Supporting Information

Cytotoxic Prenylated Stilbenes and Flavonoids from *Macaranga alnifolia* from the Madagascar Rain Forest

Brent Yoder, Shugeng Cao, Andrew Norris, James S. Miller, Fidy Ratovoson, Jeremi Razafitsalama, Rabodo Andriantsiferana, Vincent E. Rasamison, and David G. I. Kingston

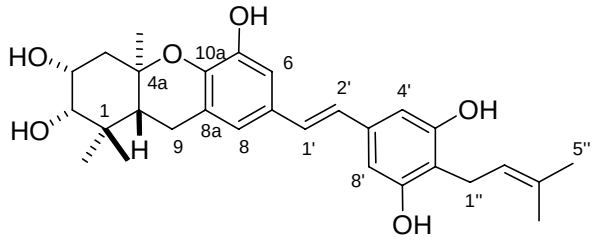
Contents:

Characterization Data for Compounds 6-10

NCI 60-Cell Line Data for Compound 1

^{1}H and ^{13}C NMR Spectra of Compounds 1-10

Characterization Data for Compounds 6-10



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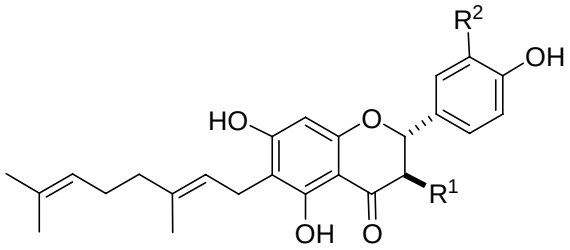

7 R^1 = OH, R^2 = H
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9 R^1 = R^2 = H
10 R^1 = H, R^2 = OH

Vedelianin (6): yellowish solid; $[\alpha]^{22}_D$ +32.9 (*c* 0.07, CH_3OH); UV (MeOH) λ_{max} 331, 224 nm; ^{1}H NMR (CD_3OD, 500 MHz) δ 6.80 (1H, d, *J* = 16.5 Hz, H-1'), 6.79 (1H, d, H-6), 6.72 (1H, d, H-8), 6.70 (1H, d, *J* = 16 Hz, H-2'), 6.44 (2H, s, H-4', 8'), 5.23 (1H, tq, *J* = 7, 1.5 Hz, H-2''), 4.15 (1H, q, *J* = 3.5 Hz, H-3), 3.30 (partially obscured by solvent, H-2, 1''), 2.75 (2H, m, H-9), 2.37 (1H, dd, *J* = 14, 3.5 Hz, H-4), 1.96 (1H, dd, *J* = 14.5, 3.5 Hz, H-4), 1.76 (3H, s, H-4''), 1.75 (1H, m, H-9a), 1.65 (3H, s, H-5''), 1.42 (3H, s, H-13), 1.11 (3H, s, H-12), 1.09 (3H, s, H-11); ^{13}C NMR (CD_3OD, 125 MHz) δ 157.3 (C-5', 7'), 147.2 (C-5), 137.6 (C-10a), 131.1 (C-3''), 130.9 (C-7), 128.6 (C-1'), 127.4 (C-2'), 124.6 (C-2''), 124.2 (C-8a), 120.4 (C-8), 115.9 (C-6'), 111.1 (C-6), 105.7 (C-4', 8'), 78.9 (C-2), 78.1 (C-4a), 71.8 (C-3), 44.8 (C-4), 39.2 (C-1), 29.4 (C-12), 26.0 (C-5''), 23.9 (C-9), 23.3 (C-1''), 22.0 (C-13), 17.9 (C-4''), 16.6 (C-11); HRFABMS *m/z* 480.2519 $[M]^+$ (calcd for $C_{25}H_{36}O_6$, 480.2512).

Bonanniol A (7): yellowish-brown solid; $[\alpha]^{23}_D$ +21.7 (*c* 0.27, CH_3OH); UV (MeOH) λ_{max} 296, 206 nm; ^{1}H NMR (CD_3OD, 500 MHz) δ 7.33 (2H, d, *J* = 8.5 Hz, H-2', 6'), 6.82 (2H, d, *J* = 8.5 Hz, H-3', 5'), 5.92 (1H, s, H-8), 5.19 (2H, t, H-2''), 5.05 (2H, t, H-7''), 4.92 (1H, d, *J* = 11.5 Hz, H-2), 4.51 (1H, d, *J* = 11.5 Hz, H-3), 3.21 (2H, d, H-1''), 2.03 (2H, q, H-6''), 1.94 (2H, t, *J* = 8 Hz, H-5''), 1.74 (3H, s, H-4''), 1.61 (3H, s, H-9''), 1.55 (3H, s, H-10''); ^{13}C NMR (CD_3OD, 125 MHz) δ 197.2 (C-4), 165.0 (C-7), 160.9 (C-5), 160.9 (C-9), 157.8 (C-4'), 134.0 (C-3''), 130.7 (C-8''), 129.0 (C-2', 6'), 128.1 (C-1'), 124.2 (C-7''),

122.5 (C-2''), 114.8 (C-3'), 114.8 (C-5'), 108.8 (C-6), 100.3 (C-10), 94.3 (C-8), 83.6 (C-2), 72.4 (C-3), 39.6 (C-5''), 26.4 (C-6''), 24.5 (C-9''), 20.5 (C-1''), 16.4 (C-10''), 14.9 (C-4''); HRFABMS *m/z* 425.1929 $[M+H]^+$ (calcd for $C_{25}H_{29}O_6$, 425.1964).

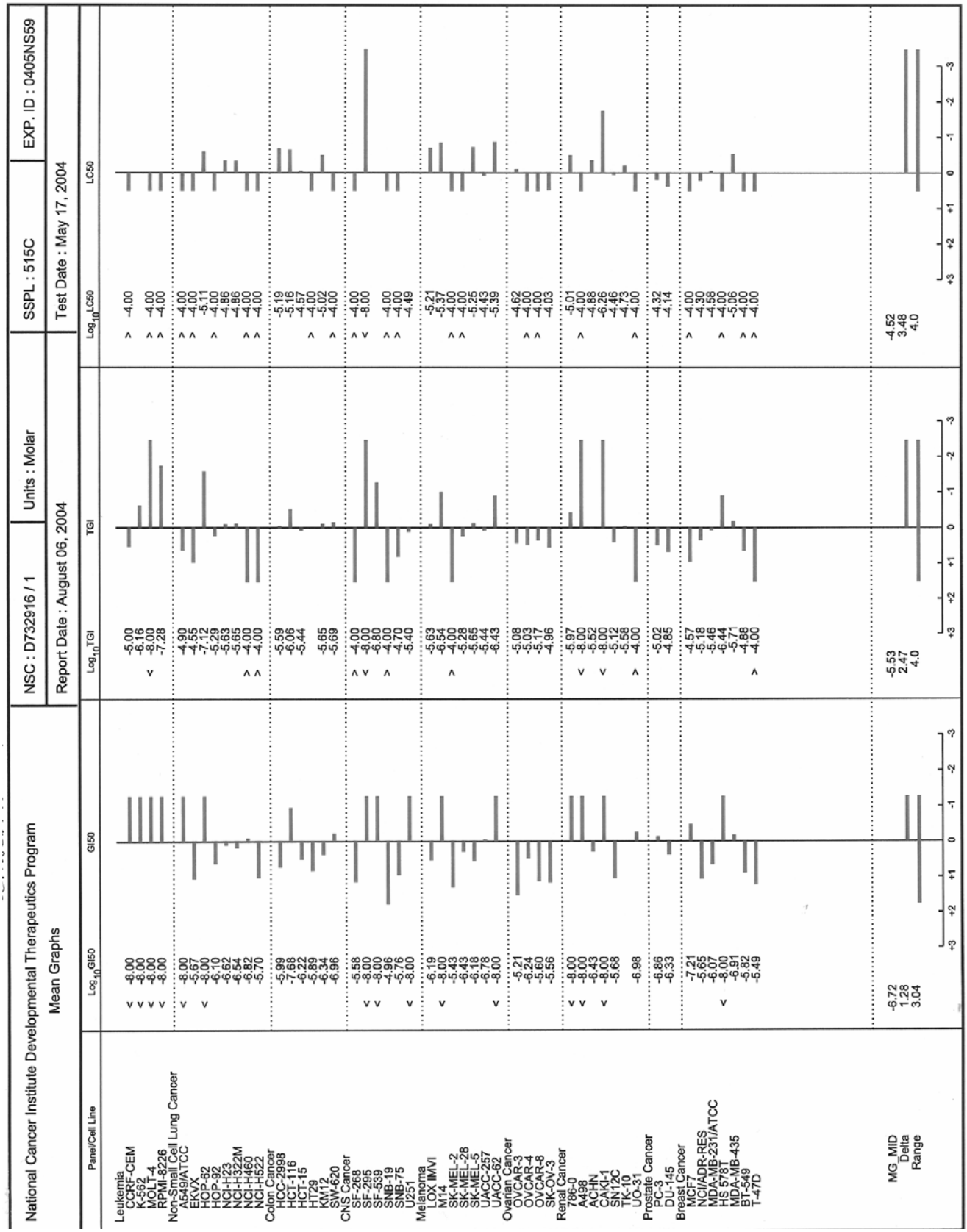
Diplacol (8): yellowish-brown solid; $[\alpha]^{23}_D$ +18.6 (*c* 0.44, CH_3OH); UV (MeOH) λ_{max} 295, 215 nm; ^1H NMR (CD_3OD, 500 MHz) δ 6.95 (1H, s, H-2'), 6.83 (1H, dd, H-5'), 6.79 (1H, d, H-6'), 5.91 (1H, s, H-8), 5.19 (2H, t, H-2''), 5.06 (2H, t, H-7''), 4.47 (1H, d, *J* = 11.5 Hz, H-3), 3.22 (2H, d, *J* = 7 Hz, H-1''), 2.04 (2H, q, H-6''), 1.95 (2H, t, *J* = 8 Hz, H-5''), 1.75 (3H, s, H-4''), 1.61 (3H, s, H-9''), 1.56 (3H, s, H-10''); ^{13}C NMR (CD_3OD, 125 MHz) δ 197.1 (C-4), 165.0 (C-7), 160.9 (C-5), 160.9 (C-9), 145.8 (C-4'), 145.0 (C-3'), 134.1 (C-3''), 130.7 (C-8''), 128.7 (C-1'), 124.2 (C-7''), 122.5 (C-2''), 119.6 (C-6'), 114.8 (C-5'), 114.6 (C-2'), 108.7 (C-6), 100.4 (C-10), 94.2 (C-8), 83.8 (C-2), 72.5 (C-3), 39.6 (C-5''), 26.4 (C-6''), 24.5 (C-9''), 20.5 (C-1''), 16.4 (C-10''), 14.9 (C-4''); HRFABMS *m/z* 425.1948 $[M+H]^+$ (calcd for $C_{25}H_{29}O_6$, 425.1964).

Bonannione A (9): yellowish-brown solid; $[\alpha]^{23}_D$ 0 (*c* 0.08, CH_3OH); UV (MeOH) λ_{max} 294, 207 nm; ^1H NMR (CD_3OD, 500 MHz) δ 7.30 (2H, d, *J* = 8.5 Hz, H-2', 6'), 6.81 (2H, d, *J* = 8.5 Hz, H-3', 5'), 5.92 (1H, s, H-8), 5.30 (1H, dd, H-2), 5.18 (2H, t, H-2''), 5.06 (2H, t, H-7''), 3.20 (2H, d, *J* = 7 Hz, H-1''), 3.09 (1H, dd, *J* = 13 Hz, H-3a), 2.66 (1H, dd, *J* = 17, 3 Hz, H-3b), 2.04 (2H, q, H-6''), 1.94 (2H, t, *J* = 8 Hz, H-5''), 1.74 (3H, s, H-4''), 1.61 (3H, s, H-9''), 1.56 (3H, s, H-10''); ^{13}C NMR (CD_3OD, 125 MHz) δ 196.4 (C-4), 165.0 (C-7), 161.2 (C-5), 161.1 (C-9), 157.7 (C-4'), 133.9 (C-3''), 130.7 (C-8''), 130.0 (C-1'), 127.7 (C-2', 6'), 124.2 (C-7''), 122.7 (C-2''), 115.0 (C-3', 5'), 108.4 (C-6), 101.8 (C-10), 94.2 (C-8), 79.1 (C-2), 42.9 (C-3), 39.6 (C-5''), 26.4 (C-6''), 24.5 (C-9''), 20.5 (C-1''), 16.4 (C-10''), 14.9 (C-4''); HRFABMS *m/z* 409.1813 $[M+H]^+$ (calcd for $C_{25}H_{29}O_5$, 409.2015).

Diplacone (10): yellowish-brown solid; $[\alpha]^{23}_D$ –13.2 (*c* 0.33, CH_3OH); UV (MeOH) λ_{max} 292, 207 nm; ^1H NMR (CD_3OD, 500 MHz) δ 6.90 (1H, s, H-2'), 6.77 (2H, s, H-5', 6'), 5.93 (1H, s, H-8), 5.23

(1H, dd, H-2), 5.18 (2H, t, H-2''), 5.05 (2H, t, H-7''), 3.20 (2H, d, *J* = 7.5 Hz, H-1''), 3.03 (1H, dd, *J* = 17, 13 Hz, H-3a), 2.66 (1H, dd, *J* = 17, 3 Hz, H-3b), 2.04 (2H, q, *J* = 7.5 Hz, H-6''), 1.94 (2H, t, *J* = 8 Hz, H-5''), 1.74 (3H, s, H-4''), 1.61 (3H, s, H-9''), 1.55 (3H, s, H-10''); ^{13}C NMR (CD_3OD, 125 MHz) δ 196.5 (C-4), 164.7 (C-7), 161.2 (C-5), 161.2 (C-9), 145.5 (C-4'), 145.2 (C-3'), 133.9 (C-3''), 130.6 (C-8''), 127.7 (C-1'), 124.2 (C-7''), 122.6 (C-2''), 117.9 (C-6'), 114.9 (C-5'), 113.4 (C-2'), 108.4 (C-6), 101.9 (C-10), 94.1 (C-8), 79.1 (C-2), 42.9 (C-3), 39.6 (C-5''), 26.4 (C-6''), 24.5 (C-9''), 20.5 (C-1''), 16.4 (C-10''), 14.9 (C-4''); HRFABMS *m/z* 441.1911 $[M+H]^+$ (calcd for $C_{25}H_{29}O_7$, 449.1913).

NCI 60-Cell Line Data for Compound 1



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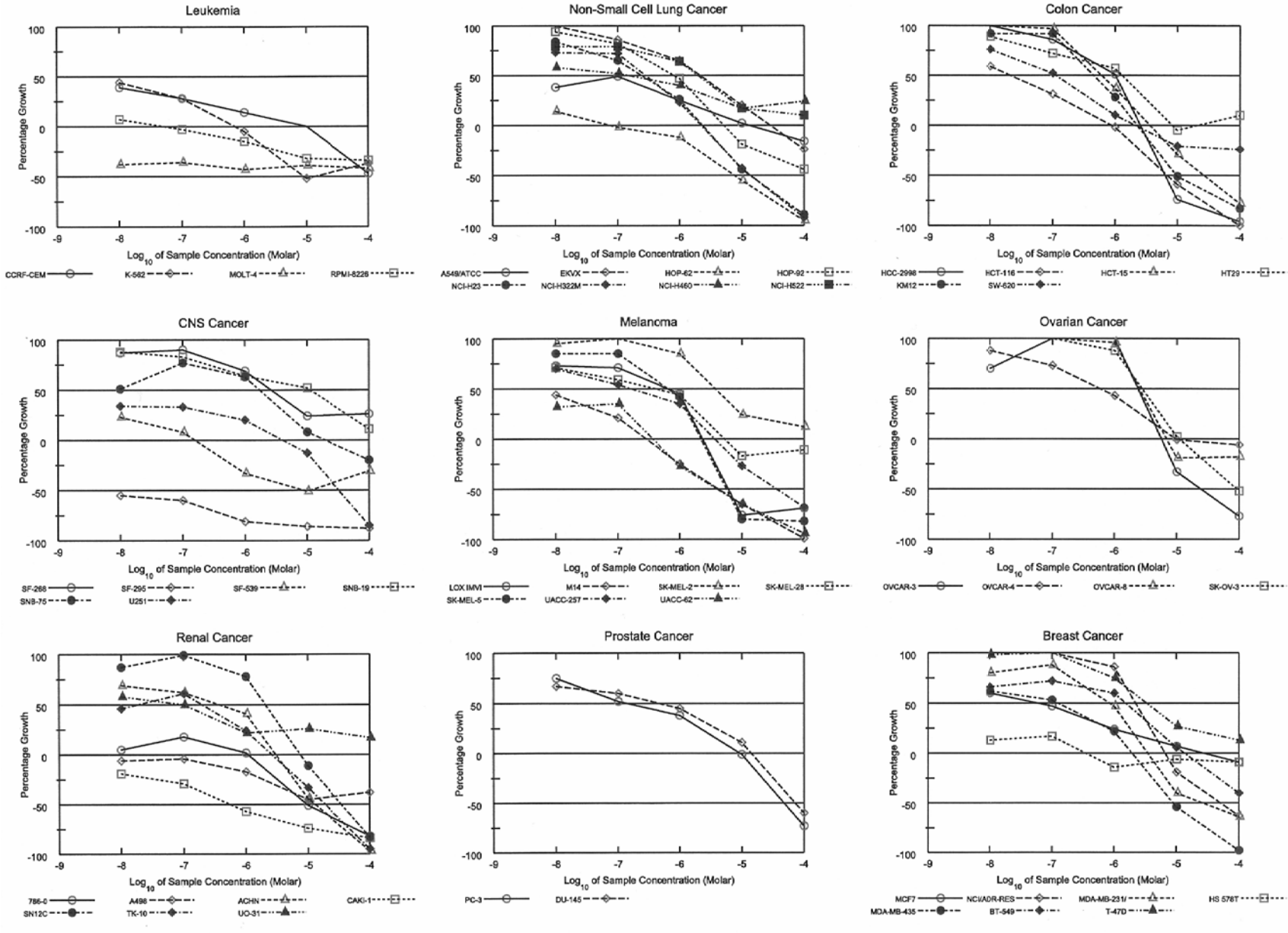

^{1}H and ^{13}C NMR Spectra of Compounds 1-10

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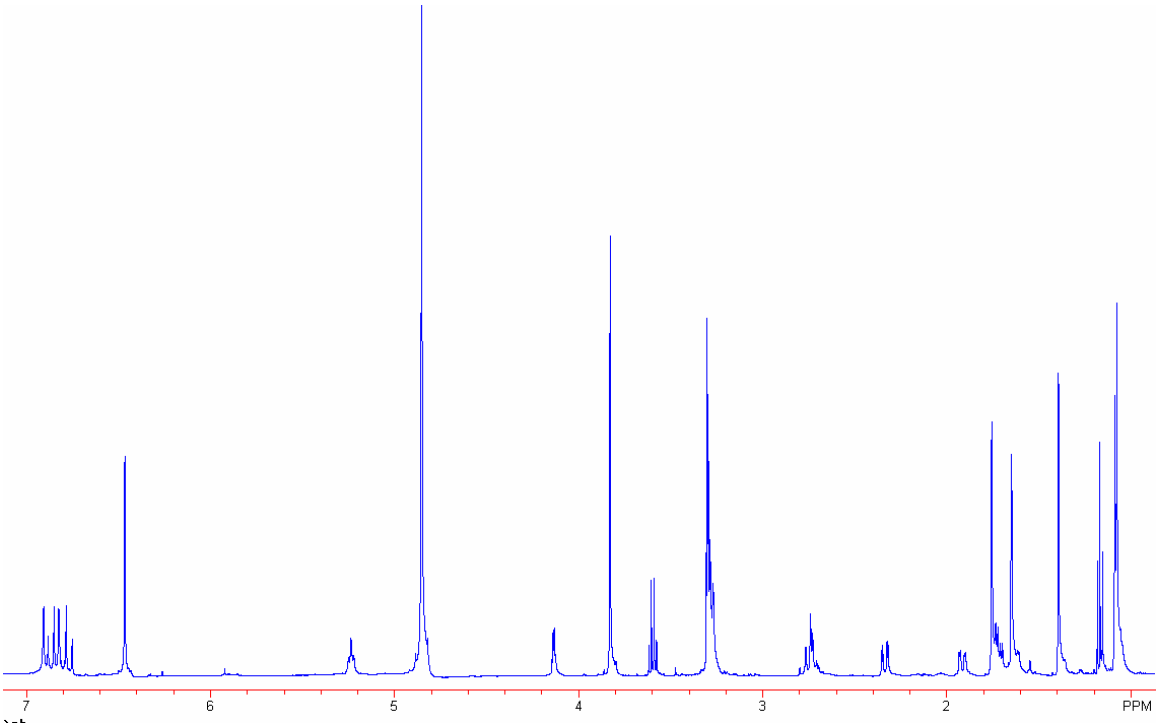

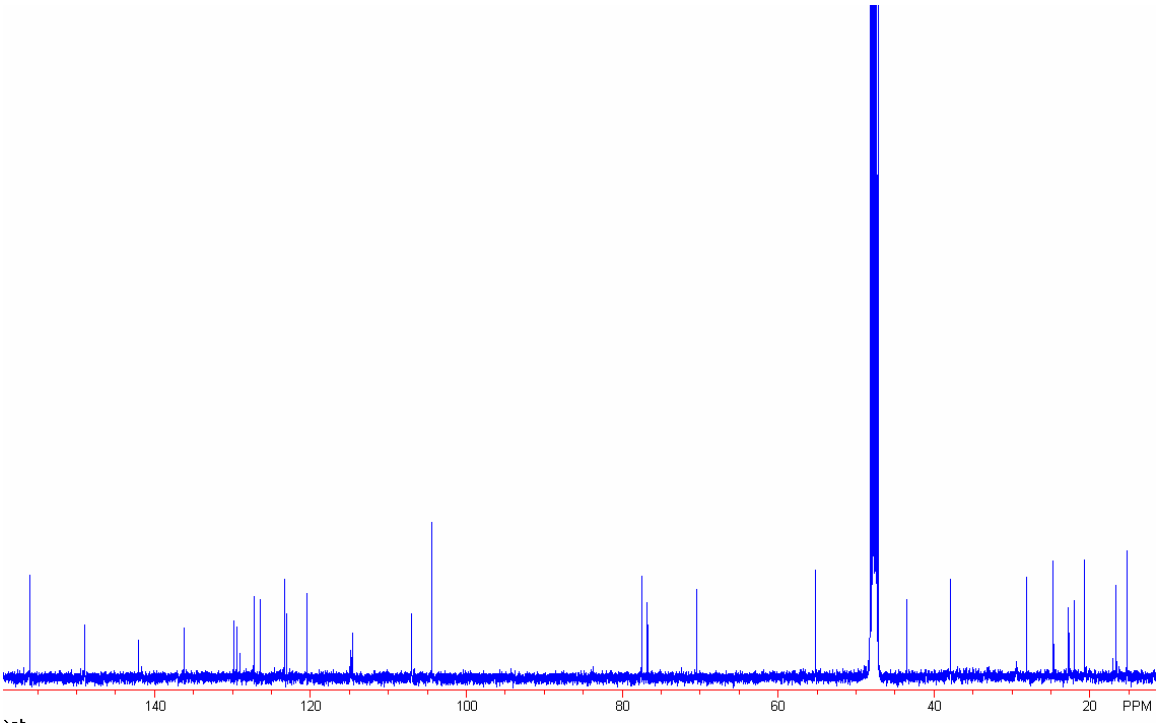

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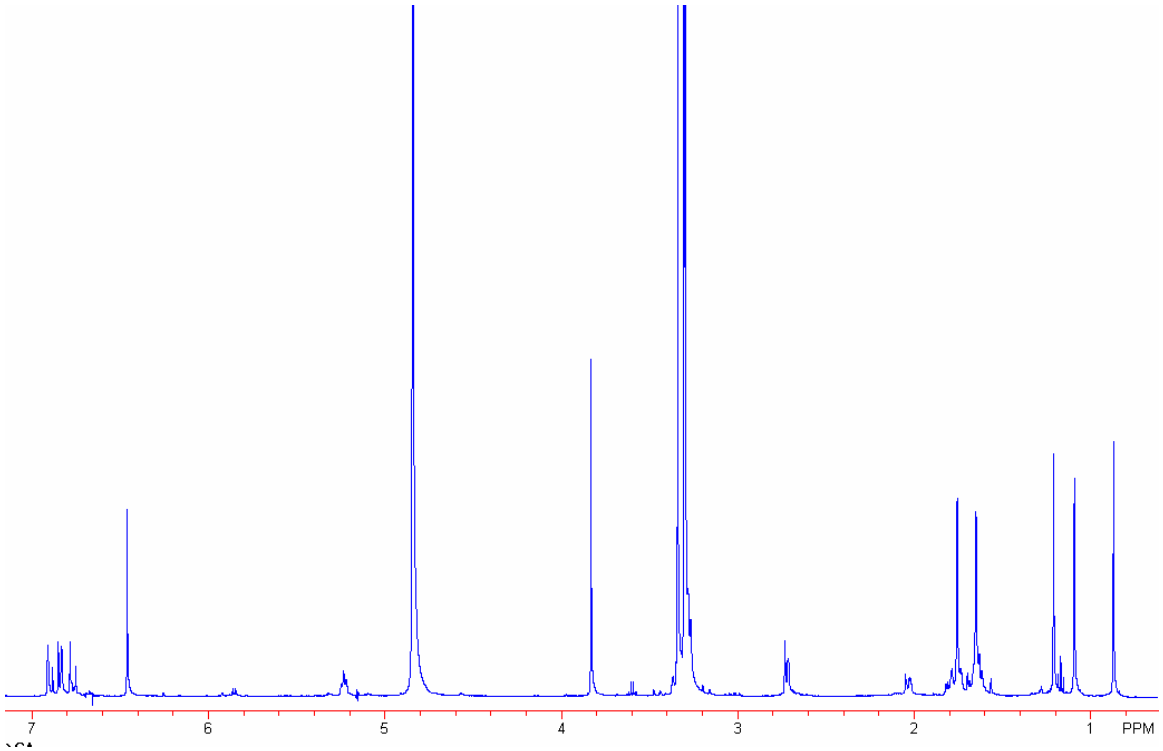

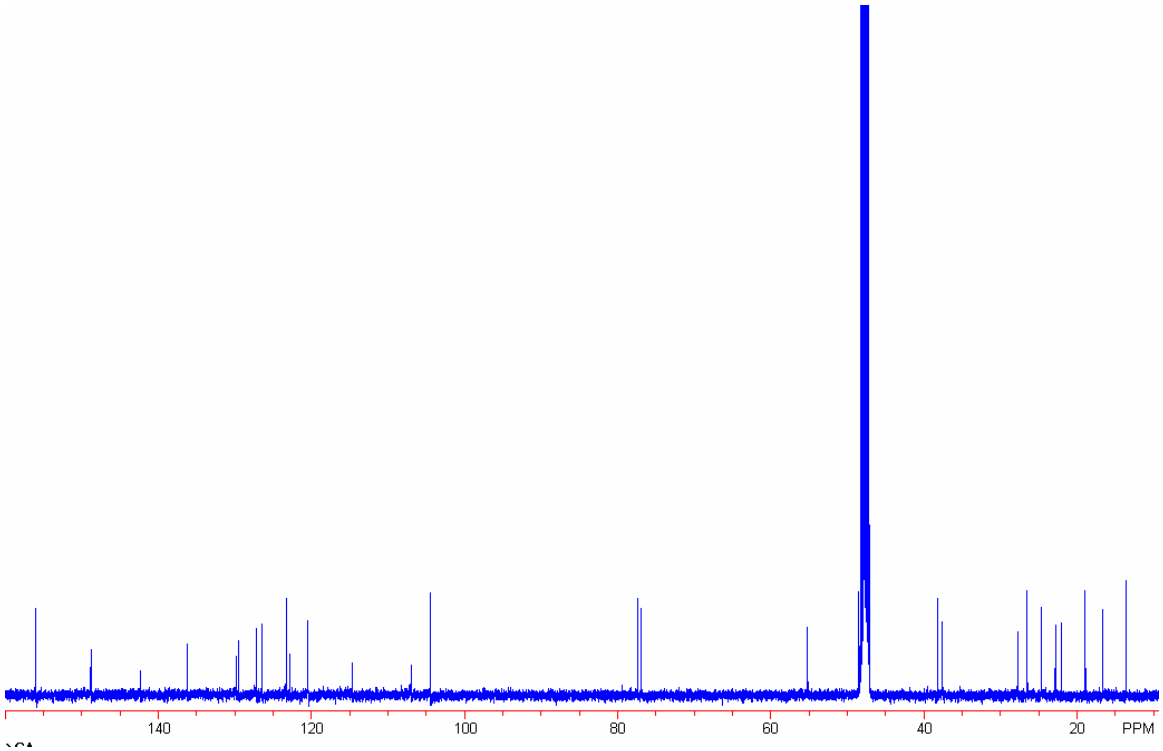

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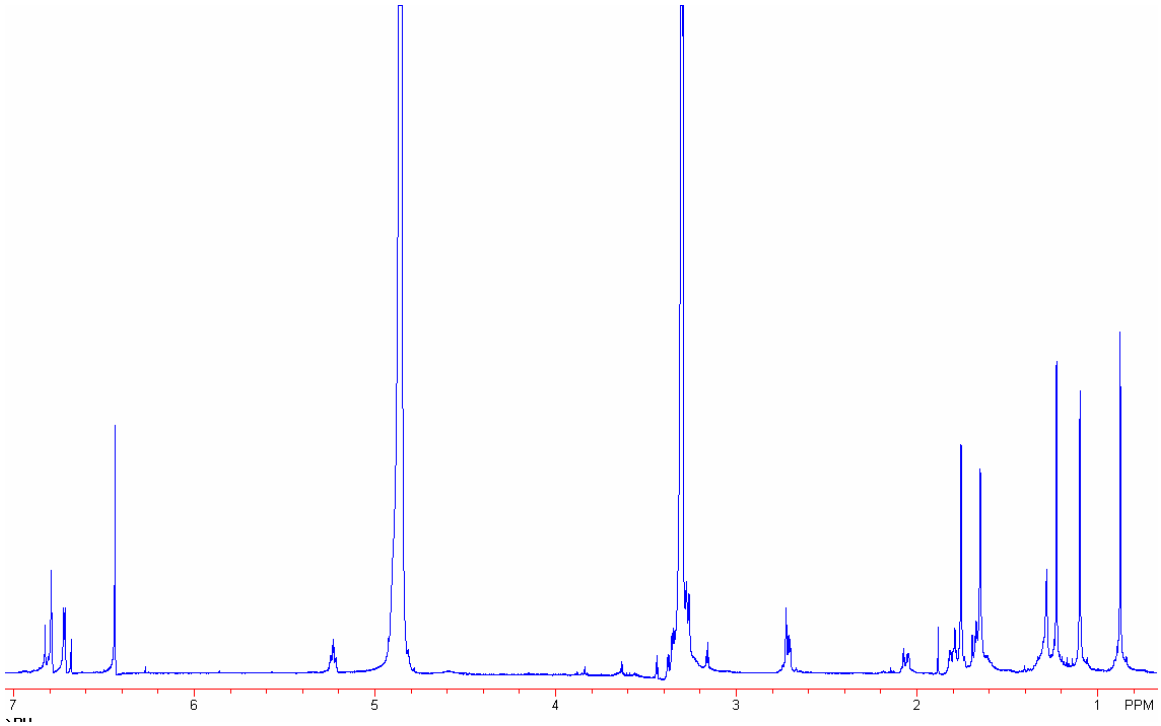

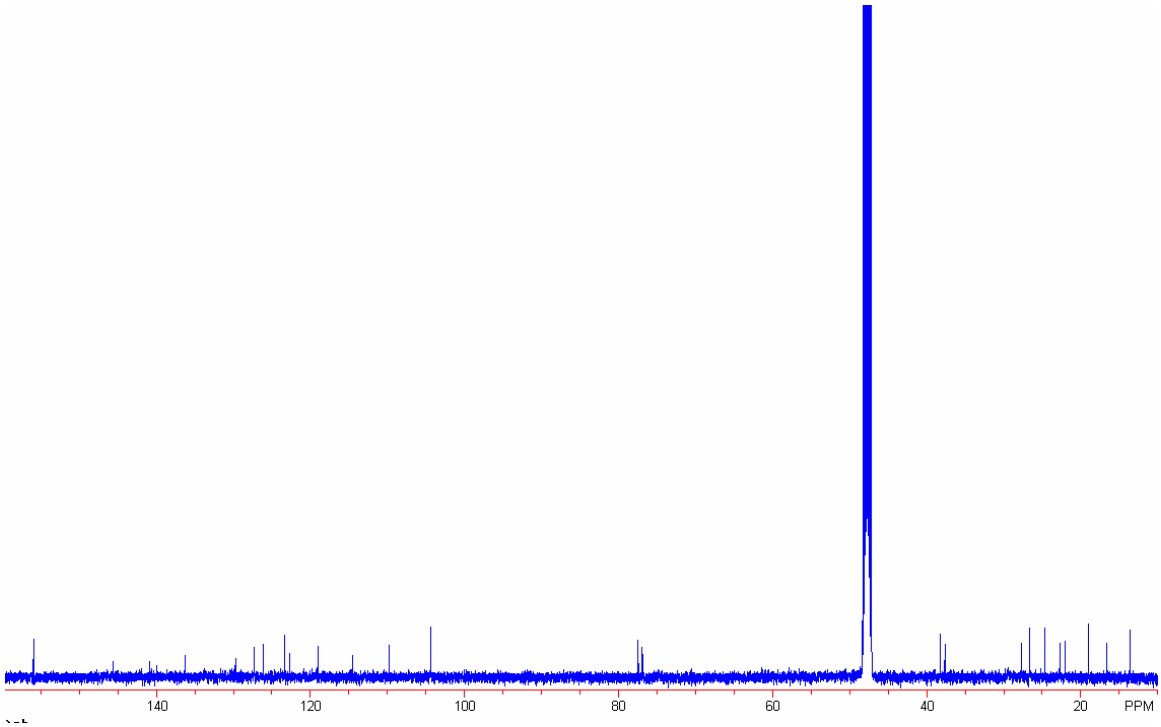

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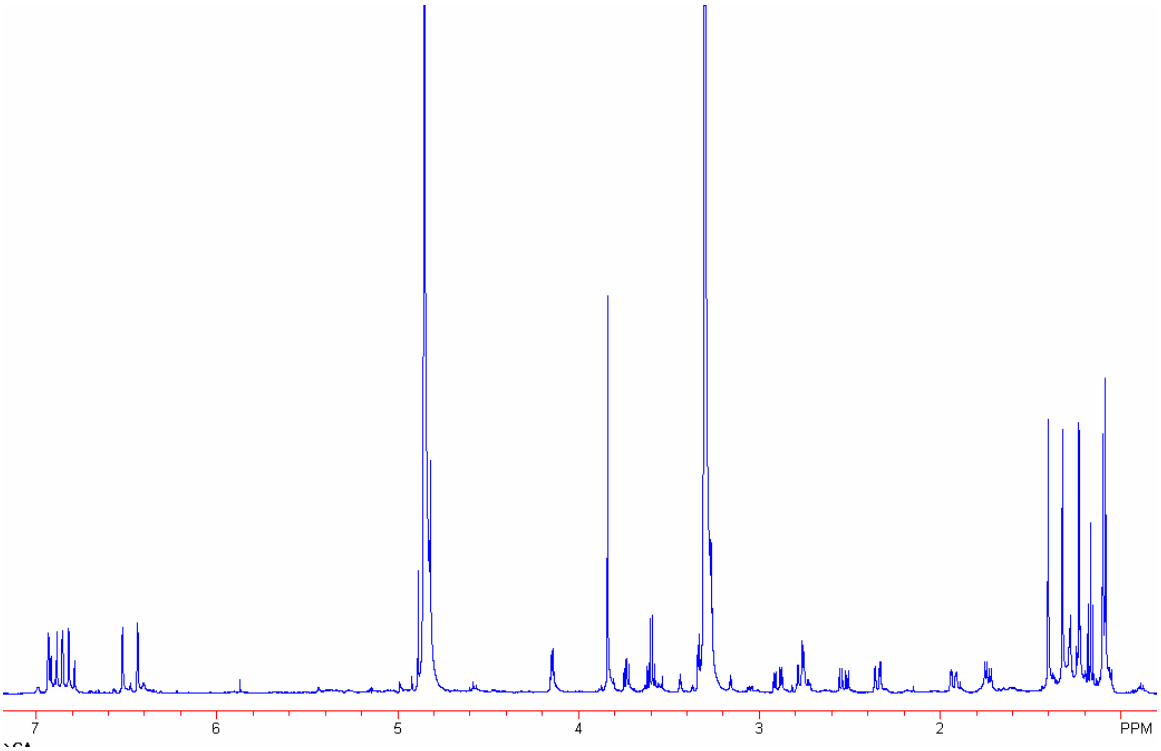

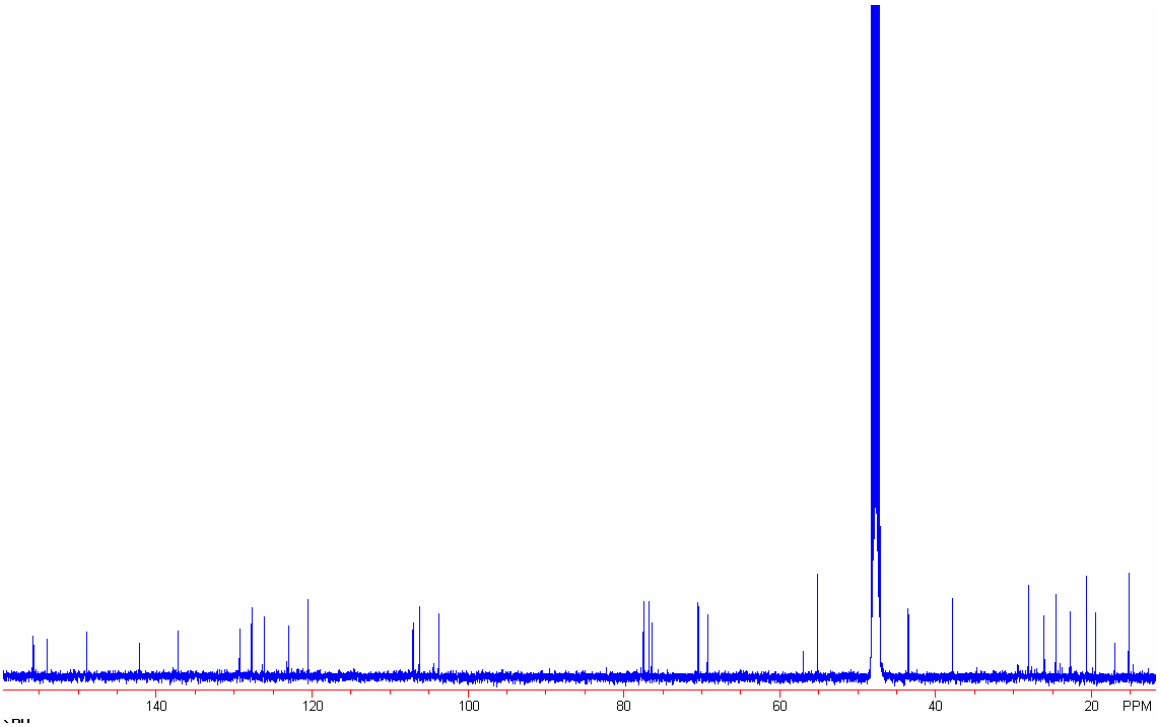

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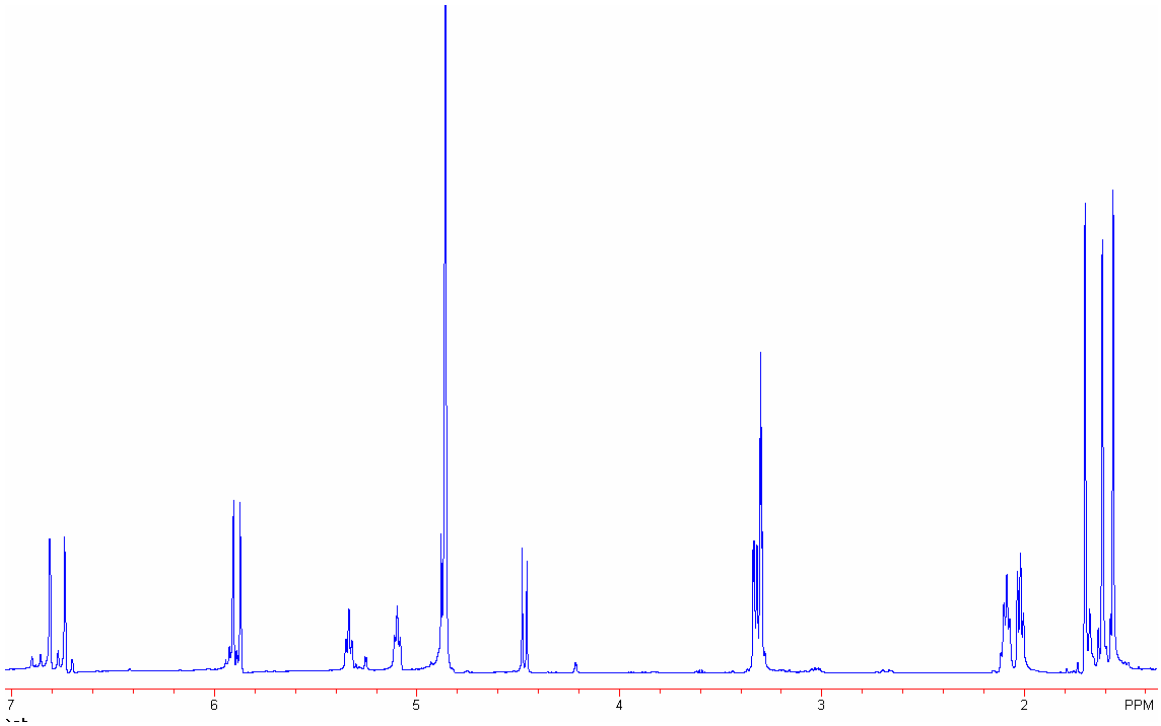

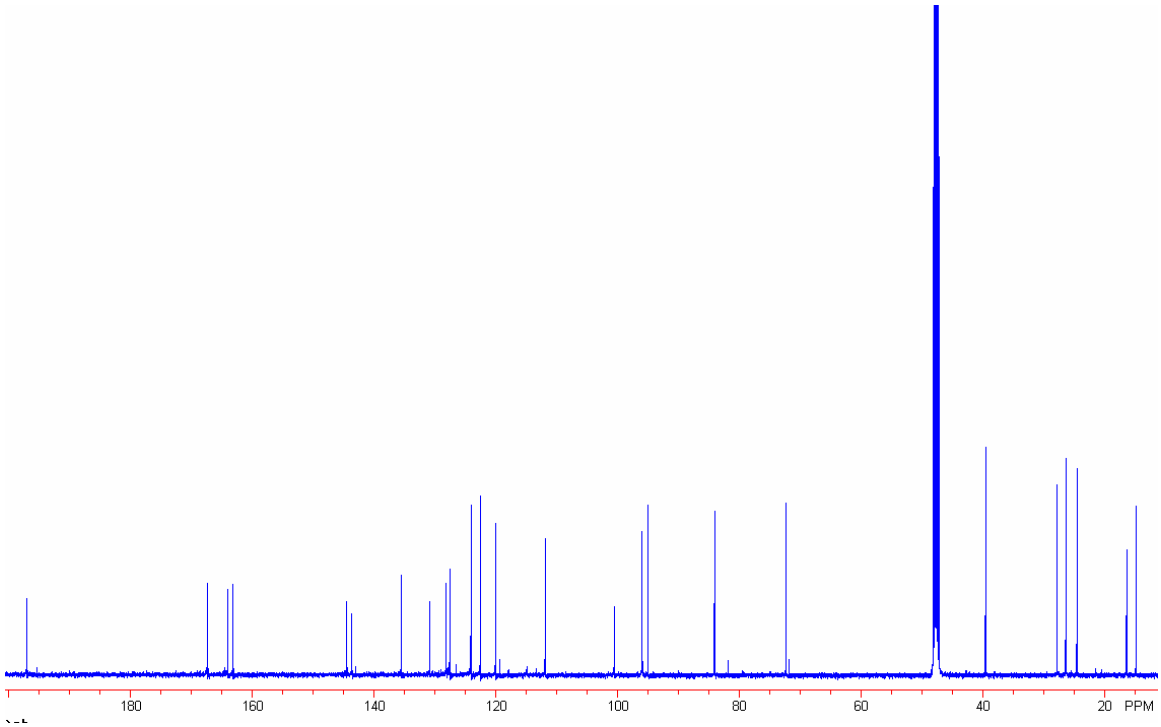

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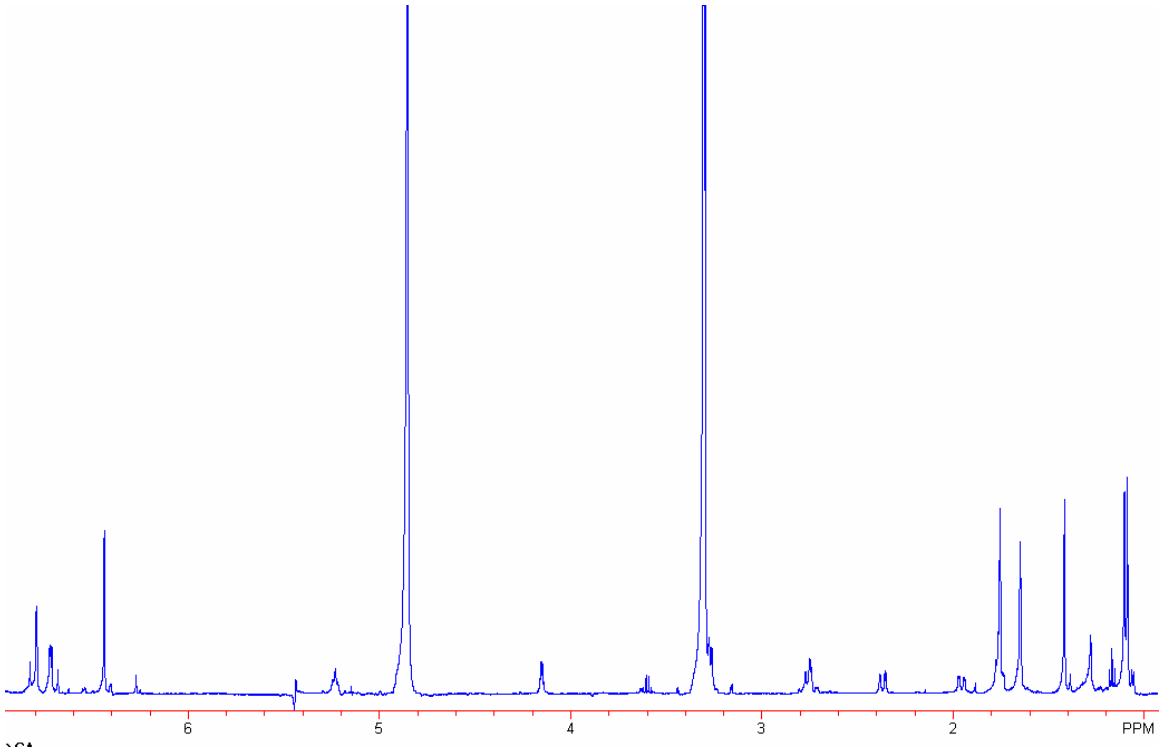

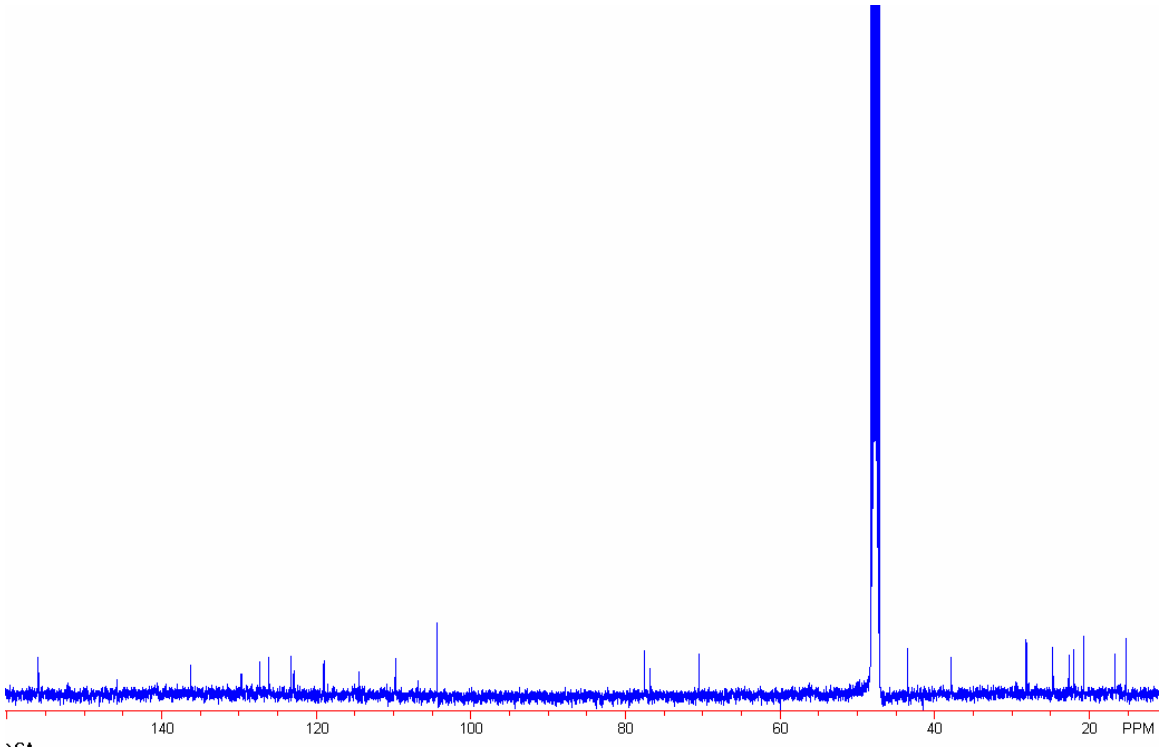

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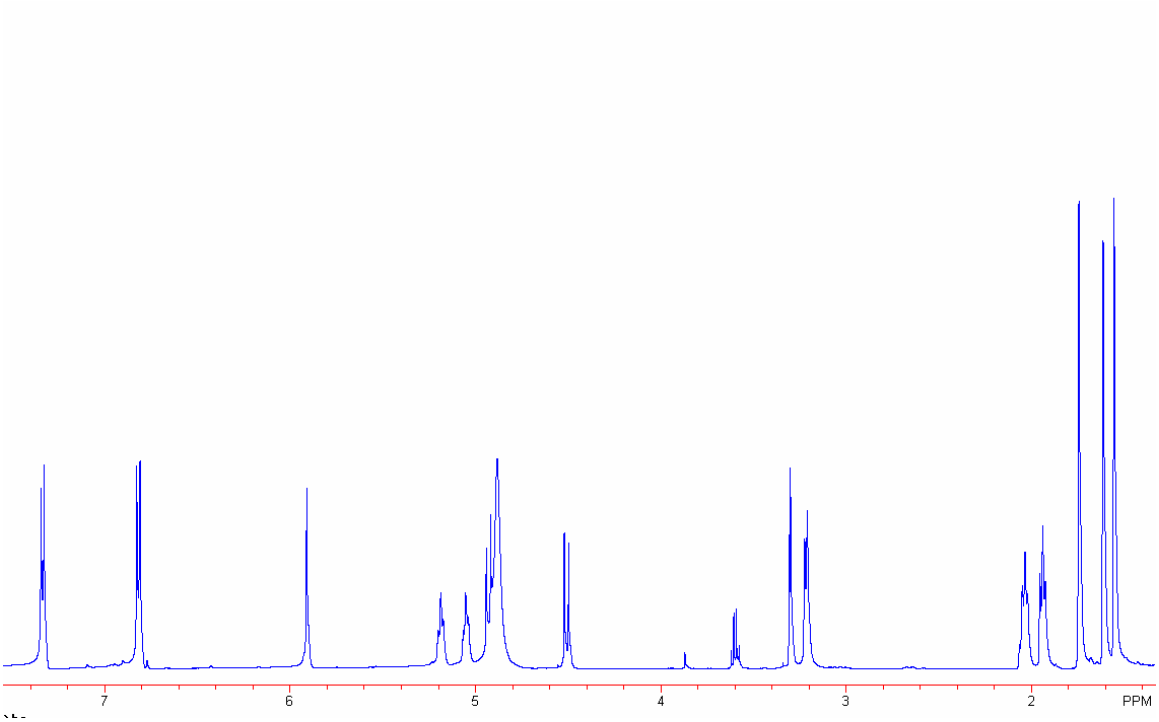

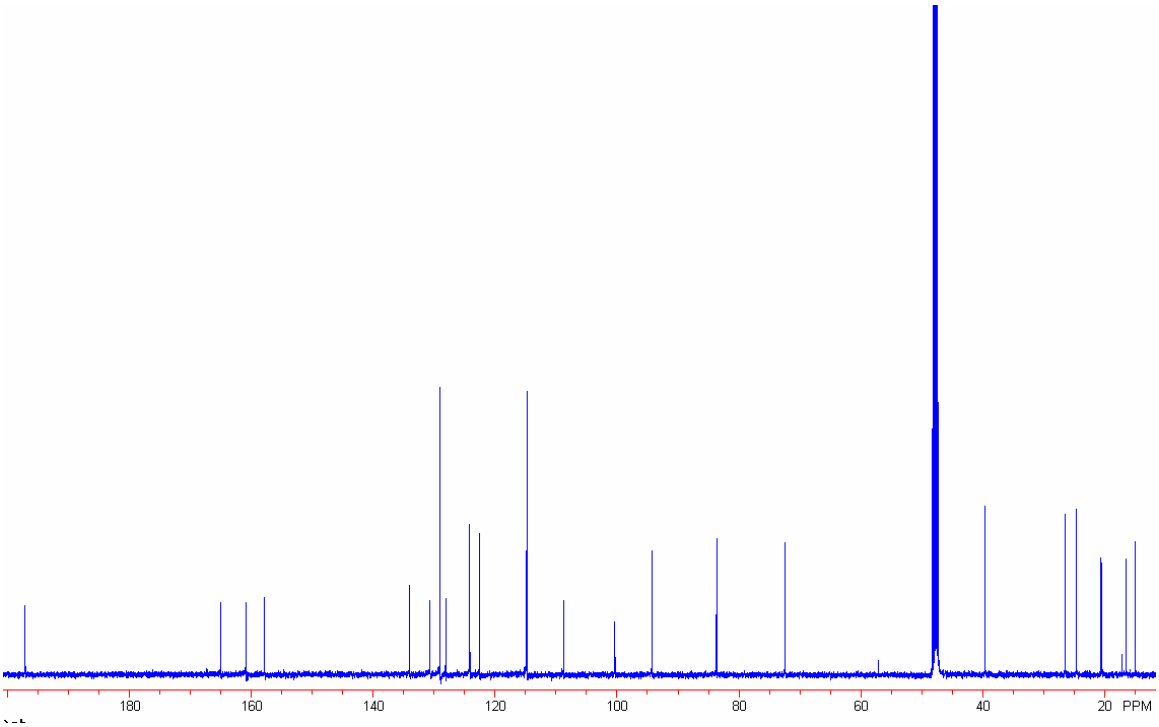

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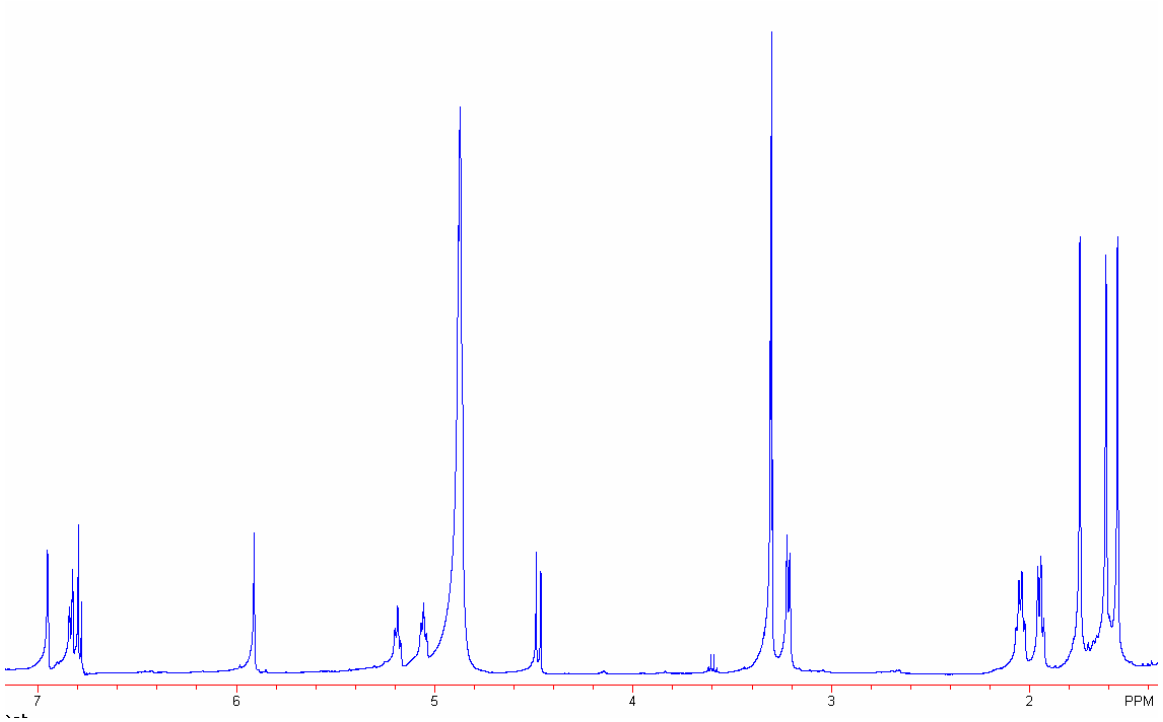
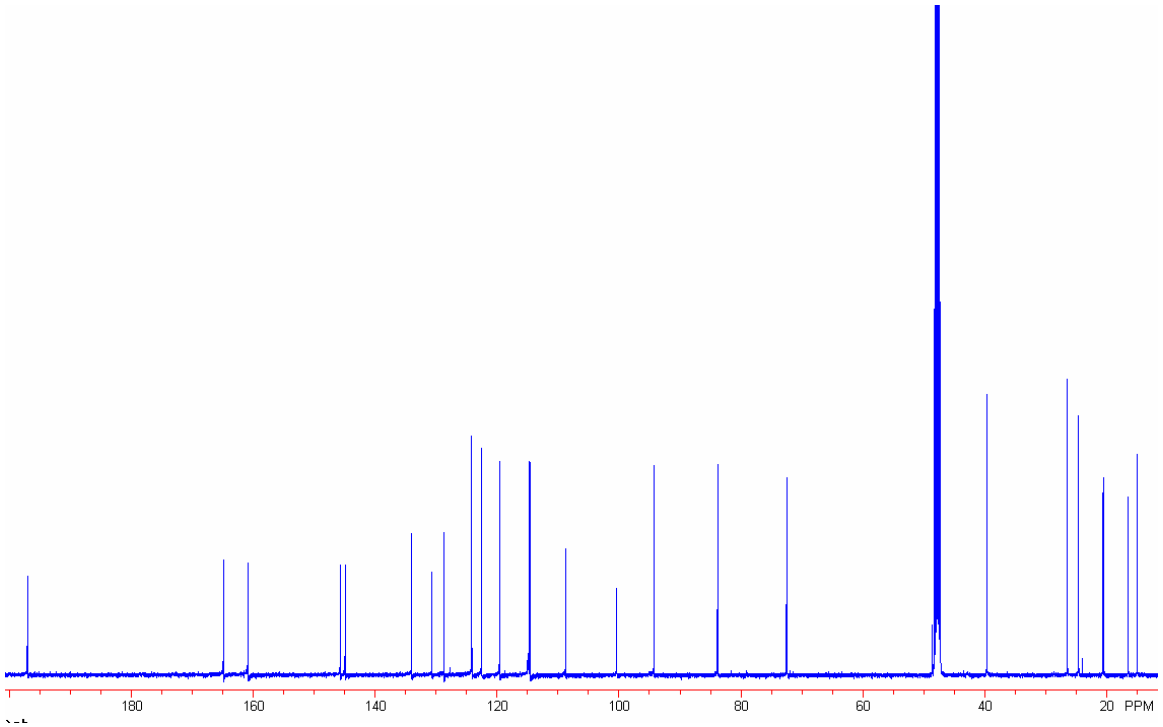
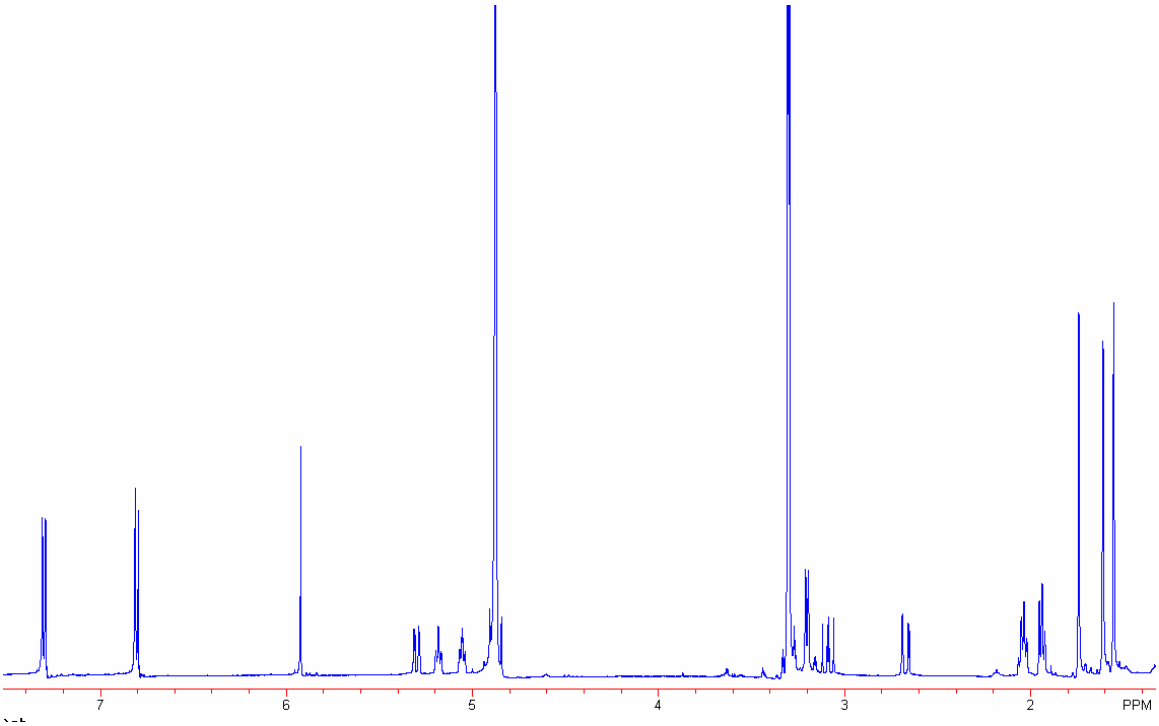
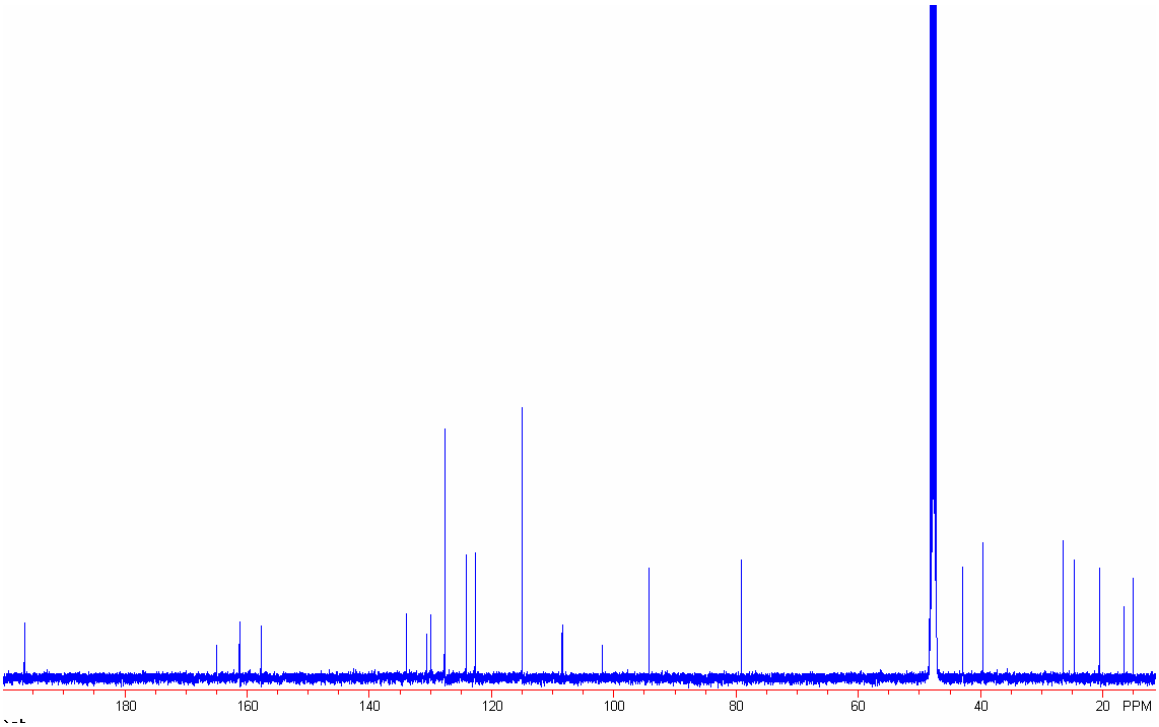


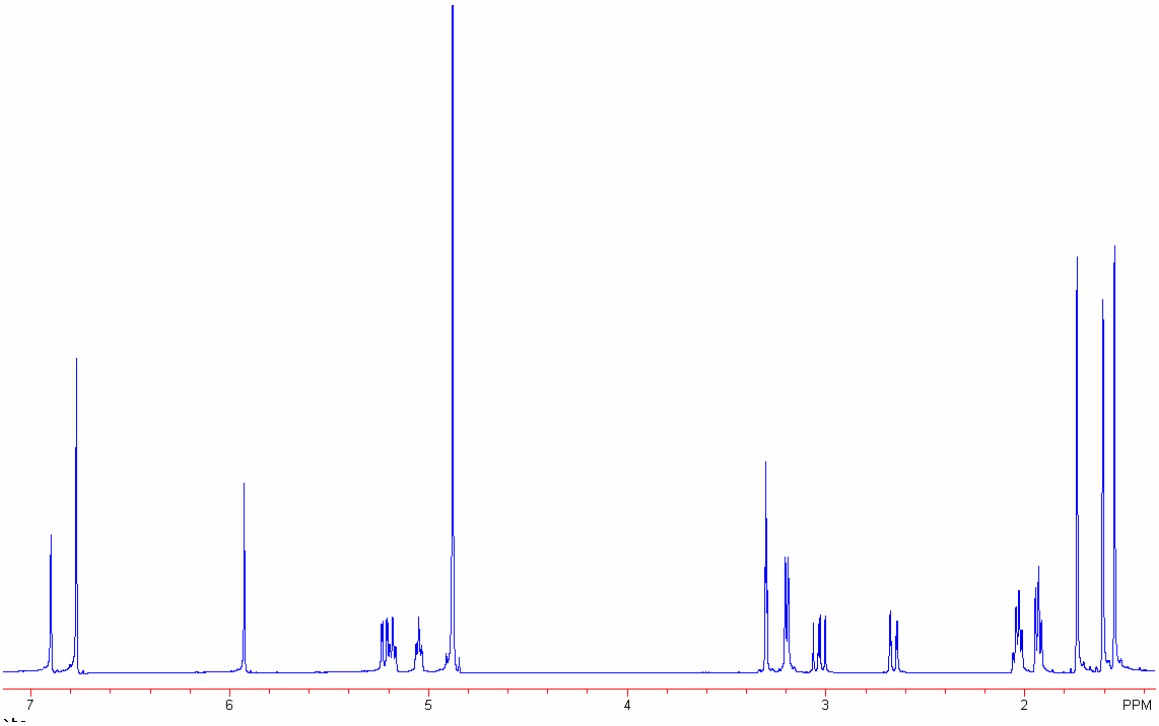


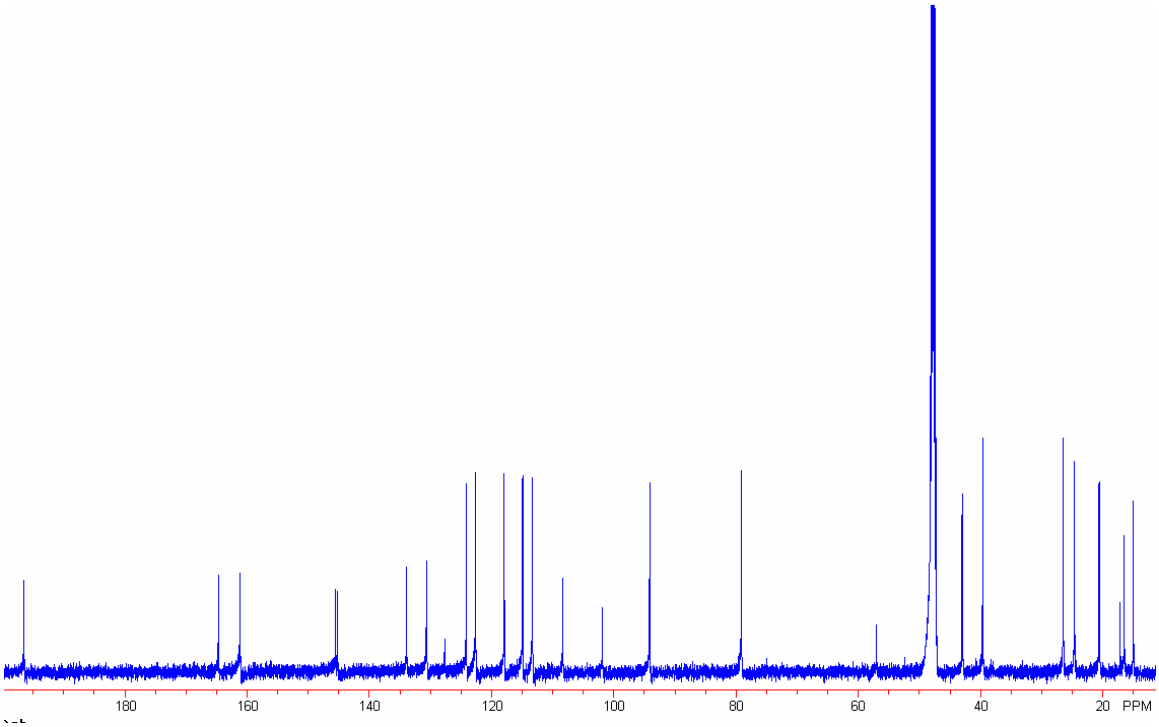
Bonannione A (**9**)





Diplacone (**10**)





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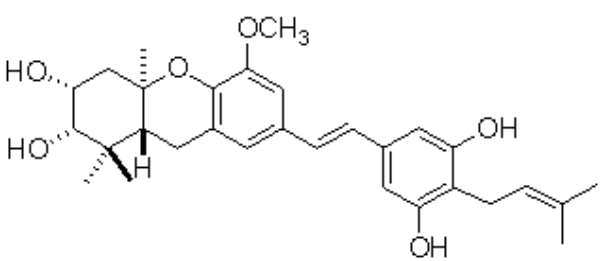
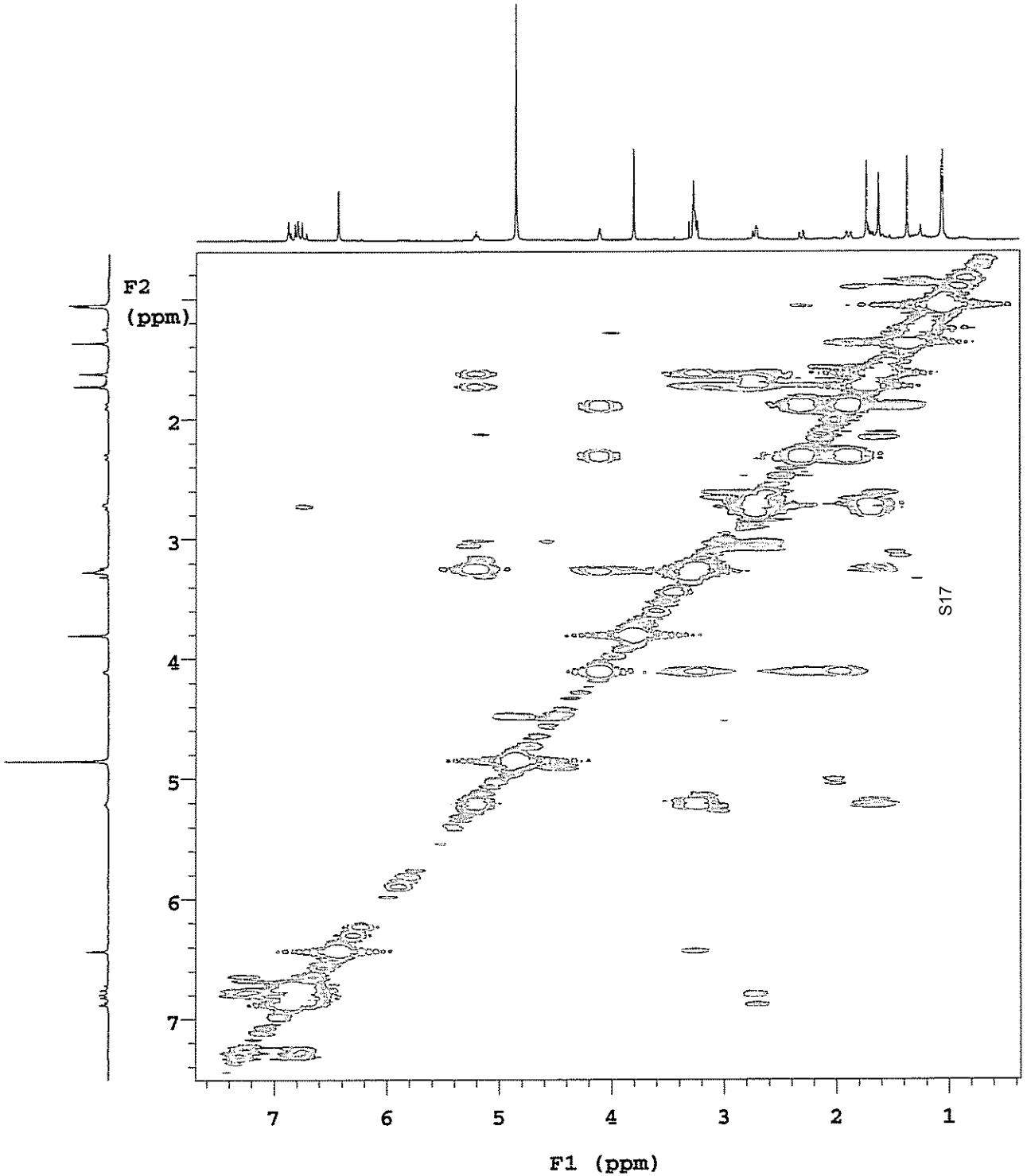
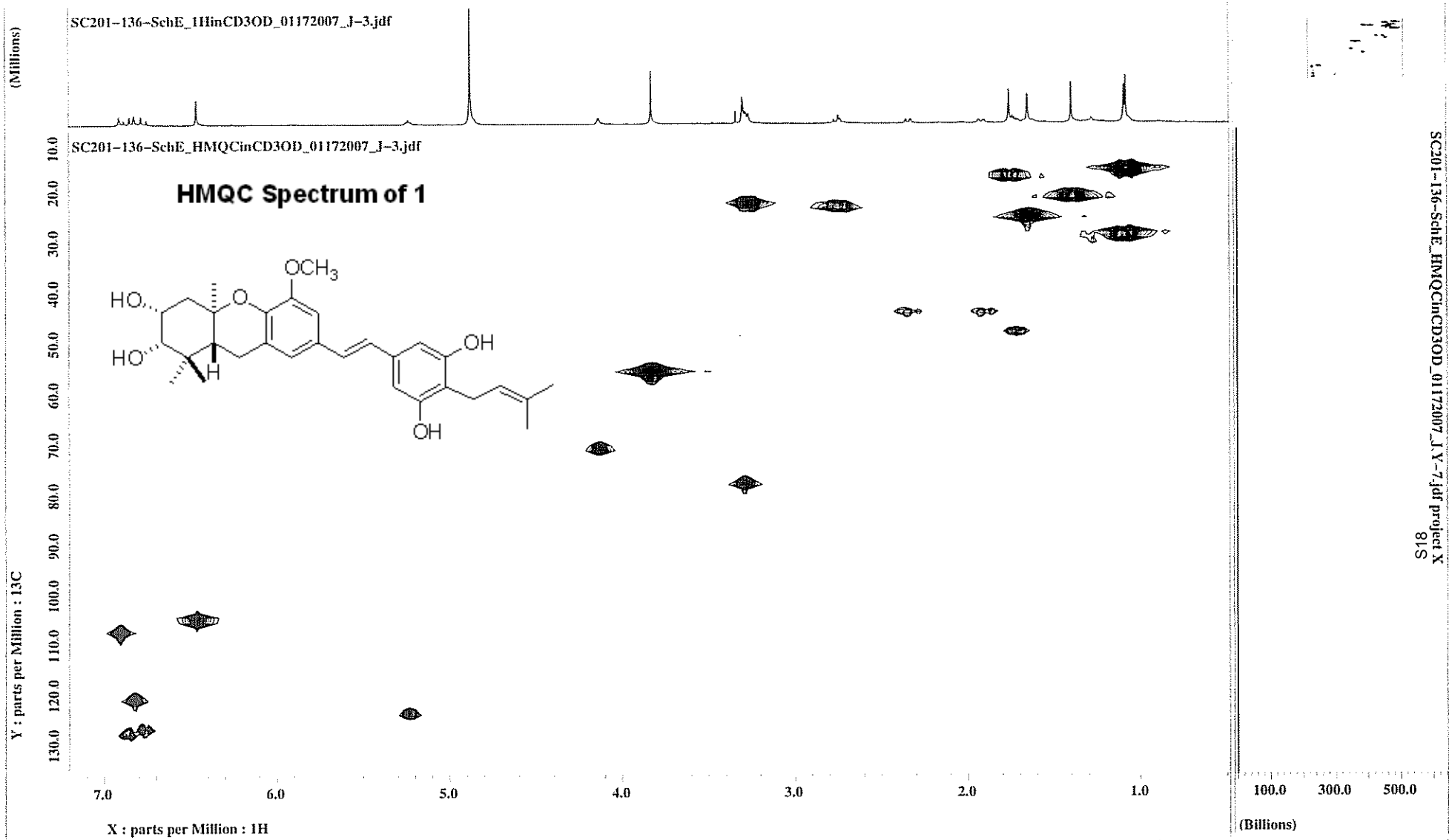
Jan 17 2007
VA Tech Chemistry NMR Lab

gCOSY Spectrum of 1







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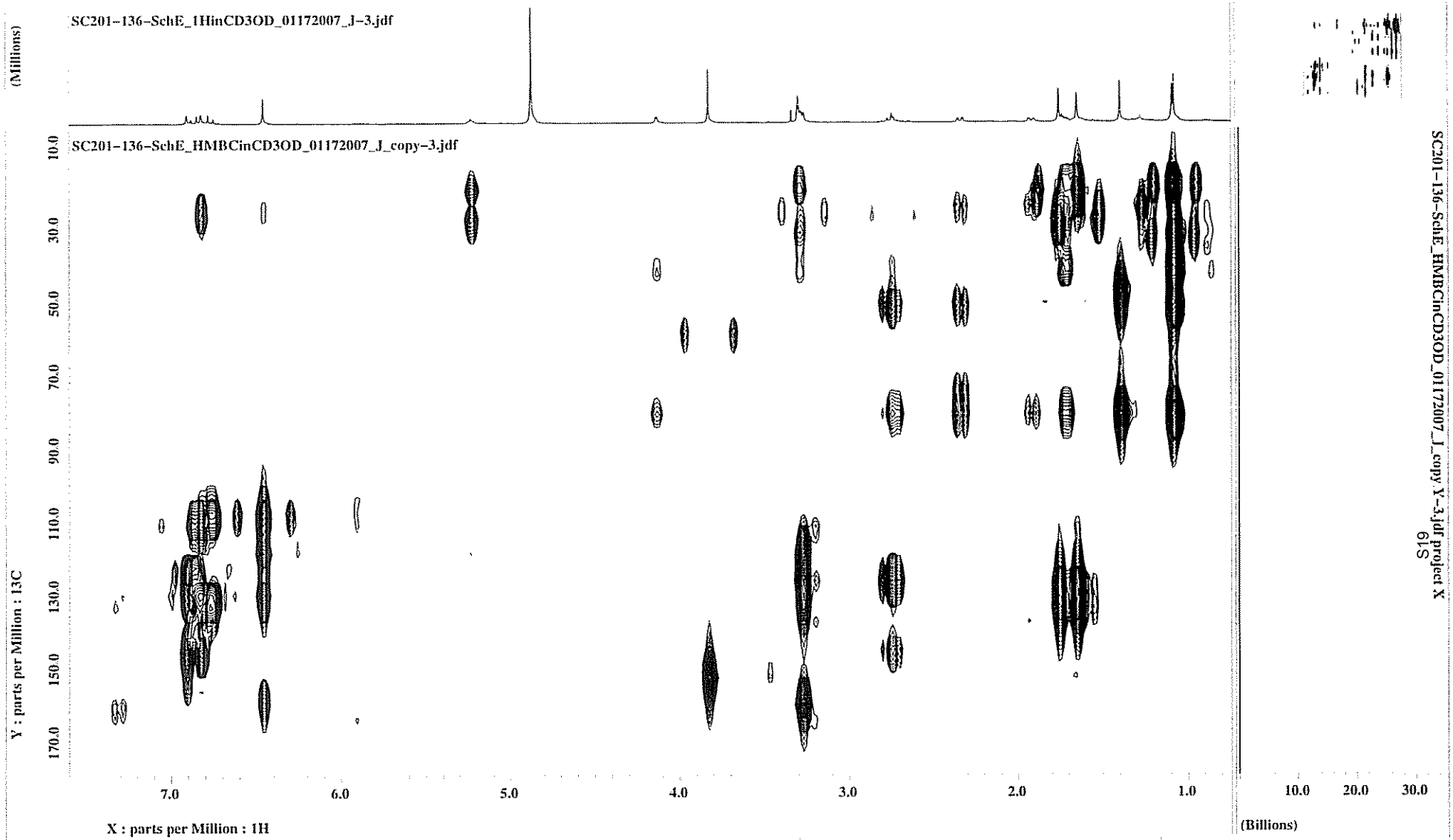
JEOL



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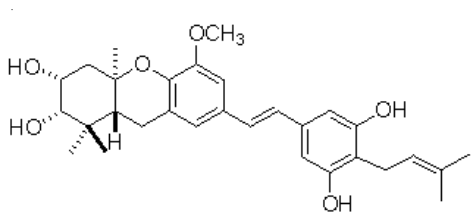
HMBC Spectrum of 1



JEOL

STANDARD 1H OBSERVE

Pulse Sequence: ROESY

Solvent: CD3OD
Ambient temperature
File: SC201-136-SchE_ROESY_011807_1
INOVA-400 "inova400alt"

Relax. delay 1.000 sec
Mixing 0.200 sec
Acq. time 0.158 sec
Width 6499.8 Hz
2D Width 6499.8 Hz
10 repetitions
2 x 200 increments
OBSERVE H1, 399.9456944 MHz
DATA PROCESSING
Gauss apodization 0.073 sec
F1 DATA PROCESSING
Gauss apodization 0.028 sec
FT size 2048 x 2048
Total time 1 hr, 33 min, 42 sec
Jan 18 2007
VA Tech Chemistry NMR Lab

ROESY Spectrum of 1