

Ground State - DFT/B3LYP/6-31G(d,p)

L-Anti (ACN)

C -2.31346800 3.72510700 0.28559600
C -3.44743700 3.86339300 -0.51698400
C -4.39437000 2.84031400 -0.57360100
C -4.21127500 1.66065400 0.16411900
C -3.06584100 1.52835200 0.96690200
C -2.12792900 2.55680400 1.03006500
C -5.25279800 0.59706600 0.15251000
C -6.58281800 0.95120700 0.33743700
C -7.66376400 0.00432600 0.39180100
O -7.47872600 -1.23953300 0.35359400
N -4.89864100 -0.71073000 0.05126300
C -9.07276600 0.50836600 0.52500300
C -9.44649900 1.82898900 0.22701900
C -10.77451900 2.23565700 0.35697200
C -11.74677800 1.33148800 0.79073800
C -11.38651700 0.01315700 1.08484100
C -10.06203200 -0.39470900 0.94692400
C -3.71510200 -1.29900300 -0.44933600
C -3.35387500 -2.55977600 0.04358900
C -2.22871000 -3.21602800 -0.45424900
C -1.42920200 -2.63562400 -1.44538200
C -1.80542700 -1.37612400 -1.93607000
C -2.93485700 -0.71645200 -1.46144100
C -0.19895900 -3.34612400 -1.98477300
C 1.11004100 -2.63316300 -1.68519100
C 1.93799900 -2.17246900 -2.71506500
C 3.14699000 -1.53405200 -2.44078100
C 3.55730900 -1.33237300 -1.11640100
C 2.72397100 -1.76840300 -0.07351000
C 1.52665400 -2.41542400 -0.36322700
N 4.76445600 -0.62970100 -0.89929100
O 5.93717700 1.66920700 -1.50733800
C 6.65310100 1.50042600 -0.48666700
C 6.56609200 0.32411800 0.33594000
C 5.63726700 -0.68953400 0.14018400
C 7.65331000 2.56549500 -0.13704800
C 5.67394900 -1.88703700 1.02387700
C 7.99582800 3.50292500 -1.12499200
C 8.91383000 4.51568300 -0.85806500
C 9.49683300 4.61534700 0.40859300
C 9.15390300 3.69738800 1.40390800

C 8.24096100 2.67789100 1.13359100
C 5.78274400 -1.73876100 2.41508900
C 5.87657300 -2.85998200 3.24013600
C 5.87492800 -4.14087900 2.68470800
C 5.77580600 -4.29682500 1.29925000
C 5.67010900 -3.17965700 0.47333300
H -1.57809300 4.52254400 0.33199600
H -3.59610400 4.76655500 -1.10084400
H -5.27223600 2.94541100 -1.20305000
H -2.92089000 0.62632500 1.55219500
H -1.25259300 2.44755000 1.66300800
H -6.78880800 1.99695600 0.51404200
H -5.70367800 -1.33020700 0.21199100
H -8.70960400 2.53961700 -0.13124800
H -11.05032800 3.25772000 0.11536700
H -12.77942200 1.65099900 0.89518000
H -12.13872600 -0.69451500 1.42072000
H -9.76890200 -1.41576000 1.16508800
H -3.95501500 -3.02072500 0.82187300
H -1.96978000 -4.19507300 -0.06007600
H -1.21206900 -0.90755300 -2.71679900
H -3.21814800 0.24015900 -1.88399900
H -0.29242200 -3.46471400 -3.07047400
H -0.16652400 -4.35878300 -1.56592100
H 1.64170400 -2.32180500 -3.74988000
H 3.78216800 -1.19536000 -3.25406400
H 3.00552500 -1.59142800 0.95769400
H 0.89353800 -2.74153400 0.45764400
H 4.95895400 0.17744500 -1.50616800
H 7.29886400 0.17048000 1.11484400
H 7.53069500 3.41718300 -2.10085700
H 9.17550100 5.22777100 -1.63516900
H 10.21091600 5.40583400 0.61966100
H 9.59416300 3.77704900 2.39329600
H 7.97130900 1.98705400 1.92507700
H 5.77720200 -0.74347100 2.84780100
H 5.94970200 -2.73155000 4.31569600
H 5.95122500 -5.01331200 3.32647500
H 5.78360600 -5.29015200 0.86107000
H 5.60045800 -3.30559900 -0.60207100

L-Syn (ACN)

C 3.79957700 3.42321200 2.85512900
C 5.04848300 2.87342900 3.15014000
C 5.57794600 1.86543900 2.34375000

C 4.85755300 1.38725500 1.23849500
C 3.60025200 1.94405800 0.95018200
C 3.07955900 2.95854200 1.75086300
C 5.44981800 0.35535000 0.34370900
C 6.75577800 0.51381000 -0.10018900
C 7.41271400 -0.39714200 -0.99873500
O 6.82092000 -1.37401600 -1.52603200
N 4.69308500 -0.68122500 -0.10351500
C 8.85632500 -0.17014500 -1.34719800
C 9.71030500 0.64694000 -0.58850800
C 11.04689700 0.80674300 -0.95443900
C 11.54833400 0.15746000 -2.08491400
C 10.70812500 -0.66210000 -2.84428900
C 9.37587500 -0.82782900 -2.47402300
C 3.51351600 -1.24556500 0.43266200
C 2.65002700 -1.91206900 -0.45225100
C 1.50112500 -2.53697200 0.02049400
C 1.17062800 -2.51509700 1.38377700
C 2.04259900 -1.85426700 2.25657800
C 3.20599000 -1.23463800 1.79939100
C -0.08713100 -3.19963900 1.89351700
C -1.37706000 -2.61202300 1.34452100
C -2.24537100 -3.37486300 0.55557000
C -3.42602500 -2.83323100 0.04816600
C -3.77365400 -1.50517400 0.32776500
C -2.92339900 -0.73682200 1.13947400
C -1.74063600 -1.28613400 1.62463100
N -5.00914500 -1.02859400 -0.16646900
O -7.59600800 -1.60836000 -0.12234600
C -7.80711900 -0.39567800 -0.38251600
C -6.74356200 0.54416500 -0.61354000
C -5.39592200 0.23412000 -0.48567300
C -9.23188500 0.07196600 -0.47557300
C -4.37978200 1.27698400 -0.79601100
C -10.23922500 -0.89773900 -0.60668100
C -11.57884600 -0.52653200 -0.69112000
C -11.93514800 0.82405000 -0.63431500
C -10.94363400 1.79733300 -0.49093300
C -9.60131500 1.42559900 -0.41432300
C -4.52117300 2.57739500 -0.28780400
C -3.60263600 3.57187200 -0.62500800
C -2.53960400 3.28215500 -1.48247500
C -2.39670300 1.99164500 -1.99993200
C -3.30552300 0.99314900 -1.65588300

H 3.38892000 4.20987000 3.48072100
H 5.61161100 3.22703600 4.00835400
H 6.54558900 1.43321900 2.57770400
H 3.04104700 1.59088500 0.09008500
H 2.11200500 3.38895000 1.51134900
H 7.27048400 1.41172500 0.20972800
H 5.18555500 -1.21873600 -0.82872400
H 9.34501400 1.14263600 0.30432700
H 11.69757000 1.43524300 -0.35387300
H 12.58822100 0.28621600 -2.37022000
H 11.09312700 -1.17078600 -3.72318200
H 8.71345900 -1.46554000 -3.04895900
H 2.88568100 -1.93095900 -1.51242200
H 0.84555900 -3.04306900 -0.68304000
H 1.82256400 -1.83739400 3.32078000
H 3.87514900 -0.75835100 2.50580100
H -0.09737500 -3.14389500 2.98831800
H -0.05137500 -4.26541200 1.63941400
H -1.99686900 -4.40808000 0.32831000
H -4.08076100 -3.43702200 -0.57349800
H -3.19299000 0.27982800 1.39976600
H -1.09335400 -0.67431600 2.24738600
H -5.81277000 -1.66920500 -0.13075200
H -6.98394800 1.53572300 -0.96879600
H -9.94794600 -1.94173600 -0.64255100
H -12.34578500 -1.28761600 -0.80056000
H -12.97927000 1.11591300 -0.69747500
H -11.21524400 2.84714300 -0.43431500
H -8.84789300 2.19441300 -0.28179000
H -5.34342700 2.80131800 0.38423800
H -3.71787800 4.57119100 -0.21663800
H -1.82642900 4.05675300 -1.74750300
H -1.57734600 1.76315500 -2.67463300
H -3.19421500 -0.00542900 -2.06533100

L-Anti (DCM)

C -2.36346900 3.78122000 0.19697400
C -3.51390600 3.90327400 -0.58432400
C -4.44945900 2.86898200 -0.61962100
C -4.23903400 1.69437400 0.11878900
C -3.07751800 1.57887600 0.90047800
C -2.15055800 2.61809300 0.94202600
C -5.26699900 0.61769200 0.12682600
C -6.59785100 0.95515100 0.33402700
C -7.66509100 -0.00659000 0.40977800

O -7.46331300 -1.24720600 0.36863200
N -4.89964800 -0.68618100 0.02053100
C -9.07836600 0.47726400 0.57030500
C -9.47589800 1.79480900 0.29093400
C -10.80682500 2.18138600 0.44831700
C -11.75823200 1.25971900 0.89096200
C -11.37433300 -0.05590500 1.16612600
C -10.04704500 -0.44353200 1.00104100
C -3.71672200 -1.26530500 -0.49038500
C -3.35003200 -2.52860900 -0.00763500
C -2.22452100 -3.17800600 -0.51289500
C -1.42855300 -2.58794800 -1.50103500
C -1.81018900 -1.32648200 -1.98185800
C -2.94066900 -0.67373000 -1.50052900
C -0.19610900 -3.28952100 -2.04622600
C 1.11288200 -2.58472200 -1.72690800
C 1.95788600 -2.12724900 -2.74408600
C 3.16912600 -1.50142500 -2.45178900
C 3.56500900 -1.30976900 -1.12162700
C 2.71398500 -1.74148600 -0.09138100
C 1.51428800 -2.37541600 -0.39900800
N 4.77740100 -0.62263200 -0.88671100
O 5.98938400 1.65542600 -1.47760800
C 6.69605500 1.47409700 -0.45327200
C 6.58295900 0.29776600 0.36705200
C 5.63989300 -0.70024000 0.16025500
C 7.71082400 2.52334600 -0.09700100
C 5.65010100 -1.90062800 1.04077900
C 8.04898500 3.47353100 -1.07402100
C 8.97901400 4.47393700 -0.80301500
C 9.57996600 4.54779900 0.45685300
C 9.24230800 3.61666700 1.44142200
C 8.31639200 2.61013400 1.16705700
C 5.75630800 -1.75738900 2.43270400
C 5.82757700 -2.88151400 3.25591200
C 5.80472300 -4.16104000 2.69806100
C 5.70711700 -4.31236600 1.31214700
C 5.62477600 -3.19200300 0.48811200
H -1.63634600 4.58702100 0.22616000
H -3.68379800 4.80229700 -1.16888700
H -5.33970000 2.96075300 -1.23366700
H -2.91106600 0.68056100 1.48568500
H -1.26196100 2.52098100 1.55823500
H -6.81370800 1.99816200 0.51488000

H -5.69687800 -1.31324400 0.19337400
H -8.75553800 2.51890000 -0.07400900
H -11.10139300 3.20159900 0.22117200
H -12.79326100 1.56367900 1.01662700
H -12.11046200 -0.77733000 1.50843500
H -9.73458100 -1.46202900 1.20357400
H -3.94809700 -2.99695100 0.76869200
H -1.96256700 -4.15960300 -0.12692800
H -1.21928000 -0.85033700 -2.75984900
H -3.22740700 0.28476400 -1.91616600
H -0.28346500 -3.38926800 -3.13438200
H -0.16687400 -4.30978200 -1.64552400
H 1.67342600 -2.26969400 -3.78325800
H 3.81780400 -1.16489500 -3.25529300
H 2.98487400 -1.57195100 0.94393900
H 0.86712500 -2.69787500 0.41228600
H 4.99011900 0.18534700 -1.48696400
H 7.30705400 0.12861300 1.15076800
H 7.56889800 3.40706600 -2.04405500
H 9.23608800 5.19673300 -1.57178500
H 10.30383800 5.32852000 0.67118500
H 9.69679200 3.67595900 2.42586200
H 8.05181700 1.90908700 1.95119900
H 5.76671300 -0.76281000 2.86708700
H 5.89918700 -2.75646200 4.33203400
H 5.86317800 -5.03594300 3.33841800
H 5.69807300 -5.30484200 0.87199800
H 5.55581900 -3.31454200 -0.58770200

L-Syn (DCM)

C 3.87187600 3.29734700 3.06582300
C 5.11685900 2.72056800 3.32211700
C 5.62869600 1.74871500 2.46199100
C 4.89496700 1.33413700 1.34016400
C 3.64141600 1.91725000 1.09169800
C 3.13809100 2.89549100 1.94639700
C 5.46955000 0.34257600 0.38954700
C 6.77069800 0.51356800 -0.06111000
C 7.40789100 -0.35702100 -1.01445700
O 6.80024900 -1.30131700 -1.57837300
N 4.69987200 -0.66578900 -0.09919700
C 8.84780700 -0.12433600 -1.37493400
C 9.71567300 0.66831800 -0.60678300
C 11.04696000 0.83480000 -0.98791600
C 11.52935100 0.21573900 -2.14300500

C 10.67536500 -0.58006700 -2.91172600
C 9.34830700 -0.75191000 -2.52689200
C 3.51940800 -1.24417300 0.41801500
C 2.64596700 -1.86299300 -0.49150400
C 1.49320700 -2.49747500 -0.04266000
C 1.16827200 -2.53384900 1.32144400
C 2.04960300 -1.92018900 2.21846800
C 3.21673600 -1.29109200 1.78491600
C -0.09198100 -3.23105200 1.80588500
C -1.38192700 -2.63003000 1.27162300
C -2.28418700 -3.39423700 0.52355400
C -3.46842500 -2.84332400 0.03587400
C -3.78628800 -1.50333500 0.29400500
C -2.90043200 -0.73266000 1.06429300
C -1.71487300 -1.29204900 1.52992300
N -5.02540100 -1.01858200 -0.18021400
O -7.61065400 -1.58030200 -0.08918500
C -7.82070900 -0.37052600 -0.35645600
C -6.75500900 0.56276500 -0.61191300
C -5.40842100 0.24441800 -0.50491600
C -9.24479200 0.10231400 -0.43224200
C -4.39115600 1.27726500 -0.84445800
C -10.25703700 -0.86620800 -0.52453600
C -11.59647300 -0.49189400 -0.59188500
C -11.94736700 0.86058700 -0.55695100
C -10.95053800 1.83298500 -0.45237300
C -9.60854200 1.45788200 -0.39255800
C -4.51255300 2.58235300 -0.34354200
C -3.59482400 3.56792800 -0.70746400
C -2.55188800 3.26441400 -1.58424900
C -2.42832900 1.96901400 -2.09369700
C -3.33655500 0.97971000 -1.72332700
H 3.47473600 4.05595100 3.73352200
H 5.69063800 3.02501100 4.19219600
H 6.59325000 1.29450900 2.66550600
H 3.07109200 1.61196100 0.22070800
H 2.17275700 3.34644000 1.73733600
H 7.29434000 1.39361200 0.28315000
H 5.18363000 -1.17213600 -0.85310700
H 9.36527900 1.13987200 0.30493700
H 11.70861600 1.44478200 -0.38010200
H 12.56541700 0.34935400 -2.44008300
H 11.04578700 -1.06600500 -3.80963300
H 8.67404800 -1.37186400 -3.10731200

H 2.87777700 -1.83624900 -1.55239100
H 0.82921200 -2.96405100 -0.76533300
H 1.83352800 -1.94837400 3.28337400
H 3.89215000 -0.85150100 2.50889800
H -0.10539800 -3.20832600 2.90225900
H -0.05590000 -4.28983900 1.52302400
H -2.05974800 -4.43666600 0.31325000
H -4.15027500 -3.44879700 -0.55430600
H -3.14413900 0.29463200 1.30725500
H -1.03884700 -0.67766200 2.11858200
H -5.83539500 -1.65046400 -0.12171400
H -6.99484800 1.55123700 -0.97611300
H -9.96749300 -1.91104700 -0.54266500
H -12.36783900 -1.25238800 -0.67069900
H -12.99162400 1.15487300 -0.60692900
H -11.21790300 2.88477900 -0.41298900
H -8.84978500 2.22612200 -0.29011000
H -5.31925000 2.81620700 0.34394200
H -3.69492400 4.57130800 -0.30477300
H -1.83916000 4.03203900 -1.87026100
H -1.62410100 1.72915900 -2.78256600
H -3.24004200 -0.02326800 -2.12558700

L-Anti (CYH)

C -2.34633500 3.79317400 0.23570700
C -3.49579700 3.92976800 -0.54391500
C -4.43310000 2.89803200 -0.59603100
C -4.22654900 1.71179700 0.12411100
C -3.06600000 1.58229000 0.90436900
C -2.13681100 2.61829900 0.96231400
C -5.25625000 0.63652900 0.11207200
C -6.58478500 0.97156800 0.32774200
C -7.65187600 0.00542500 0.39275000
O -7.44667400 -1.23131500 0.32902300
N -4.89162800 -0.66687500 -0.01974500
C -9.06561600 0.48183400 0.57003500
C -9.46750000 1.80622700 0.33608600
C -10.79898900 2.18323100 0.50844100
C -11.74630400 1.24419900 0.92093000
C -11.35783900 -0.07843900 1.15040600
C -10.03005400 -0.45620700 0.97057700
C -3.71255400 -1.24150600 -0.54037300
C -3.36823900 -2.52648400 -0.09951500
C -2.24464500 -3.17212200 -0.61255300
C -1.42683800 -2.55797200 -1.56708700

C -1.78559300 -1.27537100 -2.00656300
C -2.91420900 -0.62556000 -1.51825000
C -0.19568200 -3.25497600 -2.11982300
C 1.11734800 -2.56740400 -1.78024100
C 1.99949300 -2.15149800 -2.78316800
C 3.21528600 -1.54501100 -2.47190300
C 3.57965200 -1.32988500 -1.13616200
C 2.69096000 -1.71975800 -0.12116000
C 1.48686300 -2.33486700 -0.44746600
N 4.79944100 -0.66384200 -0.88660500
O 6.07190000 1.56076100 -1.52072300
C 6.73890900 1.41276100 -0.46776100
C 6.57675800 0.27059600 0.39571000
C 5.62367400 -0.71652200 0.19360900
C 7.75631600 2.46206700 -0.11902200
C 5.58087600 -1.88310200 1.11786600
C 8.11452900 3.38545800 -1.11382500
C 9.04789200 4.38508200 -0.85381500
C 9.63274000 4.48468100 0.41144200
C 9.27518000 3.58025200 1.41311100
C 8.34518700 2.57486200 1.15022900
C 5.64227000 -1.68961100 2.50617600
C 5.66361700 -2.78227400 3.37294800
C 5.63386100 -4.08109500 2.86309300
C 5.57948300 -4.28290300 1.48160200
C 5.54753200 -3.19370900 0.61395200
H -1.61687000 4.59641400 0.27717500
H -3.66308600 4.83817100 -1.11483200
H -5.32272000 2.99944500 -1.20963600
H -2.90173600 0.67339600 1.47356500
H -1.24793500 2.50900500 1.57618100
H -6.79876700 2.01039800 0.53350600
H -5.69368500 -1.29299000 0.14029800
H -8.74949700 2.54416400 -0.00523100
H -11.09746100 3.20972200 0.31671200
H -12.78222400 1.54047100 1.05834800
H -12.09148600 -0.81356300 1.46837000
H -9.71087100 -1.47936000 1.13536500
H -3.98378900 -3.01428400 0.65087200
H -2.00114900 -4.17087300 -0.25928600
H -1.17551100 -0.77821700 -2.75613200
H -3.18128600 0.35133200 -1.90242100
H -0.27754200 -3.33347300 -3.21053100
H -0.17579700 -4.28458900 -1.74165300

H 1.73972300 -2.31120700 -3.82650700
H 3.89259400 -1.23940300 -3.26418300
H 2.93609500 -1.53084700 0.91711100
H 0.80874400 -2.62145100 0.35188500
H 5.04986700 0.11971100 -1.50609500
H 7.27355300 0.11655700 1.20681400
H 7.64413600 3.29699400 -2.08679100
H 9.32014800 5.08803800 -1.63579100
H 10.35979400 5.26504500 0.61688200
H 9.71755600 3.65964600 2.40181100
H 8.06473100 1.89450700 1.94708700
H 5.65711100 -0.67886600 2.90163400
H 5.70144200 -2.61784800 4.44563800
H 5.65314400 -4.93202800 3.53742800
H 5.56446600 -5.29119800 1.07890900
H 5.51065200 -3.35450400 -0.45833400

L-Syn (CYH)

C 3.90739000 3.22595400 3.17801800
C 5.15097300 2.63804100 3.41352800
C 5.65544000 1.68753300 2.52586900
C 4.91648500 1.30577200 1.39605700
C 3.66417700 1.89975600 1.16915700
C 3.16785500 2.85633400 2.05159800
C 5.48382300 0.33805900 0.41667600
C 6.78350400 0.51491300 -0.03264900
C 7.41061400 -0.33259300 -1.01554400
O 6.79301000 -1.25451400 -1.60165800
N 4.70692000 -0.65212100 -0.09887300
C 8.85014100 -0.10046300 -1.37796900
C 9.72471800 0.67890700 -0.60454800
C 11.05446300 0.84546800 -0.99018600
C 11.52849000 0.23896400 -2.15498600
C 10.66777300 -0.54417400 -2.92874300
C 9.34213100 -0.71566800 -2.53986800
C 3.52597300 -1.23925000 0.40528000
C 2.64755100 -1.82884400 -0.51888200
C 1.49203200 -2.46865000 -0.08606300
C 1.16863300 -2.54032300 1.27682700
C 2.05434400 -1.95567900 2.18833800
C 3.22422600 -1.32135300 1.77065000
C -0.09369000 -3.24469700 1.74389500
C -1.38339100 -2.63577900 1.21797800
C -2.30747500 -3.40177700 0.49933100
C -3.49415800 -2.84620600 0.02426200

C -3.79372500 -1.49864800 0.26532600
C -2.88442500 -0.72539300 1.00511100
C -1.69677300 -1.29009500 1.45831700
N -5.03550400 -1.01074600 -0.19572500
O -7.61500500 -1.56508100 -0.06725900
C -7.82915900 -0.35793100 -0.33548900
C -6.76505400 0.57452000 -0.60967700
C -5.41908600 0.25263600 -0.52132000
C -9.25416700 0.11443700 -0.39294600
C -4.40373800 1.27981800 -0.88363000
C -10.26629600 -0.85623900 -0.45413200
C -11.60671900 -0.48378900 -0.50439300
C -11.95843100 0.86852000 -0.48328900
C -10.96136400 1.84306500 -0.40930900
C -9.61843900 1.46976900 -0.36649200
C -4.51215900 2.58831200 -0.38916400
C -3.59775400 3.56867500 -0.77442600
C -2.57027600 3.25640100 -1.66585300
C -2.45895400 1.95738100 -2.16819000
C -3.36416600 0.97364700 -1.77695500
H 3.51572800 3.96789400 3.86745000
H 5.72935500 2.91704500 4.28919000
H 6.61883700 1.22366600 2.71277500
H 3.08914300 1.61881800 0.29312800
H 2.20298600 3.31564900 1.85879300
H 7.31204700 1.38395600 0.33151000
H 5.18920000 -1.14011200 -0.86682800
H 9.38039600 1.14012300 0.31480100
H 11.72158900 1.44563200 -0.37840600
H 12.56364700 0.37238300 -2.45565900
H 11.03211900 -1.02092100 -3.83411900
H 8.66122600 -1.32618500 -3.12246900
H 2.87866200 -1.77432600 -1.57890200
H 0.82357900 -2.91108700 -0.81975900
H 1.83932300 -2.01133900 3.25251000
H 3.90250400 -0.90421700 2.50515900
H -0.11024300 -3.24285200 2.84080200
H -0.05707700 -4.29885900 1.44335200
H -2.09815600 -4.45012500 0.30260000
H -4.19345400 -3.45355400 -0.54320300
H -3.11134800 0.30889300 1.23386700
H -1.00202800 -0.67322100 2.02202300
H -5.84933000 -1.63721800 -0.12019900
H -7.00805600 1.56026400 -0.97924500

H -9.97365400 -1.90031700 -0.46104800
H -12.37864300 -1.24594600 -0.55891200
H -13.00378300 1.16121800 -0.52015600
H -11.22936900 2.89515300 -0.38070900
H -8.85834500 2.23960100 -0.28778300
H -5.30696500 2.82819900 0.31010100
H -3.68829400 4.57510300 -0.37680100
H -1.85998900 4.01999900 -1.96853300
H -1.66633100 1.71019800 -2.86793300
H -3.27724000 -0.03265500 -2.17297600

L-Anti-1SPT (ACN)

C -2.08591200 3.56573800 0.35753100
C -3.21032100 3.79305300 -0.43814900
C -4.20785800 2.82186900 -0.53405900
C -4.08213300 1.60225300 0.14871400
C -2.94774900 1.38258800 0.94646000
C -1.96047800 2.36036500 1.05377000
C -5.17193500 0.57894500 0.07679600
C -6.52030300 1.03821300 0.28868800
C -7.60205800 0.17985900 0.27045700
O -7.43652700 -1.12444800 0.07808100
N -4.97998000 -0.70978900 -0.10659000
C -9.00127600 0.60905900 0.48423500
C -9.39456800 1.95246900 0.35068300
C -10.71918800 2.32562700 0.56487000
C -11.67384800 1.36582700 0.91318600
C -11.29536400 0.02737700 1.04017100
C -9.97135500 -0.34979600 0.82417800
C -3.77615600 -1.32389900 -0.49721500
C -3.42516900 -2.53998200 0.10891500
C -2.28274800 -3.23173500 -0.29269000
C -1.46691300 -2.74952100 -1.32310400
C -1.83665500 -1.54606700 -1.94327900
C -2.96897500 -0.84248900 -1.54585500
C -0.22697600 -3.50824000 -1.76974700
C 1.07306400 -2.76097900 -1.52125800
C 1.84376100 -2.26932100 -2.58101700
C 3.03650000 -1.58443500 -2.35111400
C 3.48858000 -1.36875900 -1.04276100
C 2.71433700 -1.83888800 0.03014000
C 1.53189800 -2.53020900 -0.21557800
N 4.67578400 -0.62081500 -0.86834600
O 5.72916100 1.73238600 -1.48456900
C 6.50298600 1.57039800 -0.50571800

C 6.50100400 0.37635100 0.29514000
C 5.60057100 -0.66747800 0.12548400
C 7.48064300 2.66537300 -0.18532400
C 5.72427300 -1.87826100 0.98268200
C 7.72756100 3.63999500 -1.16580500
C 8.62022300 4.68168700 -0.92564400
C 9.27360600 4.77300400 0.30683300
C 9.02624200 3.81757700 1.29519100
C 8.13826100 2.76976800 1.05131900
C 5.90703500 -1.75007500 2.36819700
C 6.08422100 -2.88118900 3.16556200
C 6.09219800 -4.15199900 2.58741400
C 5.91901200 -4.28785300 1.20717800
C 5.73062900 -3.16104700 0.40954700
H -1.31289900 4.32400100 0.43801400
H -3.31407000 4.72686000 -0.98236200
H -5.08107600 3.00244700 -1.15349900
H -2.84705000 0.44946000 1.49062300
H -1.09342300 2.18234400 1.68262100
H -6.67258500 2.08246000 0.51882600
H -6.40511000 -1.25119800 -0.01650500
H -8.67166700 2.70572600 0.05660800
H -11.00876300 3.36591400 0.45222500
H -12.70595600 1.65947900 1.07901500
H -12.03195700 -0.72388500 1.30856200
H -9.67397800 -1.38740500 0.92293800
H -4.05397500 -2.93162800 0.90295700
H -2.02916100 -4.16807700 0.19792000
H -1.22988600 -1.15520700 -2.75625400
H -3.24339300 0.07531600 -2.05466600
H -0.30274700 -3.73474900 -2.83968200
H -0.19896900 -4.47249800 -1.24974600
H 1.51554500 -2.43114900 -3.60426000
H 3.62787100 -1.22169800 -3.18676100
H 3.03058300 -1.65481400 1.05015100
H 0.94408700 -2.88320100 0.62771700
H 4.80905000 0.20537900 -1.46617300
H 7.27784800 0.23522000 1.03253500
H 7.20850200 3.56002700 -2.11459900
H 8.80756000 5.42285200 -1.69703700
H 9.96810600 5.58592500 0.49705900
H 9.52145200 3.88993500 2.25882200
H 7.94319000 2.04969500 1.83863300
H 5.89392900 -0.76301700 2.81921900

H 6.21436100 -2.76838100 4.23749200
H 6.23315900 -5.03201000 3.20753200
H 5.93365100 -5.27284400 0.75073200
H 5.60406800 -3.27160300 -0.66233700

L-Syn-1SPT (ACN)

C 3.60434500 3.11014000 3.16437100
C 4.88892200 2.62230400 3.41119600
C 5.46332400 1.69289000 2.54304600
C 4.75055100 1.22377500 1.42900200
C 3.45904100 1.71965000 1.18902700
C 2.89373300 2.66041300 2.04803800
C 5.38560700 0.25839500 0.47743400
C 6.71510100 0.56802800 0.01847600
C 7.39263800 -0.23795700 -0.87482300
O 6.82696000 -1.33250400 -1.37328600
N 4.79714700 -0.81327500 -0.00821600
C 8.75811700 0.04189100 -1.36977500
C 9.61909500 0.93628400 -0.70935200
C 10.89722400 1.18279200 -1.20461900
C 11.33940100 0.53982600 -2.36437400
C 10.49521900 -0.35690600 -3.02315300
C 9.21647400 -0.60736800 -2.52919100
C 3.58776600 -1.37267600 0.44266100
C 2.68504700 -1.86180000 -0.51900100
C 1.50755900 -2.49366600 -0.13290000
C 1.19690300 -2.68626100 1.22212600
C 2.11062900 -2.21946900 2.17469900
C 3.28917600 -1.57435000 1.80032800
C -0.07641300 -3.40410600 1.63963400
C -1.35487900 -2.75535500 1.13613000
C -2.24455900 -3.45032000 0.30912700
C -3.41817000 -2.85575000 -0.15303800
C -3.73683700 -1.54083100 0.21057800
C -2.86499200 -0.84093700 1.06050600
C -1.68995600 -1.44240900 1.50068200
N -4.96582200 -1.01110400 -0.24400300
O -7.56038900 -1.55059800 -0.23454700
C -7.75197700 -0.32120800 -0.42177900
C -6.67348600 0.61430400 -0.59287900
C -5.33097400 0.27485300 -0.48530600
C -9.16906000 0.17296200 -0.49198200
C -4.29758700 1.31750900 -0.73291000
C -10.18971700 -0.77059900 -0.69251400
C -11.52286800 -0.37388100 -0.76202300

C -11.85931400 0.97554200 -0.62009900
C -10.85454300 1.92200200 -0.40658500
C -9.51862500 1.52527300 -0.34504600
C -4.41316200 2.58475600 -0.14128800
C -3.47717700 3.58177300 -0.41777000
C -2.42277400 3.32844900 -1.29711200
C -2.30592000 2.07173500 -1.89768200
C -3.23207400 1.07007200 -1.61453400
H 3.15994400 3.83906500 3.83532200
H 5.44665100 2.96677900 4.27676400
H 6.46303400 1.31664800 2.73751000
H 2.90451700 1.37527200 0.32242300
H 1.89847400 3.04418300 1.84518900
H 7.16775300 1.48954900 0.35393400
H 5.87350100 -1.35571100 -0.95319500
H 9.30101500 1.42426800 0.20557800
H 11.55234500 1.87176500 -0.68033900
H 12.33658200 0.73333700 -2.74795700
H 10.83258300 -0.86152600 -3.92345700
H 8.55828100 -1.30164300 -3.03856600
H 2.91935100 -1.73034100 -1.57126300
H 0.81967600 -2.84840700 -0.89603700
H 1.90410600 -2.37023800 3.23139900
H 3.98651500 -1.23771000 2.55985900
H -0.10272900 -3.46074600 2.73444400
H -0.04661400 -4.44022000 1.28136600
H -2.01798000 -4.47171900 0.01523500
H -4.08941400 -3.40697300 -0.80516300
H -3.11129900 0.16323600 1.38454500
H -1.02497300 -0.88295000 2.15324500
H -5.78073000 -1.63850700 -0.24625300
H -6.89747100 1.62943200 -0.88701800
H -9.91418300 -1.81449700 -0.79454700
H -12.30028000 -1.11421900 -0.92623200
H -12.89841100 1.28698300 -0.67161200
H -11.11083300 2.96995900 -0.28341700
H -8.75447400 2.27166900 -0.15725600
H -5.22890200 2.77985300 0.54749700
H -3.57220900 4.55459800 0.05474100
H -1.69617100 4.10528900 -1.51491200
H -1.49325800 1.87222900 -2.58945500
H -3.14109800 0.09815700 -2.08812900
L-Anti-1SPT (DCM)
C -2.11668700 3.61760400 0.36507100

C -3.25083400 3.85097600 -0.41466300
C -4.24127000 2.87358400 -0.51936600
C -4.09893300 1.64211800 0.13823000
C -2.95499200 1.41666000 0.92024800
C -1.97467700 2.40021600 1.03648100
C -5.18060400 0.61093100 0.05532700
C -6.53006800 1.05390900 0.29244400
C -7.60522000 0.18719700 0.26658300
O -7.43190800 -1.11022400 0.04161300
N -4.98027100 -0.67152700 -0.15978000
C -9.00536900 0.59943200 0.50659500
C -9.41026700 1.94292000 0.41789100
C -10.73532200 2.29918900 0.65603100
C -11.67922300 1.32191300 0.98394900
C -11.28933600 -0.01661300 1.06619800
C -9.96481500 -0.37675800 0.82626600
C -3.77677000 -1.26930500 -0.57488700
C -3.42384300 -2.50467600 -0.01028700
C -2.28254500 -3.18251200 -0.43730200
C -1.46863700 -2.66595800 -1.45236700
C -1.83977700 -1.44241700 -2.03093000
C -2.97159500 -0.75313400 -1.60855000
C -0.23023900 -3.40826400 -1.92655400
C 1.07594600 -2.68578100 -1.63697100
C 1.92479700 -2.27606100 -2.67118800
C 3.13143400 -1.63016700 -2.40416500
C 3.51880400 -1.37055900 -1.08314000
C 2.66394000 -1.75397800 -0.03715900
C 1.46877400 -2.40795900 -0.31911500
N 4.72726800 -0.66742700 -0.87496800
O 5.92641000 1.59446700 -1.55346200
C 6.62889100 1.45998000 -0.51914200
C 6.52147000 0.31629300 0.34668400
C 5.58598800 -0.69580900 0.17750900
C 7.63245800 2.53147500 -0.19865200
C 5.60039600 -1.85875400 1.10689600
C 7.96664400 3.44707000 -1.20949400
C 8.88636200 4.46548700 -0.97241200
C 9.48078100 4.59238200 0.28631400
C 9.14697700 3.69607300 1.30397100
C 8.23139300 2.67152100 1.06383100
C 5.70395900 -1.65754700 2.49184800
C 5.77884600 -2.74630700 3.36092700
C 5.76207400 -4.04784800 2.85635400

C 5.66700600 -4.25687400 1.47774500
C 5.58099600 -3.17194000 0.60796000
H -1.34864100 4.38020800 0.45204200
H -3.36741800 4.79415700 -0.93988500
H -5.12203500 3.05828700 -1.12690300
H -2.84096100 0.47350200 1.44407600
H -1.09942400 2.21688200 1.65231200
H -6.68751200 2.09100400 0.54982500
H -6.40121400 -1.22687100 -0.06784600
H -8.69587900 2.71033600 0.14003300
H -11.03378300 3.34018500 0.57801800
H -12.71188700 1.60223800 1.16858000
H -12.01763400 -0.78156100 1.31823700
H -9.65815300 -1.41438400 0.88966900
H -4.05159100 -2.92268600 0.77103800
H -2.02866000 -4.13538100 0.02040400
H -1.23399200 -1.02454700 -2.83111100
H -3.24698700 0.18073000 -2.08648100
H -0.29990200 -3.58536600 -3.00619900
H -0.21099100 -4.39714500 -1.45324600
H 1.64693300 -2.47225500 -3.70338000
H 3.78327900 -1.33128400 -3.21992500
H 2.92872200 -1.53138600 0.98973000
H 0.81801600 -2.69245300 0.50343300
H 4.93690700 0.11609800 -1.50764800
H 7.24377900 0.18460800 1.13918900
H 7.49194200 3.33968300 -2.17850800
H 9.14051800 5.16111300 -1.76679300
H 10.19657500 5.38728600 0.47404400
H 9.59639000 3.79661700 2.28739200
H 7.96969600 1.99809200 1.87280800
H 5.70939100 -0.64572800 2.88447500
H 5.84839900 -2.57663100 4.43105200
H 5.82324700 -4.89530200 3.53239900
H 5.66267000 -5.26676600 1.07908100
H 5.51370100 -3.33880800 -0.46194700

L-Syn-1SPT (DCM)

C 3.62310300 3.02172700 3.25937100
C 4.90946700 2.52969300 3.48634300
C 5.47931800 1.62265100 2.59220400
C 4.76098100 1.18028700 1.47101100
C 3.46743700 1.67971300 1.25183500
C 2.90639800 2.59811500 2.13706300
C 5.39227400 0.23920500 0.49236800

C 6.71875200 0.56292600 0.03477500
C 7.39457400 -0.22029900 -0.88010300
O 6.83171100 -1.30522300 -1.39935500
N 4.80311300 -0.82125300 -0.01536000
C 8.75619700 0.07583900 -1.37667100
C 9.61189700 0.97265500 -0.71326700
C 10.88541800 1.23484800 -1.21158100
C 11.32865100 0.60494400 -2.37778300
C 10.49011000 -0.29452900 -3.03938700
C 9.21585500 -0.56041000 -2.54246900
C 3.59377100 -1.38925600 0.42412900
C 2.68760300 -1.85019900 -0.54798600
C 1.50762700 -2.48512700 -0.17611600
C 1.19820800 -2.71023700 1.17392200
C 2.11556700 -2.27232200 2.13620400
C 3.29629100 -1.62334100 1.77650500
C -0.07818200 -3.43139200 1.57465500
C -1.35487700 -2.76980500 1.08334600
C -2.26749200 -3.46081900 0.27871800
C -3.44150500 -2.85616200 -0.16802700
C -3.73869400 -1.53417000 0.18890500
C -2.84260700 -0.83777600 1.01609900
C -1.66739400 -1.44961800 1.44044000
N -4.96851400 -0.99638600 -0.25103500
O -7.55901000 -1.53628400 -0.23632500
C -7.75396000 -0.30730000 -0.41263000
C -6.67634200 0.63222900 -0.57889400
C -5.33412100 0.29188300 -0.48164100
C -9.17229300 0.18424300 -0.47644400
C -4.30282300 1.33669800 -0.73002200
C -10.19049500 -0.76216300 -0.67346300
C -11.52465700 -0.36903900 -0.73902000
C -11.86452700 0.97922000 -0.59671400
C -10.86207600 1.92837000 -0.38611500
C -9.52518000 1.53516400 -0.32850300
C -4.41360500 2.59897500 -0.12734400
C -3.48191200 3.59950600 -0.40495100
C -2.43572800 3.35447300 -1.29600200
C -2.32279800 2.10248400 -1.90651500
C -3.24495700 1.09762500 -1.62265800
H 3.18173300 3.73319600 3.95087800
H 5.47187500 2.85333800 4.35705100
H 6.48028100 1.24185500 2.77132400
H 2.90742600 1.35391800 0.38168300

H 1.90884300 2.98422600 1.95027800
H 7.16840100 1.47975100 0.38661100
H 5.88139200 -1.34310400 -0.97743300
H 9.29306800 1.45086900 0.20659900
H 11.53637400 1.92605400 -0.68485700
H 12.32246000 0.81064100 -2.76400800
H 10.82856400 -0.78978200 -3.94455800
H 8.56150600 -1.25753800 -3.05276800
H 2.92187000 -1.69345400 -1.59677600
H 0.81558400 -2.81583800 -0.94624100
H 1.90979100 -2.44878300 3.18917300
H 3.99597300 -1.30799900 2.54293500
H -0.10631800 -3.51065100 2.66833300
H -0.05138100 -4.46096400 1.19713900
H -2.05881700 -4.48777500 -0.00953100
H -4.13113200 -3.40483800 -0.80301100
H -3.06968400 0.17254400 1.33451200
H -0.98252600 -0.89183300 2.07350100
H -5.78637900 -1.62101400 -0.25040900
H -6.90182300 1.64837100 -0.86843800
H -9.91028000 -1.80483000 -0.77455500
H -12.30058400 -1.11169400 -0.90023500
H -12.90472500 1.28779200 -0.64526400
H -11.12109200 2.97569900 -0.26233900
H -8.76208900 2.28326500 -0.14295900
H -5.22321600 2.78668100 0.57079700
H -3.57379900 4.56868300 0.07588700
H -1.71223700 4.13399400 -1.51501000
H -1.51575400 1.90882500 -2.60654500
H -3.15672700 0.12887600 -2.10308700

L-Anti-1SPT (CYH)

C -2.11158900 3.64065500 0.32801600
C -3.25668800 3.87713600 -0.43381900
C -4.24448100 2.89703900 -0.53441800
C -4.08971300 1.66008900 0.10937600
C -2.93454200 1.43186300 0.87317800
C -1.95646400 2.41761000 0.98521400
C -5.16906100 0.62559000 0.02887100
C -6.51574100 1.06308400 0.28888600
C -7.59040600 0.19529100 0.26560100
O -7.42090800 -1.09711800 0.01978500
N -4.96810000 -0.65301900 -0.20509800
C -8.98766700 0.60208000 0.53121500
C -9.39424800 1.94661300 0.48339600

C -10.71613800 2.29590700 0.74604800
C -11.65577700 1.30985900 1.05784200
C -11.26447500 -0.02972300 1.09878400
C -9.94303500 -0.38267700 0.83449600
C -3.76829700 -1.24423600 -0.63787500
C -3.41982900 -2.49338600 -0.10176700
C -2.28124600 -3.16529800 -0.54372100
C -1.46459300 -2.62851300 -1.54548300
C -1.83113900 -1.39115700 -2.09598600
C -2.96074300 -0.70823400 -1.65936300
C -0.22702500 -3.36167800 -2.03362800
C 1.08278600 -2.65876900 -1.71258400
C 1.97849000 -2.29400700 -2.72336600
C 3.19046000 -1.67241400 -2.42707300
C 3.53718300 -1.39025900 -1.09920300
C 2.63484900 -1.72820500 -0.07774100
C 1.43473600 -2.35879600 -0.38861900
N 4.75451400 -0.71282000 -0.86690200
O 6.03667000 1.48130400 -1.58888300
C 6.68744300 1.38437100 -0.52003300
C 6.51349500 0.28415800 0.39397200
C 5.56341000 -0.71220800 0.22589000
C 7.69824700 2.45084300 -0.20528300
C 5.50755200 -1.83261700 1.20501200
C 8.07075700 3.32742200 -1.23650000
C 8.99906900 4.33965500 -1.00911200
C 9.56442300 4.49910400 0.25885400
C 9.19250400 3.64170600 1.29605400
C 8.26753000 2.62370400 1.06614000
C 5.54491300 -1.57170100 2.58306100
C 5.55342300 -2.62076800 3.50233800
C 5.53509200 -3.94290200 3.05596700
C 5.50473800 -4.21177000 1.68515600
C 5.48504500 -3.16618600 0.76502000
H -1.34448500 4.40473600 0.41111200
H -3.38334900 4.82474000 -0.94894300
H -5.13395900 3.08267700 -1.12907200
H -2.80948800 0.48293800 1.38378500
H -1.07122700 2.23084900 1.58563100
H -6.66981800 2.09532100 0.56698500
H -6.39491100 -1.21451000 -0.10569000
H -8.68267100 2.72105000 0.21786100
H -11.01579400 3.33860000 0.69973000
H -12.68648700 1.58445100 1.26175000

H -11.98994000 -0.80181100 1.33737000
H -9.63344200 -1.42083900 0.86406200
H -4.05081000 -2.92632800 0.66869800
H -2.03185000 -4.13023800 -0.10896000
H -1.22160000 -0.95645600 -2.88425900
H -3.23197400 0.23726200 -2.11597500
H -0.28930900 -3.50578600 -3.11886800
H -0.21716000 -4.36629100 -1.59297500
H 1.73249100 -2.50634500 -3.76065000
H 3.87852200 -1.40722100 -3.22466900
H 2.86600000 -1.48673000 0.95284100
H 0.74536500 -2.60428000 0.41473400
H 5.01292600 0.03972200 -1.52035500
H 7.19839600 0.16995100 1.22170300
H 7.61546300 3.19293400 -2.21137000
H 9.28259000 5.00588400 -1.81876100
H 10.28750000 5.28943700 0.43868100
H 9.61965400 3.76780300 2.28660300
H 7.97540600 1.98075700 1.88942200
H 5.55132600 -0.54287000 2.92908000
H 5.57261200 -2.40416400 4.56622500
H 5.54455200 -4.76002900 3.77108600
H 5.49848700 -5.23847300 1.33172400
H 5.46648700 -3.37900300 -0.29862300

L-Syn-1SPT (CYH)

C -3.60108100 -2.94656500 3.31847500
C -4.88967600 -2.45787100 3.53811200
C -5.46509000 -1.56972700 2.62896300
C -4.75095900 -1.14305700 1.49928100
C -3.45487700 -1.63868300 1.28812100
C -2.88801300 -2.53816000 2.18856300
C -5.38922800 -0.22266300 0.50501800
C -6.71459000 -0.56247700 0.05662100
C -7.39788800 0.20067200 -0.86990100
O -6.84579000 1.28063700 -1.40764900
N -4.80673000 0.83158800 -0.02188700
C -8.75799400 -0.11389900 -1.35958400
C -9.60161000 -1.01681700 -0.68970500
C -10.87306600 -1.29641100 -1.18308300
C -11.32648800 -0.67775700 -2.35105800
C -10.50025900 0.22801300 -3.01891500
C -9.22805300 0.51116200 -2.52697100
C -3.59717700 1.40983800 0.40250300
C -2.69464400 1.85172900 -0.58165000

C -1.51292300 2.49222800 -0.22666600
C -1.19833300 2.74301200 1.11743000
C -2.11231100 2.32482800 2.09119500
C -3.29443400 1.66956400 1.74875200
C 0.08094200 3.46886800 1.49859500
C 1.35536400 2.79360500 1.01984800
C 2.28537100 3.47599700 0.22826800
C 3.45860800 2.86020600 -0.20397900
C 3.73863000 1.53479600 0.15475600
C 2.82399000 0.84681000 0.96852700
C 1.64971000 1.46989600 1.37811500
N 4.96786300 0.98701300 -0.27164000
O 7.55453700 1.51800000 -0.24216600
C 7.75026400 0.28891000 -0.40485500
C 6.67100700 -0.65128900 -0.57090600
C 5.33035100 -0.30528400 -0.48804800
C 9.16884400 -0.20399200 -0.45173700
C 4.29731900 -1.34839700 -0.73746000
C 10.18893600 0.74432300 -0.62649500
C 11.52371300 0.35201600 -0.67639500
C 11.86217700 -0.99705800 -0.54108500
C 10.85756300 -1.94813400 -0.35267700
C 9.52013200 -1.55560700 -0.31013300
C 4.39781800 -2.60598600 -0.12366800
C 3.46583900 -3.60592900 -0.40171400
C 2.42856600 -3.36489000 -1.30379800
C 2.32505000 -2.11740700 -1.92455300
C 3.24794600 -1.11348000 -1.64078800
H -3.15494000 -3.64330400 4.02193000
H -5.44936400 -2.76930700 4.41512000
H -6.46784900 -1.19065300 2.80207700
H -2.89719400 -1.32317600 0.41277100
H -1.88803300 -2.92109700 2.00789300
H -7.15562300 -1.47796200 0.42252000
H -5.89614300 1.33457700 -0.99109200
H -9.27460200 -1.48662200 0.23166300
H -11.51465600 -1.99259900 -0.65125600
H -12.31888700 -0.89697700 -2.73368900
H -10.84698600 0.71518800 -3.92542300
H -8.58243200 1.21382000 -3.04065500
H -2.93402700 1.67508900 -1.62609700
H -0.82247000 2.80666200 -1.00501500
H -1.90238700 2.52179900 3.13979000
H -3.99125600 1.36866400 2.52350800

H 0.11200600 3.57312900 2.59037400
H 0.05623000 4.49036600 1.09911900
H 2.09092300 4.50558500 -0.06100500
H 4.16223600 3.40240500 -0.82917500
H 3.03589500 -0.16646500 1.28776900
H 0.94965000 0.91788000 1.99948700
H 5.79068900 1.60637200 -0.26735800
H 6.89546800 -1.66961100 -0.85350400
H 9.90731200 1.78713800 -0.72154000
H 12.30166500 1.09631300 -0.81979300
H 12.90316600 -1.30495500 -0.57774400
H 11.11540600 -2.99650100 -0.23446000
H 8.75463300 -2.30531900 -0.14155100
H 5.20062100 -2.78956200 0.58347300
H 3.55045200 -4.57167300 0.08755100
H 1.70459200 -4.14393700 -1.52331400
H 1.52440000 -1.92641700 -2.63271500
H 3.16692400 -0.14772800 -2.12838100

L-Anti-2SPT (ACN)

C 2.41748700 3.78001700 -0.27596800
C 3.56066100 3.90583100 0.51553600
C 4.48936200 2.86634700 0.57502500
C 4.27871300 1.68269900 -0.14885300
C 3.12457800 1.56337900 -0.94106000
C 2.20477200 2.60785800 -1.00703500
C 5.30032300 0.59998700 -0.13226600
C 6.63518700 0.92715400 -0.33331500
C 7.69741600 -0.04045400 -0.38711300
O 7.48985200 -1.28006100 -0.32738900
N 4.92394000 -0.69942900 -0.01000700
C 9.11355700 0.43480900 -0.54837800
C 9.51616600 1.75318600 -0.27944800
C 10.84915600 2.13267300 -0.43760000
C 11.79759300 1.20321100 -0.87071600
C 11.40868600 -0.11320000 -1.13549700
C 10.07932000 -0.49377200 -0.96945000
C 3.72891100 -1.26084000 0.49422100
C 3.34378300 -2.51796900 0.01023600
C 2.20319200 -3.14659700 0.50855800
C 1.41099300 -2.54138600 1.49080500
C 1.81291500 -1.28707400 1.97456300
C 2.95822900 -0.65516400 1.50004900
C 0.15839200 -3.21665600 2.02266300
C -1.13258100 -2.49047100 1.67685200

C -2.00042000 -2.03679400 2.67733300
C -3.18689900 -1.37550300 2.36111700
C -3.55593000 -1.16801400 1.02313700
C -2.67907000 -1.60682100 0.01261400
C -1.49223700 -2.25403600 0.34101700
N -4.72346300 -0.42816800 0.76032800
O -5.79415600 1.78918000 1.18518200
C -6.69200600 1.49112700 0.25188400
C -6.64434600 0.28469200 -0.41858200
C -5.61648200 -0.69257300 -0.16887000
C -7.72503300 2.52514300 0.02423600
C -5.68430100 -1.96917500 -0.94720800
C -7.89049200 3.55198600 0.97005500
C -8.86081300 4.53523700 0.78684100
C -9.67799000 4.51337500 -0.34554000
C -9.51528700 3.50250700 -1.29720800
C -8.54705300 2.51786900 -1.11673600
C -5.88133100 -1.94296900 -2.33638500
C -5.98384300 -3.13201000 -3.05964400
C -5.91299800 -4.36069200 -2.40052700
C -5.73284300 -4.39559500 -1.01494800
C -5.61306000 -3.20946300 -0.29300500
H 1.69621400 4.59011200 -0.32435300
H 3.73054900 4.81201500 1.08884700
H 5.37407100 2.96195400 1.19636100
H 2.95860200 0.65848100 -1.51623000
H 1.32249000 2.50796700 -1.63181400
H 6.85838400 1.96653400 -0.52573100
H 5.71685400 -1.33525700 -0.16790500
H 8.79832100 2.48358800 0.07773400
H 11.14756500 3.15349300 -0.21860100
H 12.83405300 1.50174200 -0.99716400
H 12.14229900 -0.84047600 -1.47062400
H 9.76381300 -1.51277800 -1.16482000
H 3.93781800 -2.99719600 -0.76248000
H 1.92539600 -4.12300000 0.12072400
H 1.22600700 -0.80037500 2.74909100
H 3.26033700 0.29818600 1.91700600
H 0.22704600 -3.30869400 3.11280600
H 0.11786000 -4.23967700 1.62963300
H -1.74464800 -2.19780500 3.72153700
H -3.84435600 -1.01967300 3.14878600
H -2.92682300 -1.42469800 -1.02763400
H -0.82658600 -2.57421000 -0.45648000

H -5.17574000 0.95123700 1.23896600
H -7.42323300 0.03406100 -1.12355200
H -7.25652500 3.56559000 1.84897000
H -8.97988200 5.31845900 1.52941900
H -10.43294800 5.28043000 -0.48913100
H -10.13868000 3.48555700 -2.18591100
H -8.41860400 1.75571800 -1.87765200
H -5.93839400 -0.98930400 -2.85222400
H -6.12267800 -3.09712300 -4.13594700
H -6.00065600 -5.28614000 -2.96163700
H -5.68741500 -5.34806800 -0.49559100
H -5.47568600 -3.24158200 0.78269500

L-Syn-2SPT (ACN)

C 3.82929700 3.30593100 3.00048400
C 5.07721400 2.73463000 3.25612400
C 5.58782100 1.75653700 2.40217700
C 4.84924300 1.32996600 1.28783100
C 3.59293200 1.90780500 1.03947200
C 3.09111200 2.89266100 1.88780300
C 5.42169600 0.33153000 0.34354000
C 6.72277200 0.49904300 -0.11163500
C 7.36097700 -0.38012900 -1.05412500
O 6.75523200 -1.33189800 -1.61077600
N 4.65152900 -0.68084000 -0.13452200
C 8.80144200 -0.14950200 -1.41350000
C 9.67049600 0.63580000 -0.63849800
C 11.00309800 0.80059200 -1.01655200
C 11.48570400 0.18785900 -2.17526000
C 10.63052900 -0.60019900 -2.95109000
C 9.30219600 -0.77081900 -2.56911700
C 3.47463500 -1.25803700 0.39434200
C 2.59340100 -1.87971600 -0.50543800
C 1.44714100 -2.51711700 -0.04292500
C 1.13719800 -2.55292400 1.32478800
C 2.02613800 -1.93517300 2.21197400
C 3.18680600 -1.30329800 1.76464100
C -0.11699500 -3.25303100 1.82345900
C -1.41107300 -2.62506600 1.33247900
C -2.26098000 -3.30552800 0.45222000
C -3.45231000 -2.73233000 0.00862400
C -3.82149300 -1.44149900 0.41745200
C -2.97884700 -0.75852600 1.31554500
C -1.79712000 -1.34451600 1.75774000
N -5.07159700 -0.94571600 0.00477800

O -7.51486900 -1.46663200 0.06082600
C -7.74904300 -0.22246100 -0.34313800
C -6.70904000 0.65416900 -0.58213200
C -5.33147100 0.28435300 -0.38305300
C -9.17654000 0.11599800 -0.53199600
C -4.29479100 1.31677900 -0.69825700
C -10.12321800 -0.91942600 -0.61985100
C -11.47383200 -0.63117500 -0.80574700
C -11.90252200 0.69477000 -0.90010300
C -10.97073800 1.73226300 -0.80364200
C -9.61988100 1.44759200 -0.61970400
C -4.43494600 2.62993700 -0.22351500
C -3.49072200 3.60482300 -0.54800400
C -2.40735700 3.28448900 -1.36830200
C -2.26908900 1.98311900 -1.85887600
C -3.20172200 1.00380400 -1.52216100
H 3.43342500 4.06940700 3.66323800
H 5.65435700 3.04821700 4.12058800
H 6.55481400 1.30761800 2.60541300
H 3.01954000 1.59467000 0.17323200
H 2.12412700 3.34001000 1.67901700
H 7.24793300 1.38047700 0.22668300
H 5.13058300 -1.19259700 -0.88686500
H 9.32026100 1.10230000 0.27583500
H 11.66543100 1.40428600 -0.40341100
H 12.52254300 0.32041600 -2.46976800
H 11.00077200 -1.08052800 -3.85200900
H 8.62842100 -1.38451300 -3.15685300
H 2.81360800 -1.85429400 -1.56879700
H 0.77756100 -2.98782600 -0.75774200
H 1.82204000 -1.96307600 3.27913000
H 3.86943600 -0.86188500 2.48084200
H -0.10385000 -3.25637000 2.91942400
H -0.09568900 -4.30348500 1.51044500
H -1.99528900 -4.30453600 0.11593400
H -4.10713700 -3.27739300 -0.66471100
H -3.26409100 0.22410600 1.67562700
H -1.16387800 -0.79873100 2.45281200
H -6.47557100 -1.54157700 0.10600400
H -6.92026700 1.63700200 -0.97711800
H -9.78713300 -1.94729500 -0.54774700
H -12.19214200 -1.44225800 -0.87785700
H -12.95518800 0.91948400 -1.04273700
H -11.29805700 2.76570800 -0.86364300

H -8.91401800 2.26519000 -0.52152800
H -5.27685500 2.88307000 0.41361000
H -3.60434600 4.61362700 -0.16287700
H -1.67642500 4.04446000 -1.62748300
H -1.43454700 1.73107200 -2.50615900
H -3.09149900 -0.00447800 -1.90718500

L-Anti-2SPT (DCM)

C 2.43883200 3.80294700 -0.27582500
C 3.58446800 3.92585600 0.51235700
C 4.50845200 2.88232100 0.57251200
C 4.29090400 1.69765300 -0.14747000
C 3.13437200 1.58148700 -0.93639000
C 2.21913100 2.62976500 -1.00289400
C 5.30730900 0.61004300 -0.12913000
C 6.64282700 0.93005200 -0.33478700
C 7.70008200 -0.04383800 -0.38899300
O 7.48551500 -1.28135700 -0.32503200
N 4.92553600 -0.68745400 -0.00062300
C 9.11859400 0.42245200 -0.55561100
C 9.52925600 1.74054200 -0.29876100
C 10.86421000 2.11075500 -0.46127900
C 11.80659500 1.17190500 -0.88679500
C 11.40959400 -0.14432800 -1.13950000
C 10.07825500 -0.51553100 -0.96912900
C 3.73037200 -1.24344300 0.50810400
C 3.34853100 -2.50707600 0.03844900
C 2.20762400 -3.13150500 0.54085800
C 1.41121400 -2.51587900 1.51297800
C 1.80945400 -1.25511600 1.98225200
C 2.95513900 -0.62711400 1.50393700
C 0.15878300 -3.18709400 2.04989300
C -1.13369100 -2.46706100 1.69685500
C -2.01243800 -2.02411300 2.69242200
C -3.20146000 -1.37076100 2.37002300
C -3.56217100 -1.16100500 1.03022100
C -2.67424200 -1.58870100 0.02478900
C -1.48483400 -2.22753300 0.35949700
N -4.73385600 -0.42992500 0.76203000
O -5.82728300 1.77735500 1.18754900
C -6.71632900 1.47412100 0.24825700
C -6.65333400 0.27070900 -0.42646700
C -5.61823300 -0.69807900 -0.17405300
C -7.75771200 2.49938600 0.01865000
C -5.66927900 -1.97158500 -0.95905900

C -7.93229600 3.52496600 0.96394900
C -8.91026800 4.50023500 0.77965000
C -9.72624700 4.47167500 -0.35325400
C -9.55457700 3.46203700 -1.30444800
C -8.57859000 2.48545800 -1.12287400
C -5.85878300 -1.94044500 -2.34910700
C -5.94606100 -3.12654300 -3.07898200
C -5.86699600 -4.35773200 -2.42578300
C -5.69380400 -4.39782900 -1.03960600
C -5.58941700 -3.21443300 -0.31103600
H 1.72078000 4.61592200 -0.32438600
H 3.75967800 4.83285300 1.08287800
H 5.39501400 2.97501500 1.19172200
H 2.96259100 0.67522900 -1.50762800
H 1.33437500 2.53169200 -1.62445300
H 6.87018100 1.96739700 -0.53331600
H 5.71657900 -1.32644400 -0.15712200
H 8.81593700 2.47825700 0.05249500
H 11.16897900 3.13173100 -0.25167600
H 12.84477400 1.46311000 -1.01662400
H 12.13866300 -0.87901700 -1.46844800
H 9.75549300 -1.53413500 -1.15429900
H 3.94611900 -2.99479000 -0.72624400
H 1.93302100 -4.11336500 0.16446700
H 1.21848500 -0.75938400 2.74789000
H 3.25351800 0.33199500 1.90996800
H 0.22667800 -3.26927600 3.14098700
H 0.12009400 -4.21426600 1.66712800
H -1.76312300 -2.18725700 3.73793600
H -3.86750800 -1.02253200 3.15386100
H -2.91553500 -1.40414100 -1.01652700
H -0.80996200 -2.53808900 -0.43399600
H -5.20130900 0.94604100 1.24280300
H -7.42627400 0.01473000 -1.13601400
H -7.29853000 3.54353600 1.84286100
H -9.03612800 5.28275100 1.52191300
H -10.48729100 5.23260400 -0.49768500
H -10.17712500 3.43984400 -2.19370300
H -8.44327400 1.72412700 -1.88345500
H -5.92176800 -0.98454600 -2.86020300
H -6.07926800 -3.08753300 -4.15590900
H -5.94266700 -5.28115000 -2.99202700
H -5.64150200 -5.35243600 -0.52479400
H -5.45673900 -3.25052000 0.76508000

L-Syn-2SPT (DCM)

C 3.90888400 3.17559700 3.19732800
C 5.15576800 2.58517800 3.40973800
C 5.64833300 1.64430200 2.50509200
C 4.89333800 1.27455700 1.38164900
C 3.63794300 1.87093000 1.17770800
C 3.15377700 2.81829300 2.07698100
C 5.44668900 0.31756700 0.38421600
C 6.74275700 0.49642300 -0.07873600
C 7.35895700 -0.34210600 -1.07340300
O 6.73560100 -1.25987100 -1.66362700
N 4.66219200 -0.66493600 -0.13191600
C 8.79588600 -0.10809700 -1.44555300
C 9.67992300 0.65348000 -0.66449400
C 11.00720800 0.82272600 -1.05818300
C 11.46970700 0.23711300 -2.23855600
C 10.59968700 -0.52799900 -3.02034700
C 9.27650800 -0.70232800 -2.62339200
C 3.48385700 -1.25305100 0.38043300
C 2.58386300 -1.81509200 -0.53968900
C 1.43262300 -2.45757200 -0.09809500
C 1.13635600 -2.55898300 1.26913000
C 2.04354900 -2.00038600 2.17632400
C 3.20905600 -1.36370000 1.74945800
C -0.12062300 -3.26878100 1.74574700
C -1.41464800 -2.63203400 1.26667100
C -2.28833700 -3.31538700 0.41288300
C -3.48277500 -2.73661600 -0.01405900
C -3.83172900 -1.43720400 0.38489500
C -2.96406600 -0.75071400 1.25593700
C -1.77946700 -1.34211500 1.68149300
N -5.08505300 -0.93684000 -0.01070000
O -7.53121700 -1.44812300 0.08300700
C -7.76531000 -0.20659800 -0.32523000
C -6.72541600 0.66533300 -0.58260200
C -5.34670100 0.29194500 -0.40042900
C -9.19410700 0.13533400 -0.49814000
C -4.31212300 1.32126500 -0.73380800
C -10.14494100 -0.89790800 -0.55708800
C -11.49698100 -0.60788500 -0.72748700
C -11.92309400 0.71759000 -0.83505600
C -10.98702200 1.75313500 -0.76713900
C -9.63480200 1.46654100 -0.59864400
C -4.44370500 2.63636200 -0.26241400

C -3.50330400 3.60895000 -0.60367900
C -2.43183900 3.28413900 -1.43732100
C -2.30159100 1.98067700 -1.92370400
C -3.23046600 1.00392800 -1.57049500
H 3.52679600 3.91005000 3.89991700
H 5.74602700 2.85473500 4.28030400
H 6.61434800 1.17929200 2.67446700
H 3.05061200 1.60069600 0.30646100
H 2.18663400 3.27976300 1.90209600
H 7.27829300 1.35857400 0.29141600
H 5.13137900 -1.14618900 -0.91109700
H 9.34541900 1.09829200 0.26641600
H 11.68135700 1.40852600 -0.44038300
H 12.50274400 0.37271000 -2.54516300
H 10.95454100 -0.98806600 -3.93796500
H 8.59003000 -1.29875900 -3.21404000
H 2.79392200 -1.73780200 -1.60263200
H 0.74715600 -2.87921100 -0.82828800
H 1.84948600 -2.07922400 3.24293400
H 3.90494400 -0.96762200 2.47933200
H -0.11084100 -3.29895900 2.84169200
H -0.09826200 -4.31253000 1.41015500
H -2.03916200 -4.32156700 0.08504000
H -4.15692700 -3.28358700 -0.66643000
H -3.23197900 0.23964800 1.60774700
H -1.12545600 -0.79280200 2.35410800
H -6.49321800 -1.52834100 0.11535400
H -6.93813400 1.64551100 -0.98334100
H -9.80955200 -1.92505900 -0.47358800
H -12.21876100 -1.41767800 -0.77691000
H -12.97712200 0.94362200 -0.96566900
H -11.31215000 2.78672800 -0.83741300
H -8.92477400 2.28293800 -0.52240700
H -5.27653200 2.89217200 0.38566100
H -3.61050200 4.61956500 -0.22111500
H -1.70363800 4.04222100 -1.70975000
H -1.47555200 1.72451300 -2.58025500
H -3.12589900 -0.00659300 -1.95101500

L-Anti-2SPT (CYH)

C -2.43057900 3.79096000 0.41335100
C -3.56066900 3.94052900 -0.39175200
C -4.48926100 2.90466200 -0.49442400
C -4.29290500 1.70147900 0.19989700
C -3.15180600 1.55904400 1.00607200

C -2.23157600 2.59899700 1.11460000
C -5.31505100 0.62080000 0.13459800
C -6.65026600 0.94278600 0.32950500
C -7.71216300 -0.03064900 0.34735700
O -7.49870100 -1.26406800 0.25299100
N -4.93945900 -0.67598000 -0.02474700
C -9.13165300 0.43297000 0.51303500
C -9.53789500 1.76026400 0.30461200
C -10.87414400 2.12545700 0.46512100
C -11.82198700 1.17143400 0.84037700
C -11.42909400 -0.15407900 1.04415800
C -10.09641200 -0.51991000 0.87592100
C -3.74182600 -1.22909600 -0.52697800
C -3.39582000 -2.51959600 -0.10441600
C -2.25173900 -3.14227100 -0.60049400
C -1.41550900 -2.49977900 -1.51975600
C -1.77673200 -1.21197900 -1.94191100
C -2.92493400 -0.58448500 -1.47034100
C -0.16290000 -3.17269200 -2.05394800
C 1.13178100 -2.45728000 -1.70179500
C 2.02407200 -2.04078800 -2.69620900
C 3.21567200 -1.39282000 -2.37431200
C 3.56562900 -1.16241900 -1.03525800
C 2.66401900 -1.56359900 -0.03137200
C 1.47194900 -2.19640500 -0.36600700
N 4.74280200 -0.43976600 -0.77035300
O 5.87424200 1.74701900 -1.22897500
C 6.75008500 1.44665700 -0.27868300
C 6.66283300 0.25804300 0.41944700
C 5.61535600 -0.69985300 0.17815600
C 7.80648600 2.45945800 -0.06175000
C 5.64096100 -1.95596800 0.99288700
C 7.99312800 3.47083200 -1.01930700
C 8.98489500 4.43409200 -0.84856700
C 9.80294400 4.40790200 0.28237900
C 9.61924700 3.41263700 1.24579500
C 8.62937300 2.44823500 1.07773700
C 5.82172700 -1.89512000 2.38287800
C 5.88603400 -3.06404300 3.14171300
C 5.79164100 -4.30888500 2.51798200
C 5.62598400 -4.37915400 1.13251600
C 5.54503100 -3.21254600 0.37510500
H -1.70799200 4.59742700 0.49422500
H -3.71971700 4.86242300 -0.94309400

H -5.36392900 3.01645800 -1.12742100
H -2.99562700 0.63671000 1.55555800
H -1.35784000 2.47920000 1.74793100
H -6.87475000 1.97451400 0.55855400
H -5.74064900 -1.31116700 0.09951600
H -8.81899300 2.51013400 -0.00759700
H -11.17587800 3.15453100 0.29333200
H -12.86166600 1.45843400 0.96883900
H -12.16307100 -0.90077300 1.33310000
H -9.77349700 -1.54489900 1.02104000
H -4.02527000 -3.02924300 0.61947300
H -2.00586600 -4.14514700 -0.26080700
H -1.15154800 -0.69238800 -2.66322000
H -3.19208000 0.39802700 -1.84001900
H -0.22997100 -3.25760300 -3.14540500
H -0.12782700 -4.20055100 -1.67160200
H 1.78279400 -2.22038600 -3.74109500
H 3.89266700 -1.06350900 -3.15690000
H 2.89738400 -1.36250300 1.00862400
H 0.78468300 -2.48423900 0.42537700
H 5.23540400 0.92886000 -1.27605100
H 7.42872000 0.00196900 1.13652400
H 7.35559800 3.48647000 -1.89542800
H 9.11976600 5.20614000 -1.60031700
H 10.57506200 5.15978300 0.41600100
H 10.24361400 3.39240100 2.13400800
H 8.48439500 1.69781500 1.84743700
H 5.89592500 -0.92761700 2.87040300
H 6.01292000 -3.00125000 4.21843300
H 5.84905500 -5.21961100 3.10667500
H 5.56057800 -5.34491700 0.64034600
H 5.41632400 -3.27181300 -0.70037800

L-Syn-2SPT (CYH)

C -4.07923500 -2.61490500 3.78870300
C -5.31834300 -1.97676900 3.85973000
C -5.76387800 -1.19286400 2.79537400
C -4.96985900 -1.02949100 1.65032400
C -3.72261900 -1.67255300 1.58912100
C -3.28516500 -2.46323100 2.64910600
C -5.47482500 -0.24564700 0.48926100
C -6.75871300 -0.48304700 0.02176500
C -7.32410300 0.17429000 -1.12936400
O -6.66405200 0.96271700 -1.84886900
N -4.65754600 0.62407100 -0.16226900

C -8.74975100 -0.10921500 -1.50845200
C -9.68289600 -0.67103900 -0.62322000
C -10.99717800 -0.89893500 -1.02999400
C -11.39561300 -0.57397000 -2.32808100
C -10.47571600 -0.00888000 -3.21542100
C -9.16609800 0.22699100 -2.80612300
C -3.48130300 1.27288200 0.27228100
C -2.56279100 1.67735700 -0.71061100
C -1.40774000 2.36515100 -0.35764900
C -1.12432400 2.67001700 0.98170100
C -2.04965900 2.26831900 1.95090100
C -3.21974700 1.58910200 1.61149300
C 0.13622600 3.42970500 1.36069600
C 1.42894900 2.74403800 0.95093200
C 2.33115300 3.35843800 0.07513800
C 3.52835300 2.73983600 -0.28180100
C 3.85119500 1.46666200 0.21157800
C 2.95326500 0.84890900 1.10283500
C 1.76675700 1.48046100 1.45866100
N 5.10724700 0.92665200 -0.11703100
O 7.56211700 1.39781500 0.03227200
C 7.78289700 0.13294800 -0.30149400
C 6.73459200 -0.73245900 -0.54706800
C 5.35857100 -0.32565900 -0.42952500
C 9.20966800 -0.24415800 -0.40509400
C 4.31509900 -1.35491400 -0.73577100
C 10.18337300 0.76723600 -0.46295300
C 11.53464200 0.44474400 -0.56628700
C 11.93700800 -0.89149200 -0.60736100
C 10.97762600 -1.90516600 -0.54035500
C 9.62631700 -1.58609800 -0.43843700
C 4.41128700 -2.64500400 -0.19256500
C 3.46313000 -3.61904300 -0.50624700
C 2.41857900 -3.32165800 -1.38273300
C 2.32322200 -2.04396900 -1.93968200
C 3.25996900 -1.06522000 -1.61487100
H -3.73326300 -3.22736500 4.61598900
H -5.93897000 -2.08682800 4.74394500
H -6.72375800 -0.68934900 2.85264500
H -3.10512900 -1.56091200 0.70411900
H -2.32364400 -2.96365900 2.58486500
H -7.32163500 -1.26425700 0.51202500
H -5.09748400 0.96887300 -1.02716300
H -9.39523500 -0.90973700 0.39514500

H -11.71097400 -1.32659200 -0.33205000
H -12.41841600 -0.75590200 -2.64520700
H -10.78180500 0.24840600 -4.22531700
H -8.44070800 0.67283100 -3.47767000
H -2.76237800 1.44109200 -1.75199000
H -0.70738900 2.66102400 -1.13401400
H -1.86590800 2.50652200 2.99554200
H -3.92909700 1.31856600 2.38424200
H 0.13481200 3.58964600 2.44585500
H 0.11045600 4.42812600 0.90706900
H 2.10193200 4.34285500 -0.32566200
H 4.22535000 3.23388900 -0.95207700
H 3.19975300 -0.11950500 1.52457700
H 1.08832900 0.98393900 2.14785600
H 6.52809100 1.50162500 0.02656900
H 6.94031300 -1.73562900 -0.89032300
H 9.86481100 1.80249400 -0.42981100
H 12.27466700 1.23803100 -0.61500100
H 12.99058300 -1.14278100 -0.68576600
H 11.28374400 -2.94684300 -0.55951600
H 8.89679300 -2.38510400 -0.36178600
H 5.22297700 -2.87865500 0.48991200
H 3.54300800 -4.60967800 -0.06844100
H 1.68407200 -4.08123000 -1.63351100
H 1.51759400 -1.80925600 -2.62886500
H 3.18215700 -0.07415400 -2.04896600

L-Anti-DPT (ACN)

C -2.17355400 3.60287200 0.49918600
C -3.29174900 3.84313600 -0.30143900
C -4.27552700 2.86332900 -0.44190600
C -4.14163800 1.62277300 0.20030600
C -3.01364200 1.39021000 1.00336500
C -2.04047300 2.37614000 1.15554500
C -5.21731600 0.58891700 0.08135300
C -6.57322700 1.02304900 0.29849100
C -7.64341700 0.15205000 0.24196200
O -7.45948100 -1.14228400 0.00388900
N -5.00700600 -0.68965200 -0.14683200
C -9.04952900 0.55499000 0.46163200
C -9.45917500 1.89746300 0.37677900
C -10.78986600 2.24558000 0.59540000
C -11.73459300 1.26128200 0.89959000
C -11.33982600 -0.07617900 0.97796900
C -10.00960800 -0.42822700 0.75759700

C -3.79101600 -1.27385500 -0.54600000
C -3.42878500 -2.50455200 0.02270300
C -2.27213600 -3.16596800 -0.38921700
C -1.45199600 -2.63778800 -1.39344800
C -1.83354000 -1.41988900 -1.97754800
C -2.98043900 -0.74648400 -1.56970600
C -0.19436100 -3.36016600 -1.84816800
C 1.09321700 -2.60875500 -1.54846600
C 1.93766500 -2.17333000 -2.57668100
C 3.11608300 -1.48001600 -2.30095900
C 3.50111700 -1.22225100 -0.97645300
C 2.64849100 -1.64400600 0.06168700
C 1.46891200 -2.32258300 -0.22683400
N 4.65889800 -0.45384400 -0.75413800
O 5.67444200 1.77686100 -1.24234600
C 6.59584900 1.51541000 -0.32101300
C 6.58702800 0.32124000 0.37239500
C 5.57427500 -0.68112700 0.16293300
C 7.61052500 2.57484200 -0.13113500
C 5.68202500 -1.93889900 0.96690900
C 7.74183400 3.58467000 -1.10025300
C 8.69517300 4.59018600 -0.95159500
C 9.52875600 4.60787700 0.16889400
C 9.39955500 3.61435700 1.14366700
C 8.44848100 2.60761600 0.99774200
C 5.91093100 -1.87820100 2.35011800
C 6.05286700 -3.04864700 3.09665000
C 5.98962900 -4.29289400 2.46659500
C 5.77756300 -4.36201800 1.08685400
C 5.61854100 -3.19469700 0.34214800
H -1.41138500 4.36758000 0.61458500
H -3.40148600 4.79365000 -0.81466900
H -5.14417800 3.05410600 -1.06472300
H -2.90705900 0.44028900 1.51647900
H -1.17835400 2.18766100 1.78812900
H -6.74062700 2.05640000 0.56452100
H -6.42603800 -1.25240400 -0.08764200
H -8.74405200 2.67054000 0.11718300
H -11.09182800 3.28575900 0.52063400
H -12.77148100 1.53536000 1.06904500
H -12.06853700 -0.84639800 1.21196400
H -9.69975800 -1.46507100 0.81916100
H -4.06002200 -2.93142200 0.79641300
H -2.00996500 -4.11440100 0.07284600

H -1.22346000 -0.99377900 -2.77011900
H -3.26319700 0.18355800 -2.05110000
H -0.24838600 -3.54575200 -2.92732600
H -0.16272600 -4.34498500 -1.36713600
H 1.66971200 -2.37443900 -3.61084000
H 3.75531300 -1.13920800 -3.11000300
H 2.90989400 -1.42440300 1.09135700
H 0.82148300 -2.62935900 0.59078100
H 5.07322500 0.92525400 -1.26818100
H 7.38526500 0.10086000 1.06577600
H 7.09502300 3.56726500 -1.96971300
H 8.78815500 5.35989500 -1.71181900
H 10.27039000 5.39232600 0.28543600
H 10.03563800 3.62829800 2.02339600
H 8.34545700 1.85933600 1.77611600
H 5.96253200 -0.91237700 2.84344600
H 6.21640300 -2.98711100 4.16828400
H 6.10789000 -5.20379200 3.04560900
H 5.73782100 -5.32650100 0.58966400
H 5.45677200 -3.25361600 -0.72899800

L-Syn-DPT (ACN)

C 3.52072700 3.01291800 3.21113700
C 4.80849500 2.53039300 3.45174000
C 5.39361300 1.62529800 2.56527200
C 4.68874700 1.17526800 1.43837700
C 3.39387400 1.66549500 1.20491200
C 2.81771500 2.58216800 2.08256900
C 5.33583000 0.23750700 0.46763000
C 6.66570000 0.56699400 0.02346800
C 7.35416500 -0.21466800 -0.88312800
O 6.79895800 -1.30194900 -1.40820800
N 4.75790800 -0.82652000 -0.04648300
C 8.72072500 0.08476300 -1.36367900
C 9.56908600 0.97672200 -0.68388000
C 10.84834800 1.24199100 -1.16629300
C 11.30449800 0.62045800 -2.33231200
C 10.47307500 -0.27381700 -3.01034200
C 9.19315600 -0.54291500 -2.52937000
C 3.54988300 -1.40553600 0.38322300
C 2.65371600 -1.87173500 -0.59577000
C 1.47979800 -2.52335700 -0.23248900
C 1.16680200 -2.75998000 1.11494100
C 2.07397800 -2.31530500 2.08418400
C 3.24832800 -1.64935900 1.73319600

C -0.10527400 -3.49633600 1.50454900
C -1.38443400 -2.80252900 1.06662100
C -2.24821900 -3.39021500 0.13460300
C -3.42910400 -2.75942900 -0.25580400
C -3.77316500 -1.50093000 0.26086400
C -2.91594800 -0.91087900 1.20962300
C -1.74524100 -1.55442400 1.59779800
N -5.01515800 -0.94923800 -0.10313000
O -7.46820300 -1.42044700 -0.06282200
C -7.67830700 -0.14472600 -0.36996800
C -6.62122200 0.72497600 -0.55280900
C -5.25064200 0.31176000 -0.39505800
C -9.09968600 0.23746100 -0.51718000
C -4.19307500 1.34163800 -0.64129700
C -10.07106300 -0.76812400 -0.66317100
C -11.41698800 -0.43791000 -0.80932800
C -11.81608700 0.90052000 -0.80582800
C -10.85938900 1.90793500 -0.65168300
C -9.51325700 1.58141100 -0.50698200
C -4.30046500 2.61932700 -0.07081200
C -3.33578300 3.59378600 -0.32984700
C -2.26444800 3.30989100 -1.17886800
C -2.15879600 2.04515300 -1.76424400
C -3.11196800 1.06517200 -1.49348200
H 3.06791200 3.72302200 3.89649600
H 5.36033300 2.86014400 4.32677100
H 6.39576400 1.25313700 2.75493700
H 2.84521600 1.33594200 0.32889400
H 1.81994900 2.96198700 1.88470100
H 7.10978000 1.48392900 0.38210700
H 5.84264600 -1.34014500 -0.99411000
H 9.24047000 1.44850400 0.23579600
H 11.49346300 1.92895300 -0.62717600
H 12.30256500 0.82861200 -2.70580500
H 10.82130600 -0.76202400 -3.91555300
H 8.54494900 -1.23550400 -3.05363900
H 2.89058900 -1.70750300 -1.64285400
H 0.79671200 -2.86018500 -1.00800100
H 1.86621300 -2.50079400 3.13510700
H 3.94116100 -1.33069300 2.50460600
H -0.11420900 -3.62686000 2.59308300
H -0.08934900 -4.50491700 1.07433700
H -2.00177500 -4.36215000 -0.28533000
H -4.09488100 -3.23332900 -0.97096100

H -3.18185400 0.04372300 1.65099200
H -1.10022600 -1.08099400 2.33383500
H -6.43023200 -1.52058000 -0.03324000
H -6.81374300 1.73908200 -0.87069800
H -9.75788400 -1.80572500 -0.66681200
H -12.15463100 -1.22600900 -0.92680200
H -12.86501300 1.15790000 -0.91746500
H -11.16349600 2.95006100 -0.63602800
H -8.78782100 2.37472900 -0.36312800
H -5.13282700 2.84406400 0.58910700
H -3.42403800 4.57402600 0.12869000
H -1.51768100 4.07016600 -1.38704100
H -1.33364900 1.82234400 -2.43389600
H -3.02718900 0.08556200 -1.95188600

L-Anti-DPT (DCM)

C -2.21293900 3.65211800 0.45875600
C -3.34347700 3.88235600 -0.32711900
C -4.31810100 2.89229300 -0.45802400
C -4.16314400 1.65160100 0.17904300
C -3.02284900 1.42935500 0.96725700
C -2.05860600 2.42524000 1.10984500
C -5.22887200 0.60643200 0.06874500
C -6.58666100 1.02594200 0.30189200
C -7.64886100 0.14458400 0.25275000
O -7.45521300 -1.14625400 0.00682000
N -5.00828300 -0.66901300 -0.16656200
C -9.05659100 0.53252200 0.48912200
C -9.47988800 1.87161700 0.42239300
C -10.81157000 2.20478600 0.65694600
C -11.74401800 1.20842600 0.95918000
C -11.33580800 -0.12579400 1.01934800
C -10.00453000 -0.46278600 0.78311100
C -3.79177400 -1.24200000 -0.57933800
C -3.42330100 -2.47888100 -0.02828700
C -2.26641900 -3.13117600 -0.45325300
C -1.45145000 -2.58709400 -1.45303400
C -1.83867800 -1.36259000 -2.01900300
C -2.98628400 -0.69858900 -1.59863600
C -0.19389700 -3.29937900 -1.92222400
C 1.09597400 -2.55970300 -1.60269400
C 1.96747100 -2.14667900 -2.61728300
C 3.15152700 -1.47072000 -2.32397800
C 3.51481600 -1.20845500 -0.99430500
C 2.63442300 -1.60629100 0.02980300

C 1.44959900 -2.26734700 -0.27653300
N 4.68186300 -0.45921400 -0.75609500
O 5.75000600 1.74531800 -1.24912800
C 6.64850000 1.47680300 -0.30836400
C 6.60257100 0.29154900 0.39902300
C 5.57444500 -0.69310500 0.18137300
C 7.68043200 2.51852800 -0.11250600
C 5.64125600 -1.94259100 1.00285500
C 7.83839700 3.52131100 -1.08475000
C 8.80747800 4.51081300 -0.93172500
C 9.63084700 4.51940900 0.19617500
C 9.47551700 3.53278800 1.17396400
C 8.50844500 2.54219100 1.02372700
C 5.84474600 -1.86872700 2.38934100
C 5.94826900 -3.03177400 3.15338500
C 5.87130200 -4.28253700 2.53821500
C 5.68403500 -4.36522900 1.15578400
C 5.56371100 -3.20490100 0.39332400
H -1.45727700 4.42441900 0.56627200
H -3.46964800 4.83287800 -0.83667500
H -5.19619500 3.07465400 -1.07012000
H -2.89910100 0.47881100 1.47526900
H -1.18615200 2.24397200 1.73023900
H -6.76107700 2.05611000 0.57562100
H -6.42222800 -1.24640400 -0.09620300
H -8.77440700 2.65409400 0.16449200
H -11.12407700 3.24280700 0.59612100
H -12.78189000 1.47070700 1.14109700
H -12.05504500 -0.90550600 1.25139300
H -9.68367600 -1.49699900 0.82989200
H -4.05101300 -2.91797300 0.74144000
H -2.00026100 -4.08544400 -0.00553200
H -1.23209500 -0.92360800 -2.80719600
H -3.27321600 0.23676100 -2.06687900
H -0.24592700 -3.45956600 -3.00559900
H -0.16475700 -4.29615700 -1.46564800
H 1.71649400 -2.35184200 -3.65497700
H 3.81209400 -1.14665700 -3.12269700
H 2.87859700 -1.38170000 1.06259900
H 0.78007300 -2.55464600 0.53020000
H 5.13217200 0.90579500 -1.27679800
H 7.38321100 0.06278400 1.10944200
H 7.19873800 3.51078900 -1.95952100
H 8.92059000 5.27537700 -1.69446600

H 10.38492400 5.29145500 0.31609900
H 10.10384200 3.53968900 2.05940400
H 8.38562000 1.79928700 1.80441600
H 5.90641000 -0.89756200 2.87100400
H 6.09238000 -2.95955800 4.22719600
H 5.95948200 -5.18803200 3.13097200
H 5.63327900 -5.33511000 0.67018700
H 5.42048000 -3.27444400 -0.67978100

L-Syn-DPT (DCM)

C -3.49628200 -2.90634500 3.30305600
C -4.78830200 -2.42889200 3.52910900
C -5.37898000 -1.55165100 2.61892200
C -4.67650500 -1.12469400 1.48180300
C -3.37703500 -1.60913100 1.26379300
C -2.79496000 -2.49796100 2.16548100
C -5.33085800 -0.21758400 0.48668600
C -6.65772700 -0.56952200 0.05154100
C -7.35233600 0.18375600 -0.87469200
O -6.80766500 1.26266400 -1.42399100
N -4.76159600 0.83736700 -0.05432300
C -8.71517200 -0.14034300 -1.35045700
C -9.55054300 -1.03792900 -0.66262900
C -10.82539800 -1.32693800 -1.14234200
C -11.29044300 -0.72349600 -2.31403800
C -10.47233900 0.17658400 -2.99991700
C -9.19678200 0.46917700 -2.52170000
C -3.55438300 1.43201300 0.35573200
C -2.66152500 1.87068200 -0.63864800
C -1.48593900 2.53025600 -0.29729600
C -1.16855100 2.80364700 1.04184700
C -2.07328800 2.38788200 2.02560400
C -3.24885700 1.71315700 1.69713700
C 0.10678600 3.54651700 1.40606800
C 1.38347200 2.83659800 0.98671000
C 2.26722100 3.41262400 0.06667500
C 3.44751700 2.76915700 -0.30347800
C 3.77102200 1.50902000 0.22206200
C 2.89298100 0.93041200 1.15844400
C 1.72311100 1.58645600 1.52629200
N 5.01239900 0.94467300 -0.12321100
O 7.46846800 1.40010600 -0.06225000
C 7.67281200 0.12202900 -0.35773500
C 6.61201900 -0.74307500 -0.54300800
C 5.24292200 -0.32010700 -0.40137900

C 9.09326600 -0.26966400 -0.48956200
C 4.18202500 -1.34717200 -0.64699600
C 10.07164000 0.73029500 -0.62369500
C 11.41698700 0.39262700 -0.75516700
C 11.80861900 -0.94770300 -0.74875000
C 10.84481400 -1.94967600 -0.60621100
C 9.49931900 -1.61553500 -0.47606300
C 4.27952100 -2.62040700 -0.06520700
C 3.31358900 -3.59349300 -0.32371400
C 2.25004500 -3.31257000 -1.18304800
C 2.15338600 -2.05212500 -1.77849300
C 3.10802300 -1.07367300 -1.50862000
H -3.03848600 -3.59460200 4.00726900
H -5.33881400 -2.74066900 4.41167700
H -6.38429900 -1.18216300 2.79728500
H -2.82864700 -1.29518500 0.38202300
H -1.79287700 -2.87258300 1.97963600
H -7.09194800 -1.48308000 0.43020700
H -5.85212300 1.32043000 -1.01096600
H -9.21499300 -1.49631100 0.26137100
H -11.46038500 -2.01851500 -0.59693400
H -12.28526300 -0.95007900 -2.68572100
H -10.82776000 0.65154000 -3.90946100
H -8.55832300 1.16699000 -3.05083000
H -2.90258300 1.67735700 -1.67978600
H -0.80350600 2.84319900 -1.08331400
H -1.86202800 2.60273500 3.07031800
H -3.93913000 1.41525000 2.47902500
H 0.11887100 3.71012400 2.49038400
H 0.09346500 4.54252000 0.94706900
H 2.03690500 4.38592800 -0.35957200
H 4.12959800 3.23379900 -1.00927700
H 3.14177300 -0.02600900 1.60560400
H 1.06045400 1.12055900 2.25131100
H 6.43154600 1.50795200 -0.04257300
H 6.80075700 -1.75991800 -0.85431600
H 9.76278400 1.76909200 -0.62844000
H 12.16031800 1.17681300 -0.86321900
H 12.85734300 -1.21090100 -0.84898500
H 11.14304900 -2.99356600 -0.58832600
H 8.76755400 -2.40460400 -0.34082700
H 5.10590300 -2.84192900 0.60341800
H 3.39460300 -4.57041400 0.14346200
H 1.50199500 -4.07176200 -1.39106600

H 1.33333600 -1.83093600 -2.45494400
H 3.02952500 -0.09671800 -1.97353000

L-Anti-DPT (CYH)

C -2.23955100 3.67107500 0.48534300
C -3.37379300 3.90536200 -0.29321500
C -4.34327800 2.91190800 -0.43318700
C -4.18060000 1.66423300 0.18755600
C -3.03622200 1.43826500 0.96809300
C -2.07675500 2.43691800 1.11948400
C -5.24180600 0.61509300 0.06598900
C -6.60052600 1.02725800 0.30541800
C -7.66054500 0.14369000 0.24468500
O -7.46599800 -1.14156000 -0.01999500
N -5.01637700 -0.65583500 -0.18577100
C -9.06920800 0.52442500 0.48833800
C -9.49593000 1.86312000 0.45453100
C -10.82820300 2.18750500 0.69587000
C -11.75834900 1.18200900 0.97194500
C -11.34684600 -0.15185500 0.99865500
C -10.01489100 -0.47983100 0.75574200
C -3.79817400 -1.22082200 -0.60286100
C -3.43629700 -2.46937800 -0.07466000
C -2.27733300 -3.11467800 -0.50323400
C -1.45291200 -2.55158800 -1.48396400
C -1.83256200 -1.31470500 -2.02669400
C -2.98244200 -0.65792000 -1.60303700
C -0.19440600 -3.25740200 -1.95921400
C 1.09665700 -2.52441400 -1.62993000
C 1.98491900 -2.12942600 -2.63659700
C 3.17189000 -1.46340000 -2.33452700
C 3.52158400 -1.19393300 -1.00289300
C 2.62400400 -1.57308900 0.01296300
C 1.43610500 -2.22325200 -0.30249400
N 4.69545600 -0.45832800 -0.75770100
O 5.81190200 1.72634800 -1.26034300
C 6.69429600 1.44776600 -0.30940000
C 6.61747300 0.27122100 0.40979200
C 5.57375200 -0.69650300 0.19105500
C 7.74548800 2.47063300 -0.11495300
C 5.60957100 -1.93704700 1.02898700
C 7.91797500 3.46976800 -1.08787500
C 8.90451300 4.44191300 -0.93825700
C 9.73149400 4.43689900 0.18646300
C 9.56195200 3.45392300 1.16498000

C 8.57726700 2.48083100 1.01811200
C 5.79982100 -1.84923800 2.41627400
C 5.87465100 -3.00327500 3.19663100
C 5.78119300 -4.26013000 2.59732200
C 5.60599100 -4.35727800 1.21467300
C 5.51472500 -3.20556400 0.43593400
H -1.48676800 4.44538200 0.59924000
H -3.50631200 4.86153900 -0.79075400
H -5.22436000 3.09592100 -1.04069800
H -2.90495000 0.48079700 1.46079800
H -1.19987600 2.25138200 1.73240000
H -6.77673100 2.05184100 0.59831500
H -6.43581100 -1.24103000 -0.12600200
H -8.79141000 2.65278400 0.21638400
H -11.14323200 3.22610600 0.66066500
H -12.79717000 1.43719000 1.15924400
H -12.06467000 -0.93901300 1.20954800
H -9.68951100 -1.51339100 0.77478200
H -4.07267200 -2.92274900 0.67948100
H -2.01725000 -4.07941300 -0.07433400
H -1.21636900 -0.85936900 -2.79791700
H -3.26286900 0.28795300 -2.05343800
H -0.24501200 -3.40582000 -3.04464300
H -0.16670800 -4.26055900 -1.51578800
H 1.74444700 -2.34105300 -3.67565500
H 3.84600100 -1.15176800 -3.12681100
H 2.85784500 -1.34195400 1.04665300
H 0.75153700 -2.49402200 0.49723800
H 5.17758800 0.90366300 -1.28955300
H 7.38819300 0.03230700 1.12761000
H 7.27350900 3.46881500 -1.95903800
H 9.02825000 5.20431000 -1.70168400
H 10.49953800 5.19568700 0.30353200
H 10.19340600 3.45012100 2.04840300
H 8.44366700 1.74021000 1.79928500
H 5.87340900 -0.87237400 2.88486800
H 6.00888900 -2.91950700 4.27104000
H 5.84665900 -5.15928100 3.20274400
H 5.54115900 -5.33242200 0.74127300
H 5.37865700 -3.28596100 -0.63725600

L-Syn-DPT (CYH)

C -3.39828900 -2.73534400 3.41191400
C -4.69692200 -2.27296400 3.62944500
C -5.30906700 -1.44100700 2.69161200

C -4.62279800 -1.04443600 1.53398500
C -3.31622200 -1.51294700 1.32539500
C -2.71228500 -2.35670400 2.25518700
C -5.30135500 -0.18754600 0.51033400
C -6.62542400 -0.58026800 0.10194000
C -7.34319900 0.12285300 -0.84570500
O -6.82808800 1.19103800 -1.44053600
N -4.75557400 0.85504200 -0.07549200
C -8.70223300 -0.24818900 -1.29754800
C -9.51157000 -1.14048600 -0.57338800
C -10.78235200 -1.47556700 -1.03280100
C -11.26941300 -0.92371200 -2.22055200
C -10.47762000 -0.02877600 -2.94248300
C -9.20622100 0.30973800 -2.48466500
C -3.55167700 1.47996800 0.29695300
C -2.67411500 1.88665100 -0.72414300
C -1.50014900 2.56731400 -0.42256300
C -1.16986300 2.89518100 0.90094500
C -2.06090100 2.51346500 1.91024400
C -3.23417100 1.81706100 1.62229300
C 0.10748400 3.65393500 1.22025900
C 1.38172900 2.91691200 0.84097900
C 2.29251500 3.46221600 -0.07092000
C 3.47113300 2.79587200 -0.40317100
C 3.76514800 1.54185800 0.15299800
C 2.85961600 0.99442900 1.08151900
C 1.69203600 1.67341300 1.41189400
N 5.00330700 0.95149600 -0.15789500
O 7.47199700 1.35811100 -0.05353900
C 7.65341100 0.07321800 -0.32996500
C 6.57853200 -0.77220000 -0.52411400
C 5.21572100 -0.32058400 -0.41353800
C 9.06786100 -0.34882000 -0.43052800
C 4.14046400 -1.33259800 -0.66248600
C 10.06906400 0.63085900 -0.54095900
C 11.40954100 0.26582700 -0.64330400
C 11.77359800 -1.08190200 -0.63117000
C 10.78677800 -2.06394000 -0.51183700
C 9.44619100 -1.70236300 -0.41057200
C 4.20583500 -2.59863500 -0.06123200
C 3.22778100 -3.55877500 -0.32154200
C 2.18321700 -3.27221900 -1.20161300
C 2.11779800 -2.01893000 -1.81551500
C 3.08492900 -1.05347900 -1.54448400

H -2.92324400 -3.38843600 4.13796900
H -5.23576500 -2.56119200 4.52720600
H -6.31955100 -1.08229500 2.86314900
H -2.77894200 -1.22056200 0.42960100
H -1.70430600 -2.71894900 2.07640400
H -7.03663000 -1.48869100 0.51691400
H -5.87273400 1.28643900 -1.04304700
H -9.15846200 -1.55858400 0.36316200
H -11.39720900 -2.16268400 -0.45922100
H -12.26124900 -1.18589100 -2.57672000
H -10.85064900 0.40673900 -3.86472000
H -8.58733300 1.00410800 -3.04072800
H -2.92626600 1.65053200 -1.75374600
H -0.82782200 2.85307100 -1.22746100
H -1.83985300 2.77191600 2.94307500
H -3.91336500 1.54444500 2.42284600
H 0.12189400 3.88037700 2.29349600
H 0.09727800 4.62226100 0.70525000
H 2.08424500 4.42981000 -0.52114300
H 4.17472800 3.23634600 -1.10328800
H 3.08504600 0.04285900 1.55083000
H 1.00631400 1.23005400 2.12950400
H 6.44117400 1.49108200 -0.05411000
H 6.75189500 -1.79593100 -0.82145000
H 9.78030000 1.67530800 -0.54904500
H 12.17103700 1.03486900 -0.73285700
H 12.81874100 -1.36646900 -0.70887000
H 11.06320800 -3.11383600 -0.48972600
H 8.69532700 -2.47624700 -0.29317900
H 5.01745000 -2.82363500 0.62422300
H 3.28444900 -4.53028000 0.16054700
H 1.42554100 -4.02149400 -1.41118900
H 1.31194400 -1.79289600 -2.50732700
H 3.03018800 -0.08137500 -2.02262900

Molecular Structures:

Excited State - TD-DFT/B3LYP/6-31G(d,p)

L-Anti (ACN)

C -3.17407200 4.35273400 3.12003000
C -4.28614000 4.56342200 2.29433300
C -4.95061400 3.49719000 1.70284700
C -4.51962200 2.15688100 1.89921800
C -3.39416600 1.96568100 2.74327400
C -2.74297000 3.04179200 3.33958400
C -5.19717800 1.04506300 1.26409700
C -6.27056000 1.10565100 0.37161600
C -7.05812000 -0.01844800 -0.00899300
O -6.90840700 -1.17043000 0.51665100
N -4.74260900 -0.27725800 1.62667400
C -8.13956800 0.16456800 -1.03046800
C -8.21830000 1.26630700 -1.90375800
C -9.25407700 1.37276900 -2.83150900
C -10.23356100 0.37893200 -2.91650200
C -10.16115200 -0.72728800 -2.06457700
C -9.12588400 -0.83356900 -1.13854400
C -3.79057300 -0.98352900 0.98813600
C -3.50459000 -2.31311400 1.41547600
C -2.52592800 -3.04450800 0.77772600
C -1.79225200 -2.49950700 -0.29751400
C -2.07770600 -1.17836500 -0.71318500
C -3.05285700 -0.42665500 -0.09758000
C -0.72603100 -3.30996000 -1.00140400
C 0.63654400 -2.63597300 -1.01091200
C 1.22206800 -2.19853000 -2.20423200
C 2.47576400 -1.59032800 -2.20927200
C 3.17539500 -1.39490000 -1.00992200
C 2.58594100 -1.80875100 0.19574700
C 1.33963800 -2.42736800 0.18491600
N 4.41472100 -0.72336800 -1.07640500
O 5.46743300 1.53138100 -1.98745900
C 6.38046500 1.37541100 -1.13692800
C 6.45214500 0.22173200 -0.27933800
C 5.48847400 -0.77580300 -0.24290900
C 7.44696800 2.42811600 -1.03868500
C 5.69453200 -1.95221700 0.64536800
C 7.58273400 3.33413100 -2.10310000
C 8.54958300 4.33574700 -2.06621600
C 9.39085900 4.45531400 -0.95610400
C 9.25678300 3.56852200 0.11468300

C 8.29400800 2.55996000 0.07377700
C 6.09870700 -1.77327700 1.97728500
C 6.34917300 -2.87656200 2.79372700
C 6.21039000 -4.16982900 2.28634400
C 5.81664300 -4.35640000 0.95827000
C 5.55453100 -3.25704000 0.14341400
H -2.66191900 5.19016400 3.58297000
H -4.64537800 5.57371000 2.11682300
H -5.82090900 3.70011600 1.08836900
H -3.02824100 0.96309700 2.93499100
H -1.88674400 2.85140900 3.98125600
H -6.55302300 2.08496700 0.00647400
H -5.26080000 -0.77288900 2.34576900
H -7.45472600 2.03716000 -1.87879200
H -9.29095400 2.23053300 -3.49747200
H -11.03796700 0.46278400 -3.64134500
H -10.91430000 -1.50854900 -2.12390800
H -9.05676800 -1.68921400 -0.47558000
H -4.06709200 -2.73792600 2.24006300
H -2.31637100 -4.05731500 1.10513800
H -1.51302000 -0.74948700 -1.53416700
H -3.27293400 0.58182100 -0.42213500
H -1.04683700 -3.48124100 -2.03603400
H -0.65602500 -4.29513300 -0.52930100
H 0.70013200 -2.34424000 -3.14585700
H 2.92279400 -1.27093200 -3.14593400
H 3.09321400 -1.63724900 1.13726300
H 0.90074200 -2.74073900 1.12840500
H 4.49146800 0.06135700 -1.73692900
H 7.33196400 0.07239900 0.32968700
H 6.91869400 3.23272900 -2.95450000
H 8.64872500 5.02364300 -2.90069500
H 10.14380400 5.23722700 -0.92422800
H 9.89940100 3.66406100 0.98469700
H 8.19071300 1.89385800 0.92349700
H 6.19972100 -0.76818800 2.37407500
H 6.65126700 -2.72451200 3.82535400
H 6.40850500 -5.02826900 2.92088100
H 5.71654600 -5.35968500 0.55562100
H 5.25680100 -3.40671500 -0.88917600

L-Syn (ACN)

C -4.55980300 5.26740600 -0.83106300
C -5.84231900 4.74723300 -1.04877700
C -6.16039400 3.44763100 -0.67700100

C -5.19541800 2.59332400 -0.07723300
C -3.90389100 3.14187000 0.13835700
C -3.60006600 4.44982100 -0.22858000
C -5.51837600 1.22968500 0.29090800
C -6.72579000 0.55910000 0.08099600
C -7.06644800 -0.68147000 0.69233900
O -6.32826100 -1.23628200 1.57160100
N -4.49248100 0.49515300 0.99387800
C -8.36231900 -1.34053600 0.32819100
C -9.11979900 -1.01009700 -0.81200000
C -10.31954300 -1.66429600 -1.08990500
C -10.79085300 -2.67034700 -0.24132700
C -10.04279100 -3.01877100 0.88719400
C -8.84412100 -2.36528100 1.16418700
C -3.54968300 -0.27979900 0.42501500
C -2.63663200 -0.99389000 1.25826400
C -1.65738500 -1.77383900 0.69125100
C -1.53892900 -1.89273100 -0.71482900
C -2.44508600 -1.18779300 -1.53184300
C -3.43480800 -0.39229900 -0.98967600
C -0.45594200 -2.76020900 -1.31719300
C 0.94572000 -2.31058800 -0.93479600
C 1.77316700 -3.10884300 -0.13703800
C 3.05351000 -2.68810000 0.21781800
C 3.54235900 -1.45082500 -0.22489100
C 2.72819900 -0.65271100 -1.04507700
C 1.44682800 -1.07833900 -1.38012800
N 4.86623800 -1.10501300 0.12089100
O 7.33715000 -2.05017300 -0.05601200
C 7.73143300 -0.85909200 0.02736700
C 6.82841700 0.24461500 0.22336000
C 5.44701000 0.11895800 0.24560500
C 9.20668600 -0.59117100 -0.05723100
C 4.61240600 1.32334200 0.50697300
C 10.08727100 -1.66895600 0.13020400
C 11.46546600 -1.48307800 0.05688100
C 11.98648400 -0.21524900 -0.21798400
C 11.12057400 0.86204700 -0.41945500
C 9.74037300 0.67746500 -0.33711200
C 4.87028400 2.52558800 -0.16947500
C 4.12591500 3.67051800 0.11609300
C 3.12431900 3.63090400 1.08794600
C 2.86741200 2.43968200 1.77249400
C 3.60090600 1.29134400 1.48159100

H -4.31921600 6.28553300 -1.11995200
H -6.60776700 5.36779300 -1.50732400
H -7.17056900 3.08931200 -0.84257300
H -3.13187700 2.53707600 0.60102300
H -2.59974500 4.83182900 -0.04270500
H -7.46432200 1.05614000 -0.53499600
H -4.54258400 0.46732100 2.00777700
H -8.76328500 -0.25344800 -1.50355400
H -10.88404000 -1.39377400 -1.97805200
H -11.72447900 -3.17987300 -0.46092300
H -10.39602100 -3.80253400 1.55207900
H -8.25347400 -2.63096300 2.03422300
H -2.72853300 -0.91237400 2.33617700
H -0.96208300 -2.30939800 1.32895000
H -2.36237600 -1.27252900 -2.61027500
H -4.12800200 0.14844900 -1.62039100
H -0.56584900 -2.76610400 -2.40629600
H -0.60490700 -3.79242600 -0.97952700
H 1.41565400 -4.07244300 0.21509800
H 3.67873000 -3.31595300 0.84558500
H 3.10028400 0.28852300 -1.43086800
H 0.83369300 -0.44612000 -2.01680300
H 5.57070200 -1.85412700 0.10541100
H 7.23267200 1.22475200 0.43136600
H 9.66795800 -2.64765000 0.33601600
H 12.13438800 -2.32423000 0.21300000
H 13.06081300 -0.06861200 -0.27825200
H 11.51939600 1.84647900 -0.64492900
H 9.08295900 1.52129800 -0.51669100
H 5.64380100 2.55466700 -0.93019200
H 4.32841000 4.59154500 -0.42182000
H 2.54722000 4.52278600 1.31229400
H 2.09631500 2.40570600 2.53605800
H 3.40267700 0.37066700 2.02046400

L-Anti (DCM)

C -3.19899100 4.31789500 3.20212300
C -4.31209800 4.53605300 2.37999800
C -4.96789800 3.47674000 1.76740600
C -4.52608900 2.13607800 1.93633100
C -3.39998700 1.93723300 2.77800000
C -2.75823000 3.00611900 3.39632100
C -5.19295300 1.03484600 1.27520300
C -6.25515900 1.10549700 0.37001500
C -7.05041300 -0.01196700 -0.01723400

O -6.92265100 -1.16293000 0.51423400
N -4.74316600 -0.29555200 1.62109600
C -8.11544900 0.18190000 -1.05345500
C -8.15521400 1.27166200 -1.94350300
C -9.17641900 1.39003000 -2.88572900
C -10.17957300 0.42018900 -2.96730000
C -10.14564800 -0.67440500 -2.09807000
C -9.12465700 -0.79284800 -1.15807400
C -3.79476700 -0.99543600 0.97454900
C -3.53474900 -2.34363000 1.36212200
C -2.55587700 -3.06774800 0.71735000
C -1.79532900 -2.49890100 -0.32670100
C -2.05412700 -1.16000700 -0.70278600
C -3.02886200 -0.41471800 -0.08011000
C -0.73112900 -3.30349100 -1.04013400
C 0.63490500 -2.63720300 -1.03996600
C 1.22694400 -2.19374200 -2.22770800
C 2.48266300 -1.59026100 -2.22382300
C 3.17897100 -1.40485100 -1.02053000
C 2.58312300 -1.82592100 0.17963200
C 1.33482700 -2.43997900 0.15945900
N 4.41952200 -0.73712500 -1.08042400
O 5.48591000 1.49962900 -2.01787100
C 6.38415500 1.36288700 -1.14997800
C 6.44237300 0.22613400 -0.26716900
C 5.48094900 -0.77226300 -0.22925700
C 7.44915700 2.41730500 -1.05698300
C 5.67762800 -1.93416500 0.68031400
C 7.60540600 3.29666800 -2.14048700
C 8.57303900 4.29757500 -2.11026000
C 9.39337000 4.44380900 -0.98787200
C 9.23795900 3.58424900 0.10188400
C 8.27504900 2.57572600 0.06758300
C 6.04799900 -1.73362600 2.01883100
C 6.28975700 -2.82334600 2.85581700
C 6.17676100 -4.12445100 2.36267000
C 5.81717100 -4.33239100 1.02823100
C 5.56309100 -3.24673100 0.19285400
H -2.69364300 5.14988900 3.68203300
H -4.67985700 5.54674400 2.22321100
H -5.84154700 3.68340900 1.15904000
H -3.02581500 0.93392700 2.94906700
H -1.90115200 2.80997200 4.03521600
H -6.52775200 2.08781800 0.00493400

H -5.29062500 -0.80978700 2.30454300
H -7.37133300 2.02206400 -1.92029700
H -9.18348000 2.23776800 -3.56546600
H -10.97298500 0.51296000 -3.70319500
H -10.91789900 -1.43702800 -2.15502700
H -9.08287300 -1.63928400 -0.48112500
H -4.11967900 -2.78720500 2.16075100
H -2.36732500 -4.09430700 1.01347600
H -1.46730500 -0.71285000 -1.49803800
H -3.22892900 0.60710000 -0.37388800
H -1.05244800 -3.45914100 -2.07737900
H -0.66773200 -4.29637800 -0.58292800
H 0.70796700 -2.33032700 -3.17241800
H 2.93375900 -1.26503800 -3.15656100
H 3.08643700 -1.66343100 1.12461000
H 0.89188000 -2.75846800 1.09943200
H 4.50558600 0.03674000 -1.75277600
H 7.31340900 0.08841800 0.35705000
H 6.95600800 3.17464000 -3.00041000
H 8.68864900 4.96468200 -2.95939600
H 10.14668800 5.22561600 -0.96122900
H 9.86422200 3.70102200 0.98123900
H 8.15460700 1.93041000 0.93100800
H 6.12923900 -0.72221500 2.40406800
H 6.56551800 -2.65453200 3.89226100
H 6.36872500 -4.97234500 3.01313800
H 5.73739000 -5.34188900 0.63660800
H 5.29164600 -3.41286100 -0.84452800

L-Syn (DCM)

C -5.78354300 5.30830900 -1.07964400
C -6.96247200 4.55283900 -1.11816000
C -6.98219700 3.23370400 -0.68635700
C -5.80609500 2.59465300 -0.20655100
C -4.62391100 3.38065300 -0.17068300
C -4.61972000 4.70584300 -0.59434900
C -5.82075600 1.21187300 0.21575800
C -6.88815600 0.31222200 0.15247200
C -6.92821300 -0.92917000 0.85357600
O -6.02978100 -1.27248300 1.68810000
N -4.60542100 0.70386800 0.81812200
C -8.09212300 -1.84856700 0.63948800
C -8.99178700 -1.74376800 -0.43783600
C -10.05552500 -2.63526100 -0.57243000
C -10.24331500 -3.65868000 0.36055000

C -9.34920700 -3.78368000 1.42779200
C -8.28701400 -2.89320800 1.56167700
C -3.61912400 0.06449000 0.17026000
C -2.55170000 -0.52007600 0.91956600
C -1.52971500 -1.16990500 0.27028800
C -1.51235900 -1.27819200 -1.14113400
C -2.56432300 -0.69193900 -1.87690300
C -3.60121400 -0.03216700 -1.25282600
C -0.41160900 -2.03954000 -1.84710600
C 0.98832900 -1.73975900 -1.34365000
C 1.75061000 -2.71417300 -0.68991100
C 3.03752100 -2.43544800 -0.23524800
C 3.60285200 -1.16684600 -0.43127300
C 2.85292400 -0.18768100 -1.10368800
C 1.56312600 -0.47530800 -1.53866100
N 4.93150000 -0.97294200 -0.00275400
O 7.32145200 -2.07178500 -0.27286300
C 7.80526000 -0.94410800 -0.00561800
C 6.98304100 0.18886000 0.33906100
C 5.59747700 0.17098100 0.31728700
C 9.29828600 -0.78747100 -0.02550800
C 4.84801700 1.38328600 0.74598400
C 10.08479700 -1.95040200 -0.00638700
C 11.47453300 -1.86926900 -0.02954800
C 12.10162800 -0.62125400 -0.08444300
C 11.32989300 0.54212100 -0.11774600
C 9.93797300 0.46096100 -0.08584000
C 5.21194500 2.64977600 0.26379000
C 4.54951300 3.79340600 0.71036300
C 3.52402000 3.68650700 1.65137300
C 3.16061200 2.42954400 2.14231900
C 3.81252600 1.28437900 1.69024700
H -5.77647300 6.34100000 -1.41338200
H -7.88290500 5.00394000 -1.47972900
H -7.92071000 2.69050100 -0.70435700
H -3.70005200 2.94656400 0.19550200
H -3.69375600 5.27304600 -0.54677900
H -7.76238000 0.62394300 -0.40524700
H -4.58364100 0.64290200 1.83158900
H -8.85093400 -0.97679300 -1.19274500
H -10.73493500 -2.53612000 -1.41471300
H -11.07136300 -4.35327100 0.25270700
H -9.48181700 -4.57886800 2.15675100
H -7.58273100 -2.98212200 2.38156900

H -2.57039900 -0.45358300 2.00217700
H -0.72299600 -1.61182800 0.84474200
H -2.55573700 -0.76447100 -2.95955700
H -4.40532900 0.41616400 -1.82070900
H -0.47715400 -1.83742600 -2.92176600
H -0.61348300 -3.11232200 -1.72832300
H 1.33669600 -3.70632300 -0.53174200
H 3.61206800 -3.20139500 0.27711600
H 3.28181800 0.78689300 -1.30111500
H 1.00111700 0.29522000 -2.05999700
H 5.58348400 -1.76069100 -0.12093300
H 7.45430700 1.08978700 0.70466600
H 9.58224000 -2.91067100 0.02838900
H 12.07031400 -2.77698700 -0.00579600
H 13.18551500 -0.55599500 -0.10517200
H 11.81158500 1.51378600 -0.17279700
H 9.35409200 1.37378600 -0.13380500
H 6.00422900 2.73176300 -0.47350400
H 4.83432400 4.76635400 0.32169300
H 3.01077500 4.57692100 2.00160300
H 2.37025500 2.34156100 2.88159900
H 3.53321600 0.31117500 2.08048200

L-Anti (CYH)

C -3.44327200 4.34204600 3.37055400
C -4.52329500 4.54451900 2.50193600
C -5.11673600 3.48097800 1.83740600
C -4.63993300 2.15037200 1.99617100
C -3.54800600 1.96743100 2.88611200
C -2.97150200 3.03997800 3.55762600
C -5.23486200 1.05223000 1.27506400
C -6.24393600 1.10171600 0.30954400
C -7.03040600 -0.02572000 -0.07866400
O -6.93884600 -1.15773200 0.49603800
N -4.78974500 -0.28682900 1.62483200
C -8.04270200 0.14017100 -1.16949500
C -8.03803100 1.20450800 -2.08946000
C -9.01467300 1.29876300 -3.07992300
C -10.01535700 0.32899300 -3.17948200
C -10.02361400 -0.74158300 -2.28061000
C -9.04736000 -0.83633400 -1.29266100
C -3.82912200 -0.97436700 0.99716400
C -3.66966000 -2.36911600 1.27268900
C -2.67263500 -3.08481000 0.65069800
C -1.78882100 -2.46772800 -0.26261300

C -1.94438600 -1.08528900 -0.52630600
C -2.93427600 -0.34532800 0.07543600
C -0.72010300 -3.27457400 -0.96729900
C 0.65046500 -2.62167800 -0.98175000
C 1.23522500 -2.18421900 -2.17512600
C 2.49591000 -1.59259100 -2.18427000
C 3.20760800 -1.41217000 -0.98860400
C 2.61930000 -1.82906500 0.21707400
C 1.36562300 -2.43158400 0.20927100
N 4.45190100 -0.75838300 -1.06559400
O 5.51348000 1.44639800 -2.05365600
C 6.40852600 1.34154500 -1.18167600
C 6.46905800 0.22609000 -0.26654700
C 5.51195000 -0.77217000 -0.20846400
C 7.46592100 2.40458400 -1.11485500
C 5.70983600 -1.91548500 0.72417200
C 7.60185900 3.26772400 -2.21354500
C 8.56196900 4.27563700 -2.21008400
C 9.39464500 4.44512500 -1.10055000
C 9.25890900 3.60216100 0.00411900
C 8.30330200 2.58667000 -0.00311000
C 6.07627000 -1.68867000 2.05932400
C 6.32020600 -2.76090900 2.91766000
C 6.21198300 -4.07137700 2.44986300
C 5.85497200 -4.30581900 1.11952500
C 5.59967100 -3.23755000 0.26287300
H -2.98761000 5.17772900 3.89190000
H -4.91657300 5.54668400 2.35199800
H -5.97246300 3.67088600 1.19879300
H -3.15079900 0.97200300 3.05167200
H -2.14005900 2.85590100 4.23314200
H -6.50171000 2.07653700 -0.08595800
H -5.44831200 -0.84261000 2.16399600
H -7.25277900 1.95297300 -2.05087100
H -8.98898200 2.12758000 -3.78235100
H -10.77477500 0.40290400 -3.95265800
H -10.79458500 -1.50436700 -2.35243000
H -9.03452500 -1.66317100 -0.59108900
H -4.35516800 -2.85040300 1.96153600
H -2.56576000 -4.14480700 0.85790000
H -1.26033300 -0.60171900 -1.21530400
H -3.05215900 0.71018000 -0.12867500
H -1.04767300 -3.44155500 -2.00217900
H -0.66305000 -4.26645600 -0.50527200

H 0.70559300 -2.31586700 -3.11494100
H 2.94042800 -1.27109200 -3.12145900
H 3.13327900 -1.67226600 1.15699500
H 0.92982500 -2.74628200 1.15405500
H 4.54266700 0.00384800 -1.75252900
H 7.34209500 0.10302600 0.35806100
H 6.94062600 3.12632500 -3.06126100
H 8.66182100 4.93103200 -3.07033400
H 10.14244200 5.23279300 -1.09513200
H 9.89491200 3.73750800 0.87389700
H 8.19712900 1.95425300 0.87170000
H 6.15277400 -0.66921200 2.42408700
H 6.59382800 -2.57129100 3.95119200
H 6.40568500 -4.90599400 3.11690800
H 5.77875000 -5.32305200 0.74741500
H 5.33017000 -3.42349300 -0.77163800

L-Syn (CYH)

C -6.11052500 5.29318300 -1.02170400
C -7.24512800 4.47182000 -1.02781900
C -7.17418100 3.14944200 -0.61420500
C -5.94595400 2.57182300 -0.18822200
C -4.80960800 3.42450900 -0.18446900
C -4.89724500 4.75255200 -0.58720700
C -5.86757400 1.18653300 0.20515700
C -6.87904000 0.22306600 0.16689200
C -6.83858000 -1.00464000 0.89569600
O -5.91168200 -1.28038700 1.72265500
N -4.60691600 0.73070200 0.76745000
C -7.95488100 -1.98791500 0.72166900
C -8.87242000 -1.95662900 -0.34441000
C -9.89171300 -2.90297400 -0.43989900
C -10.01460400 -3.90832300 0.52235600
C -9.10081700 -3.96020500 1.57884200
C -8.08298100 -3.01518700 1.67378800
C -3.62308800 0.13409900 0.08503200
C -2.54835000 -0.48780500 0.79775400
C -1.52143300 -1.08867900 0.11196900
C -1.50239700 -1.11236300 -1.30379500
C -2.55991200 -0.49012100 -2.00385000
C -3.60136900 0.12314200 -1.34392000
C -0.39681000 -1.82307200 -2.05385000
C 0.99916100 -1.56951700 -1.51582400
C 1.73788400 -2.58554800 -0.89960600
C 3.01786900 -2.34628900 -0.40579400

C 3.60205800 -1.07611700 -0.52416500
C 2.87617000 -0.05538000 -1.16064200
C 1.59239500 -0.30453400 -1.63462100
N 4.92094500 -0.92221600 -0.05656000
O 7.28957300 -2.05527200 -0.31359100
C 7.79256600 -0.95039600 0.00106900
C 6.98488000 0.18973500 0.36581500
C 5.60167700 0.19889200 0.31567600
C 9.28846900 -0.82820700 0.01990300
C 4.86532000 1.40896100 0.77297100
C 10.04504300 -2.01029500 -0.01104700
C 11.43617500 -1.96392000 0.00043900
C 12.09495000 -0.73179700 0.03172200
C 11.35345800 0.45106700 0.04892400
C 9.95984900 0.40434400 0.04542500
C 5.25579100 2.68430200 0.33772400
C 4.60476000 3.82342200 0.81142500
C 3.56361500 3.70283400 1.73300500
C 3.17334300 2.43680400 2.17710900
C 3.81404200 1.29666200 1.69773200
H -6.17451000 6.32866500 -1.34026900
H -8.20279000 4.87441700 -1.34765100
H -8.08003700 2.55321700 -0.60117800
H -3.84955700 3.03886800 0.14069800
H -4.00442400 5.37219700 -0.56408300
H -7.78222500 0.47826300 -0.37337800
H -4.59933600 0.58050200 1.77259300
H -8.77934000 -1.20411700 -1.12111700
H -10.58704700 -2.86082400 -1.27401000
H -10.80820100 -4.64606100 0.44554700
H -9.18377300 -4.74124300 2.33015100
H -7.36229000 -3.04367800 2.48355800
H -2.57250700 -0.49208400 1.88205800
H -0.71126600 -1.55878100 0.65860200
H -2.54862500 -0.49648700 -3.08914100
H -4.40652900 0.60309000 -1.88322900
H -0.45157900 -1.54169900 -3.11139800
H -0.60471300 -2.90113800 -2.01870100
H 1.31057900 -3.58010100 -0.80260100
H 3.57403500 -3.14469500 0.07641900
H 3.31936500 0.92267300 -1.29968200
H 1.04962600 0.49888700 -2.12609900
H 5.56362200 -1.71638700 -0.18887300
H 7.46449900 1.06709000 0.77519000

H 9.51591700 -2.95617400 -0.04346200
H 12.00869800 -2.88668900 -0.01598300
H 13.18037200 -0.69360500 0.03853700
H 11.86036900 1.41138700 0.06130600
H 9.40038800 1.33358700 0.03802300
H 6.06050400 2.77630100 -0.38489000
H 4.91066300 4.80383200 0.45902000
H 3.05905700 4.58961800 2.10452700
H 2.37051000 2.33786100 2.90150400
H 3.51404900 0.31550100 2.05101300

L-Anti-1SPT (ACN)

C -3.26604300 4.46316100 2.99165700
C -4.38349000 4.62378700 2.16195500
C -5.01994600 3.52131800 1.60739600
C -4.54797900 2.20514900 1.84657000
C -3.42118400 2.06411300 2.69400700
C -2.79712000 3.17450200 3.25613500
C -5.17514000 1.02889000 1.25930000
C -6.24245900 1.08633400 0.35610100
C -7.07289100 0.02049300 -0.00606800
O -6.98976000 -1.19097100 0.60294500
N -4.74991400 -0.24868200 1.72446200
C -8.13258200 0.11244800 -1.00427700
C -8.23249600 1.20178700 -1.89961300
C -9.26311300 1.26745800 -2.83106000
C -10.21710400 0.24701900 -2.90977100
C -10.12327400 -0.84441200 -2.04160800
C -9.09785800 -0.91508100 -1.10317100
C -3.80113700 -0.89488000 1.03537800
C -3.45929400 -2.22142700 1.47167900
C -2.49294200 -2.95923000 0.82209400
C -1.79916800 -2.43393100 -0.28798000
C -2.11489800 -1.12554200 -0.72272700
C -3.08096300 -0.37102600 -0.09587800
C -0.74027000 -3.24605700 -1.00336900
C 0.63090900 -2.58846400 -1.00961700
C 1.23379800 -2.17686700 -2.20340100
C 2.49583300 -1.58515300 -2.20669900
C 3.18688100 -1.38072100 -1.00446500
C 2.58104600 -1.76799600 0.20179100
C 1.32681000 -2.37048300 0.18880500
N 4.43614000 -0.72518100 -1.06791300
O 5.52870100 1.50806800 -1.98554900
C 6.43557100 1.34134700 -1.13007500

C 6.48447500 0.19212300 -0.26600300
C 5.50436200 -0.78999100 -0.22932200
C 7.51752800 2.37842900 -1.03128200
C 5.68667500 -1.96394800 0.66743500
C 7.67300600 3.27651000 -2.09972100
C 8.65531600 4.26302500 -2.06326300
C 9.49267600 4.37553900 -0.94947000
C 9.33907100 3.49683200 0.12535800
C 8.36076700 2.50330300 0.08484800
C 6.08708000 -1.78296600 2.00025100
C 6.31505400 -2.88471200 2.82530700
C 6.15757000 -4.17889000 2.32579100
C 5.76762500 -4.36772700 0.99691900
C 5.52774600 -3.26965100 0.17352400
H -2.77607300 5.32855900 3.42672900
H -4.76728100 5.61888800 1.95574000
H -5.89856800 3.68288800 0.99298400
H -3.04096000 1.07281200 2.90998800
H -1.93634300 3.03110800 3.90317900
H -6.50345300 2.05363800 -0.05202800
H -6.29701900 -1.13289100 1.29916900
H -7.48836600 1.99058500 -1.88351800
H -9.31628400 2.11465600 -3.50853400
H -11.01717500 0.29996300 -3.64158500
H -10.85539600 -1.64511200 -2.09448900
H -9.03610500 -1.76108600 -0.42920600
H -3.99024200 -2.62108000 2.32902000
H -2.25819600 -3.96158000 1.16755300
H -1.57710700 -0.70948700 -1.56963000
H -3.30847400 0.62807000 -0.44690700
H -1.05863500 -3.40872300 -2.04017800
H -0.67621000 -4.23565100 -0.53840600
H 0.71797700 -2.32935100 -3.14743600
H 2.95512700 -1.28510800 -3.14392400
H 3.08243800 -1.58819000 1.14508900
H 0.87420000 -2.66200600 1.13284500
H 4.52692700 0.05617100 -1.73056300
H 7.35836100 0.03225900 0.34886100
H 7.01186800 3.18076700 -2.95403100
H 8.76944200 4.94473300 -2.90091300
H 10.25763600 5.14572000 -0.91785000
H 9.97863000 3.58693400 0.99821500
H 8.24280500 1.84364200 0.93768200
H 6.20267500 -0.77709900 2.39103400

H 6.61431700 -2.73074000 3.85747900
H 6.33823300 -5.03623500 2.96699400
H 5.65292800 -5.37188200 0.60035800
H 5.23254100 -3.42138100 -0.85948600

L-Syn-1SPT (ACN)

C -4.45740100 5.24145300 -0.76003800
C -5.73263400 4.72736800 -1.02906100
C -6.06399500 3.42737300 -0.67076700
C -5.11888000 2.57688400 -0.04171100
C -3.83738000 3.11810200 0.22725100
C -3.51811100 4.42707500 -0.12374600
C -5.42393000 1.20018100 0.32420400
C -6.64031000 0.57051000 0.03747200
C -7.10780500 -0.61600600 0.61224000
O -6.44526500 -1.22939100 1.62718900
N -4.47121800 0.50404100 1.12263100
C -8.35826000 -1.26811100 0.23923400
C -9.07005100 -0.92104500 -0.93170200
C -10.26807000 -1.55099300 -1.25130100
C -10.78777400 -2.55299400 -0.42457000
C -10.08773700 -2.91843400 0.72872700
C -8.89077600 -2.28940700 1.05816900
C -3.56835500 -0.27021600 0.50825400
C -2.67290300 -1.02771700 1.34387700
C -1.70351900 -1.83568400 0.79967900
C -1.55182400 -1.95161400 -0.60293000
C -2.41863400 -1.21533500 -1.43562200
C -3.39984700 -0.39571100 -0.91392400
C -0.47210600 -2.83838500 -1.18582800
C 0.93411000 -2.37339300 -0.83787000
C 1.77500900 -3.14160500 -0.02503500
C 3.05790000 -2.70446700 0.30143600
C 3.53615600 -1.48099100 -0.18719100
C 2.70969000 -0.71381600 -1.02411900
C 1.42610200 -1.15514300 -1.32939200
N 4.86287800 -1.11653700 0.13203500
O 7.34201100 -2.04148300 -0.04688200
C 7.72486400 -0.84485700 0.01020400
C 6.81296100 0.25342400 0.18995400
C 5.43253100 0.11449800 0.22623200
C 9.19720700 -0.56476700 -0.08975200
C 4.58862000 1.31681100 0.46770800
C 10.08894900 -1.63078900 0.11147200
C 11.46491200 -1.43390800 0.02550200

C 11.97257200 -0.16671000 -0.27590000
C 11.09545300 0.89875900 -0.49132000
C 9.71754500 0.70319500 -0.39652200
C 4.83063800 2.50617200 -0.23682400
C 4.07836300 3.65061000 0.02934200
C 3.08454800 3.62370700 1.00956600
C 2.84329300 2.44556200 1.72185100
C 3.58472100 1.29752200 1.45043800
H -4.20624200 6.26035000 -1.03764400
H -6.47795100 5.35185800 -1.51339200
H -7.06920100 3.07335500 -0.87039300
H -3.09464100 2.50189300 0.71967500
H -2.52697600 4.81182200 0.09942300
H -7.32234100 1.07608200 -0.63302000
H -5.65933700 -0.68130200 1.85049200
H -8.67447300 -0.17092700 -1.60781300
H -10.79460600 -1.26670900 -2.15765600
H -11.72093600 -3.04524700 -0.68024000
H -10.47828200 -3.69731900 1.37736700
H -8.35808800 -2.57380900 1.95766400
H -2.79164900 -0.93598300 2.41830600
H -1.03807800 -2.39383000 1.45149900
H -2.30808600 -1.29623100 -2.51311800
H -4.05125800 0.16465000 -1.57325000
H -0.59173100 -2.87998000 -2.27363000
H -0.61003900 -3.86046000 -0.81426700
H 1.42571400 -4.09438000 0.36314800
H 3.69286000 -3.30824600 0.94302100
H 3.07365500 0.21601200 -1.44422500
H 0.80149500 -0.54610800 -1.97746100
H 5.57396000 -1.85935500 0.12394600
H 7.20872500 1.24174800 0.37388800
H 9.67985900 -2.60927800 0.33781200
H 12.14248300 -2.26601600 0.19249900
H 13.04510300 -0.01146800 -0.34598100
H 11.48369800 1.88248500 -0.73746800
H 9.05132900 1.53760700 -0.58731100
H 5.59815300 2.52541100 -1.00391600
H 4.26863600 4.56130300 -0.53022100
H 2.50122900 4.51522800 1.21878100
H 2.07810900 2.42151000 2.49171400
H 3.39826400 0.38715700 2.01053300
L-Anti-1SPT (DCM)
C -3.27147700 4.43871900 3.02477300

C -4.39029700 4.60545500 2.19848400
C -5.02649800 3.50718200 1.63568400
C -4.55252300 2.18959900 1.86199900
C -3.42505300 2.04234100 2.70713400
C -2.80138000 3.14827900 3.27784800
C -5.17792200 1.01858700 1.26301900
C -6.24215200 1.08375900 0.35822100
C -7.07546500 0.02138900 -0.01097600
O -6.99671700 -1.19252800 0.59247600
N -4.75304700 -0.26446300 1.71736500
C -8.13319100 0.12209900 -1.00913300
C -8.22566900 1.21393900 -1.90226400
C -9.25571700 1.28868200 -2.83342300
C -10.21668100 0.27511900 -2.91403900
C -10.13005200 -0.81890300 -2.04836100
C -9.10533900 -0.89880300 -1.11035900
C -3.80561300 -0.90266800 1.02310400
C -3.46760700 -2.23656600 1.44393200
C -2.50056200 -2.96831000 0.78934700
C -1.79935300 -2.43051700 -0.31014400
C -2.10999000 -1.11546400 -0.72947000
C -3.07743500 -0.36685800 -0.09882600
C -0.73899100 -3.23596400 -1.03068600
C 0.63304200 -2.58013500 -1.02913000
C 1.24202100 -2.16712200 -2.21919200
C 2.50530500 -1.57847700 -2.21584600
C 3.19234600 -1.37857100 -1.01044900
C 2.58027500 -1.76749600 0.19214800
C 1.32458800 -2.36645400 0.17240800
N 4.44330000 -0.72703600 -1.06891400
O 5.54526300 1.49624600 -1.99439000
C 6.44523700 1.33612800 -1.13160300
C 6.48699400 0.19242100 -0.25829000
C 5.50582800 -0.78780700 -0.22217700
C 7.52842300 2.37201600 -1.03468400
C 5.68097700 -1.95681100 0.68267000
C 7.68679400 3.26492200 -2.10676700
C 8.67038100 4.25006800 -2.07290700
C 9.50605100 4.36630600 -0.95837900
C 9.34935800 3.49288400 0.12011500
C 8.36961700 2.50081200 0.08231800
C 6.07039200 -1.76853100 2.01758300
C 6.29209500 -2.86555500 2.85052000
C 6.13882400 -4.16239900 2.35696600

C 5.75930600 -4.35854100 1.02625600
C 5.52593500 -3.26514500 0.19493300
H -2.78152600 5.30078200 3.46650500
H -4.77573400 5.60192900 2.00201100
H -5.90749400 3.67245200 1.02565400
H -3.04425700 1.04948500 2.91429800
H -1.93985100 3.00014300 3.92285200
H -6.50288300 2.05437100 -0.04237800
H -6.30410600 -1.14007500 1.28902100
H -7.47517200 1.99673000 -1.88471200
H -9.30306500 2.13748200 -3.50940000
H -11.01649400 0.33504900 -3.64563800
H -10.86775900 -1.61439300 -2.10290900
H -9.04854800 -1.74635600 -0.43794500
H -4.00356700 -2.64509400 2.29390000
H -2.27025600 -3.97589600 1.12274400
H -1.56542200 -0.68957800 -1.56713100
H -3.29963400 0.63742700 -0.43784500
H -1.05539100 -3.38945600 -2.06967400
H -0.67675200 -4.23031400 -0.57530200
H 0.72977500 -2.31602600 -3.16584800
H 2.96908100 -1.27685200 -3.15037400
H 3.07783600 -1.59134800 1.13806600
H 0.86729000 -2.65841700 1.11410200
H 4.54044900 0.05088200 -1.73511100
H 7.35752500 0.03449400 0.36182800
H 7.02590400 3.16605800 -2.96088200
H 8.78673700 4.92807900 -2.91328400
H 10.27212400 5.13553000 -0.92896900
H 9.98753400 3.58623900 0.99370200
H 8.24862100 1.84521900 0.93788100
H 6.18219800 -0.76025200 2.40333200
H 6.58302200 -2.70584900 3.88425400
H 6.31452000 -5.01618600 3.00432600
H 5.64772200 -5.36492300 0.63438400
H 5.23850000 -3.42221700 -0.83944800

L-Syn-1SPT (DCM)

C -4.96895900 5.27137700 -1.00782000
C -6.21595500 4.65663900 -1.17784100
C -6.42611700 3.35057700 -0.75665900
C -5.38330500 2.59425300 -0.16316600
C -4.13279600 3.23756900 0.00769800
C -3.93483900 4.55190500 -0.40531600
C -5.56130400 1.21265000 0.26138400

C -6.73528800 0.48308800 0.05684200
C -7.08441000 -0.71342300 0.69604400
O -6.33532900 -1.22998200 1.70312000
N -4.51668800 0.61588900 1.02949700
C -8.29156300 -1.47394000 0.40088800
C -9.07505900 -1.22920900 -0.75015600
C -10.23110400 -1.96156800 -0.99538000
C -10.63642200 -2.96771300 -0.11198800
C -9.86383600 -3.23284600 1.02225100
C -8.70850800 -2.50116700 1.27775300
C -3.59891600 -0.11220000 0.39069300
C -2.61163400 -0.78460700 1.19946500
C -1.62316000 -1.54978900 0.63018600
C -1.53645300 -1.70485500 -0.77440200
C -2.48715000 -1.04669900 -1.58205900
C -3.48993300 -0.27211600 -1.03631400
C -0.45215700 -2.56458500 -1.38862800
C 0.95709000 -2.15450100 -0.99295900
C 1.78658500 -3.01271400 -0.26313300
C 3.07760100 -2.63240600 0.09884000
C 3.57744400 -1.37567800 -0.26973700
C 2.76115400 -0.51529100 -1.02198100
C 1.46919400 -0.90228700 -1.36299100
N 4.91110100 -1.07258100 0.07803200
O 7.35444900 -2.05550000 -0.17256300
C 7.77728900 -0.88243700 -0.01992300
C 6.89996300 0.22884800 0.24538300
C 5.51688100 0.13017700 0.27134400
C 9.25855300 -0.64543600 -0.09375300
C 4.70935900 1.33344600 0.61191600
C 10.11142600 -1.75560600 0.01363000
C 11.49354400 -1.59965900 -0.05139000
C 12.04644200 -0.32949000 -0.23749600
C 11.20810500 0.78064000 -0.35976500
C 9.82403000 0.62528300 -0.28604900
C 4.98521700 2.56782500 0.00435600
C 4.26866500 3.70916500 0.36495700
C 3.27636400 3.63319000 1.34379700
C 3.00084500 2.40925000 1.95939700
C 3.70696800 1.26537700 1.59371600
H -4.81210900 6.29494700 -1.33355500
H -7.03469200 5.20735700 -1.63234100
H -7.41321100 2.91804500 -0.87587800
H -3.31812800 2.69596800 0.47300700

H -2.96398300 5.01638400 -0.25696400
H -7.48633200 0.91099300 -0.59380500
H -5.58520000 -0.61611900 1.86914400
H -8.76578100 -0.47861400 -1.46939900
H -10.81444000 -1.75475700 -1.88795200
H -11.53728300 -3.54042100 -0.30953100
H -10.16545000 -4.01404100 1.71420700
H -8.11816100 -2.70707100 2.16244100
H -2.68148300 -0.66254500 2.27511100
H -0.89011100 -2.04224200 1.26194300
H -2.42361300 -1.15426300 -2.66122200
H -4.20453500 0.22784100 -1.67802600
H -0.55464300 -2.54096200 -2.47921200
H -0.61433900 -3.60694100 -1.08660100
H 1.42155400 -3.99331200 0.03027200
H 3.70387500 -3.30747700 0.67461400
H 3.13981300 0.44506500 -1.34999300
H 0.85294400 -0.22132900 -1.94412200
H 5.60325700 -1.83092600 0.00724600
H 7.32629200 1.18503100 0.51244100
H 9.66615700 -2.73489000 0.15015900
H 12.14105900 -2.46657300 0.04193300
H 13.12415300 -0.20619900 -0.29094800
H 11.63151600 1.76821900 -0.51677300
H 9.18778300 1.49575600 -0.40423800
H 5.75142800 2.62486200 -0.76226100
H 4.48531600 4.65601900 -0.12022100
H 2.72057600 4.52201700 1.62668400
H 2.23618100 2.34602900 2.72760800
H 3.49463900 0.31863200 2.07929200

L-Anti-1SPT (CYH)

C -3.35741600 3.87570600 3.76550200
C -4.39166500 4.20161100 2.87965600
C -5.00761300 3.21933700 2.11676400
C -4.59586400 1.86437400 2.19258300
C -3.55480600 1.55511000 3.10161900
C -2.95278100 2.54389900 3.87357900
C -5.19905800 0.81635100 1.38205300
C -6.18118700 1.04767400 0.42001300
C -7.02016700 0.08079900 -0.15546200
O -7.03503500 -1.20258600 0.28488100
N -4.84159800 -0.53933000 1.67561800
C -7.98462900 0.36236400 -1.20694100
C -7.97048000 1.57053100 -1.94206600

C -8.91829800 1.81730900 -2.92807100
C -9.90100500 0.86694600 -3.22419300
C -9.91862300 -0.33930600 -2.51814400
C -8.97763000 -0.59246300 -1.52622800
C -3.86745400 -1.09563200 0.96367800
C -3.59436700 -2.49296700 1.20550100
C -2.60245600 -3.15784500 0.52140600
C -1.80523000 -2.49447600 -0.43606300
C -2.04648500 -1.11972800 -0.67709800
C -3.03559700 -0.43270900 -0.01462200
C -0.72907100 -3.23508900 -1.20104900
C 0.63655100 -2.56952300 -1.16411700
C 1.25817600 -2.12136700 -2.33436900
C 2.51732900 -1.52624000 -2.29999700
C 3.18954800 -1.35283200 -1.08161900
C 2.56409300 -1.77809900 0.10182500
C 1.31300800 -2.38395900 0.05016500
N 4.43524200 -0.69384400 -1.11280700
O 5.53451700 1.52257700 -2.03985500
C 6.40942500 1.39340300 -1.15038900
C 6.44052700 0.26406800 -0.25329000
C 5.47453300 -0.72860200 -0.23369700
C 7.47578900 2.44512700 -1.04341400
C 5.64324300 -1.88616000 0.68744900
C 7.64756600 3.32094300 -2.12683500
C 8.61769400 4.31854100 -2.08678700
C 9.42467900 4.46500400 -0.95524300
C 9.25309000 3.60931300 0.13456900
C 8.28749000 2.60418500 0.09061600
C 5.97926500 -1.67945000 2.03378700
C 6.19571200 -2.76440600 2.88346300
C 6.09046700 -4.06785500 2.39590600
C 5.76401200 -4.28235000 1.05441500
C 5.53595800 -3.20124800 0.20621600
H -2.88304800 4.64709400 4.36417600
H -4.72823900 5.23102800 2.79385500
H -5.82697000 3.50384800 1.46617400
H -3.22702800 0.52756400 3.20045900
H -2.15903700 2.27140300 4.56358500
H -6.38654700 2.07429900 0.14723000
H -6.40336800 -1.27573500 1.03359300
H -7.19834800 2.30965300 -1.75762100
H -8.88380400 2.75289300 -3.47898200
H -10.63658700 1.06190300 -3.99852300

H -10.67426300 -1.08739300 -2.74095300
H -9.00147200 -1.52565200 -0.97670700
H -4.20397300 -2.99605500 1.94816700
H -2.42440100 -4.21110700 0.71908300
H -1.42452100 -0.59938900 -1.39944900
H -3.19935300 0.61802900 -0.21636000
H -1.04549200 -3.33106800 -2.24813700
H -0.65737900 -4.25716700 -0.81137200
H 0.75793100 -2.24625600 -3.29113200
H 2.98996900 -1.19553700 -3.22022000
H 3.04734200 -1.62449600 1.05866100
H 0.84598600 -2.70240200 0.97848500
H 4.54304100 0.08055300 -1.78306900
H 7.29749900 0.12459800 0.38981100
H 7.00559500 3.19731400 -2.99200900
H 8.74535500 4.98378700 -2.93578200
H 10.18017700 5.24461000 -0.92129200
H 9.86888800 3.72666000 1.02139100
H 8.15331800 1.96150900 0.95409200
H 6.05329000 -0.66537300 2.41371700
H 6.44534500 -2.59014200 3.92576000
H 6.26240600 -4.91244800 3.05636000
H 5.68963900 -5.29407700 0.66720000
H 5.28904300 -3.37188600 -0.83649700

L-Syn-1SPT (CYH)

C -5.47115600 5.27103500 -1.15794500
C -6.66854500 4.55426200 -1.27303500
C -6.75834100 3.24595000 -0.81859300
C -5.63938800 2.58853800 -0.24653600
C -4.44073200 3.33427600 -0.13192400
C -4.36378100 4.65046700 -0.57664400
C -5.69266000 1.20828600 0.21227500
C -6.81164100 0.38759100 0.07729200
C -7.04442300 -0.81273000 0.76649100
O -6.22486400 -1.23178300 1.76315800
N -4.56883300 0.70808300 0.94710500
C -8.19350200 -1.67415800 0.53650700
C -9.03473100 -1.52754800 -0.59084300
C -10.13566000 -2.35602500 -0.77248300
C -10.42755100 -3.36413700 0.15228500
C -9.59631500 -3.53289700 1.26330200
C -8.49580500 -2.70517000 1.45592300
C -3.63859100 0.03386000 0.28011400
C -2.56794200 -0.55132500 1.05591000

C -1.55746600 -1.26429200 0.45999200
C -1.52369800 -1.44988200 -0.94331200
C -2.55185300 -0.87340500 -1.72120700
C -3.57855700 -0.15410700 -1.14999600
C -0.42918900 -2.26983700 -1.59270000
C 0.97841500 -1.91897400 -1.14315200
C 1.78624100 -2.85344300 -0.48666200
C 3.08059900 -2.53130700 -0.08418200
C 3.60812400 -1.25704500 -0.33687500
C 2.81234600 -0.31772200 -1.01307400
C 1.51640900 -0.64874200 -1.39508500
N 4.94412500 -1.01713100 0.04383700
O 7.34958900 -2.05929400 -0.26449700
C 7.81234900 -0.91558200 -0.03716200
C 6.97117700 0.20616600 0.30230300
C 5.58693000 0.15127400 0.31929600
C 9.30039300 -0.72476200 -0.10046100
C 4.81701100 1.35370900 0.74016300
C 10.11262300 -1.86948000 -0.08211800
C 11.49883400 -1.75795100 -0.14441100
C 12.09610000 -0.49796000 -0.23809100
C 11.29807600 0.64717400 -0.27111700
C 9.90988400 0.53569500 -0.20028600
C 5.13696100 2.61746800 0.22140800
C 4.45736300 3.75452600 0.65829400
C 3.45724900 3.64421300 1.62548600
C 3.13693300 2.39038300 2.15228800
C 3.80667900 1.25170900 1.71063100
H -5.40851500 6.29647900 -1.50867800
H -7.54387400 5.02699100 -1.70971300
H -7.71106100 2.73368800 -0.89326500
H -3.57096400 2.87102500 0.31747500
H -3.42978500 5.19509800 -0.46941500
H -7.62199500 0.73922500 -0.54745900
H -5.52008400 -0.55778200 1.88272800
H -8.81067600 -0.77746100 -1.34153900
H -10.76475700 -2.22316500 -1.64802000
H -11.28594000 -4.01212900 0.00421100
H -9.80980000 -4.31473000 1.98675800
H -7.85931200 -2.83583600 2.32264400
H -2.59872500 -0.40453500 2.13017300
H -0.76474500 -1.69076100 1.06687200
H -2.52658000 -1.00227600 -2.79982800
H -4.35027500 0.28269800 -1.77054900

H -0.50919500 -2.16635100 -2.68111100
H -0.61394700 -3.33083900 -1.37701000
H 1.40130900 -3.84951200 -0.28416600
H 3.69037000 -3.26658900 0.43261000
H 3.21011400 0.66101000 -1.25148200
H 0.91689800 0.09319400 -1.91609800
H 5.61603600 -1.78829100 -0.07804600
H 7.42853900 1.12590200 0.63764100
H 9.63080600 -2.83883500 -0.01802700
H 12.11538600 -2.65181200 -0.12132500
H 13.17741500 -0.40927600 -0.28927500
H 11.75631200 1.62809200 -0.35633500
H 9.30398600 1.43408000 -0.24920500
H 5.90926100 2.70083300 -0.53673600
H 4.70862600 4.72513900 0.24137300
H 2.92980700 4.52944300 1.96786500
H 2.36540700 2.29973000 2.91091700
H 3.56010400 0.28089800 2.12774400

L-Anti-2SPT (ACN)

C -3.35142300 4.42335100 3.08767500
C -4.45542200 4.59686600 2.24270600
C -5.08718200 3.50727500 1.65801600
C -4.62958700 2.18001500 1.88078900
C -3.51336800 2.02649300 2.74454700
C -2.89509400 3.12571300 3.33372000
C -5.27197200 1.04449400 1.25109700
C -6.32522800 1.06907200 0.33339600
C -7.08361600 -0.07560900 -0.04582300
O -6.93112400 -1.21459900 0.50635000
N -4.79956900 -0.26222400 1.64583900
C -8.13859300 0.07113300 -1.10057500
C -8.20140500 1.14921100 -2.00406300
C -9.21169700 1.22286200 -2.96256800
C -10.18058700 0.21879600 -3.04851900
C -10.12319400 -0.86461700 -2.16655600
C -9.11320800 -0.93812600 -1.20990900
C -3.82163400 -0.96028400 1.03867000
C -3.51506400 -2.27511400 1.49681700
C -2.50825600 -2.99610800 0.89203700
C -1.76624000 -2.45598900 -0.18013300
C -2.07313600 -1.14974100 -0.62696300
C -3.07600000 -0.40849900 -0.04441800
C -0.66888400 -3.25540900 -0.84767600
C 0.67621500 -2.54708800 -0.85061700

C 1.26168400 -2.10549500 -2.04309200
C 2.49106100 -1.44883000 -2.04079000
C 3.18539700 -1.23235100 -0.83954100
C 2.59197500 -1.66067900 0.36341400
C 1.35937500 -2.30533900 0.35112500
N 4.38141600 -0.49628300 -0.88649400
O 5.31446100 1.71849100 -1.58256600
C 6.41639100 1.42263300 -0.90160900
C 6.53688700 0.22052100 -0.23192600
C 5.48025100 -0.75639700 -0.21040700
C 7.47601500 2.45322100 -0.94882800
C 5.74180600 -2.03051600 0.52973800
C 7.41612900 3.45627900 -1.93183400
C 8.40494300 4.43516300 -2.00643000
C 9.46524500 4.43288300 -1.09728400
C 9.52861900 3.44609900 -0.10924400
C 8.54305300 2.46501900 -0.03299800
C 6.28417600 -2.00086000 1.82373000
C 6.56289200 -3.18848100 2.50131700
C 6.32390900 -4.41871200 1.88582700
C 5.79922500 -4.45696300 0.59109400
C 5.50434100 -3.27222500 -0.08109700
H -2.86475500 5.27877100 3.54519800
H -4.83443200 5.59609400 2.04484400
H -5.95304100 3.68106900 1.02858300
H -3.12800200 1.03533600 2.95650100
H -2.04458000 2.96408100 3.99070600
H -6.61620800 2.03623400 -0.05682500
H -5.32252500 -0.75489700 2.36347800
H -7.44424600 1.92636200 -1.97809800
H -9.23664500 2.06254800 -3.65173000
H -10.96517900 0.27689600 -3.79722400
H -10.86822500 -1.65359100 -2.22643000
H -9.05459700 -1.77576500 -0.52332200
H -4.08327100 -2.69665500 2.31917000
H -2.28235600 -3.99731600 1.24340400
H -1.50250200 -0.72452500 -1.44566800
H -3.31286300 0.58801000 -0.39321900
H -0.96837300 -3.45795200 -1.88314400
H -0.58350000 -4.22770400 -0.35177200
H 0.75121600 -2.27531100 -2.98735700
H 2.93174200 -1.10497600 -2.97153700
H 3.09577100 -1.47415700 1.30551200
H 0.91937600 -2.62350200 1.29287600

H 4.70075600 0.88503800 -1.47623700
H 7.46886700 -0.02752100 0.25428100
H 6.59299000 3.45426700 -2.63684200
H 8.34835400 5.19971900 -2.77534000
H 10.23466300 5.19690500 -1.15394900
H 10.34329100 3.44537800 0.60837900
H 8.59358900 1.72139800 0.75494200
H 6.47203600 -1.04604700 2.30519400
H 6.96937100 -3.15147100 3.50744000
H 6.54812700 -5.34280800 2.40998300
H 5.62168500 -5.41060300 0.10328100
H 5.10103300 -3.30690100 -1.08766300

L-Syn-2SPT (ACN)

C -5.05214700 5.24671600 -1.38556500
C -6.29901900 4.61318100 -1.46810900
C -6.48516900 3.33172100 -0.96659500
C -5.41734300 2.61035400 -0.36644000
C -4.16394200 3.27273200 -0.28870400
C -3.99242000 4.56180700 -0.78504600
C -5.60322800 1.26483600 0.13687400
C -6.76202800 0.48727200 0.06812300
C -6.96521000 -0.71430300 0.80590200
O -6.13854300 -1.12916500 1.68341200
N -4.47801100 0.67400700 0.82369800
C -8.22116800 -1.50097400 0.58023600
C -9.05448900 -1.34615500 -0.54412600
C -10.21019400 -2.11270500 -0.69085900
C -10.56001300 -3.05862600 0.27723100
C -9.73498100 -3.23300800 1.39238600
C -8.58029100 -2.46748200 1.53812400
C -3.52159900 -0.08357100 0.25495700
C -2.51608800 -0.67480700 1.07816900
C -1.52966900 -1.44468800 0.50984100
C -1.49154500 -1.67096700 -0.88766900
C -2.48410000 -1.08024000 -1.69547200
C -3.48464000 -0.29992700 -1.15231400
C -0.41532700 -2.54424000 -1.49282900
C 0.99694900 -2.12563000 -1.11883800
C 1.83909200 -2.98024000 -0.39760500
C 3.14240300 -2.60452700 -0.07682800
C 3.63490200 -1.34271200 -0.44610700
C 2.79476700 -0.48438100 -1.18088800
C 1.50004400 -0.87436300 -1.50745100
N 4.98053400 -1.04487800 -0.17084800

O 7.31241800 -1.81894800 -0.63704400
C 7.75071700 -0.66162800 -0.15325900
C 6.86849100 0.29085900 0.31860200
C 5.44235500 0.09881200 0.28811400
C 9.22139200 -0.50571800 -0.14282500
C 4.59145600 1.19568700 0.84669800
C 10.03455200 -1.64013000 -0.31079000
C 11.42315500 -1.52510400 -0.29632000
C 12.02254300 -0.27590900 -0.12036500
C 11.22317300 0.85992600 0.03720400
C 9.83507600 0.74838600 0.02463100
C 4.83069400 2.53150600 0.48907700
C 4.06382000 3.55942800 1.03892200
C 3.06385300 3.26705200 1.96840800
C 2.82950500 1.94084400 2.34183400
C 3.58299700 0.91110400 1.78127100
H -4.91440400 6.25032600 -1.77508800
H -7.14031700 5.13019000 -1.92215500
H -7.47104100 2.88407300 -1.02937800
H -3.31723000 2.77244300 0.16809300
H -3.01710800 5.03420900 -0.70278400
H -7.57532200 0.86776600 -0.53695600
H -4.46757600 0.72083100 1.83804200
H -8.79016200 -0.64005000 -1.32469300
H -10.83495300 -1.97752900 -1.56952000
H -11.45926600 -3.65620200 0.15991000
H -9.99374300 -3.96860100 2.14942400
H -7.92985400 -2.59755800 2.39624300
H -2.54694400 -0.51206200 2.15030200
H -0.76635600 -1.88980000 1.13894300
H -2.46063900 -1.24427300 -2.76766500
H -4.24461800 0.15154600 -1.77623700
H -0.53249600 -2.54967900 -2.58163500
H -0.58100100 -3.57603200 -1.15889000
H 1.47731800 -3.95867000 -0.09276000
H 3.79045000 -3.28255000 0.47001400
H 3.16856100 0.48006200 -1.50736400
H 0.87333100 -0.19758700 -2.08271100
H 6.27739400 -1.77791300 -0.53618600
H 7.25038400 1.19388500 0.77163300
H 9.56636600 -2.60832000 -0.44521800
H 12.03774200 -2.41144500 -0.42134900
H 13.10455600 -0.18598100 -0.11089300
H 11.68203300 1.83584700 0.16246200

H 9.23054300 1.64335200 0.12336000
H 5.60804000 2.76286700 -0.23268100
H 4.25060800 4.58738500 0.74346100
H 2.47236700 4.06753700 2.40236900
H 2.06053200 1.70834000 3.07227200
H 3.40017200 -0.11651900 2.07714200

L-Anti-2SPT (DCM)

C -3.43580200 4.48753100 3.05851600
C -4.53738300 4.63830000 2.20628600
C -5.14891800 3.53568700 1.62500100
C -4.67168200 2.21693400 1.85796100
C -3.55768000 2.08668800 2.72870300
C -2.96059500 3.19866100 3.31495000
C -5.29179100 1.06920800 1.23110600
C -6.34128800 1.06868700 0.30874000
C -7.09034300 -0.08940600 -0.05099500
O -6.92780000 -1.21687500 0.52000100
N -4.80543900 -0.23069500 1.63786400
C -8.14787900 0.03022600 -1.10635700
C -8.23114800 1.09790600 -2.02010000
C -9.24554800 1.14550300 -2.97581700
C -10.19797400 0.12502600 -3.04842400
C -10.11970000 -0.94852900 -2.15624900
C -9.10585000 -0.99588300 -1.20243600
C -3.82550600 -0.92575500 1.03519500
C -3.53565100 -2.25071200 1.47804700
C -2.52646500 -2.97120100 0.87781200
C -1.76333700 -2.42132600 -0.17471300
C -2.05114400 -1.10456700 -0.60472000
C -3.05635700 -0.36356800 -0.02725500
C -0.66679200 -3.22245600 -0.84118200
C 0.68153500 -2.52083700 -0.84336800
C 1.27889300 -2.09852400 -2.03676100
C 2.51236000 -1.44995200 -2.03329000
C 3.19923200 -1.22269300 -0.82982100
C 2.59392400 -1.63165700 0.37388900
C 1.35744800 -2.26839600 0.36015600
N 4.40084400 -0.49642300 -0.87780900
O 5.35911000 1.70324500 -1.59338600
C 6.45585900 1.40197900 -0.90749800
C 6.56135100 0.20585600 -0.22432100
C 5.49479400 -0.75969700 -0.19535100
C 7.52766900 2.41940300 -0.96386300
C 5.74161200 -2.02745400 0.56090300

C 7.47585900 3.41903400 -1.95065900
C 8.47655600 4.38500300 -2.03367300
C 9.54103800 4.37308700 -1.12971500
C 9.59656400 3.38974900 -0.13798900
C 8.59903400 2.42184000 -0.05324900
C 6.28351900 -1.98674500 1.85473100
C 6.54992900 -3.16791400 2.54814200
C 6.29829800 -4.40346600 1.94889600
C 5.77358200 -4.45313300 0.65466200
C 5.49097200 -3.27452300 -0.03325400
H -2.96537700 5.35324200 3.51363400
H -4.93116100 5.63024800 2.00057700
H -6.01489200 3.69139700 0.99093900
H -3.15786200 1.10289500 2.94834200
H -2.11143900 3.05454900 3.97782500
H -6.64215700 2.02732500 -0.09488600
H -5.34960100 -0.73572300 2.33064800
H -7.48690800 1.88773200 -2.00418700
H -9.28678400 1.97800000 -3.67296000
H -10.98596500 0.16298800 -3.79492900
H -10.85174900 -1.75030600 -2.20603900
H -9.02997800 -1.82492500 -0.50730800
H -4.12249400 -2.68032700 2.28292100
H -2.31575900 -3.98043500 1.21565400
H -1.46222100 -0.67152600 -1.40619700
H -3.27794200 0.64091100 -0.36253400
H -0.96683600 -3.42375800 -1.87703200
H -0.58591100 -4.19629300 -0.34707000
H 0.77447300 -2.27680400 -2.98278800
H 2.96254700 -1.12052100 -2.96467000
H 3.09200000 -1.43650000 1.31726400
H 0.90803200 -2.57167700 1.30245300
H 4.73586300 0.87922500 -1.48068300
H 7.48988400 -0.04796700 0.26540200
H 6.64900700 3.42417000 -2.65123800
H 8.42578900 5.14722300 -2.80533100
H 10.31975400 5.12712400 -1.19323900
H 10.41460700 3.38156000 0.57580000
H 8.64429200 1.68119600 0.73778600
H 6.48109000 -1.02748600 2.32337400
H 6.95681400 -3.12181500 3.55376500
H 6.51278700 -5.32295600 2.48513700
H 5.58600700 -5.41124500 0.17946900
H 5.08661100 -3.31812700 -1.03902400

L-Syn-2SPT (DCM)

C -5.38726800 5.26857000 -1.33651000
C -6.60790700 4.58130400 -1.34310600
C -6.70220500 3.28486700 -0.85611000
C -5.56358400 2.59984500 -0.34984800
C -4.33794200 3.31730400 -0.34713400
C -4.25882000 4.62109700 -0.82629800
C -5.65648000 1.23891300 0.12924000
C -6.77586200 0.40263000 0.10771800
C -6.89240100 -0.79827400 0.86819100
O -6.01463600 -1.16298000 1.71540500
N -4.47236800 0.68794900 0.75546000
C -8.12094700 -1.64091500 0.70526300
C -8.99815200 -1.54818200 -0.39134000
C -10.12565400 -2.36416300 -0.47757100
C -10.40156400 -3.29735000 0.52546400
C -9.53149500 -3.40963600 1.61395300
C -8.40500100 -2.59530300 1.69893800
C -3.52026100 -0.02847500 0.13822200
C -2.48860600 -0.64021600 0.91620000
C -1.49573000 -1.35981200 0.29739900
C -1.47302800 -1.51560000 -1.11025500
C -2.49168400 -0.90738600 -1.87371100
C -3.49943900 -0.17694100 -1.28038500
C -0.39008100 -2.33658100 -1.77433100
C 1.01837700 -1.96325000 -1.34509200
C 1.82956900 -2.86673400 -0.64875600
C 3.12784600 -2.52635300 -0.27384000
C 3.64750900 -1.25439100 -0.56327400
C 2.83858100 -0.34726600 -1.27416800
C 1.54823200 -0.70108600 -1.65353900
N 4.98841800 -0.99467700 -0.23583100
O 7.32184900 -1.80301700 -0.65305900
C 7.76560600 -0.67437600 -0.11323100
C 6.88710900 0.28023500 0.36263800
C 5.45983900 0.12110400 0.27866700
C 9.23776200 -0.55039400 -0.04719800
C 4.61558600 1.21813700 0.84783100
C 10.03242700 -1.69500600 -0.23102800
C 11.42153400 -1.61070800 -0.16550100
C 12.04004200 -0.38257300 0.07780600
C 11.25947500 0.76362300 0.25145600
C 9.87087600 0.68262900 0.18827200
C 4.89096300 2.55856500 0.53718400

C 4.13004500 3.58574000 1.09622800
C 3.09927100 3.28704600 1.98894400
C 2.82836200 1.95577300 2.31567700
C 3.57592700 0.92741700 1.74517700
H -5.32151300 6.28417900 -1.71346700
H -7.50179000 5.06900700 -1.72326300
H -7.67027100 2.79595300 -0.85130900
H -3.43971000 2.84664200 0.03709200
H -3.30173900 5.13572500 -0.80273700
H -7.63214600 0.74067700 -0.46251600
H -4.45733800 0.66550300 1.77056500
H -8.78921400 -0.85226300 -1.19771700
H -10.78623200 -2.27753600 -1.33605800
H -11.27923700 -3.93340800 0.45556700
H -9.73343900 -4.13513500 2.39762500
H -7.71795100 -2.67452400 2.53434800
H -2.51044100 -0.53519900 1.99575600
H -0.71377700 -1.81934400 0.89222800
H -2.48010700 -1.01773000 -2.95309700
H -4.27726200 0.29006400 -1.86945900
H -0.49187300 -2.24558200 -2.86107700
H -0.56799500 -3.39351100 -1.53768800
H 1.44829600 -3.85560000 -0.40742800
H 3.75326800 -3.24090800 0.25233100
H 3.23342100 0.62693000 -1.54075700
H 0.94547300 0.01344000 -2.20856300
H 6.28703600 -1.74550600 -0.58737300
H 7.27193400 1.15604900 0.86386700
H 9.54814000 -2.64615900 -0.41874700
H 12.02184800 -2.50488200 -0.30380200
H 13.12277300 -0.31669800 0.12692700
H 11.73383000 1.72401100 0.42884800
H 9.28113900 1.58596400 0.30037700
H 5.69271100 2.79398000 -0.15616800
H 4.34538800 4.61793800 0.83697700
H 2.51228100 4.08657000 2.43082300
H 2.03519900 1.71814400 3.01817600
H 3.36427700 -0.10468300 2.00408100

L-Anti-2SPT (CYH)

C -3.74107900 4.53196400 3.22278800
C -4.80160500 4.65809600 2.31655800
C -5.33738700 3.54652600 1.68221000
C -4.81915500 2.24202300 1.91176500
C -3.74747000 2.13683200 2.83812800

C -3.22910800 3.25699100 3.47854900
C -5.35521800 1.09243700 1.22498200
C -6.34273400 1.06372200 0.23672500
C -7.07644100 -0.10776000 -0.12364800
O -6.95602600 -1.21121000 0.49915400
N -4.87028700 -0.21213600 1.64416700
C -8.06601200 -0.02650700 -1.24482400
C -8.09565400 1.01091800 -2.19480600
C -9.05053500 1.02454700 -3.21053000
C -9.99429700 -0.00112300 -3.30674400
C -9.96710900 -1.04580400 -2.37839200
C -9.01304200 -1.05956100 -1.36469200
C -3.87305500 -0.89273200 1.06809100
C -3.67019200 -2.26602400 1.41404300
C -2.63910400 -2.97554900 0.84292400
C -1.76226700 -2.37289600 -0.08665700
C -1.95932600 -1.01028500 -0.41809400
C -2.98373500 -0.27718700 0.13202200
C -0.65786500 -3.17574200 -0.73802000
C 0.69282600 -2.48275500 -0.76273600
C 1.29059500 -2.09877200 -1.96849600
C 2.52957200 -1.46181800 -1.98638700
C 3.22259200 -1.20781600 -0.79183200
C 2.61671300 -1.57830300 0.42388700
C 1.37493100 -2.20373800 0.43098400
N 4.43027900 -0.49587700 -0.86384300
O 5.41622600 1.67918600 -1.63492300
C 6.50909300 1.37925100 -0.94593600
C 6.60100700 0.19839100 -0.23348000
C 5.52351600 -0.75210000 -0.17765700
C 7.59362400 2.38099900 -1.03007600
C 5.75713200 -2.00171300 0.61319000
C 7.54237400 3.36522900 -2.03171100
C 8.55408800 4.31637600 -2.14166300
C 9.62895200 4.30507300 -1.25070400
C 9.68393800 3.33737800 -0.24424100
C 8.67543300 2.38427300 -0.13266100
C 6.29995000 -1.93131400 1.90510000
C 6.55349900 -3.09498900 2.63151200
C 6.28751400 -4.34365700 2.06759500
C 5.76102000 -4.42347800 0.77604800
C 5.49141900 -3.26191800 0.05532800
H -3.33081300 5.40486200 3.72030400
H -5.22536500 5.63804100 2.11248900

H -6.17999800 3.67844800 1.01226500
H -3.32068300 1.16431500 3.05754100
H -2.41166800 3.13197200 4.18399800
H -6.62652700 2.01140200 -0.20419800
H -5.51894200 -0.76641000 2.19655300
H -7.35396900 1.80260600 -2.15891000
H -9.05205500 1.83446900 -3.93513200
H -10.73656400 0.01014600 -4.09976900
H -10.69305000 -1.85182900 -2.44727000
H -8.97317500 -1.86529800 -0.63999200
H -4.35019100 -2.73714300 2.11531800
H -2.49930900 -4.01991700 1.10298200
H -1.27955000 -0.53733800 -1.11859200
H -3.13388800 0.76268700 -0.12451100
H -0.96421100 -3.39913400 -1.76884000
H -0.57817300 -4.14384500 -0.23076000
H 0.78166900 -2.29794700 -2.90822900
H 2.98011800 -1.16068400 -2.92702600
H 3.11992900 -1.36254300 1.35986000
H 0.92587000 -2.47691800 1.38276400
H 4.78161300 0.87165400 -1.50378000
H 7.52898800 -0.05736000 0.25617600
H 6.70560400 3.36930400 -2.72025800
H 8.50350300 5.06739800 -2.92432000
H 10.41641500 5.04799300 -1.33545000
H 10.51041400 3.33010600 0.45993400
H 8.72004300 1.65563900 0.66954200
H 6.50806200 -0.96089200 2.34558900
H 6.96167000 -3.02534400 3.63538000
H 6.49212500 -5.25013800 2.62939400
H 5.56174000 -5.39245900 0.32827500
H 5.08444100 -3.32847200 -0.94808400

L-Syn-2SPT (CYH)

C -6.04139900 5.26106100 -1.30991200
C -7.17971600 4.44771200 -1.24008700
C -7.10172800 3.14601900 -0.76641700
C -5.86305300 2.58148400 -0.35340700
C -4.72294700 3.42589600 -0.42717700
C -4.81718700 4.73387500 -0.88981400
C -5.77835900 1.21632000 0.10368800
C -6.79565500 0.25904500 0.14758300
C -6.74144300 -0.92594700 0.94333600
O -5.79128100 -1.16484800 1.75526700
N -4.50387400 0.78151900 0.65155700

C -7.87295000 -1.90405800 0.86262200
C -8.81223800 -1.93500800 -0.18422700
C -9.84424100 -2.87242100 -0.19260000
C -9.95879500 -3.80590000 0.84048900
C -9.02397100 -3.79548800 1.87972600
C -7.99299000 -2.86002700 1.88724500
C -3.54218400 0.14693500 -0.02792000
C -2.45428700 -0.45146000 0.68519600
C -1.44610000 -1.08511500 0.00160100
C -1.45832700 -1.16528200 -1.41243800
C -2.53087000 -0.56984300 -2.11309700
C -3.55501700 0.07422600 -1.45533300
C -0.36687200 -1.90313500 -2.15582600
C 1.03901500 -1.62262100 -1.65738300
C 1.81781400 -2.62839200 -1.07366200
C 3.11475900 -2.37066600 -0.63452600
C 3.66648200 -1.08404300 -0.74366600
C 2.89040000 -0.07300500 -1.34196300
C 1.60121200 -0.34377600 -1.78701800
N 5.00460700 -0.90057700 -0.36086600
O 7.33813900 -1.69265000 -0.83557400
C 7.78609600 -0.65528100 -0.14101900
C 6.91238300 0.24509000 0.43900700
C 5.48563800 0.12666500 0.30622400
C 9.25796900 -0.57026300 -0.02699900
C 4.64872000 1.15625100 0.99969800
C 10.03711900 -1.69299900 -0.35403200
C 11.42520200 -1.64661700 -0.24734700
C 12.05828900 -0.47816200 0.18064700
C 11.29347700 0.64740200 0.49785100
C 9.90592300 0.60389100 0.39403100
C 4.94950000 2.52032600 0.86826100
C 4.19558100 3.48037900 1.54355500
C 3.14602000 3.08767900 2.37548700
C 2.84942700 1.73062300 2.52409700
C 3.58999600 0.77119700 1.83676100
H -6.11067700 6.28066400 -1.67516400
H -8.14535200 4.84094200 -1.54736300
H -8.00954200 2.55697800 -0.69490200
H -3.75504500 3.04979900 -0.11450500
H -3.92108900 5.34815000 -0.92534500
H -7.71398900 0.49064000 -0.37786600
H -4.47144200 0.67584700 1.66193300
H -8.72530600 -1.23971300 -1.01324100

H -10.55615500 -2.88000900 -1.01365600
H -10.76234700 -4.53677800 0.83160200
H -9.10077600 -4.52056500 2.68577600
H -7.25591300 -2.84132700 2.68254300
H -2.45383900 -0.41103300 1.76902000
H -0.62493900 -1.53638200 0.54764500
H -2.54419400 -0.62047400 -3.19718500
H -4.37104200 0.53462000 -1.99541000
H -0.44587800 -1.66636300 -3.22293100
H -0.56928900 -2.97960500 -2.07161900
H 1.41199200 -3.63177400 -0.97226600
H 3.71528200 -3.16243500 -0.19755300
H 3.31037100 0.91856700 -1.46975200
H 1.02457800 0.45187100 -2.25232200
H 6.30589200 -1.62763400 -0.78709900
H 7.29987500 1.03726900 1.06239400
H 9.54018600 -2.59706900 -0.68567800
H 12.01355300 -2.52414400 -0.49819100
H 13.14053600 -0.44168700 0.26191900
H 11.77975000 1.56333100 0.81968900
H 9.32864900 1.49388200 0.62014700
H 5.76655600 2.82802800 0.22263100
H 4.43102200 4.53348000 1.42244000
H 2.56436200 3.83393300 2.90831000
H 2.04151900 1.41891400 3.17934500
H 3.35852700 -0.28193300 1.95685800

L-Anti-DPT (ACN)

C -3.46495500 4.50576900 3.00439700
C -4.56614900 4.63562700 2.14800800
C -5.16531500 3.51518400 1.58788400
C -4.67020400 2.21163200 1.84827000
C -3.56113900 2.10159500 2.72311200
C -2.97452900 3.22973600 3.29023200
C -5.25749900 1.01794200 1.25482400
C -6.29478500 1.04720400 0.31615200
C -7.09393400 -0.03696800 -0.06154500
O -7.01328600 -1.23928500 0.56583000
N -4.82445800 -0.24684300 1.74659400
C -8.11873400 0.02577400 -1.09763600
C -8.19353300 1.09574500 -2.01826500
C -9.19114700 1.13517500 -2.98642900
C -10.13531900 0.10665100 -3.07708300
C -10.06518500 -0.96630500 -2.18388100
C -9.07293600 -1.01067400 -1.20889300

C -3.84295000 -0.88225500 1.09397500
C -3.48846200 -2.19682800 1.55572900
C -2.48829400 -2.92198100 0.94419500
C -1.77196500 -2.39597600 -0.15124200
C -2.10001100 -1.09888600 -0.61007800
C -3.09907100 -0.35698900 -0.02108800
C -0.67940000 -3.19691800 -0.82803800
C 0.67305100 -2.50202100 -0.83275800
C 1.26464100 -2.07201000 -2.02637400
C 2.50085500 -1.42745300 -2.02719200
C 3.19724500 -1.21346700 -0.82721900
C 2.59900500 -1.63017300 0.37728900
C 1.35944100 -2.26166100 0.36737700
N 4.40225400 -0.49053000 -0.87606700
O 5.36180300 1.71117800 -1.57451800
C 6.46136500 1.40172700 -0.89547700
C 6.56814500 0.19844000 -0.22608300
C 5.49859900 -0.76488400 -0.20216400
C 7.53366700 2.41923400 -0.94416200
C 5.74517700 -2.04169300 0.53871300
C 7.48556800 3.42246900 -1.92758700
C 8.48637700 4.38905600 -2.00332500
C 9.54723800 4.37413500 -1.09495900
C 9.59907900 3.38706800 -0.10652700
C 8.60143600 2.41835300 -0.02912100
C 6.28959500 -2.01789000 1.83193100
C 6.55547700 -3.20835300 2.50974100
C 6.30142900 -4.43601700 1.89520000
C 5.77453500 -4.46868100 0.60120500
C 5.49252500 -3.28088600 -0.07113900
H -3.00412700 5.38493100 3.44371200
H -4.96695800 5.62044900 1.92545200
H -6.03360800 3.65205000 0.95300400
H -3.16428300 1.12062700 2.95569600
H -2.12606600 3.11024100 3.95807200
H -6.55795100 2.00521800 -0.11217300
H -6.34486400 -1.16187200 1.28352600
H -7.45426900 1.88888700 -1.99230300
H -9.22557700 1.96757700 -3.68318600
H -10.90954100 0.13884100 -3.83736400
H -10.79009400 -1.77290600 -2.24576500
H -9.02896300 -1.84197400 -0.51543700
H -4.03722700 -2.59763500 2.40125800
H -2.24415700 -3.91539900 1.30853300

H -1.54513100 -0.68175500 -1.44526400
H -3.33584400 0.63320700 -0.39075800
H -0.97818400 -3.39568300 -1.86461600
H -0.59699200 -4.17196000 -0.33586600
H 0.75251800 -2.24047900 -2.97011000
H 2.94476300 -1.09170400 -2.95947500
H 3.10467900 -1.44462200 1.31868900
H 0.91491800 -2.56937400 1.31051500
H 4.73771200 0.88478600 -1.46591300
H 7.49771800 -0.06122100 0.25869400
H 6.66193400 3.43018700 -2.63198400
H 8.43867400 5.15391000 -2.77255800
H 10.32598800 5.12858200 -1.15252500
H 10.41416400 3.37657900 0.61056800
H 8.64317000 1.67455100 0.75917500
H 6.48940300 -1.06511900 2.31265700
H 6.96375500 -3.17558100 3.51529200
H 6.51559400 -5.36243500 2.41947300
H 5.58515700 -5.42040300 0.11407200
H 5.08737000 -3.31134200 -1.07709500

L-Syn-DPT (ACN)

C -5.08582400 5.22231300 -1.43332900
C -6.32173000 4.56924100 -1.52804700
C -6.48988900 3.29059900 -1.01339200
C -5.41439900 2.60119600 -0.39648400
C -4.17494900 3.28184800 -0.30493600
C -4.01916300 4.56905300 -0.81204600
C -5.54862900 1.24988700 0.12997300
C -6.71436600 0.48360500 0.01841400
C -7.01098400 -0.67263700 0.74784200
O -6.21377500 -1.10574000 1.75875600
N -4.47016300 0.72997200 0.90264200
C -8.21076100 -1.47843000 0.54995700
C -9.03220700 -1.33817600 -0.59172500
C -10.17764600 -2.11174500 -0.74577300
C -10.53363800 -3.05623000 0.22311900
C -9.72315100 -3.21759200 1.35044800
C -8.57795700 -2.44383000 1.51447000
C -3.55127700 -0.02353100 0.28628200
C -2.53079600 -0.62234900 1.10696500
C -1.54669100 -1.40963900 0.55844100
C -1.49971100 -1.65583700 -0.83478200
C -2.48416300 -1.06694300 -1.65420100
C -3.48430500 -0.27409200 -1.12783300

C -0.42509700 -2.54363400 -1.42498700
C 0.99223400 -2.12526100 -1.06902200
C 1.84960400 -2.98697000 -0.37480700
C 3.15797800 -2.61313300 -0.07124400
C 3.64127600 -1.34556700 -0.43132800
C 2.78681400 -0.47961800 -1.13997200
C 1.48731500 -0.86826200 -1.44920700
N 4.99088700 -1.04651700 -0.17293400
O 7.31798500 -1.80581000 -0.68032300
C 7.75944400 -0.65456800 -0.18479000
C 6.88081900 0.28789800 0.31261000
C 5.45465300 0.09119000 0.29803100
C 9.22982500 -0.49437600 -0.19071600
C 4.60804400 1.17638900 0.88554700
C 10.04394700 -1.62355700 -0.38681100
C 11.43233900 -1.50475000 -0.38796100
C 12.03056100 -0.25681100 -0.19964300
C 11.23011000 0.87403300 -0.01404900
C 9.84226100 0.75864700 -0.01107900
C 4.83661000 2.51830600 0.54422100
C 4.07498400 3.53504000 1.12159600
C 3.09108900 3.22498700 2.06240300
C 2.86750800 1.89245000 2.41951300
C 3.61566600 0.87406900 1.83168300
H -4.96202100 6.22423500 -1.83222900
H -7.16424400 5.06836400 -1.99824700
H -7.46819600 2.82780800 -1.07986800
H -3.33464300 2.79189500 0.17226700
H -3.05600500 5.06367300 -0.72324000
H -7.49584800 0.84766100 -0.63530800
H -5.47234300 -0.46566900 1.85447200
H -8.76157400 -0.63770700 -1.37419800
H -10.79081800 -1.98574400 -1.63329100
H -11.42594200 -3.66145600 0.09671700
H -9.98648700 -3.94976900 2.10841400
H -7.95859600 -2.56987600 2.39446600
H -2.56998000 -0.43182200 2.17428600
H -0.78825000 -1.85020000 1.19827900
H -2.45100900 -1.24345500 -2.72544400
H -4.22772000 0.17112800 -1.77756300
H -0.54493300 -2.56850200 -2.51387500
H -0.58749500 -3.57079900 -1.07474800
H 1.49490900 -3.96995700 -0.07599800
H 3.81622500 -3.29671800 0.45634000

H 3.15285500 0.49036400 -1.45904500
H 0.84832000 -0.18445400 -2.00224800
H 6.28339900 -1.76831900 -0.56561600
H 7.26567300 1.18539100 0.77410000
H 9.57666400 -2.59084200 -0.53062500
H 12.04769200 -2.38723300 -0.53472300
H 13.11236500 -0.16390900 -0.20220900
H 11.68784200 1.84918600 0.12101900
H 9.23657000 1.65015400 0.10952000
H 5.60160600 2.76339900 -0.18617300
H 4.25333000 4.56801300 0.83862400
H 2.50359800 4.01657000 2.51761200
H 2.11089900 1.64611400 3.15828100
H 3.44093100 -0.15854700 2.11473700

L-Anti-DPT (DCM)

C -3.50058600 4.50009800 3.02728300
C -4.59999000 4.63014300 2.16897600
C -5.19254300 3.51048600 1.60063800
C -4.69207900 2.20769700 1.85382800
C -3.58492000 2.09753500 2.73082400
C -3.00527300 3.22460100 3.30664000
C -5.27152500 1.01517100 1.25085100
C -6.30885700 1.04491300 0.31362800
C -7.10545900 -0.04110800 -0.06793400
O -7.01684600 -1.24568200 0.55262100
N -4.83078100 -0.25202500 1.73343900
C -8.13385200 0.02265100 -1.09919000
C -8.22758700 1.10378500 -2.00521200
C -9.23001500 1.14292500 -2.96810500
C -10.16093900 0.10339300 -3.06852800
C -10.07207800 -0.98039200 -2.19029800
C -9.07508700 -1.02476000 -1.22062500
C -3.84850700 -0.87584700 1.07545300
C -3.49275400 -2.19677300 1.52191500
C -2.49126600 -2.91374000 0.90396600
C -1.77122400 -2.37337400 -0.18217700
C -2.09793500 -1.06976800 -0.62463000
C -3.09949600 -0.33611200 -0.03078900
C -0.67727500 -3.16552400 -0.86635900
C 0.67651300 -2.47318000 -0.86072300
C 1.28689500 -2.06091100 -2.05093300
C 2.52659200 -1.42343300 -2.04216800
C 3.20770800 -1.19894900 -0.83549000
C 2.59018200 -1.59706400 0.36548000

C 1.34751300 -2.22169100 0.34569600
N 4.41826800 -0.48521900 -0.87727600
O 5.40770700 1.70006500 -1.59191100
C 6.49743800 1.38617900 -0.90013600
C 6.58458300 0.19026100 -0.21471000
C 5.50505800 -0.76177400 -0.18940200
C 7.58245500 2.38996000 -0.95289700
C 5.73224300 -2.03111100 0.57062300
C 7.54954300 3.38704100 -1.94301900
C 8.56302800 4.33991500 -2.02293500
C 9.62180100 4.31732400 -1.11251400
C 9.65859800 3.33653300 -0.11739700
C 8.64818100 2.38177700 -0.03573900
C 6.26843800 -1.99478500 1.86691900
C 6.51744600 -3.17784400 2.56362500
C 6.25390900 -4.41133100 1.96529800
C 5.73472000 -4.45687900 0.66867300
C 5.46952300 -3.27616100 -0.02254200
H -3.04497500 5.37865500 3.47326200
H -5.00492300 5.61448400 1.95163400
H -6.06047900 3.64716500 0.96530000
H -3.18497500 1.11685600 2.95887100
H -2.15833300 3.10480600 3.97637800
H -6.57916800 2.00446300 -0.10673500
H -6.34662500 -1.16868500 1.26864200
H -7.49921500 1.90669200 -1.97203800
H -9.27895300 1.98431700 -3.65317600
H -10.93912400 0.13560500 -3.82478300
H -10.78635700 -1.79584100 -2.25997200
H -9.01655000 -1.86475500 -0.53896300
H -4.04362200 -2.60774000 2.36114300
H -2.24827800 -3.91204300 1.25582400
H -1.53840900 -0.64104600 -1.45087200
H -3.33365100 0.65928300 -0.38756800
H -0.97407300 -3.35244400 -1.90588000
H -0.59644600 -4.14697000 -0.38629200
H 0.78684700 -2.23759400 -2.99971900
H 2.98553000 -1.10107700 -2.97188400
H 3.08370600 -1.40257700 1.31150000
H 0.88762700 -2.51479300 1.28613100
H 4.77353700 0.88334300 -1.47958200
H 7.50728800 -0.07440600 0.28029900
H 6.72707600 3.40041600 -2.64863900
H 8.52668700 5.10025400 -2.79728400

H 10.41049900 5.06112800 -1.17363500
H 10.47206000 3.32015900 0.60149300
H 8.67895100 1.64320900 0.75794500
H 6.47526300 -1.03714800 2.33491500
H 6.91997700 -3.13484500 3.57114900
H 6.45464500 -5.33241300 2.50414400
H 5.53762900 -5.41349200 0.19428400
H 5.06882900 -3.31656900 -1.02989200

L-Syn-DPT (DCM)

C -5.16003000 5.22885100 -1.41310800
C -6.38614500 4.55879800 -1.51080900
C -6.53586700 3.27596200 -1.00169000
C -5.45082300 2.59861700 -0.38860700
C -4.22180600 3.29682500 -0.29334800
C -4.08469300 4.58819300 -0.79397200
C -5.56532100 1.24283700 0.12923700
C -6.71968000 0.46298100 0.01917500
C -7.00096400 -0.69400800 0.75705100
O -6.19485800 -1.10810600 1.76689100
N -4.47485300 0.73024400 0.89555400
C -8.19143800 -1.51273000 0.56912500
C -9.02332300 -1.38508200 -0.56668600
C -10.16173500 -2.17041200 -0.70909900
C -10.50080200 -3.11464000 0.26584900
C -9.67977200 -3.26386500 1.38717900
C -8.54155500 -2.47866400 1.53974600
C -3.55810800 -0.01137200 0.27072900
C -2.52587900 -0.60652400 1.08372700
C -1.53883200 -1.38385900 0.52841900
C -1.49666300 -1.62605300 -0.86590200
C -2.48988000 -1.04057200 -1.67863600
C -3.49283000 -0.25689600 -1.14679900
C -0.42027700 -2.50616400 -1.46418800
C 0.99693100 -2.09447200 -1.10056300
C 1.85000500 -2.96343400 -0.41066700
C 3.15781100 -2.59480400 -0.09945500
C 3.64547900 -1.32579000 -0.44818300
C 2.79520300 -0.45284300 -1.15303800
C 1.49609100 -0.83597700 -1.46909100
N 4.99431200 -1.03338000 -0.18076100
O 7.31840500 -1.80840000 -0.66924800
C 7.76448000 -0.66150600 -0.17207700
C 6.88894300 0.28904500 0.31696500
C 5.46233800 0.10228600 0.29127200

C 9.23617100 -0.51273100 -0.16677000
C 4.61878800 1.19591500 0.86788100
C 10.04153200 -1.64645600 -0.37046500
C 11.43064400 -1.53957200 -0.36195900
C 12.03848800 -0.29935800 -0.15626700
C 11.24687400 0.83609100 0.03701300
C 9.85836600 0.73247500 0.03034700
C 4.85996200 2.53447200 0.52269400
C 4.10131400 3.55949600 1.08873400
C 3.10698800 3.26112000 2.02194400
C 2.87017000 1.93208400 2.38244800
C 3.61572100 0.90562700 1.80602900
H -5.05051700 6.23435500 -1.80729700
H -7.23600900 5.04830800 -1.97806200
H -7.50799400 2.80019200 -1.06774200
H -3.37580700 2.81658400 0.18327800
H -3.12906400 5.09669000 -0.70155800
H -7.51010800 0.81865600 -0.62835100
H -5.45946900 -0.45841100 1.85147800
H -8.76482500 -0.68522100 -1.35389200
H -10.78310300 -2.05396200 -1.59233500
H -11.38809000 -3.72910500 0.14859700
H -9.93004200 -3.99601000 2.14967900
H -7.91318900 -2.59432500 2.41464000
H -2.56180900 -0.41809200 2.15146200
H -0.77239900 -1.81915700 1.16238700
H -2.45949200 -1.21325900 -2.75077100
H -4.24067200 0.18601300 -1.79252800
H -0.53795400 -2.51866100 -2.55376400
H -0.58416400 -3.53806500 -1.12774500
H 1.49249000 -3.94859400 -0.12199000
H 3.81355200 -3.28366800 0.42430700
H 3.16415500 0.51886500 -1.46292200
H 0.85989900 -0.14605500 -2.01779500
H 6.28276700 -1.76312800 -0.56327800
H 7.27635700 1.18307100 0.78291100
H 9.56526300 -2.60700000 -0.52863000
H 12.03929400 -2.42567400 -0.51520700
H 13.12112800 -0.21583100 -0.15133100
H 11.71227800 1.80570600 0.18581400
H 9.25944900 1.62770600 0.15740000
H 5.63275000 2.76971900 -0.20286800
H 4.28967000 4.58993100 0.80264900
H 2.52120600 4.05905500 2.46829300

H 2.10447900 1.69466400 3.11479400

H 3.43013100 -0.12464300 2.09057500

L-Anti-DPT (CYH)

C -3.60431200 4.29466000 3.36378900

C -4.66686300 4.47937000 2.47065100

C -5.23553300 3.39816200 1.81204100

C -4.74577000 2.08097700 2.00376200

C -3.67820200 1.91503400 2.91956900

C -3.12337600 3.00296800 3.58640000

C -5.29942600 0.93280100 1.30200200

C -6.28467900 1.02519800 0.32000000

C -7.08563600 -0.02681300 -0.15047800

O -7.05814500 -1.25588300 0.42470500

N -4.88893100 -0.37252200 1.72888500

C -8.05417500 0.10744100 -1.22673900

C -8.06986000 1.22476300 -2.09363900

C -9.02155100 1.33388700 -3.10059900

C -9.97853200 0.33083200 -3.28665200

C -9.96595200 -0.78830200 -2.44915600

C -9.02062500 -0.90354600 -1.43596100

C -3.88895600 -0.95490500 1.07732400

C -3.56728000 -2.31326500 1.44880000

C -2.54909800 -3.00267000 0.83115800

C -1.76974200 -2.40244000 -0.18128400

C -2.05519500 -1.06357300 -0.54598400

C -3.07241700 -0.35457900 0.04646600

C -0.66578600 -3.17192100 -0.87439900

C 0.68272600 -2.47082300 -0.87161000

C 1.29228500 -2.06393600 -2.06365200

C 2.52909400 -1.42150400 -2.05860700

C 3.20844300 -1.18622100 -0.85315800

C 2.59125400 -1.57890800 0.34948100

C 1.35140800 -2.20818100 0.33322300

N 4.41606700 -0.46910100 -0.89883500

O 5.40393500 1.72106000 -1.61831700

C 6.48929800 1.41184700 -0.92116400

C 6.57760100 0.21824200 -0.23096000

C 5.50129600 -0.73622100 -0.20528800

C 7.57060500 2.41979500 -0.97163400

C 5.72904200 -1.99979300 0.56522000

C 7.53391200 3.41566700 -1.96215600

C 8.54227500 4.37348900 -2.04059800

C 9.59913500 4.35737800 -1.12842200

C 9.63936100 3.37790900 -0.13266600

C 8.63414000 2.41801800 -0.05271700
C 6.25566900 -1.95288800 1.86480500
C 6.50421600 -3.12976100 2.57148100
C 6.24951300 -4.36805100 1.98016100
C 5.73888000 -4.42433400 0.68107000
C 5.47461600 -3.24978300 -0.02018500
H -3.16722700 5.14316300 3.88097000
H -5.06336600 5.47608200 2.29809900
H -6.08027400 3.57359600 1.15514500
H -3.29035800 0.92104500 3.10575700
H -2.30656700 2.83986100 4.28397200
H -6.52423300 2.00959900 -0.06016400
H -6.42481600 -1.22721000 1.17498700
H -7.31703300 1.99939900 -1.99473700
H -9.01020200 2.20177700 -3.75381500
H -10.71749300 0.41766900 -4.07728100
H -10.70120300 -1.57638900 -2.58569100
H -9.02054400 -1.76965400 -0.78526900
H -4.16379700 -2.76726700 2.23254900
H -2.33621500 -4.02674600 1.12450000
H -1.44527900 -0.58963700 -1.30934100
H -3.27039500 0.66740000 -0.24998800
H -0.96594400 -3.35448700 -1.91468200
H -0.57503400 -4.15901000 -0.40650400
H 0.79335700 -2.24886900 -3.01171900
H 2.98750200 -1.10174900 -2.98940400
H 3.08370700 -1.37627400 1.29420100
H 0.89154900 -2.49550000 1.27548800
H 4.77011800 0.90798000 -1.50878800
H 7.50080400 -0.04351300 0.26465100
H 6.71079800 3.42328900 -2.66693900
H 8.50318000 5.13359000 -2.81516300
H 10.38389200 5.10560300 -1.18830700
H 10.45149600 3.36678500 0.58800300
H 8.66556100 1.67976100 0.74133600
H 6.45444800 -0.99056100 2.32689000
H 6.89922100 -3.07849000 3.58173700
H 6.44999200 -5.28462400 2.52693400
H 5.54764800 -5.38500400 0.21234800
H 5.07964300 -3.29776900 -1.02939300
L-Syn-DPT (CYH)
C -5.16003000 5.22885100 -1.41310800
C -6.38614500 4.55879800 -1.51080900
C -6.53586700 3.27596200 -1.00169000

C -5.45082300 2.59861700 -0.38860700
C -4.22180600 3.29682500 -0.29334800
C -4.08469300 4.58819300 -0.79397200
C -5.56532100 1.24283700 0.12923700
C -6.71968000 0.46298100 0.01917500
C -7.00096400 -0.69400800 0.75705100
O -6.19485800 -1.10810600 1.76689100
N -4.47485300 0.73024400 0.89555400
C -8.19143800 -1.51273000 0.56912500
C -9.02332300 -1.38508200 -0.56668600
C -10.16173500 -2.17041200 -0.70909900
C -10.50080200 -3.11464000 0.26584900
C -9.67977200 -3.26386500 1.38717900
C -8.54155500 -2.47866400 1.53974600
C -3.55810800 -0.01137200 0.27072900
C -2.52587900 -0.60652400 1.08372700
C -1.53883200 -1.38385900 0.52841900
C -1.49666300 -1.62605300 -0.86590200
C -2.48988000 -1.04057200 -1.67863600
C -3.49283000 -0.25689600 -1.14679900
C -0.42027700 -2.50616400 -1.46418800
C 0.99693100 -2.09447200 -1.10056300
C 1.85000500 -2.96343400 -0.41066700
C 3.15781100 -2.59480400 -0.09945500
C 3.64547900 -1.32579000 -0.44818300
C 2.79520300 -0.45284300 -1.15303800
C 1.49609100 -0.83597700 -1.46909100
N 4.99431200 -1.03338000 -0.18076100
O 7.31840500 -1.80840000 -0.66924800
C 7.76448000 -0.66150600 -0.17207700
C 6.88894300 0.28904500 0.31696500
C 5.46233800 0.10228600 0.29127200
C 9.23617100 -0.51273100 -0.16677000
C 4.61878800 1.19591500 0.86788100
C 10.04153200 -1.64645600 -0.37046500
C 11.43064400 -1.53957200 -0.36195900
C 12.03848800 -0.29935800 -0.15626700
C 11.24687400 0.83609100 0.03701300
C 9.85836600 0.73247500 0.03034700
C 4.85996200 2.53447200 0.52269400
C 4.10131400 3.55949600 1.08873400
C 3.10698800 3.26112000 2.02194400
C 2.87017000 1.93208400 2.38244800
C 3.61572100 0.90562700 1.80602900

H -5.05051700 6.23435500 -1.80729700
H -7.23600900 5.04830800 -1.97806200
H -7.50799400 2.80019200 -1.06774200
H -3.37580700 2.81658400 0.18327800
H -3.12906400 5.09669000 -0.70155800
H -7.51010800 0.81865600 -0.62835100
H -5.45946900 -0.45841100 1.85147800
H -8.76482500 -0.68522100 -1.35389200
H -10.78310300 -2.05396200 -1.59233500
H -11.38809000 -3.72910500 0.14859700
H -9.93004200 -3.99601000 2.14967900
H -7.91318900 -2.59432500 2.41464000
H -2.56180900 -0.41809200 2.15146200
H -0.77239900 -1.81915700 1.16238700
H -2.45949200 -1.21325900 -2.75077100
H -4.24067200 0.18601300 -1.79252800
H -0.53795400 -2.51866100 -2.55376400
H -0.58416400 -3.53806500 -1.12774500
H 1.49249000 -3.94859400 -0.12199000
H 3.81355200 -3.28366800 0.42430700
H 3.16415500 0.51886500 -1.46292200
H 0.85989900 -0.14605500 -2.01779500
H 6.28276700 -1.76312800 -0.56327800
H 7.27635700 1.18307100 0.78291100
H 9.56526300 -2.60700000 -0.52863000
H 12.03929400 -2.42567400 -0.51520700
H 13.12112800 -0.21583100 -0.15133100
H 11.71227800 1.80570600 0.18581400
H 9.25944900 1.62770600 0.15740000
H 5.63275000 2.76971900 -0.20286800
H 4.28967000 4.58993100 0.80264900
H 2.52120600 4.05905500 2.46829300
H 2.10447900 1.69466400 3.11479400
H 3.43013100 -0.12464300 2.09057500

L-Anti-TS1 (ACN)

C -3.38466800 5.17885300 1.54624900
C -4.58261800 5.10611300 0.81941500
C -5.18875700 3.88405700 0.56920400
C -4.60526300 2.67028800 1.02389900
C -3.39136700 2.76400600 1.75349000
C -2.80282300 3.99861200 2.01465300
C -5.19931500 1.38633300 0.74848700
C -6.39092900 1.12503300 0.06971300
C -7.13553800 -0.05894000 0.31699000

O -6.73588100 -0.94510600 1.19591700
N -4.62801900 0.20000700 1.36654800
C -8.43901300 -0.29602000 -0.33355900
C -8.87239800 0.42602000 -1.46514500
C -10.11616400 0.17362900 -2.03835100
C -10.95676500 -0.80819300 -1.50429200
C -10.53438100 -1.54114600 -0.39088600
C -9.29136100 -1.29287400 0.18442900
C -3.70675100 -0.51785500 0.69138700
C -3.45563400 -1.86429300 1.11232900
C -2.51041100 -2.63309800 0.46942400
C -1.75701800 -2.11571500 -0.60730600
C -1.98944700 -0.78191300 -1.01505400
C -2.93565500 0.00531800 -0.39693000
C -0.71631200 -2.96090400 -1.30860900
C 0.68719100 -2.38176300 -1.21763600
C 1.35030500 -1.90221700 -2.35291200
C 2.63955600 -1.38048400 -2.26624500
C 3.29855500 -1.31660000 -1.03023600
C 2.63267400 -1.77304800 0.11896900
C 1.35058300 -2.30377700 0.01589500
N 4.58042400 -0.72687700 -1.00086900
O 5.81466000 1.50835600 -1.70964100
C 6.67800900 1.23419700 -0.83727800
C 6.63827000 0.02275900 -0.06125700
C 5.61162900 -0.90808400 -0.13274600
C 7.80499200 2.20363400 -0.62369500
C 5.70335700 -2.15351500 0.67714900
C 8.04697900 3.16701500 -1.61649400
C 9.07538500 4.09491600 -1.47225900
C 9.87287000 4.08244200 -0.32411800
C 9.63308700 3.13819500 0.67680600
C 8.60857900 2.20325100 0.52815300
C 6.06062100 -2.09335400 2.03290500
C 6.20413200 -3.26401700 2.77823600
C 6.00433400 -4.50745900 2.17560100
C 5.65698500 -4.57616600 0.82345500
C 5.50138300 -3.40872600 0.07903400
H -2.91910900 6.13940200 1.74292000
H -5.05097100 6.01660900 0.45601300
H -6.12746200 3.86158400 0.02597700
H -2.92011400 1.85866900 2.11864700
H -1.87771700 4.03727700 2.58310400
H -6.84864200 1.91051900 -0.51840000

H -5.56689600 -0.44330700 1.63458300
H -8.22645200 1.17145000 -1.91665900
H -10.42731500 0.73924600 -2.91189200
H -11.92467800 -1.00448000 -1.95548800
H -11.17693200 -2.31013800 0.02868000
H -8.95855900 -1.85980300 1.04632700
H -4.03002400 -2.26400900 1.94077700
H -2.33971300 -3.65516600 0.79271500
H -1.40237000 -0.37037000 -1.83011400
H -3.09957600 1.02626800 -0.71659100
H -0.99287300 -3.05593100 -2.36542800
H -0.73253100 -3.97133800 -0.88752800
H 0.86105300 -1.94718400 -3.32198800
H 3.14603100 -1.02780700 -3.15973400
H 3.10925000 -1.70248300 1.08908900
H 0.85221000 -2.65127000 0.91690700
H 4.73599900 0.09433400 -1.60032400
H 7.47944100 -0.22653000 0.56929900
H 7.41606300 3.16849500 -2.49853900
H 9.25646900 4.82809800 -2.25266400
H 10.67372200 4.80673100 -0.20855100
H 10.24132200 3.13153200 1.57625100
H 8.42397800 1.49110900 1.32512300
H 6.20911000 -1.12670300 2.50346300
H 6.47062600 -3.20320100 3.82890900
H 6.11922800 -5.41848800 2.75494400
H 5.50990100 -5.54069700 0.34720800
H 5.23911900 -3.46740100 -0.97219500

L-Syn-TS1 (ACN)

C -5.64907600 5.29046500 -1.05721300
C -6.81986600 4.53287700 -1.21259600
C -6.85397000 3.19499200 -0.84904800
C -5.70064500 2.54786600 -0.32774700
C -4.52470300 3.32950500 -0.18253900
C -4.50895700 4.67700200 -0.53324500
C -5.70242100 1.15102100 0.02728400
C -6.77444600 0.25817800 -0.02656100
C -6.82588000 -0.88421500 0.81546900
O -5.87300400 -1.13916800 1.67838600
N -4.53085000 0.59053000 0.68280000
C -7.99843100 -1.78080400 0.82324800
C -8.97003300 -1.77981300 -0.19930300
C -10.06437600 -2.63921900 -0.14355500

C -10.21577900 -3.52572200 0.92742700
C -9.25356600 -3.54662300 1.94174600
C -8.15750400 -2.69007100 1.88934200
C -3.57404800 0.00398800 -0.06516500
C -2.65329600 -0.88428600 0.58418200
C -1.64600300 -1.48820700 -0.12831100
C -1.48327200 -1.24812600 -1.51565200
C -2.37599200 -0.36501600 -2.15515000
C -3.39994200 0.25262200 -1.46385400
C -0.37423400 -1.93028800 -2.28595800
C 1.01059300 -1.66930300 -1.71563300
C 1.77158400 -2.70017600 -1.15292400
C 3.03882000 -2.45487100 -0.62758200
C 3.58248800 -1.16284400 -0.65799800
C 2.83629700 -0.12535100 -1.24079800
C 1.56615600 -0.38143400 -1.74774400
N 4.89288000 -0.99183700 -0.16269800
O 7.33555500 -1.96983600 -0.47260000
C 7.76267500 -0.87792600 -0.01766600
C 6.88572800 0.16691800 0.44108100
C 5.50215800 0.11112900 0.34908200
C 9.24850300 -0.67793600 0.07024300
C 4.69190200 1.22761900 0.90800300
C 10.07524100 -1.81013900 -0.01303700
C 11.46062200 -1.68646800 0.05718800
C 12.04391800 -0.42399900 0.19979900
C 11.23284200 0.71098300 0.26985600
C 9.84486800 0.58604200 0.20844000
C 5.03235900 2.56006100 0.62862600
C 4.30996900 3.60829900 1.19949500
C 3.24781700 3.33813300 2.06440700
C 2.90801300 2.01376700 2.35458100
C 3.61985000 0.96437100 1.77719900
H -5.63179300 6.33860300 -1.33860600
H -7.71665700 4.99880900 -1.61145600
H -7.78071300 2.64179700 -0.95802300
H -3.62750400 2.86994900 0.21601300
H -3.59536200 5.25018000 -0.40177900
H -7.66164900 0.52933800 -0.58471600
H -4.98712700 -0.15058900 1.46414200
H -8.85997500 -1.12325000 -1.05582200
H -10.79793200 -2.62392900 -0.94447600
H -11.06859900 -4.19666800 0.96614600
H -9.35834000 -4.23503300 2.77563200

H -7.40774700 -2.70432700 2.67209600
H -2.77726800 -1.07236000 1.64501300
H -0.95887100 -2.16018800 0.37588200
H -2.25156100 -0.16403500 -3.21468600
H -4.07028700 0.93780100 -1.96619300
H -0.41602600 -1.60897300 -3.33187500
H -0.56103600 -3.01131600 -2.28416100
H 1.37183000 -3.70995300 -1.12185800
H 3.61173100 -3.26470900 -0.18577300
H 3.25266000 0.87215500 -1.31078900
H 1.00467100 0.43444000 -2.19504700
H 5.57350600 -1.73737800 -0.36016900
H 7.30650800 1.02174300 0.95058200
H 9.60884200 -2.78215000 -0.13039500
H 12.08678600 -2.57195500 0.00055200
H 13.12410300 -0.32516200 0.25214600
H 11.68068400 1.69522400 0.36837300
H 9.23209800 1.48026000 0.24345100
H 5.85345900 2.77040000 -0.04918800
H 4.57704800 4.63458500 0.96697300
H 2.68775900 4.15399900 2.51106700
H 2.08909500 1.79789300 3.03392700
H 3.35726500 -0.06201500 2.01151700

L-Anti-TS1 (DCM)

C -3.43306100 5.15553200 1.73615800
C -4.60928500 5.09624800 0.97379100
C -5.20154600 3.87853800 0.67487300
C -4.62447400 2.65583300 1.11369200
C -3.43259900 2.73621800 1.88027900
C -2.85876500 3.96606700 2.19041600
C -5.20181000 1.37790400 0.78541100
C -6.36593600 1.12621600 0.05683300
C -7.12224900 -0.05829100 0.26567900
O -6.75830700 -0.95433700 1.14839700
N -4.65165200 0.17740700 1.39898500
C -8.40217400 -0.28330800 -0.43464600
C -8.78710300 0.44528400 -1.57905100
C -10.01079000 0.20495400 -2.19874500
C -10.87841700 -0.77109900 -1.69900100
C -10.50352600 -1.51061000 -0.57308800
C -9.28073200 -1.27452000 0.04841500
C -3.72493300 -0.53680500 0.73058000
C -3.50595100 -1.89862100 1.12073600
C -2.55477800 -2.66404500 0.48313500

C -1.76293700 -2.12935400 -0.55695700
C -1.96281700 -0.78079100 -0.93303700
C -2.91419000 0.00392300 -0.32037100
C -0.72050500 -2.97489000 -1.25560600
C 0.68314300 -2.39553100 -1.17827200
C 1.34711500 -1.94458800 -2.32453800
C 2.63782200 -1.42481200 -2.25098500
C 3.29822600 -1.33374800 -1.01736500
C 2.63145700 -1.76147100 0.14238400
C 1.34793900 -2.29078000 0.05241300
N 4.58135900 -0.74757000 -1.00396100
O 5.81752500 1.46128200 -1.77898300
C 6.67894000 1.21579100 -0.89733300
C 6.63742400 0.02866500 -0.08307500
C 5.61074700 -0.90290100 -0.12793300
C 7.80491900 2.19206900 -0.71241100
C 5.69992900 -2.12319500 0.71972000
C 8.04249400 3.12846900 -1.73155200
C 9.06968700 4.06140700 -1.61509400
C 9.87029500 4.08120300 -0.46937400
C 9.63483200 3.16414100 0.55730800
C 8.61142200 2.22415800 0.43672000
C 6.05334200 -2.02195200 2.07395400
C 6.19470000 -3.16921100 2.85511200
C 5.99612800 -4.43034000 2.29026800
C 5.65212900 -4.54010500 0.94011000
C 5.49894100 -3.39600000 0.15997600
H -2.97844000 6.11272200 1.97114800
H -5.07248500 6.01390100 0.62179900
H -6.12581900 3.86523600 0.10707900
H -2.96711100 1.82347800 2.23428600
H -1.95065000 3.99429000 2.78630000
H -6.80114500 1.91968700 -0.53786500
H -5.59937200 -0.46198700 1.63591700
H -8.11787000 1.18598700 -2.00382400
H -10.28482200 0.77533300 -3.08165100
H -11.83065000 -0.95810500 -2.18620500
H -11.16760600 -2.27528800 -0.17989000
H -8.98350300 -1.84598600 0.92025400
H -4.11087300 -2.31167400 1.92024200
H -2.40912400 -3.69751500 0.78180800
H -1.34397100 -0.35586300 -1.71708100
H -3.05158900 1.03681100 -0.61280200
H -1.00299400 -3.07953400 -2.31040900

H -0.73392000 -3.98315900 -0.82857000
H 0.85689900 -2.01036600 -3.29203600
H 3.14454100 -1.09388600 -3.15263600
H 3.10858800 -1.66952900 1.11036600
H 0.84917100 -2.61508200 0.96186900
H 4.73979800 0.05600200 -1.62671200
H 7.47839400 -0.20242300 0.55466800
H 7.40836700 3.10477500 -2.61097600
H 9.24733300 4.77375700 -2.41537100
H 10.67031600 4.80962500 -0.37561700
H 10.24556300 3.18280900 1.45495400
H 8.42978300 1.53366700 1.25322600
H 6.20044600 -1.04117900 2.51486800
H 6.45847000 -3.07643100 3.90418100
H 6.10934700 -5.32332200 2.89742700
H 5.50582000 -5.51871400 0.49318600
H 5.23907300 -3.48636900 -0.88958600

L-Syn-TS1 (DCM)

C 5.91701000 5.29311000 1.05586300
C 7.05120600 4.47935400 1.19541500
C 7.01442100 3.14118300 0.83458100
C 5.82279600 2.54966400 0.33329600
C 4.68463800 3.38814200 0.20381900
C 4.74067500 4.73510900 0.55005400
C 5.75028000 1.15456600 -0.01233500
C 6.76985900 0.20209800 0.04337900
C 6.76995200 -0.92451600 -0.82302900
O 5.81815400 -1.11201300 -1.70058300
N 4.54998000 0.65203200 -0.66999200
C 7.89487200 -1.88103500 -0.83383600
C 8.84434200 -1.95860200 0.20553300
C 9.89559100 -2.86971000 0.14417500
C 10.02349000 -3.73060100 -0.94994700
C 9.08101700 -3.67416700 -1.98112100
C 8.02807200 -2.76600000 -1.92289700
C 3.59075800 0.07348300 0.07541500
C 2.65054400 -0.79520800 -0.57499400
C 1.63844300 -1.38805600 0.13918600
C 1.48848400 -1.15710000 1.52952900
C 2.39847200 -0.29145400 2.16988500
C 3.42683900 0.31593400 1.47765500
C 0.37714700 -1.83151400 2.30336000
C -1.00788700 -1.58759900 1.72706400
C -1.77264700 -2.63530900 1.20244300

C -3.04148500 -2.40596900 0.67463200
C -3.58464300 -1.11313800 0.66415400
C -2.83369800 -0.05801900 1.20816900
C -1.56199400 -0.29908200 1.71780500
N -4.89582800 -0.96022300 0.16864300
O -7.32271000 -1.95224900 0.50871700
C -7.76530200 -0.87453000 0.03916100
C -6.90053600 0.17233000 -0.44334700
C -5.51727300 0.12969900 -0.35905200
C -9.25377800 -0.69264700 -0.04094200
C -4.71924000 1.24210300 -0.94332800
C -10.06565900 -1.83030000 0.09385800
C -11.45271300 -1.72546600 0.03285200
C -12.05254700 -0.47667600 -0.15275000
C -11.25622900 0.66402100 -0.27444600
C -9.86659400 0.55767600 -0.22153600
C -5.06598000 2.57660800 -0.68295800
C -4.35530300 3.62021900 -1.27624900
C -3.29799800 3.34314200 -2.14453600
C -2.95145300 2.01667900 -2.41536000
C -3.65190800 0.97225800 -1.81591300
H 5.95541000 6.34153000 1.33420900
H 7.97627100 4.90209600 1.57775500
H 7.91510100 2.54337900 0.92557600
H 3.76031300 2.97108500 -0.17926800
H 3.85478300 5.35270600 0.42973500
H 7.66543900 0.41654200 0.61323200
H 4.97077900 -0.07955200 -1.47404200
H 8.74826000 -1.32276300 1.07931000
H 10.61326700 -2.91491200 0.95838700
H 10.84269400 -4.44206300 -0.99365200
H 9.16772100 -4.34278600 -2.83307800
H 7.29211000 -2.71857700 -2.71725800
H 2.76792200 -0.97899600 -1.63709100
H 0.93648100 -2.04439900 -0.36521600
H 2.28161600 -0.09489800 3.23129000
H 4.10783500 0.99180600 1.97797400
H 0.41438800 -1.49676400 3.34560300
H 0.56974700 -2.91180900 2.31923400
H -1.37482600 -3.64649600 1.20415900
H -3.61781400 -3.22927600 0.26307800
H -3.24762600 0.94207000 1.24597800
H -0.99687400 0.53077000 2.13399600
H -5.57227000 -1.70542200 0.38457800

H -7.33147000 1.01239200 -0.96865800
H -9.58438400 -2.79027700 0.24460000
H -12.06765200 -2.61532100 0.13037400
H -13.13437600 -0.39258800 -0.19830200
H -11.71700000 1.63838200 -0.40678900
H -9.26516400 1.45709600 -0.29702100
H -5.88317200 2.79157600 -0.00174900
H -4.62752100 4.64849000 -1.05850900
H -2.74679200 4.15530000 -2.60872800
H -2.13587200 1.79525000 -3.09700200
H -3.38417300 -0.05624100 -2.03455400

L-Anti-TS1 (CYH)

C -3.60635800 5.05104700 2.26910400
C -4.69949700 5.03512100 1.39054800
C -5.24167000 3.83712500 0.95241500
C -4.69274000 2.59075300 1.36103100
C -3.58399900 2.62802300 2.24688500
C -3.06368300 3.83714700 2.69701500
C -5.21243600 1.33857300 0.88533600
C -6.28607800 1.12234600 0.01851600
C -7.07480400 -0.05784000 0.11273600
O -6.81880900 -0.98417300 0.99689000
N -4.72768600 0.09614300 1.48268100
C -8.27676700 -0.23874900 -0.72622000
C -8.52080300 0.51881700 -1.88927700
C -9.67764200 0.32168000 -2.63866600
C -10.61584700 -0.63932900 -2.25185900
C -10.37925100 -1.40784200 -1.10825400
C -9.22367400 -1.21514300 -0.35775500
C -3.78034300 -0.60641000 0.84323800
C -3.64634200 -2.00451400 1.14185800
C -2.67309200 -2.75946600 0.52811600
C -1.77333700 -2.18425300 -0.39714300
C -1.88648400 -0.80227600 -0.67854100
C -2.85612000 -0.02452900 -0.08797700
C -0.72265600 -3.03079900 -1.08305900
C 0.67774700 -2.44393000 -1.04891800
C 1.33030200 -2.05154400 -2.22259700
C 2.62077900 -1.52833800 -2.18882500
C 3.29482100 -1.37354600 -0.96863800
C 2.63899900 -1.74245500 0.21752800
C 1.35554000 -2.27626900 0.16722600
N 4.57634100 -0.78934900 -1.00204500
O 5.79356700 1.35675600 -1.93667700

C 6.65896900 1.18748200 -1.04453200
C 6.62812100 0.06184400 -0.14189300
C 5.60900900 -0.87559900 -0.11762300
C 7.77634200 2.18466500 -0.93865200
C 5.70824800 -2.03345300 0.81274100
C 7.97832000 3.06295200 -2.01504500
C 8.99528600 4.01269500 -1.97580900
C 9.82139900 4.10759500 -0.85261400
C 9.62152500 3.24881500 0.22989300
C 8.60785800 2.29218600 0.18718300
C 6.05964400 -1.83590600 2.15658400
C 6.21089900 -2.92452100 3.01557200
C 6.02316000 -4.22321000 2.54014600
C 5.67992700 -4.42910700 1.20145900
C 5.51759900 -3.34361600 0.34377800
H -3.19144700 5.99310600 2.61335300
H -5.14004600 5.97143000 1.05876900
H -6.10852700 3.85374300 0.30035100
H -3.14257800 1.69618400 2.58140800
H -2.22080900 3.83139600 3.38283600
H -6.64981600 1.94073700 -0.59078800
H -5.69677900 -0.52712100 1.62673200
H -7.79091300 1.24756700 -2.22607300
H -9.84350700 0.91400600 -3.53416500
H -11.51607400 -0.79280800 -2.83960000
H -11.09964900 -2.16148300 -0.80225900
H -9.03042400 -1.80759600 0.52909100
H -4.33824600 -2.44889700 1.84810400
H -2.59295500 -3.81837200 0.75482300
H -1.18033100 -0.34703800 -1.36557400
H -2.92325700 1.03458500 -0.29882100
H -1.02238900 -3.17130000 -2.13022700
H -0.72285900 -4.02958900 -0.63209000
H 0.83025000 -2.16582700 -3.18079900
H 3.11784300 -1.24205500 -3.11097300
H 3.12511200 -1.60122600 1.17485200
H 0.86591100 -2.55314900 1.09726800
H 4.73155100 -0.02753800 -1.67782200
H 7.47466300 -0.12005800 0.50437800
H 7.32208100 2.97987800 -2.87429300
H 9.14489800 4.68059800 -2.81909000
H 10.61385100 4.84962200 -0.81946200
H 10.25265300 3.32618000 1.11027000
H 8.45359900 1.64774600 1.04590700

H 6.19741200 -0.82502200 2.52711300
H 6.47374000 -2.75686000 4.05566700
H 6.14396600 -5.07092000 3.20787600
H 5.54145700 -5.43768400 0.82379800
H 5.25773000 -3.50778800 -0.69678100

L-Syn-TS1 (CYH)

C -6.12439600 5.28807500 -1.03274000
C -7.22690600 4.43093200 -1.16379500
C -7.13306800 3.09345400 -0.81268000
C -5.91238300 2.54524300 -0.33140800
C -4.80699300 3.42801000 -0.20976900
C -4.92109300 4.77356000 -0.54441500
C -5.78120800 1.15284700 -0.00274200
C -6.75758400 0.15576900 -0.06298800
C -6.72226400 -0.95596200 0.82353700
O -5.77519100 -1.09430900 1.71166000
N -4.56053600 0.69110400 0.65511500
C -7.81192400 -1.95305800 0.83761300
C -8.73699100 -2.09239100 -0.21634400
C -9.75658600 -3.03824300 -0.14926600
C -9.87526400 -3.87240800 0.96583400
C -8.95552500 -3.75456500 2.01203300
C -7.93416400 -2.81194300 1.94790900
C -3.60124600 0.11726000 -0.08642600
C -2.65212100 -0.74426300 0.56417400
C -1.63668700 -1.32988500 -0.15014800
C -1.49000400 -1.10039700 -1.54126000
C -2.40734200 -0.24155100 -2.18183400
C -3.43852600 0.35986000 -1.49046400
C -0.37528700 -1.76836700 -2.31579300
C 1.00847000 -1.53472100 -1.73268700
C 1.77196600 -2.59082700 -1.22382800
C 3.03979600 -2.37090900 -0.69050100
C 3.58507700 -1.07901000 -0.65848800
C 2.83462000 -0.01523300 -1.18649600
C 1.56371300 -0.24739100 -1.70149600
N 4.89401600 -0.93741800 -0.15769800
O 7.30661900 -1.94804900 -0.50306700
C 7.76259000 -0.87513400 -0.03995000
C 6.90822500 0.18163000 0.44599300
C 5.52591300 0.14959800 0.36719900
C 9.25289000 -0.70658000 0.02919200
C 4.73791100 1.26727800 0.95511200
C 10.05201800 -1.85019000 -0.12682500

C 11.44016900 -1.75914700 -0.07671200
C 12.05360500 -0.51884200 0.11927600
C 11.26982900 0.62772000 0.26198500
C 9.87909100 0.53521100 0.21966800
C 5.09173200 2.59943600 0.69307800
C 4.39069900 3.64779800 1.28912500
C 3.33525300 3.37797400 2.16153300
C 2.98109200 2.05402800 2.43357600
C 3.67225100 1.00507800 1.83172400
H -6.20764300 6.33604400 -1.30288000
H -8.17321200 4.81965800 -1.53017000
H -8.01108500 2.46118200 -0.89168000
H -3.86232700 3.04485300 0.15886500
H -4.05931300 5.42548200 -0.42926300
H -7.65612900 0.32675900 -0.64314600
H -4.95547200 -0.02837700 1.47707700
H -8.64444400 -1.47753100 -1.10551000
H -10.45629700 -3.13156200 -0.97506300
H -10.66990600 -4.61103300 1.01445300
H -9.03557300 -4.40243400 2.88059000
H -7.21427000 -2.71495400 2.75236800
H -2.77060300 -0.92998400 1.62558300
H -0.92817500 -1.97975400 0.35360900
H -2.29090900 -0.04419700 -3.24334000
H -4.12221300 1.03470500 -1.98806500
H -0.40799400 -1.42432500 -3.35549500
H -0.57034900 -2.84832700 -2.34438900
H 1.37394500 -3.60194000 -1.24297400
H 3.61543500 -3.20104200 -0.29179300
H 3.24854600 0.98519300 -1.20750900
H 0.99949200 0.58986300 -2.10409500
H 5.56709200 -1.68613700 -0.37566400
H 7.34805100 1.01639000 0.97244100
H 9.55813500 -2.80231700 -0.28591800
H 12.04573100 -2.65347200 -0.19110300
H 13.13662900 -0.44571800 0.15649800
H 11.74136300 1.59584500 0.40256500
H 9.28680400 1.43923700 0.31133600
H 5.90739300 2.80804000 0.00795900
H 4.66880300 4.67431200 1.07016700
H 2.79123000 4.19380400 2.62784800
H 2.16655900 1.83818200 3.11834000
H 3.39884600 -0.02185300 2.05069700

L-Anti-TS2 (ACN)

C -3.43496200 4.43686100 3.08316900
C -4.53875300 4.58503500 2.23311200
C -5.14026500 3.47689500 1.65147500
C -4.64504000 2.16790500 1.88286900
C -3.53273500 2.03926300 2.75113600
C -2.94403000 3.15493800 3.34035800
C -5.23483600 0.98684400 1.26710300
C -6.28326300 1.03450300 0.34147900
C -7.08324200 -0.04349400 -0.05205100
O -6.98756400 -1.26089300 0.54312400
N -4.79326400 -0.28784600 1.72481700
C -8.12386400 0.03972400 -1.07079200
C -8.22605600 1.13707600 -1.95598500
C -9.23890900 1.19430400 -2.90730600
C -10.17190600 0.15737400 -3.01641700
C -10.07501800 -0.94198300 -2.15861800
C -9.06739800 -1.00442900 -1.20056000
C -3.81638200 -0.90483200 1.04826100
C -3.45746700 -2.23067300 1.47293700
C -2.46220200 -2.93931300 0.83472000
C -1.75419400 -2.38385500 -0.25151900
C -2.08604000 -1.07521800 -0.67355600
C -3.08119600 -0.34970600 -0.05815500
C -0.66483800 -3.16470700 -0.95600200
C 0.69264000 -2.47992100 -0.92553200
C 1.29969700 -2.01780400 -2.09895600
C 2.54383900 -1.38935100 -2.06743200
C 3.22745500 -1.21832000 -0.85392800
C 2.61374400 -1.66459600 0.33141400
C 1.36948200 -2.28508600 0.28834000
N 4.44449200 -0.51300700 -0.87137100
O 5.33881000 1.62298500 -1.58341000
C 6.43170700 1.39055100 -0.89439400
C 6.57595300 0.20354300 -0.18047800
C 5.53371400 -0.77244700 -0.16285400
C 7.47674700 2.44044000 -0.95269800
C 5.76704400 -2.04184600 0.58765800
C 7.38387000 3.44209000 -1.93411900
C 8.35131000 4.44085500 -2.02200400
C 9.42380600 4.45937000 -1.12705800
C 9.52071900 3.47360200 -0.14091800
C 8.55614000 2.47246300 -0.05246700
C 6.30163300 -2.00833900 1.88482800
C 6.56140400 -3.19378800 2.57346400

C 6.30896000 -4.42571800 1.96690900
C 5.79074100 -4.46791900 0.66956200
C 5.51539700 -3.28536300 -0.01439900
H -2.97244400 5.30645400 3.53941400
H -4.93960400 5.57448600 2.03223600
H -6.00992800 3.62785100 1.02182300
H -3.13575300 1.05342900 2.96192600
H -2.09356400 3.02105000 4.00289200
H -6.55577000 2.00148000 -0.05997600
H -6.31022700 -1.19776800 1.25392600
H -7.49709000 1.93911100 -1.91601500
H -9.29429800 2.04795100 -3.57645800
H -10.95805400 0.20379300 -3.76360200
H -10.79086100 -1.75540000 -2.23507200
H -9.00321200 -1.85678000 -0.53484400
H -3.99953800 -2.65390800 2.31181600
H -2.21546200 -3.94207900 1.17050100
H -1.53742100 -0.63568700 -1.50143600
H -3.32066200 0.64999300 -0.39947400
H -0.95956000 -3.31871400 -2.00115900
H -0.59082800 -4.15936000 -0.50337900
H 0.79584800 -2.15104200 -3.05263500
H 3.00276400 -1.03430100 -2.98515400
H 3.10968100 -1.51162600 1.28358100
H 0.91216900 -2.61762600 1.21673200
H 4.71540900 0.68996100 -1.41871800
H 7.50394000 -0.02315800 0.32249200
H 6.54927500 3.42158400 -2.62545000
H 8.26908700 5.20468000 -2.78938000
H 10.17710500 5.23853300 -1.19394700
H 10.34576800 3.48837900 0.56464400
H 8.63551600 1.72866600 0.73286400
H 6.49820000 -1.05177000 2.35897300
H 6.96292700 -3.15373800 3.58141400
H 6.51737800 -5.34837900 2.50000100
H 5.60271800 -5.42321300 0.18902200
H 5.11749600 -3.32317000 -1.02296300

L-Syn-TS2 (ACN)

C -4.89249900 5.22604600 -1.15883000
C -6.14467600 4.61494200 -1.30548600
C -6.36125200 3.32205300 -0.84764300
C -5.31999600 2.57593900 -0.23821800
C -4.06378500 3.21496700 -0.09246900
C -3.85925600 4.51638900 -0.54298300

C -5.50513800 1.20815700 0.22756400
C -6.68668200 0.47989600 0.04948800
C -7.03523000 -0.69935500 0.71641000
O -6.27954600 -1.19966400 1.72836600
N -4.46319500 0.62873700 1.00756800
C -8.24922000 -1.46205900 0.44788700
C -9.03843500 -1.24126200 -0.70387100
C -10.19877100 -1.97529900 -0.92502600
C -10.60227000 -2.95924000 -0.01585700
C -9.82415900 -3.20037200 1.12000400
C -8.66439700 -2.46648200 1.35124100
C -3.54479400 -0.12207100 0.38716900
C -2.55841100 -0.77156800 1.21120000
C -1.57425900 -1.55614700 0.65924700
C -1.49499200 -1.75185400 -0.74052800
C -2.44738900 -1.11593100 -1.56252100
C -3.44593800 -0.32292700 -1.03293000
C -0.41257200 -2.62869100 -1.33372900
C 0.99748100 -2.17514500 -0.99004000
C 1.84910800 -2.97218800 -0.21648900
C 3.14512800 -2.55772500 0.08784100
C 3.62273700 -1.31715500 -0.36155900
C 2.77645500 -0.51864900 -1.15352100
C 1.48691000 -0.94449000 -1.45443700
N 4.96228900 -0.98375500 -0.09070700
O 7.19398100 -1.86927600 -0.41646400
C 7.69962600 -0.70076700 -0.09663700
C 6.86402500 0.35934600 0.24572200
C 5.44409000 0.20779700 0.23154500
C 9.17895000 -0.60503700 -0.10240400
C 4.60512900 1.37105600 0.64613200
C 9.93960200 -1.78613000 -0.14162300
C 11.33188700 -1.73325200 -0.14263600
C 11.98715500 -0.49988500 -0.11131700
C 11.24034900 0.68122800 -0.08213200
C 9.84822600 0.63108800 -0.07838800
C 4.87670400 2.65322500 0.14420100
C 4.12281100 3.75053700 0.56184900
C 3.10255400 3.58287200 1.50006300
C 2.83544400 2.31168100 2.01600400
C 3.57641200 1.21151100 1.58871800
H -4.73079800 6.23904400 -1.51375100
H -6.96193100 5.15797800 -1.77157700
H -7.35113900 2.89232500 -0.95253600

H -3.24885500 2.68080200 0.38122300
H -2.88418000 4.97766100 -0.41403200
H -7.43758900 0.89372000 -0.61032700
H -5.52505700 -0.58549100 1.87489300
H -8.73194600 -0.50823800 -1.44211300
H -10.78654800 -1.78711200 -1.81869300
H -11.50615500 -3.53322600 -0.19473900
H -10.12423600 -3.96391100 1.83196100
H -8.07044500 -2.65470800 2.23758600
H -2.62250200 -0.61963500 2.28348900
H -0.84088200 -2.03360000 1.30197300
H -2.39050700 -1.25528700 -2.63822800
H -4.16434400 0.15904800 -1.68456900
H -0.53883300 -2.66270500 -2.42124900
H -0.55184400 -3.65483900 -0.97210000
H 1.49993600 -3.93482500 0.14757100
H 3.79746700 -3.18895500 0.68357900
H 3.13924100 0.42611300 -1.54312800
H 0.85223400 -0.31297900 -2.07084900
H 6.07585900 -1.71365500 -0.31347800
H 7.28009600 1.29622900 0.58439800
H 9.42485800 -2.73975500 -0.16578300
H 11.90616000 -2.65447900 -0.16720100
H 13.07217600 -0.45808600 -0.11399300
H 11.74317700 1.64337500 -0.06887800
H 9.28485400 1.55787200 -0.07830700
H 5.66896800 2.78614400 -0.58593700
H 4.33483000 4.73501500 0.15607700
H 2.52017100 4.43767700 1.83030300
H 2.05026700 2.17734200 2.75375400
H 3.36838000 0.22747800 1.99535800

L-Anti-TS2 (DCM)

C -3.45304000 4.41188900 3.12806500
C -4.55572300 4.56564000 2.27792100
C -5.15307700 3.46179500 1.68426500
C -4.65448200 2.15202000 1.90277300
C -3.54378300 2.01768900 2.77190800
C -2.95932800 3.12878200 3.37332800
C -5.23945800 0.97616800 1.27307100
C -6.28183800 1.03134300 0.34254100
C -7.08307400 -0.04311300 -0.06119400
O -6.99379600 -1.26296800 0.52865400
N -4.79891500 -0.30361900 1.72143700
C -8.11746700 0.04864500 -1.08432500

C -8.21255200 1.15113700 -1.96403000
C -9.22062400 1.21655500 -2.91960600
C -10.15605400 0.18306300 -3.03870000
C -10.06605800 -0.92136000 -2.18669000
C -9.06339300 -0.99215400 -1.22445900
C -3.82131000 -0.91266200 1.04295100
C -3.46571600 -2.24483500 1.45471000
C -2.46877700 -2.94804400 0.81398900
C -1.75340300 -2.38205600 -0.26208800
C -2.08013100 -1.06748300 -0.67069500
C -3.07717700 -0.34697400 -0.05357000
C -0.66297200 -3.15805400 -0.97007900
C 0.69483200 -2.47420000 -0.93663100
C 1.30546700 -2.01382300 -2.10870700
C 2.55030700 -1.38715700 -2.07458800
C 3.23110900 -1.21592900 -0.85958300
C 2.61374100 -1.66059200 0.32439400
C 1.36893900 -2.27939800 0.27859400
N 4.44910900 -0.51270400 -0.87529300
O 5.34824100 1.61838400 -1.59311000
C 6.43747300 1.38886700 -0.89952000
C 6.57829000 0.20474200 -0.17892500
C 5.53547500 -0.76963800 -0.16104100
C 7.48348600 2.43796500 -0.95834200
C 5.76412200 -2.03565500 0.59675500
C 7.38945800 3.44030200 -1.93872600
C 8.35721300 4.43853600 -2.02735700
C 9.43118200 4.45586400 -1.13434600
C 9.52922000 3.46943100 -0.14917800
C 8.56430600 2.46885200 -0.06006500
C 6.29204600 -1.99625700 1.89638800
C 6.54766900 -3.17831200 2.59219300
C 6.29742500 -4.41295300 1.99054800
C 5.78543600 -4.46111800 0.69107500
C 5.51437700 -3.28189800 -0.00010800
H -2.99367000 5.27806400 3.59396100
H -4.95936300 5.55595500 2.08690900
H -6.02330200 3.61612100 1.05615300
H -3.14508400 1.03078300 2.97374600
H -2.10984900 2.99052000 4.03625600
H -6.55253600 2.00158000 -0.05229900
H -6.31965700 -1.20528800 1.24275400
H -7.48086200 1.95031500 -1.91646600
H -9.27049500 2.07398100 -3.58443000

H -10.93865300 0.23587600 -3.78922000
H -10.78388100 -1.73229400 -2.27106300
H -9.00402500 -1.84807600 -0.56295700
H -4.01313600 -2.67547200 2.28627000
H -2.22591600 -3.95519900 1.13965800
H -1.52435200 -0.61943200 -1.48919300
H -3.31141100 0.65730300 -0.38447200
H -0.95744700 -3.30745500 -2.01617600
H -0.58914900 -4.15545300 -0.52306200
H 0.80377200 -2.14703100 -3.06361900
H 3.01211400 -1.03298400 -2.99119100
H 3.10733600 -1.50753700 1.27769700
H 0.90868900 -2.61026400 1.20615900
H 4.72214900 0.68535900 -1.42587000
H 7.50453000 -0.02127500 0.32750300
H 6.55295000 3.42047400 -2.62770900
H 8.27395100 5.20320900 -2.79382100
H 10.18477400 5.23475000 -1.20185500
H 10.35553300 3.48320200 0.55500000
H 8.64458200 1.72423800 0.72441300
H 6.48645600 -1.03724000 2.36654600
H 6.94415400 -3.13359600 3.60199100
H 6.50254600 -5.33314000 2.52923500
H 5.59877000 -5.41867200 0.21446200
H 5.12076300 -3.32410000 -1.01016000

L-Syn-TS2 (DCM)

C -5.04363400 5.22111200 -1.24672700
C -6.28272600 4.57905000 -1.36597200
C -6.46113200 3.28752900 -0.88900400
C -5.39325300 2.57327200 -0.28796200
C -4.15107300 3.24390100 -0.16935100
C -3.98484500 4.54380300 -0.63821600
C -5.53816100 1.20720200 0.19536000
C -6.70407100 0.45133600 0.04711300
C -7.01959700 -0.72255100 0.74308400
O -6.23999700 -1.18575300 1.75295900
N -4.46741800 0.65907100 0.96367100
C -8.22169200 -1.51166400 0.50842700
C -9.03124200 -1.33115100 -0.63636900
C -10.18170400 -2.08908000 -0.82343900
C -10.55537400 -3.05788300 0.11397600
C -9.75677400 -3.25959800 1.24326500
C -8.60678300 -2.50195300 1.44056600
C -3.55102200 -0.07946500 0.33505000

C -2.53596000 -0.70276000 1.14880100
C -1.54681400 -1.47449900 0.58972100
C -1.48628600 -1.68470500 -0.80915500
C -2.46436400 -1.07460000 -1.62198700
C -3.46870500 -0.29497500 -1.08645000
C -0.40163600 -2.55234200 -1.41136200
C 1.00922900 -2.11532700 -1.05168600
C 1.86314700 -2.94638700 -0.31801400
C 3.16056800 -2.54703600 -0.00070100
C 3.63799400 -1.28842200 -0.39673700
C 2.78925400 -0.45528700 -1.14919700
C 1.49834800 -0.86616600 -1.46315400
N 4.97791300 -0.96875200 -0.11394000
O 7.20525500 -1.84887700 -0.46971400
C 7.71528700 -0.69783700 -0.10577700
C 6.88351000 0.35408200 0.27418600
C 5.46440100 0.20850700 0.25301100
C 9.19534800 -0.60897200 -0.10457400
C 4.62894500 1.35871900 0.70935500
C 9.94855800 -1.79059000 -0.20745800
C 11.34089400 -1.74631700 -0.20393000
C 12.00373100 -0.52097000 -0.10396100
C 11.26435800 0.66120200 -0.01094500
C 9.87218500 0.61936000 -0.01188300
C 4.90460000 2.65707300 0.25387500
C 4.15458000 3.74127000 0.71034200
C 3.13343300 3.54357100 1.64133700
C 2.86166200 2.25572100 2.11067500
C 3.59900800 1.16923300 1.64461300
H -4.91161900 6.23332800 -1.61603700
H -7.12015800 5.09720300 -1.82470400
H -7.44259800 2.83391700 -0.97038900
H -3.31754000 2.73506000 0.29945900
H -3.01947400 5.03006000 -0.52903400
H -7.47645800 0.84030500 -0.60300600
H -5.49632800 -0.55407300 1.87627400
H -8.74649300 -0.61130400 -1.39605800
H -10.78539400 -1.93194200 -1.71260700
H -11.45195800 -3.65081500 -0.03817800
H -10.03378900 -4.01126000 1.97696700
H -7.99623400 -2.65828400 2.32169900
H -2.58560900 -0.53829400 2.21993900
H -0.79262100 -1.92943000 1.22469500
H -2.42105500 -1.22425300 -2.69714000

H -4.20461400 0.16734600 -1.73230600
H -0.52187900 -2.56628000 -2.50039400
H -0.54844000 -3.58579300 -1.07258900
H 1.51459100 -3.92421000 0.00418400
H 3.81505900 -3.20414800 0.56382100
H 3.15109300 0.50574800 -1.49736200
H 0.86116300 -0.20704900 -2.04724800
H 6.08374500 -1.69172800 -0.36279500
H 7.30245700 1.27488400 0.65109400
H 9.42618400 -2.73704600 -0.28541400
H 11.90953100 -2.66839900 -0.27879400
H 13.08907600 -0.48585500 -0.10287500
H 11.77326800 1.61799100 0.05614200
H 9.31432700 1.54811400 0.03883800
H 5.69749300 2.81245500 -0.47125300
H 4.37003900 4.73904200 0.34016500
H 2.55361500 4.38788400 2.00186700
H 2.07497400 2.09756900 2.84212200
H 3.38697900 0.17163200 2.01435000

L-Anti-TS2 (CYH)

C -3.65003500 3.40251900 4.27604100
C -4.62813700 3.82214400 3.36611100
C -5.18052700 2.93021900 2.45749400
C -4.75764200 1.57747900 2.40638000
C -3.77444800 1.17170800 3.34159100
C -3.23654300 2.06911300 4.25889300
C -5.29420600 0.62593700 1.44434700
C -6.20977700 0.96220700 0.44837300
C -6.99897200 0.06497800 -0.28784000
O -7.03339800 -1.25965300 0.00547100
N -4.94616300 -0.75382800 1.60941500
C -7.88997700 0.46091400 -1.36671600
C -7.83668700 1.74412300 -1.95904800
C -8.71555400 2.09819900 -2.97571700
C -9.66522000 1.18487300 -3.44545700
C -9.71959600 -0.09337100 -2.88241500
C -8.84790200 -0.45444600 -1.86103900
C -3.92124200 -1.22664400 0.90873800
C -3.65345500 -2.64214100 1.01304500
C -2.61317200 -3.22635400 0.32806900
C -1.75982700 -2.46124500 -0.49682100
C -1.99462200 -1.06836400 -0.59927900
C -3.03045000 -0.45927000 0.06847400
C -0.63905900 -3.11886700 -1.27368700

C 0.70252200 -2.41370700 -1.17421000
C 1.32943900 -1.88319200 -2.30701100
C 2.56474900 -1.24466500 -2.21517700
C 3.21978100 -1.12855600 -0.97962700
C 2.58507800 -1.64340100 0.16606200
C 1.35099000 -2.27566500 0.06226500
N 4.42726500 -0.41058300 -0.93839600
O 5.31431300 1.74846300 -1.57461400
C 6.38575100 1.51721000 -0.86117000
C 6.52578200 0.31586600 -0.16513200
C 5.49913200 -0.67167500 -0.20223700
C 7.41936400 2.58049300 -0.86742800
C 5.72661400 -1.95547700 0.52580000
C 7.33347600 3.60567400 -1.82391000
C 8.28931000 4.61783700 -1.86503700
C 9.34222700 4.62650000 -0.94769300
C 9.43126800 3.61736400 0.01444900
C 8.47837300 2.60266300 0.05576300
C 6.21458400 -1.94479000 1.84119800
C 6.47030200 -3.14132300 2.51122300
C 6.25942700 -4.36202000 1.86838200
C 5.78631500 -4.38143500 0.55392100
C 5.51555900 -3.18807700 -0.11201100
H -3.22574500 4.10290600 4.98871100
H -4.97140000 4.85289400 3.37571400
H -5.95960300 3.28244800 1.79062900
H -3.44069900 0.14130400 3.34453700
H -2.48620200 1.72369700 4.96463500
H -6.40336000 2.01290200 0.27764500
H -6.45264900 -1.41519000 0.78229100
H -7.08679100 2.45946900 -1.63906800
H -8.65223100 3.08995500 -3.41435400
H -10.34683200 1.46394000 -4.24307000
H -10.44970900 -0.81354400 -3.24095900
H -8.89953100 -1.44397800 -1.42343100
H -4.30640500 -3.22439300 1.65407400
H -2.43926800 -4.29464400 0.42128500
H -1.33034800 -0.47122000 -1.21662700
H -3.18734700 0.60758400 -0.02524600
H -0.93236300 -3.17074800 -2.33100300
H -0.54092200 -4.15809700 -0.93823700
H 0.84711500 -1.96951100 -3.27741700
H 3.03920000 -0.83480300 -3.10154900
H 3.05675300 -1.53407000 1.13609500

H 0.87738600 -2.66051600 0.96193600
H 4.69392900 0.79850300 -1.44660600
H 7.44415400 0.08697700 0.35412800
H 6.51127900 3.59068600 -2.52993900
H 8.21301500 5.40096800 -2.61350600
H 10.08659700 5.41666800 -0.97830700
H 10.24113600 3.62443600 0.73776200
H 8.54949200 1.83919500 0.82294800
H 6.37735800 -0.99559600 2.34250400
H 6.83599700 -3.11883700 3.53343300
H 6.46455700 -5.29372400 2.38707600
H 5.62955600 -5.32813000 0.04570500
H 5.15087700 -3.20715600 -1.13353200

L-Syn-TS2 (CYH)

C -5.36313600 5.22081100 -1.30737300
C -6.57029700 4.51553100 -1.38612300
C -6.66917200 3.22184900 -0.89335400
C -5.55026400 2.56736500 -0.31772700
C -4.34174100 3.30196000 -0.23941600
C -4.25546600 4.60393400 -0.72269600
C -5.61305400 1.20056000 0.17857000
C -6.74241800 0.38924900 0.07721300
C -6.98267200 -0.78896800 0.80079800
O -6.15641200 -1.19294100 1.79845200
N -4.48697800 0.70769200 0.91447400
C -8.14651600 -1.63963800 0.60820800
C -9.00206900 -1.50883400 -0.51033200
C -10.11735900 -2.32519900 -0.65550400
C -10.41022300 -3.30575100 0.29809500
C -9.56511300 -3.45931300 1.40082800
C -8.45005700 -2.64336800 1.55696200
C -3.57009900 0.00736400 0.25603000
C -2.49852200 -0.57015200 1.03661500
C -1.49895600 -1.30444400 0.44895700
C -1.47747000 -1.52133000 -0.95039600
C -2.50743600 -0.95461700 -1.73279900
C -3.52376400 -0.21409200 -1.16975700
C -0.38856200 -2.35812400 -1.58733600
C 1.02278000 -1.96091700 -1.18927400
C 1.85861500 -2.84354200 -0.49655600
C 3.15784000 -2.48083600 -0.14576400
C 3.65657400 -1.20913800 -0.46663900
C 2.82567100 -0.32322700 -1.17753200
C 1.53238100 -0.69753700 -1.52459200

N 4.99759500 -0.92699000 -0.15428000
O 7.21009400 -1.83241800 -0.52557400
C 7.73797100 -0.71189700 -0.10544900
C 6.92253900 0.34020600 0.31316800
C 5.50293400 0.22318800 0.27114500
C 9.21960400 -0.65305200 -0.08411000
C 4.68363800 1.36694200 0.77124900
C 9.94887100 -1.84361200 -0.23891600
C 11.34140900 -1.82910000 -0.21831200
C 12.02827700 -0.62499000 -0.04944800
C 11.31287200 0.56634700 0.09526300
C 9.92043900 0.55402600 0.07759500
C 4.98539200 2.67882100 0.37559700
C 4.25057700 3.75510400 0.87317000
C 3.21813400 3.53506300 1.78610700
C 2.91990100 2.23308800 2.19579300
C 3.64226600 1.15528700 1.68855900
H -5.29317400 6.23490400 -1.68841400
H -7.44579600 4.98612200 -1.82477700
H -7.62861900 2.71899500 -0.94104100
H -3.47140200 2.84139000 0.21171600
H -3.31386100 5.14013500 -0.64316000
H -7.55465000 0.73414400 -0.54880600
H -5.44182300 -0.52537800 1.89217300
H -8.77908700 -0.78084900 -1.28283900
H -10.75729000 -2.20460200 -1.52495200
H -11.27994900 -3.94445100 0.17856100
H -9.77901700 -4.21984100 2.14653500
H -7.80279900 -2.76236300 2.41734200
H -2.51942700 -0.39881600 2.10748800
H -0.70430300 -1.72327700 1.05872600
H -2.49190300 -1.10789300 -2.80838500
H -4.29665800 0.21549100 -1.79388400
H -0.49725800 -2.31023000 -2.67699900
H -0.55013000 -3.40915900 -1.31297000
H 1.49417800 -3.83340900 -0.23368700
H 3.79871500 -3.17743600 0.38599400
H 3.20340100 0.65074400 -1.46769200
H 0.90919100 0.00253400 -2.07525300
H 6.08655300 -1.65711100 -0.42371200
H 7.35480300 1.23282500 0.73950600
H 9.40613500 -2.77236800 -0.37101000
H 11.89175100 -2.75811100 -0.33398400
H 13.11411300 -0.61312600 -0.03506900

H 11.84094100 1.50745000 0.21601300
H 9.38075700 1.49042000 0.16918400
H 5.78723200 2.85079700 -0.33593300
H 4.48650800 4.76425500 0.54895800
H 2.64975800 4.37289200 2.17867500
H 2.12379200 2.05712200 2.91291300
H 3.40964900 0.14603800 2.01129100

L-Anti-TS3 (ACN)

C -3.33230800 4.36262200 3.15846000
C -4.43513300 4.55090500 2.31512600
C -5.06610500 3.47185800 1.71032700
C -4.60892000 2.14083400 1.91062300
C -3.49321900 1.97232500 2.77229800
C -2.87584300 3.06093100 3.38177700
C -5.25129600 1.01592600 1.26212900
C -6.31298300 1.05486800 0.35465200
C -7.06784700 -0.08558000 -0.04347200
O -6.89822200 -1.23699900 0.47724500
N -4.77153500 -0.29680200 1.62710100
C -8.13929300 0.07817200 -1.07885000
C -8.23368300 1.18357800 -1.94595100
C -9.25952600 1.27091300 -2.88665700
C -10.21305000 0.25391600 -2.99114800
C -10.12445800 -0.85608200 -2.14570300
C -9.09908100 -0.94318800 -1.20677100
C -3.79508900 -0.97917600 0.99989500
C -3.48662800 -2.30430800 1.42572200
C -2.48319700 -3.01143400 0.79931900
C -1.74596700 -2.44608000 -0.26302400
C -2.05382700 -1.12928900 -0.67696400
C -3.05379600 -0.40161200 -0.07260300
C -0.65176600 -3.22945400 -0.95433900
C 0.69790100 -2.53004000 -0.92780500
C 1.29189200 -2.05289700 -2.10198800
C 2.52824700 -1.40997000 -2.07233500
C 3.21594400 -1.23789600 -0.86079300
C 2.61417400 -1.69945000 0.32491600
C 1.37774300 -2.33528000 0.28440900
N 4.42326300 -0.51780000 -0.88057600
O 5.28391600 1.63297600 -1.58747100
C 6.38110900 1.41539700 -0.90135700
C 6.54476200 0.22821100 -0.19090200
C 5.51797000 -0.76299100 -0.17430700
C 7.41028900 2.48076600 -0.95833200

C 5.77130300 -2.03142900 0.57098300
C 7.30239700 3.48213600 -1.93851900
C 8.25457100 4.49555000 -2.02478700
C 9.32636700 4.52911200 -1.12940700
C 9.43803700 3.54364600 -0.14453400
C 8.48883800 2.52777500 -0.05775300
C 6.30833400 -1.99476900 1.86708900
C 6.58630900 -3.17881900 2.55095300
C 6.34979800 -4.41207500 1.94065400
C 5.82928400 -4.45715300 0.64433100
C 5.53576300 -3.27625800 -0.03490600
H -2.84645400 5.20989400 3.63172300
H -4.81364000 5.55349600 2.13403700
H -5.93027300 3.65725700 1.08183700
H -3.10824300 0.97756500 2.96743700
H -2.02609700 2.88774200 4.03679900
H -6.61373300 2.02900900 -0.00970900
H -5.28923800 -0.80698200 2.33623700
H -7.48986600 1.97288700 -1.90583400
H -9.30883100 2.13207700 -3.54741200
H -11.00973000 0.32299300 -3.72601600
H -10.85716100 -1.65527900 -2.22025900
H -9.01698800 -1.80144700 -0.54869900
H -4.05190600 -2.74511100 2.23999500
H -2.25663300 -4.02102400 1.12529200
H -1.48657500 -0.68470500 -1.48776400
H -3.29095300 0.60332300 -0.39613600
H -0.94847900 -3.39420700 -1.99716000
H -0.57358700 -4.21851100 -0.49161900
H 0.78495300 -2.18661300 -3.05384000
H 2.97853600 -1.04427100 -2.99003900
H 3.11304900 -1.54673900 1.27546400
H 0.93056500 -2.68107500 1.21284500
H 4.67463100 0.68893000 -1.42463700
H 7.47736200 0.01392400 0.30892800
H 6.46843900 3.44980400 -2.63016900
H 8.16104600 5.25904200 -2.79118000
H 10.06773200 5.31974100 -1.19499800
H 10.26255400 3.57008500 0.56129100
H 8.57923500 1.78423000 0.72663000
H 6.49235900 -1.03716800 2.34414700
H 6.98953200 -3.13662000 3.55812600
H 6.57243100 -5.33352700 2.47006200
H 5.65372800 -5.41333200 0.16087000

H 5.13648500 -3.31625200 -1.04285100

L-Syn-TS3 (ACN)

C -4.99197200 5.24462700 -1.21820600

C -6.24487800 4.62651100 -1.32333300

C -6.44668200 3.33410800 -0.85720500

C -5.38922000 2.58577800 -0.27193300

C -4.12962000 3.23291700 -0.17040000

C -3.94234000 4.53297900 -0.63124500

C -5.59153700 1.22883500 0.19308200

C -6.75612900 0.46356900 0.09186400

C -6.97623000 -0.75485400 0.79641900

O -6.16109800 -1.19839000 1.67068100

N -4.47871000 0.61055100 0.87584200

C -8.23585600 -1.52536600 0.53880800

C -9.05920300 -1.33232700 -0.58703600

C -10.21916400 -2.08583900 -0.76444000

C -10.58327700 -3.05659600 0.17329500

C -9.76836100 -3.26890800 1.28933400

C -8.60950500 -2.51623500 1.46584100

C -3.51989400 -0.13692300 0.29775400

C -2.52570000 -0.75353700 1.11613400

C -1.53446600 -1.51004700 0.53841800

C -1.48040100 -1.69804700 -0.86418600

C -2.46289600 -1.08404100 -1.66686900

C -3.46801700 -0.31625800 -1.11411000

C -0.39463400 -2.55253900 -1.47982400

C 1.01086200 -2.11563700 -1.10052700

C 1.84923000 -2.94272100 -0.34410600

C 3.14217800 -2.54335700 -0.00976100

C 3.62910800 -1.28909400 -0.40963800

C 2.79513300 -0.45999000 -1.18317500

C 1.50844100 -0.87055800 -1.51540300

N 4.96587200 -0.97128300 -0.11184300

O 7.19612900 -1.85498700 -0.44670800

C 7.70392500 -0.70047300 -0.08432900

C 6.86951300 0.35208200 0.28544100

C 5.44990600 0.20746300 0.25363100

C 9.18353700 -0.61119500 -0.07363100

C 4.61114300 1.35905000 0.69931300

C 9.93943500 -1.79373400 -0.14685300

C 11.33184100 -1.74716100 -0.13378200

C 11.99195400 -0.51854300 -0.05421900

C 11.24998100 0.66426800 0.00909800

C 9.85768900 0.62036900 -0.00109200

C 4.89111500 2.65633500 0.24287100
C 4.13657000 3.74144100 0.69009000
C 3.10736400 3.54584700 1.61302600
C 2.83189600 2.25905900 2.08393100
C 3.57347600 1.17137800 1.62680200
H -4.84206200 6.25673500 -1.58025200
H -7.07864600 5.16426500 -1.76706500
H -7.43693300 2.89890100 -0.93593300
H -3.29034800 2.71159500 0.27645400
H -2.96260200 4.99270800 -0.53177300
H -7.55942700 0.86668400 -0.51185200
H -4.47813100 0.63190200 1.89109500
H -8.78421900 -0.60615000 -1.34525400
H -10.83607900 -1.92101300 -1.64358300
H -11.48581500 -3.64392400 0.03194400
H -10.03823000 -4.02400000 2.02291900
H -7.96696900 -2.67551400 2.32503000
H -2.56820000 -0.61961800 2.19188100
H -0.77940700 -1.97332100 1.16440900
H -2.42801900 -1.21938200 -2.74275400
H -4.22007000 0.15340800 -1.73420300
H -0.51115400 -2.54658200 -2.56847500
H -0.54578900 -3.58971400 -1.15646900
H 1.49259500 -3.91624800 -0.01861300
H 3.78543500 -3.19741800 0.57085800
H 3.16555100 0.49643300 -1.53505200
H 0.88438200 -0.21648900 -2.11894500
H 6.07660200 -1.69775100 -0.34810400
H 7.28646000 1.27529300 0.65878300
H 9.42086600 -2.74358600 -0.20842600
H 11.90243600 -2.66956000 -0.18507800
H 13.07711800 -0.48160000 -0.04589700
H 11.75676300 1.62306700 0.05999000
H 9.29830900 1.54915400 0.02602100
H 5.69035400 2.81090300 -0.47528300
H 4.35509600 4.73822200 0.31935200
H 2.52461600 4.39107200 1.96645000
H 2.03992700 2.10278700 2.81001500
H 3.35931400 0.17506600 1.99895200
L-Anti-TS3 (DCM)
C -3.39459300 4.40161800 3.15848300
C -4.49844200 4.57479600 2.31349100
C -5.11320400 3.48766300 1.70699600
C -4.63731200 2.16290900 1.90617000

C -3.52076300 2.00983600 2.76987700
C -2.92038200 3.10620900 3.38158100
C -5.26165900 1.03166000 1.25397900
C -6.31581500 1.05507700 0.33718400
C -7.06748100 -0.09321500 -0.04730500
O -6.90223100 -1.23470500 0.49430700
N -4.77535300 -0.27836100 1.62681300
C -8.13087700 0.05305500 -1.09329700
C -8.21756600 1.14218900 -1.98100500
C -9.23708100 1.21372000 -2.92977500
C -10.19150500 0.19661600 -3.02110800
C -10.11004100 -0.89775500 -2.15489900
C -9.09100300 -0.96909300 -1.20812500
C -3.79884000 -0.96009100 1.00349200
C -3.50680700 -2.29440200 1.41552900
C -2.50138700 -3.00174600 0.79358900
C -1.74457900 -2.42903700 -0.25119200
C -2.03448100 -1.10319700 -0.65058300
C -3.03589300 -0.37477900 -0.05082900
C -0.65120100 -3.21498100 -0.94072600
C 0.70069700 -2.52037100 -0.91631200
C 1.29631000 -2.04851700 -2.09165700
C 2.53487600 -1.41012000 -2.06379500
C 3.22338100 -1.23710200 -0.85283600
C 2.62002600 -1.69362500 0.33398800
C 1.38146300 -2.32506500 0.29512200
N 4.43313100 -0.52196000 -0.87558200
O 5.30159700 1.62017400 -1.59544700
C 6.39655100 1.40458700 -0.90757900
C 6.55594000 0.22146200 -0.18784500
C 5.52655200 -0.76565500 -0.16605200
C 7.42925500 2.46633400 -0.97093300
C 5.77440900 -2.03002100 0.58805800
C 7.31912800 3.46675800 -1.95162200
C 8.27394600 4.47695500 -2.04416900
C 9.35064900 4.50824200 -1.15480100
C 9.46462400 3.52370900 -0.16945900
C 8.51277700 2.51105100 -0.07649700
C 6.30794600 -1.98648700 1.88529600
C 6.58112900 -3.16665300 2.57757600
C 6.34297700 -4.40312700 1.97474200
C 5.82549700 -4.45517800 0.67760500
C 5.53689400 -3.27807300 -0.01006700
H -2.92164900 5.25521800 3.63343300

H -4.89137200 5.57204000 2.13336600
H -5.98067800 3.66019600 1.07939000
H -3.12165600 1.02044000 2.96407400
H -2.06943200 2.94465500 4.03809900
H -6.61799200 2.02363700 -0.04093500
H -5.31564900 -0.79853500 2.31135700
H -7.47201900 1.93036600 -1.95048800
H -9.28085200 2.06248000 -3.60686100
H -10.98352500 0.25330300 -3.76214000
H -10.84365100 -1.69704400 -2.21948000
H -9.01264000 -1.81456000 -0.53333300
H -4.08910100 -2.74147600 2.21420300
H -2.28903000 -4.01821400 1.10782400
H -1.45057100 -0.65279000 -1.44616900
H -3.25920800 0.63683200 -0.36271600
H -0.94904800 -3.38103600 -1.98329100
H -0.57628300 -4.20425800 -0.47751600
H 0.78890800 -2.18295700 -3.04324200
H 2.98654300 -1.04814000 -2.98226500
H 3.11955500 -1.54046900 1.28405300
H 0.93312600 -2.66696000 1.22453100
H 4.68775800 0.67750600 -1.42612600
H 7.48773800 0.00673200 0.31320800
H 6.48063000 3.43592800 -2.63777600
H 8.17850700 5.24005000 -2.81075900
H 10.09411900 5.29652200 -1.22532400
H 10.29317000 3.54831500 0.53176900
H 8.60526500 1.76788300 0.70801200
H 6.49293800 -1.02604400 2.35631300
H 6.98194100 -3.11902400 3.58551700
H 6.56195800 -5.32172800 2.51065500
H 5.64848100 -5.41404400 0.19997400
H 5.13966000 -3.32326900 -1.01858800

L-Syn-TS3 (DCM)

C -5.37703200 5.25457000 -1.30445200
C -6.59753200 4.56733800 -1.32511300
C -6.69592700 3.26835600 -0.84577400
C -5.56164900 2.58068300 -0.33340800
C -4.33610100 3.29810700 -0.31648300
C -4.25294400 4.60440300 -0.78809500
C -5.65869600 1.21730800 0.13790000
C -6.77789700 0.38123500 0.10273800
C -6.90033500 -0.82330500 0.85638800
O -6.02917100 -1.19182100 1.70877100

N -4.48005600 0.66331400 0.77157300
C -8.12741400 -1.66525200 0.67968800
C -8.99495600 -1.56816500 -0.42419500
C -10.12174100 -2.38365200 -0.52344500
C -10.40651400 -3.32063500 0.47355100
C -9.54604800 -3.43720900 1.56919800
C -8.42024700 -2.62337400 1.66718600
C -3.52173500 -0.04894100 0.15899500
C -2.49457000 -0.66094000 0.94260400
C -1.49432800 -1.37448400 0.32864800
C -1.45991400 -1.52407400 -1.07942600
C -2.47487100 -0.91680000 -1.84832700
C -3.48965500 -0.19197800 -1.25988200
C -0.36703100 -2.33628900 -1.73798700
C 1.03583300 -1.94690900 -1.30433200
C 1.85765900 -2.84328100 -0.61176800
C 3.14877600 -2.48565100 -0.22782200
C 3.65137300 -1.20624000 -0.51219200
C 2.83388600 -0.30651000 -1.22174600
C 1.54879100 -0.67553200 -1.60391100
N 4.98553600 -0.92848100 -0.16995400
O 7.20872100 -1.81057800 -0.53949800
C 7.72464800 -0.69659400 -0.08316900
C 6.89700500 0.33735400 0.35439400
C 5.47839700 0.21325800 0.29181600
C 9.20502800 -0.62768200 -0.04381200
C 4.64553200 1.33715200 0.81323500
C 9.94645500 -1.80941800 -0.21105800
C 11.33870800 -1.78365800 -0.17432400
C 12.01310500 -0.57656500 0.02331100
C 11.28570200 0.60618700 0.18081500
C 9.89351600 0.58269600 0.14717400
C 4.94260800 2.66177600 0.45792700
C 4.19429600 3.71837600 0.97751900
C 3.15374500 3.46542200 1.87300200
C 2.86061500 2.15019900 2.24307500
C 3.59600300 1.09200100 1.71314500
H -5.30811700 6.27216000 -1.67545000
H -7.48816400 5.05704100 -1.71029000
H -7.66397300 2.77942400 -0.85180800
H -3.44112700 2.82547500 0.07289600
H -3.29612500 5.11890600 -0.75365800
H -7.62948300 0.72204800 -0.47285000
H -4.47260600 0.63767000 1.78669400

H -8.77883700 -0.86918800 -1.22602200
H -10.77474800 -2.29365600 -1.38735800
H -11.28359900 -3.95630800 0.39352700
H -9.75494700 -4.16566400 2.34828600
H -7.74063800 -2.70589300 2.50832700
H -2.52524200 -0.56047600 2.02237300
H -0.71552200 -1.83370300 0.92788800
H -2.45467400 -1.02289000 -2.92800800
H -4.26446400 0.27476800 -1.85312400
H -0.46533900 -2.24854800 -2.82531500
H -0.53451400 -3.39441100 -1.49944700
H 1.48957100 -3.83848000 -0.37648800
H 3.77975600 -3.19264400 0.30190700
H 3.21615200 0.67327700 -1.48519100
H 0.93778900 0.03371700 -2.15653700
H 6.08517500 -1.64592800 -0.44515500
H 7.31873900 1.22212600 0.80686400
H 9.41510900 -2.74150100 -0.36459800
H 11.89827100 -2.70579200 -0.29957900
H 13.09847000 -0.55576700 0.05019300
H 11.80410600 1.54940200 0.32393100
H 9.34528100 1.51297800 0.24899100
H 5.75107000 2.86027400 -0.23893100
H 4.42654400 4.73780300 0.68468900
H 2.57595100 4.28808700 2.28334600
H 2.05967600 1.94861900 2.94797200
H 3.36841800 0.07271400 2.00688500

L-Anti-TS3 (CYH)

C -3.65771900 4.40135500 3.35521600
C -4.72630900 4.56344000 2.46427100
C -5.27402800 3.47673500 1.79788700
C -4.76034200 2.16267800 1.97792400
C -3.68045900 2.02073100 2.88977500
C -3.15002600 3.11595600 3.56262600
C -5.30844600 1.03997100 1.25727800
C -6.30541100 1.04936300 0.27807800
C -7.04862600 -0.10564900 -0.11431400
O -6.92615800 -1.23144500 0.46687600
N -4.82696600 -0.28091400 1.62662800
C -8.05299700 0.02153400 -1.21784100
C -8.07766600 1.08431700 -2.13937400
C -9.04672100 1.14177800 -3.14007900
C -10.01018000 0.13591800 -3.24888300
C -9.98843900 -0.93342900 -2.34885100

C -9.01988500 -0.99123600 -1.35055600
C -3.83757300 -0.94530200 1.01899700
C -3.64204800 -2.33214100 1.31048800
C -2.61794700 -3.02534200 0.70739300
C -1.74124800 -2.39231300 -0.20180600
C -1.93151700 -1.01685400 -0.47977400
C -2.94914300 -0.29952000 0.10266400
C -0.64249300 -3.17471900 -0.88707500
C 0.71373900 -2.49202400 -0.87425100
C 1.31211000 -2.04186800 -2.05633400
C 2.55677300 -1.41593800 -2.03922900
C 3.24940400 -1.23219200 -0.83207000
C 2.64342100 -1.66787800 0.36126800
C 1.39940600 -2.28807900 0.33257700
N 4.46452500 -0.52962800 -0.86907400
O 5.34753500 1.58500900 -1.63970700
C 6.43500100 1.38580100 -0.94286400
C 6.58643500 0.22053900 -0.18777100
C 5.55419000 -0.75855100 -0.14599500
C 7.47265200 2.44136900 -1.02952800
C 5.78986500 -2.00408600 0.64273900
C 7.35833700 3.42564300 -2.02533400
C 8.31591100 4.43022100 -2.14122500
C 9.39922500 4.47199900 -1.26091400
C 9.51724500 3.50377400 -0.26063400
C 8.56261800 2.49662200 -0.14444900
C 6.31232600 -1.92942400 1.94278200
C 6.57433500 -3.09185400 2.66804700
C 6.33520900 -4.34231100 2.09612500
C 5.82775100 -4.42577200 0.79708900
C 5.55069600 -3.26615600 0.07637800
H -3.23802900 5.25483700 3.87792100
H -5.14686100 5.55184100 2.29784500
H -6.12233400 3.63536900 1.14103200
H -3.25669700 1.03922900 3.07182000
H -2.32650500 2.96305500 4.25539100
H -6.58998900 2.01270700 -0.12697700
H -5.47567600 -0.85176900 2.16184400
H -7.32098700 1.86119900 -2.09329800
H -9.04404000 1.97041300 -3.84319600
H -10.76366800 0.18139600 -4.03001100
H -10.73001300 -1.72414400 -2.42780500
H -8.98448200 -1.81648400 -0.64788300
H -4.32251700 -2.82594200 1.99550700

H -2.48384600 -4.07995900 0.92577300
H -1.25201800 -0.52099800 -1.16455300
H -3.09394000 0.75038100 -0.11279700
H -0.94658500 -3.34686400 -1.92823400
H -0.57250300 -4.16573900 -0.42490800
H 0.80150600 -2.18324900 -3.00549100
H 3.01056800 -1.06966600 -2.96260600
H 3.14583200 -1.50715600 1.30834400
H 0.94970800 -2.61340300 1.26742900
H 4.72429400 0.64464000 -1.44635000
H 7.51619700 0.01262900 0.31974800
H 6.51268600 3.38541800 -2.70204400
H 8.21723200 5.18160100 -2.91899300
H 10.14501100 5.25636700 -1.34988800
H 10.35136800 3.53687400 0.43377800
H 8.65797700 1.76562900 0.65115200
H 6.49716500 -0.95708300 2.38899300
H 6.96722000 -3.01974800 3.67777600
H 6.54553100 -5.24757600 2.65774400
H 5.64956200 -5.39611700 0.34349400
H 5.16034400 -3.33503800 -0.93348300

L-Syn-TS3 (CYH)

C -6.03532600 5.23988100 -1.30376900
C -7.17410400 4.42617200 -1.24718600
C -7.10083400 3.12384800 -0.77448100
C -5.86648800 2.55905000 -0.34912700
C -4.72589000 3.40384500 -0.40951900
C -4.81552200 4.71242500 -0.87134900
C -5.78653000 1.19324800 0.10694100
C -6.80391300 0.23549100 0.13737500
C -6.75792300 -0.95070700 0.93180900
O -5.81687900 -1.18972500 1.75428500
N -4.51831300 0.75824300 0.66876200
C -7.88706700 -1.93009000 0.83619800
C -8.81425900 -1.95981900 -0.22143300
C -9.84493300 -2.89844800 -0.24373700
C -9.97016600 -3.83434000 0.78592100
C -9.04733200 -3.82513200 1.83581200
C -8.01764500 -2.88844500 1.85727100
C -3.54822000 0.12552000 -0.00057300
C -2.46642700 -0.47005900 0.72404200
C -1.44917000 -1.10061100 0.05106200
C -1.44655900 -1.18099800 -1.36304800
C -2.51339100 -0.58898400 -2.07493200

C -3.54608200 0.05253000 -1.42791300
C -0.34421300 -1.91458500 -2.09453100
C 1.05582500 -1.61483000 -1.59061200
C 1.84479000 -2.60849500 -1.00044300
C 3.13443600 -2.33117900 -0.55155700
C 3.67010200 -1.03867300 -0.66616300
C 2.88575700 -0.03978700 -1.27308500
C 1.60166800 -0.32886400 -1.72088800
N 5.00137400 -0.83785000 -0.26729700
O 7.20788500 -1.73002200 -0.69327000
C 7.74189500 -0.69263800 -0.10447000
C 6.93092700 0.30928300 0.43344900
C 5.51348500 0.23092800 0.33114600
C 9.22252600 -0.66995200 -0.02973100
C 4.69655900 1.30928300 0.96258300
C 9.93599200 -1.84101500 -0.33475000
C 11.32704000 -1.85979600 -0.26989400
C 12.02818600 -0.70821900 0.09414700
C 11.32895600 0.46467700 0.38973000
C 9.93791600 0.48530500 0.32818600
C 5.02820700 2.65767200 0.76159600
C 4.29482200 3.66737800 1.38493900
C 3.23416500 3.34121900 2.23142300
C 2.90604100 2.00052100 2.44779700
C 3.62667600 0.99075500 1.81381800
H -6.10098600 6.25997200 -1.66832600
H -8.13651700 4.81960900 -1.56415300
H -8.00921600 2.53452900 -0.71321800
H -3.76126000 3.02760000 -0.08705300
H -3.91927000 5.32699400 -0.89644500
H -7.71610000 0.46740000 -0.39852700
H -4.49650700 0.65249800 1.67943100
H -8.71869100 -1.26250700 -1.04778700
H -10.54736000 -2.90508500 -1.07293000
H -10.77266600 -4.56616000 0.76621900
H -9.13250200 -4.55206900 2.63934000
H -7.28979700 -2.87075000 2.66104000
H -2.47760400 -0.42970800 1.80781200
H -0.63238700 -1.54924400 0.60588400
H -2.51551900 -0.64009000 -3.15907200
H -4.35780300 0.51046100 -1.97649800
H -0.41918900 -1.68731000 -3.16396600
H -0.53557000 -2.99231400 -2.00225300
H 1.45189900 -3.61675000 -0.89735500

H 3.73987500 -3.11245900 -0.10265100
H 3.29327000 0.95597600 -1.40584100
H 1.01713800 0.45763100 -2.19171600
H 6.08224600 -1.54563000 -0.60156000
H 7.36406200 1.12313600 0.99499200
H 9.38249100 -2.72880400 -0.61778600
H 11.86511000 -2.77369900 -0.50334100
H 13.11295700 -0.72223900 0.14325100
H 11.86868100 1.36633000 0.66313800
H 9.41182300 1.40992100 0.53973300
H 5.85266000 2.91222900 0.10263500
H 4.55422000 4.70737200 1.21122500
H 2.66780700 4.12658400 2.72288500
H 2.08913100 1.74109100 3.11450100
H 3.37221300 -0.04947800 1.98769000

L-Anti-TS4 (ACN)

C -3.54077200 5.16506500 1.68222400
C -4.70142200 5.08576000 0.89783100
C -5.28220000 3.85961900 0.61032500
C -4.70888300 2.64837700 1.08429900
C -3.53260600 2.74879500 1.87229800
C -2.97006700 3.98723000 2.17001900
C -5.27555100 1.36053700 0.77171400
C -6.43063700 1.09282800 0.03476500
C -7.17442200 -0.09993200 0.23808100
O -6.80769100 -0.98911600 1.12827200
N -4.72239300 0.17576700 1.40875300
C -8.44381800 -0.34406000 -0.47429200
C -8.83000000 0.38166600 -1.62052600
C -10.04311300 0.12225100 -2.25322100
C -10.89901800 -0.87035000 -1.76538700
C -10.52296200 -1.60679900 -0.63776600
C -9.31065500 -1.35158900 -0.00301200
C -3.76321700 -0.52851700 0.77310000
C -3.51815500 -1.87495600 1.19775500
C -2.53507100 -2.62982600 0.59671000
C -1.73657100 -2.09846600 -0.44016000
C -1.96387300 -0.76464800 -0.85104900
C -2.94690100 0.00893700 -0.27448500
C -0.65923300 -2.93161100 -1.09928300
C 0.72502500 -2.30813600 -1.01525000
C 1.38830300 -1.85403000 -2.16151400
C 2.65502700 -1.27822500 -2.07959200
C 3.30953300 -1.15992500 -0.84301900

C 2.63891300 -1.59987200 0.31426600
C 1.36967000 -2.16163600 0.22273500
N 4.55195500 -0.50380700 -0.80750100
O 5.65661400 1.67437700 -1.34970700
C 6.71132200 1.26738500 -0.65134400
C 6.72530000 0.02696400 -0.04394900
C 5.60470000 -0.87403600 -0.11004500
C 7.84001100 2.22219400 -0.60931500
C 5.75221500 -2.19919800 0.56949400
C 7.87439700 3.28769600 -1.52569500
C 8.92986900 4.19744700 -1.51547700
C 9.96449300 4.06250500 -0.58698100
C 9.93497300 3.01233200 0.33509500
C 8.88240200 2.10051800 0.32677800
C 6.25473500 -2.27290500 1.87777300
C 6.42924600 -3.50946700 2.50038500
C 6.12442800 -4.68741900 1.81567700
C 5.63872800 -4.62363500 0.50675600
C 5.44757800 -3.38901200 -0.11098600
H -3.09513300 6.12871600 1.90777400
H -5.16106100 5.99421300 0.51852600
H -6.19343400 3.83185900 0.02239000
H -3.07028900 1.84546100 2.25349400
H -2.07389200 4.03092500 2.78274300
H -6.86787100 1.87822400 -0.56883000
H -5.66719000 -0.47926900 1.62572700
H -8.17022000 1.13565700 -2.03645700
H -10.31792400 0.69085000 -3.13695900
H -11.84280800 -1.07214100 -2.26288600
H -11.17768100 -2.38397900 -0.25358900
H -9.01401600 -1.92105300 0.87038000
H -4.12663600 -2.28525700 1.99617300
H -2.36838900 -3.65165700 0.92284200
H -1.34230200 -0.34211000 -1.63418800
H -3.10602400 1.03017600 -0.59571600
H -0.92171200 -3.07196600 -2.15510900
H -0.65076700 -3.92792600 -0.64501300
H 0.90968700 -1.95017400 -3.13254900
H 3.15626300 -0.92395900 -2.97518100
H 3.11264300 -1.48718800 1.28339900
H 0.86973000 -2.48955700 1.13059500
H 4.98456300 0.88089900 -1.30834100
H 7.61943000 -0.31016900 0.45927100
H 7.07113500 3.38852700 -2.24626000

H 8.94525000 5.01175800 -2.23355300
H 10.78594500 4.77248000 -0.57776400
H 10.72965400 2.90784200 1.06737000
H 8.86327400 1.30631600 1.06514400
H 6.49382000 -1.35907000 2.41302700
H 6.80623700 -3.55144800 3.51772400
H 6.26742400 -5.65014000 2.29700700
H 5.41030400 -5.53675800 -0.03449700
H 5.07334300 -3.34503300 -1.12836200

L-Syn-TS4 (ACN)

C -5.40700300 5.27003100 -1.19288200
C -6.60277800 4.54816700 -1.32655200
C -6.68007300 3.22160000 -0.92964700
C -5.54722200 2.54961700 -0.39506200
C -4.34560900 3.29516700 -0.27197500
C -4.28625000 4.63224300 -0.65635800
C -5.59410600 1.16279600 -0.00529500
C -6.69457200 0.30424000 -0.03796600
C -6.78321200 -0.81458000 0.83207700
O -5.83885200 -1.07919700 1.70156700
N -4.44132500 0.58149400 0.66494900
C -7.98477800 -1.67136900 0.86138500
C -8.95572400 -1.66400500 -0.16179000
C -10.07799000 -2.48492000 -0.08535900
C -10.25882800 -3.33863900 1.00745800
C -9.29795500 -3.36578700 2.02289200
C -8.17411100 -2.54763400 1.94988300
C -3.50427100 -0.05486200 -0.06726400
C -2.61087500 -0.95330900 0.60601200
C -1.62237300 -1.60580000 -0.08953500
C -1.45316800 -1.40861000 -1.48300600
C -2.32008400 -0.51761800 -2.14660800
C -3.32415300 0.14963600 -1.47232200
C -0.35685600 -2.13571000 -2.22958600
C 1.03595600 -1.80754100 -1.71353400
C 1.81918900 -2.77280900 -1.06948200
C 3.09811500 -2.46928300 -0.60585100
C 3.62475000 -1.17565100 -0.75059000
C 2.84588800 -0.20605000 -1.41107300
C 1.57462000 -0.52221900 -1.87875000
N 4.94817700 -0.94718000 -0.33690300
O 7.29488700 -1.72773600 -0.70387900
C 7.71374300 -0.64952600 -0.05029900
C 6.81363800 0.26516100 0.46113900

C 5.39151700 0.11901700 0.29485700
C 9.18115800 -0.53763600 0.09649300
C 4.51938400 1.16447500 0.91589100
C 9.98436100 -1.66662300 -0.14116100
C 11.36895400 -1.59320700 -0.00250000
C 11.97478100 -0.39081400 0.36892800
C 11.18619000 0.74045100 0.59767400
C 9.80196600 0.67014500 0.46175700
C 4.80922100 2.52621800 0.73918800
C 4.01994700 3.50263500 1.34818700
C 2.94549600 3.12972900 2.15799300
C 2.65978900 1.77551100 2.35224700
C 3.43642700 0.79891500 1.73142600
H -5.35584800 6.30969800 -1.50038400
H -7.48492000 5.03364400 -1.73466900
H -7.62513400 2.69716400 -1.02227400
H -3.46286300 2.81616100 0.13581700
H -3.35372000 5.17780900 -0.54137100
H -7.57240700 0.58998000 -0.60359900
H -4.92195500 -0.12564200 1.46369900
H -8.82394500 -1.03325400 -1.03449100
H -10.81056100 -2.46551900 -0.88709700
H -11.13345400 -3.97972700 1.06229500
H -9.42557400 -4.02905800 2.87379900
H -7.42533400 -2.56683500 2.73343200
H -2.74022200 -1.10894800 1.67147200
H -0.95508800 -2.28405300 0.43273300
H -2.19133500 -0.35078700 -3.21155500
H -3.97460100 0.84003300 -1.99339100
H -0.42954100 -1.89527300 -3.29527000
H -0.52496300 -3.21555300 -2.13819200
H 1.43164500 -3.77977700 -0.93923900
H 3.70126700 -3.23055500 -0.12058000
H 3.24898200 0.78834600 -1.56894900
H 0.99404600 0.24132600 -2.39021000
H 6.25533600 -1.66771200 -0.68231900
H 7.17401700 1.09625600 1.04920100
H 9.51114400 -2.59860300 -0.42769400
H 11.97530600 -2.47553500 -0.18361000
H 13.05381900 -0.33305500 0.47504400
H 11.65107600 1.68149400 0.87513000
H 9.20769900 1.56363300 0.61930600
H 5.64443300 2.82000500 0.11078700
H 4.24717200 4.55284100 1.19227100

H 2.33576400 3.88904900 2.63821500
H 1.83216300 1.47949900 2.98967600
H 3.21273600 -0.25108900 1.88795100

L-Anti-TS4 (DCM)

C -3.60487600 5.16495200 1.80251000
C -4.74870200 5.08696900 0.99391300
C -5.31094000 3.86014900 0.67496700
C -4.73430900 2.64686600 1.13974500
C -3.57508500 2.74617900 1.95279700
C -3.03193600 3.98489600 2.28230300
C -5.27973800 1.35983300 0.79272700
C -6.41114400 1.09012100 0.02038400
C -7.15846600 -0.10425600 0.20368200
O -6.81542800 -0.99346500 1.10159100
N -4.73645200 0.16929000 1.43109400
C -8.40843700 -0.34799700 -0.54293100
C -8.76016900 0.37268400 -1.70294300
C -9.95674300 0.11476600 -2.36692300
C -10.82953700 -0.87137900 -1.89687800
C -10.48709700 -1.60307700 -0.75563500
C -9.29141600 -1.34944300 -0.08987000
C -3.77487200 -0.53325500 0.80041600
C -3.54966100 -1.88994600 1.20487100
C -2.56302200 -2.64281800 0.60776000
C -1.74087100 -2.10064000 -0.40477200
C -1.94757700 -0.75692300 -0.79451500
C -2.93340200 0.01541100 -0.22183200
C -0.66276400 -2.93452100 -1.06190400
C 0.72169000 -2.31107800 -0.98839100
C 1.38606200 -1.87862000 -2.14217000
C 2.65370700 -1.30374800 -2.07026400
C 3.30823800 -1.16462200 -0.83594200
C 2.63655000 -1.58294800 0.32865200
C 1.36648800 -2.14391500 0.24676000
N 4.55157100 -0.51022200 -0.81232200
O 5.66170300 1.65656500 -1.39425900
C 6.71484600 1.25965800 -0.68882900
C 6.72584000 0.03060800 -0.05836200
C 5.60337900 -0.86882800 -0.10761800
C 7.84592700 2.21224900 -0.66467100
C 5.74784200 -2.18083100 0.59795300
C 7.88120100 3.26135500 -1.59950200
C 8.93847900 4.16884600 -1.60656900
C 9.97404200 4.04809600 -0.67737900

C 9.94364300 3.01443000 0.26294700
C 8.88926700 2.10487700 0.27187100
C 6.24890600 -2.22989200 1.90785700
C 6.42064400 -3.45414500 2.55488800
C 6.11422800 -4.64467000 1.89328200
C 5.62956200 -4.60563700 0.58316100
C 5.44133600 -3.38317800 -0.05894100
H -3.17389300 6.12914500 2.05293600
H -5.21072200 5.99705700 0.62132000
H -6.21160600 3.83227600 0.07090800
H -3.11094300 1.84103100 2.32745600
H -2.14878900 4.02755900 2.91380100
H -6.83445900 1.87605300 -0.59262400
H -5.68419100 -0.48377900 1.63153500
H -8.08539900 1.12113900 -2.10475700
H -10.20518700 0.67935600 -3.26105400
H -11.76047700 -1.07211300 -2.41855200
H -11.15532200 -2.37539600 -0.38503000
H -9.01970200 -1.91465300 0.79428500
H -4.17740900 -2.30869700 1.98357500
H -2.41176500 -3.67211100 0.91777900
H -1.30565700 -0.32574100 -1.55618900
H -3.07528600 1.04491900 -0.52395600
H -0.92965600 -3.08255600 -2.11591600
H -0.65233100 -3.92889000 -0.60284200
H 0.90726300 -1.99078900 -3.11149000
H 3.15572900 -0.96554600 -2.97158600
H 3.11030600 -1.45393600 1.29568500
H 0.86559900 -2.45439800 1.16024100
H 4.98749900 0.86709800 -1.33902000
H 7.61985700 -0.29986600 0.44943400
H 7.07657200 3.35089400 -2.31996900
H 8.95440800 4.97055100 -2.33872300
H 10.79693400 4.75650700 -0.68166800
H 10.73916400 2.92125600 0.99590500
H 8.86925200 1.32373400 1.02407400
H 6.48884400 -1.30590600 2.42509700
H 6.79662900 -3.47683500 3.57325600
H 6.25502900 -5.59803600 2.39356900
H 5.39954300 -5.52880800 0.05987300
H 5.06746300 -3.35826300 -1.07705700
L-Syn-TS4 (DCM)
C -5.83802700 5.27691800 -1.21272800
C -6.98004700 4.46748000 -1.30609700

C -6.94412300 3.13955800 -0.90915200
C -5.74600400 2.55384100 -0.41666100
C -4.60018700 3.38775000 -0.33381100
C -4.65495700 4.72503200 -0.71605900
C -5.67468300 1.16805200 -0.03482900
C -6.70115300 0.22154700 -0.04513200
C -6.69191300 -0.88085700 0.85181800
O -5.72318400 -1.05202400 1.71418300
N -4.46470500 0.67617400 0.61285900
C -7.82384900 -1.82707000 0.91298100
C -8.79878900 -1.92205000 -0.10112100
C -9.85585800 -2.82181800 0.00818100
C -9.96465000 -3.65404500 1.12629500
C -8.99712600 -3.58043700 2.13287200
C -7.93831400 -2.68349800 2.02677100
C -3.52367700 0.07196600 -0.13556600
C -2.57433200 -0.78341600 0.51941700
C -1.57686200 -1.39702000 -0.19758200
C -1.45117600 -1.20185900 -1.59599500
C -2.37202000 -0.35194900 -2.24185700
C -3.38607100 0.27597200 -1.54677700
C -0.35060400 -1.89322500 -2.36972200
C 1.04312500 -1.61424400 -1.83038100
C 1.83519500 -2.63829200 -1.29830100
C 3.11827900 -2.38071900 -0.81910900
C 3.64075300 -1.07759900 -0.83382600
C 2.85231300 -0.04718900 -1.38081600
C 1.57735700 -0.31719500 -1.86604000
N 4.96738100 -0.88920100 -0.41160200
O 7.31915800 -1.61160100 -0.88029500
C 7.73573200 -0.61039900 -0.11426200
C 6.83472700 0.23804400 0.49979500
C 5.41235600 0.10351100 0.32873500
C 9.20343200 -0.50839100 0.03672100
C 4.54157300 1.07229700 1.06597000
C 10.00938500 -1.59823600 -0.33477400
C 11.39417300 -1.53535700 -0.19518000
C 11.99749000 -0.38218600 0.31095800
C 11.20608700 0.71122400 0.67342700
C 9.82171900 0.65106800 0.53678600
C 4.82425900 2.44638900 1.03302000
C 4.03747800 3.34868800 1.74960500
C 2.97233500 2.88666300 2.52460600
C 2.69347200 1.51841500 2.57545300

C 3.46761100 0.61725900 1.84714400
H -5.87558900 6.31748700 -1.51925400
H -7.91023300 4.88591300 -1.68069000
H -7.85027200 2.54569100 -0.96479400
H -3.67071700 2.97507600 0.04147500
H -3.76284900 5.33957300 -0.63128100
H -7.60635400 0.42709600 -0.60290100
H -4.87513000 -0.03293500 1.44349400
H -8.71883000 -1.30887200 -0.99252200
H -10.59333500 -2.88066500 -0.78725400
H -10.78855900 -4.35673800 1.20741000
H -9.06885600 -4.22684300 3.00317500
H -7.18316600 -2.62296400 2.80199500
H -2.67254700 -0.93924300 1.58793100
H -0.86643200 -2.04144800 0.31035500
H -2.27440000 -0.18335300 -3.31000500
H -4.07471400 0.94042800 -2.05191700
H -0.41396000 -1.59627500 -3.42219700
H -0.53166500 -2.97527800 -2.34255200
H 1.45116200 -3.65474900 -1.26945600
H 3.72868400 -3.18587300 -0.42177500
H 3.25075700 0.95991700 -1.43627200
H 0.98906600 0.49397800 -2.28757200
H 6.28195600 -1.56278600 -0.84779000
H 7.19506800 0.99912600 1.17598900
H 9.53671400 -2.49140800 -0.72622500
H 12.00288900 -2.38787500 -0.48112100
H 13.07690900 -0.33254300 0.41803200
H 11.66907800 1.61559200 1.05631900
H 9.22469100 1.51753700 0.79982400
H 5.65252800 2.80860600 0.43159100
H 4.25925700 4.41068800 1.70457200
H 2.36425900 3.58754000 3.08856600
H 1.87259300 1.15248300 3.18473700
H 3.24891300 -0.44441600 1.89154300

L-Anti-TS4 (CYH)

C -3.85348900 5.09353900 2.30740400
C -4.90241300 5.04367700 1.37771700
C -5.39590800 3.82911500 0.92770200
C -4.83961100 2.59988100 1.37622600
C -3.77574400 2.67152000 2.31345600
C -3.30490500 3.89676700 2.77433400
C -5.30794400 1.33121900 0.89084900
C -6.33247500 1.08195100 -0.02523300

C -7.10010000 -0.11355300 0.04592200
O -6.87080000 -1.02158700 0.95632700
N -4.82697400 0.10670400 1.52671200
C -8.25167500 -0.33375600 -0.85215100
C -8.45329700 0.40506600 -2.03526700
C -9.56378100 0.17048800 -2.84179200
C -10.49650200 -0.81041400 -2.49352400
C -10.30093300 -1.56077800 -1.33030900
C -9.19173000 -1.33050100 -0.52259300
C -3.83957800 -0.58522200 0.93801800
C -3.69272400 -1.97694900 1.26014000
C -2.68177600 -2.72108700 0.69680700
C -1.75491600 -2.14115400 -0.19886800
C -1.88023100 -0.76471300 -0.50119800
C -2.88691600 0.00224600 0.03968300
C -0.66769700 -2.98088400 -0.83471300
C 0.71197800 -2.34741100 -0.81988300
C 1.35021000 -1.96756300 -2.00605100
C 2.61520000 -1.38358000 -1.98819100
C 3.29431700 -1.18169800 -0.77612700
C 2.64918000 -1.54825500 0.42037000
C 1.38174100 -2.11937000 0.39155800
N 4.53280500 -0.52057100 -0.81183500
O 5.62391400 1.62107400 -1.52886500
C 6.69068200 1.26351100 -0.82625800
C 6.71923000 0.06892200 -0.13210300
C 5.60078600 -0.83527600 -0.11094500
C 7.81844200 2.21904800 -0.87562900
C 5.76634700 -2.10634600 0.66270400
C 7.82337600 3.22372700 -1.85804500
C 8.87607300 4.13265800 -1.93587400
C 9.93704200 4.05813500 -1.03144500
C 9.93668100 3.06958300 -0.04391400
C 8.88696200 2.15865900 0.03561600
C 6.29015200 -2.08068100 1.96407000
C 6.48118200 -3.26588000 2.67466000
C 6.17087500 -4.49249800 2.08561000
C 5.66276300 -4.52832100 0.78476200
C 5.45559100 -3.34463700 0.07959600
H -3.47689300 6.04830900 2.66060400
H -5.34742300 5.96623100 1.01478500
H -6.23079600 3.81914900 0.23502100
H -3.33004200 1.75344500 2.67892300
H -2.49599800 3.91728300 3.49964800

H -6.68181800 1.88457300 -0.66330500
H -5.79102600 -0.53451100 1.63206600
H -7.72539200 1.14892400 -2.34193500
H -9.69720200 0.74914400 -3.75154500
H -11.36037800 -0.99318300 -3.12576100
H -11.01700600 -2.32977500 -1.05375400
H -9.03048700 -1.90897800 0.37967400
H -4.40513000 -2.42514200 1.94322000
H -2.59197300 -3.77544100 0.94057600
H -1.15395600 -0.30523300 -1.16378900
H -2.96317200 1.05763000 -0.18633200
H -0.95514500 -3.18193500 -1.87580000
H -0.63947300 -3.95690500 -0.33680600
H 0.85191100 -2.12742200 -2.95897300
H 3.09672900 -1.08448100 -2.91409900
H 3.14220500 -1.37132700 1.36988700
H 0.90137600 -2.38894200 1.32889200
H 4.95300900 0.83871700 -1.42130500
H 7.62625300 -0.23413000 0.36964200
H 6.99715200 3.27676600 -2.55719200
H 8.86829300 4.90013100 -2.70406300
H 10.75658200 4.76808500 -1.09114000
H 10.75236200 3.01308900 0.67056700
H 8.88984500 1.41319000 0.82348700
H 6.53252700 -1.12751900 2.42432200
H 6.87507000 -3.23026100 3.68599600
H 6.32651400 -5.41601300 2.63524500
H 5.42876900 -5.48030300 0.31772000
H 5.06219300 -3.37709900 -0.93087400

L-Syn-TS4 (CYH)

C -6.03880600 5.27952700 -1.16950100
C -7.14976200 4.42745500 -1.25424500
C -7.05706100 3.09861500 -0.87147200
C -5.82961300 2.55379000 -0.40380300
C -4.71584800 3.43120900 -0.32910300
C -4.82834900 4.76871100 -0.69519900
C -5.70008200 1.16903300 -0.04348600
C -6.68427800 0.17793300 -0.05833400
C -6.63852400 -0.91031600 0.85631600
O -5.67359700 -1.03303100 1.72755400
N -4.46890300 0.71570900 0.60030400
C -7.73558100 -1.89720300 0.92038200
C -8.68287700 -2.05771600 -0.11057400
C -9.70880800 -2.99216200 0.00331100

C -9.81196700 -3.79383100 1.14349500
C -8.87030900 -3.65505900 2.16739900
C -7.84257700 -2.72376700 2.05653300
C -3.53021600 0.11579100 -0.14713700
C -2.57292300 -0.73635200 0.50407000
C -1.57516300 -1.34391000 -0.21652400
C -1.45467900 -1.14728500 -1.61536900
C -2.38153300 -0.29994800 -2.25751000
C -3.39560000 0.32297800 -1.55986200
C -0.35385700 -1.83343000 -2.39337400
C 1.04038700 -1.56595800 -1.85007000
C 1.82709200 -2.59793900 -1.32609100
C 3.11050300 -2.35040400 -0.84318200
C 3.63947400 -1.04986900 -0.84646000
C 2.85593500 -0.01148100 -1.38520000
C 1.58050000 -0.27140700 -1.87374700
N 4.96604800 -0.87218000 -0.42145800
O 7.31909800 -1.60089300 -0.89279800
C 7.73683000 -0.60764300 -0.11918600
C 6.83796800 0.24039200 0.49937500
C 5.41589800 0.11357200 0.32503000
C 9.20464500 -0.51262900 0.03494900
C 4.54910700 1.08388200 1.06555000
C 10.00637400 -1.60011000 -0.35125100
C 11.39099300 -1.54452900 -0.20941100
C 11.99837600 -0.40135900 0.31352000
C 11.21120100 0.68984200 0.69048200
C 9.82702500 0.63691600 0.55159400
C 4.83827200 2.45655800 1.03779600
C 4.05527200 3.36033300 1.75628800
C 2.98692200 2.90111600 2.52804900
C 2.70118200 1.53438600 2.57346300
C 3.47170600 0.63196200 1.84331000
H -6.12098700 6.32092300 -1.46430200
H -8.10140400 4.81374500 -1.60922400
H -7.94083700 2.47092400 -0.91485000
H -3.76570200 3.05043300 0.02771900
H -3.95978500 5.41696500 -0.61593100
H -7.59361600 0.34063200 -0.62391700
H -4.85281200 0.01814900 1.44810900
H -8.60305300 -1.46880100 -1.01832900
H -10.42573100 -3.10222400 -0.80549400
H -10.61161300 -4.52370000 1.22864800
H -8.93823600 -4.27770900 3.05523100

H -7.10597100 -2.61090300 2.84361200
H -2.67085400 -0.89641200 1.57174400
H -0.85904200 -1.98506700 0.28767600
H -2.28554000 -0.12812900 -3.32547900
H -4.08589100 0.98961300 -2.05941700
H -0.41486000 -1.52651900 -3.44339800
H -0.53892600 -2.91538400 -2.37848500
H 1.43884600 -3.61319900 -1.30736700
H 3.71759900 -3.16135200 -0.45275000
H 3.25891900 0.99420600 -1.43107500
H 0.99587200 0.54620900 -2.28807300
H 6.28422800 -1.55081600 -0.86386700
H 7.20001200 0.99324600 1.18380200
H 9.52925800 -2.48463400 -0.75653500
H 11.99672400 -2.39520300 -0.50713800
H 13.07794600 -0.35754600 0.42232100
H 11.67752600 1.58690000 1.08651200
H 9.23272400 1.50183900 0.82581600
H 5.66917300 2.81596600 0.43817500
H 4.28229300 4.42145900 1.71520900
H 2.38144900 3.60304700 3.09355800
H 1.87729800 1.17063700 3.18006900
H 3.24749400 -0.42875200 1.88253200