Supporting Information
Thermal Isomerization of Cannabinoid Analogs

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I. Figures S2, S3, S4

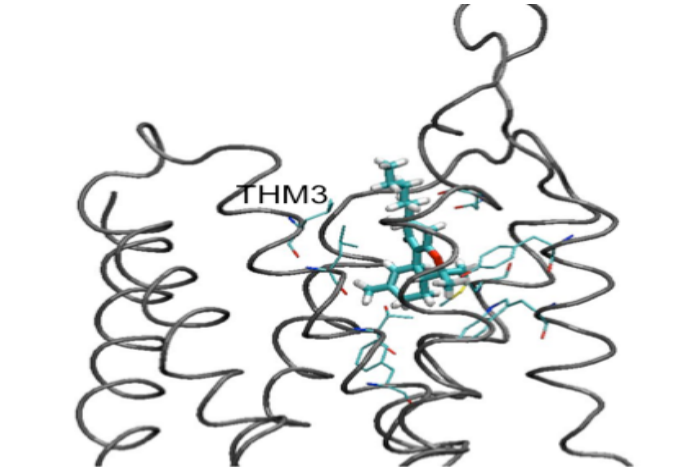


Figure S2. *trans*-(R,R)-THC$_{an}$ docked in the CB1 model (side view). The protein is represented as grey tube. Residues directly interact with the ligand are shown as thin line without explicit hydrogen atoms.

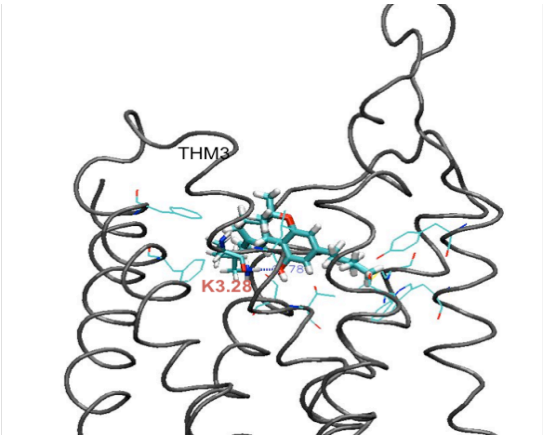


Figure S3. (R,R)-THC docked in the CB1 model (side view)A hydrogen bond between oxygen and K3.28 (192) is shown as a dash line.

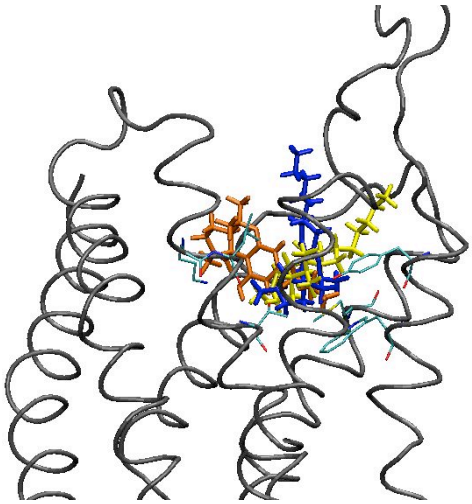
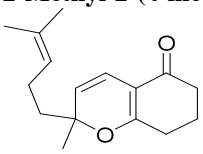


Figure S4, Docked ligands in the binding site of the CB1 model. Blue: *trans*-(R,R)-THC_{an}; yellow: *cis*-(R,S)-THC_{an}; orange: *trans*-(R,R)-THC.

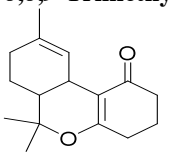
II. Experimental Procedures and Spectroscopic Data

2-Methyl-2-(4-methyl-pent-3-enyl)-2,6,7,8-tetrahydro-chromen-5-one (CBC_{an}):



To a flask containing 1,3- Cyclohexanedione (2.50g, 22.3 mmol) dissolved in THF (19 mL), was added citral (3.09g, 20.3 mmol), freshly prepared $ZnBr_2$ (20.3 mmol) in THF (20mL), and EDDA (0.63g, 3.50 mmol). Mixture was then heated using either oil bath or microwave (100 Watts) at 40 ˚C for 10 minutes. Mixture was then extracted 3x with diethyl ether and water. CBC_{an} was then purified by column chromatography using a 1:4 Ethyl Acetate: Hexane solution. (4.41g, 88%). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 6.475- 6.441 p.p.m. (d, *J* = 10.1 Hz, 1H), 5.201- 5.167 (d, *J* = 10.08 Hz, 1H), 5.086 (m, 1H), 2.425- 2.165 (m, 6H), 2.079- 1.949 (m, 4H), 1.676 (bs, 3H), 1.589 (bs, 3H), 1.365 (s, 3H). ^{13}C-NMR (400 MHz, $CDCl_3$): δ 194.76, 172.09, 132.15, 123.87, 121.85, 116.67, 110.52, 82.53, 41.91, 36.65, 28.80, 27.62, 25.86, 22.74, 20.87, 17.82. HRMS (*m/z*): $[M]^+$ calcd for $C_{16}H_{22}O_2$, 246.1620; found, 246.1701.

6,6,9-Trimethyl-3,4,6a,7,8,10a-hexahydro-2H,6H-benzo[c]chromen-1-one (THC_{an}):



CBC_{an} (1.51g) was adsorbed onto silica (3.02g) and heated to 150 ˚C by microwave, under vacuum (300 Watts), for about 60 minutes. Compound was then filtered, concentrated, and columned with 1:4 Ethyl Acetate: Hexane solution, giving 1.16g (77%) of the product. Heating CBC_{an} in the presence of EDDA decreases the rate of THC_{an} formation (**Table S1**). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 6.09 p.p.m. (m, 1H), 6.02 (m, 1H), 3.18 (bs, 1H), 2.86-2.83 (br, 1H), 2.47- 2.20 (cm, 17H), 2.13-2.10 (m, 4H), 1.94- 1.78 (cm, 15H), 1.71 (s, 1H), 1.65 (s, 11H), 1.60 (m, 2H), 1.39-1.37 (d, *J*=5.00 Hz, 12H), 1.28-1.26 (m, 4H), 1.22 (s, 6H), 1.07 (s, 6H). ^{13}C-NMR (400 MHz, $CDCl_3$): δ 198.04, 197.57, 170.94, 168.91, 133.67, 133.52, 123.84, 122.40, 114.18, 113.59, 80.84, 79.13, 45.59, 40.22, 37.65, 37.43, 32.22, 31.46, 30.17, 30.05, 29.60, 29.46, 27.21, 25.89, 25.24, 24.71, 23.68, 23.37, 20.41, 20.33, 20.00 (Ratio= 1.2:1 *trans*:*cis*). *Data is for a mixture of isomers. Isolation of isomers proved to be difficult. Due to the peak overlap, multiplicity cannot be accurately determined for individual isomers. HRMS (*m/z*): $[M]^+$ calcd for $C_{16}H_{22}O_2$, 246.1620; found, 246.1693.

Table S1. Thermal Isomerization of CBC_{an} → THC_{an}

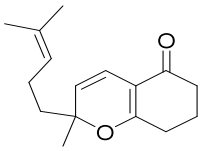
Run	Adsorbent	Time	Temperature	CBC_{an}: THC_{an}
1	silica	40 min	150 °C	0:1
2	admix mass ratio: silica(98):EDDA(8)	40 min	150 °C	1:2

III. Computational Methods

Docking. For each molecule, the Vconf package was used to search for global energy minimum for an initial conformation generated with the program Spartan.[1,2] The program Vdock was used to dock ligands to a CB1 homology model.[3-6] For each ligand-protein pair, 20 docked conformations were generated, and were scored by their computed interaction with the receptor. The potential energy of the CB1 protein is computed with the CHARMM22 force field,[7] with parameters assigned by the VMD/psfgen program.[8] The Dreiding force field was applied to the chemical compounds.[9] No detailed solvent model was used, but a distance-dependent dielectric constant (ε= 4r, where r is the distance between a pair of atoms) was employed to avoid unrealistic in vacuo Coulombic interactions.

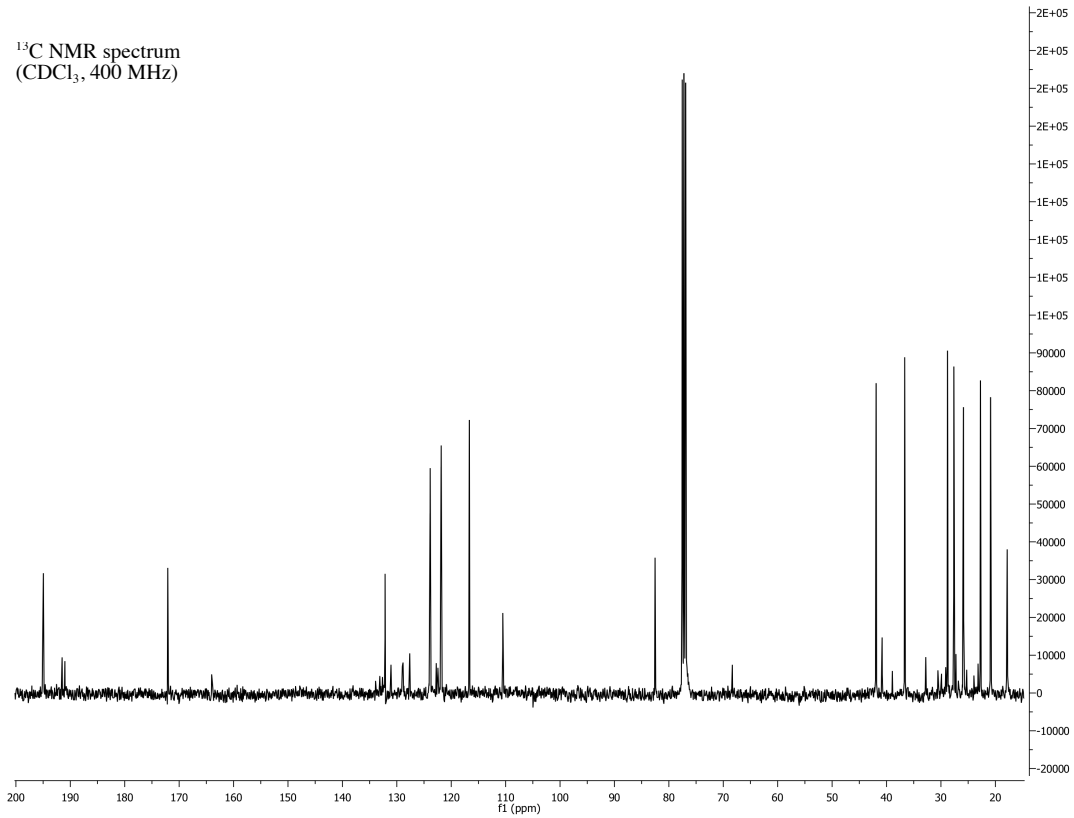
DFT. Spartan '06 molecular modeling suite[2] was used to calculate global minimum and transition state structures at the B3LYP/6-31G* level of theory. Each transition state structure was confirmed to have exactly one negative frequency.

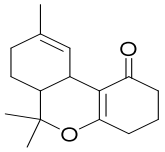
IV. ^{1}H and ^{13}C NMR Spectra of Compounds CBC_{an} and THC_{an}



^{1}H NMR Spectrum
($CDCl_3$, 300 MHz)

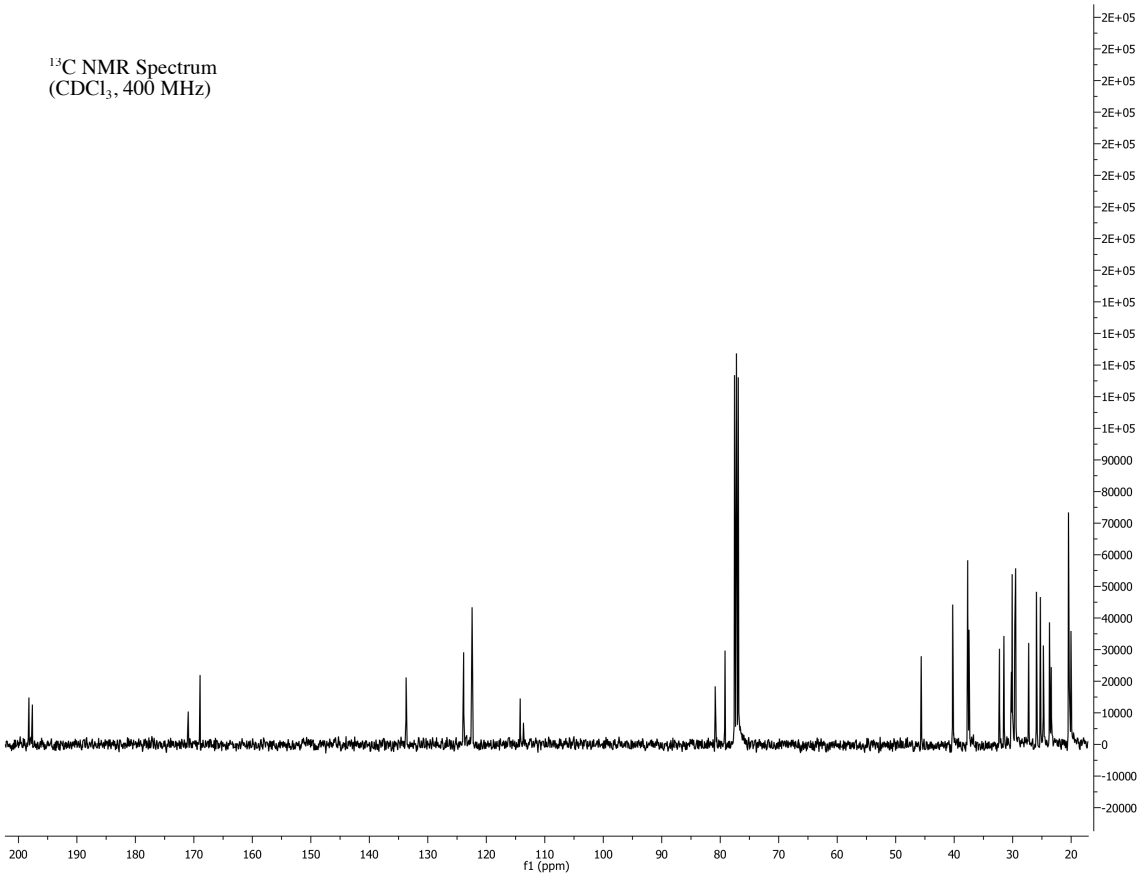
^{13}C NMR spectrum
($CDCl_3$, 400 MHz)





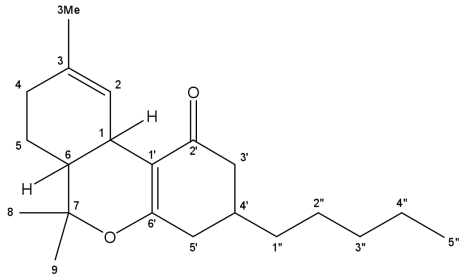
^{1}H NMR Spectrum
($CDCl_3$, 300 MHz)

^{13}C NMR Spectrum
($CDCl_3$, 400 MHz)

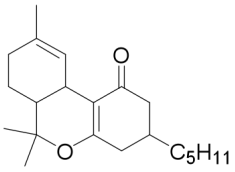


THC_{an} with C_5 alkyl chain used for NMR analysis

THC_{an} with the C_5 alkyl chain was obtained as a mixture of all stereoisomers by the same pathway as CBC_{an} to THC_{an} (with no alkyl chain). The following table gives the carbon and proton assignments for the 4 isomers produced from the reaction. The NMR spectra show groupings of four for all atoms in the structure, representing four stereoisomers. One of the key factors used in the identification of all four isomers involves the *gem*-dimethyl groups (labeled 8 and 9) and the NOESY spectrum. For the C1-C6 *cis* isomers, it was found that one of the methyl groups correlated to both protons 1 and 6, while the methyl group from the C1-C6 *trans* isomers showed correlation to only one proton, either 1 or 6. Formal designation of the chemical shifts associated with *cis* and *trans* isomers could not be assigned with absolute certainty.

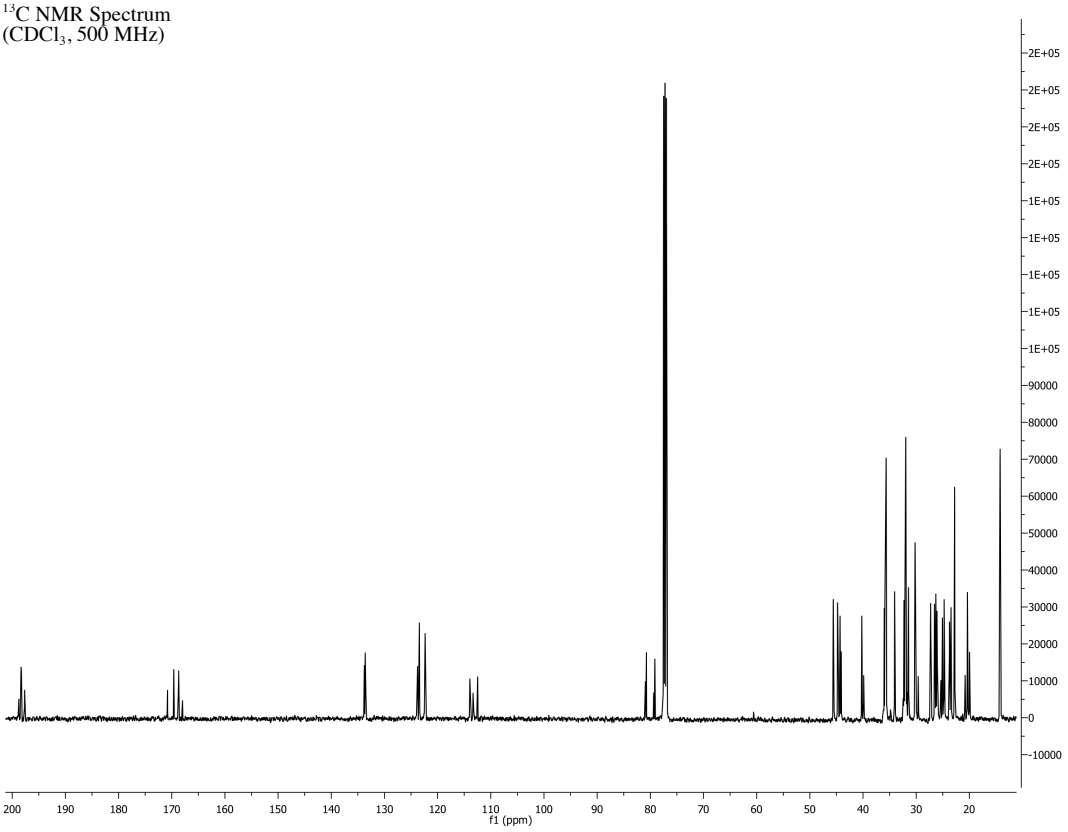


	cis I				*cis* II				*trans* I				*trans* II			
Position	^{1}H	^{13}C	NOESY	HMBC	^{1}H	^{13}C	NOESY	HMBC	^{1}H	^{13}C	NOESY	HMBC	^{1}H	^{13}C	NOESY	HMBC
1	3.14	29.97	4,5,6,9,5"	2,3,5,6,1',6'	3.15	29.79	4,5,6,8		2.81	31.90	4,5,9,5"		2.81	32.05	4,5,8	
2	6.11	122.12	1,4,3$_{Me}$	4,3$_{Me}$,6,1'	5.99	122.03	1,4,3$_{Me}$	4,3$_{Me}$,6	6.06	123.20	1,4,3$_{Me}$, 6	1,3$_{Me}$,4,6,1'	6.01	123.55	1,4,3$_{Me}$, 6	1,3$_{Me}$,4,6,1'
3		133.55				133.25				133.39				133.34		
3$_{Me}$	1.64	23.52	2,4	2,3,4	1.61	23.45	2,4	2,3,4	1.62	23.23	2,4	2,3,4	1.62	23.18	2,4	2,3,4
4	1.92	29.97	3$_{Me}$,5,6	2,3,3$_{Me}$,5,6,1'	1.91	29.39	3$_{Me}$,5,6	2,3,3$_{Me}$,5,6	2.09	31.22	3$_{Me}$,5,6	2,3,3$_{Me}$,5,6	2.10	31.24	3$_{Me}$,5,6	2,3,3$_{Me}$,5,6
5	1.23,1.80	20.08	4,6	1,3,4,6	1.31,1.84	20.57	4,6	1,4,6,7	1.33,1.79	24.53	4,6	1,3,6,7,1'	1.33,1.80	24.49	4,6	1,3,6,1'
6	1.59	39.99	1,5,8,9	1,2,5,1'	1.64	39.65	1,5,8,9	1,2,7,5,1'	1.48	45.37	5,8,9	1,2,5,7,9	1.48	45.37	5,8,9	1,2,5,7,9
7		78.92				79.13				80.50				80.70		
8	1.37	25.88	6,9	1,7,6,9	1.25	25.81	1,6,9	6,7,9	1.37	27.05	6,9	1,7,6,9	1.05	19.75	1,9	6,7,9
9	1.19	24.83	1,6,8	6,7,8	1.33	25.13	6,8	6,7,8	1.07	20.14	1,8	6,7,8	1.37	27.03	6,8	6,7,8
1'		113.71				112.99				112.25				113.10		
2'		198.03				197.44				198.11				198.51		
3'	1.92,2.44	44.09	4'	1',2',4',5'	1.92,2.44	43.87	4'	2',4',5'	2.17,2.42	44.56	4'	1',2',4',5'	2.11,2.40	44.51	4'	1',2',4',5'
4'	1.95	32.06	3',5'	2',5',1"	1.98	32.20	3',5'	5',1"	2.05	33.84	3',5'	2',3',5',6',1"	2.05	33.73	3',5'	3',5',6',1"
5'	1.90,2.36	35.79	4'	1',3',4',6'	1.92,2.36	35.90	4'	3',4',6'	2.20,2.31	35.65	4'	1',3',4',6'	2.16,2.29	35.65	4'	3',4',6'
6'		168.47				170.57				169.39				167.75		
1"	1.31	31.73	2"	3',4',5',2", 3"	1.31	31.73	2"	3',4',5',2", 3"	1.31	31.73	4'	3',4',5',2", 3"	1.31	31.73	4'	3',4',5',2", 3"
2"	1.27	26.33		1",3"	1.27	26.25		1",3"	1.27	26.08		1",3"	1.27	26.06		1",3"
3"	1.23	31.73		2",4"	1.23	31.73		2",4"	1.23	31.73		2",4"	1.23	31.73		2",4"
4"	1.27	22.53		3",5"	1.27	22.53		3",5"	1.27	22.53		3",5"	1.27	22.53		3",5"
5"	0.86	13.99	1,4"	3",4"	0.86	13.99	4"	3",4"	0.86	13.99	1,4"	3",4"	0.86	13.99	4"	3",4"

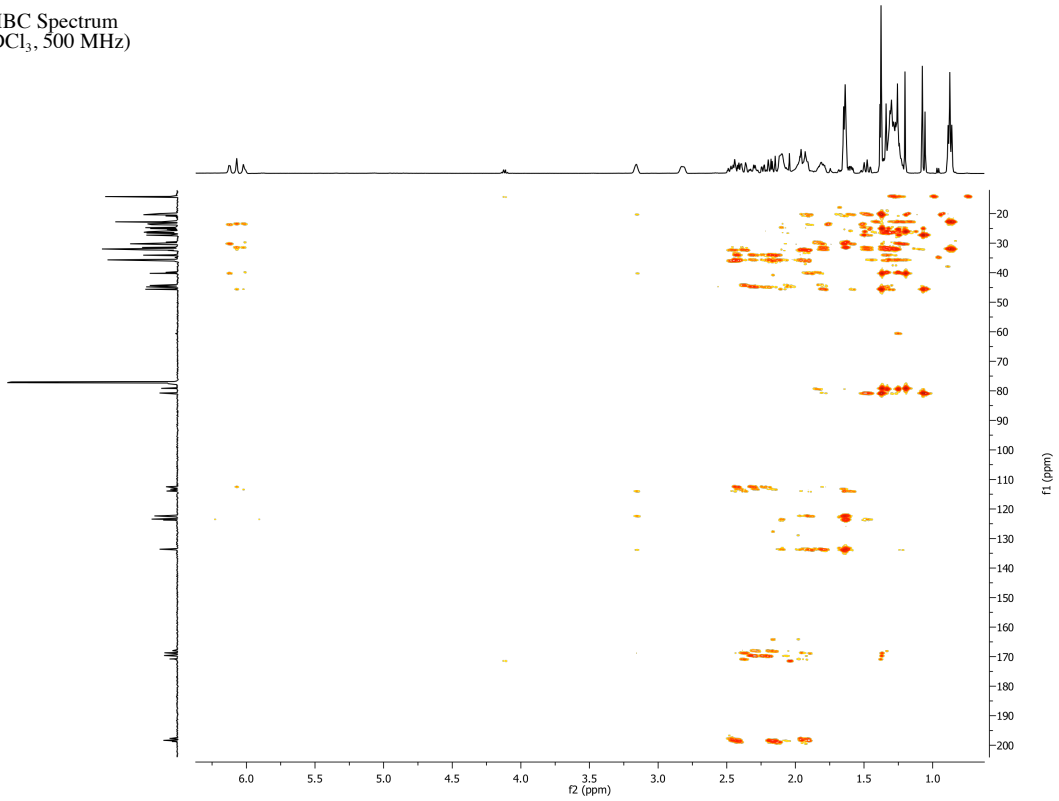


^{1}H NMR Spectrum
($CDCl_3$, 500 MHz)

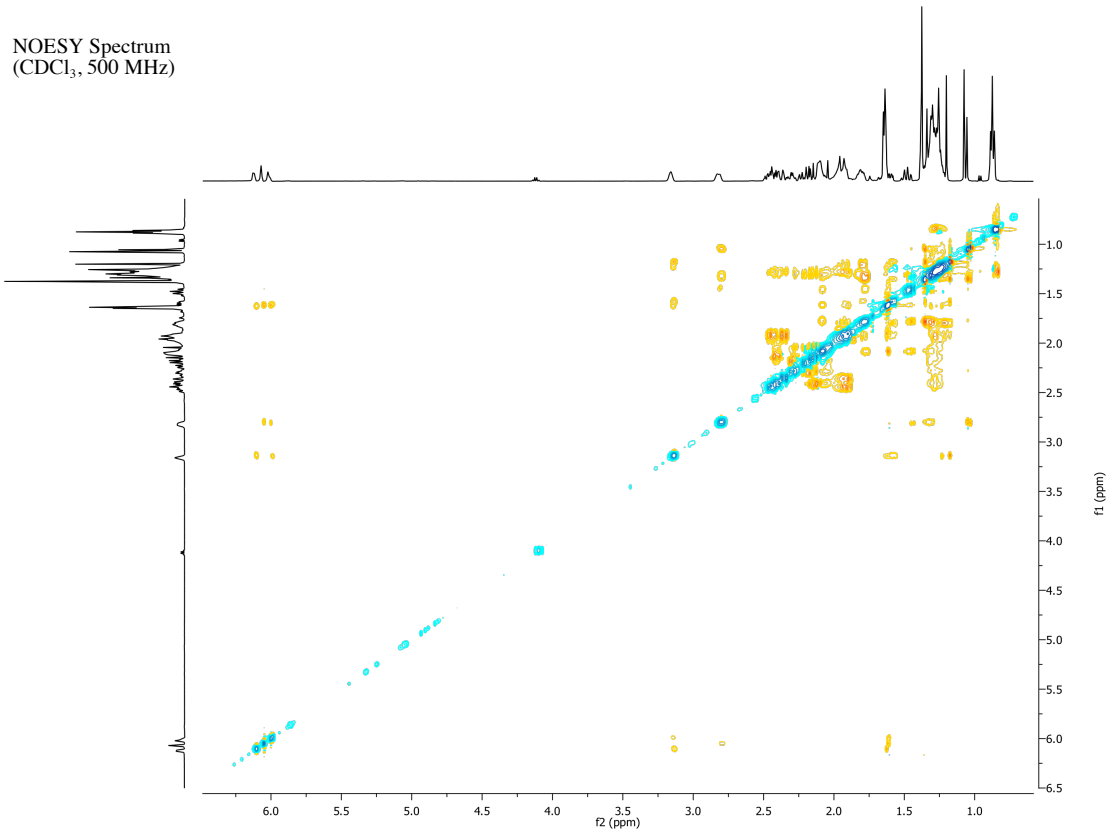
^{13}C NMR Spectrum
($CDCl_3$, 500 MHz)



HMBC Spectrum
($CDCl_3$, 500 MHz)



NOESY Spectrum
($CDCl_3$, 500 MHz)



V. Ground State and TS Coordinates (DFT B3LYP/6-31G*)

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HETATM 4 C UNK 0001 -1.282 -1.443 2.363
HETATM 5 H UNK 0001 -1.500 -0.821 3.243
HETATM 6 H UNK 0001 -1.897 -2.349 2.495
HETATM 7 C UNK 0001 -1.733 -0.707 1.094
HETATM 8 H UNK 0001 -2.830 -0.628 1.108
HETATM 9 H UNK 0001 -1.352 0.321 1.103
HETATM 10 C UNK 0001 -1.271 -1.430 -0.159
HETATM 11 H UNK 0001 -1.125 -2.503 -0.033
HETATM 12 C UNK 0001 0.803 -1.062 0.071
HETATM 13 H UNK 0001 0.986 -1.725 -0.772
HETATM 14 C UNK 0001 1.076 0.284 -0.265
HETATM 15 C UNK 0001 -1.619 -1.035 -1.449
HETATM 16 O UNK 0001 0.462 -0.290 -2.463
HETATM 17 C UNK 0001 0.902 0.604 -1.686
HETATM 18 C UNK 0001 1.446 1.344 0.624
HETATM 19 C UNK 0001 1.729 2.604 0.141
HETATM 20 H UNK 0001 2.064 3.379 0.830
HETATM 21 C UNK 0001 1.601 2.912 -1.246
HETATM 22 C UNK 0001 1.170 1.948 -2.124
HETATM 23 H UNK 0001 1.041 2.160 -3.182
HETATM 24 C UNK 0001 0.604 -2.526 3.689
HETATM 25 H UNK 0001 -0.007 -3.414 3.904
HETATM 26 H UNK 0001 0.479 -1.848 4.546

HETATM 27 H UNK 0001 1.653 -2.835 3.654
HETATM 28 C UNK 0001 -1.678 -2.044 -2.560
HETATM 29 H UNK 0001 -2.711 -2.408 -2.675
HETATM 30 H UNK 0001 -1.044 -2.912 -2.350
HETATM 31 H UNK 0001 -1.365 -1.606 -3.510
HETATM 32 C UNK 0001 -2.219 0.318 -1.691
HETATM 33 H UNK 0001 -3.233 0.371 -1.264
HETATM 34 H UNK 0001 -2.280 0.549 -2.757
HETATM 35 H UNK 0001 -1.633 1.106 -1.202
HETATM 36 C UNK 0001 1.945 4.306 -1.712
HETATM 37 H UNK 0001 3.016 4.512 -1.580
HETATM 38 H UNK 0001 1.401 5.066 -1.137
HETATM 39 H UNK 0001 1.706 4.443 -2.771
HETATM 40 O UNK 0001 1.557 1.055 1.958
HETATM 41 H UNK 0001 1.861 1.857 2.412
CONECT 1 2 4 24
CONECT 2 3 1 12
CONECT 3 2
CONECT 4 5 6 1 7
CONECT 5 4
CONECT 6 4
CONECT 7 8 9 4 10
CONECT 8 7
CONECT 9 7
CONECT 10 11 7 12 15
CONECT 11 10
CONECT 12 13 10 2 14
CONECT 13 12
CONECT 14 12 17 18
CONECT 15 10 16 28 32
CONECT 16 15 17
CONECT 17 14 16 22
CONECT 18 14 19 40
CONECT 19 20 18 21
CONECT 20 19
CONECT 21 19 22 36
CONECT 22 23 17 21
CONECT 23 22
CONECT 24 25 26 27 1
CONECT 25 24
CONECT 26 24
CONECT 27 24
CONECT 28 29 30 31 15
CONECT 29 28
CONECT 30 28
CONECT 31 28
CONECT 32 33 34 35 15
CONECT 33 32
CONECT 34 32
CONECT 35 32
CONECT 36 37 38 39 21
CONECT 37 36
CONECT 38 36
CONECT 39 36
CONECT 40 41 18
CONECT 41 40
END

TS *trans*-THC (24.1 kcal/mol)
Energy= -509175.659 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 C UNK 0001 0.874 0.658 -0.458
HETATM 2 C UNK 0001 1.558 1.701 0.241
HETATM 3 C UNK 0001 1.653 -0.501 -0.885
HETATM 4 C UNK 0001 3.073 -0.500 -0.665
HETATM 5 H UNK 0001 3.630 -1.367 -1.006
HETATM 6 C UNK 0001 3.699 0.562 -0.057
HETATM 7 C UNK 0001 2.926 1.665 0.407
HETATM 8 H UNK 0001 3.427 2.496 0.904
HETATM 9 C UNK 0001 -0.518 0.553 -0.722
HETATM 10 C UNK 0001 -1.347 -1.026 0.412
HETATM 11 H UNK 0001 -1.225 -0.482 1.348
HETATM 12 C UNK 0001 -0.517 -2.139 0.245
HETATM 13 O UNK 0001 1.041 -1.500 -1.375
HETATM 14 C UNK 0001 -2.746 -0.994 -0.182
HETATM 15 H UNK 0001 -3.338 -1.834 0.210
HETATM 16 H UNK 0001 -2.695 -1.152 -1.268
HETATM 17 C UNK 0001 -3.506 0.305 0.105
HETATM 18 H UNK 0001 -4.458 0.289 -0.445
HETATM 19 H UNK 0001 -3.797 0.336 1.168
HETATM 20 C UNK 0001 -2.777 1.589 -0.211
HETATM 21 C UNK 0001 -1.473 1.667 -0.526
HETATM 22 H UNK 0001 -1.042 2.658 -0.637
HETATM 23 H UNK 0001 -0.699 -0.105 -1.569
HETATM 24 C UNK 0001 0.568 -2.385 1.254
HETATM 25 H UNK 0001 1.361 -3.018 0.849
HETATM 26 H UNK 0001 0.151 -2.886 2.142
HETATM 27 C UNK 0001 -0.896 -3.269 -0.670
HETATM 28 H UNK 0001 -1.687 -3.880 -0.207
HETATM 29 H UNK 0001 -0.039 -3.914 -0.876
HETATM 30 H UNK 0001 -1.280 -2.902 -1.625
HETATM 31 C UNK 0001 -3.609 2.840 -0.072
HETATM 32 H UNK 0001 -4.034 2.924 0.938
HETATM 33 H UNK 0001 -4.460 2.826 -0.767
HETATM 34 H UNK 0001 -3.022 3.742 -0.270
HETATM 35 C UNK 0001 5.193 0.578 0.159
HETATM 36 H UNK 0001 5.672 -0.296 -0.293
HETATM 37 H UNK 0001 5.440 0.583 1.230
HETATM 38 H UNK 0001 5.648 1.478 -0.276
HETATM 39 H UNK 0001 1.013 -1.443 1.595
HETATM 40 O UNK 0001 0.816 2.753 0.717
HETATM 41 H UNK 0001 1.423 3.385 1.132
CONECT 1 2 3 9
CONECT 2 1 7 40

CONECT 3 1 4 13
CONECT 4 5 3 6
CONECT 5 4
CONECT 6 4 7 35
CONECT 7 8 6 2
CONECT 8 7
CONECT 9 1 10 23 21
CONECT 10 11 9 12 14
CONECT 11 10
CONECT 12 10 13 24 27
CONECT 13 12 3
CONECT 14 15 16 10 17
CONECT 15 14
CONECT 16 14
CONECT 17 18 19 14 20
CONECT 18 17
CONECT 19 17
CONECT 20 17 21 31
CONECT 21 22 20 9
CONECT 22 21
CONECT 23 9
CONECT 24 25 26 12 39
CONECT 25 24
CONECT 26 24
CONECT 27 28 29 30 12
CONECT 28 27
CONECT 29 27
CONECT 30 27
CONECT 31 32 33 34 20
CONECT 32 31
CONECT 33 31
CONECT 34 31
CONECT 35 36 37 38 6
CONECT 36 35
CONECT 37 35
CONECT 38 35
CONECT 39 24
CONECT 40 41 2
CONECT 41 40
END

CBC (-16.8 kcal/mol)
Energy= -509216.547 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 O UNK 0001 0.844 -0.324 0.872
HETATM 2 C UNK 0001 2.062 -0.170 0.281
HETATM 3 C UNK 0001 0.004 0.845 1.115
HETATM 4 C UNK 0001 0.163 1.867 0.011
HETATM 5 H UNK 0001 -0.642 2.585 -0.119
HETATM 6 C UNK 0001 1.278 1.926 -0.731
HETATM 7 H UNK 0001 1.414 2.686 -1.493
HETATM 8 C UNK 0001 2.333 0.942 -0.535
HETATM 9 C UNK 0001 3.594 1.004 -1.154
HETATM 10 C UNK 0001 4.539 -0.004 -0.967
HETATM 11 H UNK 0001 5.512 0.073 -1.452
HETATM 12 C UNK 0001 4.246 -1.112 -0.159
HETATM 13 C UNK 0001 2.999 -1.190 0.464
HETATM 14 H UNK 0001 2.738 -2.032 1.097
HETATM 15 C UNK 0001 0.421 1.449 2.468
HETATM 16 H UNK 0001 -0.202 2.317 2.711
HETATM 17 H UNK 0001 1.464 1.779 2.430
HETATM 18 H UNK 0001 0.315 0.706 3.267
HETATM 19 C UNK 0001 -1.430 0.291 1.190
HETATM 20 H UNK 0001 -2.101 1.115 1.468
HETATM 21 H UNK 0001 -1.468 -0.435 2.012
HETATM 22 C UNK 0001 -1.929 -0.372 -0.108
HETATM 23 H UNK 0001 -1.931 0.365 -0.918
HETATM 24 H UNK 0001 -1.200 -1.141 -0.394
HETATM 25 C UNK 0001 -3.281 -1.008 0.069
HETATM 26 H UNK 0001 -3.301 -1.818 0.802
HETATM 27 C UNK 0001 -4.441 -0.705 -0.535
HETATM 28 C UNK 0001 -5.702 -1.471 -0.212
HETATM 29 H UNK 0001 -6.116 -1.950 -1.111
HETATM 30 H UNK 0001 -6.487 -0.803 0.172
HETATM 31 H UNK 0001 -5.526 -2.249 0.537
HETATM 32 C UNK 0001 -4.616 0.381 -1.569
HETATM 33 H UNK 0001 -4.977 -0.040 -2.518
HETATM 34 H UNK 0001 -3.696 0.931 -1.778
HETATM 35 H UNK 0001 -5.376 1.106 -1.245
HETATM 36 C UNK 0001 5.278 -2.197 0.041
HETATM 37 H UNK 0001 4.901 -2.991 0.694
HETATM 38 H UNK 0001 6.195 -1.799 0.494
HETATM 39 H UNK 0001 5.565 -2.657 -0.913
HETATM 40 O UNK 0001 3.839 2.097 -1.943
HETATM 41 H UNK 0001 4.717 1.999 -2.342
CONECT 1 2 3
CONECT 2 1 8 13
CONECT 3 1 4 15 19
CONECT 4 5 3 6
CONECT 5 4
CONECT 6 7 4 8
CONECT 7 6
CONECT 8 6 2 9
CONECT 9 8 10 40
CONECT 10 11 9 12
CONECT 11 10
CONECT 12 10 13 36
CONECT 13 14 2 12
CONECT 14 13
CONECT 15 16 17 18 3
CONECT 16 15
CONECT 17 15
CONECT 18 15
CONECT 19 20 21 3 22
CONECT 20 19
CONECT 21 19
CONECT 22 23 24 19 25
CONECT 23 22
CONECT 24 22
CONECT 25 26 22 27
CONECT 26 25
CONECT 27 25 28 32
CONECT 28 29 30 31 27
CONECT 29 28
CONECT 30 28
CONECT 31 28
CONECT 32 33 34 35 27
CONECT 33 32
CONECT 34 32

CONECT 35 32
CONECT 36 37 38 39 12
CONECT 37 36
CONECT 38 36
CONECT 39 36
CONECT 40 41 9
CONECT 41 40
END

***cis*-THC** (-25.4 kcal/mol)
Energy= -509225.085 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 C UNK 0001 2.571 1.482 0.147
HETATM 2 C UNK 0001 1.238 1.432 0.281
HETATM 3 H UNK 0001 0.728 1.974 1.077
HETATM 4 C UNK 0001 3.174 0.602 -0.926
HETATM 5 H UNK 0001 4.265 0.561 -0.838
HETATM 6 H UNK 0001 2.958 1.014 -1.924
HETATM 7 C UNK 0001 2.581 -0.823 -0.821
HETATM 8 H UNK 0001 2.983 -1.450 -1.626
HETATM 9 H UNK 0001 2.944 -1.259 0.116
HETATM 10 C UNK 0001 1.030 -0.844 -0.858
HETATM 11 H UNK 0001 0.713 -1.190 -1.851
HETATM 12 C UNK 0001 0.426 0.584 -0.686
HETATM 13 C UNK 0001 -1.058 0.528 -0.390
HETATM 14 C UNK 0001 0.392 -1.850 0.133
HETATM 15 O UNK 0001 -1.040 -1.879 -0.101
HETATM 16 C UNK 0001 -1.709 -0.686 -0.144
HETATM 17 C UNK 0001 -1.852 1.690 -0.442
HETATM 18 C UNK 0001 -3.232 1.640 -0.260
HETATM 19 H UNK 0001 -3.798 2.566 -0.310
HETATM 20 C UNK 0001 -3.866 0.413 -0.026
HETATM 21 C UNK 0001 -3.096 -0.748 0.037
HETATM 22 H UNK 0001 -3.550 -1.716 0.224
HETATM 23 C UNK 0001 3.479 2.297 1.025
HETATM 24 H UNK 0001 4.192 1.654 1.560
HETATM 25 H UNK 0001 2.918 2.874 1.767
HETATM 26 H UNK 0001 4.080 2.999 0.431
HETATM 27 C UNK 0001 0.838 -3.282 -0.176
HETATM 28 H UNK 0001 1.904 -3.415 0.029
HETATM 29 H UNK 0001 0.649 -3.529 -1.226
HETATM 30 H UNK 0001 0.276 -3.987 0.446
HETATM 31 C UNK 0001 0.618 -1.524 1.617
HETATM 32 H UNK 0001 1.680 -1.523 1.879
HETATM 33 H UNK 0001 0.118 -2.283 2.228
HETATM 34 H UNK 0001 0.201 -0.549 1.880
HETATM 35 C UNK 0001 -5.364 0.358 0.165
HETATM 36 H UNK 0001 -5.891 0.755 -0.712
HETATM 37 H UNK 0001 -5.680 0.958 1.028
HETATM 38 H UNK 0001 -5.709 -0.668 0.326
HETATM 39 O UNK 0001 -1.305 2.921 -0.698
HETATM 40 H UNK 0001 -0.337 2.852 -0.702
HETATM 41 H UNK 0001 0.534 1.051 -1.682
CONECT 1 2 4 23
CONECT 2 3 1 12
CONECT 3 2
CONECT 4 5 6 1 7
CONECT 5 4
CONECT 6 4
CONECT 7 8 9 4 10
CONECT 8 7
CONECT 9 7
CONECT 10 11 7 12 14
CONECT 11 10
CONECT 12 10 13 41 2
CONECT 13 12 16 17
CONECT 14 10 15 27 31
CONECT 15 14 16
CONECT 16 13 15 21
CONECT 17 13 18 39
CONECT 18 19 17 20
CONECT 19 18
CONECT 20 18 21 35
CONECT 21 22 16 20
CONECT 22 21
CONECT 23 24 25 26 1
CONECT 24 23
CONECT 25 23
CONECT 26 23
CONECT 27 28 29 30 14
CONECT 28 27
CONECT 29 27
CONECT 30 27
CONECT 31 32 33 34 14
CONECT 32 31
CONECT 33 31
CONECT 34 31
CONECT 35 36 37 38 20
CONECT 36 35
CONECT 37 35
CONECT 38 35
CONECT 39 40 17
CONECT 40 39
CONECT 41 12
END

***trans*-THC** (-27.5 kcal/mol)
Energy= -509227.168 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 C UNK 0001 2.611 1.679 -0.241
HETATM 2 C UNK 0001 1.326 1.695 0.140
HETATM 3 H UNK 0001 0.800 2.642 0.195
HETATM 4 C UNK 0001 3.417 0.400 -0.321
HETATM 5 H UNK 0001 4.373 0.532 0.209
HETATM 6 H UNK 0001 3.695 0.224 -1.374
HETATM 7 C UNK 0001 2.676 -0.830 0.232
HETATM 8 H UNK 0001 3.155 -1.742 -0.141
HETATM 9 H UNK 0001 2.759 -0.851 1.327

HETATM 10 C UNK 0001 1.194 -0.766 -0.165
HETATM 11 H UNK 0001 1.150 -0.565 -1.246
HETATM 12 C UNK 0001 0.553 0.447 0.542
HETATM 13 H UNK 0001 0.686 0.318 1.630
HETATM 14 C UNK 0001 - 0.945 0.485 0.269
HETATM 15 C UNK 0001 0.364 -2.048 0.030
HETATM 16 O UNK 0001 - 0.942 -1.805 -0.564
HETATM 17 C UNK 0001 - 1.590 -0.634 -0.283
HETATM 18 C UNK 0001 - 1.772 1.574 0.606
HETATM 19 C UNK 0001 - 3.134 1.590 0.309
HETATM 20 H UNK 0001 - 3.729 2.462 0.575
HETATM 21 C UNK 0001 - 3.739 0.490 -0.312
HETATM 22 C UNK 0001 - 2.959 -0.627 -0.589
HETATM 23 H UNK 0001 - 3.389 -1.520 -1.031
HETATM 24 C UNK 0001 3.338 2.940 -0.634
HETATM 25 H UNK 0001 3.732 2.868 -1.658
HETATM 26 H UNK 0001 4.204 3.124 0.019
HETATM 27 H UNK 0001 2.684 3.816 -0.584
HETATM 28 C UNK 0001 0.908 -3.220 -0.789
HETATM 29 H UNK 0001 1.842 -3.604 -0.368
HETATM 30 H UNK 0001 1.087 -2.919 -1.827
HETATM 31 H UNK 0001 0.175 -4.033 -0.792
HETATM 32 C UNK 0001 0.169 -2.460 1.496
HETATM 33 H UNK 0001 1.133 -2.675 1.971
HETATM 34 H UNK 0001 - 0.447 -3.364 1.546
HETATM 35 H UNK 0001 - 0.331 -1.679 2.075
HETATM 36 C UNK 0001 - 5.208 0.523 -0.665
HETATM 37 H UNK 0001 - 5.390 1.147 -1.550
HETATM 38 H UNK 0001 - 5.808 0.940 0.152
HETATM 39 H UNK 0001 - 5.587 -0.480 -0.886
HETATM 40 O UNK 0001 - 1.189 2.630 1.266
HETATM 41 H UNK 0001 - 1.872 3.296 1.436
CONECT 1 2 4 24
CONECT 2 3 1 12
CONECT 3 2
CONECT 4 5 6 1 7
CONECT 5 4
CONECT 6 4
CONECT 7 8 9 4 10
CONECT 8 7
CONECT 9 7
CONECT 10 11 7 12 15
CONECT 11 10
CONECT 12 13 10 2 14
CONECT 13 12
CONECT 14 12 17 18
CONECT 15 10 16 28 32
CONECT 16 15 17
CONECT 17 14 16 22
CONECT 18 14 19 40
CONECT 19 20 18 21
CONECT 20 19
CONECT 21 19 22 36
CONECT 22 23 17 21
CONECT 23 22
CONECT 24 25 26 27 1
CONECT 25 24
CONECT 26 24
CONECT 27 24
CONECT 28 29 30 31 15
CONECT 29 28
CONECT 30 28
CONECT 31 28
CONECT 32 33 34 35 15
CONECT 33 32
CONECT 34 32
CONECT 35 32
CONECT 36 37 38 39 21
CONECT 37 36
CONECT 38 36
CONECT 39 36
CONECT 40 41 18
CONECT 41 40
END

1$_{an}$ (set to 0 kcal/mol)

Energy= -509971.466 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 C UNK 0001 3.006 -0.005 1.455
HETATM 2 C UNK 0001 4.272 -0.846 1.349
HETATM 3 H UNK 0001 4.492 -1.233 2.358
HETATM 4 H UNK 0001 5.093 -0.169 1.091
HETATM 5 C UNK 0001 1.687 -0.667 1.195
HETATM 6 C UNK 0001 1.631 -2.105 0.821
HETATM 7 C UNK 0001 4.155 -2.026 0.377
HETATM 8 H UNK 0001 3.969 -1.624 -0.631
HETATM 9 C UNK 0001 2.946 -2.877 0.783
HETATM 10 H UNK 0001 3.119 -3.286 1.793
HETATM 11 H UNK 0001 2.799 -3.735 0.119
HETATM 12 O UNK 0001 3.085 1.181 1.755
HETATM 13 O UNK 0001 0.584 -2.690 0.559
HETATM 14 C UNK 0001 0.581 0.137 1.325
HETATM 15 H UNK 0001 0.825 1.159 1.607
HETATM 16 C UNK 0001 - 0.799 -0.201 1.138
HETATM 17 H UNK 0001 - 1.014 -1.227 0.867
HETATM 18 C UNK 0001 - 1.834 0.676 1.264
HETATM 19 C UNK 0001 - 3.245 0.190 1.032
HETATM 20 H UNK 0001 - 3.836 0.368 1.944
HETATM 21 H UNK 0001 - 3.235 -0.893 0.867
HETATM 22 C UNK 0001 - 3.982 0.876 -0.151
HETATM 23 H UNK 0001 - 4.099 1.945 0.053
HETATM 24 H UNK 0001 - 5.001 0.460 -0.173
HETATM 25 C UNK 0001 - 3.312 0.634 -1.478

HETATM 26 H UNK 0001 -3.076 -0.413 -1.674
HETATM 27 C UNK 0001 -2.984 1.524 -2.427
HETATM 28 C UNK 0001 -2.316 1.074 -3.705
HETATM 29 H UNK 0001 -1.344 1.569 -3.839
HETATM 30 H UNK 0001 -2.922 1.338 -4.584
HETATM 31 H UNK 0001 -2.149 -0.008 -3.720
HETATM 32 C UNK 0001 -3.236 3.010 -2.348
HETATM 33 H UNK 0001 -2.297 3.571 -2.454
HETATM 34 H UNK 0001 -3.711 3.322 -1.414
HETATM 35 H UNK 0001 -3.884 3.336 -3.174
HETATM 36 C UNK 0001 -1.695 2.132 1.618
HETATM 37 H UNK 0001 -0.703 2.400 1.984
HETATM 38 H UNK 0001 -2.428 2.410 2.386
HETATM 39 H UNK 0001 -1.906 2.760 0.742
HETATM 40 C UNK 0001 5.442 -2.856 0.329
HETATM 41 H UNK 0001 5.675 -3.276 1.316
HETATM 42 H UNK 0001 6.297 -2.245 0.017
HETATM 43 H UNK 0001 5.349 -3.690 -0.375
CONECT 1 2 5 12
CONECT 2 3 4 1 7
CONECT 3 2
CONECT 4 2
CONECT 5 1 6 14
CONECT 6 5 9 13
CONECT 7 8 2 9 40
CONECT 8 7
CONECT 9 10 11 6 7
CONECT 10 9
CONECT 11 9
CONECT 12 1
CONECT 13 6
CONECT 14 15 5 16
CONECT 15 14
CONECT 16 17 14 18
CONECT 17 16
CONECT 18 16 19 36
CONECT 19 20 21 18 22
CONECT 20 19
CONECT 21 19
CONECT 22 23 24 19 25
CONECT 23 22
CONECT 24 22
CONECT 25 26 22 27
CONECT 26 25
CONECT 27 25 28 32
CONECT 28 29 30 31 27
CONECT 29 28
CONECT 30 28
CONECT 31 28
CONECT 32 33 34 35 27
CONECT 33 32
CONECT 34 32
CONECT 35 32
CONECT 36 37 38 39 18
CONECT 37 36
CONECT 38 36
CONECT 39 36
CONECT 40 41 42 43 7
CONECT 41 40
CONECT 42 40
CONECT 43 40
END

TS CBC$_{an}$ (17.8 kcal/mol)
Energy= -509953.660 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 O UNK 0001 -0.145 -1.172 0.724
HETATM 2 C UNK 0001 1.043 -1.297 1.120
HETATM 3 C UNK 0001 -0.984 0.722 1.286
HETATM 4 C UNK 0001 0.183 1.508 1.253
HETATM 5 H UNK 0001 0.154 2.449 0.704
HETATM 6 C UNK 0001 1.408 1.064 1.730
HETATM 7 H UNK 0001 2.218 1.779 1.865
HETATM 8 C UNK 0001 1.780 -0.294 1.845
HETATM 9 C UNK 0001 3.131 -0.578 2.368
HETATM 10 C UNK 0001 3.684 -1.985 2.169
HETATM 11 H UNK 0001 3.306 -2.627 2.982
HETATM 12 H UNK 0001 4.771 -1.932 2.282
HETATM 13 C UNK 0001 3.265 -2.580 0.817
HETATM 14 H UNK 0001 3.635 -1.910 0.026
HETATM 15 C UNK 0001 1.735 -2.603 0.741
HETATM 16 H UNK 0001 1.375 -2.881 -0.256
HETATM 17 H UNK 0001 1.349 -3.374 1.428
HETATM 18 O UNK 0001 3.790 0.277 2.955
HETATM 19 C UNK 0001 -1.435 0.072 2.566
HETATM 20 H UNK 0001 -2.144 0.758 3.055
HETATM 21 H UNK 0001 -0.606 -0.100 3.255
HETATM 22 H UNK 0001 -1.959 -0.869 2.374
HETATM 23 C UNK 0001 -2.075 0.975 0.271
HETATM 24 H UNK 0001 -2.519 1.957 0.499
HETATM 25 H UNK 0001 -2.877 0.241 0.413
HETATM 26 C UNK 0001 -1.609 0.956 -1.201
HETATM 27 H UNK 0001 -0.829 1.709 -1.350
HETATM 28 H UNK 0001 -1.135 -0.018 -1.381
HETATM 29 C UNK 0001 -2.755 1.151 -2.157
HETATM 30 H UNK 0001 -3.506 0.359 -2.123
HETATM 31 C UNK 0001 -2.964 2.156 -3.021
HETATM 32 C UNK 0001 -4.186 2.169 -3.910
HETATM 33 H UNK 0001 -3.901 2.180 -4.972
HETATM 34 H UNK 0001 -4.789 3.073 -3.743
HETATM 35 H UNK 0001 -4.827 1.298 -3.741
HETATM 36 C UNK 0001 -2.046 3.340 -3.209
HETATM 37 H UNK 0001 -1.688 3.391 -4.247
HETATM 38 H UNK 0001 -1.171 3.319 -2.555

HETATM 39 H UNK 0001 -
2.584 4.279 -3.021
HETATM 40 C UNK 0001 3.861
-3.972 0.584
HETATM 41 H UNK 0001
3.560 -4.374 -0.391
HETATM 42 H UNK 0001
3.528 -4.678 1.356
HETATM 43 H UNK 0001
4.957 -3.941 0.611
CONECT 1 2 3
CONECT 2 1 8 15
CONECT 3 1 4 19 23
CONECT 4 5 3 6
CONECT 5 4
CONECT 6 7 4 8
CONECT 7 6
CONECT 8 6 2 9
CONECT 9 8 10 18
CONECT 10 11 12 9 13
CONECT 11 10
CONECT 12 10
CONECT 13 14 10 15 40
CONECT 14 13
CONECT 15 16 17 2 13
CONECT 16 15
CONECT 17 15
CONECT 18 9
CONECT 19 20 21 22 3
CONECT 20 19
CONECT 21 19
CONECT 22 19
CONECT 23 24 25 3 26
CONECT 24 23
CONECT 25 23
CONECT 26 27 28 23 29
CONECT 27 26
CONECT 28 26
CONECT 29 30 26 31
CONECT 30 29
CONECT 31 29 32 36
CONECT 32 33 34 35 31
CONECT 33 32
CONECT 34 32
CONECT 35 32
CONECT 36 37 38 39 31
CONECT 37 36
CONECT 38 36
CONECT 39 36
CONECT 40 41 42 43 13
CONECT 41 40
CONECT 42 40
CONECT 43 40
END

TS *cis*-THC$_{an}$ (29.3 kcal/mol)
Energy= -509942.187 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 C UNK 0001 -1.290
-2.123 0.129
HETATM 2 C UNK 0001 -0.622
-3.476 0.383
HETATM 3 H UNK 0001 -1.399
-4.172 0.718
HETATM 4 H UNK 0001 -0.262
-3.860 -0.586
HETATM 5 C UNK 0001 -0.488
-0.931 0.380
HETATM 6 C UNK 0001 0.925
-0.999 0.605
HETATM 7 C UNK 0001 1.562
-2.355 0.895
HETATM 8 H UNK 0001 2.364
-2.201 1.627
HETATM 9 H UNK 0001 2.053
-2.706 -0.026
HETATM 10 C UNK 0001 0.550
-3.405 1.374
HETATM 11 H UNK 0001
0.149 -3.067 2.341
HETATM 12 O UNK 0001 -
2.453 -2.071 -0.284
HETATM 13 C UNK 0001 -
1.095 0.357 0.194
HETATM 14 H UNK 0001 -
2.168 0.240 0.028
HETATM 15 C UNK 0001 -
0.818 1.073 -1.536
HETATM 16 H UNK 0001 -
1.317 0.263 -2.070
HETATM 17 C UNK 0001 0.574
1.092 -1.766
HETATM 18 O UNK 0001
1.640 0.019 0.484
HETATM 19 C UNK 0001 1.432
2.279 -1.478
HETATM 20 H UNK 0001
1.076 3.166 -2.021
HETATM 21 H UNK 0001
2.475 2.097 -1.747
HETATM 22 H UNK 0001
1.389 2.509 -0.406
HETATM 23 C UNK 0001 1.168
-0.118 -2.409
HETATM 24 H UNK 0001
0.716 -1.025 -1.981
HETATM 25 H UNK 0001
2.253 -0.165 -2.297
HETATM 26 H UNK 0001
0.922 -0.133 -3.482
HETATM 27 C UNK 0001 1.206
-4.774 1.584
HETATM 28 H UNK 0001
1.618 -5.162 0.643
HETATM 29 H UNK 0001
0.481 -5.508 1.957
HETATM 30 H UNK 0001
2.028 -4.713 2.307
HETATM 31 C UNK 0001 -
0.742 1.460 1.133
HETATM 32 H UNK 0001 -
0.310 1.135 2.076
HETATM 33 C UNK 0001 -
0.933 2.775 0.939
HETATM 34 C UNK 0001 -
1.395 3.353 -0.375
HETATM 35 H UNK 0001 -
2.298 3.960 -0.212
HETATM 36 H UNK 0001 -
0.634 4.075 -0.707
HETATM 37 C UNK 0001 -
1.692 2.333 -1.489
HETATM 38 H UNK 0001 -
1.642 2.839 -2.462
HETATM 39 H UNK 0001 -
2.727 1.986 -1.385
HETATM 40 C UNK 0001 -
0.630 3.782 2.020
HETATM 41 H UNK 0001 -
0.252 3.300 2.927
HETATM 42 H UNK 0001 -
1.530 4.353 2.288
HETATM 43 H UNK 0001
0.117 4.517 1.688
CONECT 1 2 5 12
CONECT 2 3 4 1 10
CONECT 3 2
CONECT 4 2
CONECT 5 1 6 13
CONECT 6 5 7 18
CONECT 7 8 9 6 10
CONECT 8 7
CONECT 9 7
CONECT 10 11 7 2 27
CONECT 11 10
CONECT 12 1
CONECT 13 14 5 15 31
CONECT 14 13
CONECT 15 16 13 17 37
CONECT 16 15

CONECT 17 15 18 19 23
CONECT 18 17 6
CONECT 19 20 21 22 17
CONECT 20 19
CONECT 21 19
CONECT 22 19
CONECT 23 24 25 26 17
CONECT 24 23
CONECT 25 23
CONECT 26 23
CONECT 27 28 29 30 10
CONECT 28 27
CONECT 29 27
CONECT 30 27
CONECT 31 32 13 33
CONECT 32 31
CONECT 33 31 34 40
CONECT 34 35 36 33 37
CONECT 35 34
CONECT 36 34
CONECT 37 38 39 34 15
CONECT 38 37
CONECT 39 37
CONECT 40 41 42 43 33
CONECT 41 40
CONECT 42 40
CONECT 43 40
END

TS *trans*-THC$_{an}$ (26.9 kcal/mol)
Energy= -509944.552 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 C UNK 0001 0.683 0.542 -0.321
HETATM 2 C UNK 0001 1.262 1.661 0.425
HETATM 3 C UNK 0001 1.489 -0.582 -0.694
HETATM 4 C UNK 0001 3.002 -0.532 -0.542
HETATM 5 H UNK 0001 3.278 -1.064 0.382
HETATM 6 H UNK 0001 3.439 -1.109 -1.366
HETATM 7 C UNK 0001 3.546 0.901 -0.495
HETATM 8 C UNK 0001 2.786 1.681 0.585
HETATM 9 H UNK 0001 3.091 2.732 0.626
HETATM 10 H UNK 0001 3.018 1.254 1.574
HETATM 11 C UNK 0001 - 0.715 0.406 -0.616
HETATM 12 C UNK 0001 - 1.597 -0.968 0.494
HETATM 13 H UNK 0001 - 1.543 -0.389 1.417
HETATM 14 C UNK 0001 - 0.798 -2.124 0.486
HETATM 15 O UNK 0001 0.945 -1.642 -1.091
HETATM 16 O UNK 0001 0.596 2.567 0.930
HETATM 17 C UNK 0001 - 2.975 -0.993 -0.162
HETATM 18 H UNK 0001 - 3.576 -1.812 0.258
HETATM 19 H UNK 0001 - 2.869 -1.215 -1.231
HETATM 20 C UNK 0001 - 3.741 0.322 0.013
HETATM 21 H UNK 0001 - 4.639 0.301 -0.621
HETATM 22 H UNK 0001 - 4.123 0.395 1.045
HETATM 23 C UNK 0001 - 2.948 1.571 -0.283
HETATM 24 C UNK 0001 - 1.624 1.578 -0.509
HETATM 25 H UNK 0001 - 1.127 2.540 -0.600
HETATM 26 H UNK 0001 - 0.862 -0.218 -1.498
HETATM 27 C UNK 0001 0.223 -2.284 1.571
HETATM 28 H UNK 0001 0.970 -3.044 1.330
HETATM 29 H UNK 0001 - 0.269 -2.567 2.513
HETATM 30 C UNK 0001 - 1.129 -3.304 -0.376
HETATM 31 H UNK 0001 - 1.972 -3.859 0.066
HETATM 32 H UNK 0001 - 0.280 -3.983 -0.467
HETATM 33 H UNK 0001 - 1.432 -2.997 -1.380
HETATM 34 C UNK 0001 - 3.733 2.857 -0.230
HETATM 35 H UNK 0001 - 4.214 2.987 0.750
HETATM 36 H UNK 0001 - 4.540 2.858 -0.976
HETATM 37 H UNK 0001 - 3.097 3.728 -0.413
HETATM 38 H UNK 0001 3.332 1.374 -1.465
HETATM 39 C UNK 0001 5.061 0.934 -0.269
HETATM 40 H UNK 0001 5.593 0.393 -1.060
HETATM 41 H UNK 0001 5.323 0.468 0.690
HETATM 42 H UNK 0001 5.437 1.964 -0.253
HETATM 43 H UNK 0001 0.728 -1.327 1.761
CONECT 1 2 3 11
CONECT 2 1 8 16
CONECT 3 1 4 15
CONECT 4 5 6 3 7
CONECT 5 4
CONECT 6 4
CONECT 7 4 8 38 39
CONECT 8 9 10 7 2
CONECT 9 8
CONECT 10 8
CONECT 11 1 12 26 24
CONECT 12 13 11 14 17
CONECT 13 12
CONECT 14 12 15 27 30
CONECT 15 14 3
CONECT 16 2
CONECT 17 18 19 12 20
CONECT 18 17
CONECT 19 17
CONECT 20 21 22 17 23
CONECT 21 20
CONECT 22 20
CONECT 23 20 24 34
CONECT 24 25 23 11
CONECT 25 24
CONECT 26 11
CONECT 27 28 29 14 43
CONECT 28 27
CONECT 29 27
CONECT 30 31 32 33 14
CONECT 31 30
CONECT 32 30
CONECT 33 30
CONECT 34 35 36 37 23
CONECT 35 34
CONECT 36 34
CONECT 37 34
CONECT 38 7
CONECT 39 40 41 42 7
CONECT 40 39
CONECT 41 39
CONECT 42 39

CONECT 43 27
END

CBC$_{an}$ (-3.4 kcal/mol)
Energy= -509974.861 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 O UNK 0001 -0.690 -1.054 -0.508
HETATM 2 C UNK 0001 -1.734 -0.258 -0.791
HETATM 3 C UNK 0001 0.578 -0.970 -1.266
HETATM 4 C UNK 0001 0.720 0.370 -1.953
HETATM 5 H UNK 0001 1.711 0.618 -2.324
HETATM 6 C UNK 0001 -0.326 1.184 -2.138
HETATM 7 H UNK 0001 -0.241 2.129 -2.666
HETATM 8 C UNK 0001 -1.637 0.834 -1.603
HETATM 9 C UNK 0001 -2.810 1.672 -1.878
HETATM 10 C UNK 0001 - 4.141 1.213 -1.284
HETATM 11 H UNK 0001 - 4.619 0.536 -2.010
HETATM 12 H UNK 0001 - 4.788 2.092 -1.200
HETATM 13 C UNK 0001 - 3.983 0.488 0.061
HETATM 14 H UNK 0001 - 3.540 1.199 0.773
HETATM 15 C UNK 0001 - 2.995 -0.679 -0.093
HETATM 16 H UNK 0001 - 2.728 -1.111 0.879
HETATM 17 H UNK 0001 - 3.462 -1.494 -0.671
HETATM 18 O UNK 0001 - 2.738 2.683 -2.570
HETATM 19 C UNK 0001 0.539 -2.110 -2.294
HETATM 20 H UNK 0001 1.470 -2.131 -2.871
HETATM 21 H UNK 0001 - 0.291 -1.960 -2.992
HETATM 22 H UNK 0001 0.414 -3.077 -1.795
HETATM 23 C UNK 0001 1.684 -1.209 -0.221
HETATM 24 H UNK 0001 2.644 -1.250 -0.752
HETATM 25 H UNK 0001 1.529 -2.200 0.224
HETATM 26 C UNK 0001 1.754 -0.144 0.889
HETATM 27 H UNK 0001 1.910 0.841 0.438
HETATM 28 H UNK 0001 0.773 -0.103 1.382
HETATM 29 C UNK 0001 2.811 -0.460 1.914
HETATM 30 H UNK 0001 2.636 -1.383 2.471
HETATM 31 C UNK 0001 3.921 0.234 2.212
HETATM 32 C UNK 0001 4.868 -0.249 3.286
HETATM 33 H UNK 0001 4.973 0.498 4.085
HETATM 34 H UNK 0001 5.877 -0.413 2.881
HETATM 35 H UNK 0001 4.529 -1.185 3.741
HETATM 36 C UNK 0001 4.337 1.525 1.551
HETATM 37 H UNK 0001 4.393 2.339 2.288
HETATM 38 H UNK 0001 3.660 1.843 0.755
HETATM 39 H UNK 0001 5.343 1.432 1.118
HETATM 40 C UNK 0001 - 5.327 0.017 0.625
HETATM 41 H UNK 0001 - 5.200 -0.488 1.590
HETATM 42 H UNK 0001 - 5.818 -0.686 -0.060
HETATM 43 H UNK 0001 - 6.007 0.863 0.778
CONECT 1 2 3
CONECT 2 1 8 15
CONECT 3 1 4 19 23
CONECT 4 5 3 6
CONECT 5 4
CONECT 6 7 4 8
CONECT 7 6
CONECT 8 6 2 9
CONECT 9 8 10 18
CONECT 10 11 12 9 13
CONECT 11 10
CONECT 12 10
CONECT 13 14 10 15 40
CONECT 14 13
CONECT 15 16 17 2 13
CONECT 16 15
CONECT 17 15
CONECT 18 9
CONECT 19 20 21 22 3
CONECT 20 19
CONECT 21 19
CONECT 22 19
CONECT 23 24 25 3 26
CONECT 24 23
CONECT 25 23
CONECT 26 27 28 23 29
CONECT 27 26
CONECT 28 26
CONECT 29 30 26 31
CONECT 30 29
CONECT 31 29 32 36
CONECT 32 33 34 35 31
CONECT 33 32
CONECT 34 32
CONECT 35 32
CONECT 36 37 38 39 31
CONECT 37 36
CONECT 38 36
CONECT 39 36
CONECT 40 41 42 43 13
CONECT 41 40
CONECT 42 40
CONECT 43 40
END

***cis*-THC$_{an}$** (-16.8 kcal/mol)
Energy= -509988.300 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 C UNK 0001 -2.537 -1.884 0.033
HETATM 2 C UNK 0001 -1.559 -1.615 -0.840
HETATM 3 H UNK 0001 -1.209 -2.389 -1.516
HETATM 4 C UNK 0001 -3.031 -0.846 1.011
HETATM 5 H UNK 0001 -3.193 -1.309 1.995
HETATM 6 H UNK 0001 -4.024 -0.483 0.695
HETATM 7 C UNK 0001 -2.063 0.334 1.151
HETATM 8 H UNK 0001 -2.546 1.132 1.723
HETATM 9 H UNK 0001 -1.184 0.017 1.726

HETATM 10 C UNK 0001 -1.616 0.851 -0.230
HETATM 11 H UNK 0001 -2.521 1.117 -0.794
HETATM 12 C UNK 0001 -0.879 -0.267 -1.014
HETATM 13 C UNK 0001 0.602 -0.301 -0.643
HETATM 14 C UNK 0001 -0.743 2.125 -0.159
HETATM 15 O UNK 0001 0.521 1.800 0.507
HETATM 16 C UNK 0001 1.166 0.681 0.113
HETATM 17 C UNK 0001 1.472 -1.338 -1.215
HETATM 18 C UNK 0001 3.194 -0.738 0.584
HETATM 19 C UNK 0001 -3.209 -3.233 0.086
HETATM 20 H UNK 0001 -3.076 -3.706 1.070
HETATM 21 H UNK 0001 -2.812 -3.913 -0.674
HETATM 22 H UNK 0001 -4.294 -3.144 -0.070
HETATM 23 C UNK 0001 -0.415 2.676 -1.555
HETATM 24 H UNK 0001 -1.335 2.981 -2.066
HETATM 25 H UNK 0001 0.092 1.936 -2.179
HETATM 26 H UNK 0001 0.235 3.553 -1.469
HETATM 27 C UNK 0001 -1.342 3.239 0.702
HETATM 28 H UNK 0001 -2.344 3.501 0.344
HETATM 29 H UNK 0001 -0.713 4.133 0.648
HETATM 30 H UNK 0001 -1.412 2.943 1.751
HETATM 31 O UNK 0001 1.070 -2.139 -2.056
HETATM 32 H UNK 0001 -0.942 -0.042 -2.090
HETATM 33 C UNK 0001 2.943 -1.356 -0.795
HETATM 34 H UNK 0001 3.287 -2.394 -0.853
HETATM 35 H UNK 0001 3.511 -0.797 -1.557
HETATM 36 C UNK 0001 2.587 0.668 0.606
HETATM 37 H UNK 0001 2.600 1.098 1.616
HETATM 38 H UNK 0001 3.187 1.348 -0.020
HETATM 39 H UNK 0001 2.657 -1.344 1.329
HETATM 40 C UNK 0001 4.680 -0.726 0.956
HETATM 41 H UNK 0001 5.091 -1.742 0.968
HETATM 42 H UNK 0001 4.838 -0.289 1.949
HETATM 43 H UNK 0001 5.263 -0.138 0.235
CONECT 1 2 4 19
CONECT 2 3 1 12
CONECT 3 2
CONECT 4 5 6 1 7
CONECT 5 4
CONECT 6 4
CONECT 7 8 9 4 10
CONECT 8 7
CONECT 9 7
CONECT 10 11 7 12 14
CONECT 11 10
CONECT 12 10 13 32 2
CONECT 13 12 16 17
CONECT 14 10 15 23 27
CONECT 15 14 16
CONECT 16 13 15 36
CONECT 17 13 31 33
CONECT 18 33 39 36 40
CONECT 19 20 21 22 1
CONECT 20 19
CONECT 21 19
CONECT 22 19
CONECT 23 24 25 26 14
CONECT 24 23
CONECT 25 23
CONECT 26 23
CONECT 27 28 29 30 14
CONECT 28 27
CONECT 29 27
CONECT 30 27
CONECT 31 17
CONECT 32 12
CONECT 33 34 35 18 17
CONECT 34 33
CONECT 35 33
CONECT 36 37 38 16 18
CONECT 37 36
CONECT 38 36
CONECT 39 18
CONECT 40 41 42 43 18
CONECT 41 40
CONECT 42 40
CONECT 43 40
END

***trans*-THC$_{an}$** (-15.8 kcal/mol)
Energy= -509987.258 kcal/mol

HEADER
REMARK Spartan `06 exported M001
HETATM 1 C UNK 0001 2.824 1.728 -0.108
HETATM 2 C UNK 0001 1.542 1.730 0.282
HETATM 3 H UNK 0001 1.024 2.670 0.433
HETATM 4 C UNK 0001 3.616 0.451 -0.294
HETATM 5 H UNK 0001 4.585 0.540 0.219
HETATM 6 H UNK 0001 3.865 0.337 -1.362
HETATM 7 C UNK 0001 2.877 -0.803 0.204
HETATM 8 H UNK 0001 3.348 -1.698 -0.218
HETATM 9 H UNK 0001 2.972 -0.877 1.295
HETATM 10 C UNK 0001 1.390 -0.714 -0.171
HETATM 11 H UNK 0001 1.334 -0.465 -1.241
HETATM 12 C UNK 0001 0.755 0.466 0.594
HETATM 13 H UNK 0001 0.860 0.283 1.677
HETATM 14 C UNK 0001 -0.733 0.538 0.277
HETATM 15 C UNK 0001 0.572 -2.007 -0.012
HETATM 16 O UNK 0001 -0.788 -1.738 -0.500
HETATM 17 C UNK 0001 -1.369 -0.545 -0.254
HETATM 18 C UNK 0001 -1.529 1.720 0.642
HETATM 19 C UNK 0001 -3.669 0.418 0.156
HETATM 20 C UNK 0001 3.569 3.008 -0.393
HETATM 21 H UNK 0001 3.974 3.013 -1.416
HETATM 22 H UNK 0001 4.429 3.128 0.282

```
HETATM   23  H   UNK  0001
2.924   3.885  -0.279
HETATM   24  C   UNK  0001      1.061
-3.125  -0.934
HETATM   25  H   UNK  0001
2.021  -3.524  -0.592
HETATM   26  H   UNK  0001
1.178  -2.761  -1.960
HETATM   27  H   UNK  0001
0.334  -3.943  -0.941
HETATM   28  C   UNK  0001      0.448
-2.508   1.432
HETATM   29  H   UNK  0001
1.434  -2.765   1.836
HETATM   30  H   UNK  0001     -
0.177  -3.406   1.461
HETATM   31  H   UNK  0001     -
0.004  -1.756   2.085
HETATM   32  C   UNK  0001     -
5.110   0.492  -0.358
HETATM   33  H   UNK  0001     -
5.143   0.849  -1.396
HETATM   34  H   UNK  0001     -
5.708   1.179   0.251
HETATM   35  H   UNK  0001     -
5.594  -0.492  -0.328
HETATM   36  O   UNK  0001     -
1.068   2.641   1.313
HETATM   37  C   UNK  0001     -
2.975   1.784   0.154
HETATM   38  H   UNK  0001     -
3.501   2.512   0.779
HETATM   39  H   UNK  0001     -
2.966   2.186  -0.872
HETATM   40  H   UNK  0001     -
3.694   0.056   1.195
HETATM   41  C   UNK  0001     -
2.822  -0.569  -0.657
HETATM   42  H   UNK  0001     -
2.895  -0.324  -1.729
HETATM   43  H   UNK  0001     -
3.193  -1.594  -0.549
CONECT    1    2    4   20
CONECT    2    3    1   12
CONECT    3    2
CONECT    4    5    6    1    7
CONECT    5    4
CONECT    6    4
CONECT    7    8    9    4   10
CONECT    8    7
CONECT    9    7
CONECT   10   11    7   12   15
CONECT   11   10
CONECT   12   13   10    2   14
CONECT   13   12
CONECT   14   12   17   18
CONECT   15   10   16   24   28
CONECT   16   15   17
CONECT   17   14   16   41
CONECT   18   14   36   37
CONECT   19   32   37   40   41
CONECT   20   21   22   23    1
CONECT   21   20
CONECT   22   20
CONECT   23   20
CONECT   24   25   26   27   15
CONECT   25   24
CONECT   26   24
CONECT   27   24
CONECT   28   29   30   31   15
CONECT   29   28
CONECT   30   28
CONECT   31   28
CONECT   32   33   34   35   19
CONECT   33   32
CONECT   34   32
CONECT   35   32
CONECT   36   18
CONECT   37   38   39   19   18
CONECT   38   37
CONECT   39   37
CONECT   40   19
CONECT   41   42   43   17   19
CONECT   42   41
CONECT   43   41
END
```

References

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