

The HR-ESI-MS Spectrum of Compound 1.

Mass Spectrum SmartFormula Report

Analysis Info

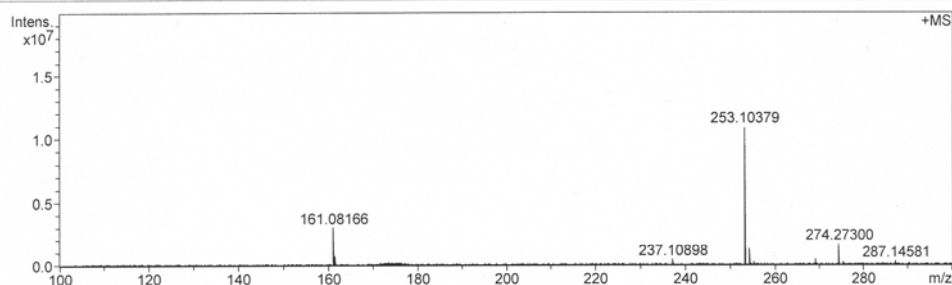
Analysis Name D:\Data\User\20111019\ZL_7_ESI_POS_000002.d
Method Metal_Trypsin digestion
Sample Name ZL_7_ESI_POS
Comment ZL_7_ESI_POS

Acquisition Date 10/19/2011 4:43:20 PM

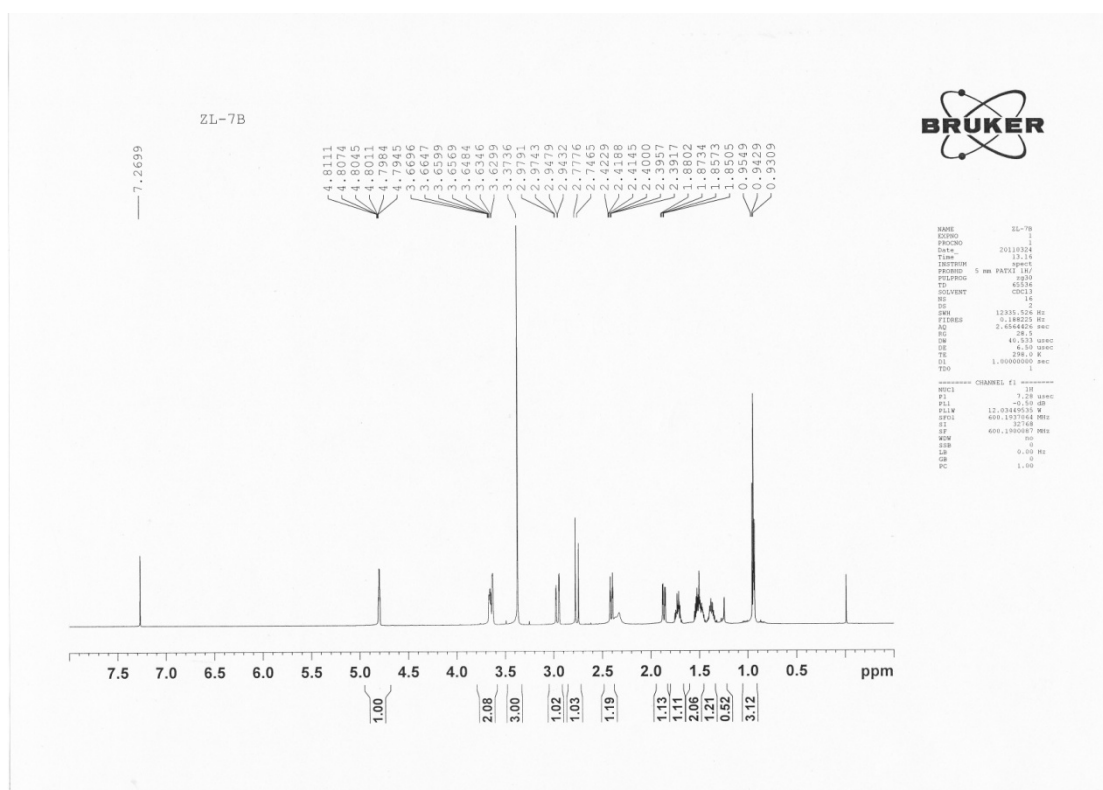
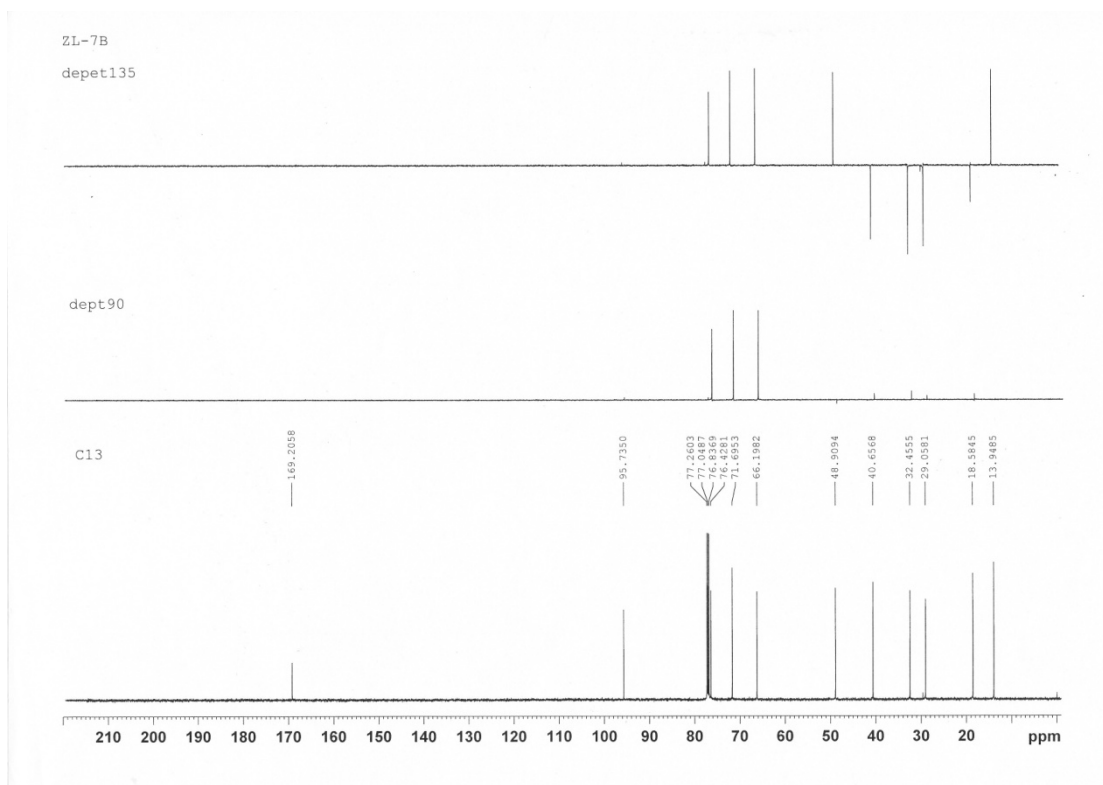
Operator
Instrument apex-Ultra

Acquisition Parameter

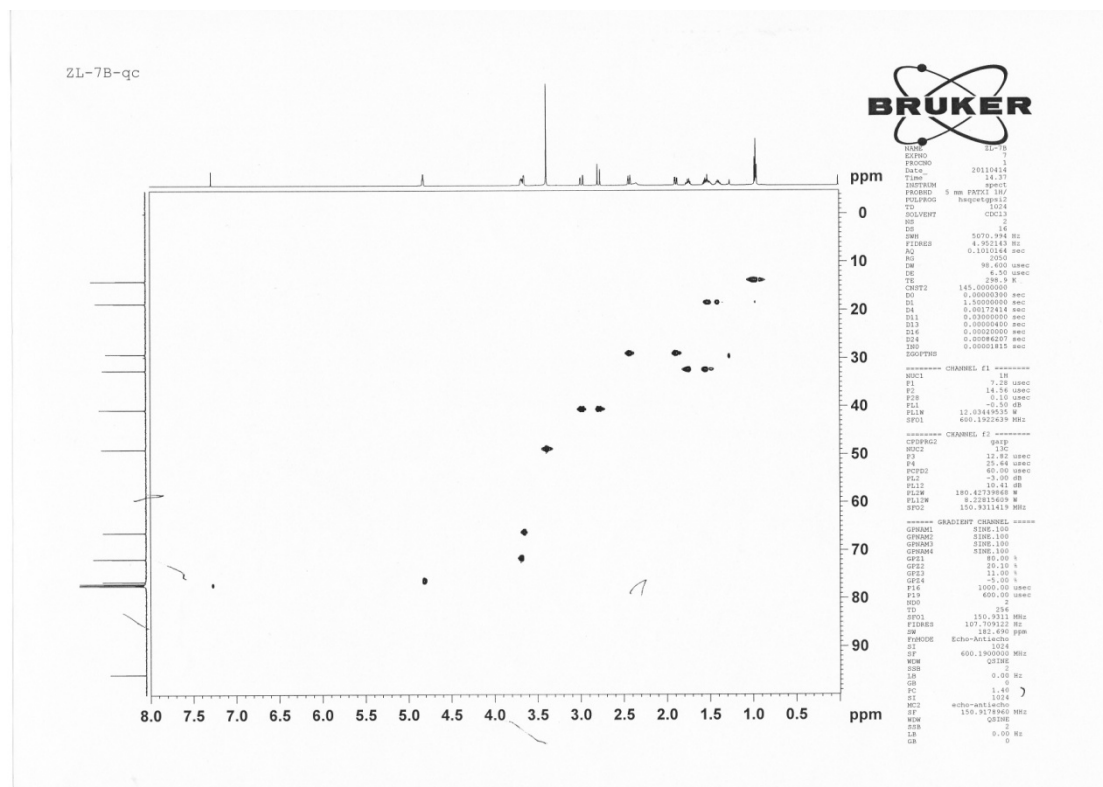
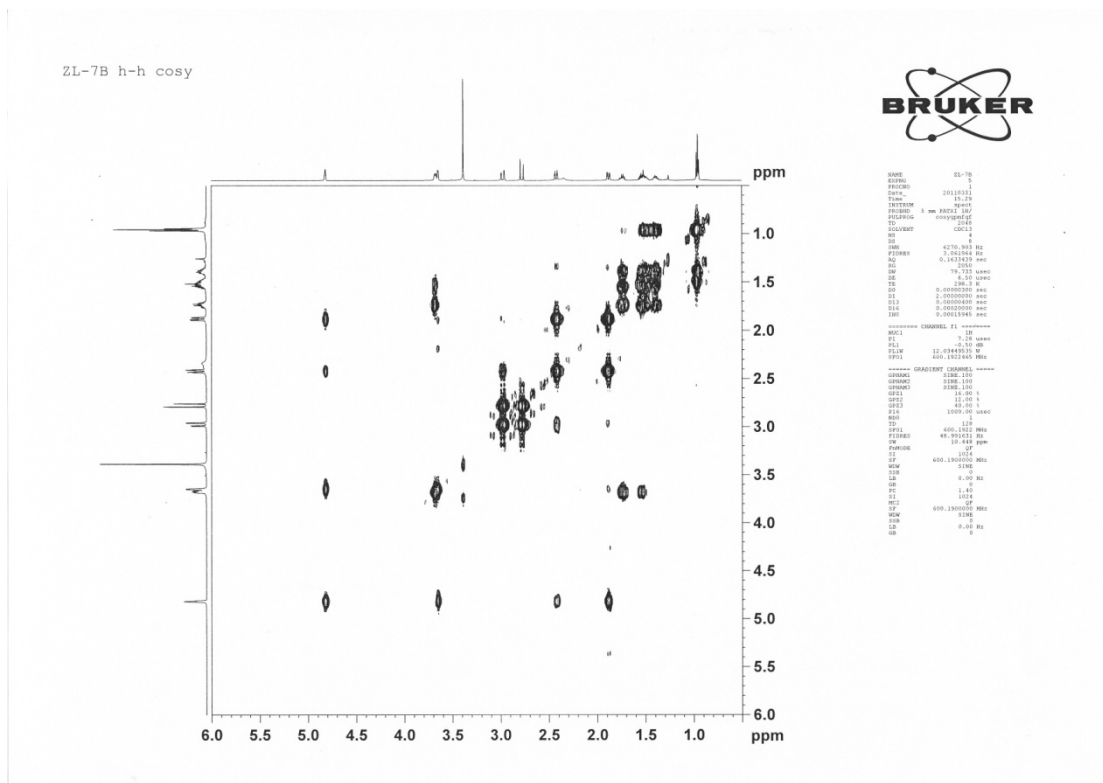
Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Oct 19 09:26:51
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	261072
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



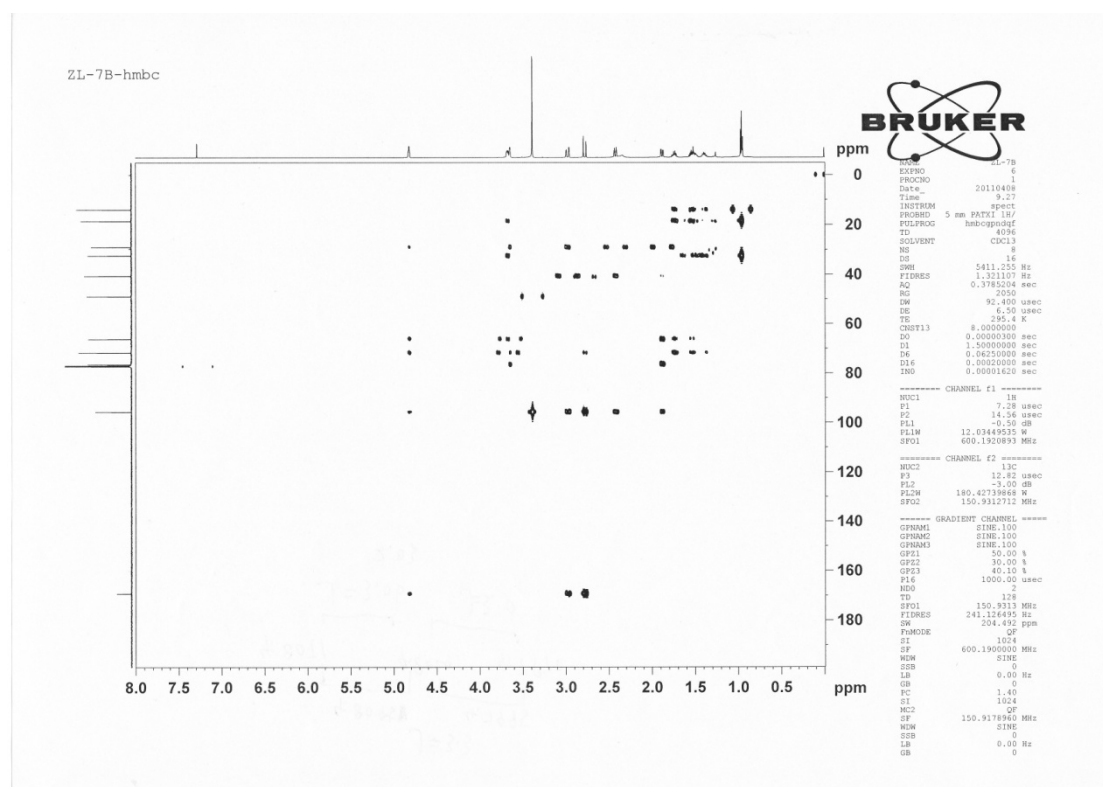
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
253.10379	1	C 11 H 18 Na O 5	100.00	253.10464	0.9	3.4	6.3	2.5	even	ok

The ^1H -NMR Spectrum of Compound 1.The ^{13}C -NMR Spectrum of Compound 1.

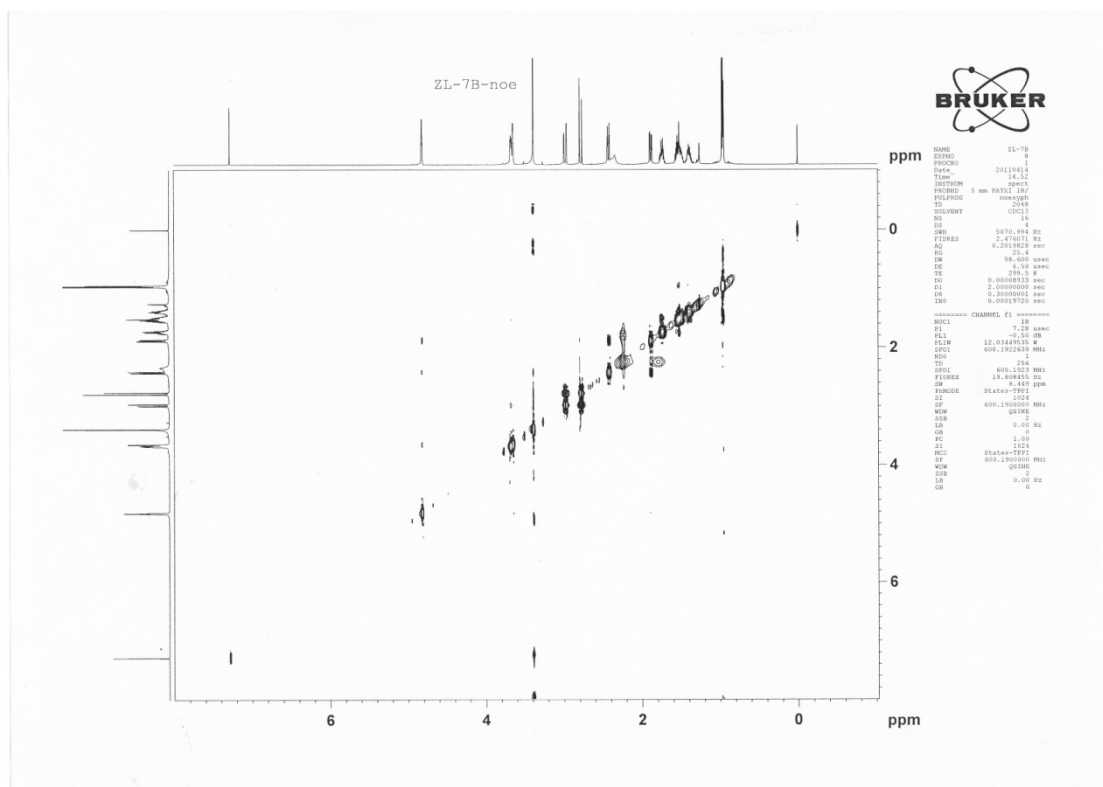
The HSQC Spectrum of Compound 1.

The ^1H - ^1H COSY spectrum of compound 1.

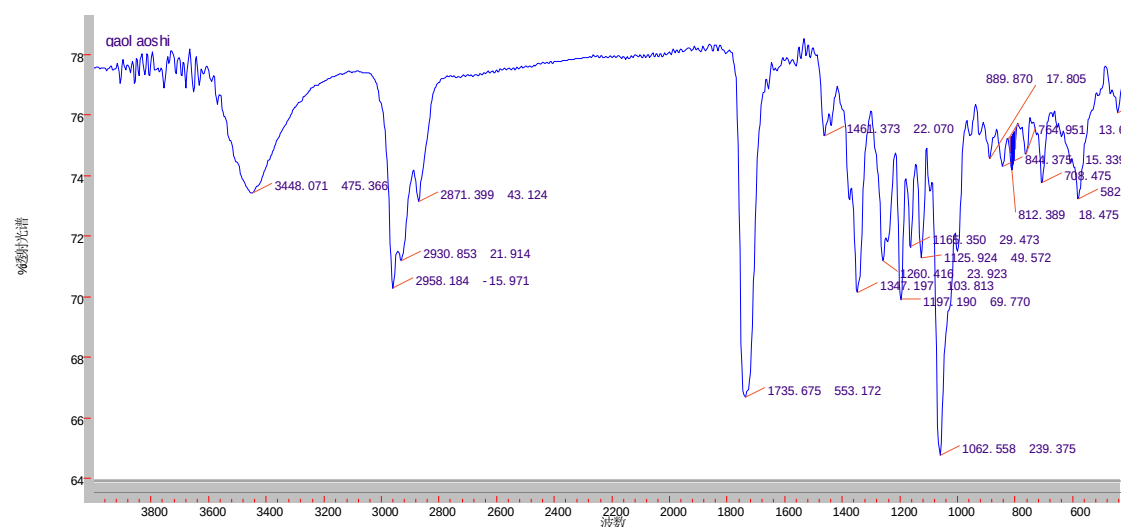
The HMBC Spectrum of Compound 1.



The NOESY Spectrum of Compound 1.



The IR Spectrum of Compound 1.



The HR-ESI-MS Spectrum of Compound 2.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\User\20111019\ZL_10_ESI_POS_000003.d
Method Metal_Trypsin digestion
Sample Name ZL_10_ESI_POS
Comment ZL_10_ESI_POS

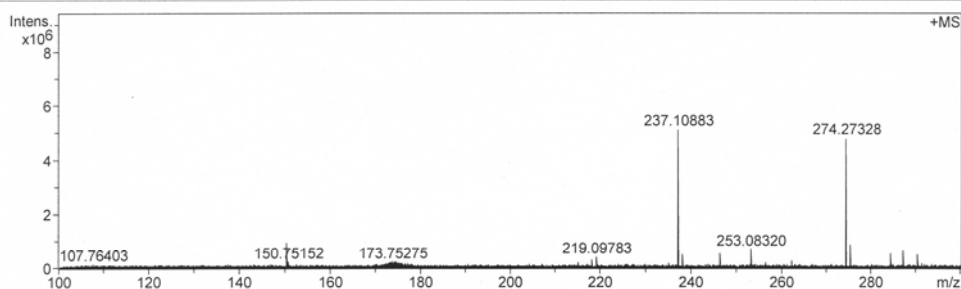
Acquisition Date 10/19/2011 4:41:52 PM

Operator

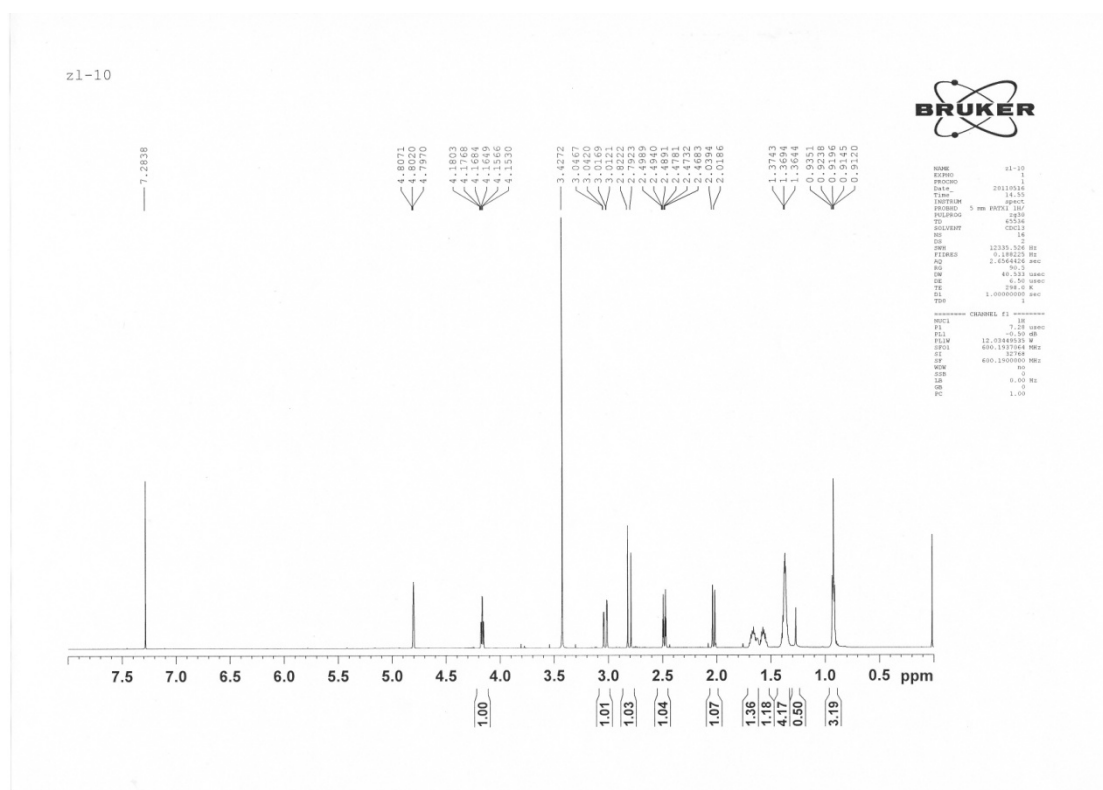
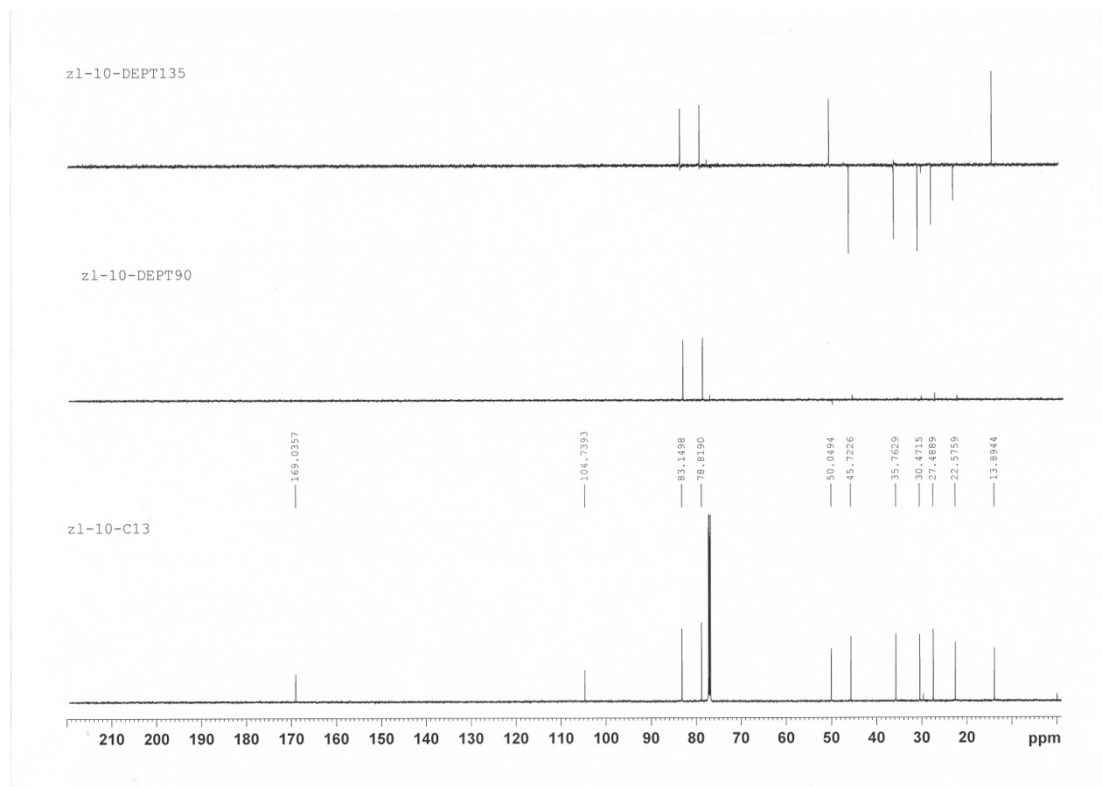
Instrument apex-Ultra

Acquisition Parameter

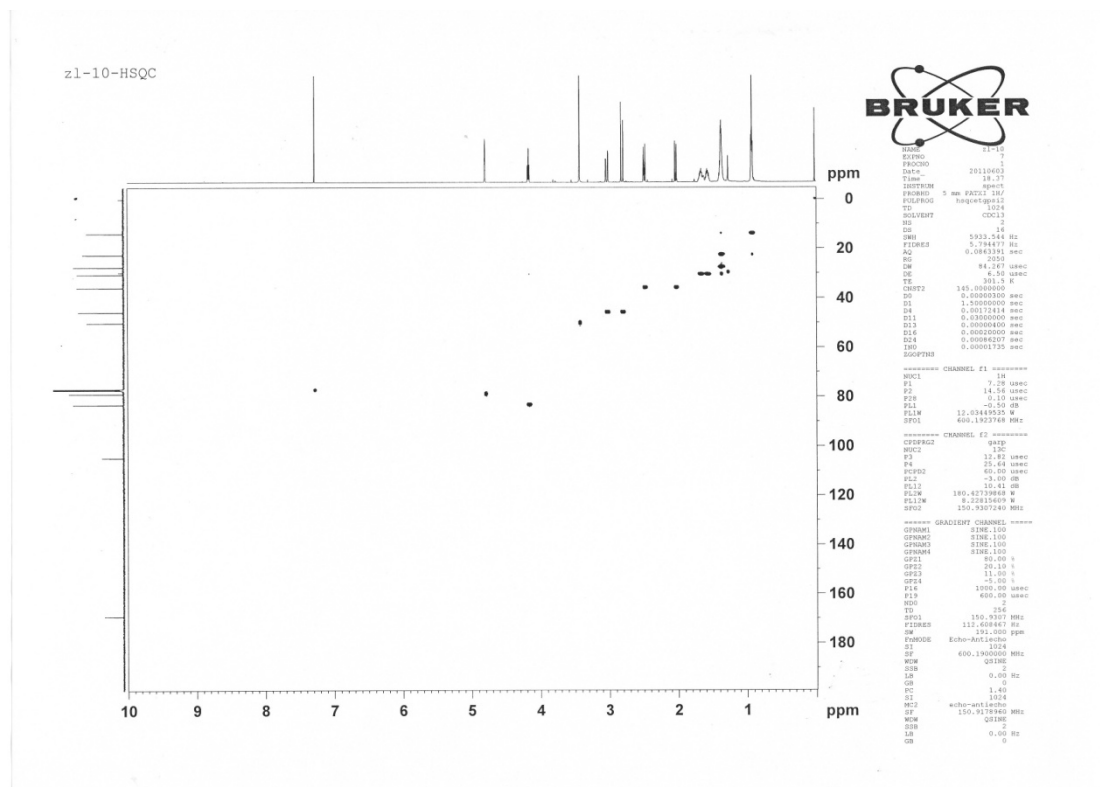
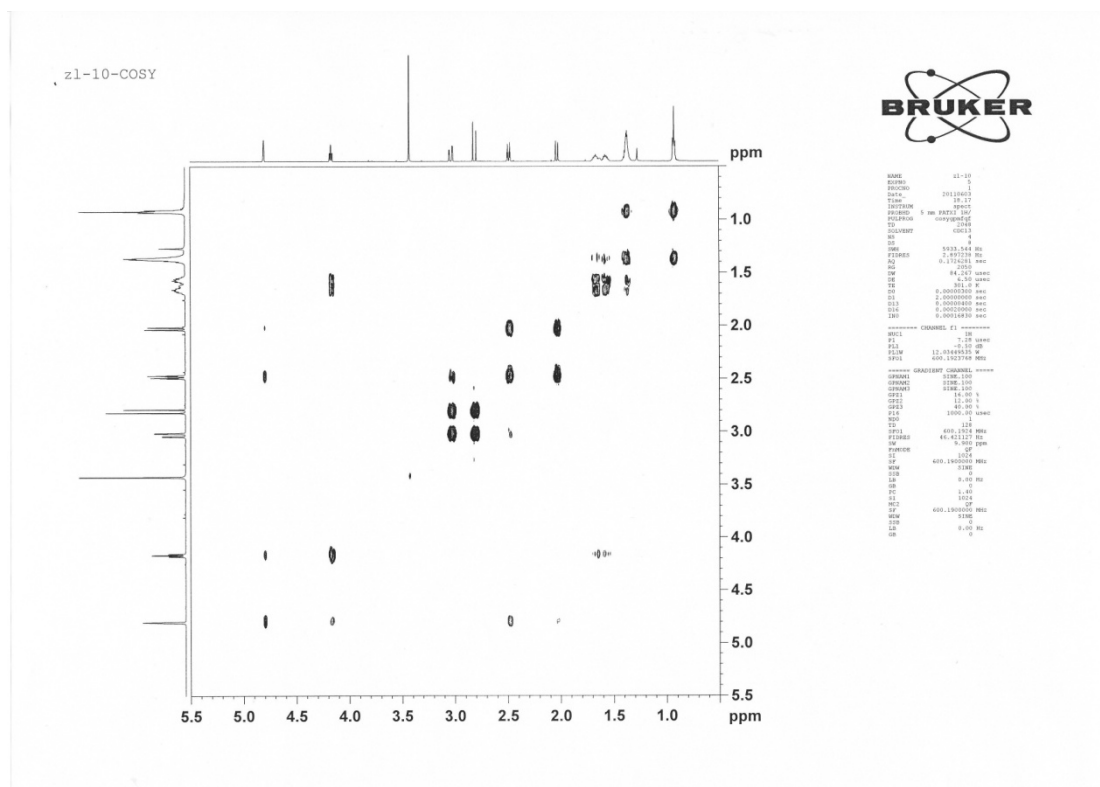
Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	2000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Wed Oct 19 09:26:51
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Data Acquisition Size	281072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				



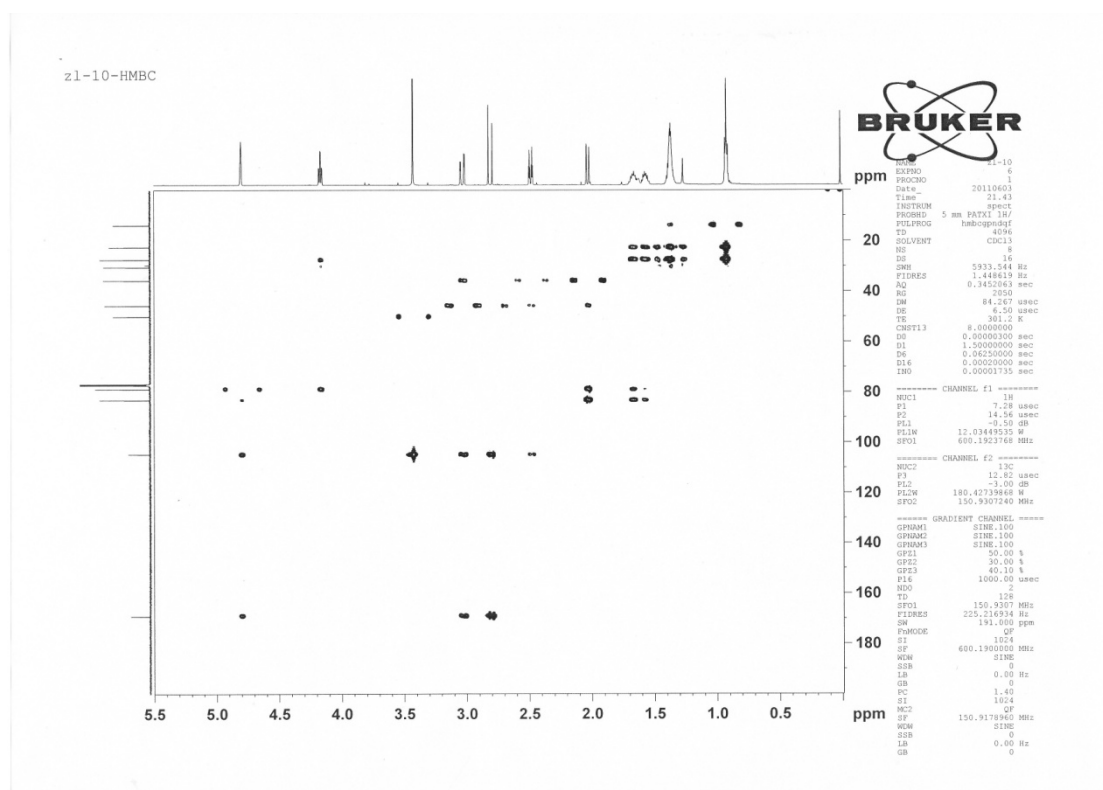
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
237.10883	1	C 11 H 18 Na O 4	100.00	237.10973	0.9	3.8	11.4	2.5	even	ok

The ^1H -NMR Spectrum of Compound 2.The ^{13}C -NMR of compound 2.

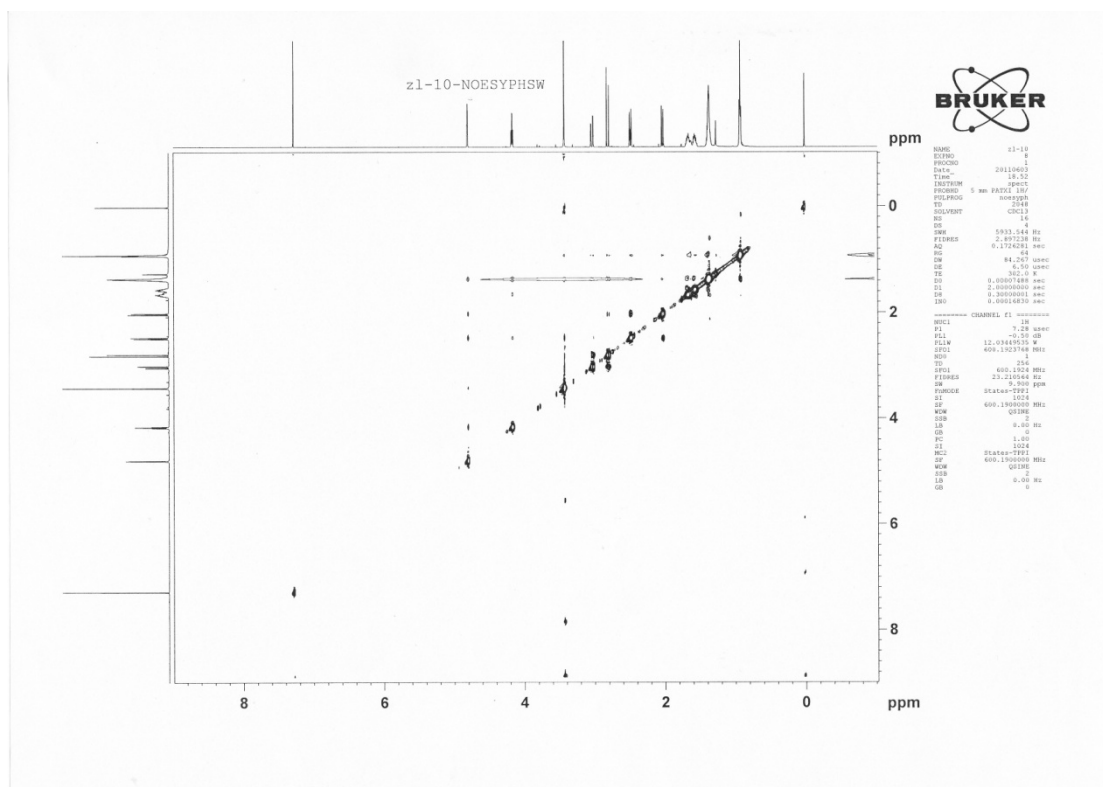
The HSQC Spectrum of Compound 2.

The ^1H - ^1H COSY Spectrum of Compound 2.

The HMBC Spectrum of Compound 2.



The NOESY Spectrum of Compound 2.



The IR Spectrum of Compound 2.

