

Supporting Information

Semisynthesis of Mallotus B from Rottlerin: Evaluation of Cytotoxicity and Apoptosis-inducing Activity

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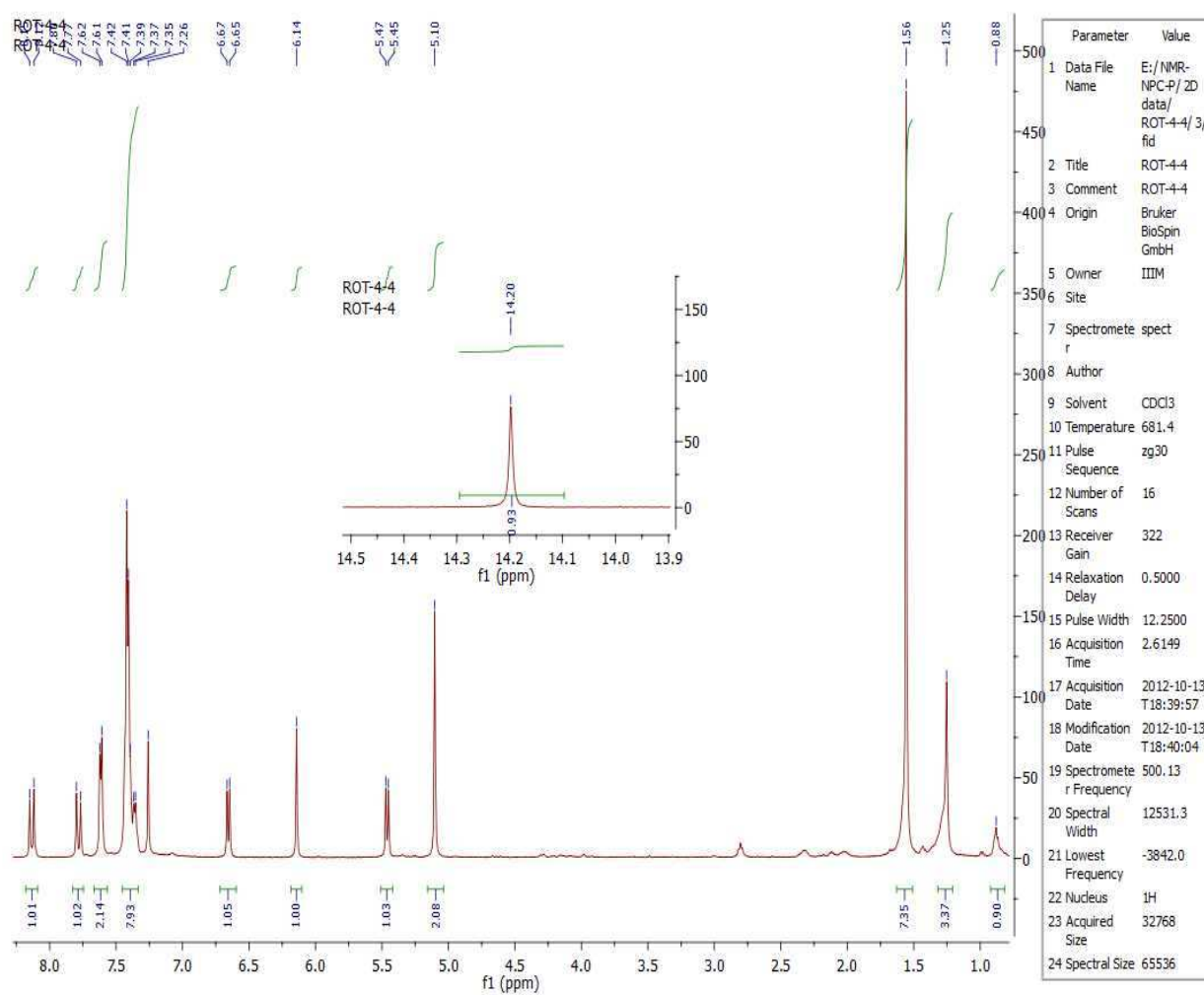
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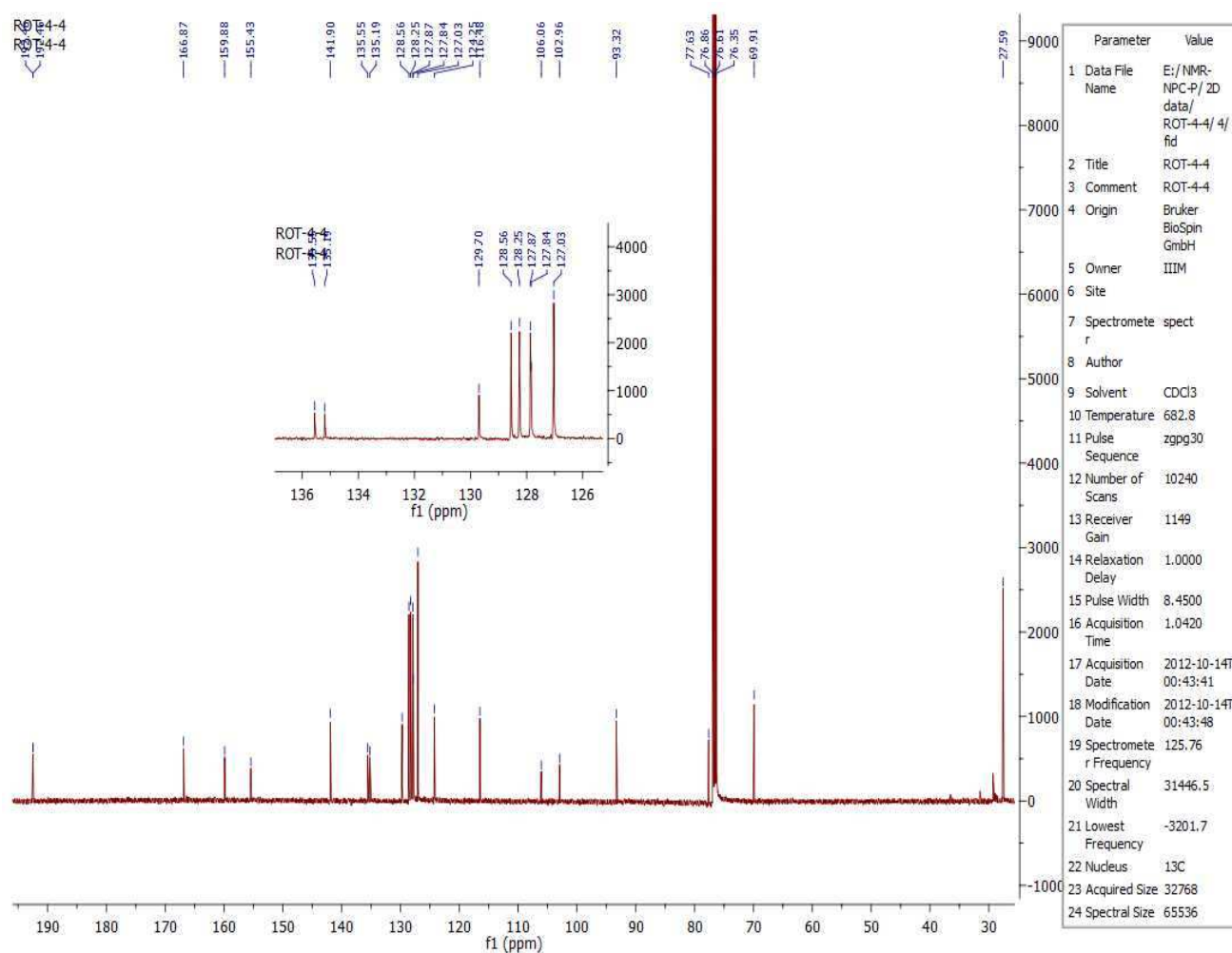
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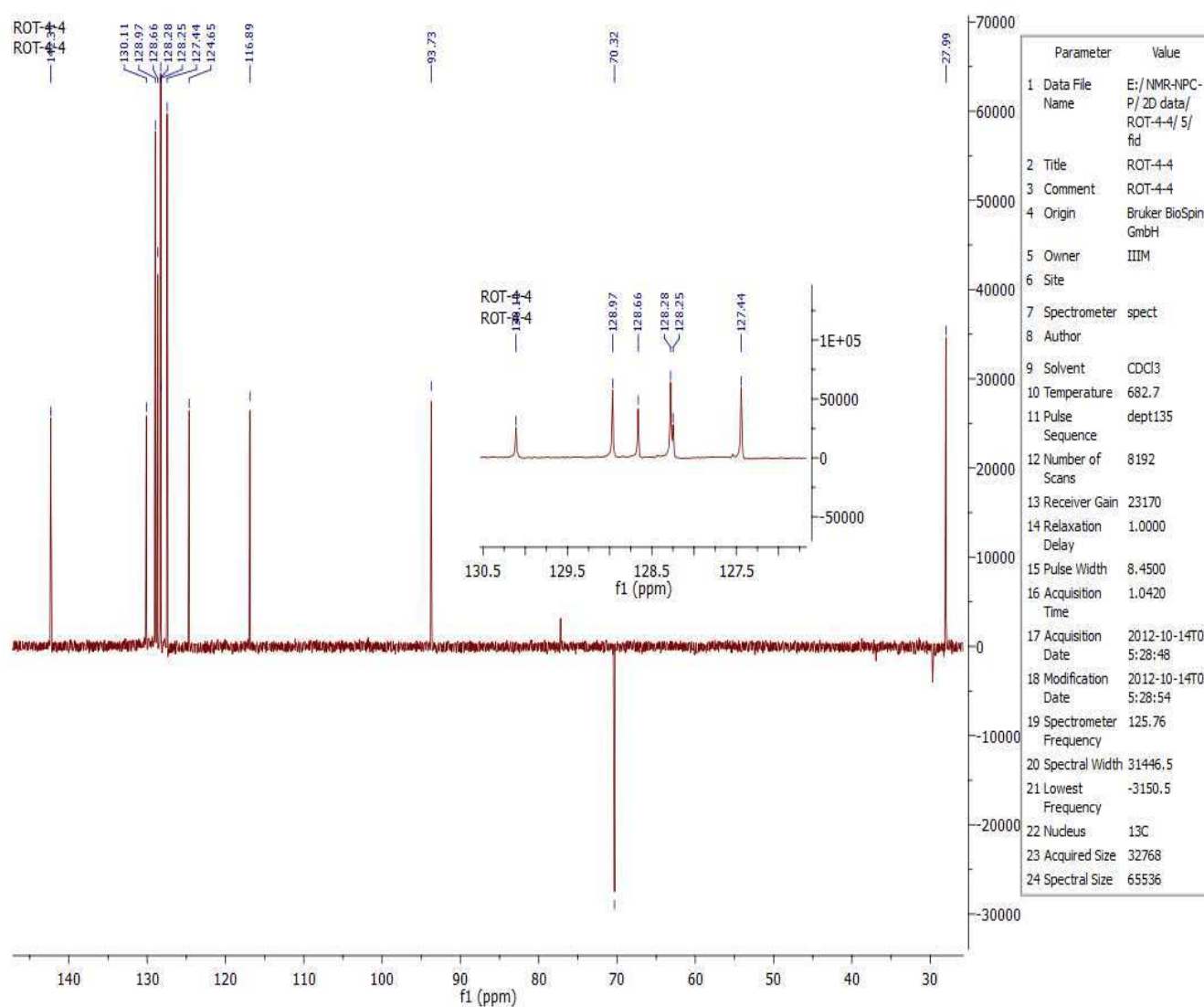
S1 HNMR Spectrum of **2a** in CDCl₃



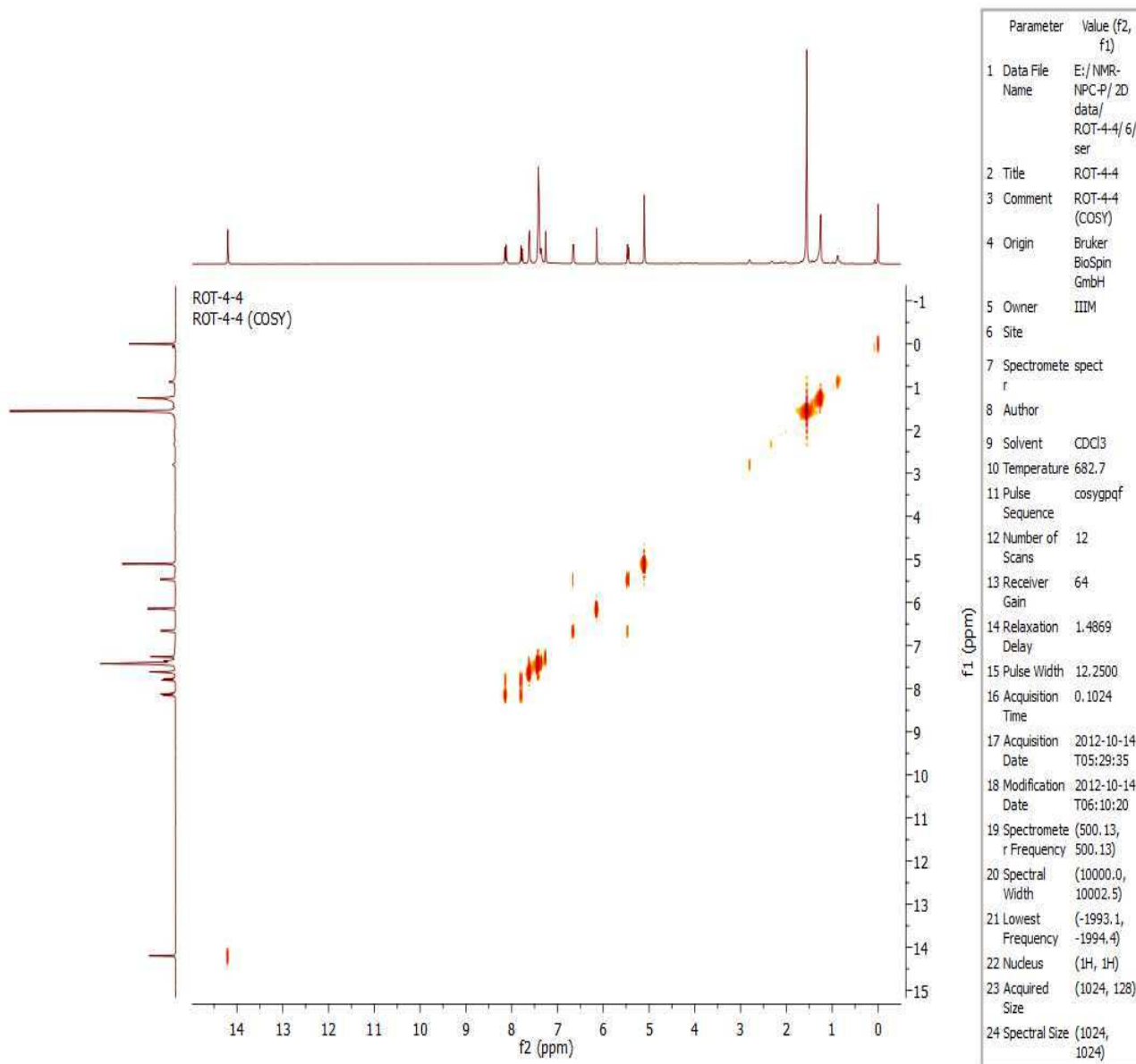
S2 ^{13}C NMR Spectrum of **2a** in CDCl_3



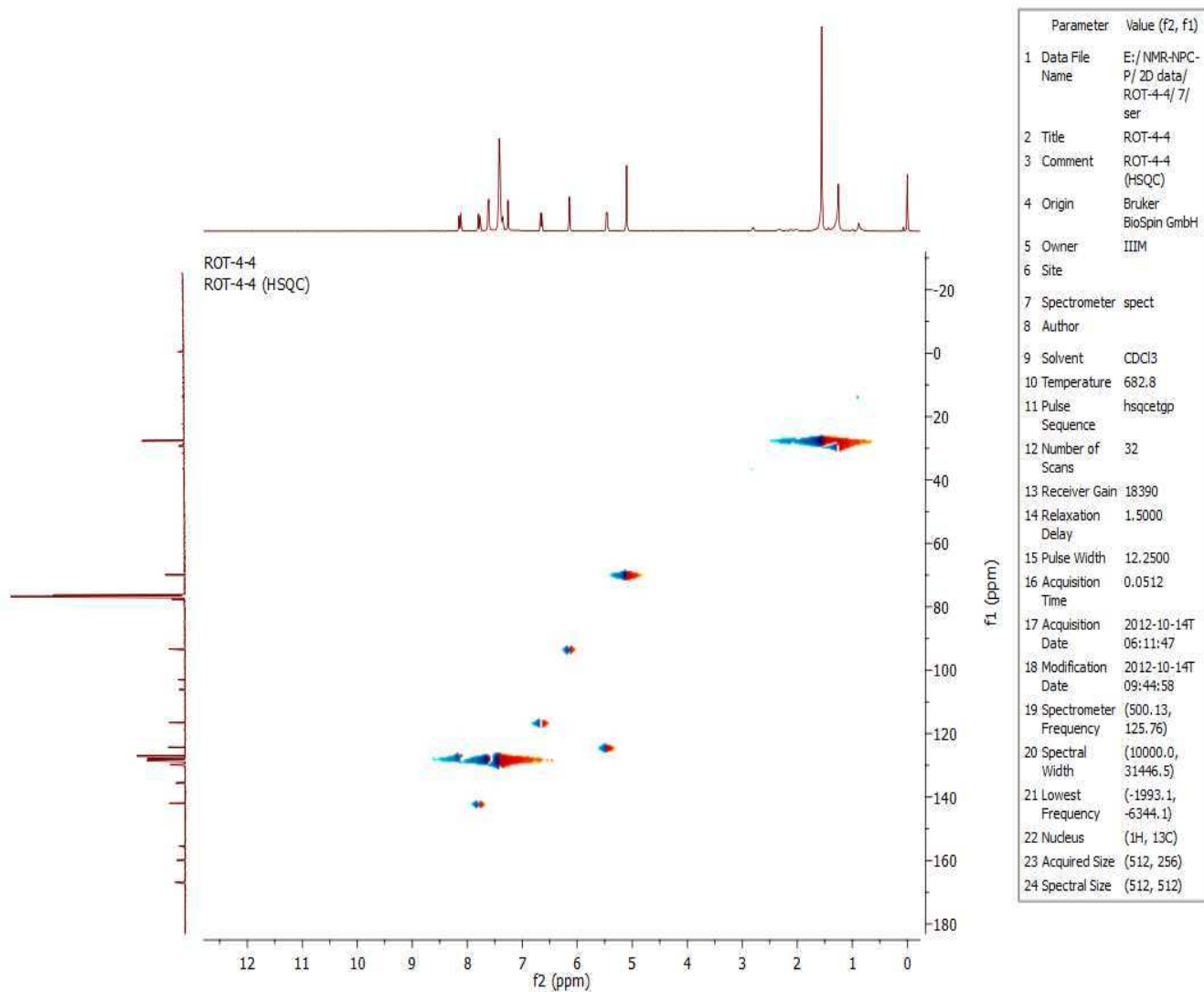
S3 DEPT-135 Spectrum of **2a** in CDCl₃



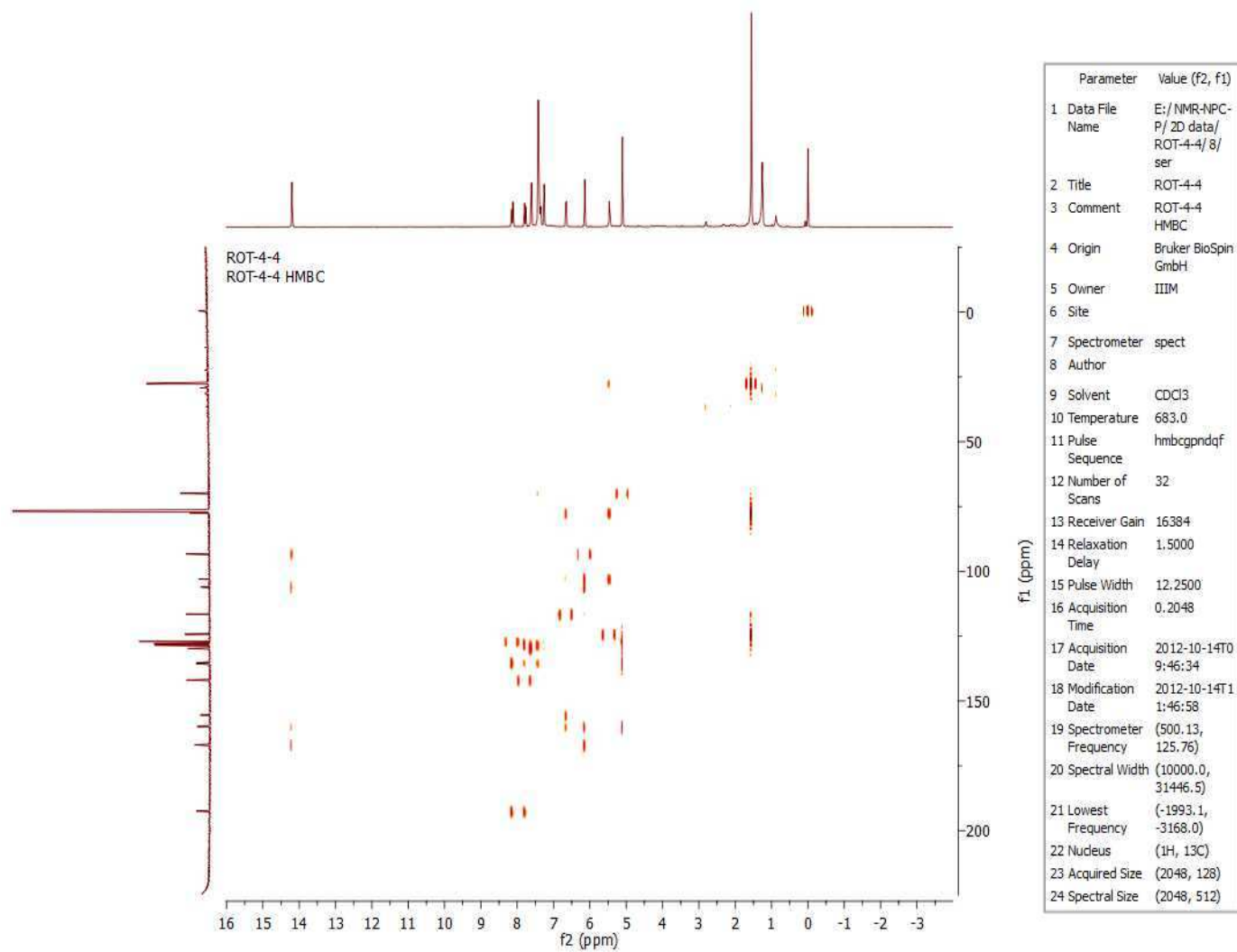
S4 COSY Spectrum of **2a** in CDCl₃



S5 HSQC Spectrum of **2a** in CDCl_3



S6 HMBC Spectrum of **2a** in CDCl₃



S7 HRMS Spectrum of 2a

Qualitative Compound Report

Data File	ROT-4-4.d	Sample Name	ROT-4-4
Sample Type	Sample	Position	Vial 31
Instrument Name	Instrument 1	User Name	
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IRM Calibration Status	Success	DA Method	SamplePurity-Default.m
Comment			

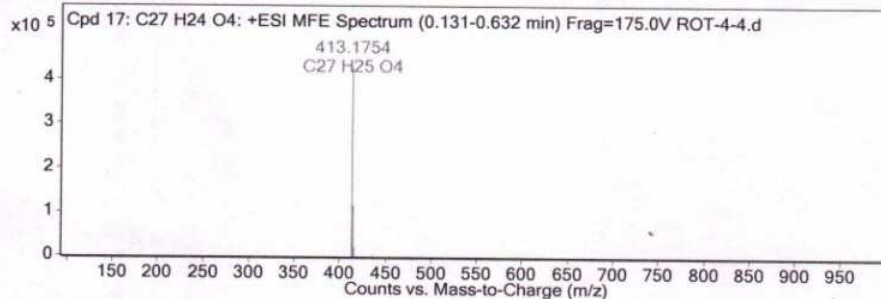
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

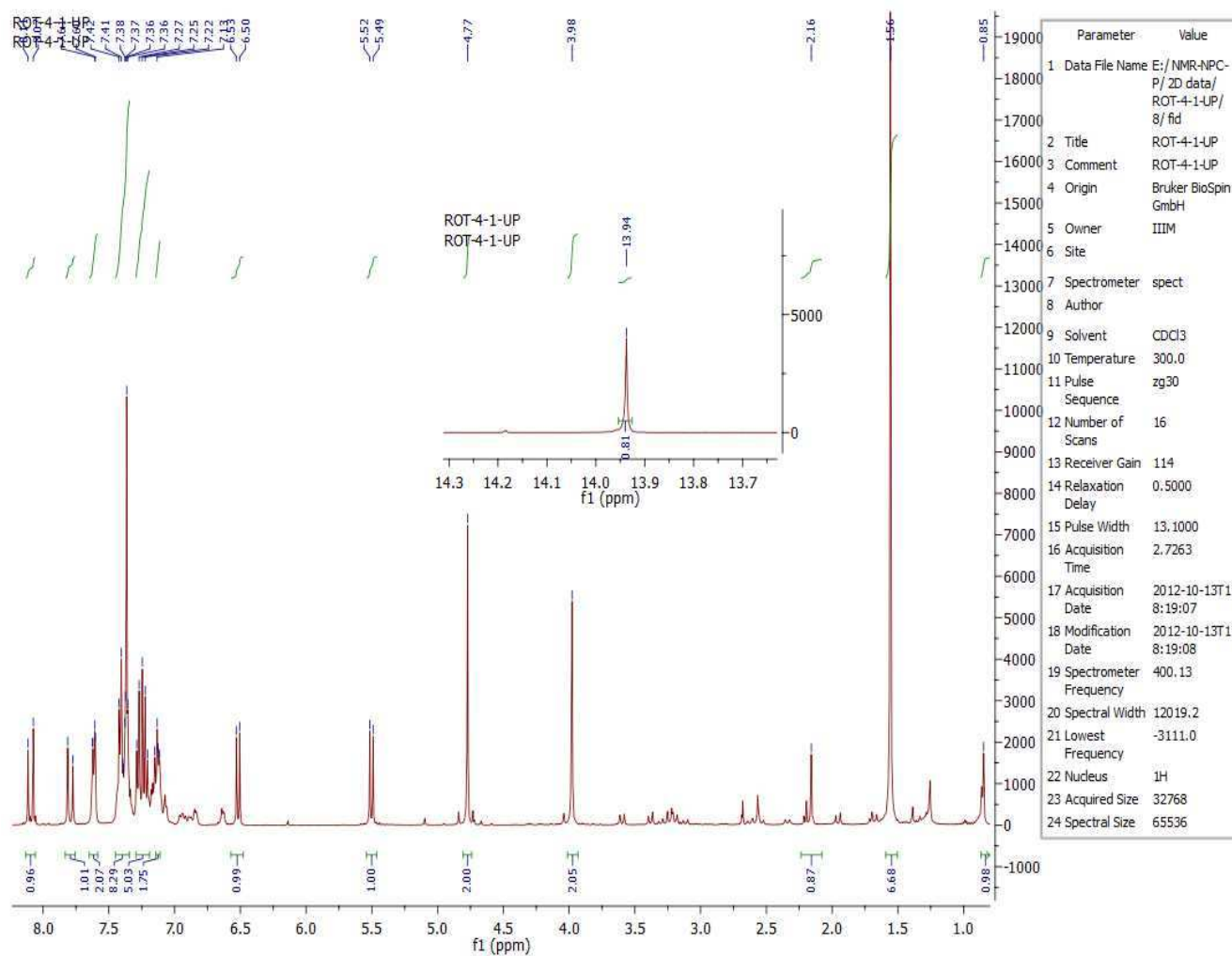
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 17: C27 H24 O4	0.187	412.168	C27 H24 O4	C27 H24 O4	-1.24	C27 H24 O4

Compound Label	m/z	RT	Algorithm	Mass
Cpd 17: C27 H24 O4	413.1754	0.187	Find by Molecular Feature	412.168

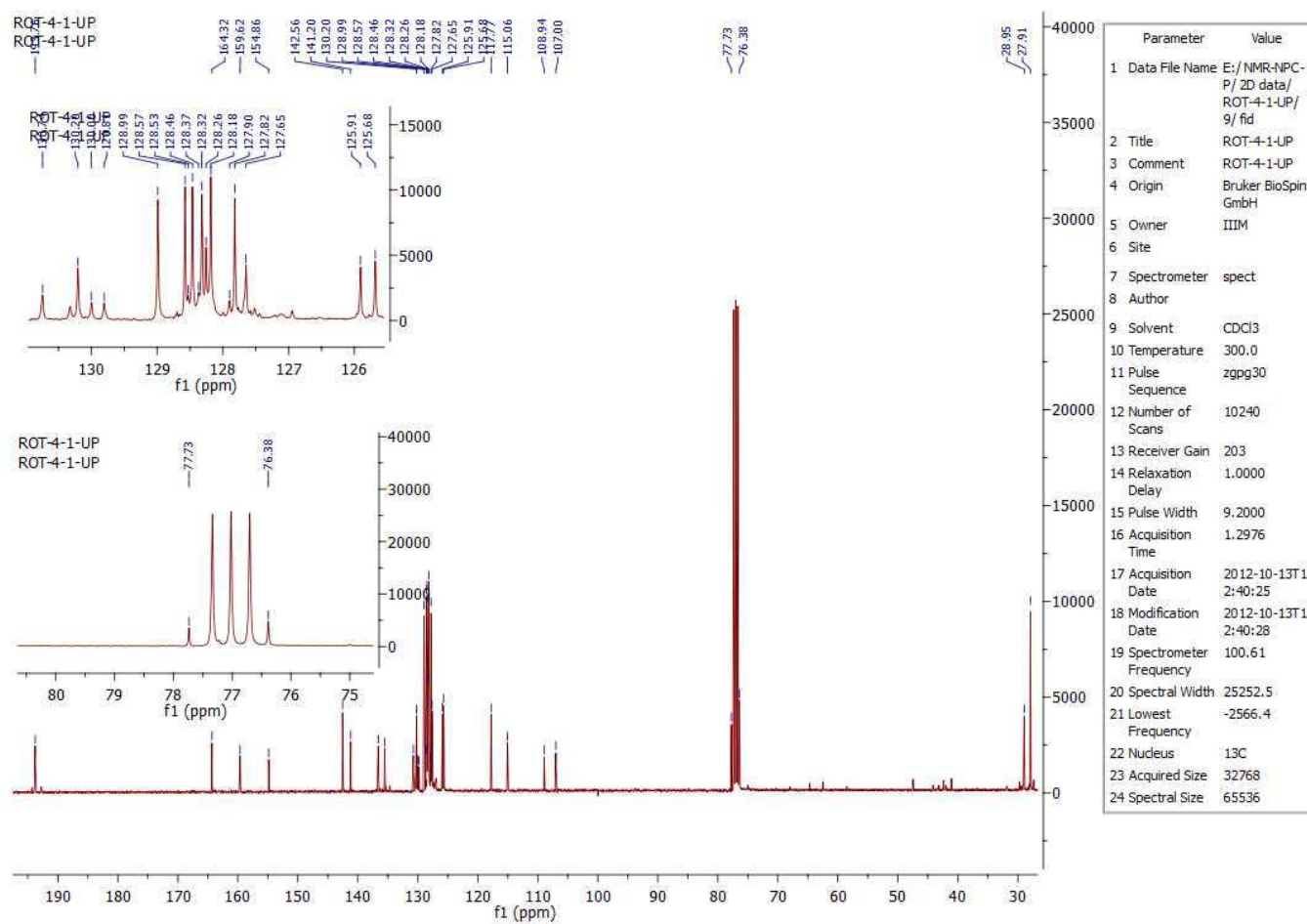
MFE MS Spectrum



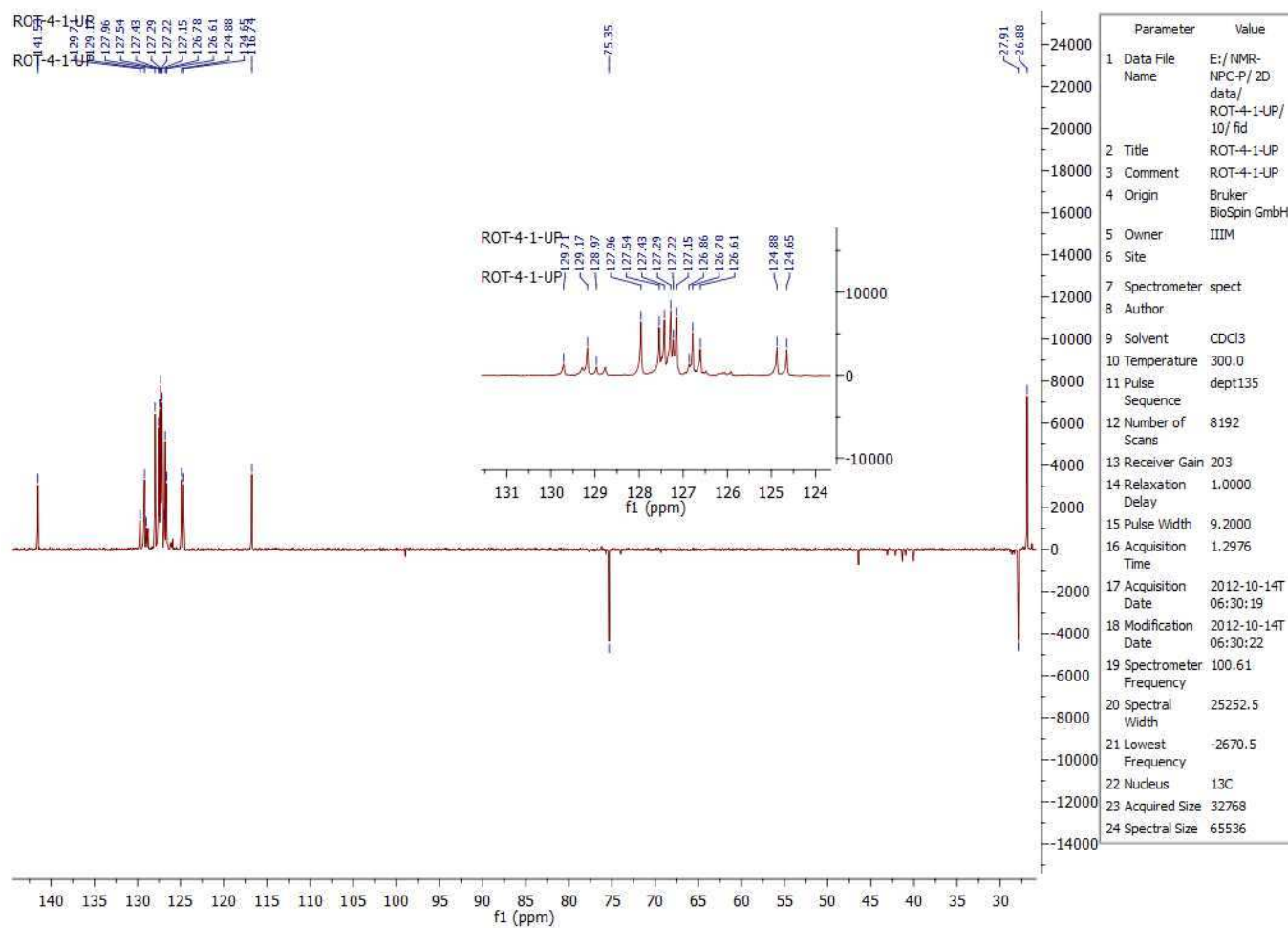
S8 ^1H NMR Spectrum of **2b** in CDCl_3



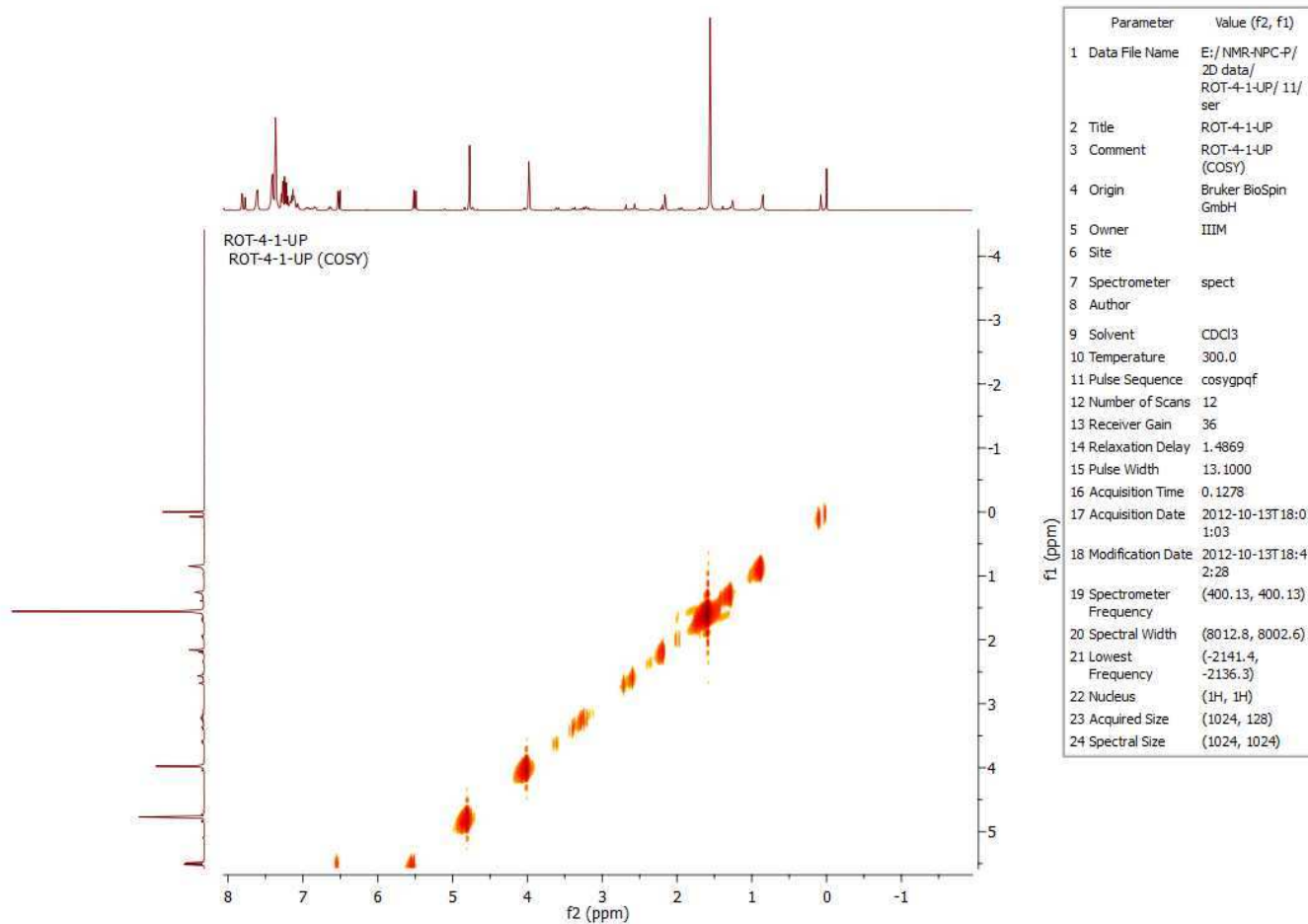
S9 ^{13}C NMR Spectrum of **2b** in CDCl_3



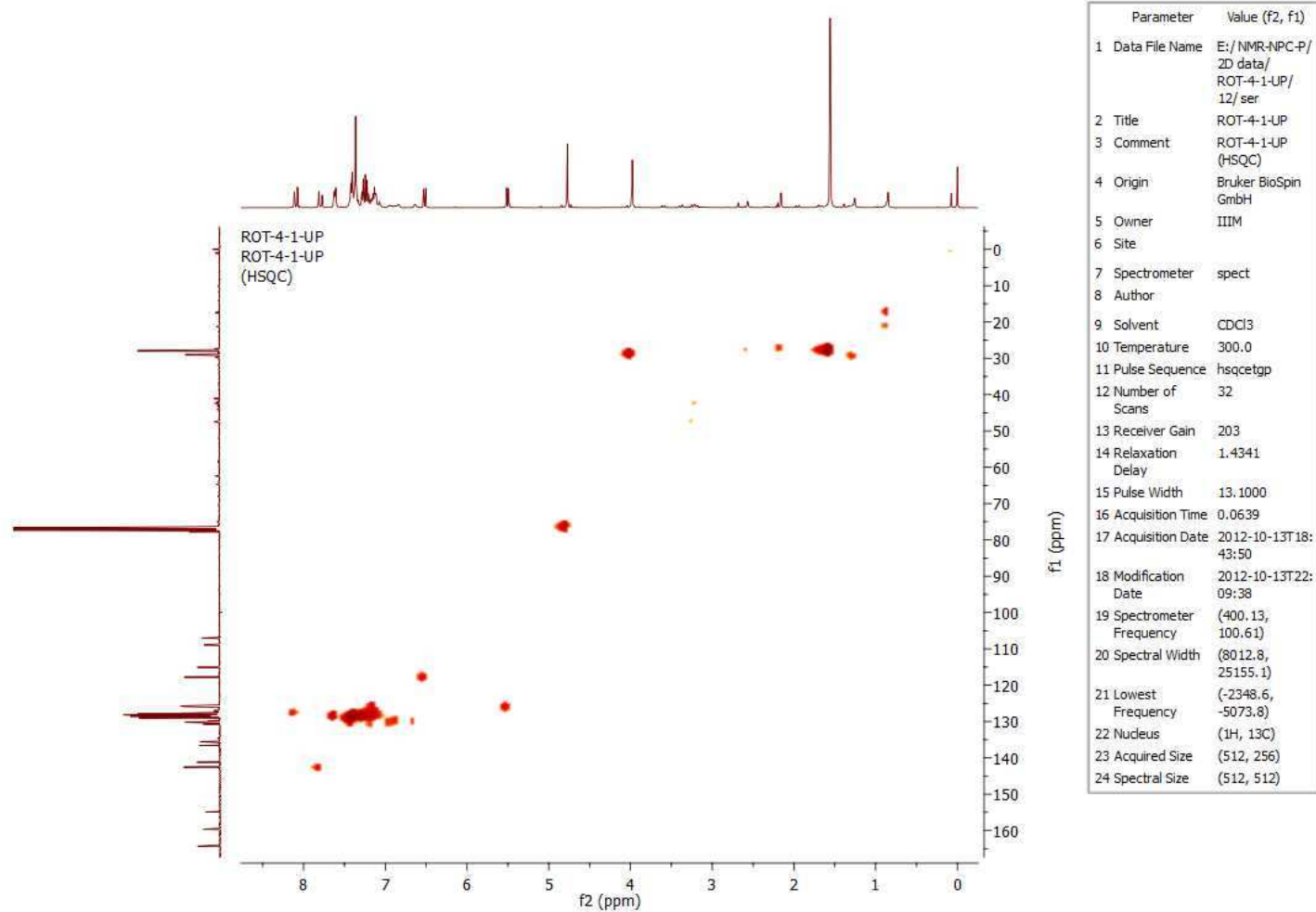
S10 DEPT-135 Spectrum of **2b** in CDCl₃



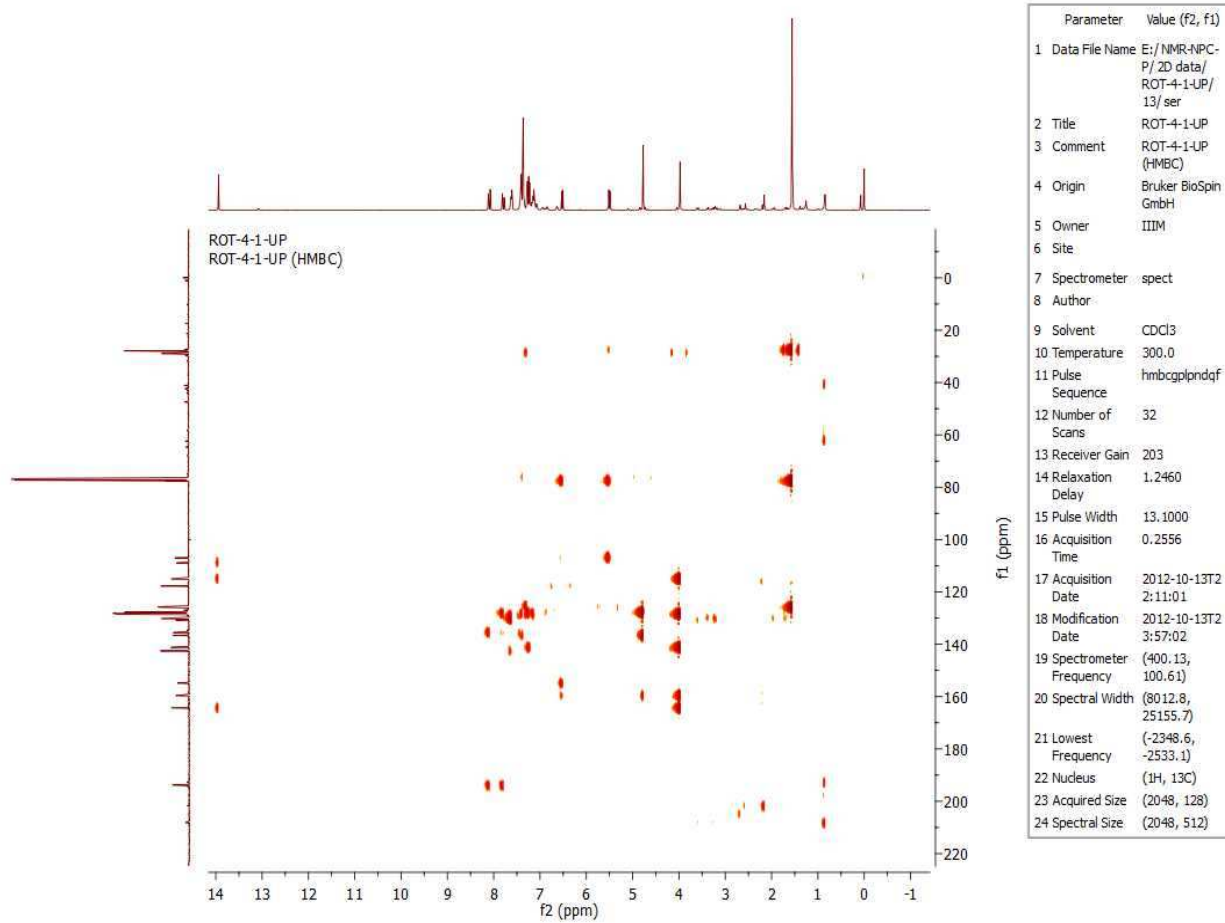
S11 COSY Spectrum of **2b** in CDCl₃



S12 HSQC Spectrum of **2b** in CDCl₃



S13 HMBC Spectrum of **2b** in CDCl₃



S14 HRMS Spectrum of 2b

Qualitative Compound Report

Data File	ROT-4-1-UP.d	Sample Name	ROT-4-1-UP
Sample Type	Sample	Position	Vial 45
Instrument Name	Instrument 1	User Name	
Acq Method	vishal_12-01-13.m	Acquired Time	13-03-2013 PM 5:06:08
IRM Calibration Status	Success	DA Method	SamplePurity-Default.m
Comment			

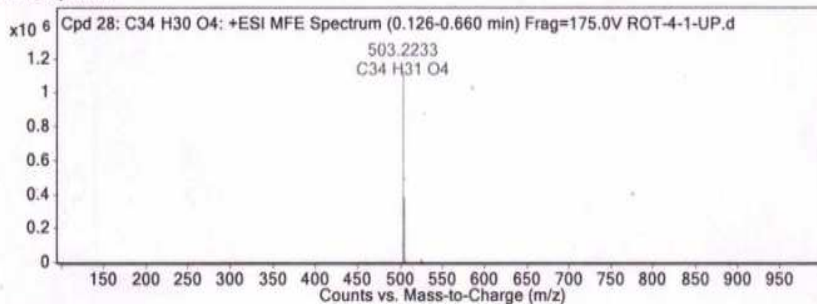
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

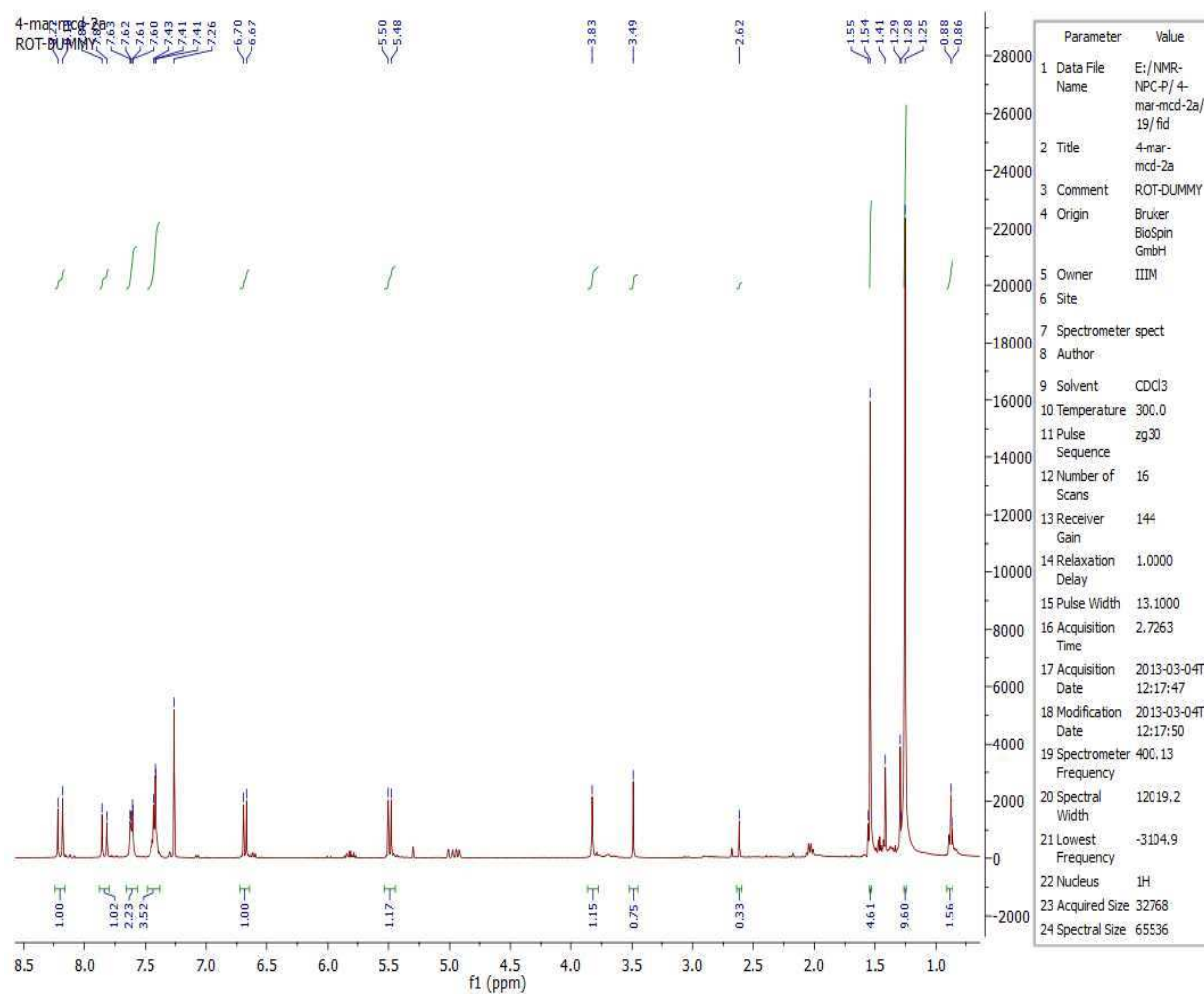
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 28: C34 H30 O4	0.188	502.2161	C34 H30 O4	C34 H30 O4	-3.39	C34 H30 O4

Compound Label	m/z	RT	Algorithm	Mass
Cpd 28: C34 H30 O4	503.2233	0.188	Find by Molecular Feature	502.2161

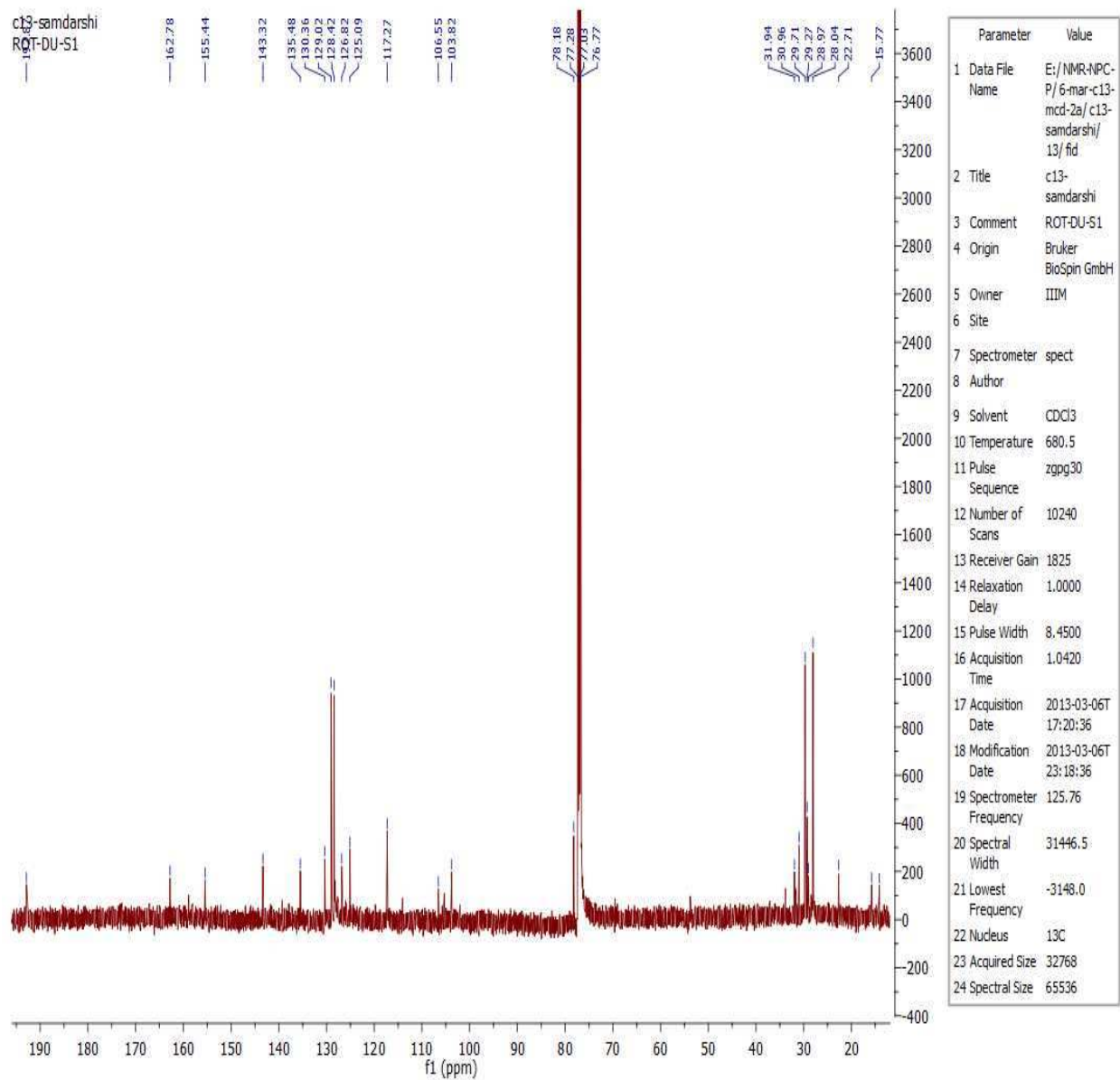
MFE MS Spectrum



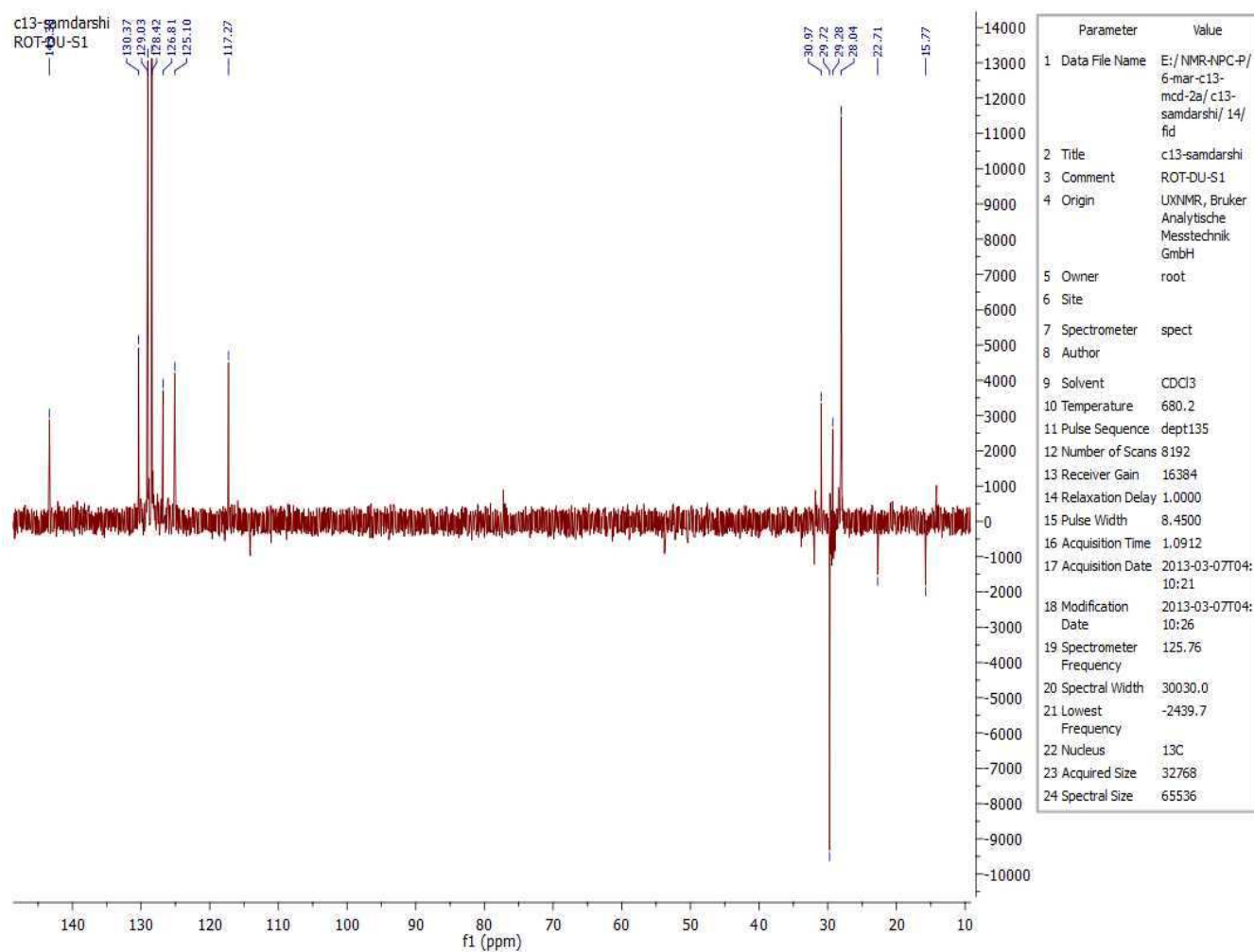
S15 ^1H NMR Spectrum of **2c** in CDCl_3



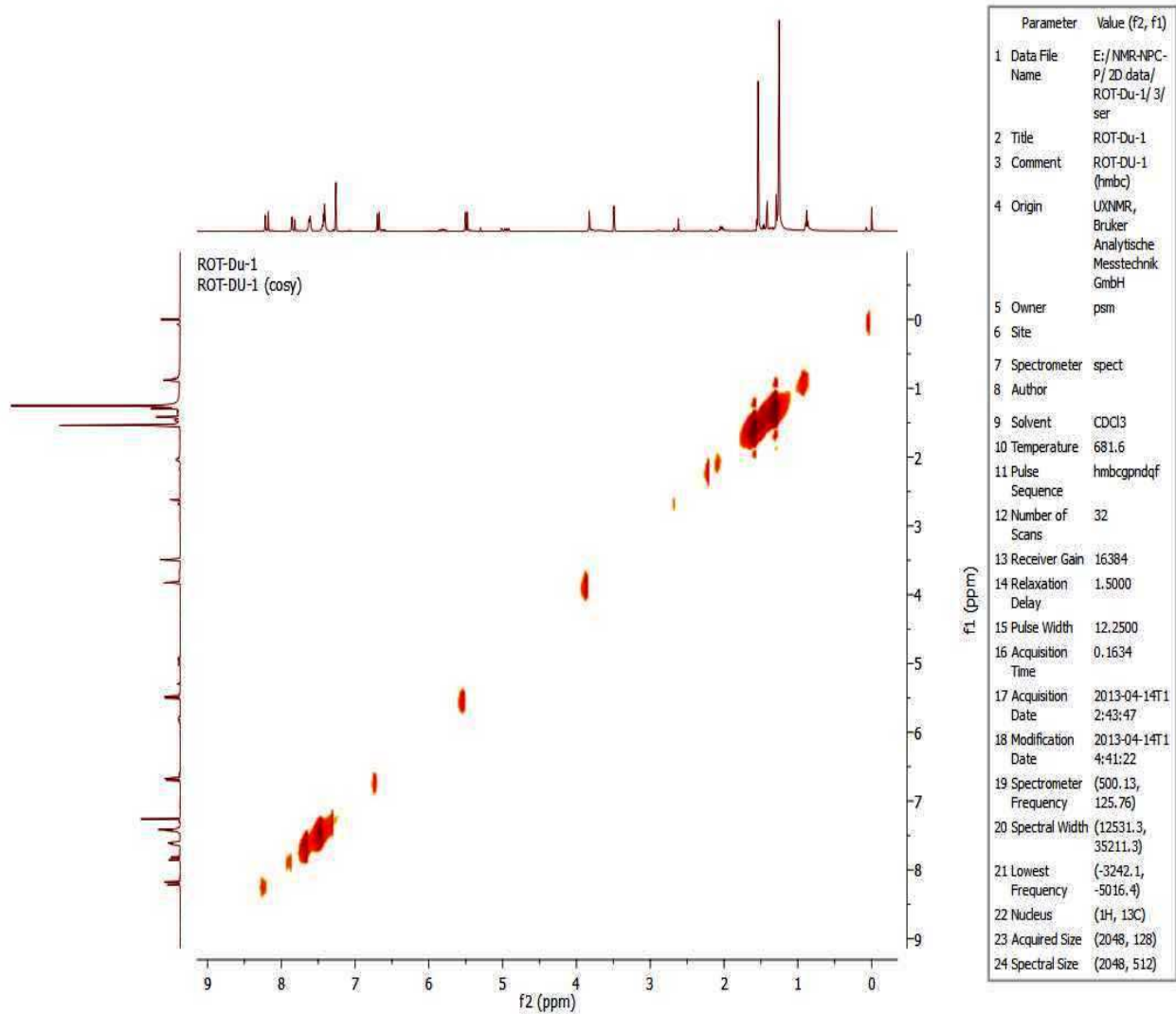
S16 ^{13}C NMR Spectrum of **2c** in CDCl_3



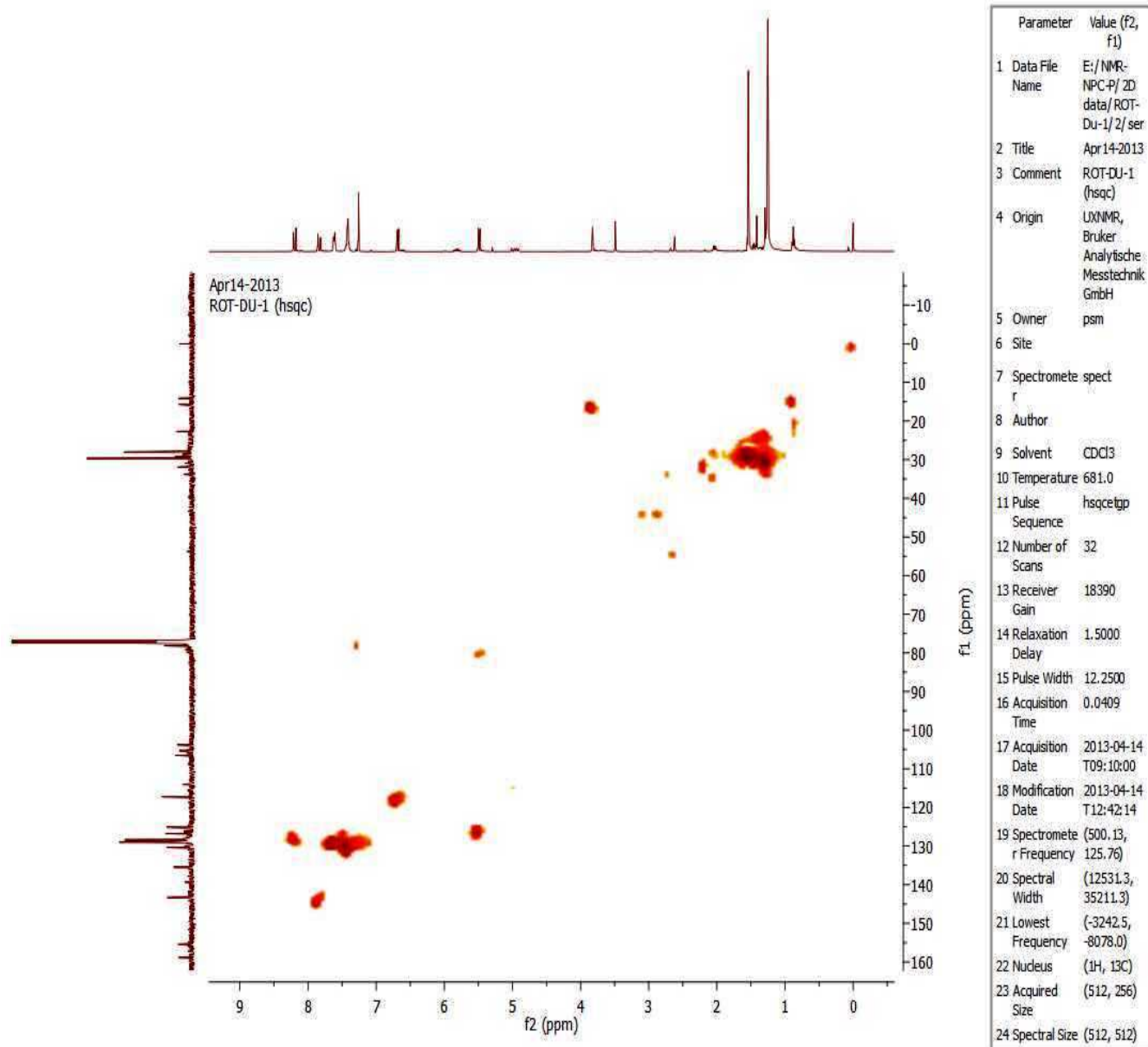
S17 DEPT-135 Spectrum of **2c** in CDCl₃



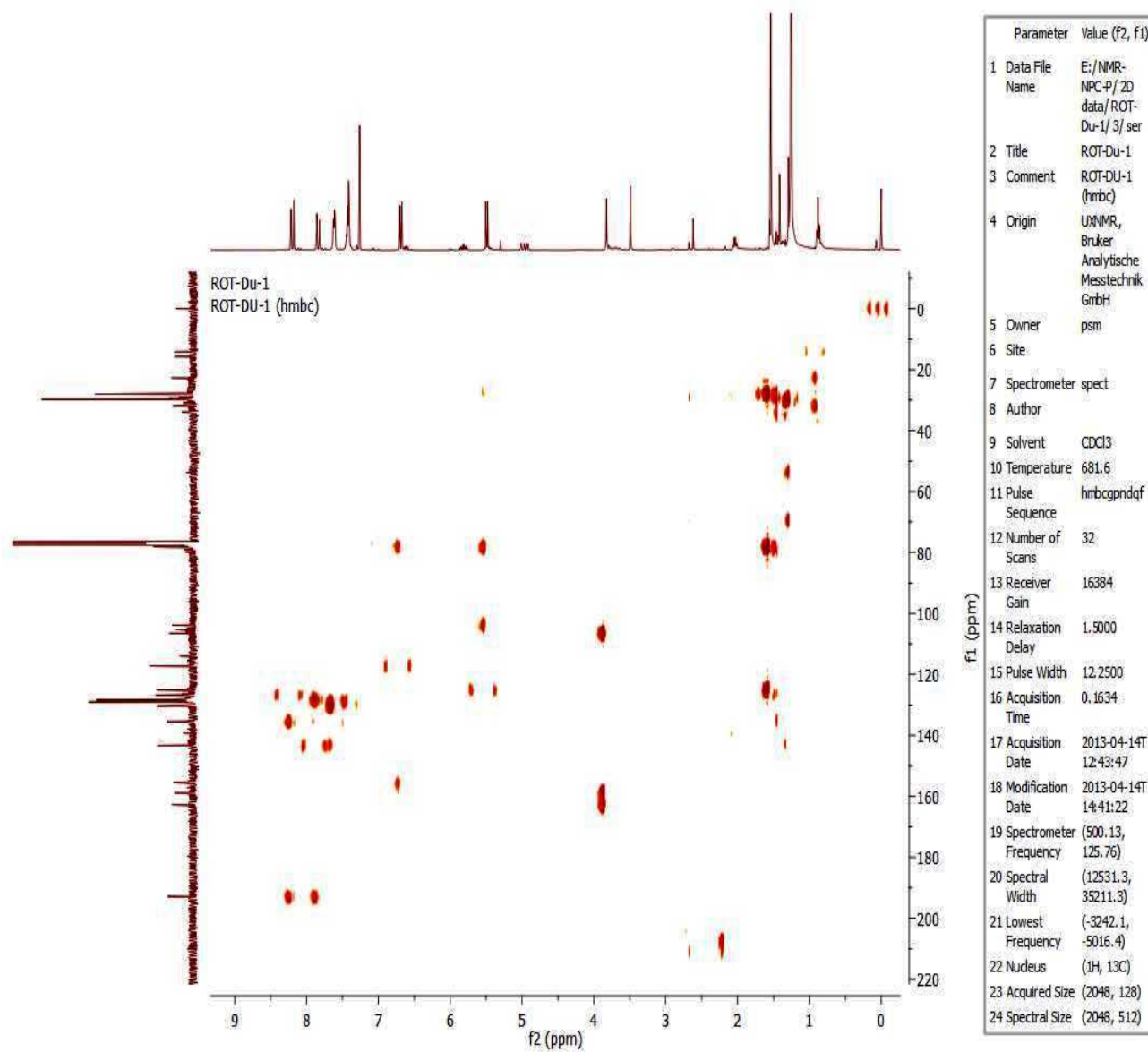
S18 COSY Spectrum of **2c** in CDCl₃



S19 HSQC Spectrum of **2c** in CDCl₃



S20 HMBC Spectrum of **2c** in CDCl₃



S21 HRMS Spectrum of 2c

Qualitative Compound Report

Data File	ROT-DU1.d	Sample Name	ROT-DU1
Sample Type	Sample	Position	Vial 53
Instrument Name	Instrument 1	User Name	
Acq Method	vishal_12-01-13.m	Acquired Time	11-03-2013 PM 4:25:08
IRM Calibration Status	Success	DA Method	SamplePurity-Default.m
Comment			

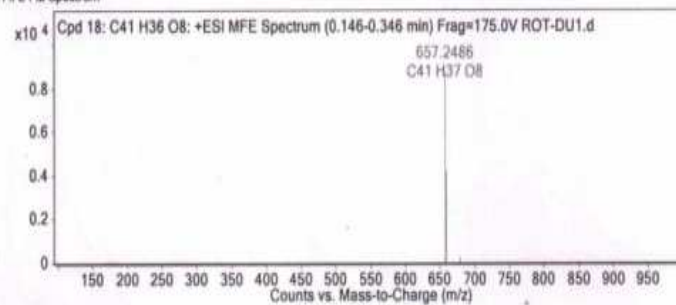
Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (85125)

Compound Table

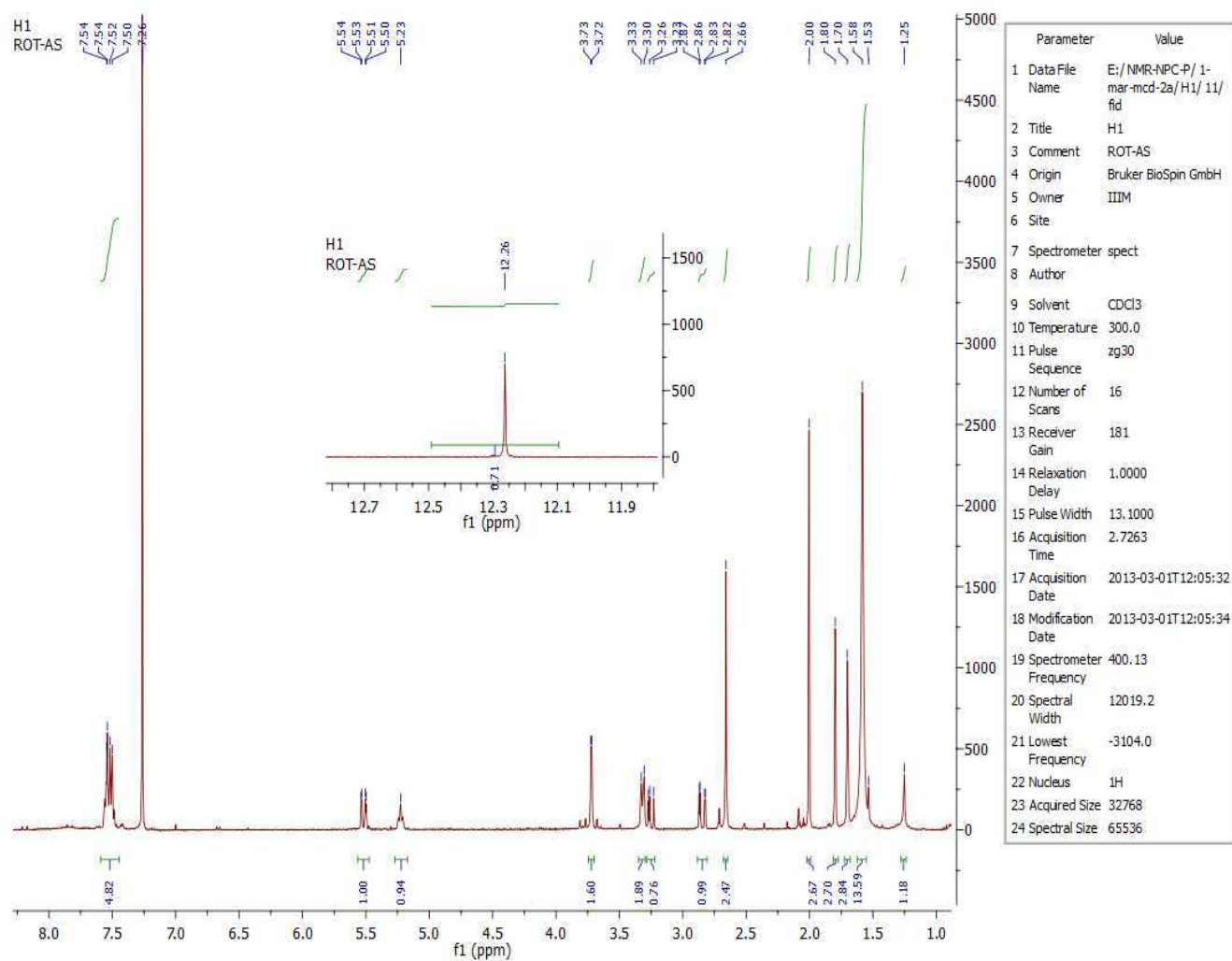
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C41 H36 O8	0.199	656.2414	C41 H36 O8	C41 H36 O8	-0.64	C41 H36 O8

Compound Label	m/z	RT	Algorithm	Mass
Cpd 18: C41 H36 O8	657.2486	0.199	Find by Molecular Feature	656.2414

MFE MS Spectrum



S22 HNMR Spectrum of **2d** in CDCl₃



S23 HRMS Spectrum of 2d

Qualitative Compound Report

Data File	ROT-AS.d	Sample Name	ROT-AS
Sample Type	Sample	Position	Vial 2
Instrument Name	Instrument 1	User Name	
Acq Method	vishal_12-01-13.m	Acquired Time	14-03-2013 PM 12:50:25
IRM Calibration Status	Success	DA Method	SamplePurity-Default.m
Comment			

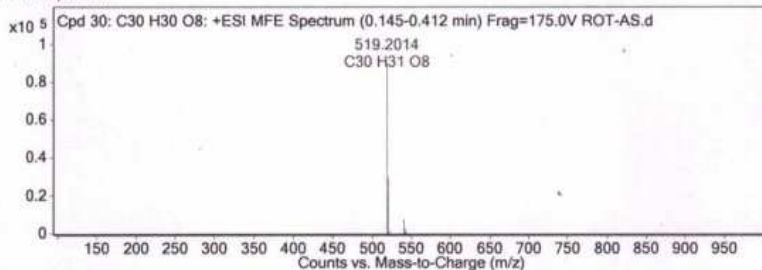
Sample Group		Info.	65:25(ACN:H2O)
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
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Compound Label	m/z	RT	Algorithm	Mass
Cpd 30: C30 H30 O8	519.2014	0.195	Find by Molecular Feature	518.194

MFE MS Spectrum



S24 ^1H NMR Spectrum of rottlerin CDCl_3

