

Supplementary Materials

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Mass Spectrum SmartFormula Report

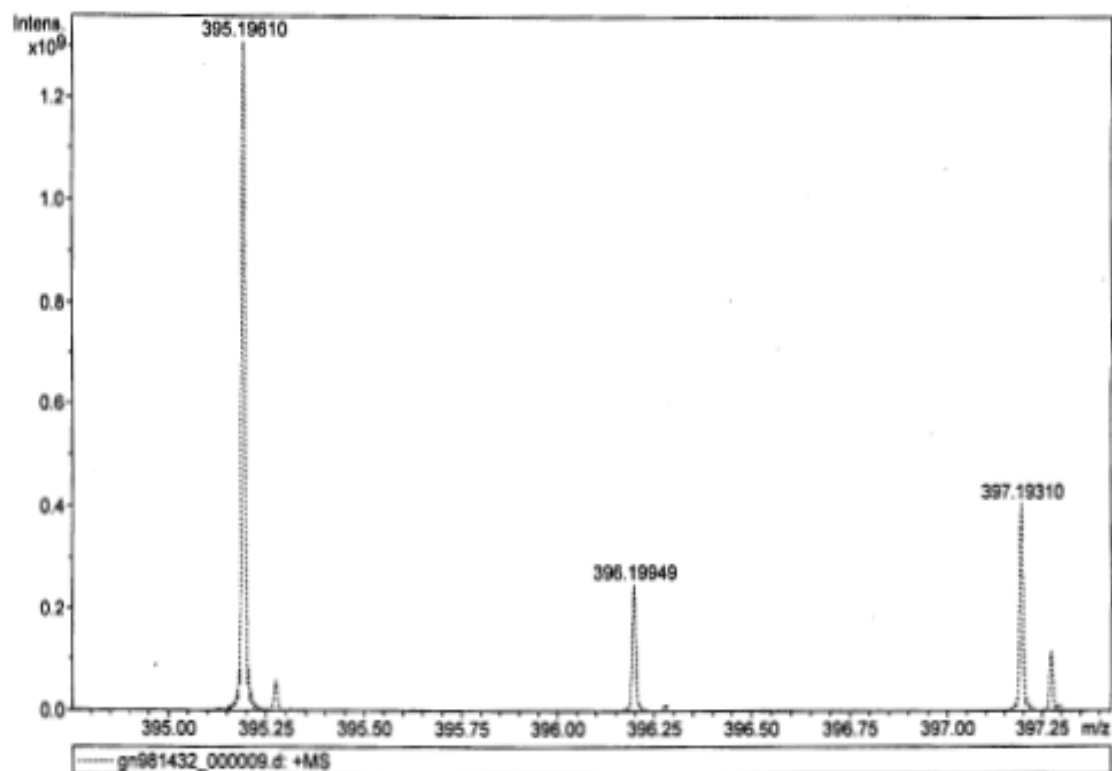
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Analysis Info

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Method broadband first signal
Sample Name GN98-14-3-2
Comment ESI Positive

11/25/2014 11:18:12 AM

Instrument: FT-MS solarix



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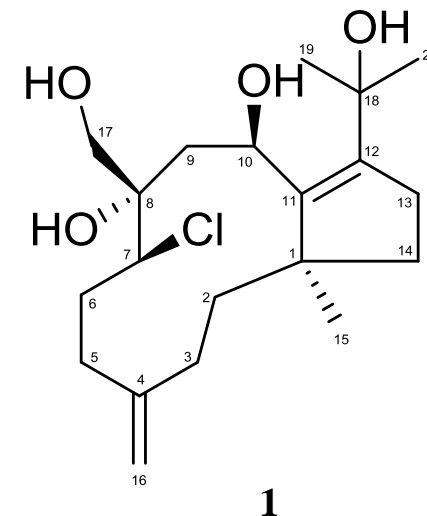
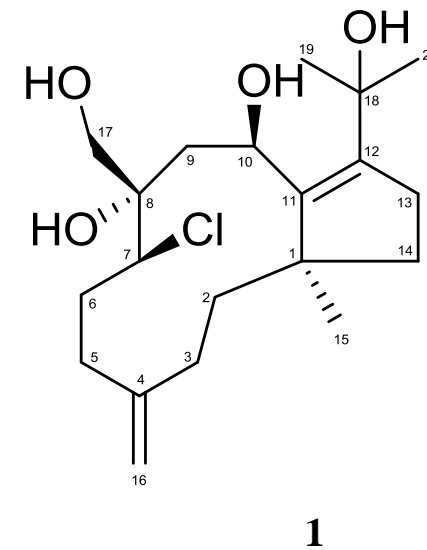
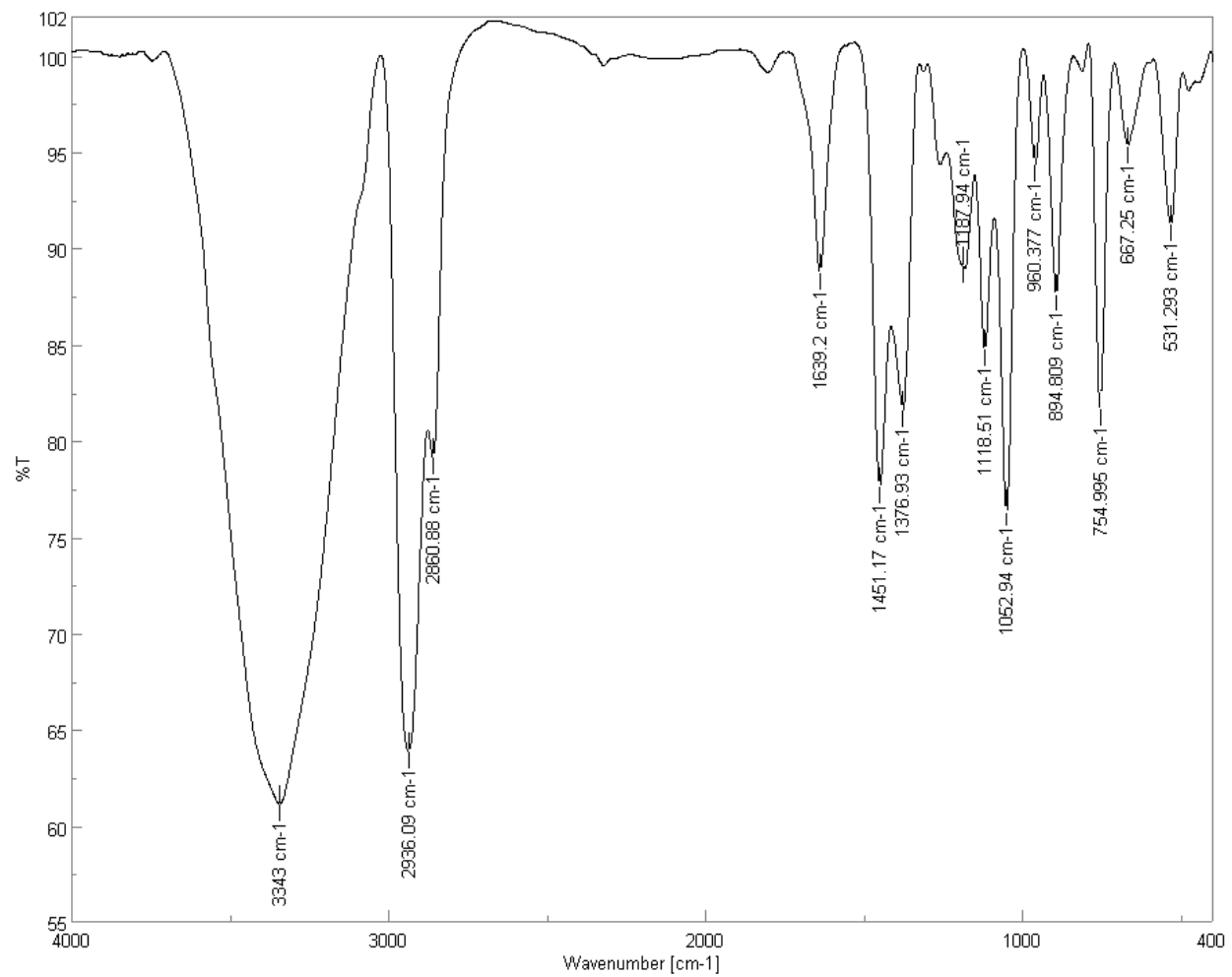


Figure S1. HRESIMS of 1

Figure S2. IR spectrum of **1**

GN98-14-3-2

4

Sample Name:
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Archive directory:
/home/duh/vnmrsys/data
Sample directory:
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FidFile: PROTON_01
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 7 2014

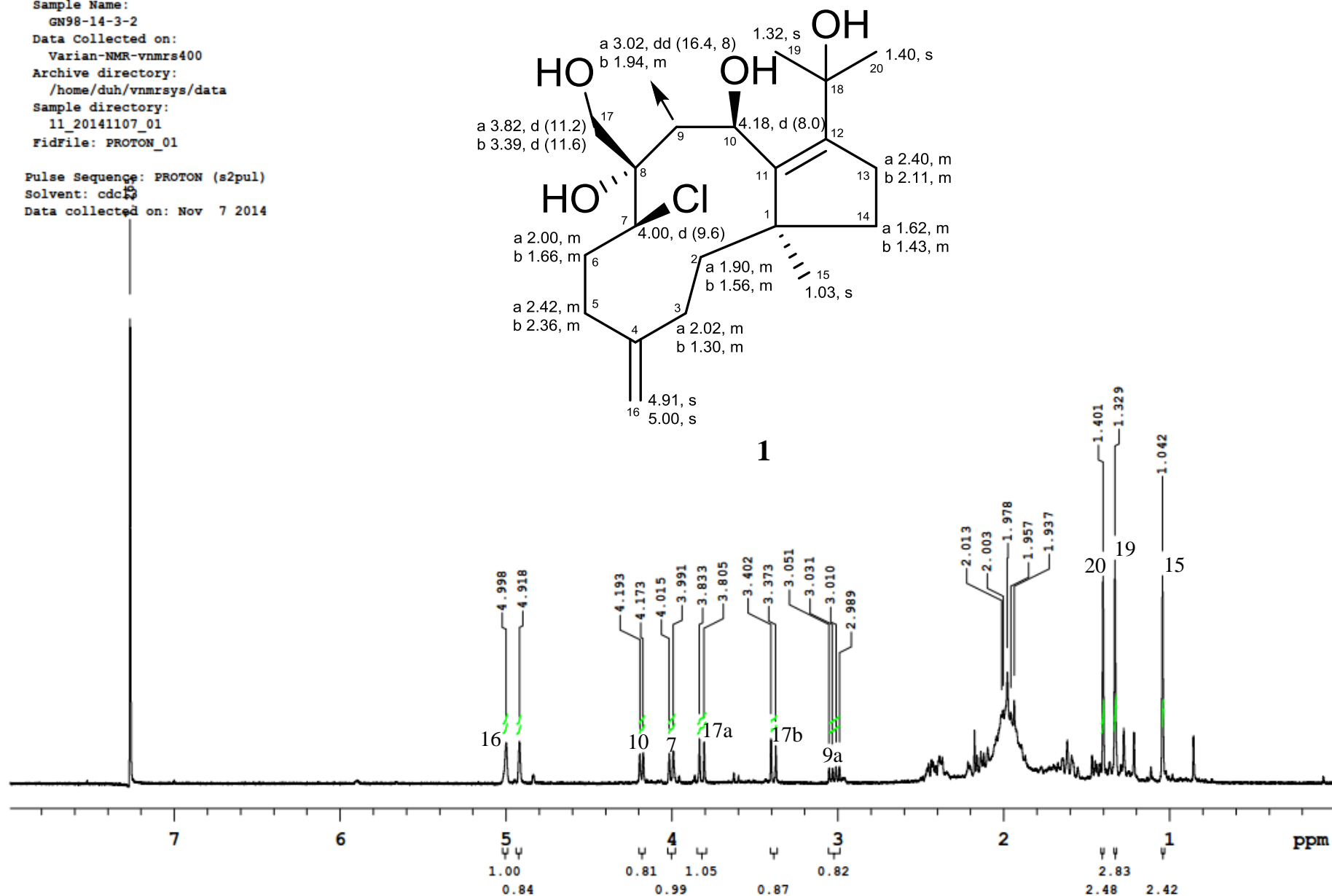
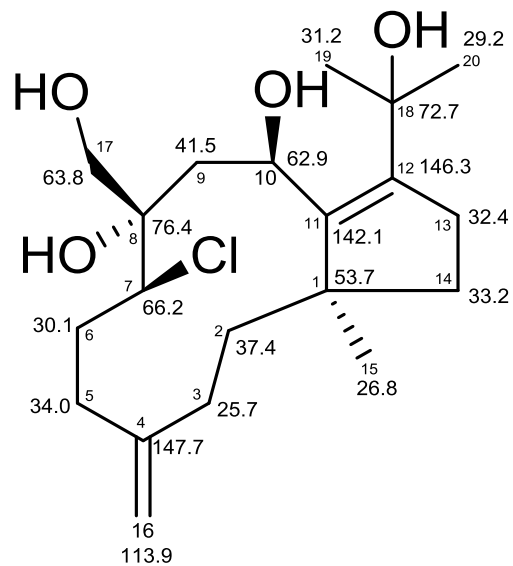


Figure S3. ¹H NMR spectrum (400 MHz) of **1** in CDCl₃

GN98-14-3-2

Sample Name:
GN98-14-3-2
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/duh/vnmrsys/data
Sample directory:
GN98-14-3-2_20141104_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 4 2014



1

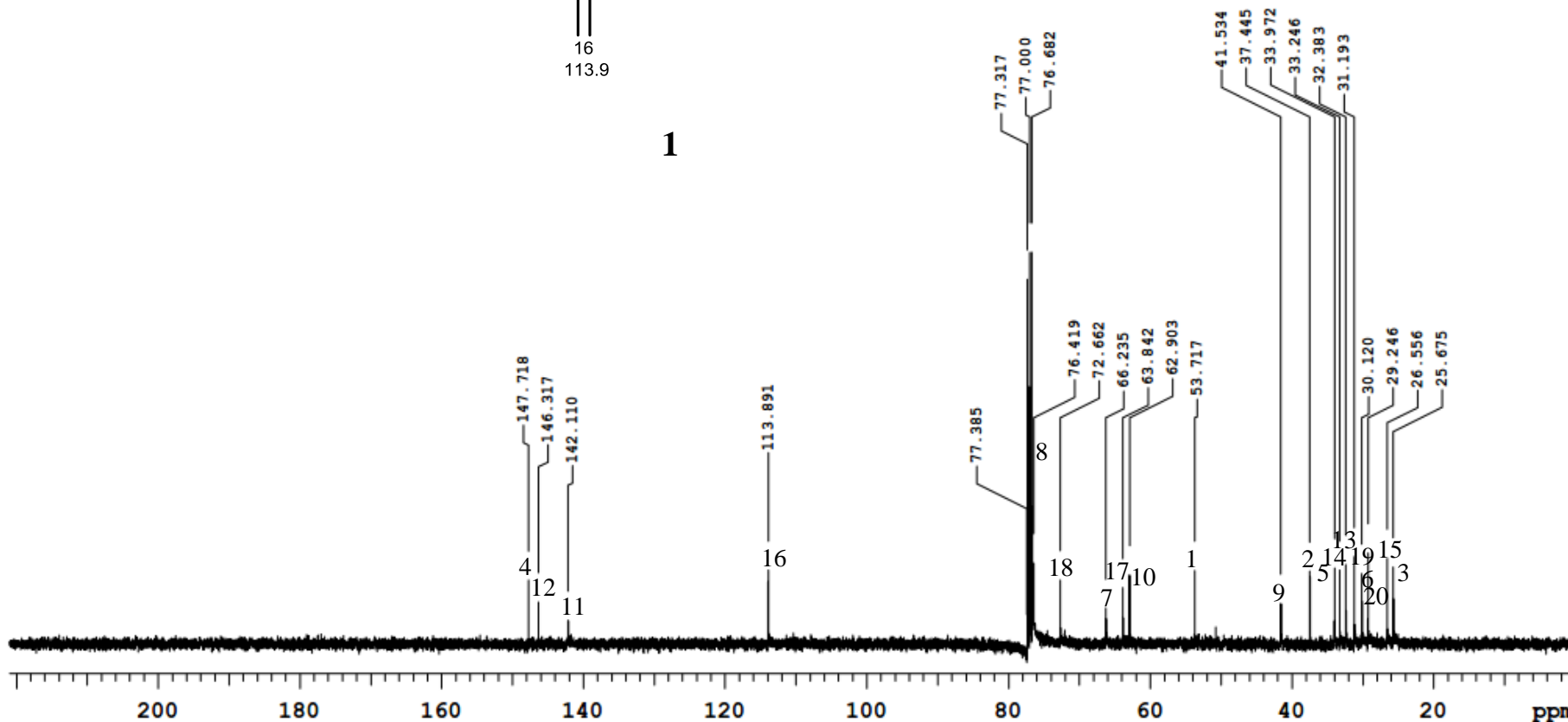


Figure S4. ¹³C NMR spectrum (100 MHz) of 1 in CDCl₃

GN98-14-3-2

Sample Name:
GN98-14-3-2
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/duh/vnmrsys/data
Sample directory:
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FidFile: gHSQCAD_01

Pulse Sequence: gHSQCAD
Solvent: cdcl3
Data collected on: Nov 4 2014

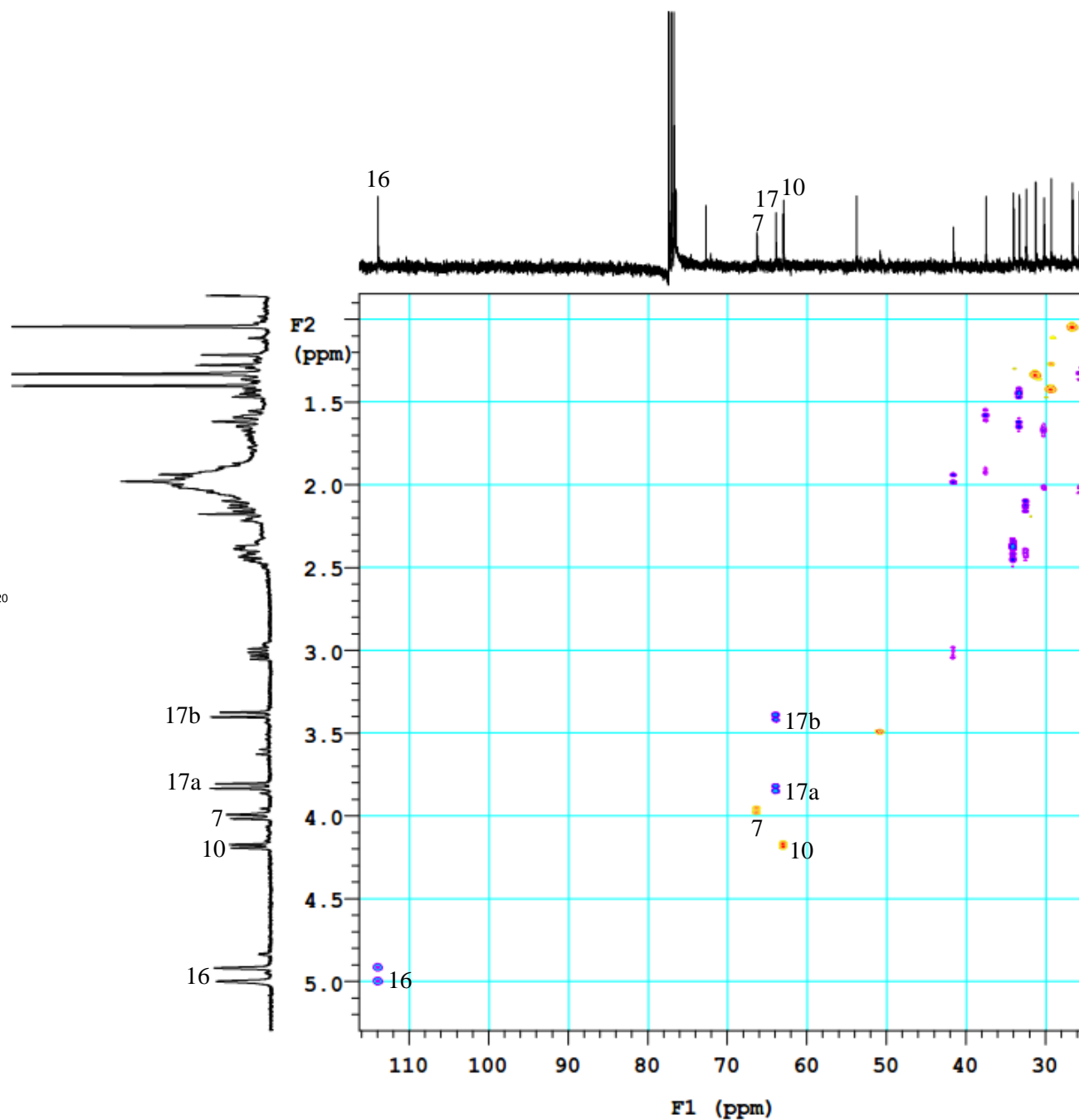
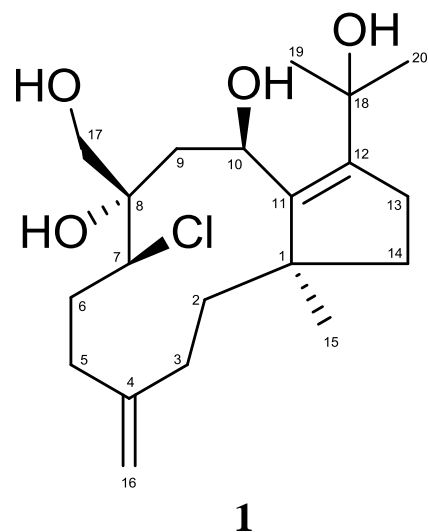
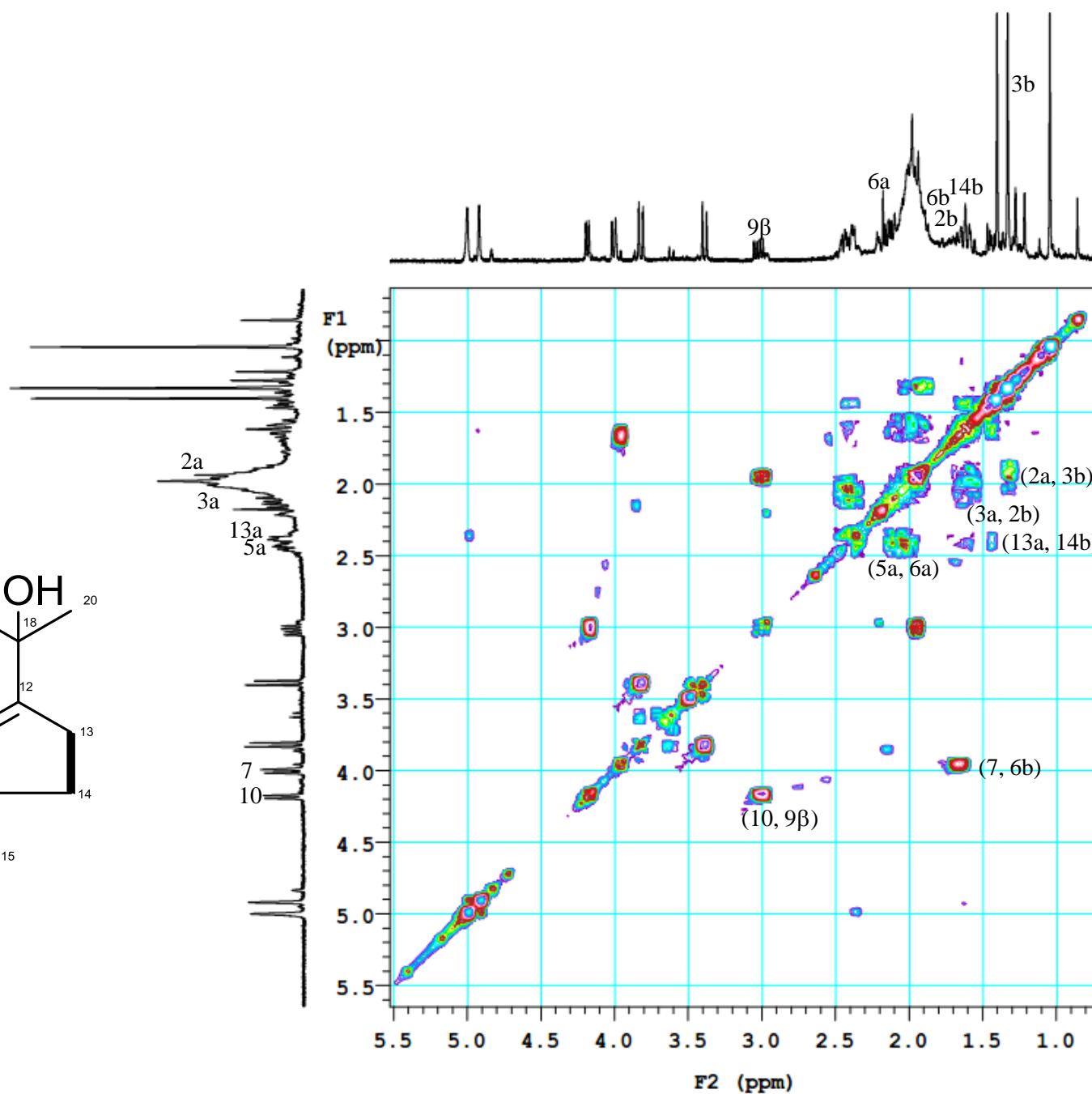
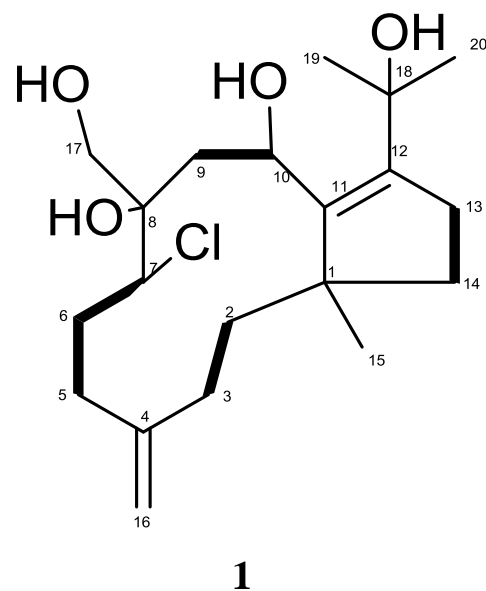


Figure S5. HSQC spectrum (400 MHz) of **1** in CDCl_3

GN98-14-3-2

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GN98-14-3-2
Data Collected on:
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Archive directory:
/home/duh/vnmrsys/data
Sample directory:
GN98-14-3-2_20141104_01
FidFile: gCOSY_01

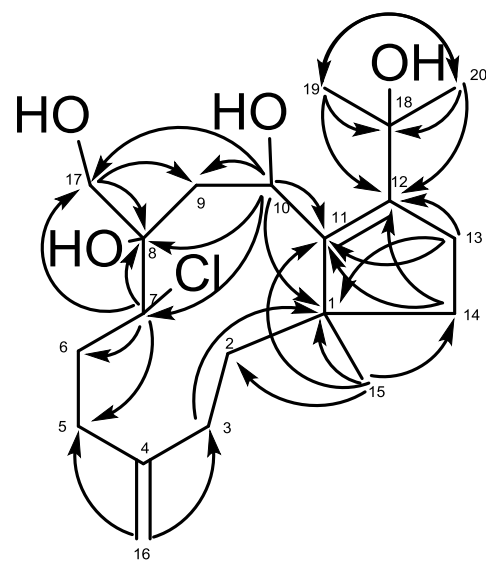
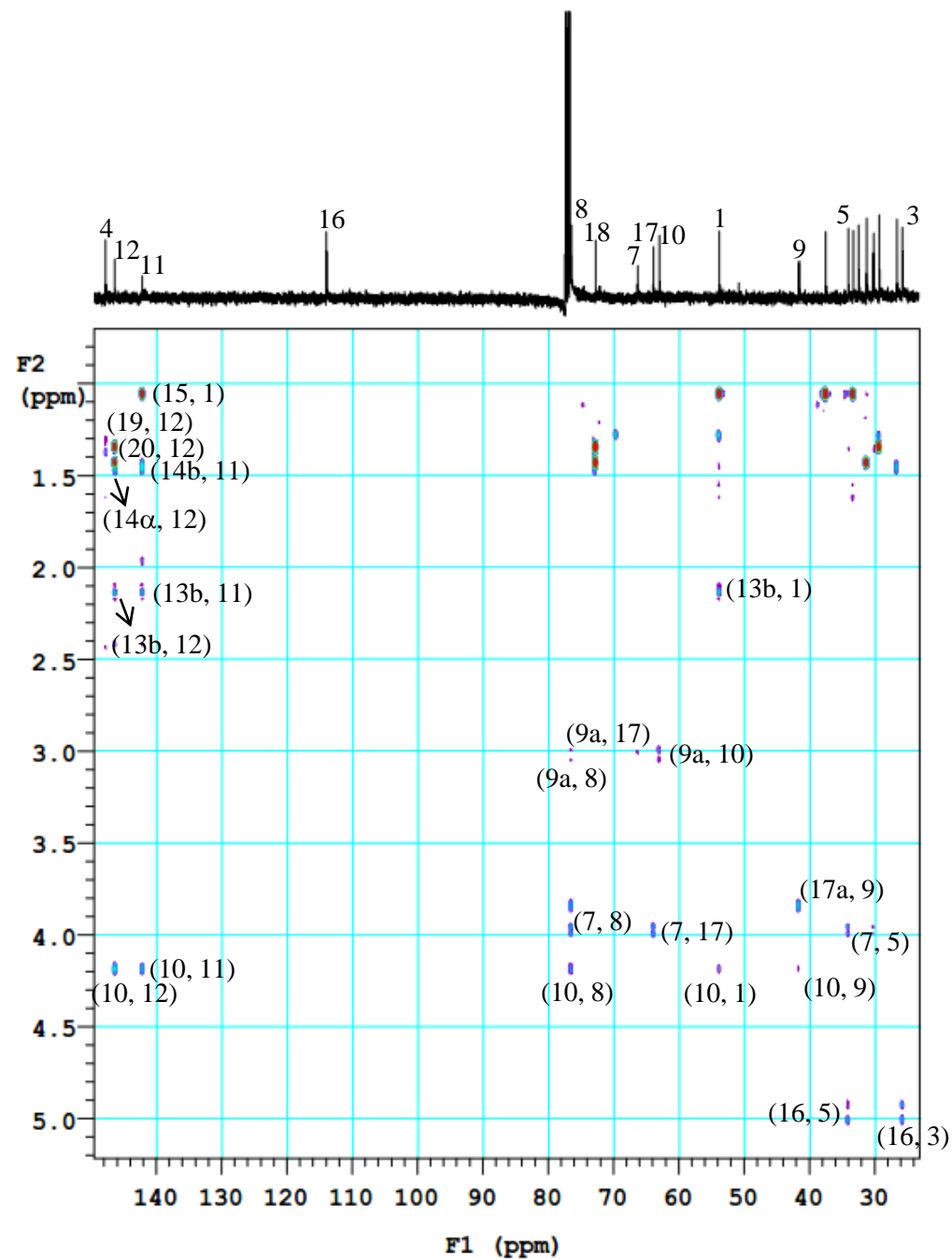
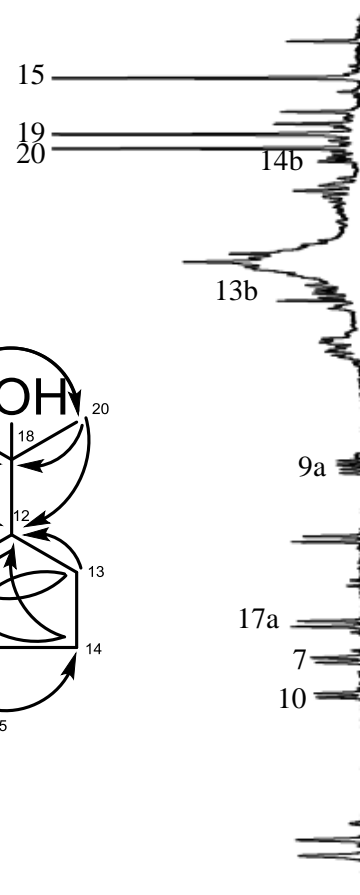
Pulse Sequence: gCOSY
Solvent: cdcl3
Data collected on: Nov 4 2014



GN98-14-3-2

Sample Name:
GN98-14-3-2
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/duh/vnmrsys/data
Sample directory:
GN98-14-3-2_20141104_01
FidFile: gHMBCAD_01

Pulse Sequence: gHMBCAD
Solvent: cdcl3
Data collected on: Nov 4 2014

**1**Figure S7. spectrum (400 MHz) of **1** in CDCl₃

GN98-14-3-2

Sample Name:
GN98-14-3-2
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/duh/vnmrsys/data
Sample directory:
GN98-14-3-2_20141104_01
Fidfile: NOESY_01

Pulse Sequence: NOESY
Solvent: cdcl3
Data collected on: Nov 4 2014

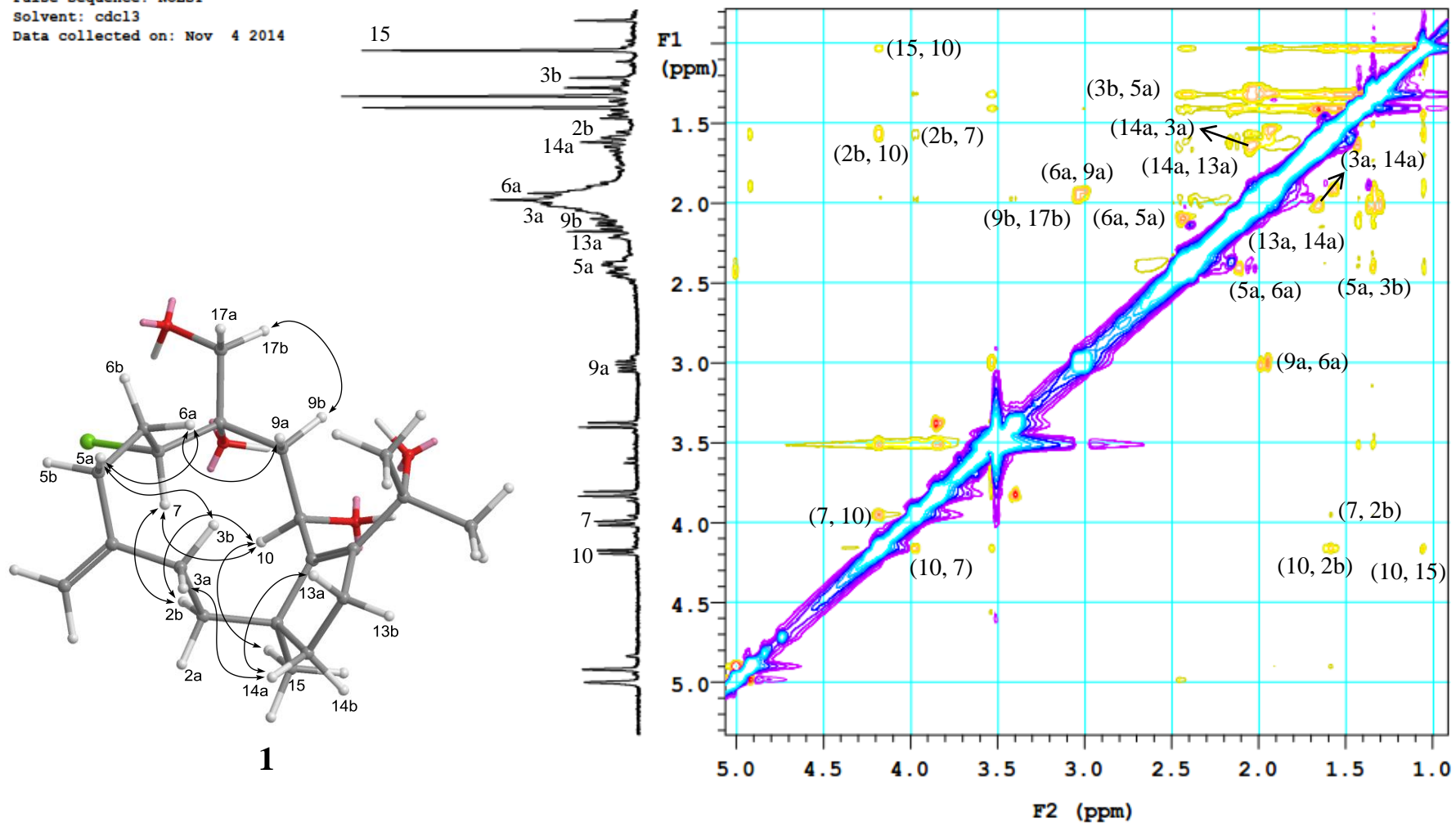


Figure S8. NOESY spectrum (400 MHz) of **1** in CDCl₃

Mass Spectrum SmartFormula Report

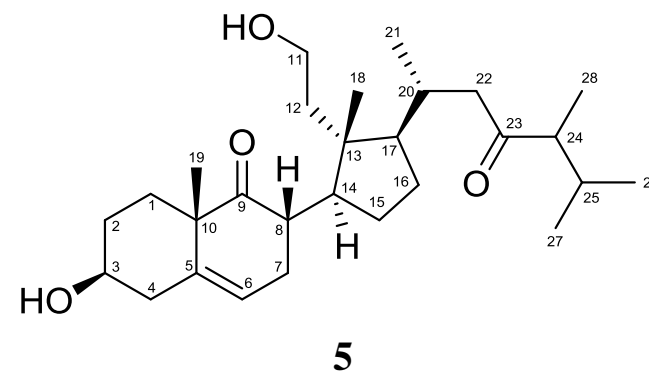
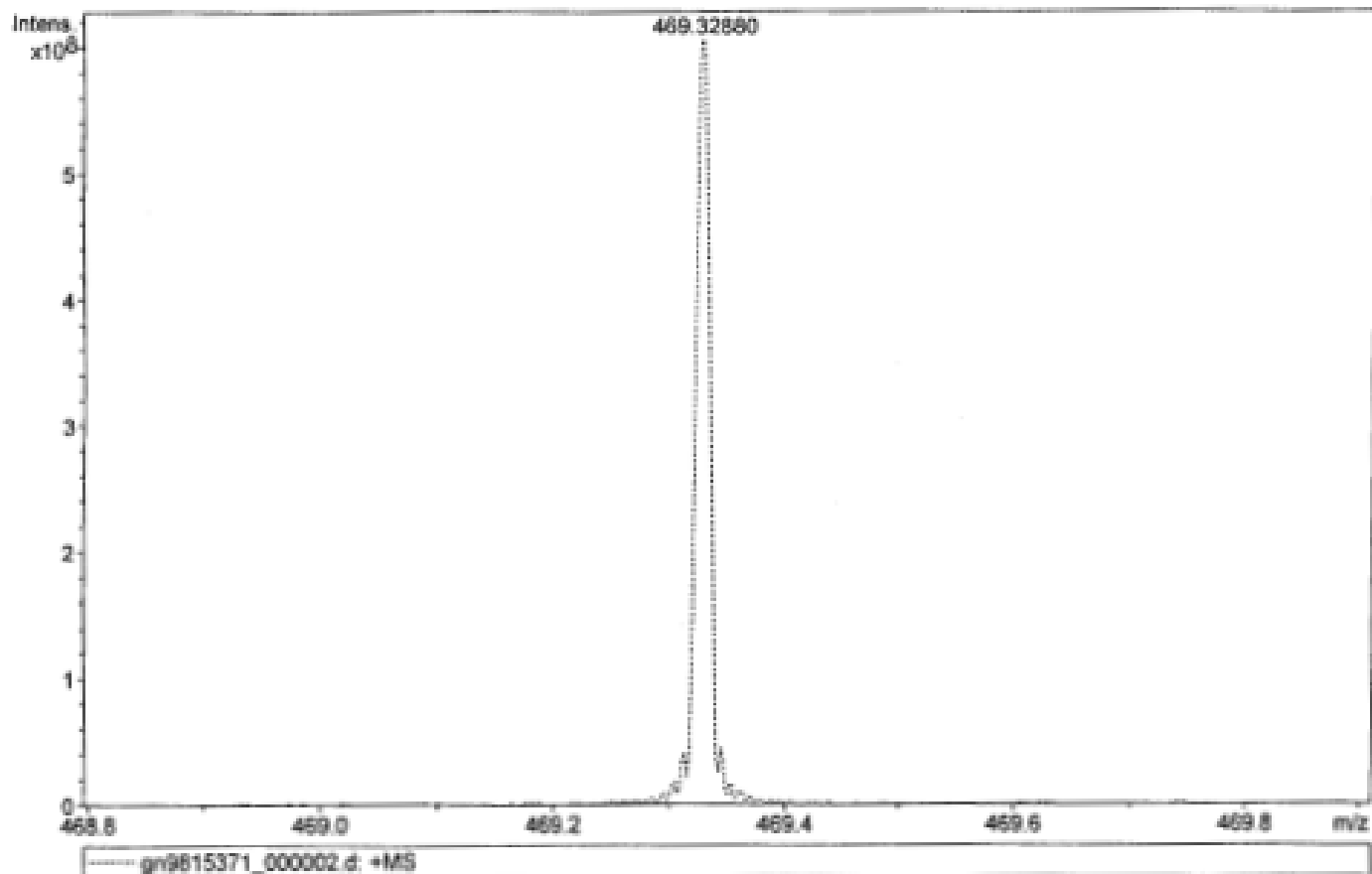
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Analysis Info

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Sample Name GN98-15-3-7-1
Comment ESI Positive

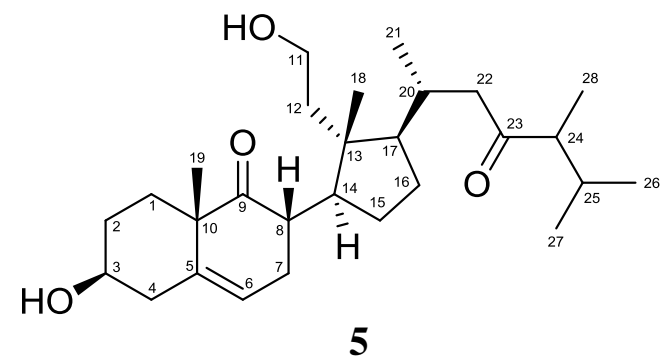
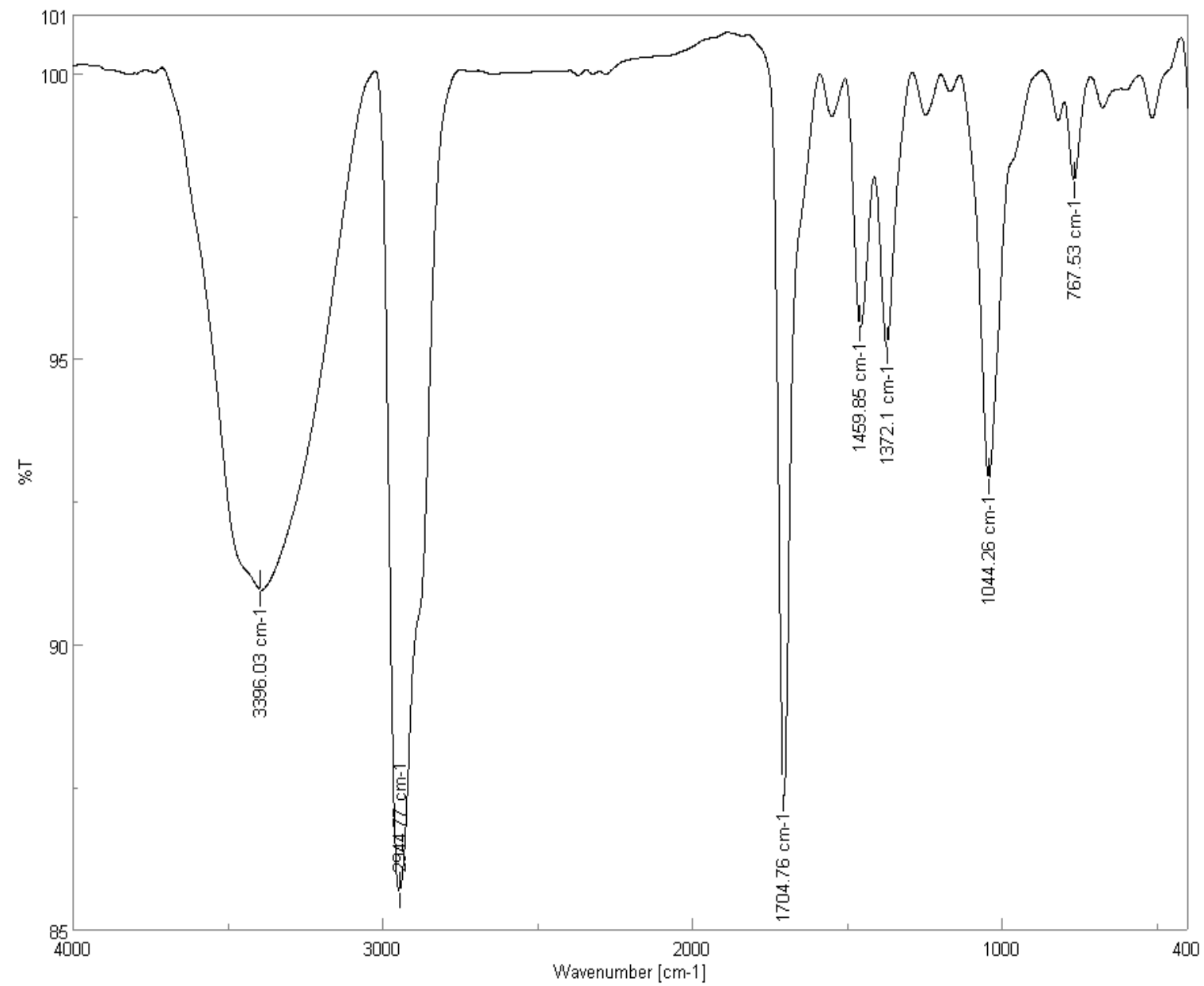
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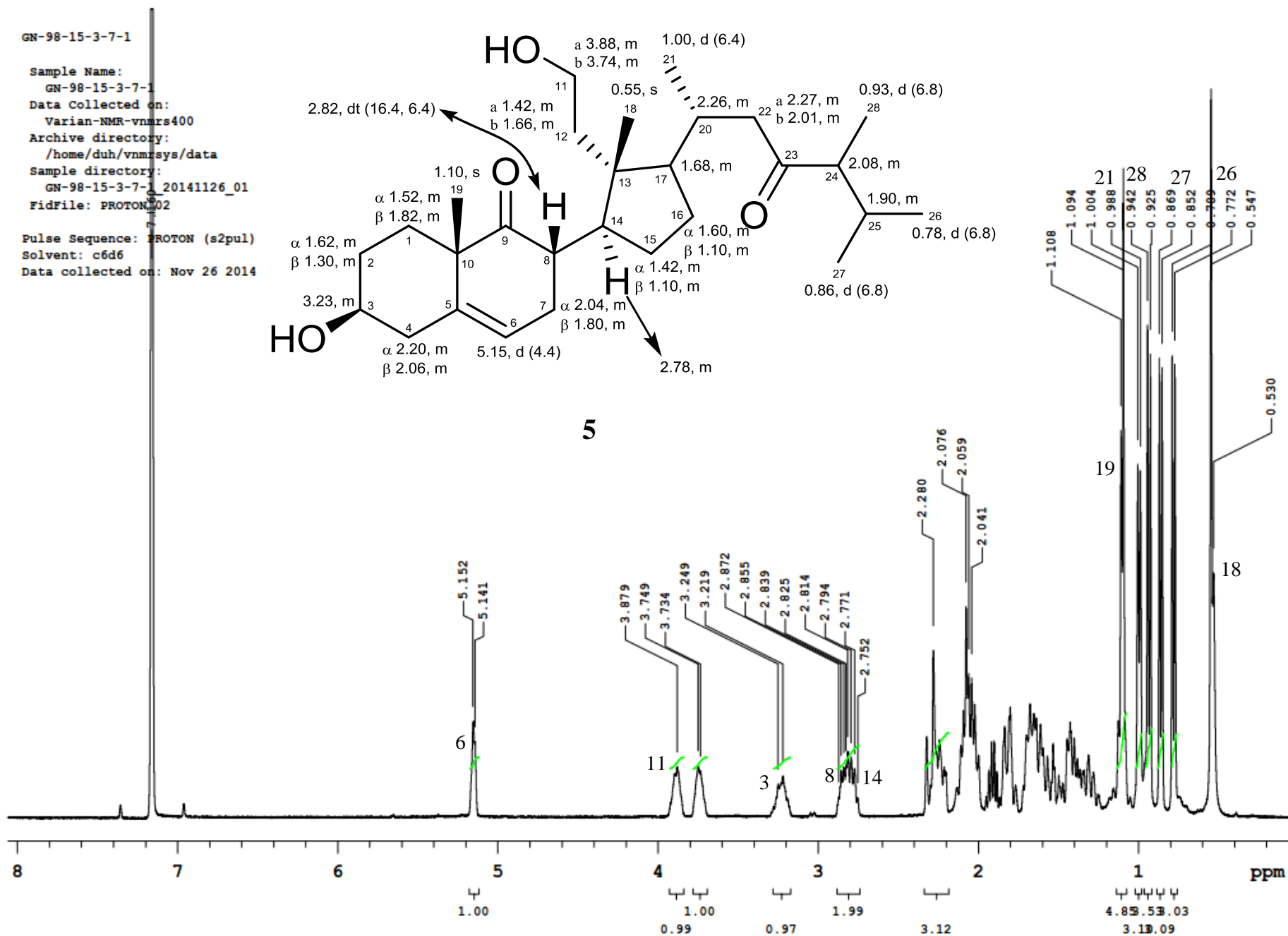
Instrument: FT-MS solarix



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
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Figure S9. HRESI of **5**

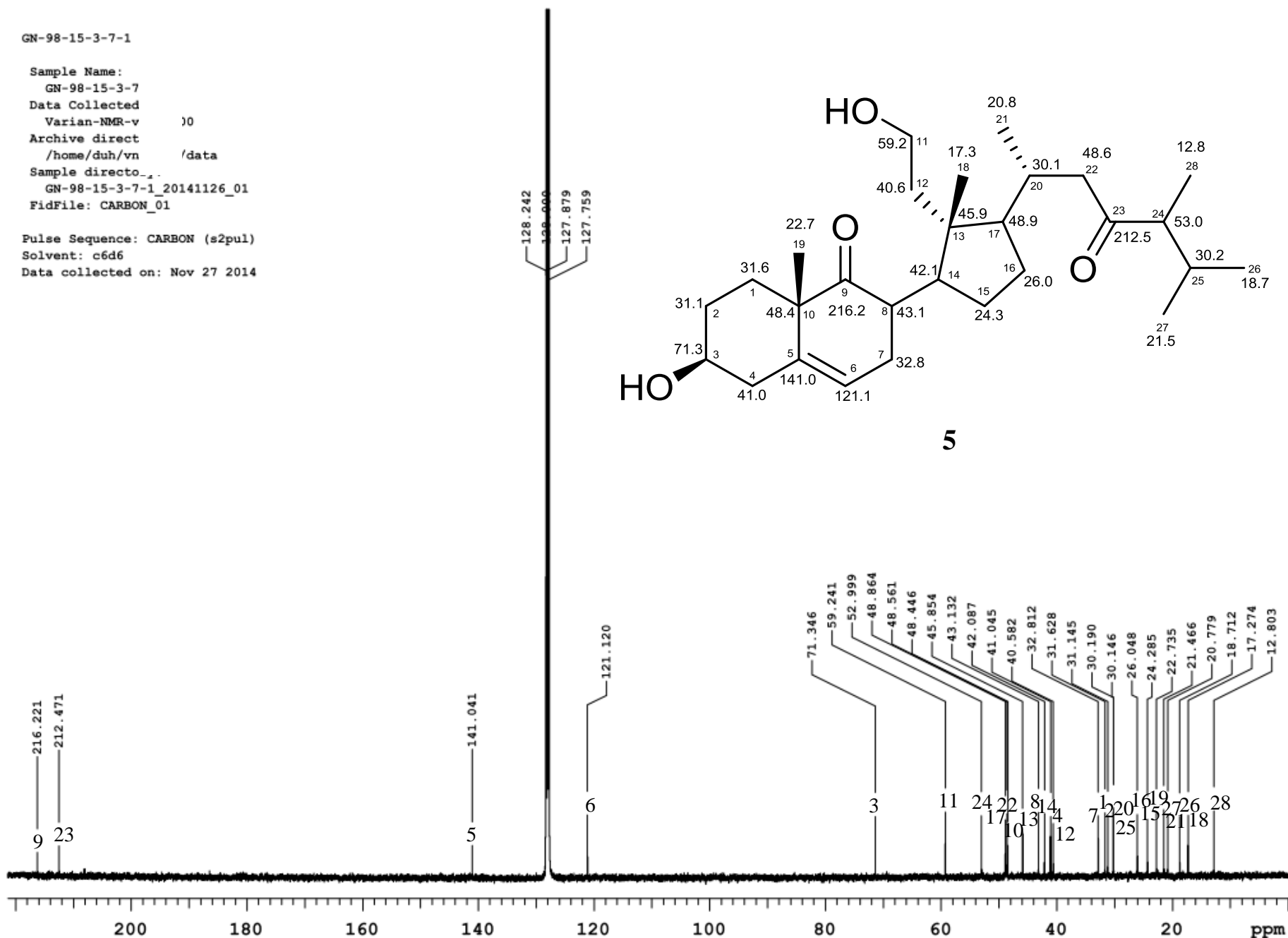
Figure S10. IR spectrum of **5**

Figure S11. ^1H NMR spectrum (400 MHz) of **5** in C_6D_6

GN-98-15-3-7-1

Sample Name:
GN-98-15-3-7
Data Collected
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Archive direct
/home/duh/vn /data
Sample directo_...
GN-98-15-3-7-1_20141126_01
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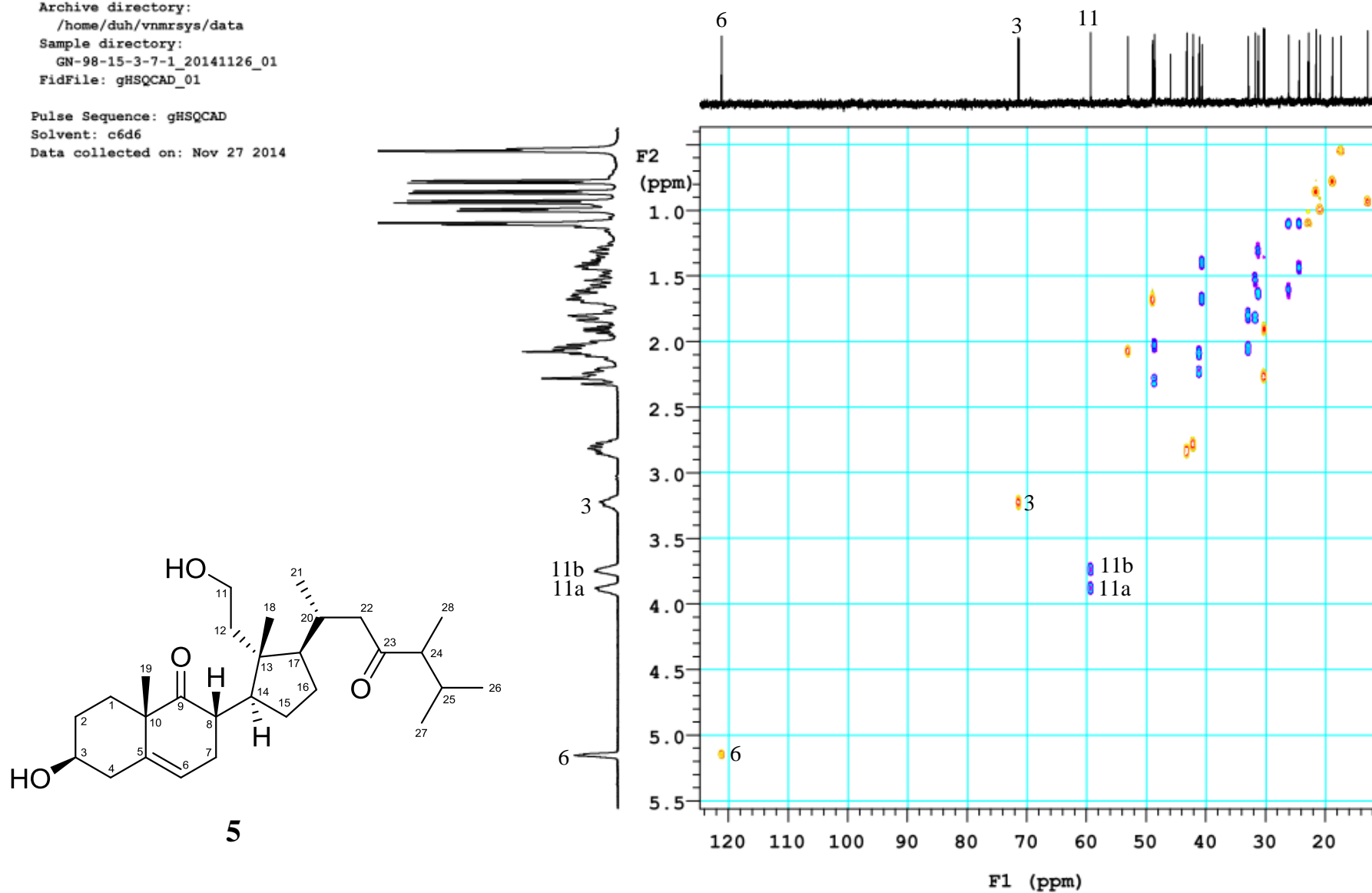
Pulse Sequence: CARBON (s2pul)
Solvent: c6d6
Data collected on: Nov 27 2014

Figure S12. ^{13}C NMR spectrum (100 MHz) of **5** in C_6D_6

GN-98-15-3-7-1

Sample Name:
GN-98-15-3-7-1
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/duh/vnmrsys/data
Sample directory:
GN-98-15-3-7-1_20141126_01
FidFile: gHSQCAD_01

Pulse Sequence: gHSQCAD
Solvent: c6d6
Data collected on: Nov 27 2014

Figure S13. HSQC spectrum (400 MHz) of **5** in C₆D₆

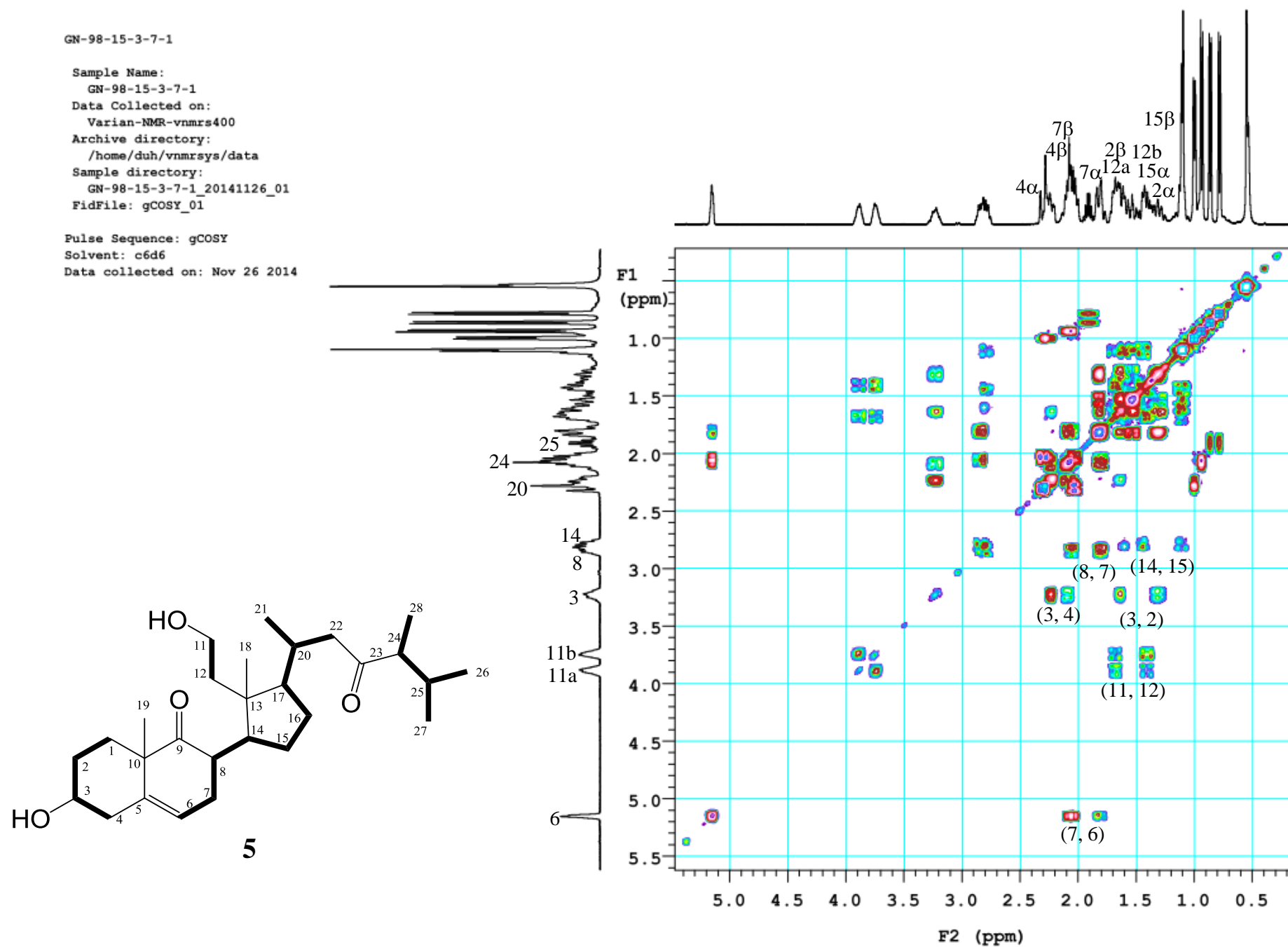
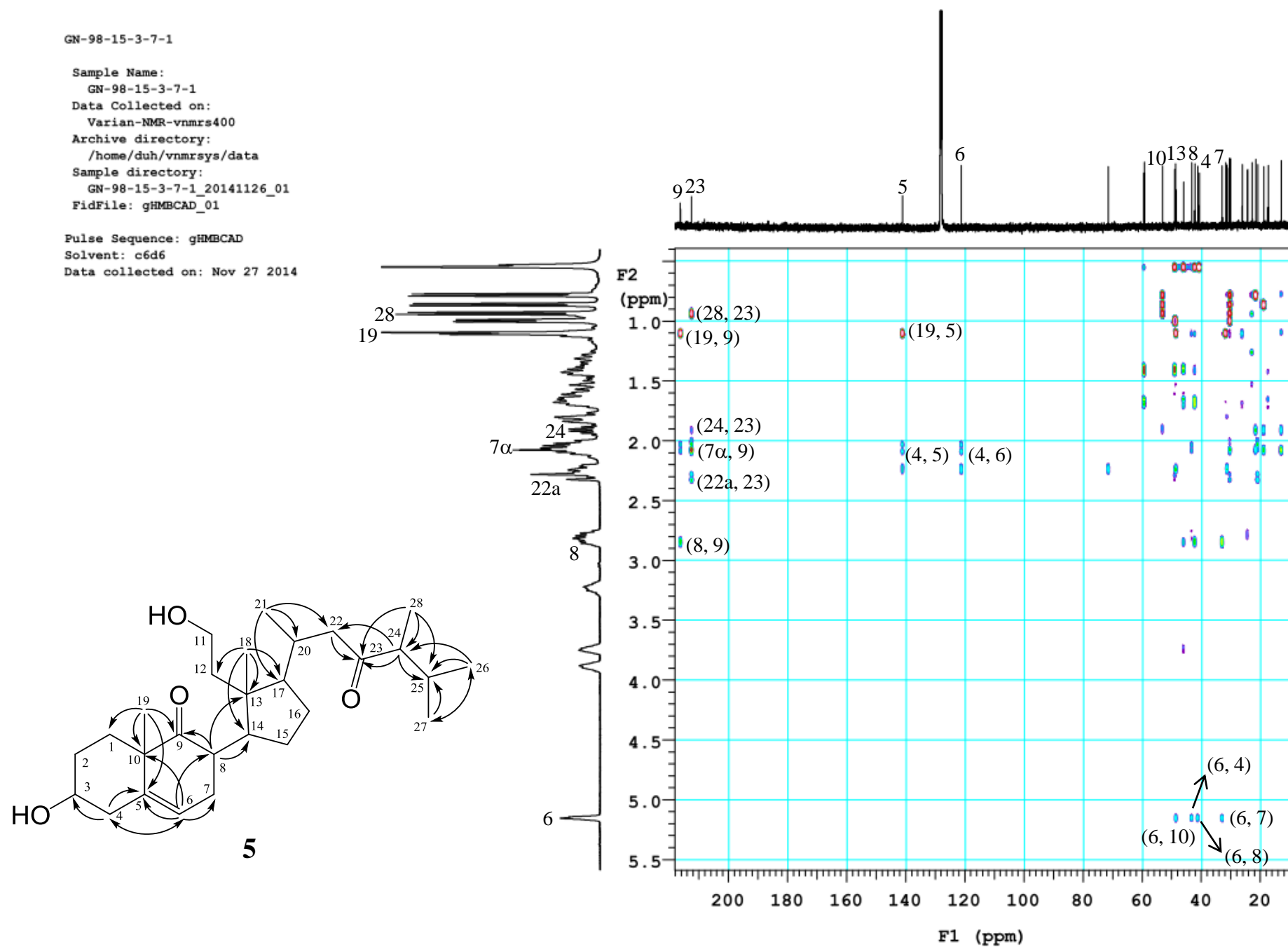
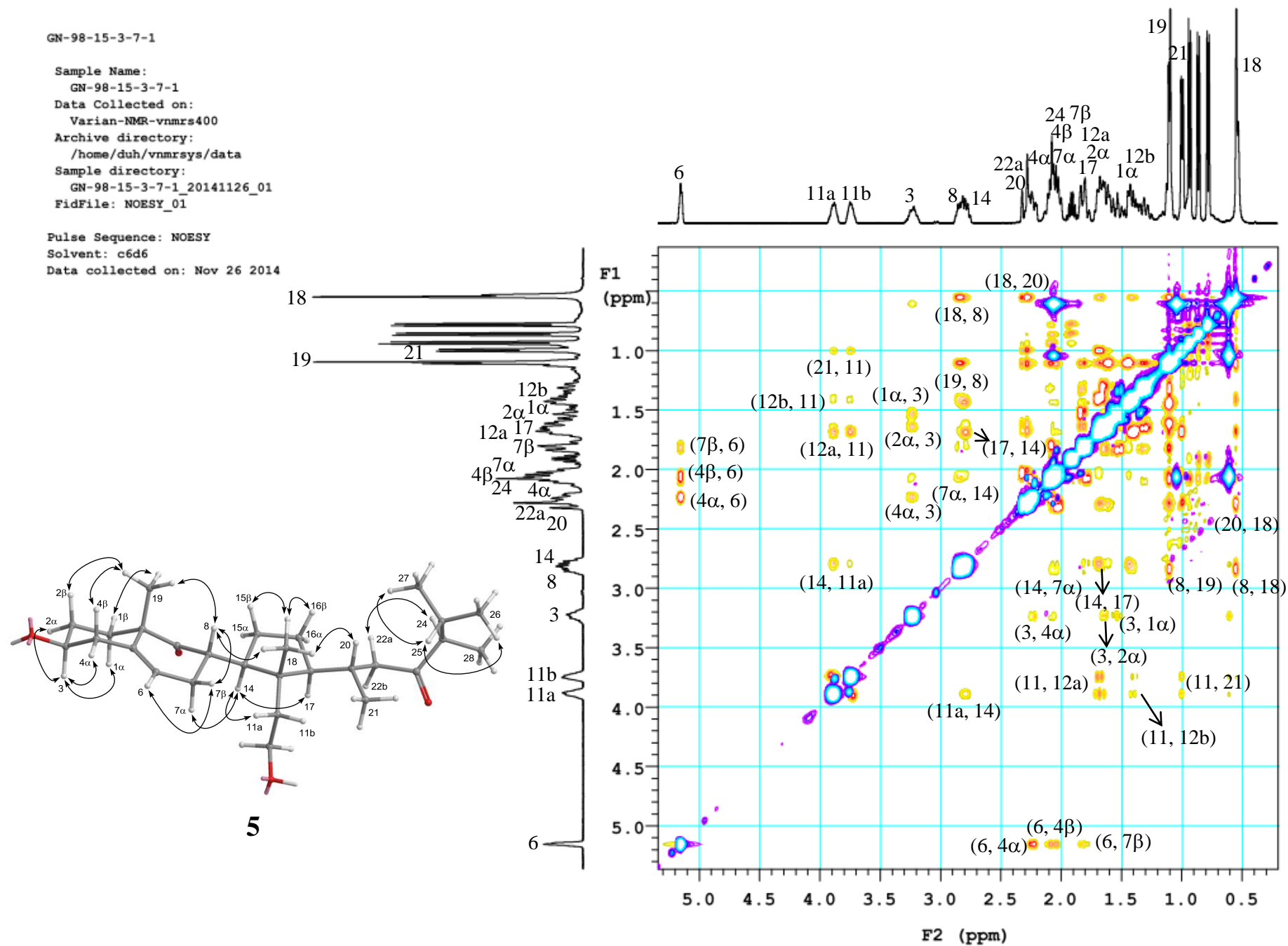


Figure S14. COSY spectrum (400 MHz) of **5** in C₆D₆





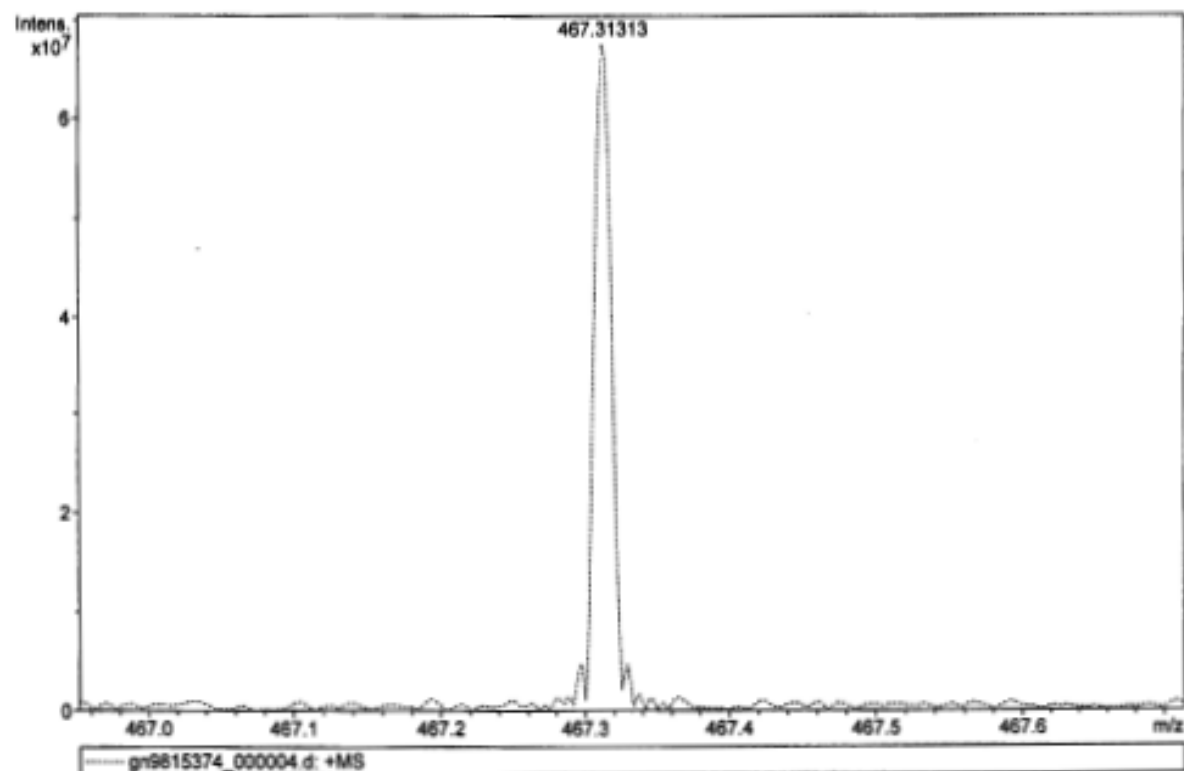
Mass Spectrum SmartFormula Report

Analysis Info

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 Sample Name GN98-15-3-7-4
 Comment ESI Positive

1/26/2015 2:35:27 PM

Instrument: FT-MS solarX



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
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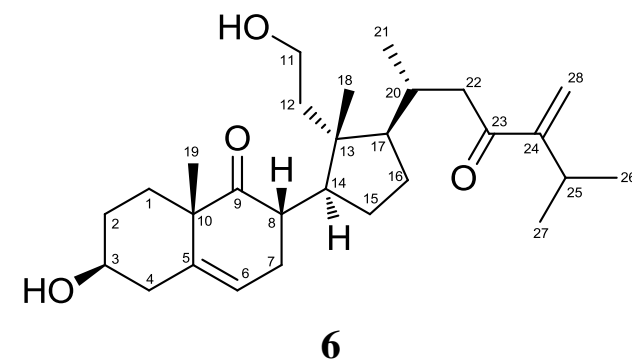
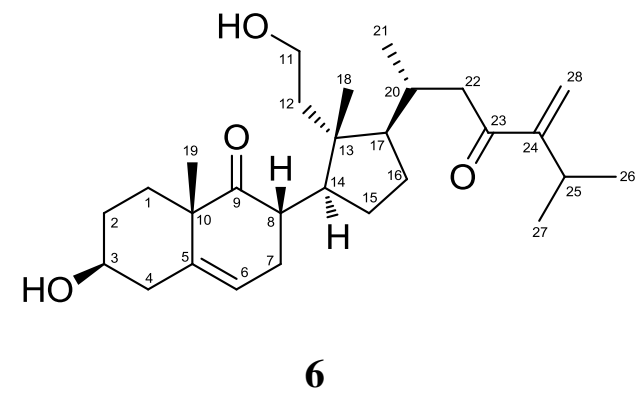
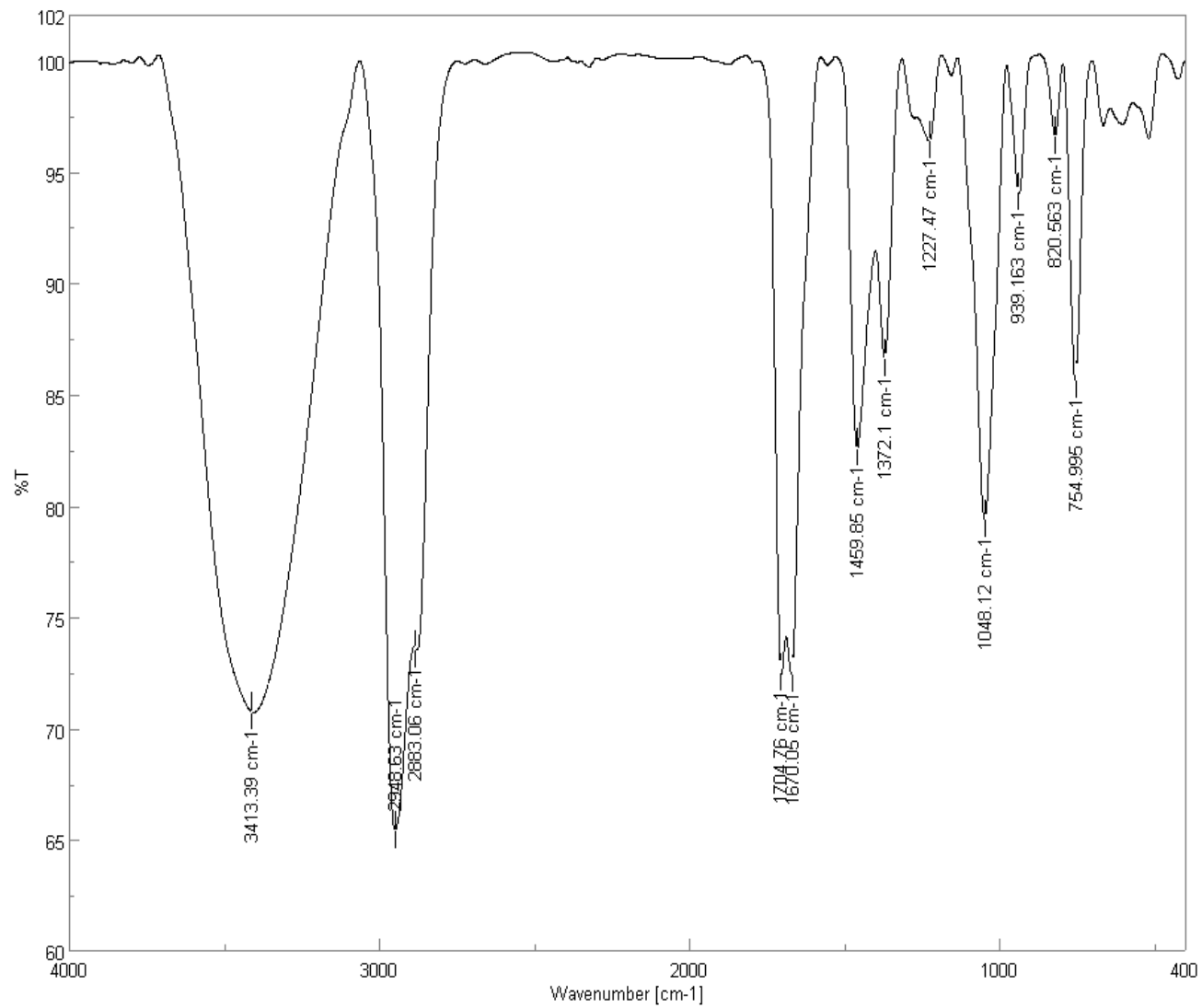


Figure S17. HRESI of **6**

Figure S18. IR spectrum of **6**

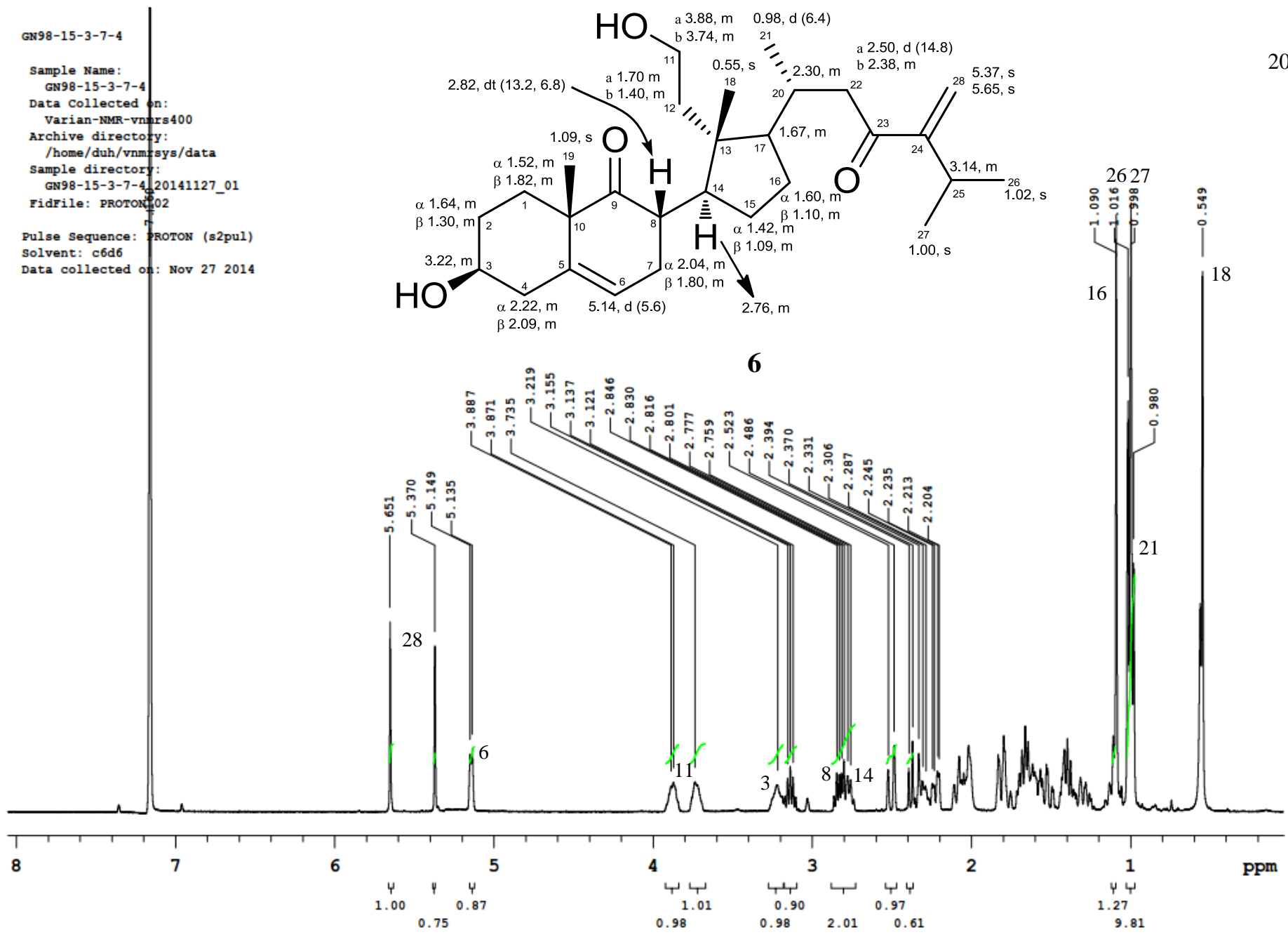


Figure S19. ^1H NMR spectrum (400 MHz) of **6** in C_6D_6

GN98-15-3-7-4

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Data Collected
Varian-NMR-v 10
Archive direct
/home/duh/vn /data
Sample directo...
GN98-15-3-7-4_20141127_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: c6d6
Data collected on: Nov 28 2014

21

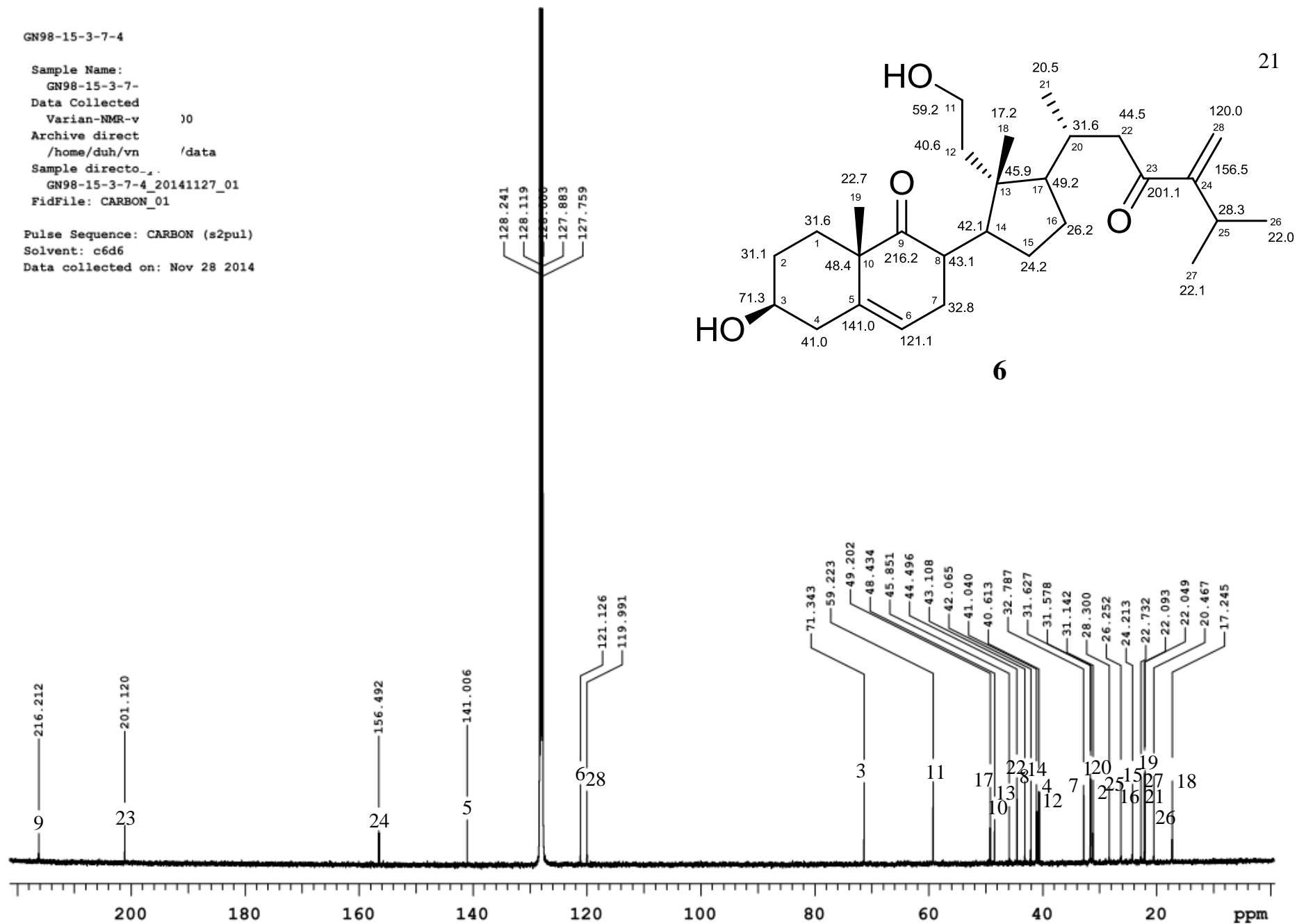


Figure S20. ¹³C NMR spectrum (100 MHz) of **6** in C₆D₆

GN98-15-3-7-4

22

Sample Name:
GN98-15-3-7-4
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/duh/vnmrsys/data
Sample directory:
GN98-15-3-7-4_20141127_01
FidFile: gHSQCAD_01

Pulse Sequence: gHSQCAD
Solvent: c6d6
Data collected on: Nov 27 2014

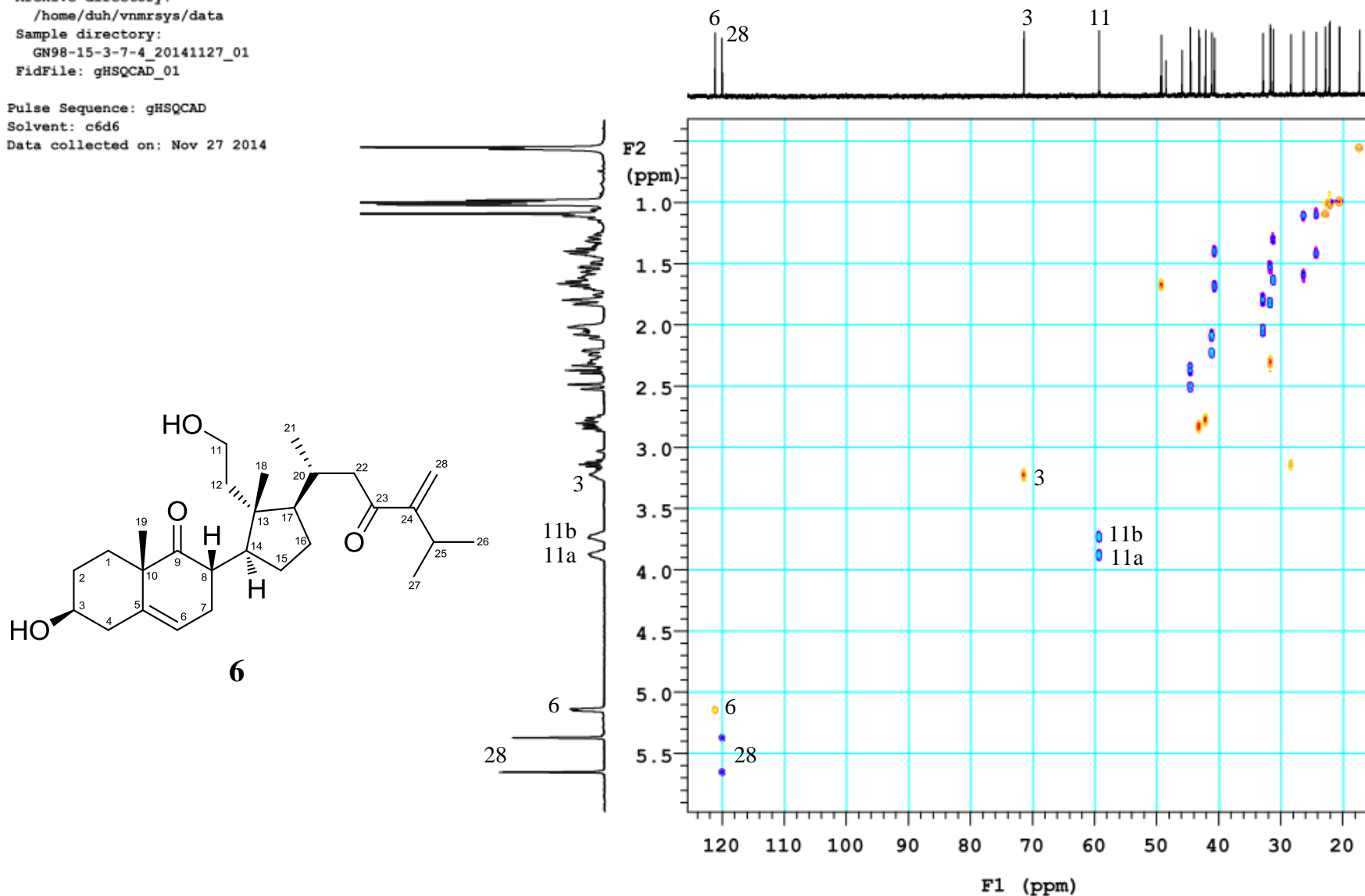
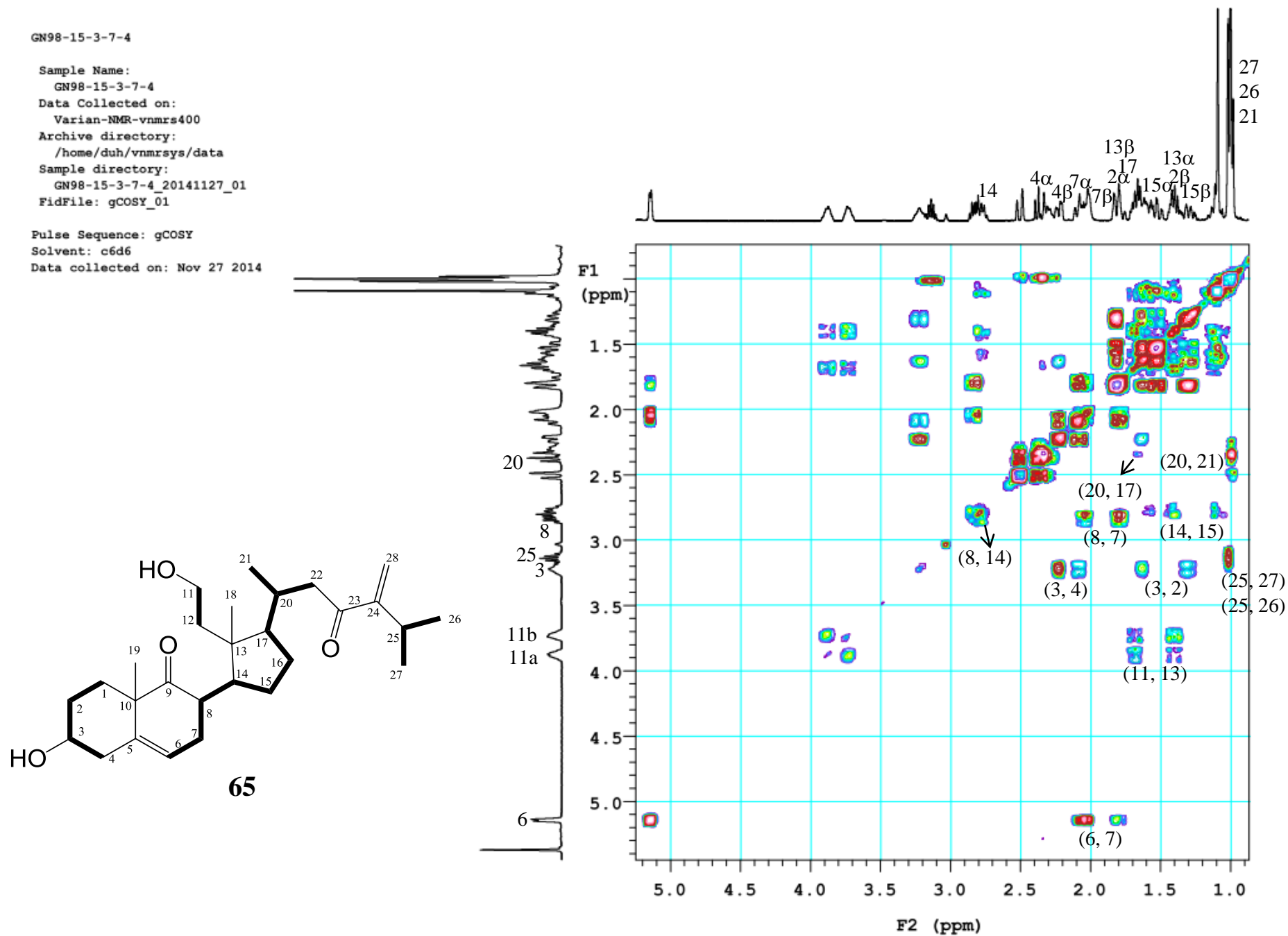


Figure S21. HSQC spectrum (400 MHz) of **6** in C₆D₆

Figure S22. COSY spectrum (400 MHz) of **6** in C₆D₆

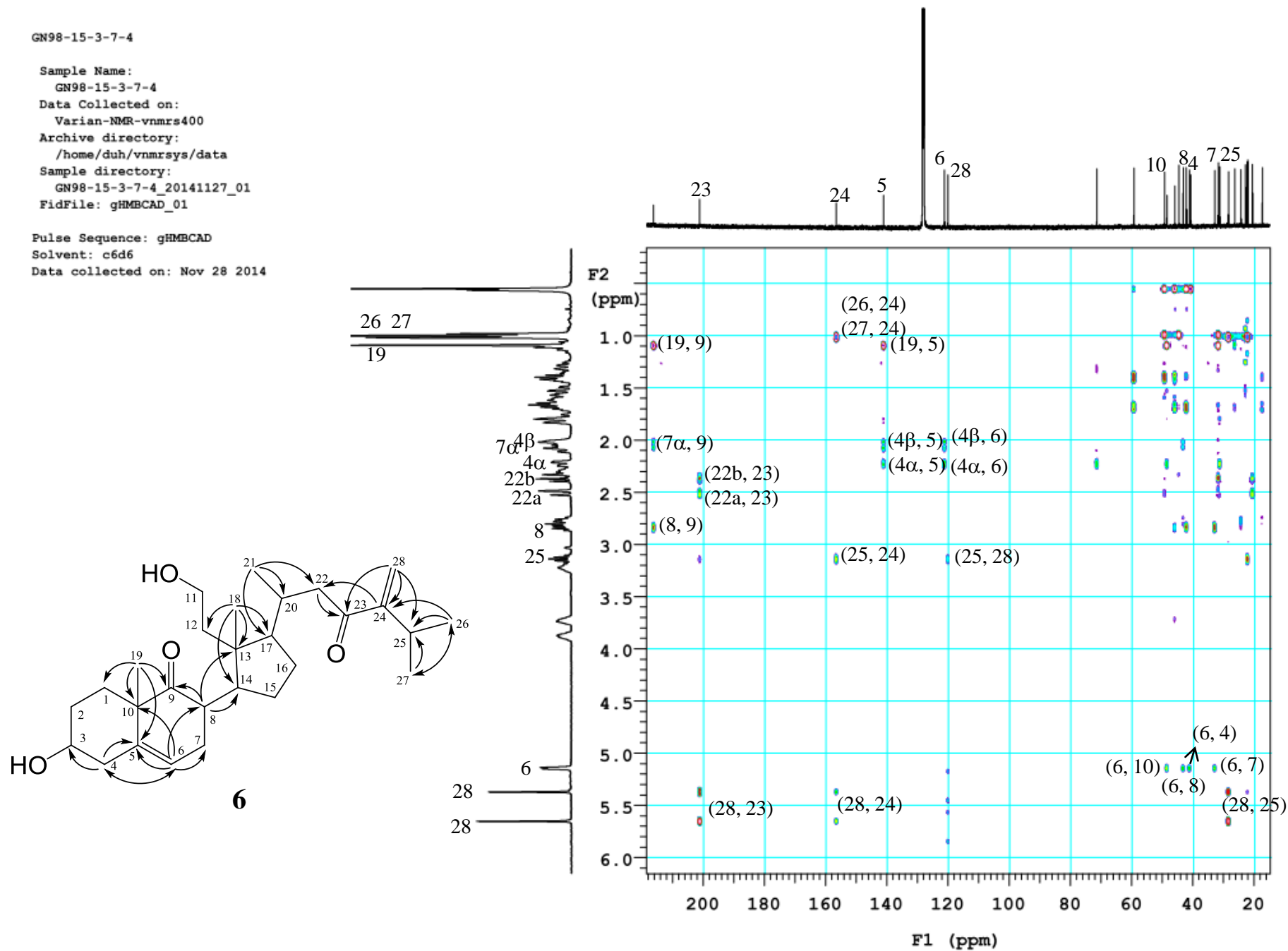


Figure S23. HMBC spectrum (400 MHz) of **6** in C_6D_6

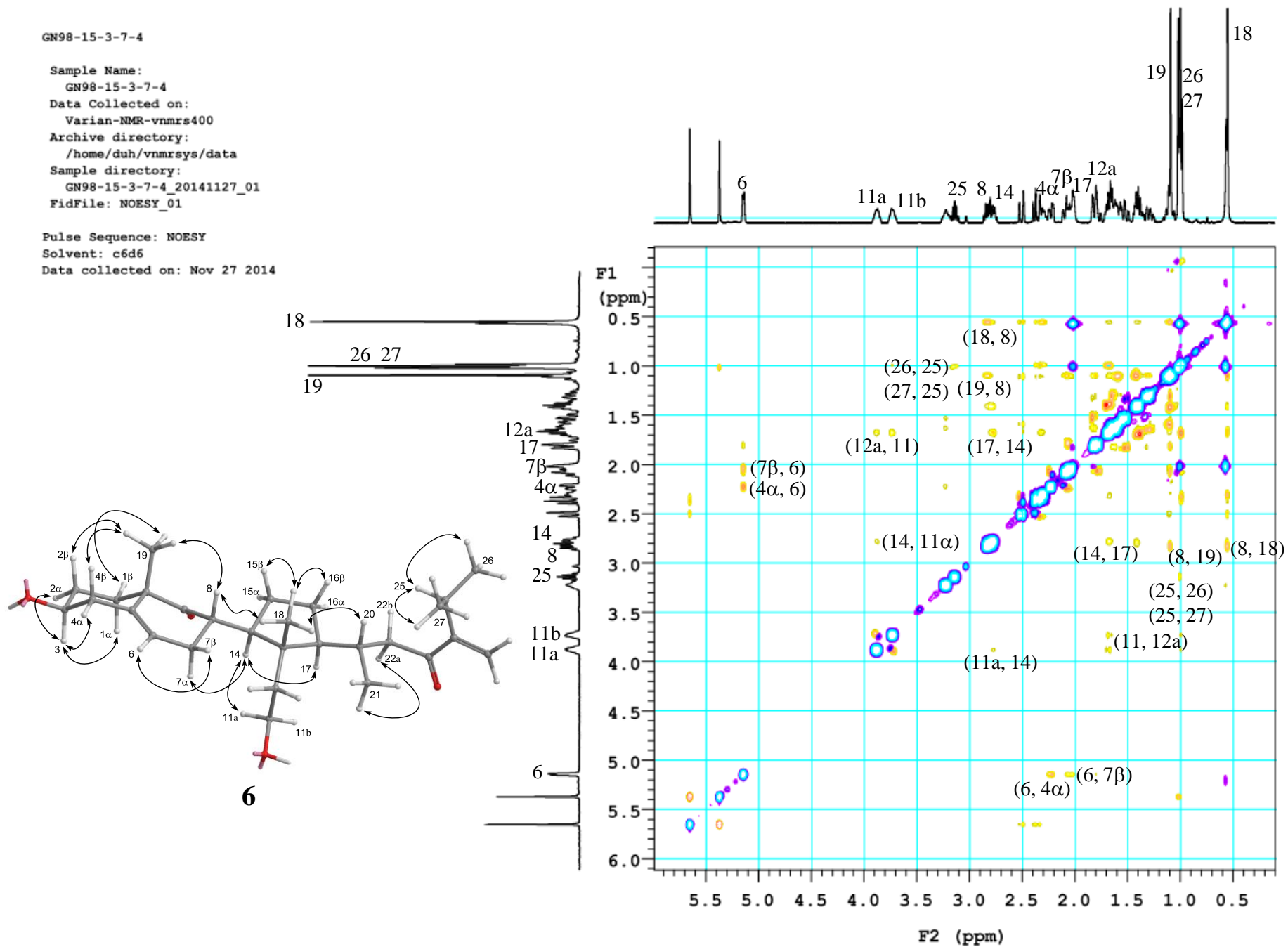


Table S1. Evaluation of ED₅₀ cytotoxicity of tested compounds against HEK293T cells

ID	Compound	M (g/mol)	MTT assay			High-content assay	
			A549	HT29	P388	Nuclear count	
			HEK293T-EGFP-UL76				
B	Bortezomib	384.243	25.7 nM	18.7 nM	1.6 nM	12.0 nM	24.3 nM
M	MG132	475.630	5.5 μ M	6.8 μ M	0.71 μ M	1.2 μ M	1.9 μ M
1	Clavinflol C	372	>50 μ g/ml (134.4 μ M)	>50 μ g/ml	>50 μ g/ml	>25 μ g/ml (67.2 μ M)	6.1 μ g/ml (16.4 μ M)
2	Stolonidiol	336	3.9 μ g/ml (11.6 μ M)	>50 μ g/ml (148.8 μ M)	0.6 μ g/ml (1.8 μ M)	>25 μ g/ml (74.4 μ M)	>25 μ g/ml
3	Stolonidiol-17-acetate	378	>50 μ g/ml (132.3 μ M)	>50 μ g/ml	>50 μ g/ml	>25 μ g/ml (66.1 μ M)	19.6 μ g/ml (51.9 μ M)
4	Clavinflol B	372	>50 μ g/ml (134.4 μ M)	>50 μ g/ml	>50 μ g/ml	>25 μ g/ml (67.2 μ M)	21.3 μ g/ml (57.3 μ M)
5	3 β ,11-dihydroxy-24-methyl-9,11-secocholest-5-en-9,23-dione	446	>50 μ g/ml (112.1 μ M)	3.2 μ g/ml (7.2 μ M)	4.6 μ g/ml (10.3 μ M)	12.3 μ g/ml (27.6 μ M)	12.1 μ g/ml (27.1 μ M)
6	3 β ,11-dihydroxy-24-methylene-9,11-secocholest-5-en-9,23-dione	444	5.3 μ g/ml (11.9 μ M)	>50 μ g/ml (112.6 μ M)	4.8 μ g/ml (10.8 μ M)	>25 μ g/ml (56.3 μ M)	10.9 μ g/ml (24.5 μ M)