Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information (SI)

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General Experimental Procedures

Optical rotation data was obtained using a Jasco P-2000 spectrophotometer. IR spectra were obtained by ATR FT-IR spectrometer Perkin Elmer SPECTRUM 2000 and UV spectra were obtained by Perkin Elmer Lambda-35 UV/vis spectrometer. 1D and 2D NMR spectra were recorded on a DRX500 (500.13 MHz; 125.77 MHz), and Brucker Avance-900 (^{1}H NMR - 900.14 MHz; ^{13}C NMR 226.36 MHz) equipped with cryoprobe in $CDCl_3$: δ in ppm, J in Hz. Low resolution electrospray ionisation mass spectrometry measurements (LRESIMS) were recorded in positive or negative ionization mode on a Bruker Esquire HCT (High Capacity 3D ion trap) instrument with a Bruker ESI source. High resolution electrospray ionisation (HRESIMS) accurate mass measurements were recorded in positive mode on a Bruker MicrOTOF-Q (quadrupole – Time of Flight) instrument with a Bruker ESI source. Accurate mass measurements were carried out with external calibration using sodium formate as the reference calibrant. HPLC instruments include HPLC Agilent 1190 and Gilson Fraction collector FC204. Column chromatography (CC): Silica gel 60 (200-300mesch, 15-40μ, Merck, Germany). Semi-preparative HPLC was carried out on a Phenomenex Luna 5u C18 (2), 250×10.00mm, 5μ micron column. HPLC separation using analytical column was made on Phenomenex Luna C18(2) 100A, 250×4.6mm 5μ.

Plant Material. Stems (less than 2cm in diameter) of *Croton insularis* Baill. (family Euphorbiaceae) were sampled from trees growing in an arboretum on the grounds of the Ecobiotics Limited research laboratories at Yungaburra in north Queensland. The arboretum specimens had been established from vegetatively propagated *Croton insularis* that were originally collected (EcoBiotics herbarium voucher specimen Reddell 1714) from a natural population of the species growing in a semi-deciduous vine forest at Iron Range (12°38.33'S, 143°22.76'E), Queensland.

Extraction and Isolation. The mulched stems of *Croton insularis* (1.6 kg) collected from Yungaburra in October 2012 were extracted) three times (3×24 h) with ethanol (3×4 L) at ambient temperature. The ethanol extract was concentrated under reduced pressure to yield a dark brown residue (~200ml). The residue was suspended in water and sequentially partitioned with petroleum spirit (PS) methylene chloride and ethyl acetate respectively. The PS layer was concentrated under reduced pressure to give a green viscous residue (6.5 g) which was applied to silica gel column chromatography (70g, 5×8.2 cm) and eluted with petroleum ether-EtOAc gradient system (9:1, 4:1, 2:1, 1:1, 1:2, 1:4, EtOAc) and then with EtOAc-MeOH gradient system (99:1, 19:1, 9:1, MeOH), to give 22 fractions. Fraction 9 (192 mg) eluted with PS-EtOAc 1:1 was subjected to semi-preparative RP HPLC (MeCN H_2O, 80% to 95% for 40 min, flow rate 2 ml/min, collection mode 0.25 min/tube) to afford compound EBC-318 (**2**) (1.0 mg, R_t 18.6 min). Compound EBC-339 (**3**) (0.26 mg, R_t 9.2 min) was isolated from fraction 11 (340 mg) eluted with PS-EtOAc 1:2 after HPLC separation on semi-preparative column (MeCN H_2O, 70% to 95% for 40 min, flow rate 2 ml/min, collection mode 0.25 min/tube).

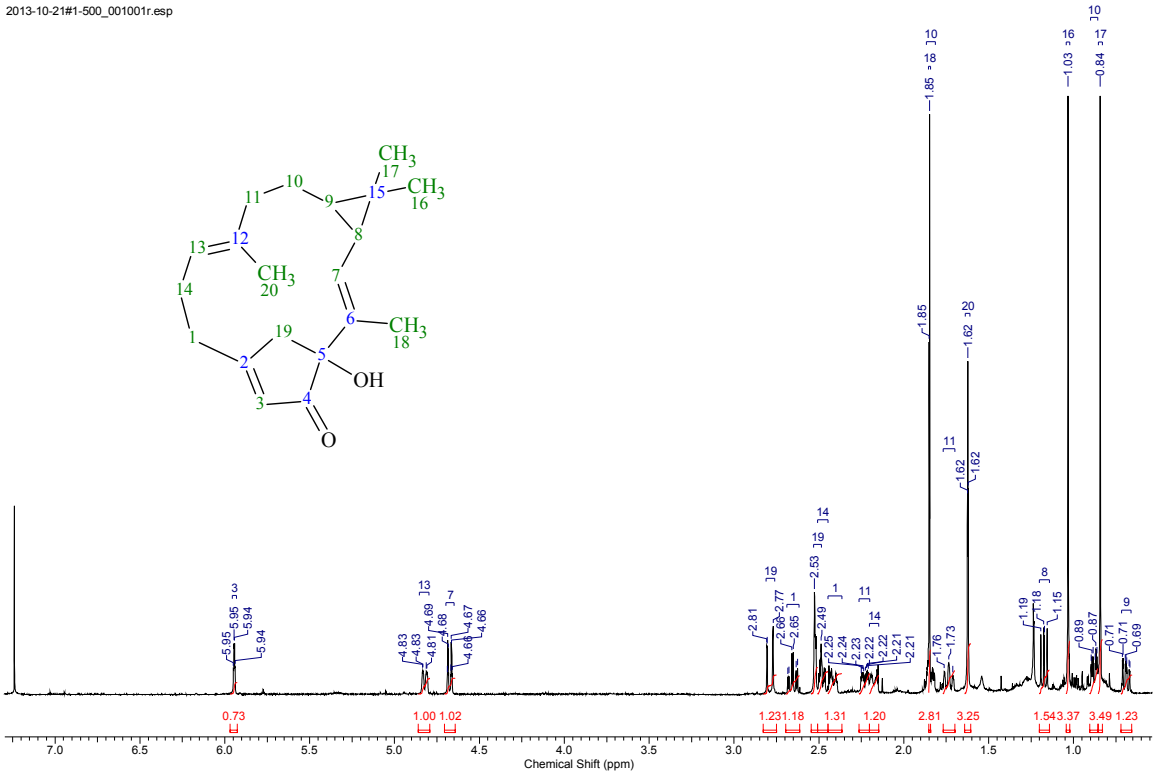
EBC-318 (2) was isolated as a colourless oil; $[\alpha]^{24.0}_D$ –23.3° (c 0.11, $CDCl_3$); UV (MeCN) λ_{max} (log ε) 205 (3.98), 227 (3.86), 243 (3.58), 276 (2.67) nm; ^{1}H NMR and ^{13}C NMR see Table 1 below on page 4 and copies of the spectra on pages 5-10; IR cm^{-1}: 3411, 3062, 2949, 2918, 2853, 1704, 1700, 1612, 1450, 1438, 1376, 1348, 1221, 1183, 1135, 1127, 1087, 1067, 954, 881, 845; positive ion HRESIMS $[M+Na]^+$*m/z* 323.1976 (calcd for $C_{20}H_{28}O_2Na$ – 323.1982).

EBC-339 (**3**) was isolated as a colourless oil; $[\alpha]^{26.4}_D$ –+51.8° (c 0.024, $CDCl_3$); UV (MeCN) λ_{max} (log ε) 206 (4.22), 218 (3.97), 234 (3.52), 283 (2.78) nm; ^{1}H NMR and ^{13}C NMR, see Table 3 below on page 11 and copies of the spectra on pages 12-16; IR cm^{-1}: 3402, 2953, 2920, 2858, 1746, 1705, 1700, 1454, 1399, 1377, 1317, 1279, 1253, 1168, 1089, 1082, 1067, 1058, 1023, 1007, 861; positive ion HRESIMS $[M+Na]^+$*m/z* 339.1944 (calcd for $C_{20}H_{28}O_3Na$ - 339.1931 Da).

Materials and Methods for Growing Cells and Cell Screening: Cells (3000-3500/well) were seeded in in 96-well plates (triplicate) in Roswell Park Memorial Institute 1640 medium containing 10% fetal calf serum, and then were treated with the compounds. After 6 days in culture at 37 degrees, the growth of treated K562 cells was compared with untreated controls by addition of MTS, and the colour change read at 490 nm in an ELISA reader. The other cell lines were fixed with ethanol *in situ*, stained with sulforhodamine B and absorbance at 564 nm determined in an ELISA reader. IC_{50} were determined by interpolation of a plot of absorbance expresses as % of untreated controls. Cell were seeded at the following densities: K562: 3500/well, MM96L: 3000/well, HeLa: 3000/well.

Table 1. ^{1}H and ^{13}C NMR Data for Compound EBC-318 (**2**) Recorded in $CDCl_3$.

Position	^{1}H, δ (ppm)	multiplicity	J, Hz	^{13}C, δ (ppm)
1	2.41	1H (m)	-	32.93
1	2.65	1H (td)	12.5, 3.6	
2				179.86
3	5.94	1H (m)	2.2, 1.3, 1.0	128.72
4				210.73
5				83.3
6				137.28
7	4.67	1H (dq)	10.3, 1.6	123.99
8	1.17	1H (dd)	10.3, 8.5	26.55
9	0.69	1H (ddd)	11.5, 8.5, 1.6	32.13
10	0.88	1H (dt)	11.5, 2.6	27.05
10	1.84	1H (m)	-	
11	1.73	1H (m)	-	39.86
11	2.23	1H (ddd)	13.1, 5.3, 2.6	
12				138.63
13	4.82	1H (m)	11.2, 1.8	123.83
14	2.17	1H (m)	-	24.71
14	2.48	1H (m)	-	
15				21.89
16	1.03	3H (s)	-	29.01
17	0.84	3H (s)	-	15.16
18	1.85	3H (d)	1.6	11.94
19	2.51	1H (m)	-	44.55
19	2.79	1H (dd)	17.6, 1.0	
20	1.62	3H (t)	1.3	18.33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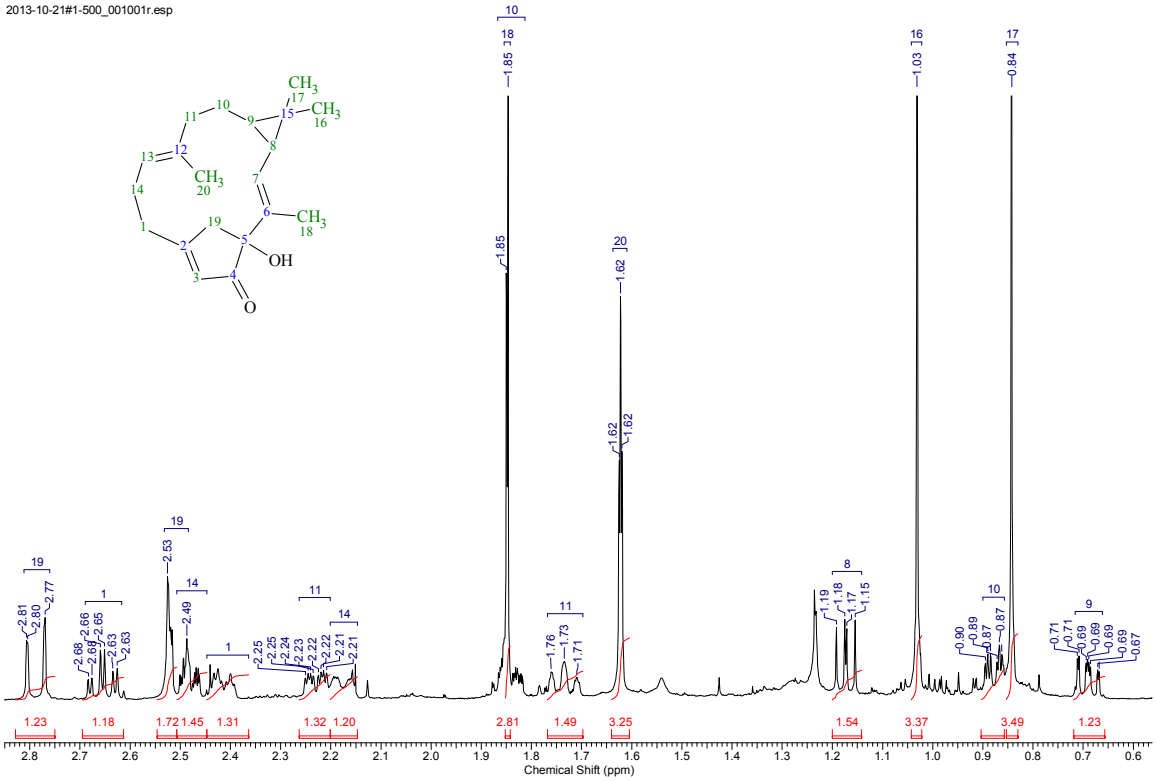
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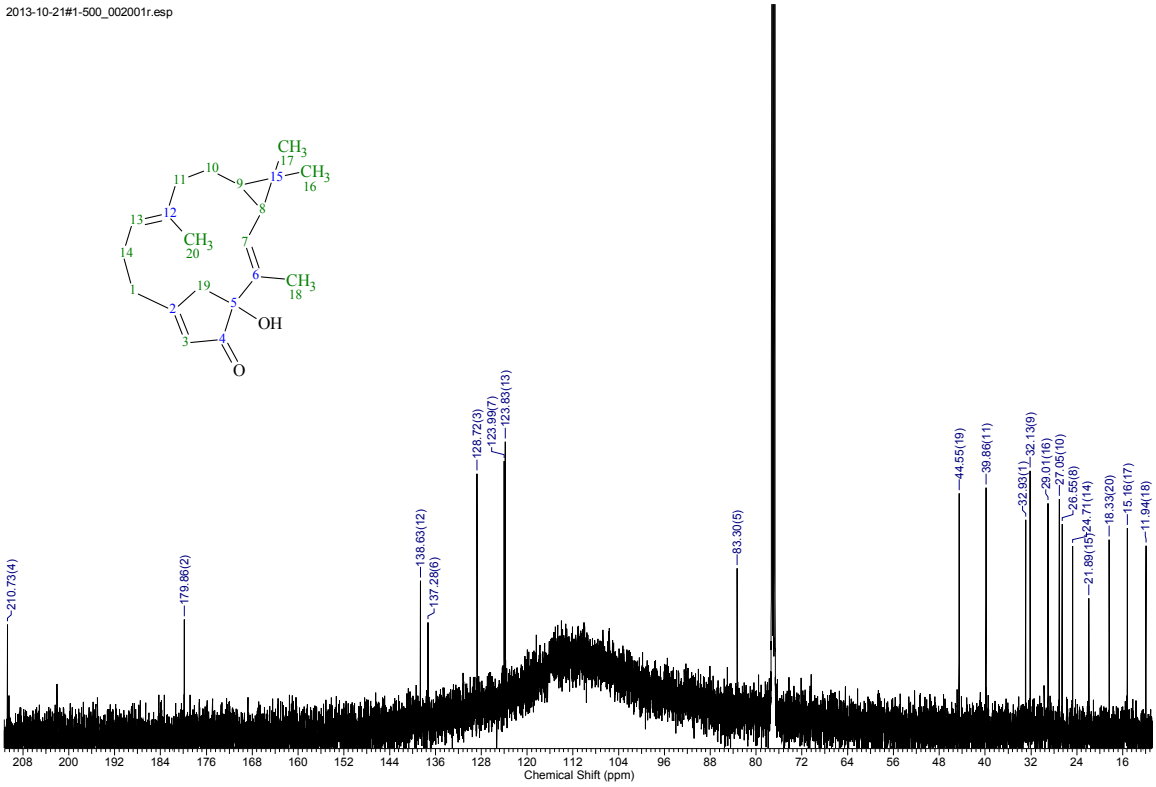
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39.86(11)
32.93(1)
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29.01(16)
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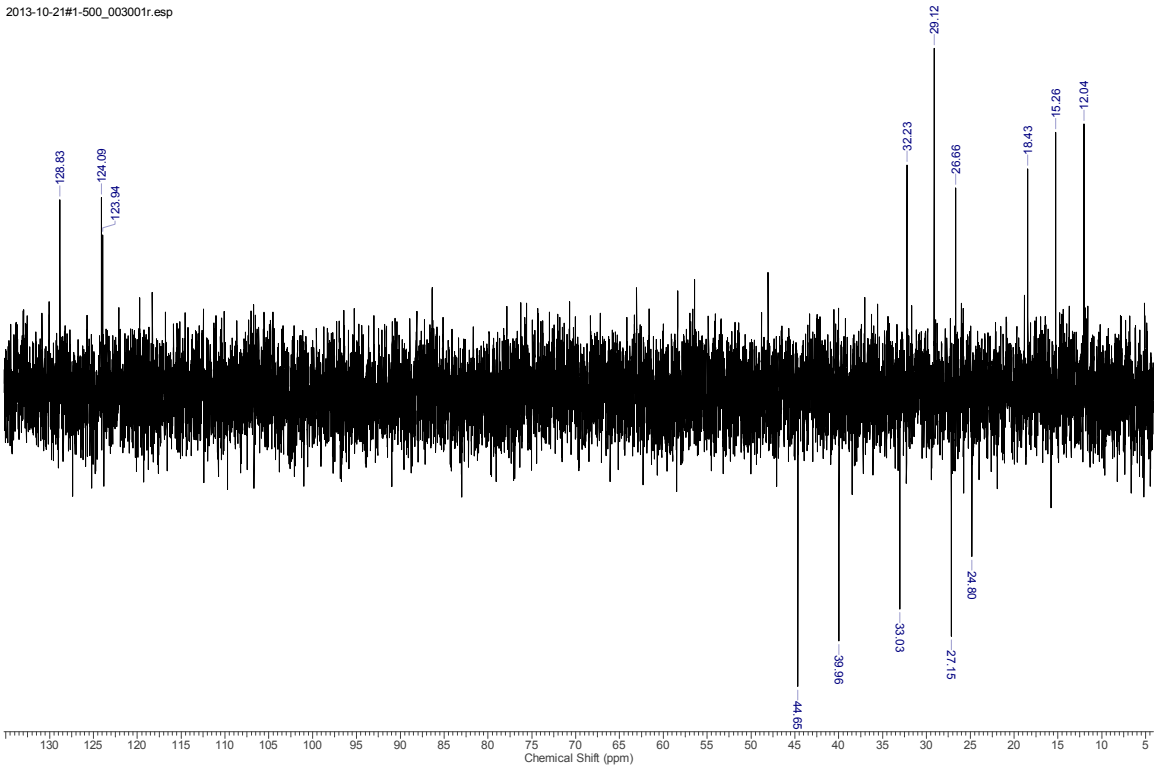
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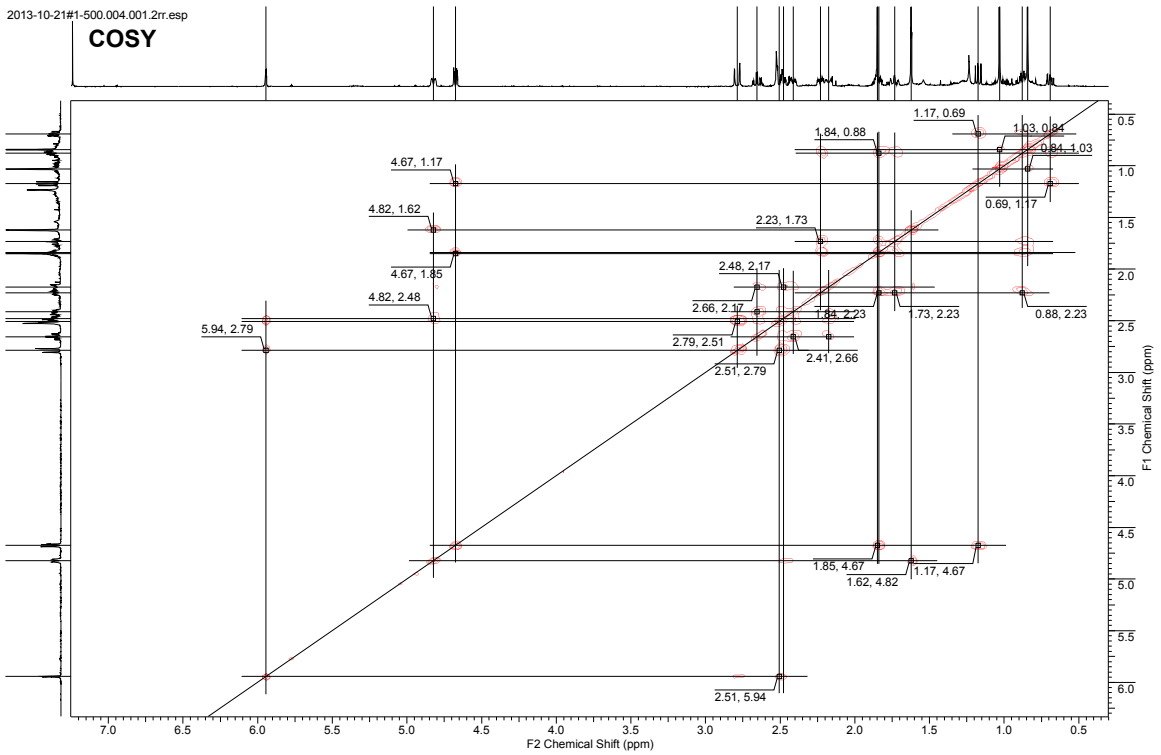
Chemical Shift (ppm)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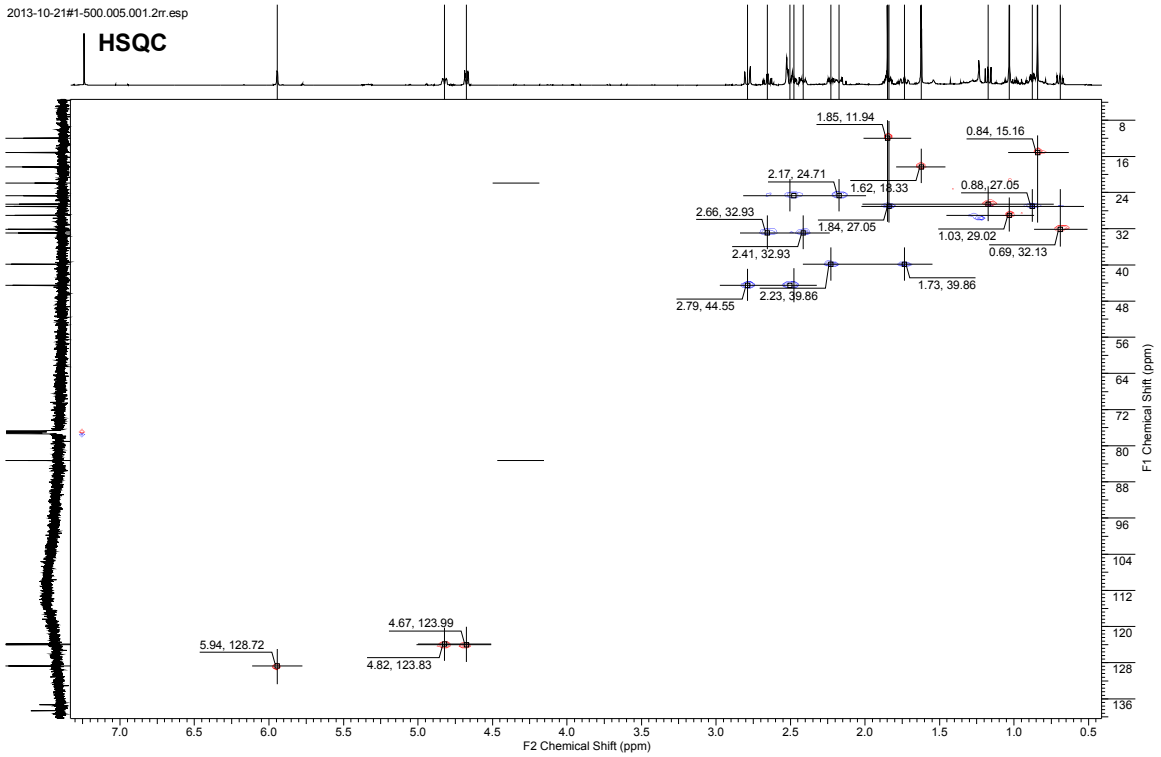
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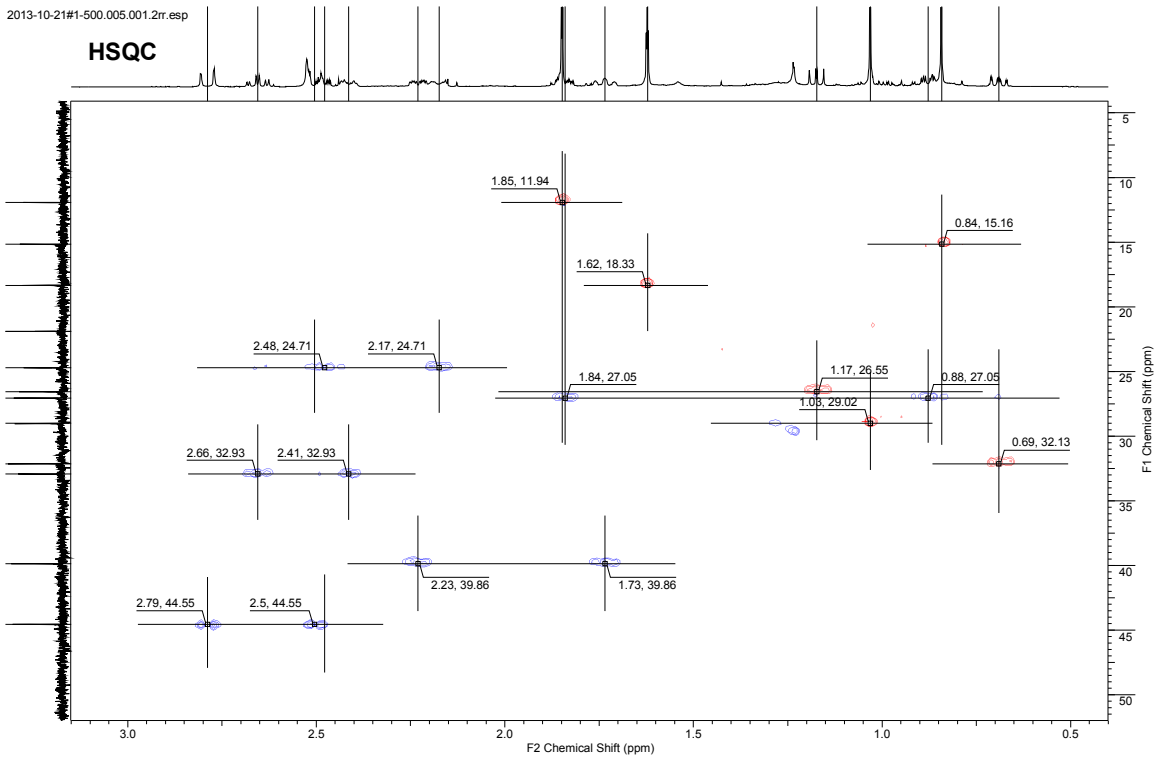
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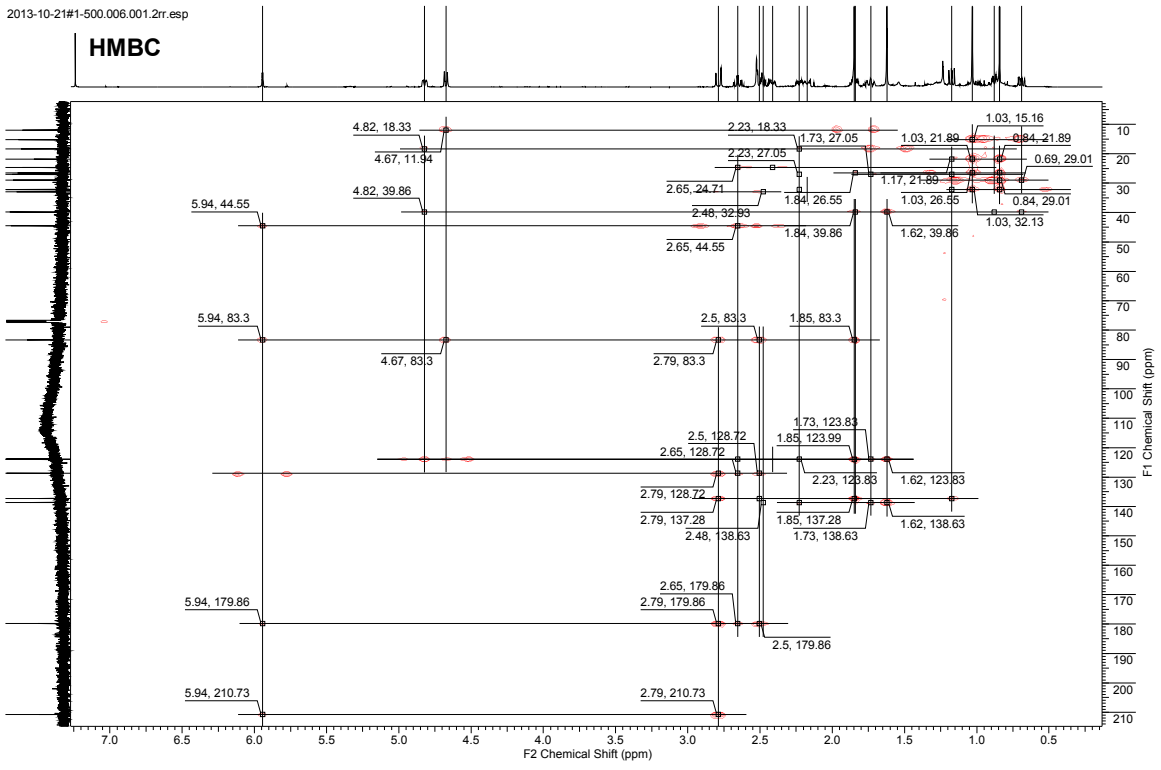
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4.82, 39.86
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2.48, 32.93
1.03, 32.13
1.84, 39.86
1.62, 39.86
2.65, 44.55
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1.62, 138.63
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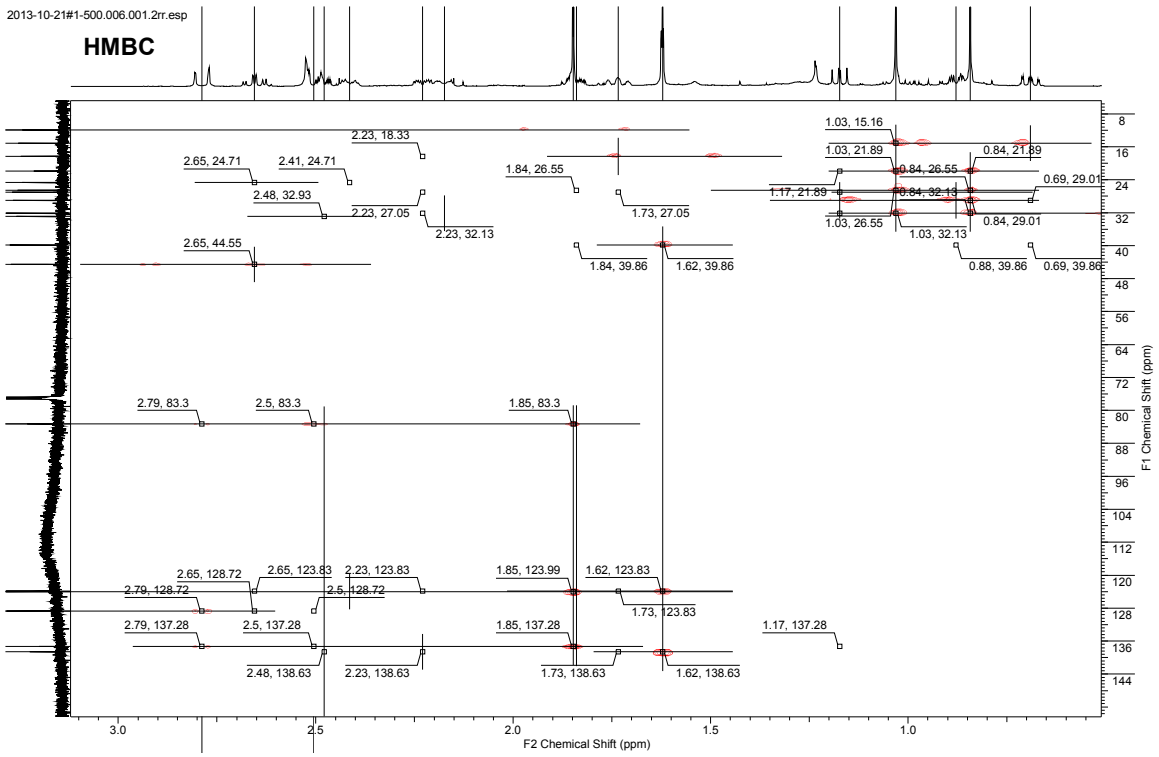
F1 Chemical Shift (ppm)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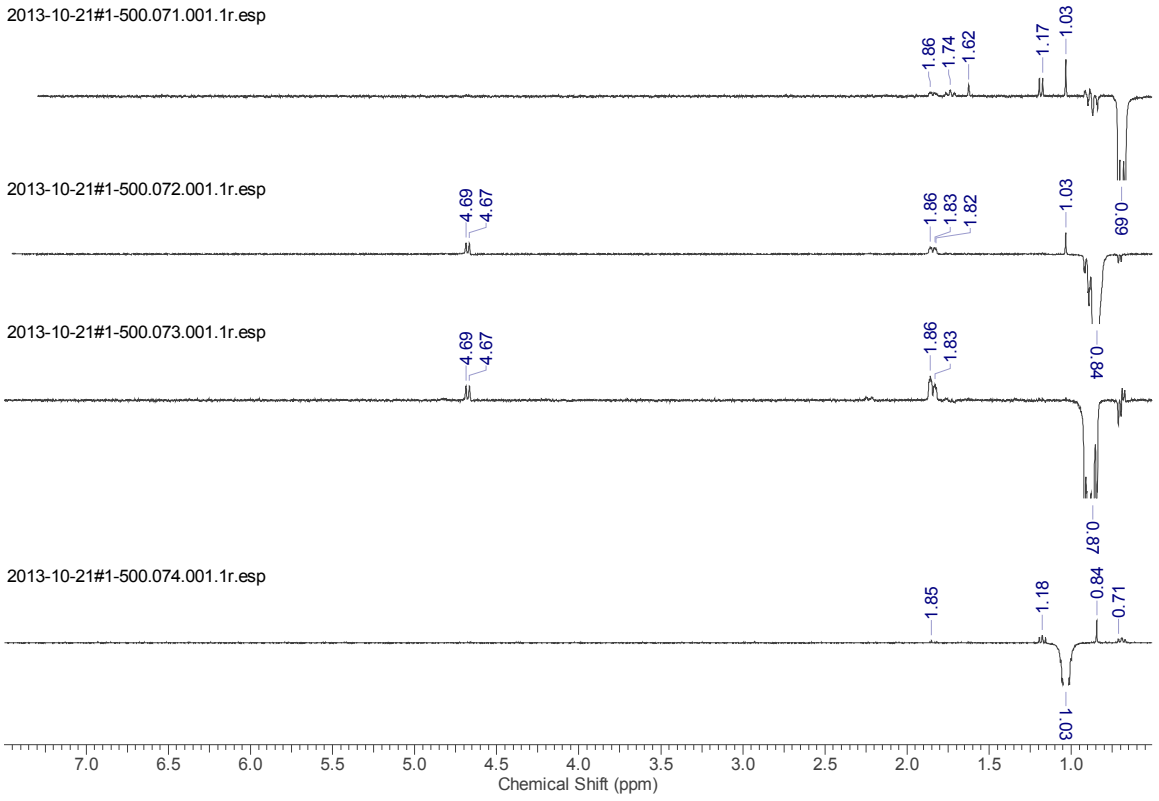
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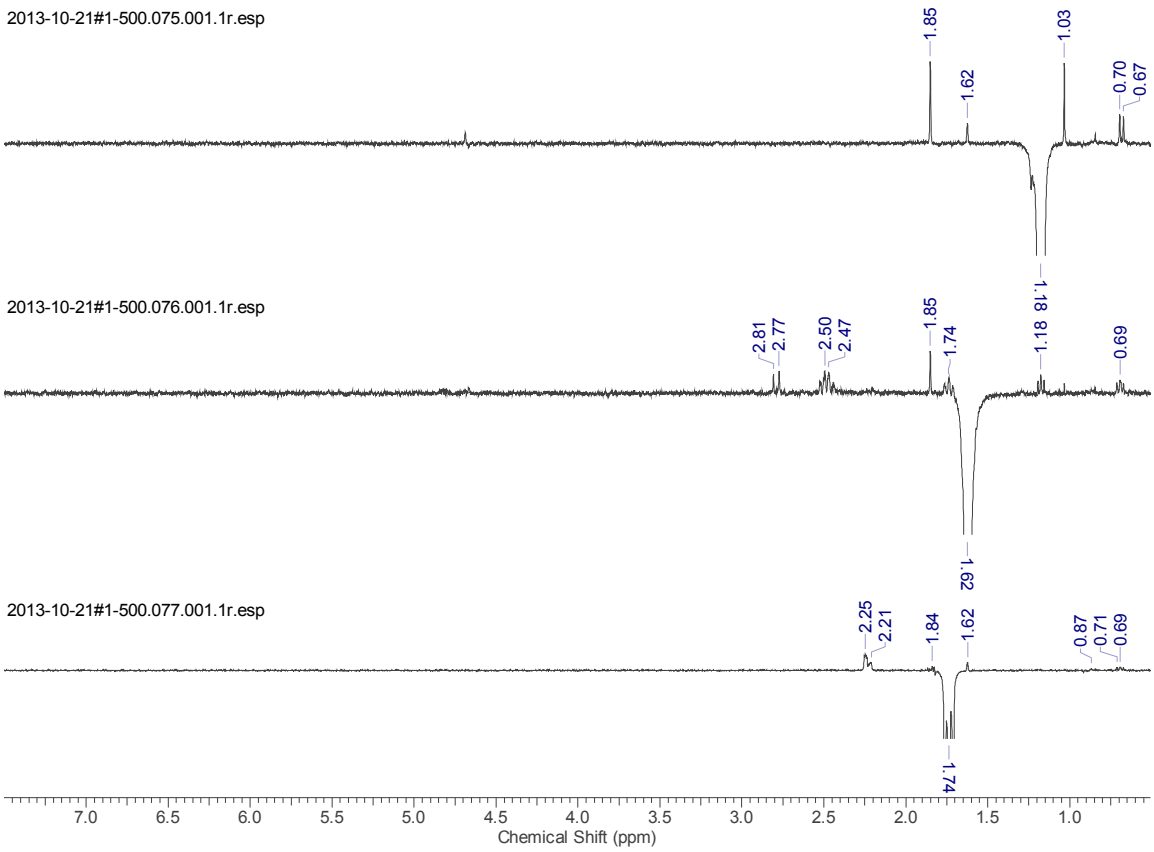
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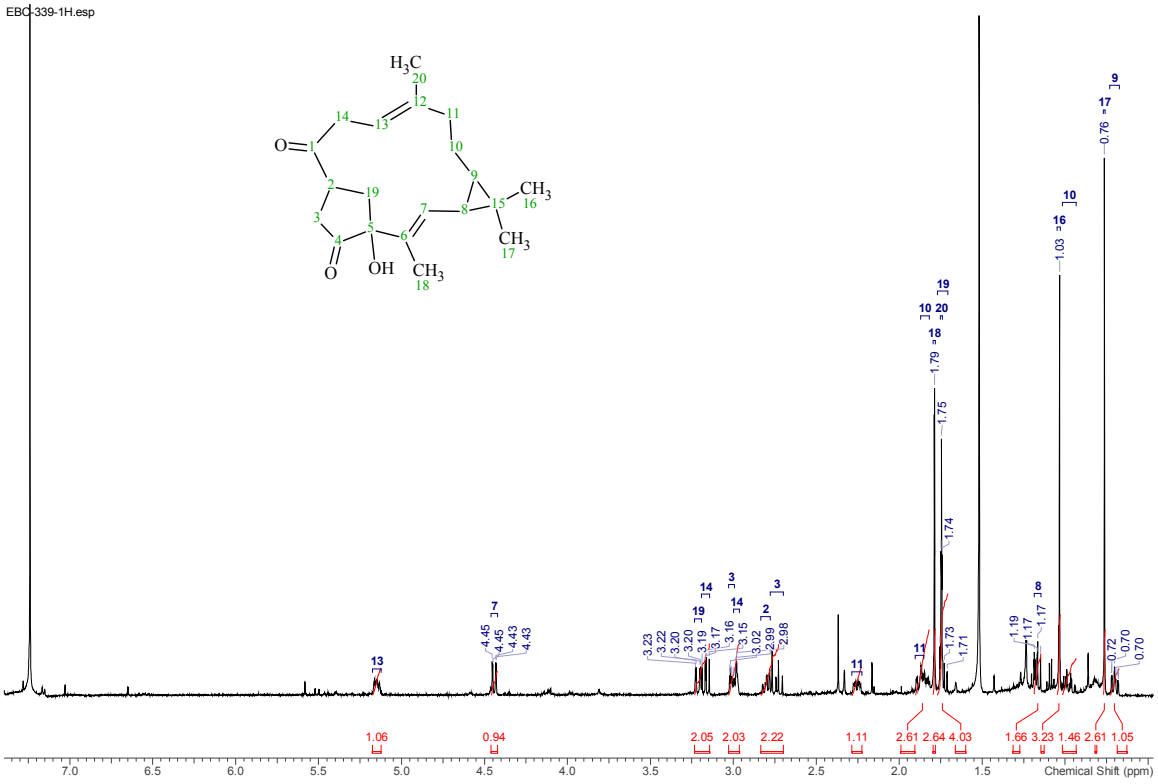
2.0
1.5
1.0
Chemical Shift (ppm)

Table 2. ^{1}H and ^{13}C NMR Data for Compound EBC-339 (**3**) Recorded in $CDCl_3$.

Position	^{1}H, δ (ppm)	multiplicity	J, Hz	^{13}C, δ (ppm)
1				205.47
2	2.79	1H (m)		42.78
3	3.01	1H (m)		36.02
3	2.74	1H (m)		36.02
4				217.84
5				83.44
6				133.08
7	4.44	1H (dq)	10.2, 1.3	126.71
8	1.17	1H (dd)	10.2, 8.3	26.31
9	0.70	1H (ddd)	11.8, 8.3, 1.6	32.32
10	1.84	1H (m)		24.24
10	0.98	1H (m)		24.24
11	2.26	1H (m)		39.05
11	1.87	1H (m)		39.05
12				141.53
13	5.15	1H (m)		116.37
14	3.17	1H (dd)	11.9, 9.9	41.37
14	2.99	1H (m)		41.37
15				21.69
16	0.76	3H (s)		15.38
17	1.03	3H (s)		29.06
18	1.79	3H (d)	1.0	12.39
19	3.21	1H (dd)	13.5, 2.6	32.76
19	1.73	1H (dd)	13.5, 8.3	32.76
20	1.75	3H (t)	1.3	19.32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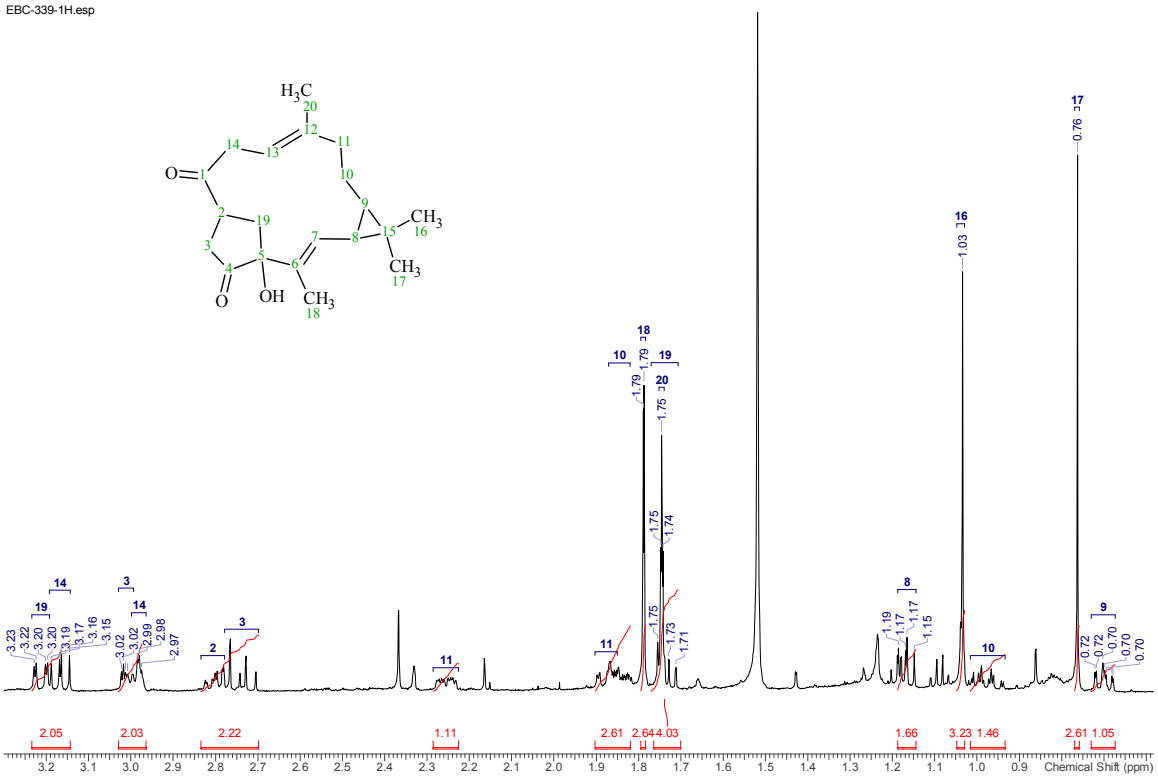
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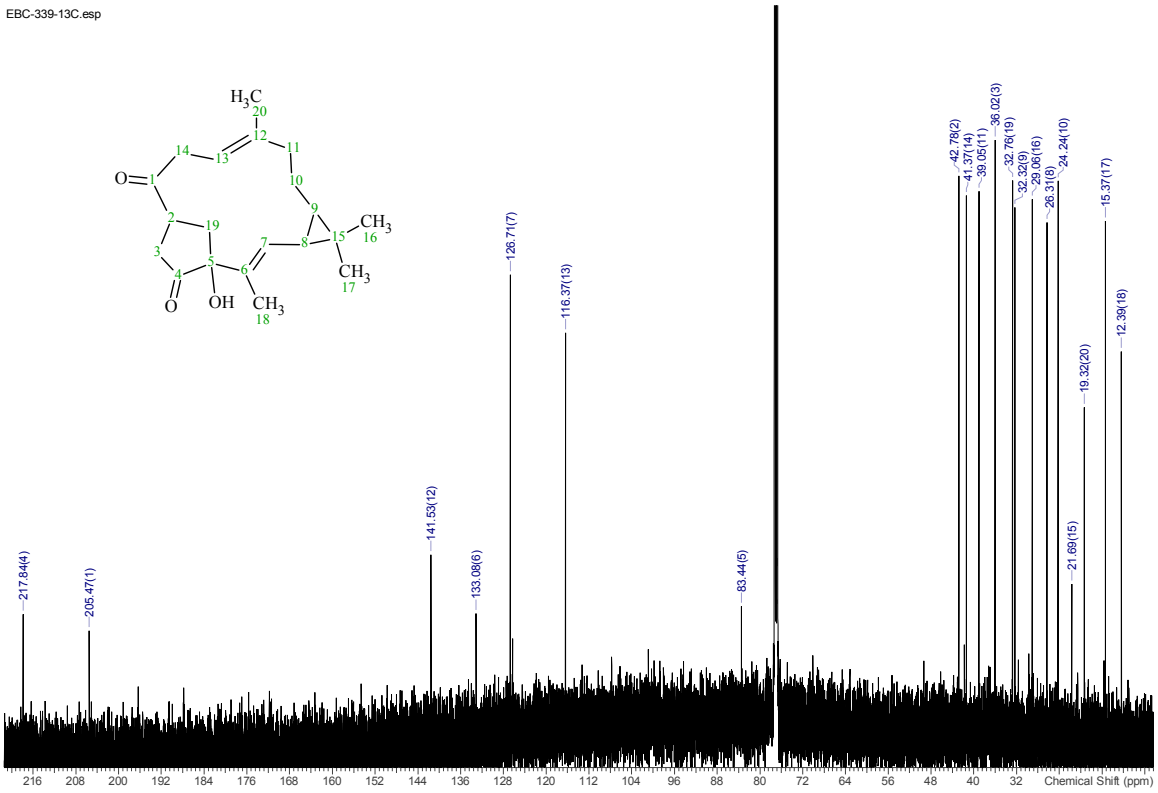
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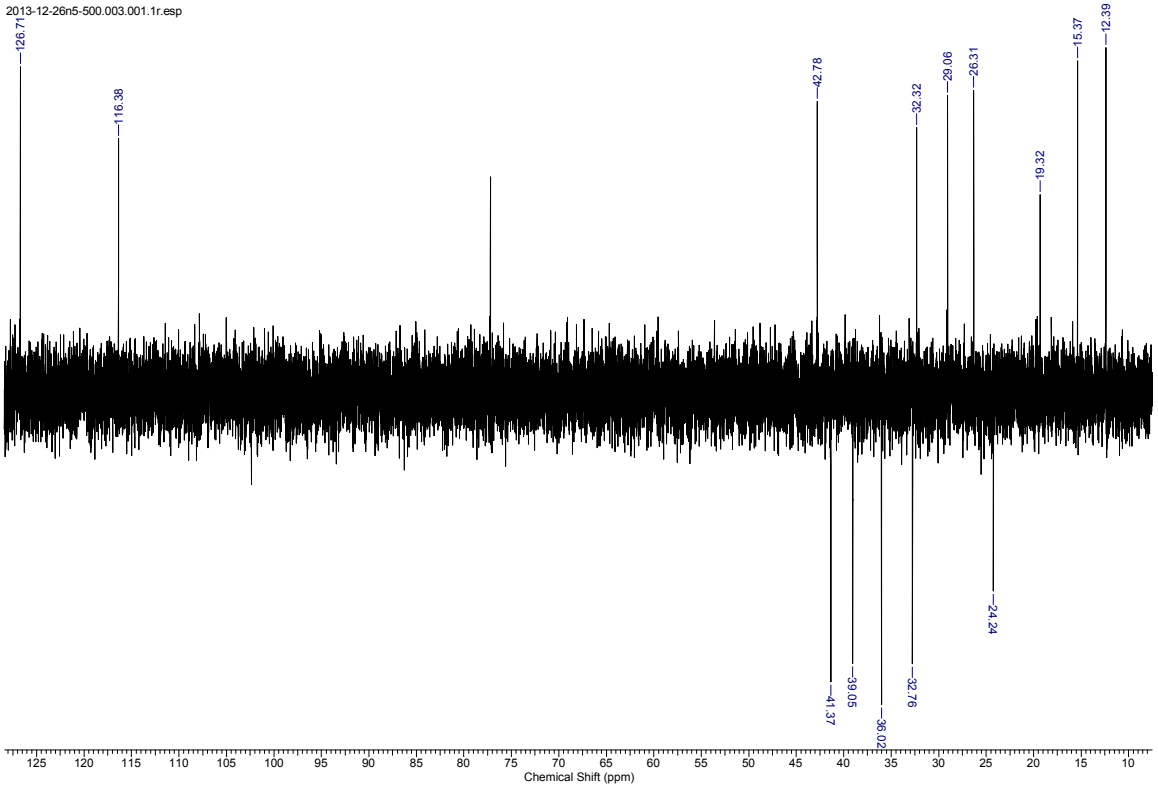
Chemical Shift (ppm)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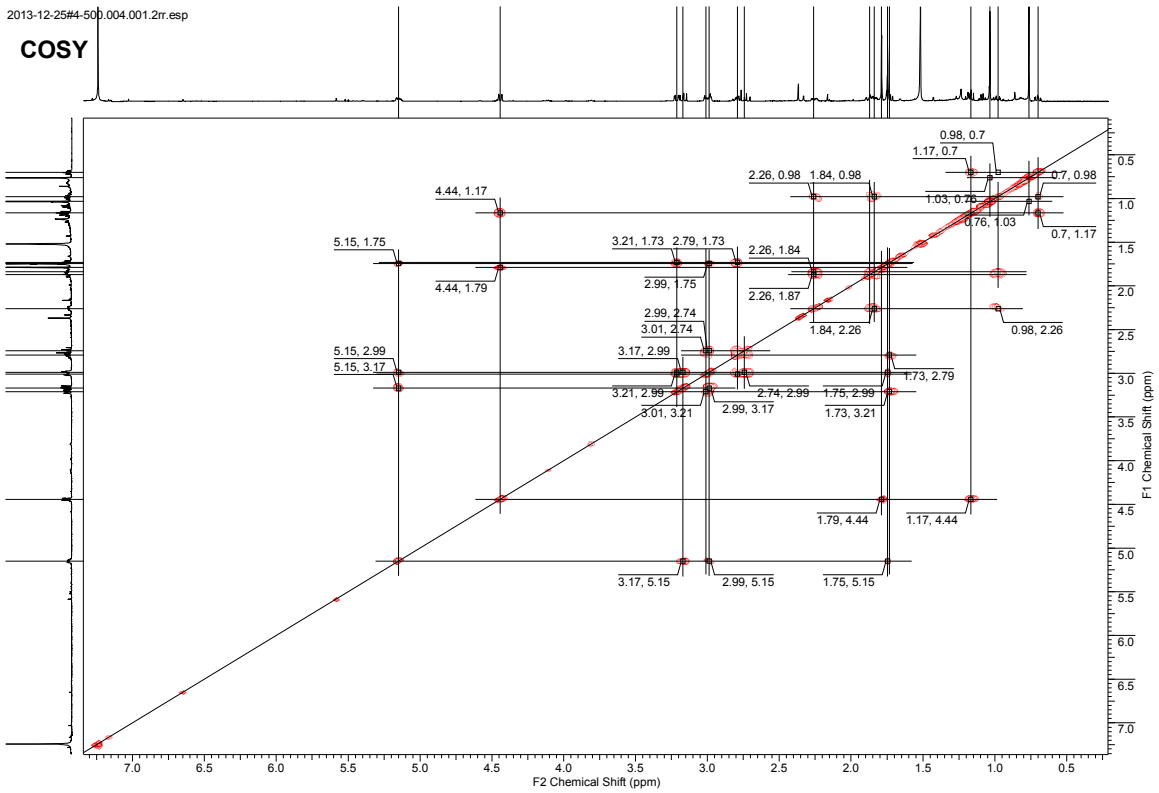
Chemical Shift (ppm)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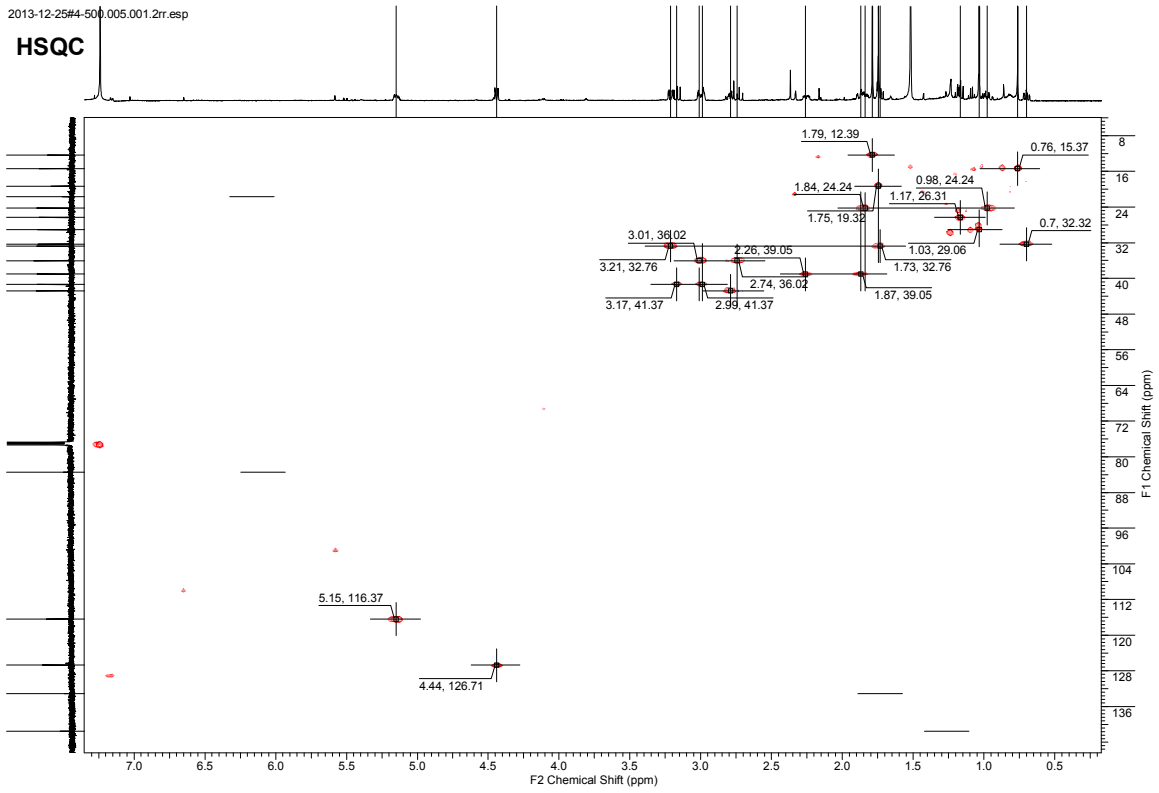
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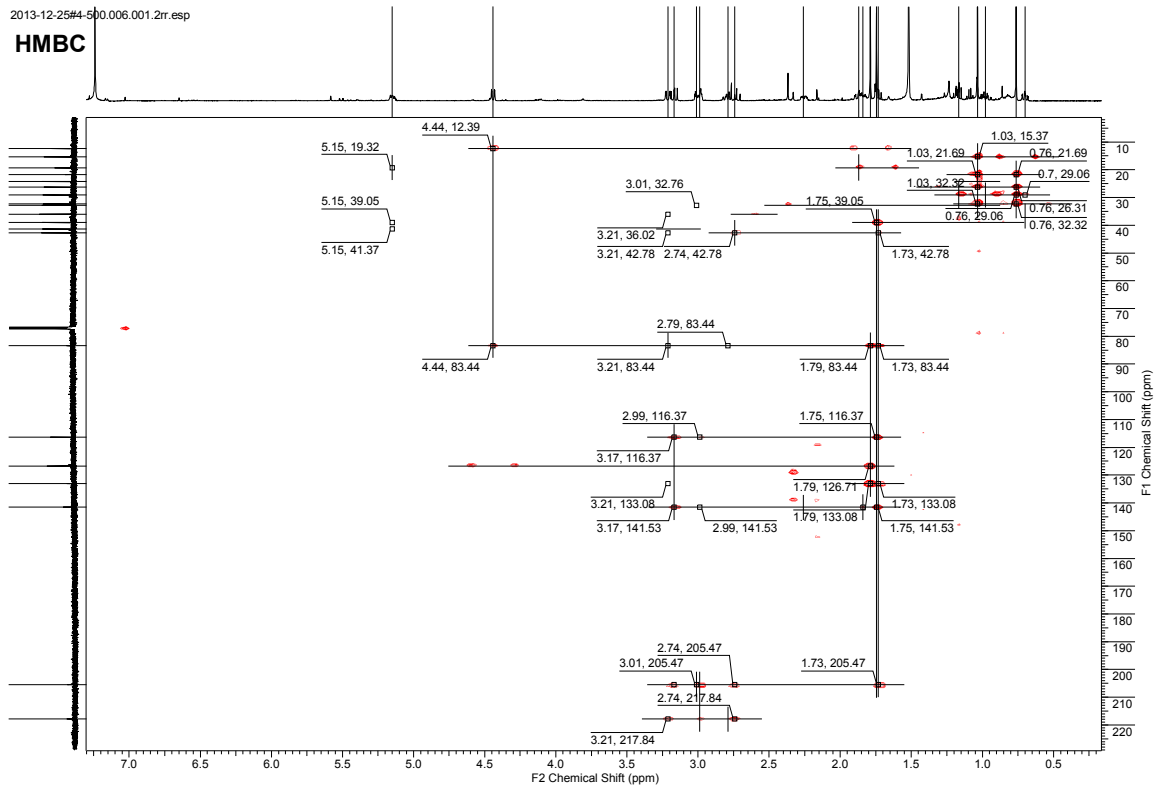
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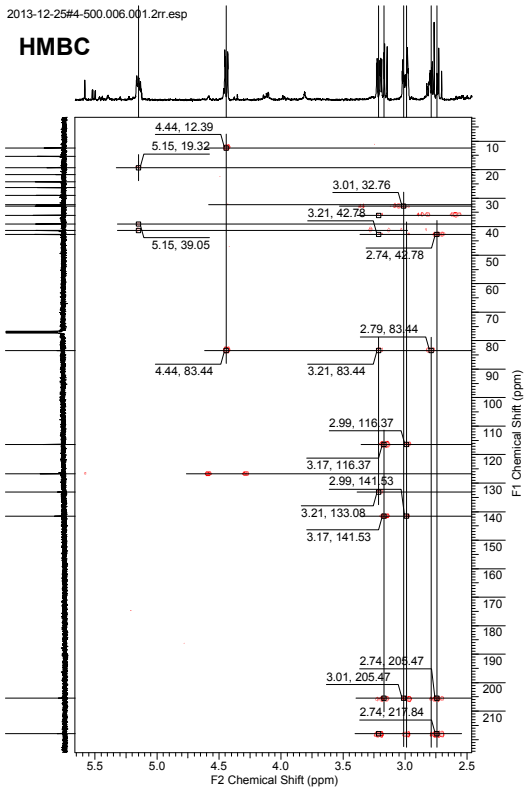
F1 Chemical Shift (ppm)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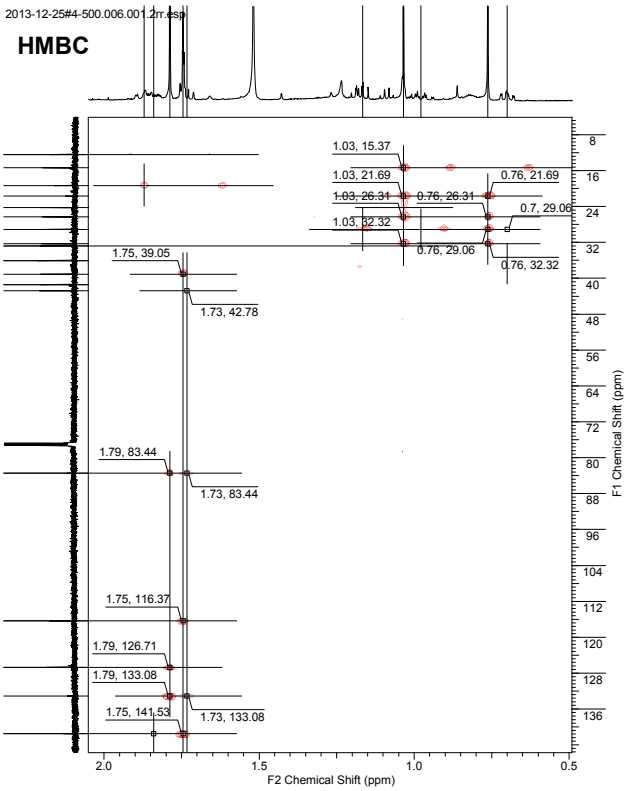
2.74, 217.84
F2 Chemical Shift (ppm)
F1 Chemical Shift (ppm)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1.73, 42.78
1.79, 83.44
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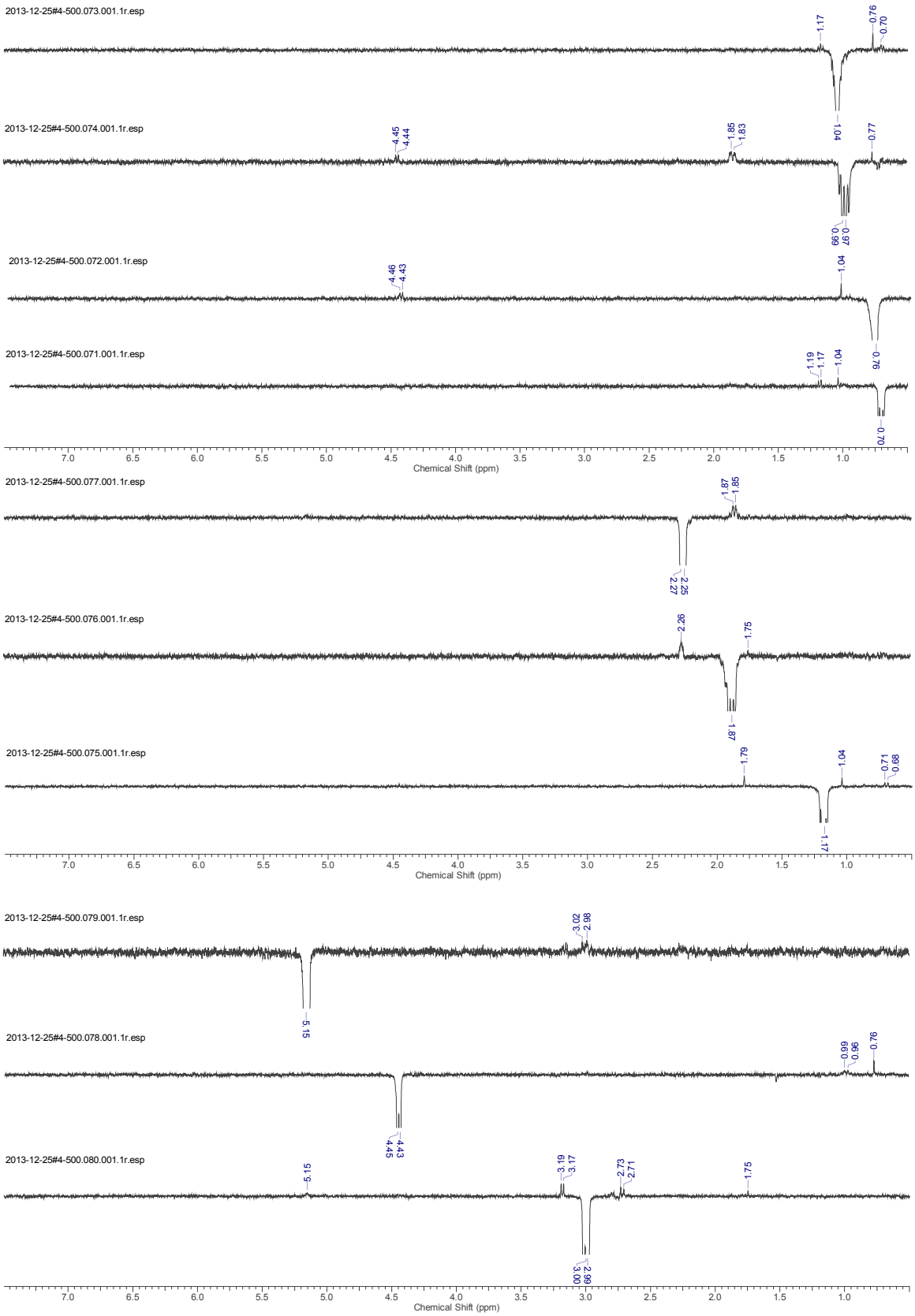
F2 Chemical Shift (ppm)
F1 Chemical Shift (ppm)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1.17
1.04
0.76
0.70
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Chemical Shift (ppm)
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1.85
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2.25
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2.26
1.75
1.87
2013-12-25#4-500.075.001.1r.esp
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1.04
0.71
0.68
1.17
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
Chemical Shift (ppm)
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4.43
2013-12-25#4-500.080.001.1r.esp
5.15
3.19
3.17
2.73
2.71
1.75
3.00
2.99
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
Chemical Shift (ppm)

Quantum Chemical Calculation of the CD Spectra for 2 and 3.

A conformer search for **2** was performed using Monte Carlo conformational searching method implemented in MacroModel v. 10.9 (Schroinger Inc) program.[1] Torsional sampling Monte Carlo Multiple Minimum (MCMM) was performed using 1000 steps per rotatable bond. Each conformer was minimized with the OPLS-2005 force field using Truncated Newton Conjugate Gradient (TNCG) method with maximum iterations of 50,000 and energy convergence threshold of 0.02. Identified low energy conformations (< 5 kcal/mol from global minimum) were further optimized using DFT calculations at the B3LYP/6-31G(**) level[2] in the gas phase by the GAUSSIAN09.[3] The B3LYP/6-31G(**) harmonic vibrational frequencies were calculated to confirm true minima. Theoretical ECD spectra of each conformer were calculated using time dependent density functional theory (TDDFT) at the same level in the gas phase and at the B3LYP/6-311++G(**)//B3LYP/6-31G** level using the "Self-Consistent Reaction Field" method (SCRF) with polarizable continuum model (PCM) model in acetonitrile for 30 electronic excitation states. Equilibrium populations of the selected conformers were calculated from DFT relative energies and free energies according to the Boltzmann distribution statistic at 298 K and 1 atm.

Comparison of Simulated ECD Spectra with Experimental Data for 2.

Boltzmann weighting of the electronic circular dichroism spectra was performed in the program SpecDis[4], using relative energies (ΔE). Calculated ECD spectra were compared with experimental data, employing Gaussian broadening σ for **2** in gas phase B3LYP/6-31G(**) σ = 0.21, acetonitrile B3LYP/6-31G(**) σ = 0.24 and B3LYP/6-311++G(**) σ = 0.22.

[1] MacroModel, version 10.9, Schrödinger, LLC, New York, NY, **2015**.

[2] C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*, **1988**, *37*, 785–789. b) A. D. Becke, *J. Chem. Phys.*, **1993**, *98*, 1372–1377. c) A. D. Becke, *J. Chem. Phys.*, **1993**, *98*, 5648–5652. (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.*, **1994**, *98*, 11623–11627.

[3] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, **2013**.

[4] T. Bruhn, A. Schaumlöffel, Y. Hemberger, G. Bringmann, SpecDis, Version 1.62, University of Wuerzburg, Germany, **2014**.

Calculated Geometries of the Lowest-Energy Conformers for Compound 2.

Optimized structures of EBC-318 (2) conformer 1-4 in the gas phase (GP).

Structures of major conformers (>99% of population) for EBC-318 (**2**) are shown in figure S1 and their calculated relative energies, Gibbs free energies and coordinate in the gas phase (GP) are listed below.

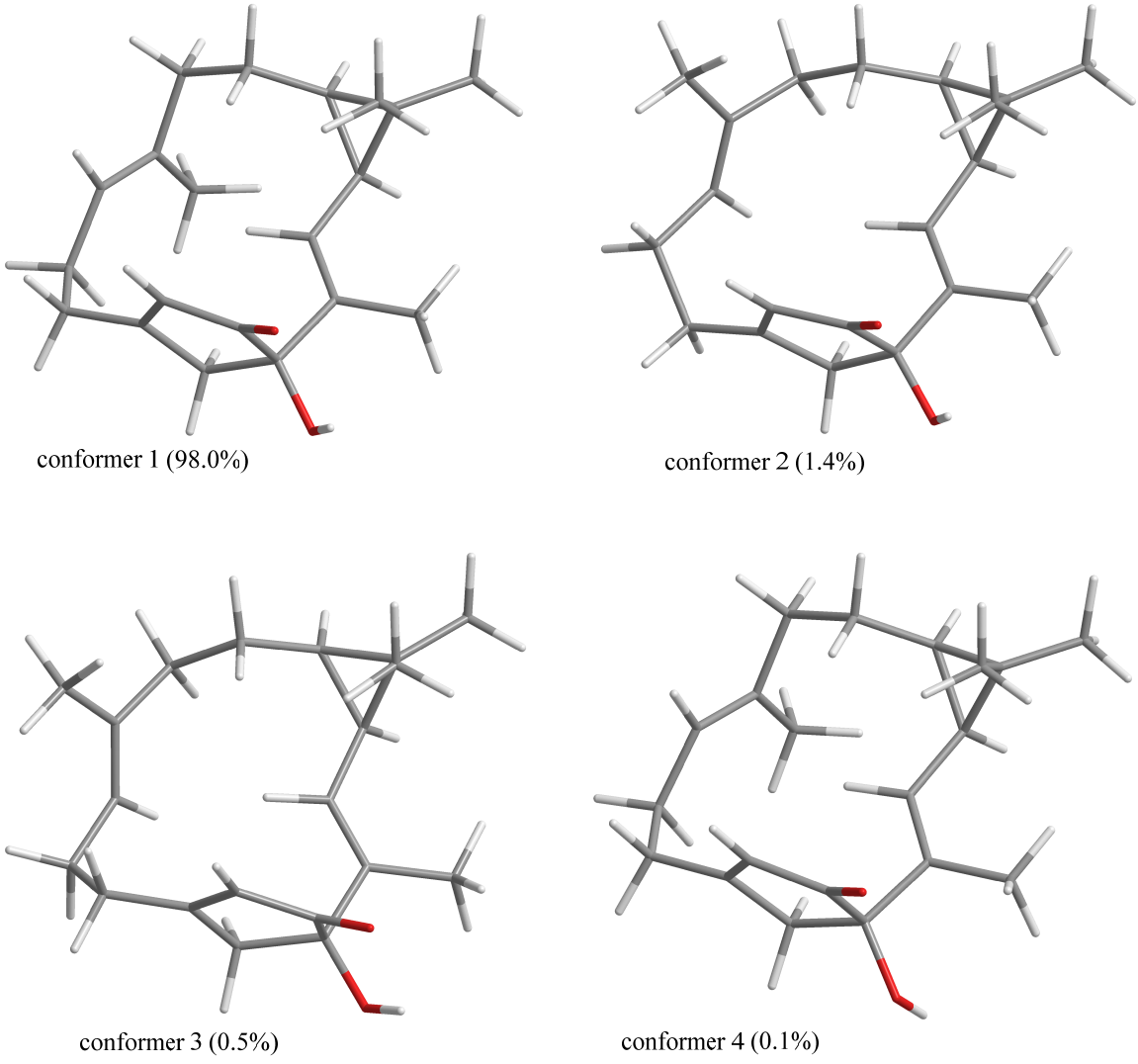

Figure S1. Four lowest energy optimized structures of EBC-318 (**2**) in the GP.

The Cartesian Coordinates and Energies of the Low-Energy Conformers of EBC-318 (2) conformer 1-4.

Conformer **1**

C	0.10766800	-3.02674900	-1.09859900
C	4.21467200	-1.74900000	-0.29554600
C	0.85150200	2.82892000	-1.73037500
C	2.47927200	-1.68589600	1.55489200
C	2.29161000	1.35868400	1.07105000
C	1.91583900	2.78933500	0.60411700
C	-1.91541400	3.05403100	-0.23935900
C	-2.43071500	-0.08765000	-0.92584200
C	-2.40341900	-0.18265200	1.44881200
C	1.95001000	-0.56727400	-0.77443000
C	2.82193800	0.41525400	0.00153500
C	-0.54029700	3.00793900	0.37352100
C	0.46893300	-0.59270800	-0.58172000
C	-2.57120700	0.64698300	0.39667600
C	2.96522800	-1.07598600	0.25046400
C	-0.35732000	-1.63494600	-0.76557300
C	0.65095100	2.88596400	-0.23621000
C	-1.87648500	-1.47821600	-0.55038500
C	-2.92437700	2.10466500	0.46232500
C	-2.14617600	-1.54803700	0.97661300
O	-2.61110800	-2.50877100	-1.19453200
O	-2.18242100	-2.60323000	1.58994200
H	1.19319500	-3.06461400	-1.20541800
H	-0.18183300	-3.72631900	-0.30393200
H	-0.35718600	-3.38603400	-2.02160700
H	5.04542800	-1.67207400	0.41683800
H	4.04053800	-2.81551400	-0.48448200
H	4.54030300	-1.29202800	-1.23579800
H	1.43352000	1.94455200	-2.01123900
H	-0.08329200	2.81404800	-2.29420600
H	1.42602100	3.70239600	-2.06565400
H	2.35585700	-2.76931800	1.44441500
H	3.20611100	-1.51944600	2.35924600
H	1.51642600	-1.28490200	1.87647200
H	1.42225300	0.92437700	1.57456700
H	3.06849600	1.46140300	1.84164300
H	2.76277600	3.21998100	0.05332200
H	1.79047200	3.40243500	1.50416200
H	-1.88390900	2.83124100	-1.30967900
H	-2.32699900	4.06999200	-0.15361200
H	-1.79958200	0.44573900	-1.64100000
H	-3.41704000	-0.21582800	-1.38887900
H	-2.50948200	0.07765300	2.49599400
H	2.26026100	-0.72711300	-1.80816000
H	3.63749400	0.85383100	-0.57498700
H	-0.53543900	3.07273900	1.46385600
H	0.02906700	0.35826800	-0.29707300

H	-3.90645400	2.24529600	-0.01153400
H	-3.03488100	2.40348400	1.51093700
H	-2.65716300	-3.23420000	-0.54926300

Electronic energies = -929.408381438
Zero-point correction= 0.438073 (Hartree/Particle)
Thermal correction to Energy= 0.460605
Thermal correction to Enthalpy= 0.461549
Thermal correction to Gibbs Free Energy= 0.388356
Sum of electronic and zero-point Energies= -928.970308
Sum of electronic and thermal Energies= -928.947776
Sum of electronic and thermal Enthalpies= -928.946832
Sum of electronic and thermal Free Energies= -929.020025

Conformer **2**

C	1.66327600	-2.84717300	-0.35809300
C	4.70511700	0.22589500	-0.36216200
C	-1.23881700	3.54731900	1.35503100
C	3.01106200	-0.11582500	1.49548300
C	1.44266500	2.28085100	0.32891200
C	0.41549600	3.07402100	-0.53788200
C	-3.30524400	1.84835700	-0.28887400
C	-1.91006400	-1.56326200	-1.16378900
C	-2.24485500	-0.85263500	1.07926600
C	2.19270800	0.12739700	-1.01205000
C	2.47756200	1.53177400	-0.49133000
C	-1.91784000	2.26096200	-0.70821100
C	0.85548800	-0.50524200	-0.77956900
C	-2.61402800	-0.62661700	-0.19998400
C	3.25261100	0.35363300	0.06967600
C	0.59616000	-1.79967000	-0.53114300
C	-0.99625600	2.93670800	-0.00330500
C	-0.84959600	-2.29575100	-0.32067900
C	-3.61319900	0.38520300	-0.70067300
C	-1.27947300	-1.95534900	1.13515000
O	-0.95627700	-3.70268000	-0.50107700
O	-0.88481900	-2.59106800	2.10022100
H	2.65760900	-2.42510100	-0.51017100
H	1.62157700	-3.27408200	0.65212000
H	1.51320600	-3.67375500	-1.05887700
H	5.36142600	0.81479600	0.29047000
H	5.04357600	-0.81656600	-0.31571900
H	4.85312200	0.57930400	-1.38795100
H	-1.07850700	4.63265300	1.31181600
H	-2.25043400	3.37855000	1.72849900
H	-0.53418800	3.15959000	2.10017200
H	3.43753700	-1.11403500	1.64484900
H	3.49579000	0.55675800	2.21355600
H	1.95115000	-0.17937600	1.74743100
H	0.89759700	1.56556900	0.95156400
H	1.95082500	2.96091100	1.02386400
H	0.44694700	2.70147200	-1.56722900

H	0.71167400	4.13121400	-0.57840200
H	-4.06662100	2.48669200	-0.76002700
H	-3.43800900	1.95755200	0.79158900
H	-1.49110600	-1.02441900	-2.01915700
H	-2.61983600	-2.30028900	-1.56005700
H	-2.62711900	-0.35687100	1.96446200
H	2.61068600	-0.08608500	-1.99718200
H	3.04296400	2.17360600	-1.16771000
H	-1.62606700	1.91410700	-1.70115400
H	0.00990800	0.17506300	-0.85396200
H	-3.65967600	0.32531900	-1.79440100
H	-4.61298000	0.11600400	-0.33570700
H	-0.72893100	-4.09217600	0.35951900

Electronic energies = -929.404366092
Zero-point correction= 0.437976 (Hartree/Particle)
Thermal correction to Energy= 0.460578
Thermal correction to Enthalpy= 0.461522
Thermal correction to Gibbs Free Energy= 0.387997
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Sum of electronic and thermal Energies= -928.943788
Sum of electronic and thermal Enthalpies= -928.942844
Sum of electronic and thermal Free Energies= -929.016369

Conformer **3**

C	1.15613100	-3.01725800	-0.96346200
C	4.63336000	-0.38129800	-0.04588300
C	-1.00384000	3.85107300	0.96022400
C	2.78963500	-0.39717500	1.69506100
C	1.71999300	2.21871500	0.34693200
C	0.84697300	3.06587800	-0.63518400
C	-2.95620400	2.07814100	-0.72461900
C	-2.17790500	-1.00099900	-0.89935700
C	-2.01579000	-0.88777300	1.46781100
C	2.17502200	-0.11654900	-0.85501300
C	2.64906400	1.24845000	-0.36544100
C	-1.49050300	2.33650500	-0.99299600
C	0.76328800	-0.55546000	-0.64551900
C	-2.46933300	-0.22961900	0.37843400
C	3.19803800	-0.00496500	0.28508600
C	0.28810900	-1.80965000	-0.73013000
C	-0.62373700	3.06092700	-0.26707700
C	-1.20220400	-2.11774300	-0.46980100
C	-3.24744200	1.05801300	0.41134400
C	-1.39487700	-2.15482000	1.06848300
O	-1.58589300	-3.36980900	-1.01648000
O	-1.10788400	-3.13063000	1.74450800
H	2.20391200	-2.73603300	-1.08356800
H	1.08665100	-3.70485000	-0.11071600
H	0.82953100	-3.57438100	-1.84669400
H	5.33732400	0.12160400	0.62890500
H	4.79263500	-1.46169200	0.05643000

H	4.89749900	-0.10012100	-1.07051500
H	-0.69603700	4.89889200	0.85065800
H	-2.07784100	3.83553000	1.15934500
H	-0.49245300	3.47099200	1.85370500
H	2.95014300	-1.47029200	1.84992200
H	3.39249400	0.13785200	2.43887300
H	1.73665000	-0.20005600	1.90442400
H	1.06215500	1.67032100	1.02724800
H	2.31966100	2.88098100	0.98349300
H	0.96142800	2.66630900	-1.64800200
H	1.22380600	4.09687100	-0.66208400
H	-3.42062000	1.71916600	-1.64955800
H	-3.48211100	3.00515500	-0.46648100
H	-1.78111300	-0.36810500	-1.69566300
H	-3.09646300	-1.46784100	-1.27624100
H	-2.14211800	-0.58298700	2.50083200
H	2.60904600	-0.44101700	-1.80045100
H	3.34612200	1.75153300	-1.03646500
H	-1.08672900	1.83030600	-1.86827200
H	0.05919800	0.23807900	-0.41561800
H	-4.31885400	0.80888300	0.37105500
H	-3.08361700	1.53270000	1.38469800
H	-1.40675300	-4.02064100	-0.31683800

Electronic energies = -929.403340965
Zero-point correction= 0.437897 (Hartree/Particle)
Thermal correction to Energy= 0.460645
Thermal correction to Enthalpy= 0.461589
Thermal correction to Gibbs Free Energy= 0.387517
Sum of electronic and zero-point Energies= -928.965444
Sum of electronic and thermal Energies= -928.942696
Sum of electronic and thermal Enthalpies= -928.941752
Sum of electronic and thermal Free Energies= -929.015824

Conformer **4**

C	0.34723600	-3.04107900	-0.96730900
C	4.33612300	-1.42933200	-0.28809500
C	0.58434500	2.90713100	-1.73159900
C	2.57521800	-1.49767500	1.53803800
C	2.16560300	1.51795600	1.05192000
C	1.68426600	2.91736700	0.58711000
C	-2.17000800	2.90004200	-0.19336500
C	-2.40736100	-0.25253500	-0.91310000
C	-2.41448500	-0.39679600	1.44971700
C	1.99618000	-0.42225200	-0.80352000
C	2.77878000	0.62164800	-0.01382100
C	-0.78444700	2.94542600	0.39561900
C	0.51659800	-0.55015800	-0.64273600
C	-2.63172700	0.44092700	0.41707200
C	3.02955700	-0.85523900	0.23738200
C	-0.22661700	-1.66248600	-0.76499700
C	0.40258900	2.92558500	-0.23390600

C	-1.74923400	-1.61095900	-0.56211700
C	-3.09512200	1.86665300	0.50410900
C	-1.99445600	-1.72828500	0.97759400
O	-2.40914600	-2.70999400	-1.17915300
O	-1.82866300	-2.73750200	1.63338800
H	1.43814900	-3.01727500	-0.95270100
H	-0.01189200	-3.71038600	-0.17848100
H	0.03104600	-3.48446300	-1.91890200
H	5.14698300	-1.28399600	0.43636500
H	4.25059300	-2.50697900	-0.47436400
H	4.63884200	-0.95077900	-1.22526400
H	1.22011400	2.06811900	-2.03586500
H	-0.35567700	2.83989200	-2.28310500
H	1.09493200	3.82194800	-2.05974400
H	2.55971500	-2.58873400	1.43774500
H	3.26490200	-1.25401300	2.35526200
H	1.57109500	-1.19049800	1.83532200
H	1.32828300	1.01623100	1.54732500
H	2.92620300	1.67720100	1.82909100
H	2.49075500	3.40550800	0.02385900
H	1.52912900	3.52259700	1.48778400
H	-2.14034600	2.70040400	-1.26841400
H	-2.65218400	3.88196800	-0.08207600
H	-1.81300500	0.34661200	-1.60904000
H	-3.37499000	-0.44801700	-1.39336700
H	-2.54584000	-0.16701000	2.50138500
H	2.33550600	-0.55527500	-1.83219500
H	3.56863700	1.12141200	-0.57625300
H	-0.76533100	2.99138100	1.48669800
H	0.00291200	0.38196500	-0.42820300
H	-4.08993000	1.93848800	0.04092100
H	-3.21923800	2.14173600	1.55772500
H	-2.18511900	-2.69371300	-2.11937200

Electronic energies = -929.401175868

Zero-point correction=	0.437694 (Hartree/Particle)
Thermal correction to Energy=	0.460382
Thermal correction to Enthalpy=	0.461327
Thermal correction to Gibbs Free Energy=	0.387999
Sum of electronic and zero-point Energies=	-928.963482
Sum of electronic and thermal Energies=	-928.940793
Sum of electronic and thermal Enthalpies=	-928.939849
Sum of electronic and thermal Free Energies=	-929.013177