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Supplementary Data

Development of Novel N-(6-Methanesulfonyl-benzothiazol-2-yl)-3-(4-substituted-piperazin-1-yl)-propionamidewithcholinesterase inhibition, anti-β-amyloid aggregation, neuroprotection and cognition enhancing properties for the therapy of Alzheimer's disease

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[c]School of Computational & Integrative Sciences, Jawaharlal Nehru University, New Delhi 110067, India.

Correspondence

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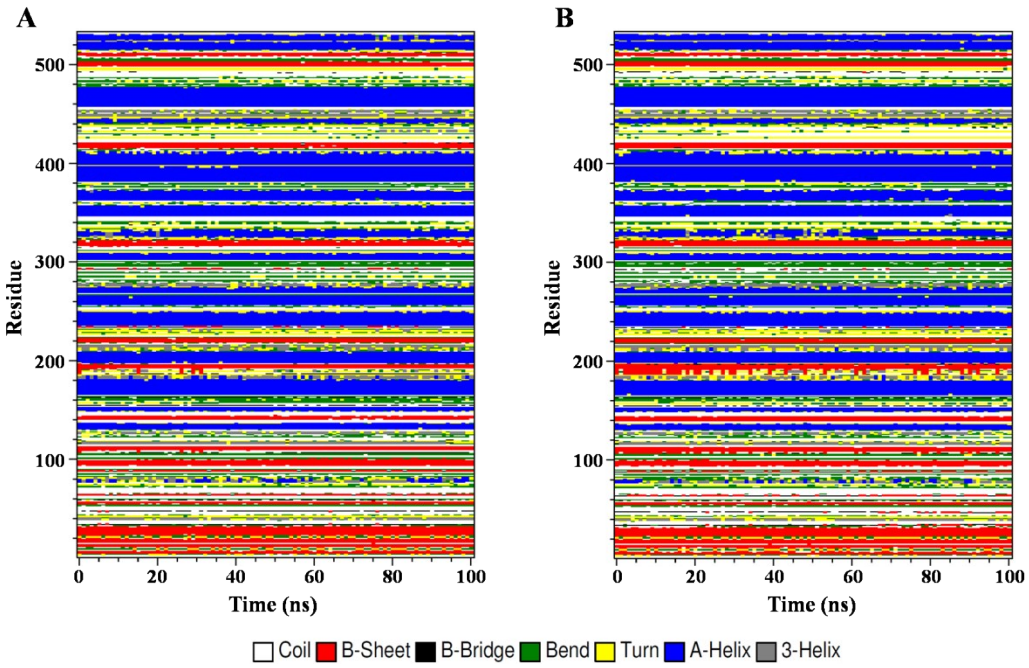
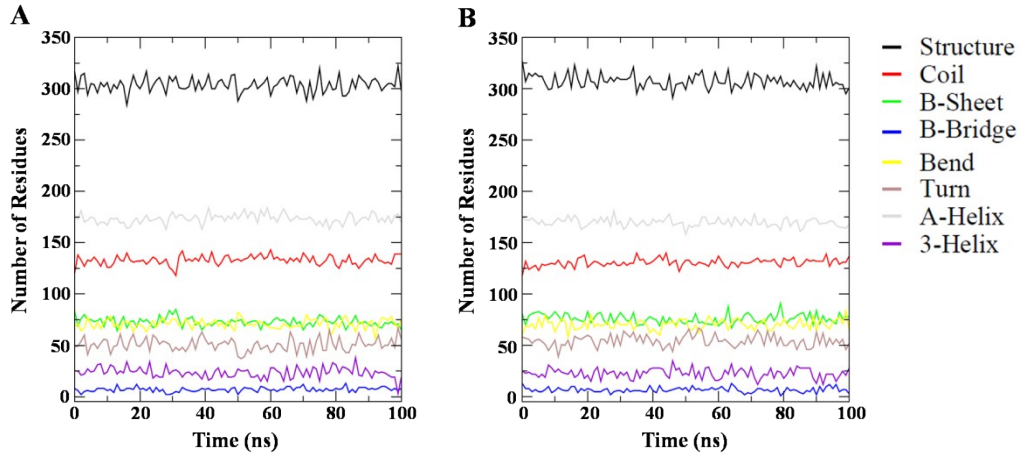
Supplementary Data

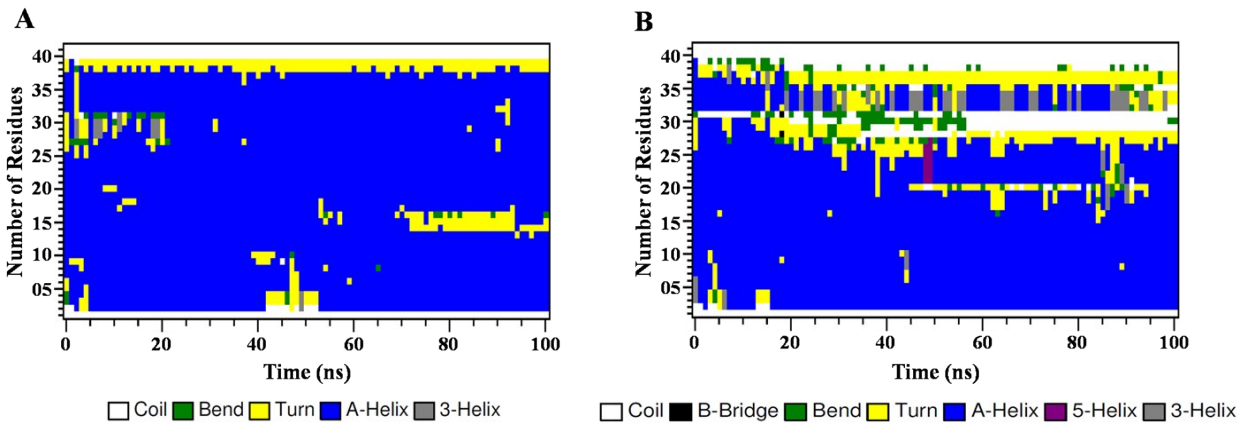


Supplementary Figure S1: Time evolution plot of secondary structures, AChE (A) and AChE-12complex (B), during the simulation in water at 300 K.

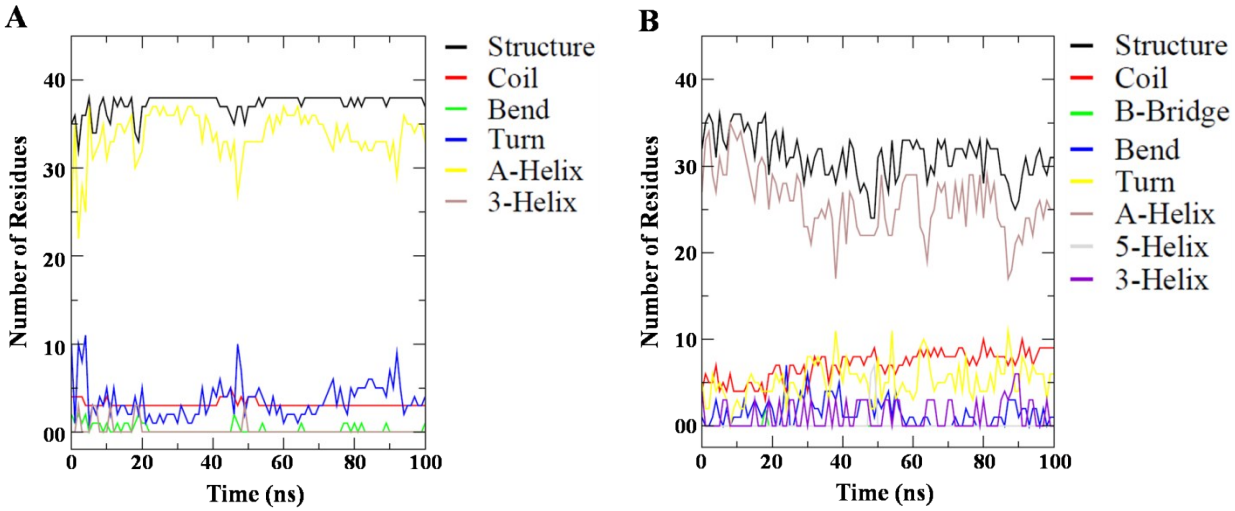


Supplementary Figure S2: Structural contents of AChE (A) and AChE-12complex (B), during the simulation in water at 300 K.

Supplementary Data



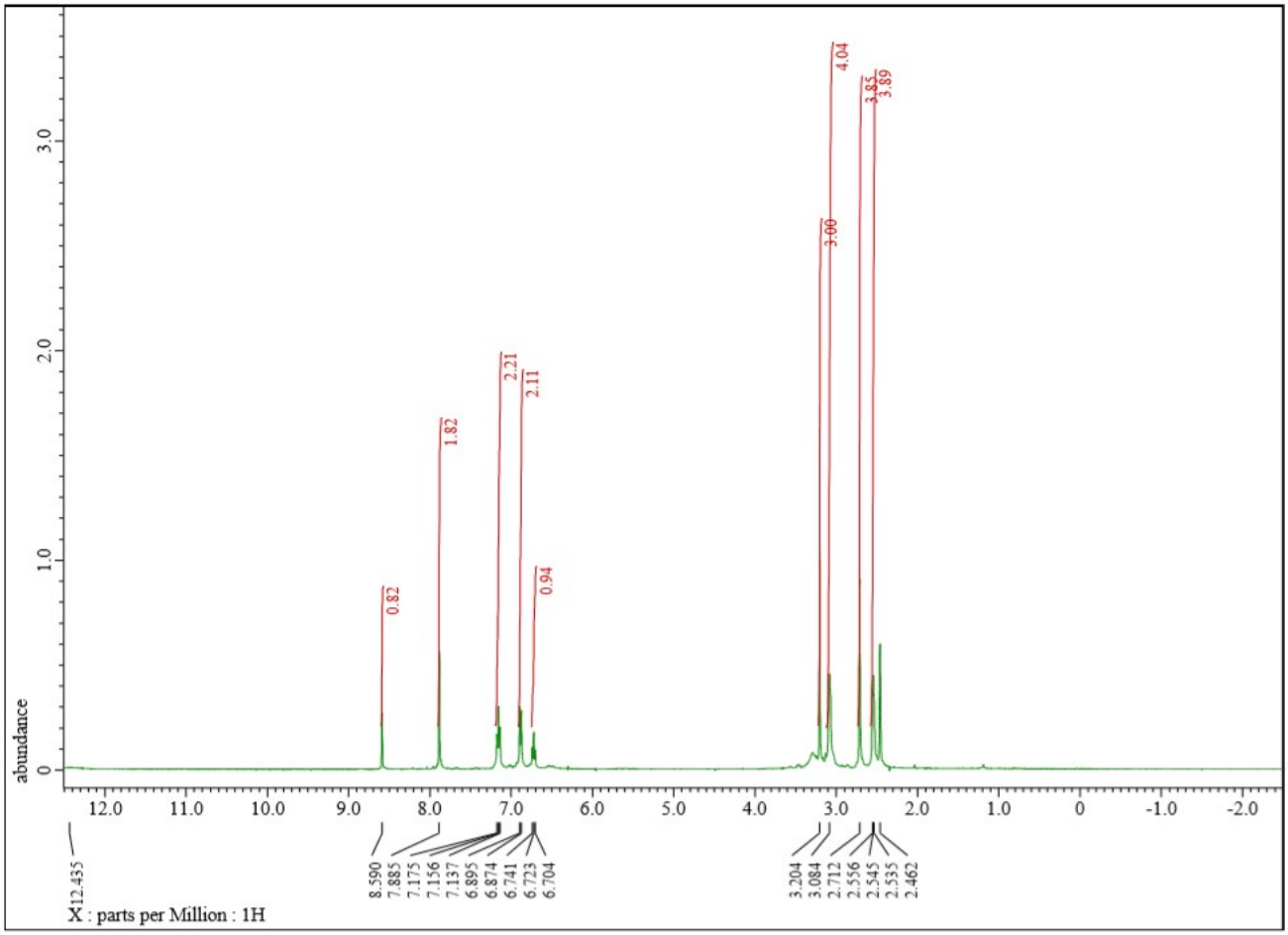
Supplementary Figure S3: Time evolution plot of secondary structures, $A\beta_{1-42}$ (A) and $A\beta_{1-42}$-12complex (B), during the simulation in water at 300 K.



Supplementary Figure S4: Structural contents of $A\beta_{1-42}$ (A) and $A\beta_{1-42}$-12complex (B), during the simulation in water at 300 K.

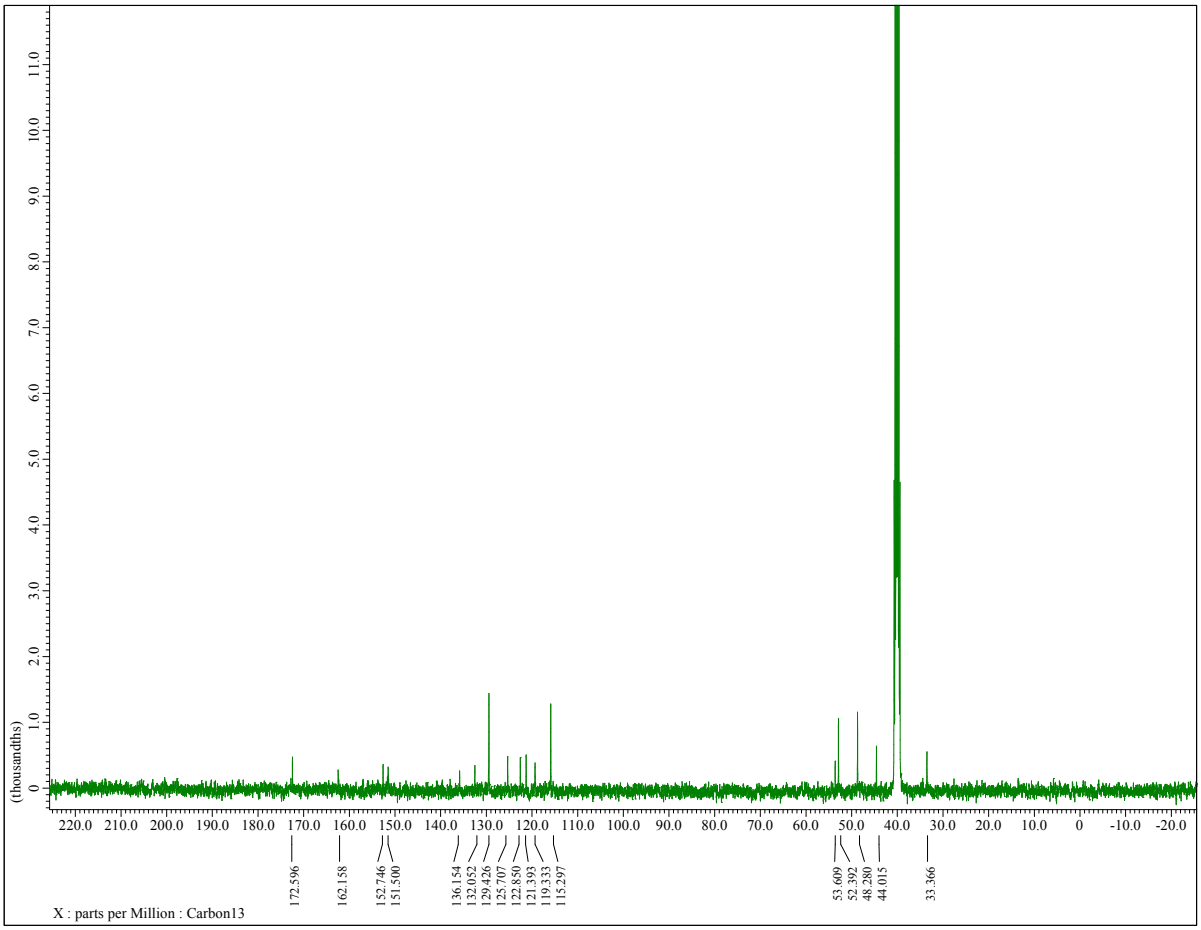
Supplementary Data

^{1}HNMR of Compound 4



Supplementary Data

^{13}C NMR of Compound 4



Supplementary Data

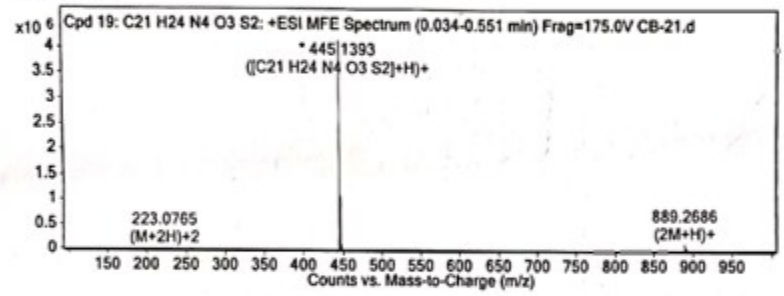
Mass spectra of compound 4

Compound Table

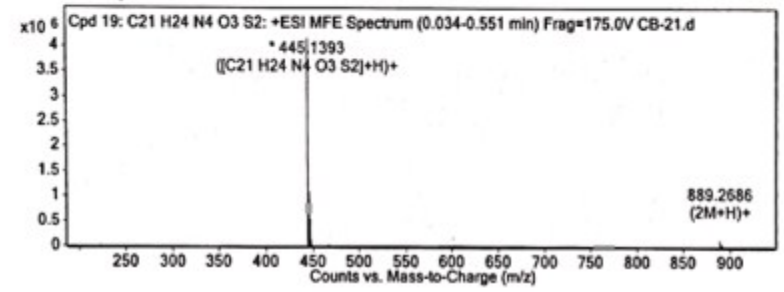
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 19: C21 H24 N4 O3 S2	0.096	444.1321	C21 H24 N4 O3 S2	C21 H24 N4 O3 S2	-6.92	C21 H24 N4 O3 S2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 19: C21 H24 N4 O3 S2	445.1393	0.096	Find by Molecular Feature	444.1321

MFE MS Spectrum

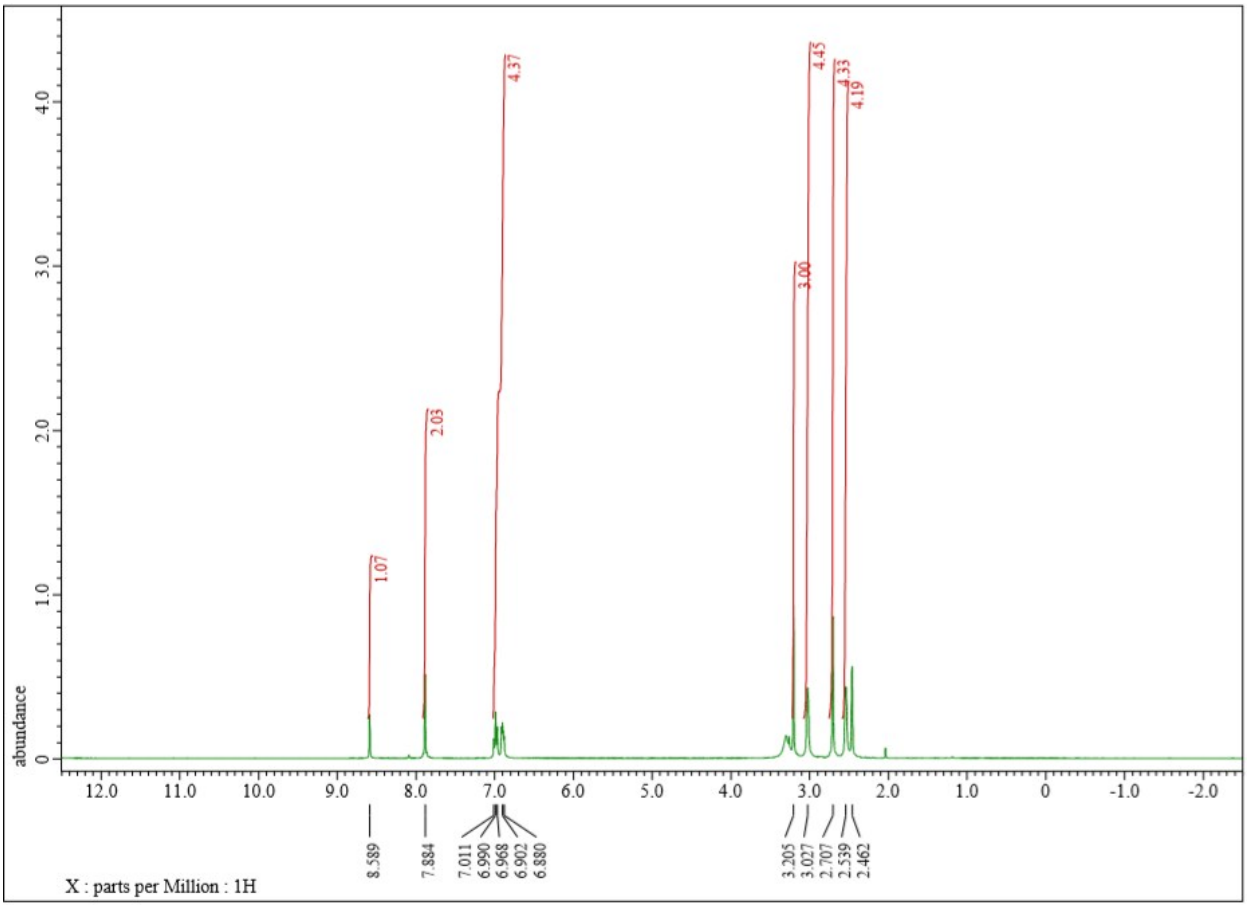


MFE MS Zoomed Spectrum



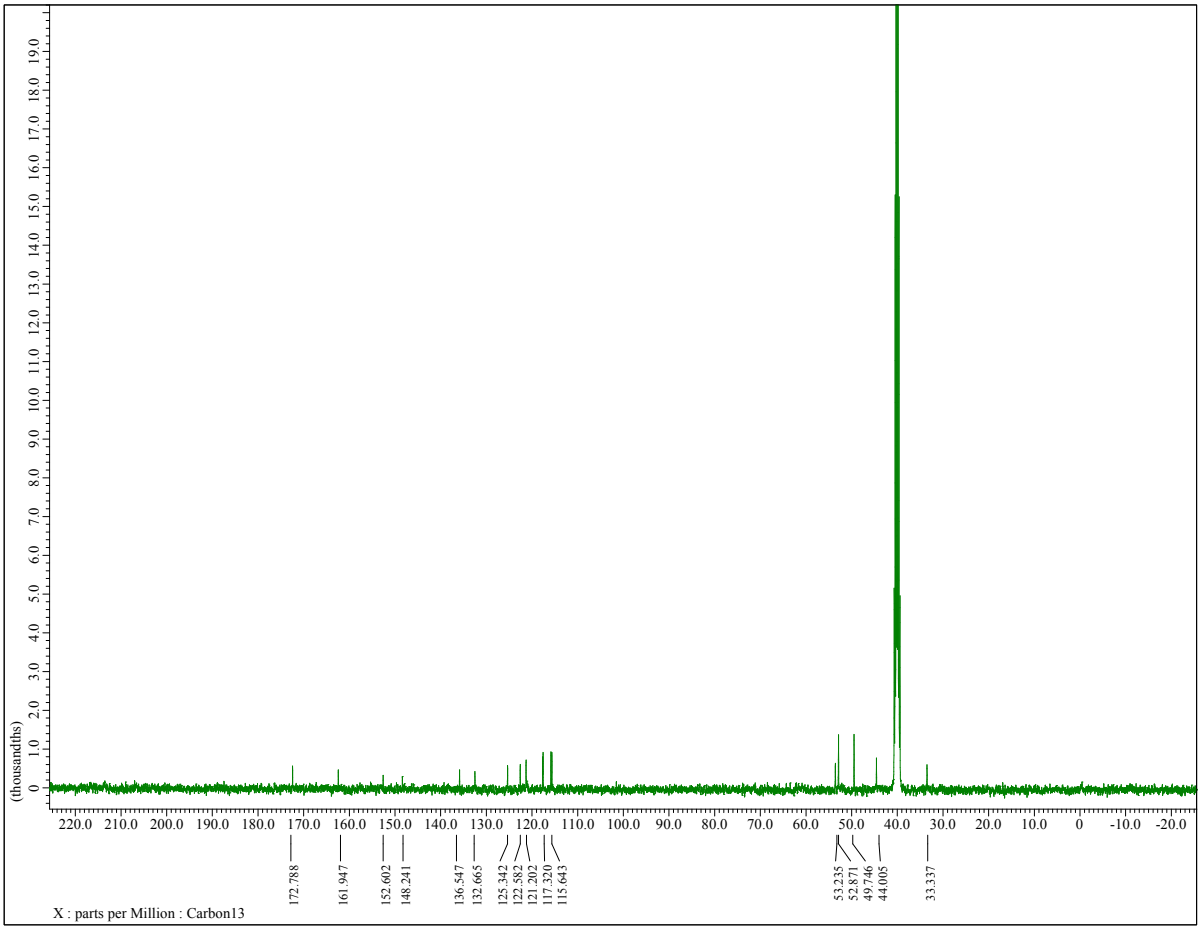
Supplementary Data

^{1}HNMR of compound 5



Supplementary Data

^{13}C NMR of compound5



Supplementary Data

Mass spectra of Compound 5

Qualitative Compound Report

Data File	CB-25.d	Sample Name	CB-25
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Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	08-07-2019 13:15:45
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C21 H23 F N4 O3 S2	0.096	462.1194	C21 H23 F N4 O3 S2	C21 H23 F N4 O3 S2	0.44	C21 H23 F N4 O3 S2

Compound Label	*m/z*	RT	Algorithm	Mass
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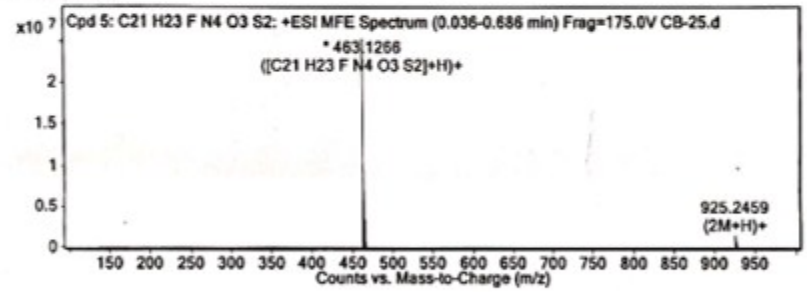
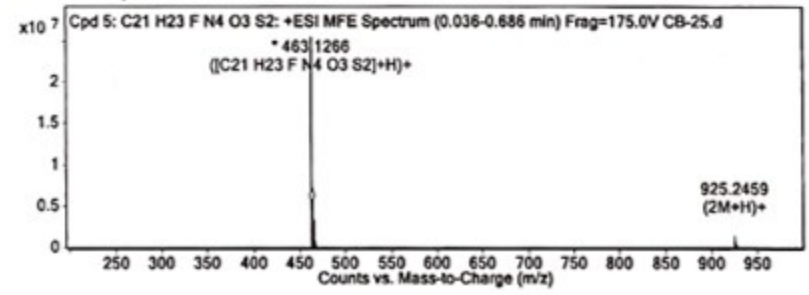
MFE MS Spectrum



MFE MS Zoomed Spectrum



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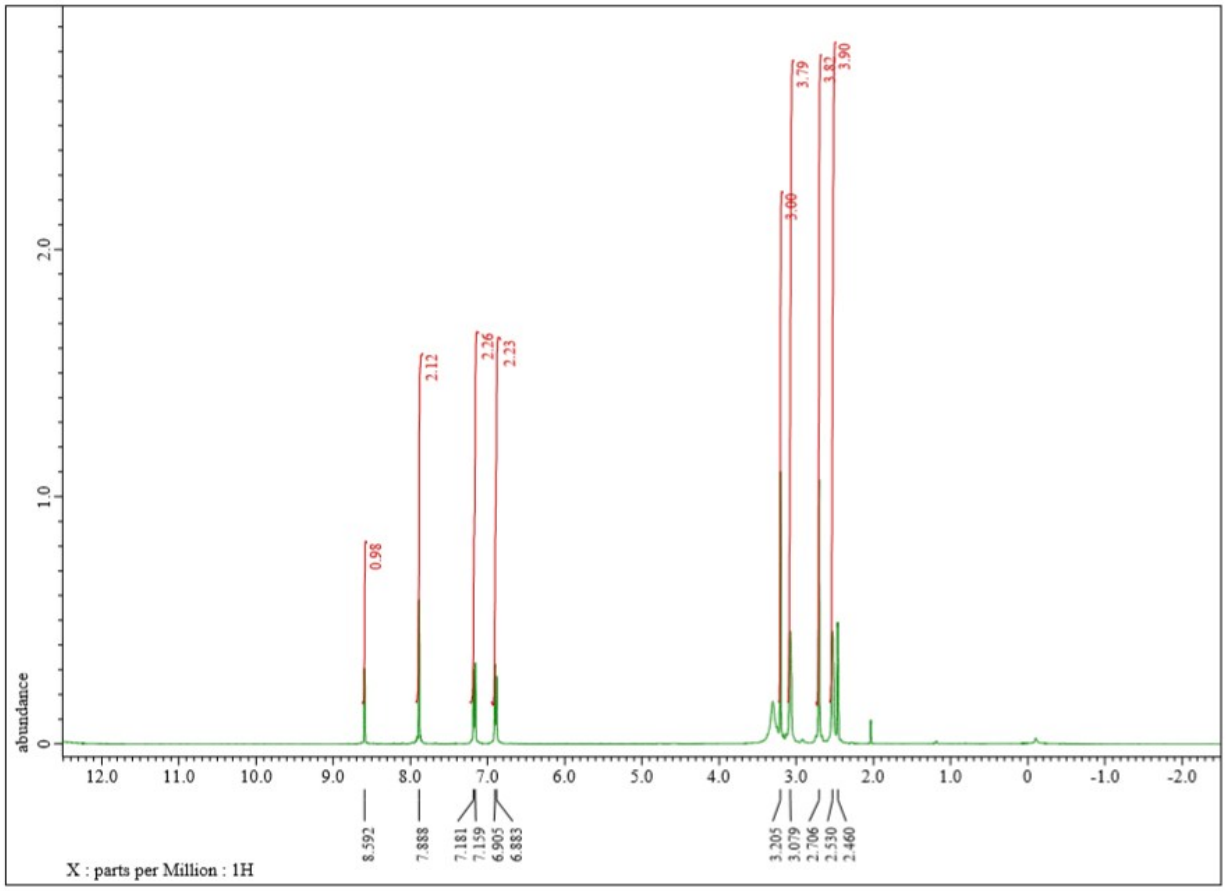
^{1}H NMR of compound 6



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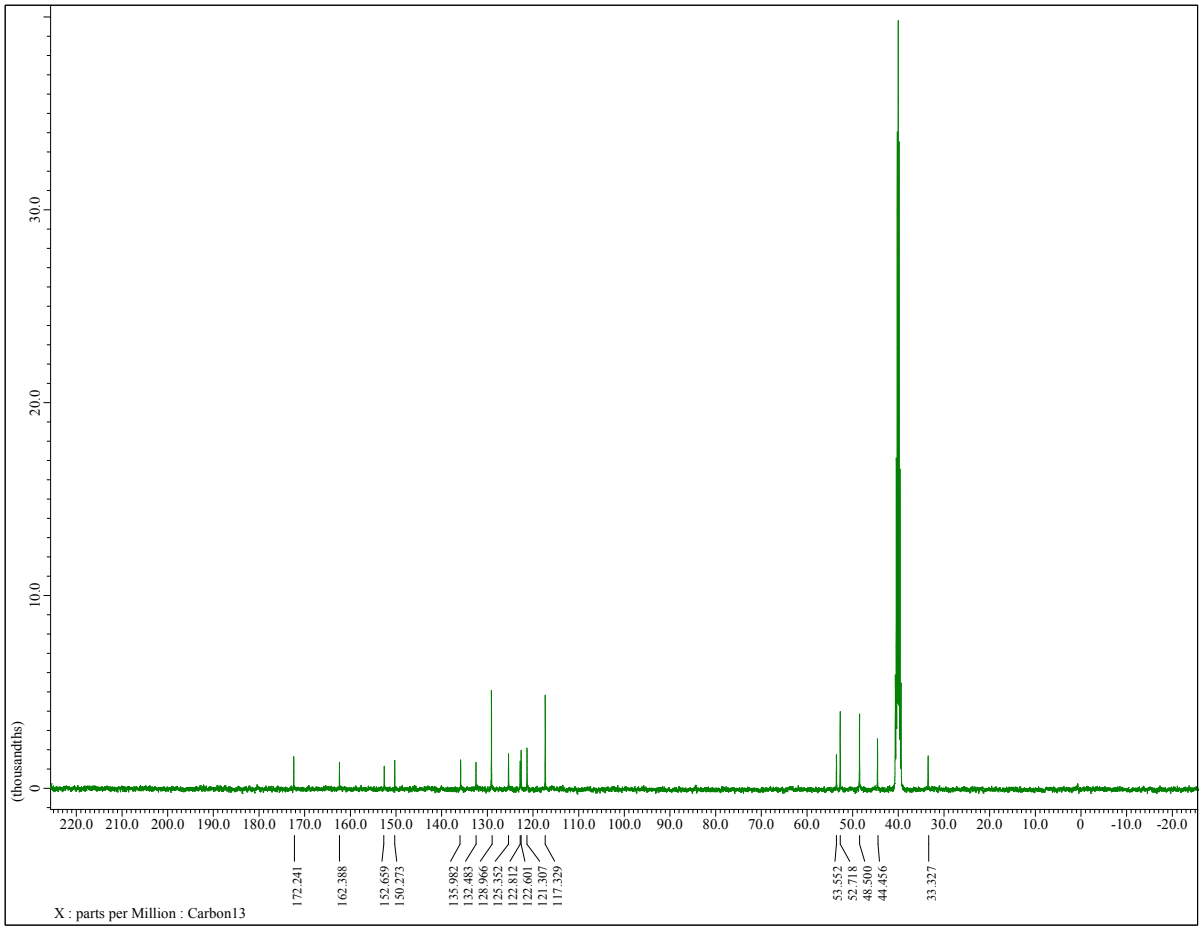
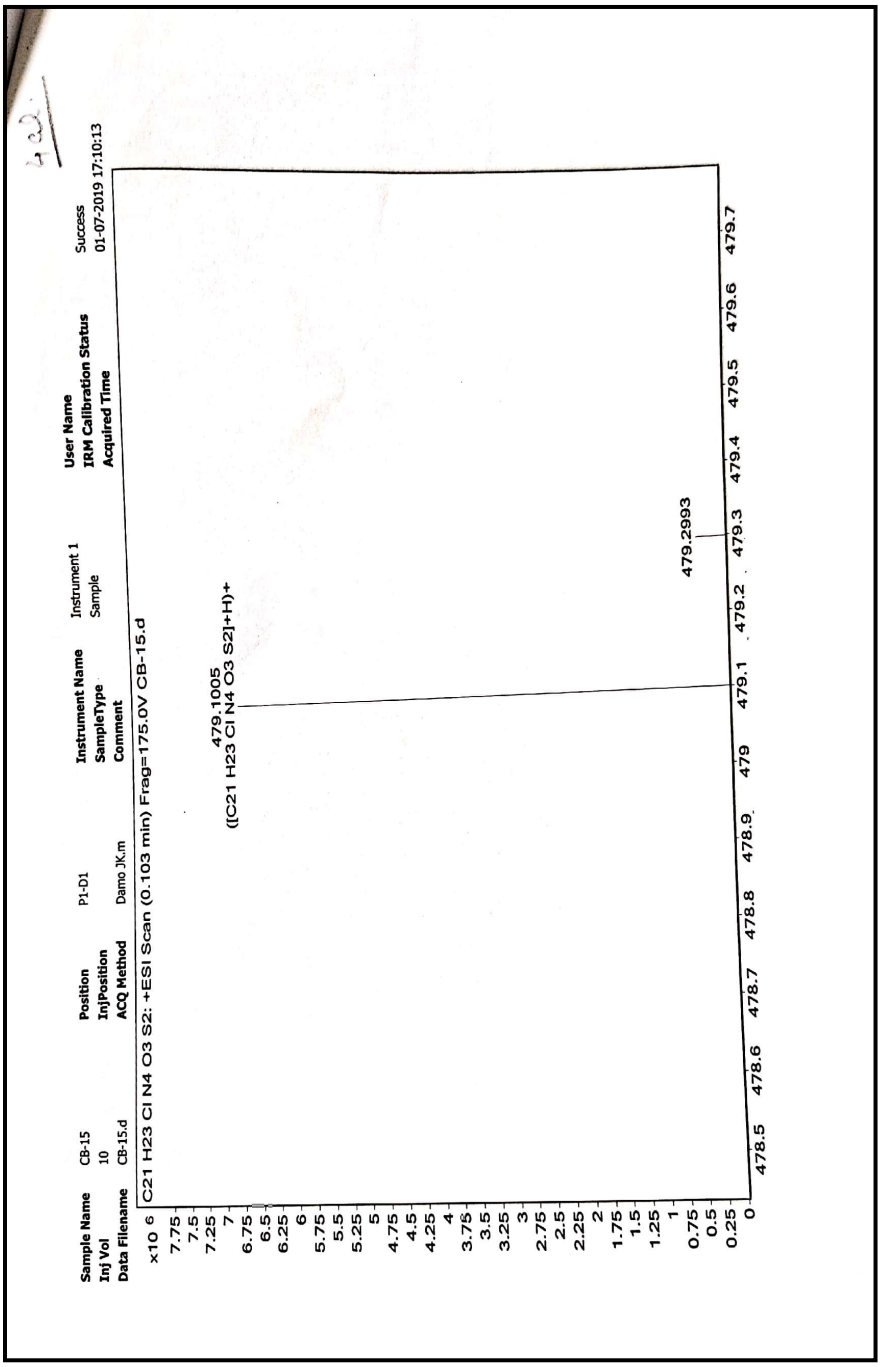
^{13}C NMR of compound 6



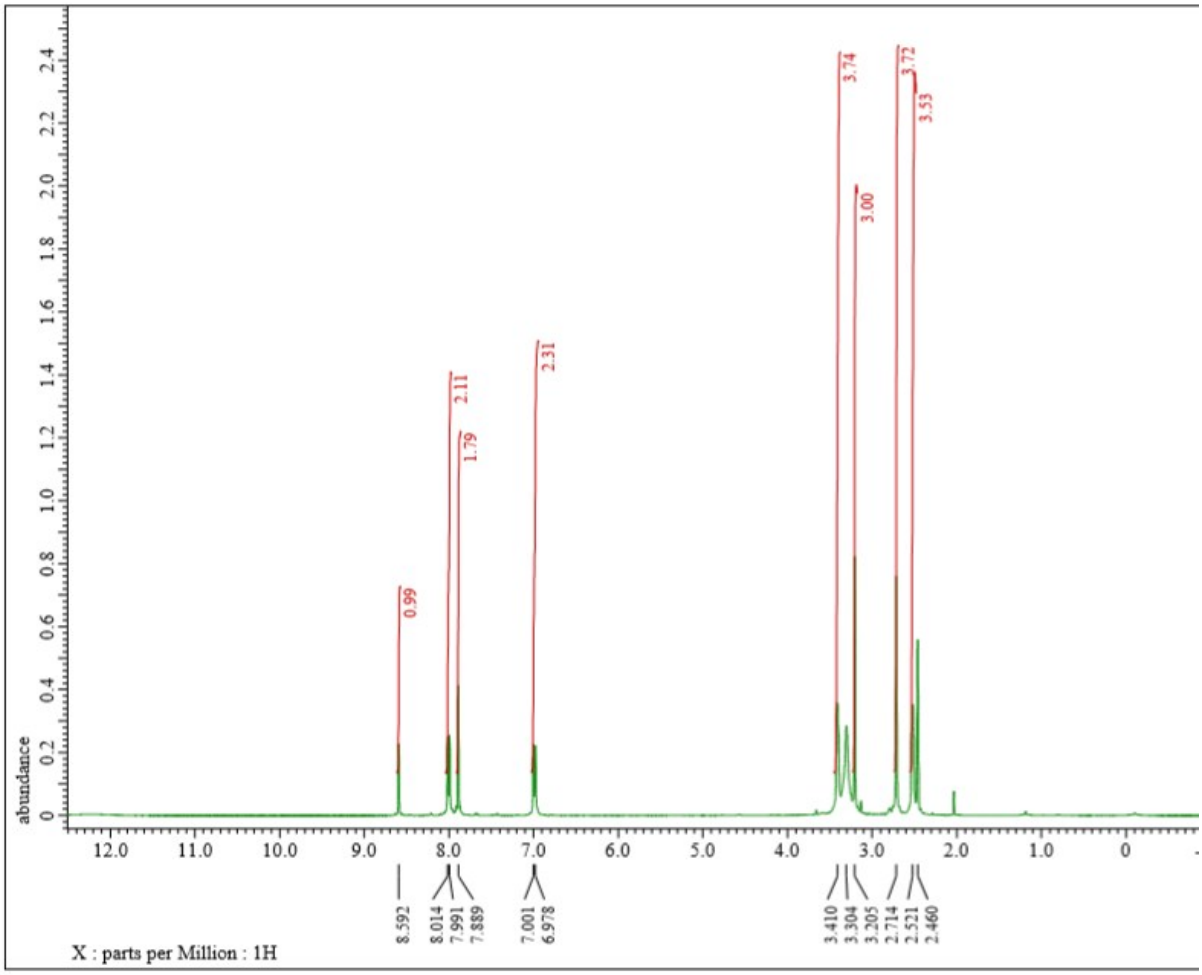
Supplementary Data

Mass spectra of Compound 6



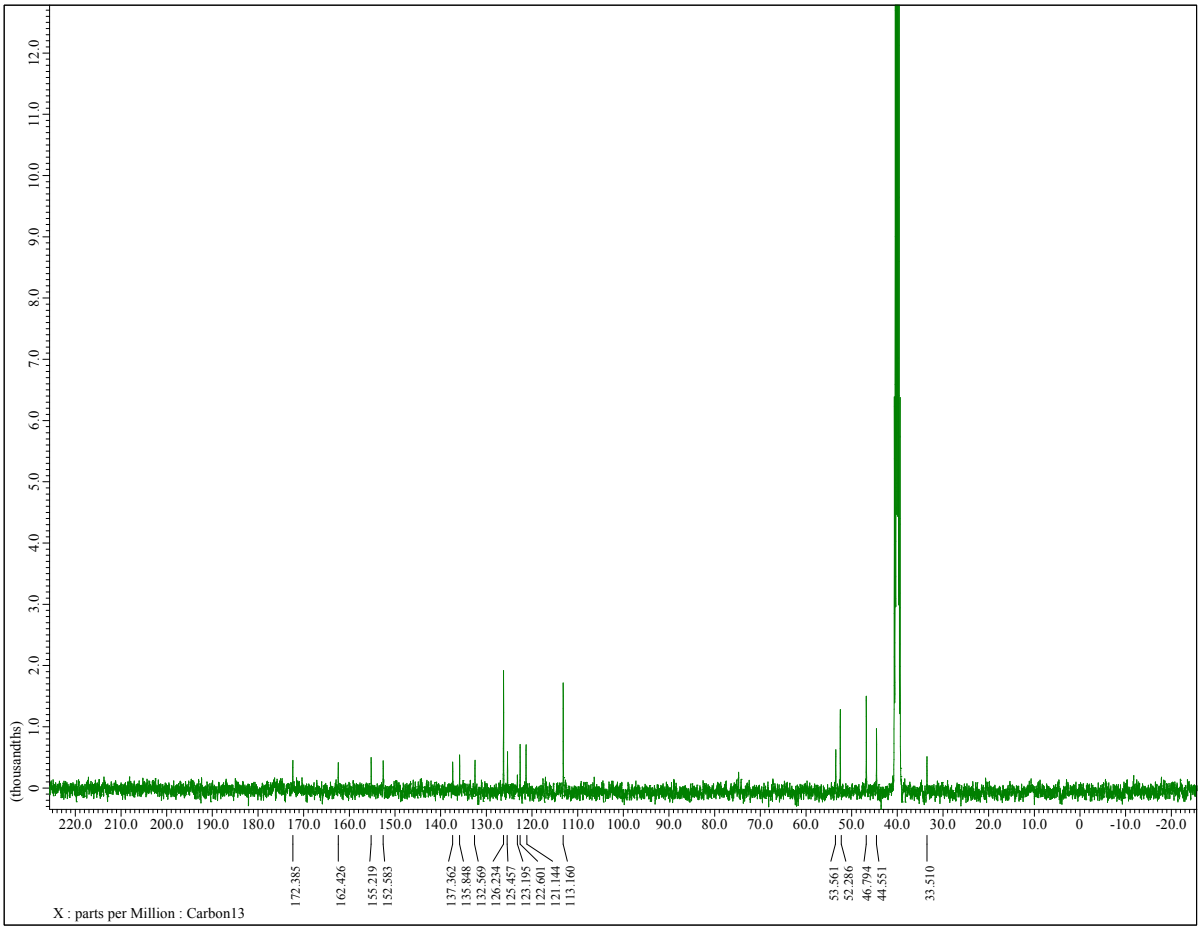
Supplementary Data

^{1}H NMR of Compound 7



Supplementary Data

^{13}C NMR of compound 7



Supplementary Data

Mass spectra of 7

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Acq Method	Damo JK.m	Acquired Time	01-07-2019 15:04:54
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

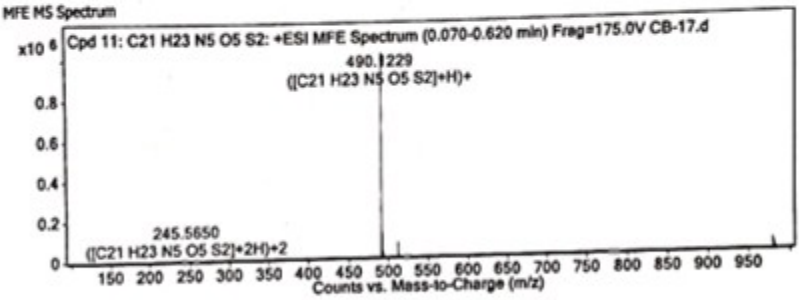
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

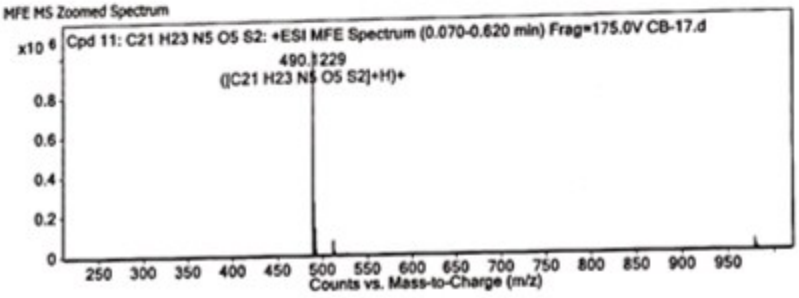
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C21 H23 N5 O5 S2	0.093	489.1153	C21 H23 N5 O5 S2	C21 H23 N5 O5 S2	-2.55	C21 H23 N5 O5 S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 11: C21 H23 N5 O5 S2	490.1229	0.093	Find by Molecular Feature	489.1153

MFE MS Spectrum

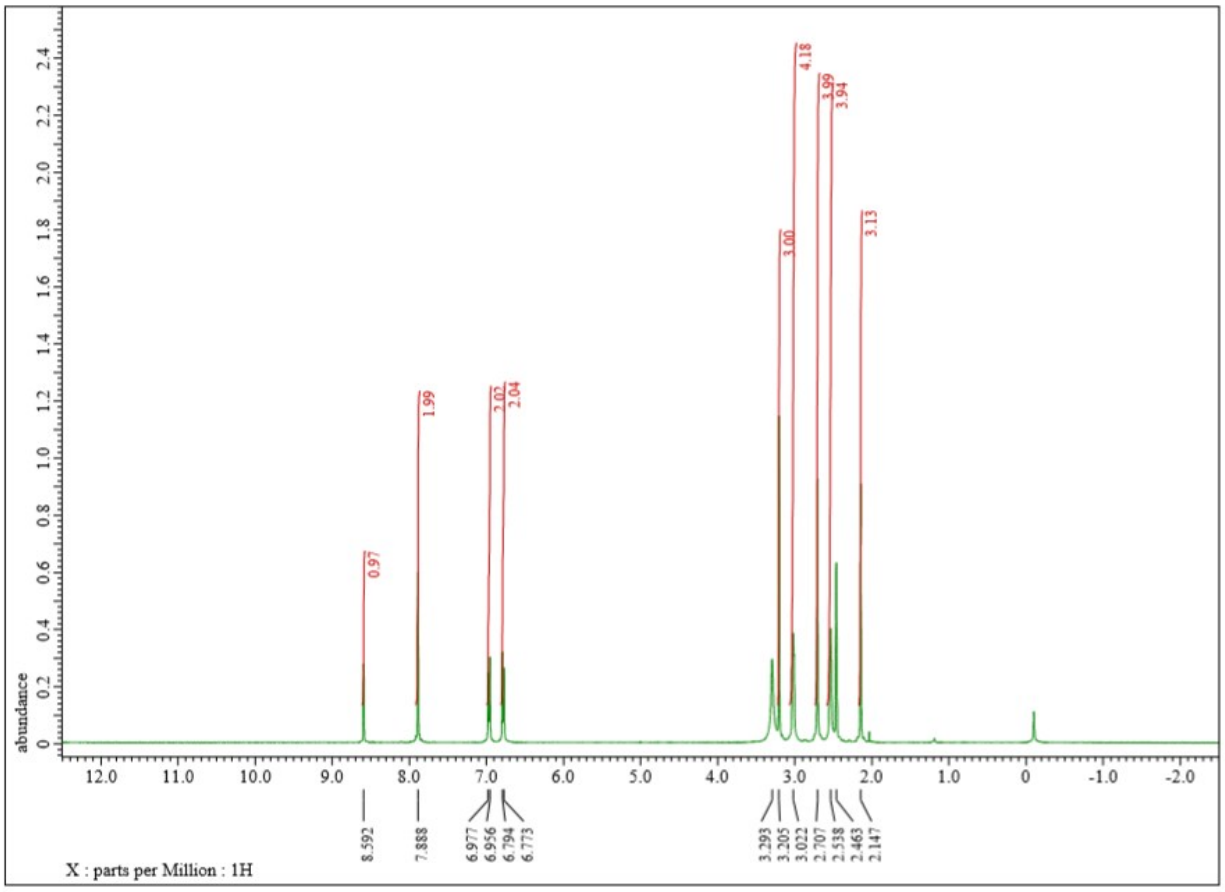


MFE MS Zoomed Spectrum



Supplementary Data

^{1}H NMR of Compound 8



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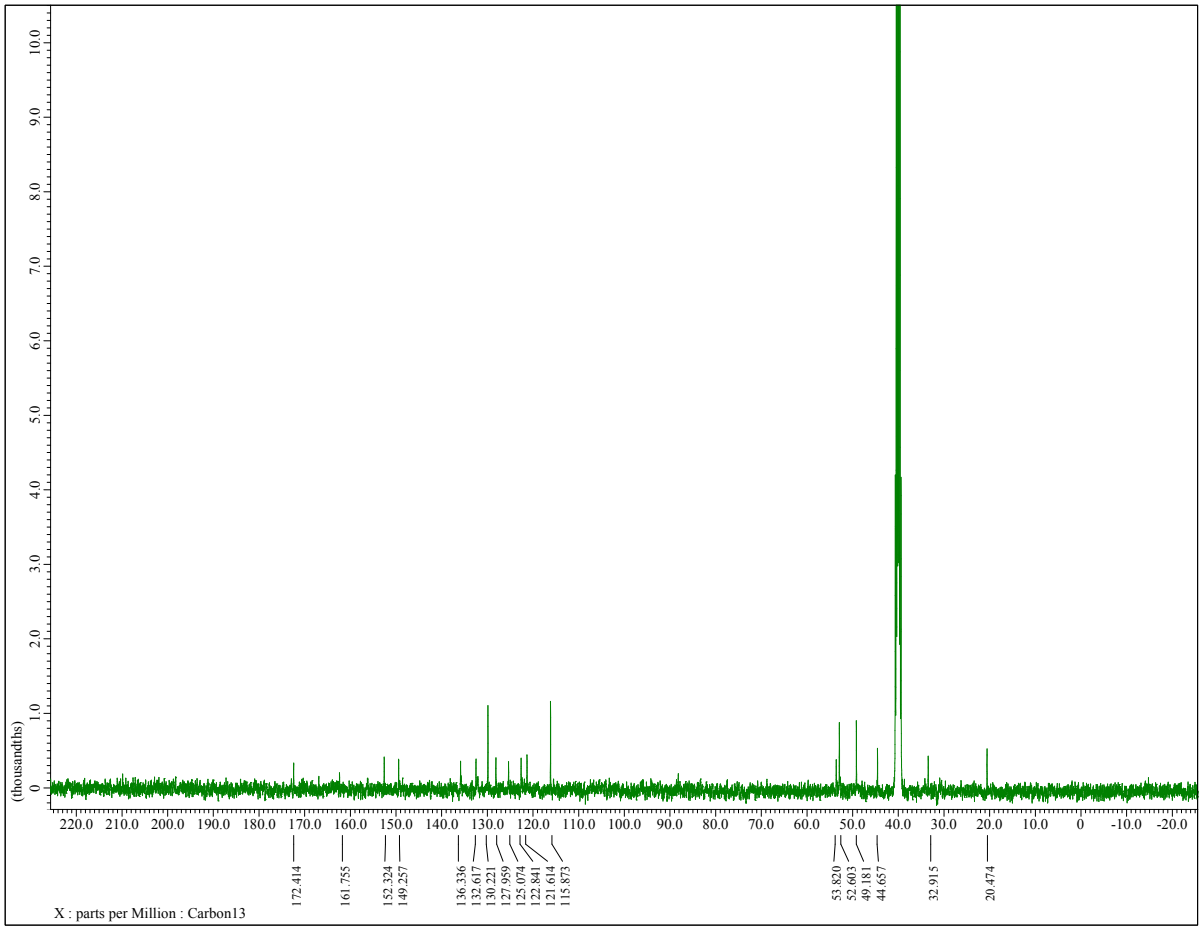
^{13}C NMR of Compound 8



Supplementary Data

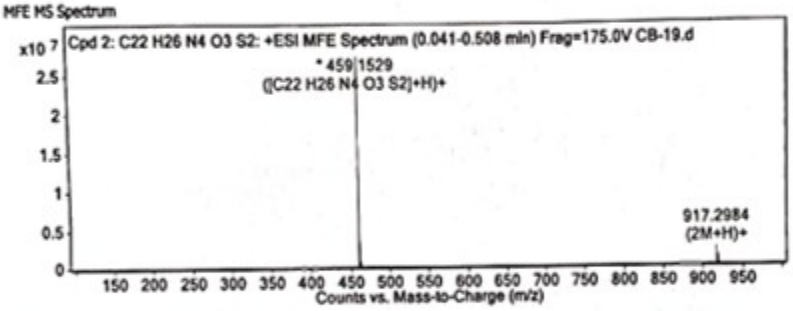
Mass spectra of Compound 8

Compound Table

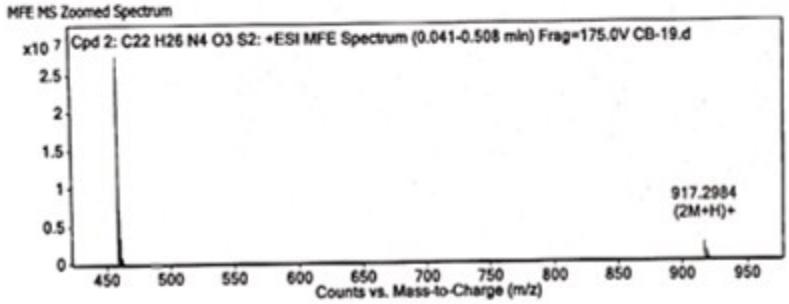
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C22 H26 N4 O3 S2	0.094	458.1457	C22 H26 N4 O3 S2	C22 H26 N4 O3 S2	-2.39	C22 H26 N4 O3 S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C22 H26 N4 O3 S2	459.1529	0.094	Find by Molecular Feature	458.1457

MFE MS Spectrum

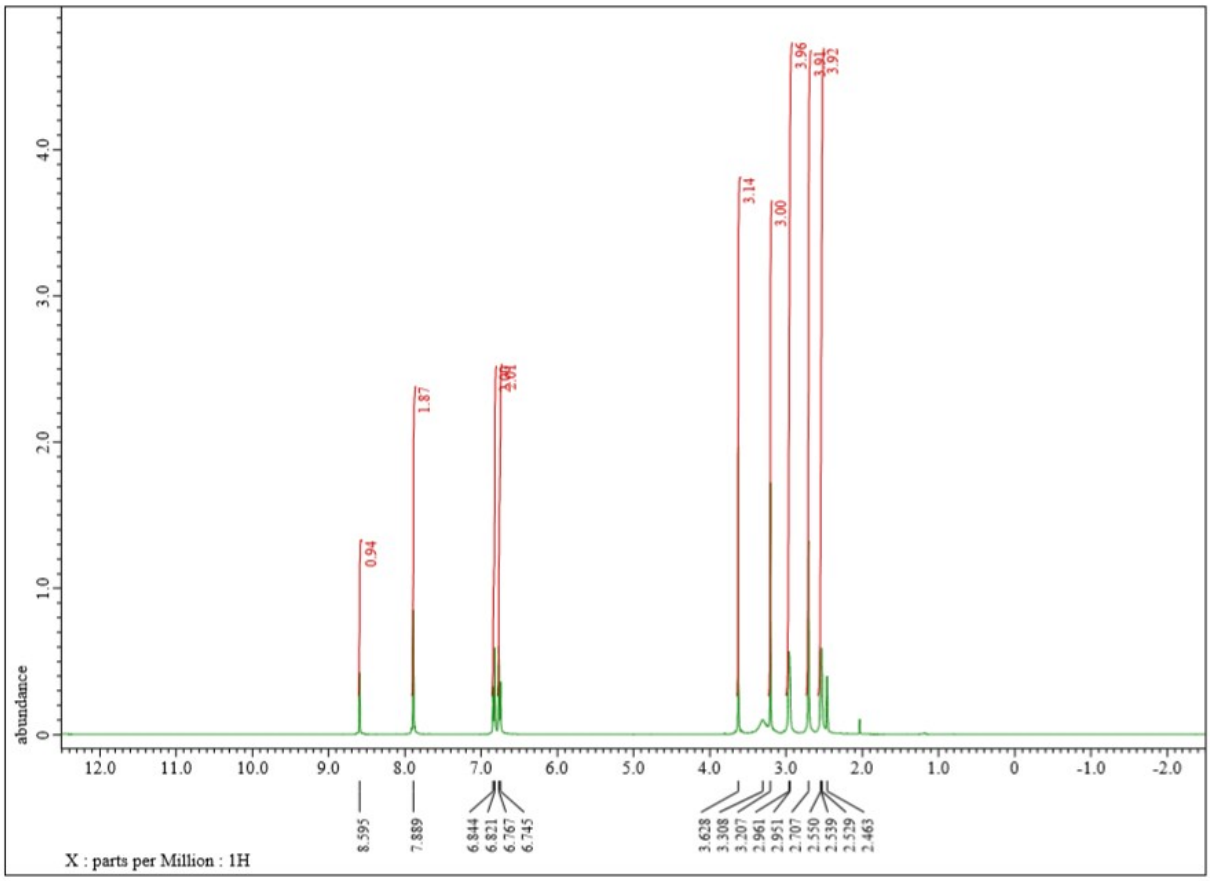


MFE MS Zoomed Spectrum



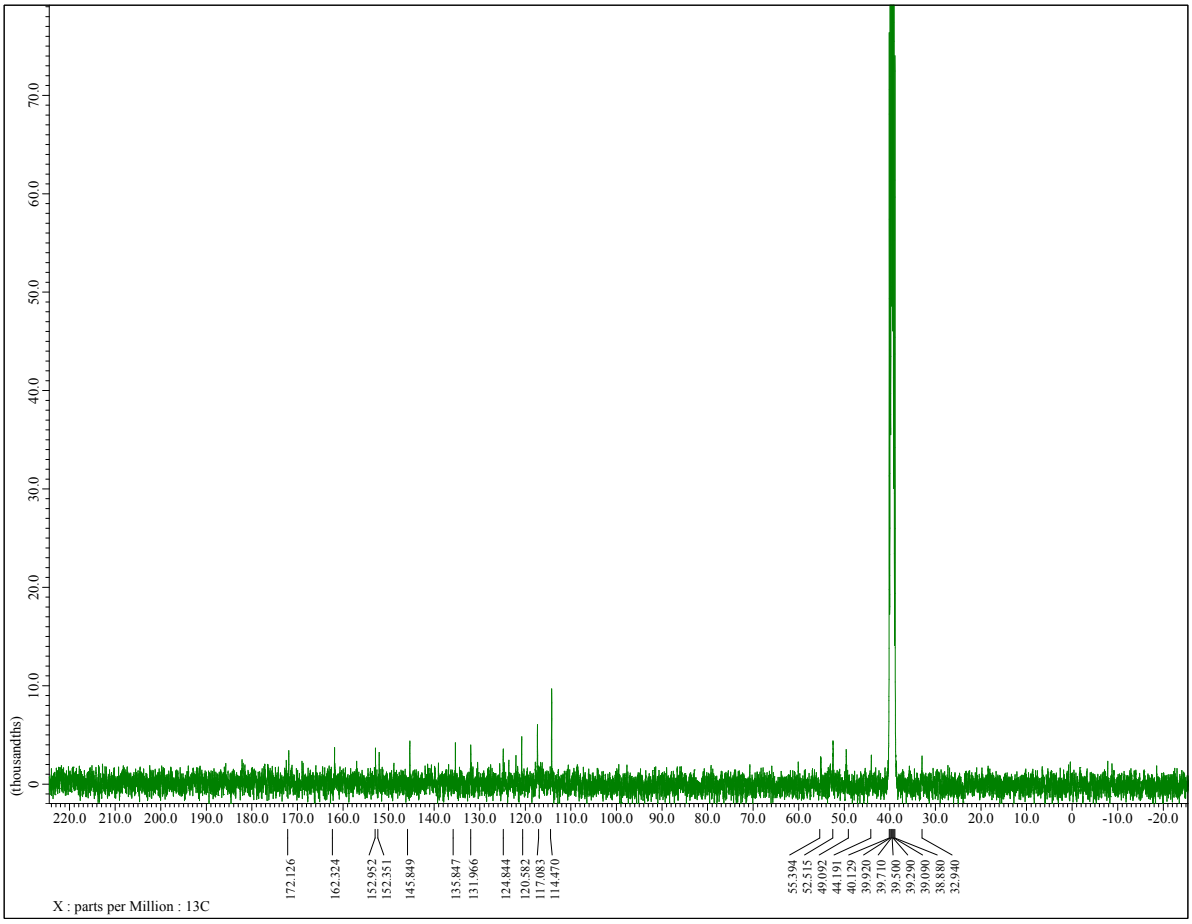
Supplementary Data

^{1}H NMR of Compound 9



Supplementary Data

^{13}C NMR of Compound 9



Supplementary Data

Mass spectra of compound 9

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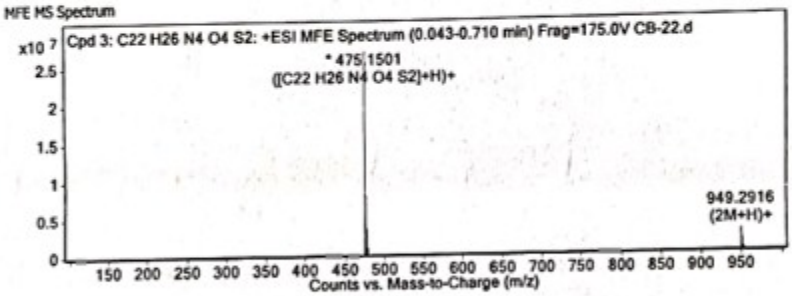
Acq Method	Damo JK.m	Acquired Time	03-07-2019 13:03:48
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

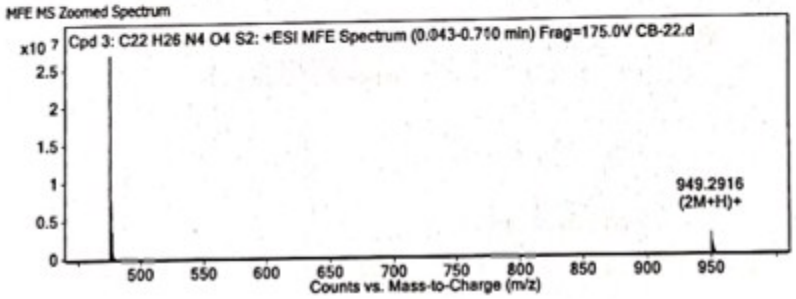
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C22 H26 N4 O4 S2	0.095	474.1429	C22 H26 N4 O4 S2	C22 H26 N4 O4 S2	-7.03	C22 H26 N4 O4 S2

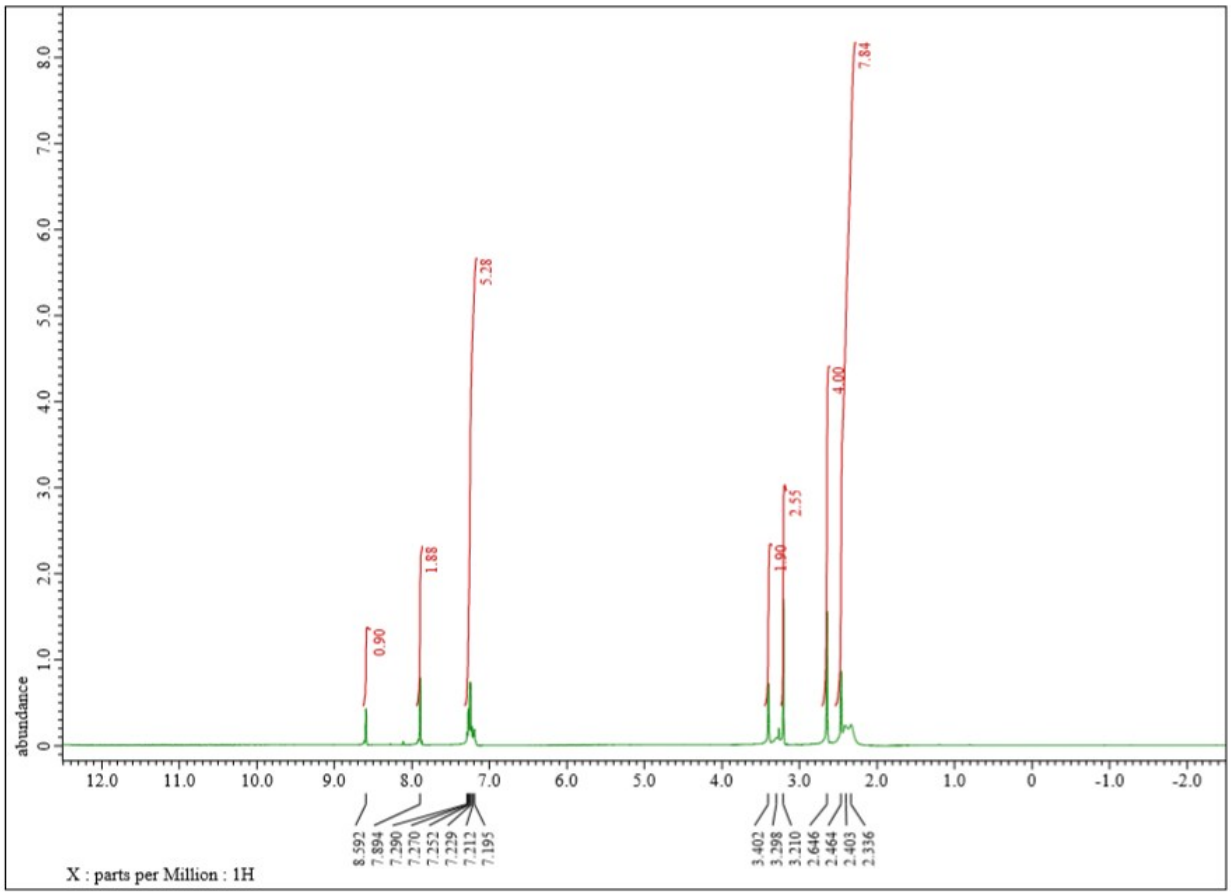
Compound Label	m/z	RT	Algorithm	Mass
Cpd 3: C22 H26 N4 O4 S2	475.1501	0.095	Find by Molecular Feature	474.1429





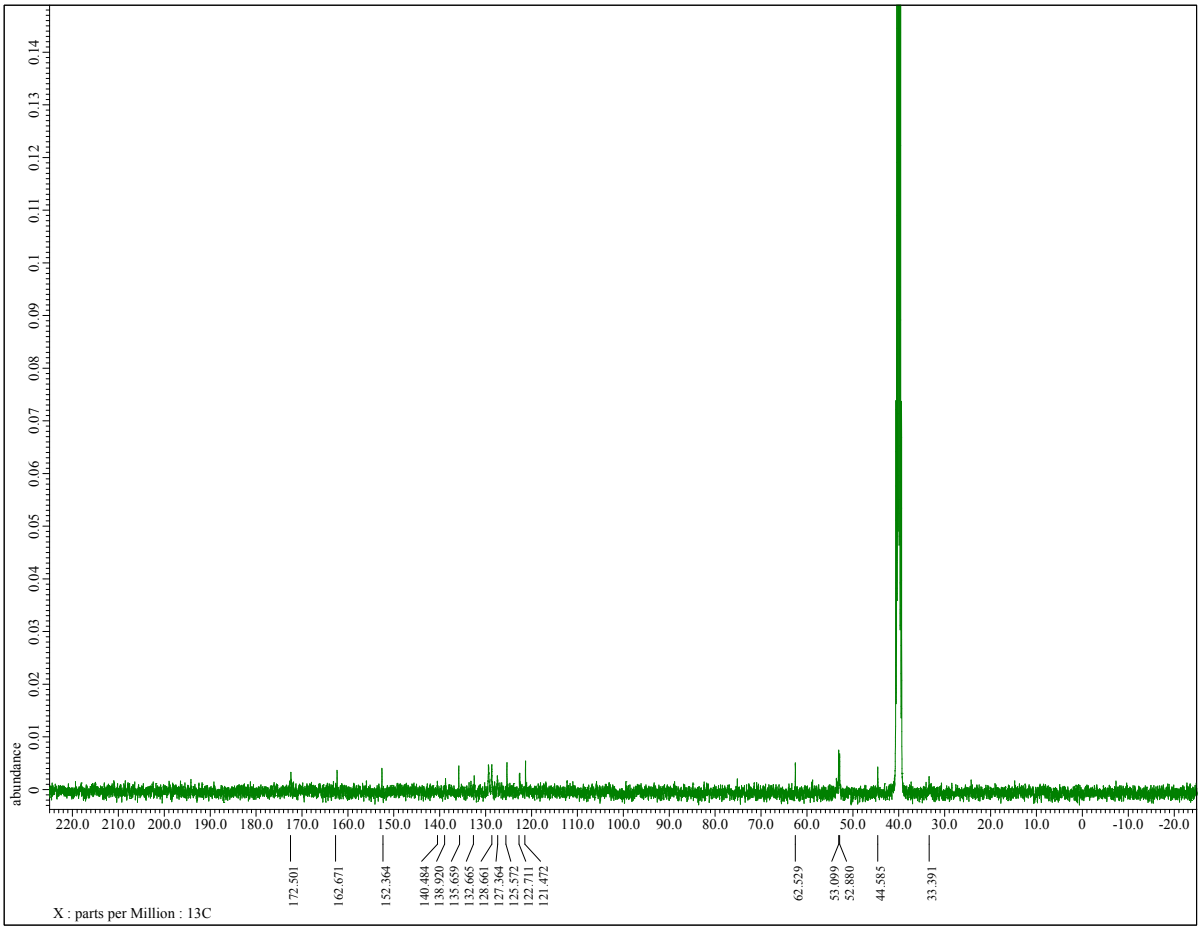
Supplementary Data

^{1}H NMR of Compound 10



Supplementary Data

^{13}C NMR of Compound 10



Supplementary Data

Mass spectra of compound 10

Qualitative Compound Report

Data File	CB-26.d	Sample Name	CB-26
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Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	08-07-2019 13:17:42
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

Sample Group Info.

Acquisition SW 6200 series TOF/6500 series

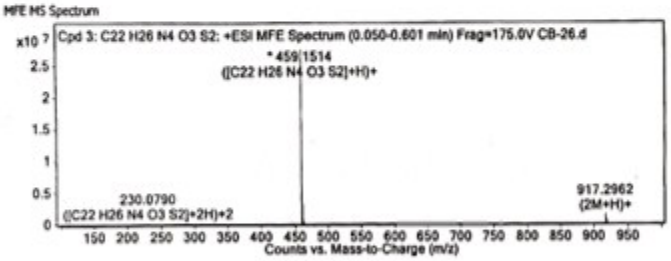
Version Q-TOF B.05.01 (B5125.1)

Compound Table

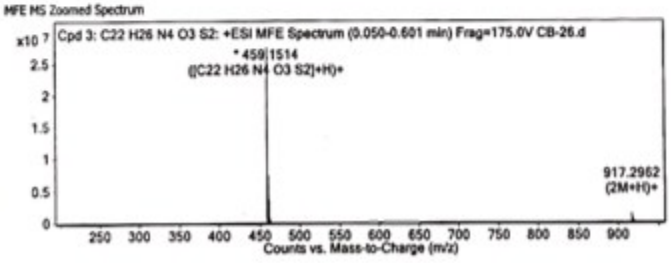
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C22 H26 N4 O3 S2	0.1	458.1442	C22 H26 N4 O3 S2	C22 H26 N4 O3 S2	0.89	C22 H26 N4 O3 S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 3: C22 H26 N4 O3 S2	459.1514	0.1	Find by Molecular Feature	458.1442

MFE MS Spectrum

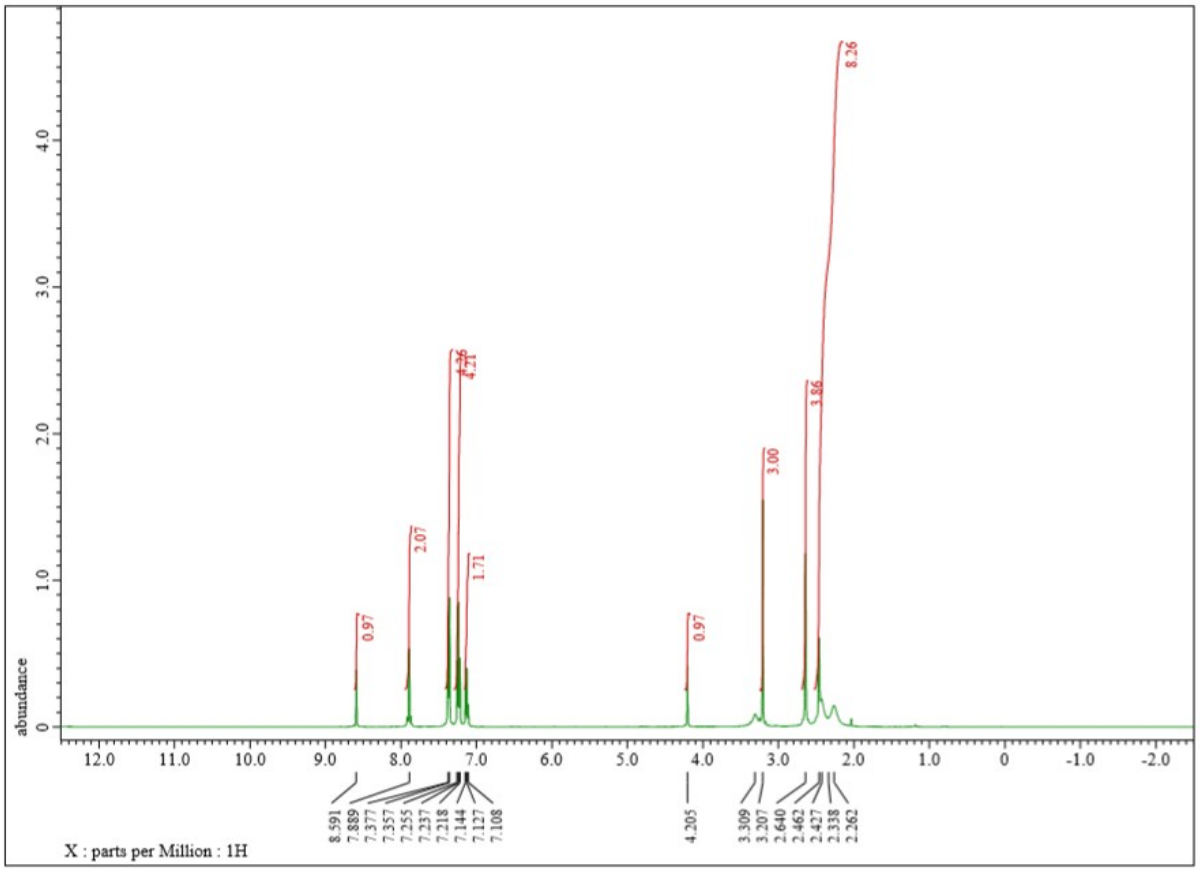


MFE MS Zoomed Spectrum



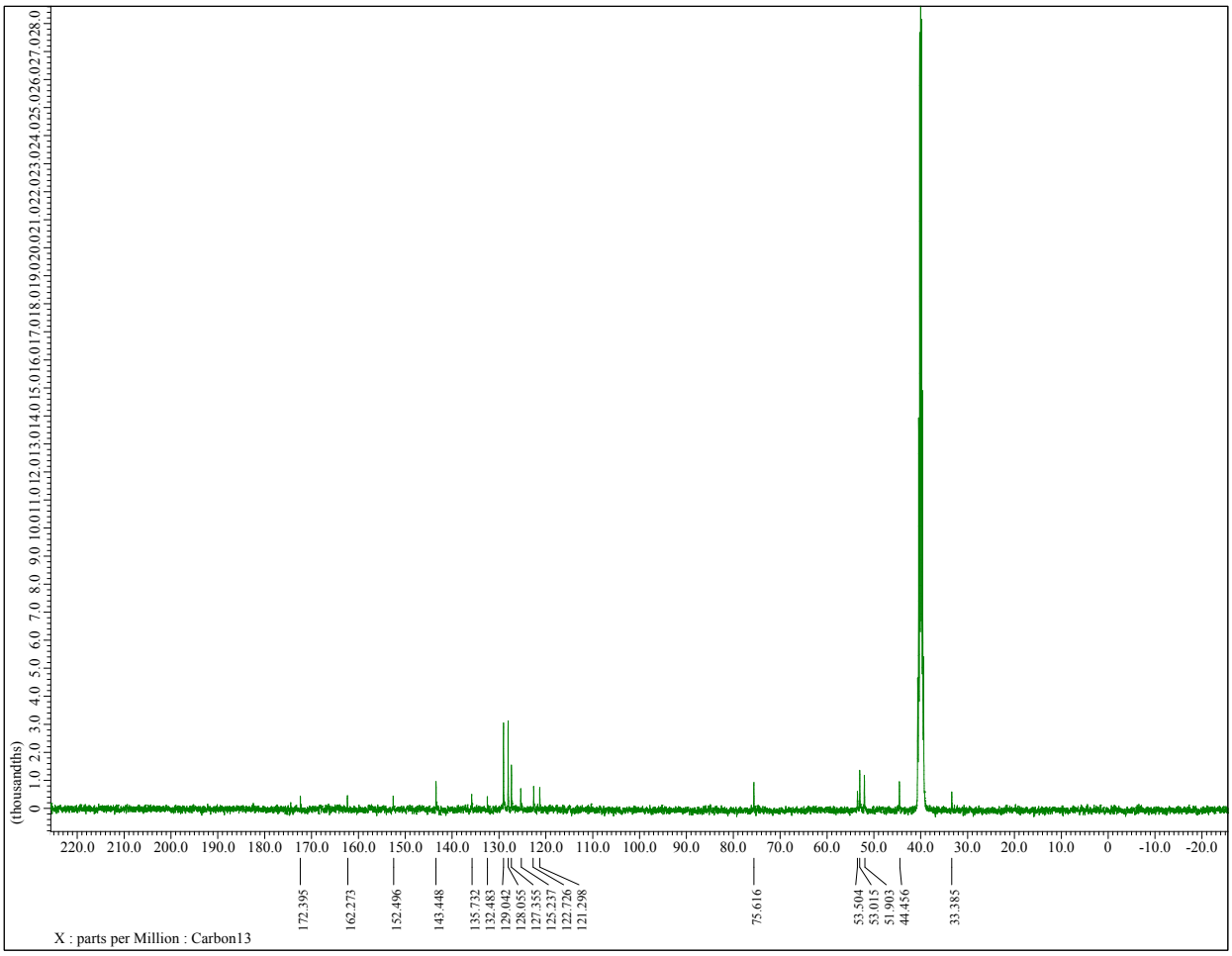
Supplementary Data

^{1}H NMR of Compound 11



Supplementary Data

^{13}C NMR of Compound 11



Supplementary Data

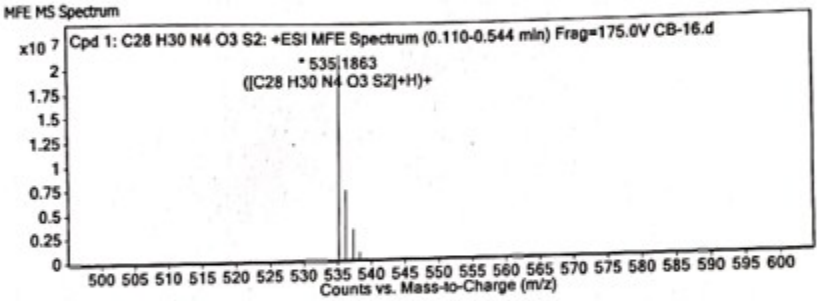
Mass spectra of compound 11

Compound Table

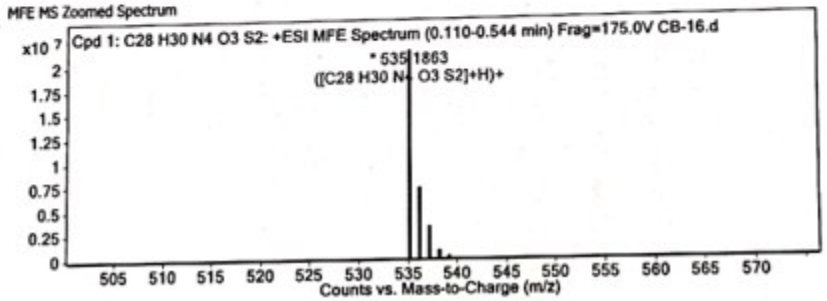
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C28 H30 N4 O3 S2	0.153	534.1792	C28 H30 N4 O3 S2	C28 H30 N4 O3 S2	-6.09	C28 H30 N4 O3 S2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H30 N4 O3 S2	535.1863	0.153	Find by Molecular Feature	534.1792

MFE MS Spectrum

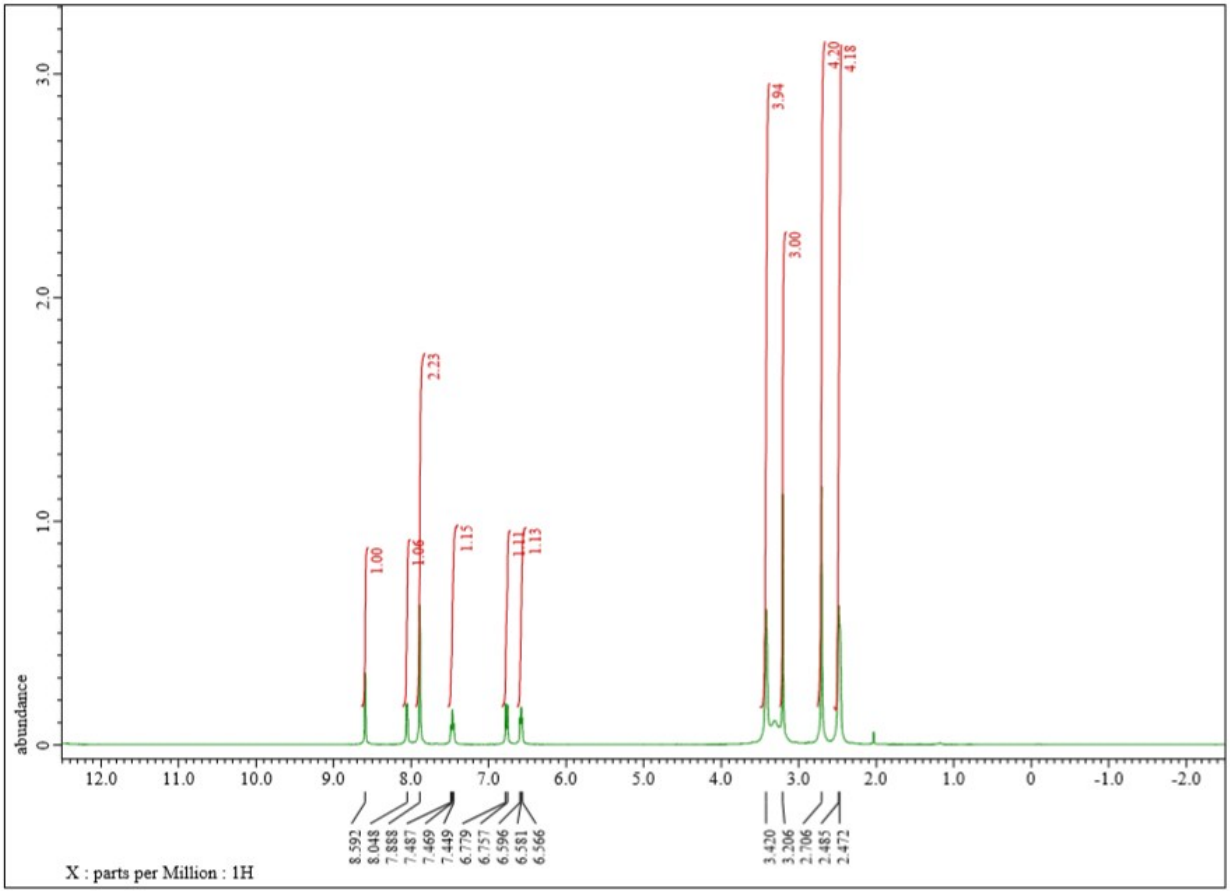


MFE MS Zoomed Spectrum



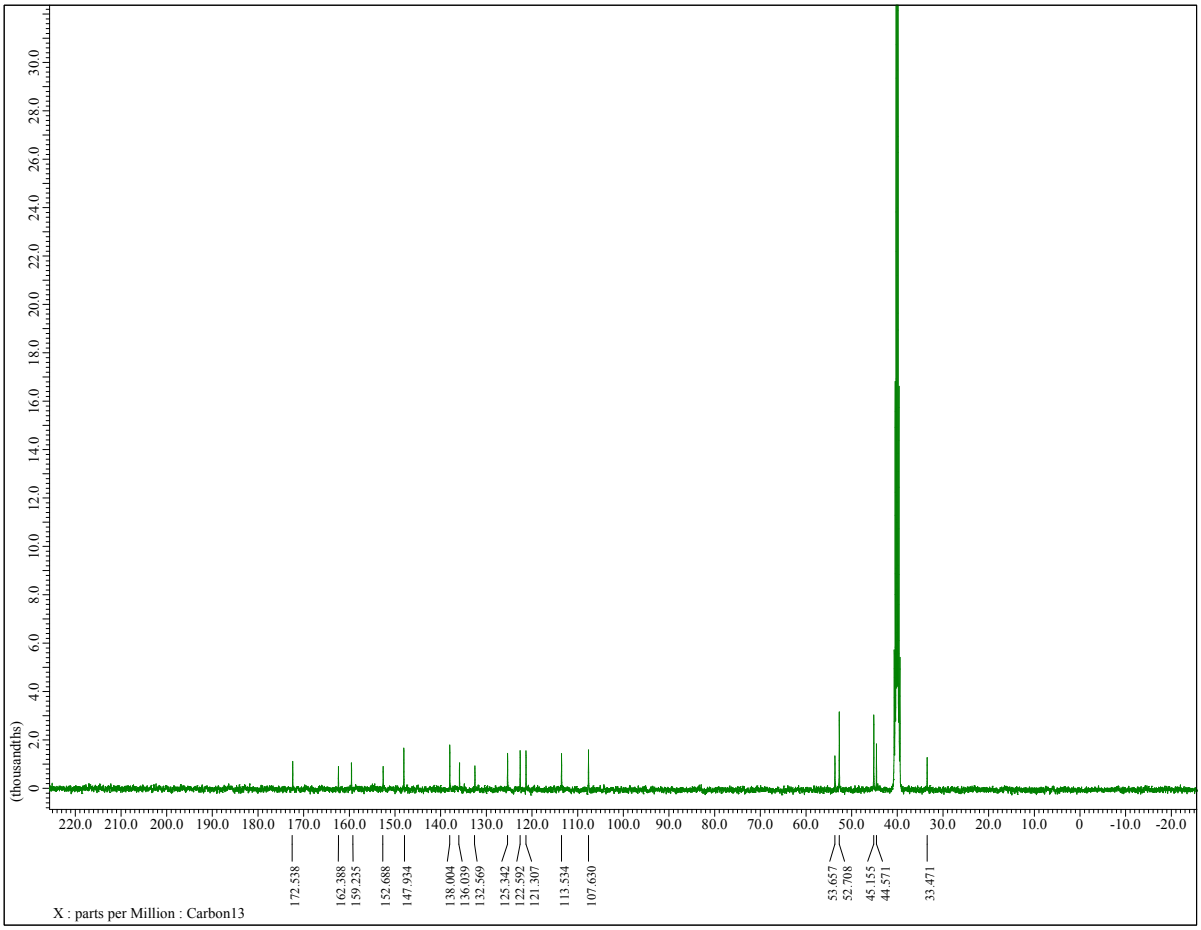
Supplementary Data

^{1}HNMR spectra of Compound 12



Supplementary Data

^{13}CNMR of Compound 12



Supplementary Data

Mass spectra of Compound 12

Qualitative Compound Report

Data File	CB-24.d	Sample Name	CB-24
Sample Type	Sample	Position	P1-C8
Instrument Name	Instrument 1	User Name	
Acq Method	Demo JK.m	Acquired Time	04-07-2019 13:44:22
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

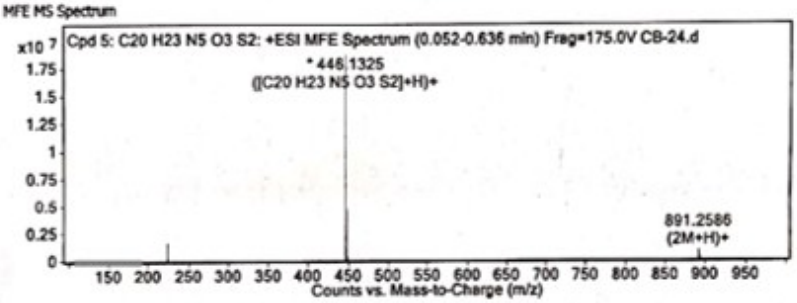
Sample Group Info.
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

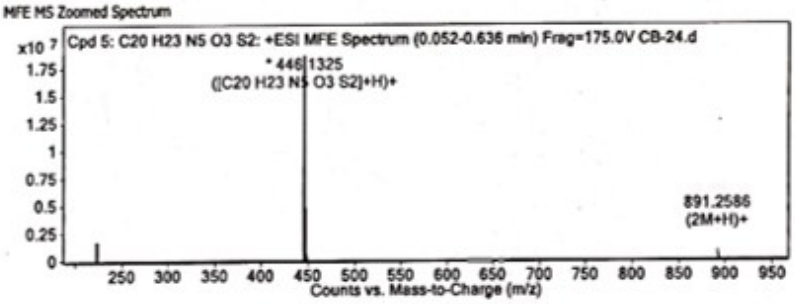
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C20 H23 N5 O3 S2	0.094	445.1259	C20 H23 N5 O3 S2	C20 H23 N5 O3 S2	-3.83	C20 H23 N5 O3 S2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C20 H23 N5 O3 S2	446.1325	0.094	Find by Molecular Feature	445.1259

MFE MS Spectrum

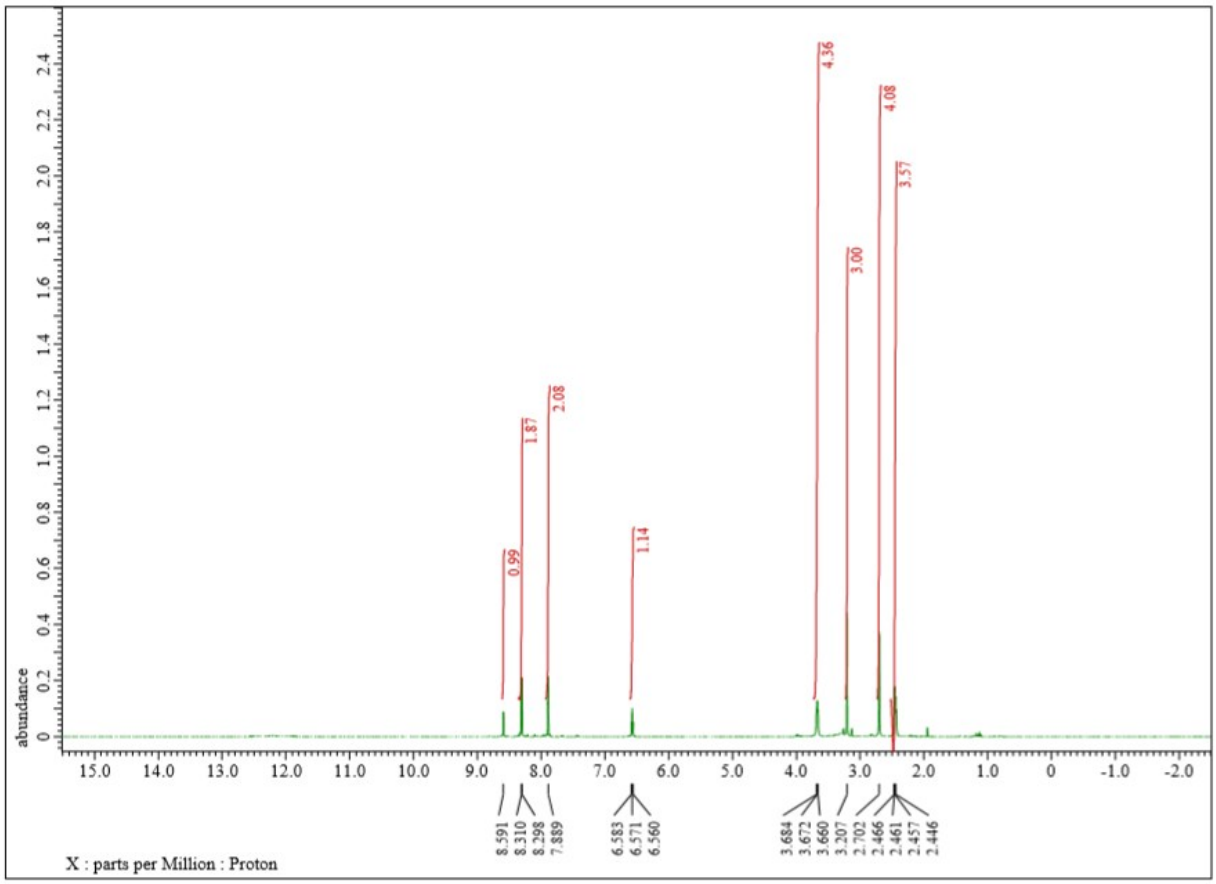


MFE MS Zoomed Spectrum



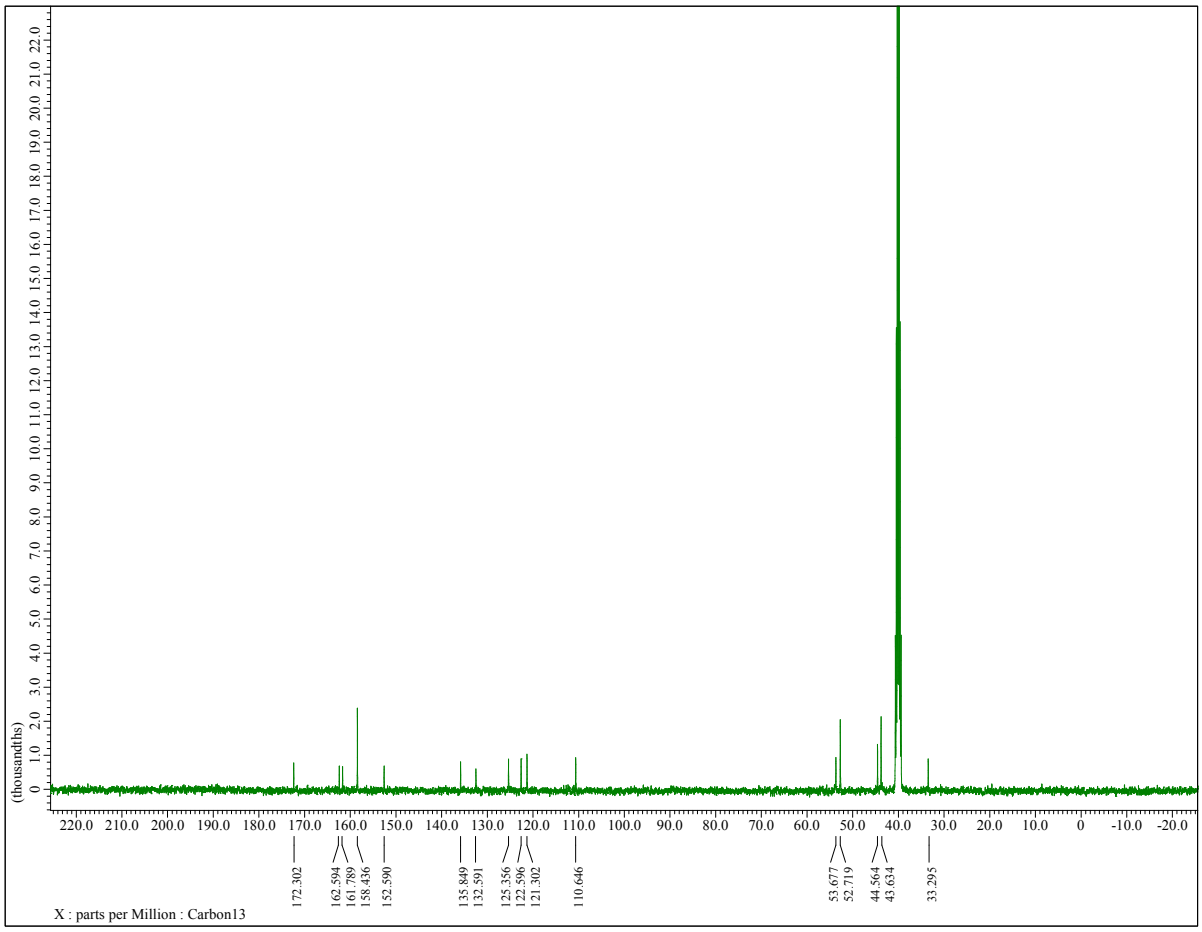
Supplementary Data

^{1}H NMR of Compound 13



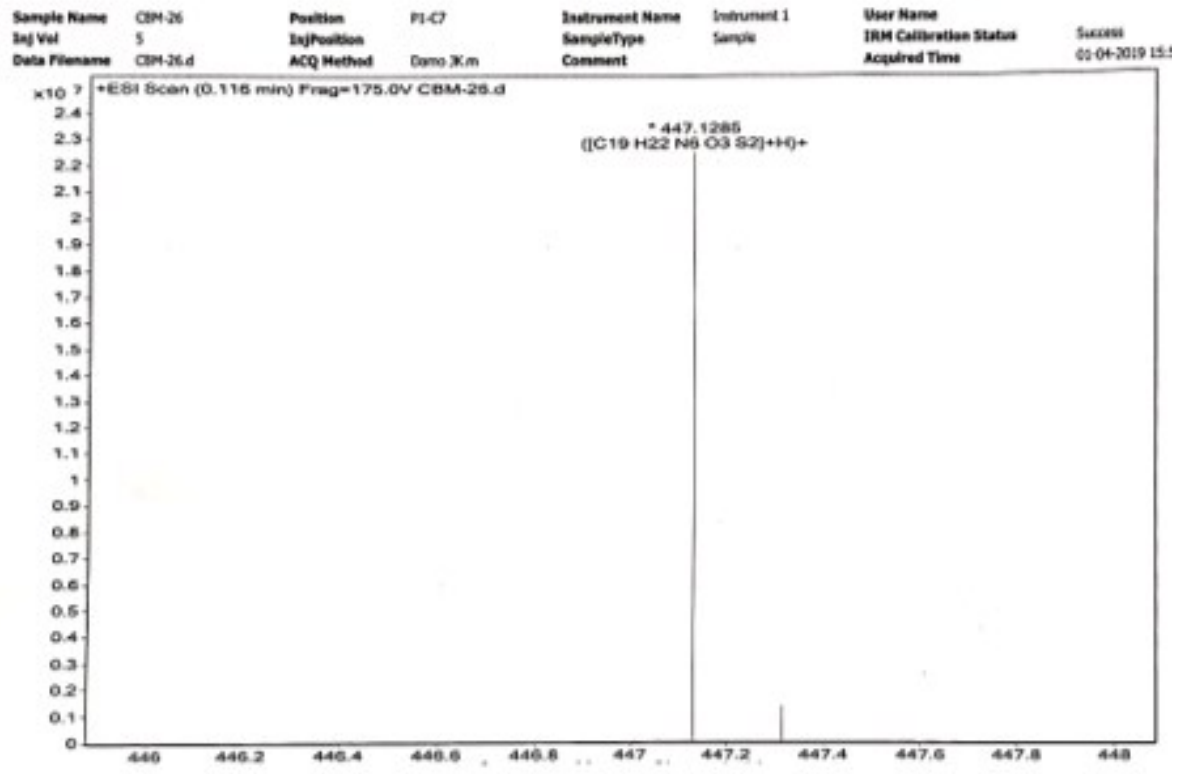
Supplementary Data

^{13}C NMR of Compound 13



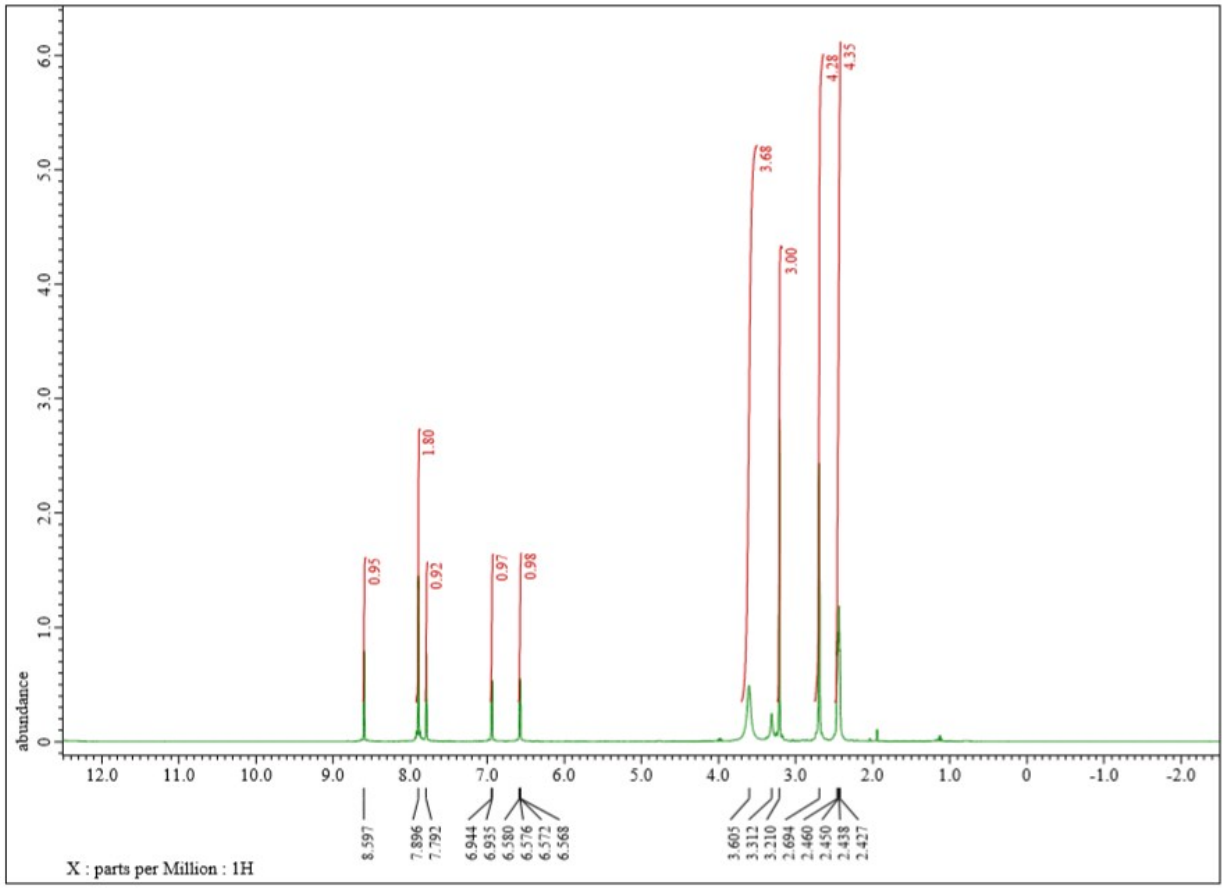
Supplementary Data

Mass spectra of Compound 13



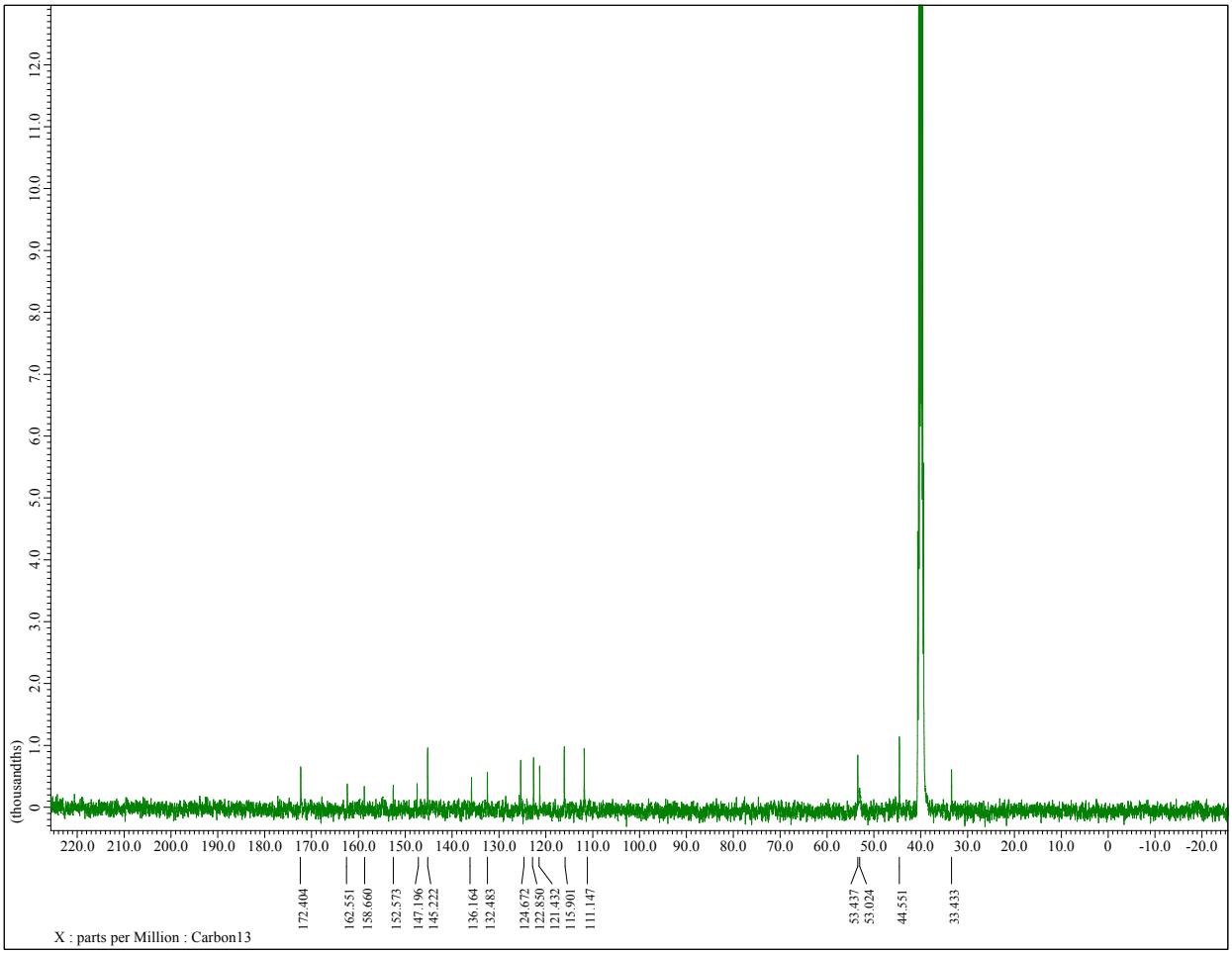
Supplementary Data

^{1}H NMR of Compound 14



Supplementary Data

^{13}C NMR of Compound 14



Supplementary Data

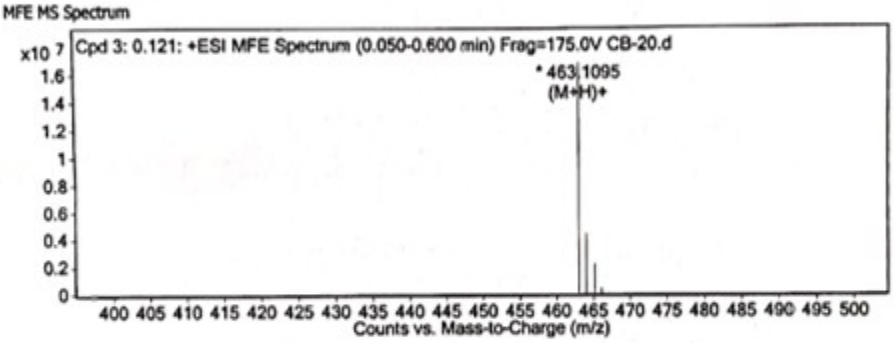
Mass spectra of Compound 14

Compound Table

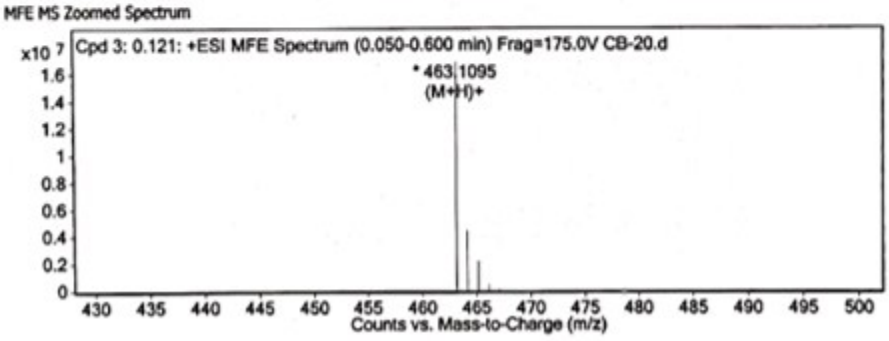
Compound Label	RT	Mass	Formula	MFG Formula	DB Formula
Cpd 3: 0.121	0.121	462.1021	C24 H14 N8 O S	C24 H14 N8 O S	C24 H14 N8 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: 0.121	463.1095	0.121	Find by Molecular Feature	462.1021

MFE MS Spectrum

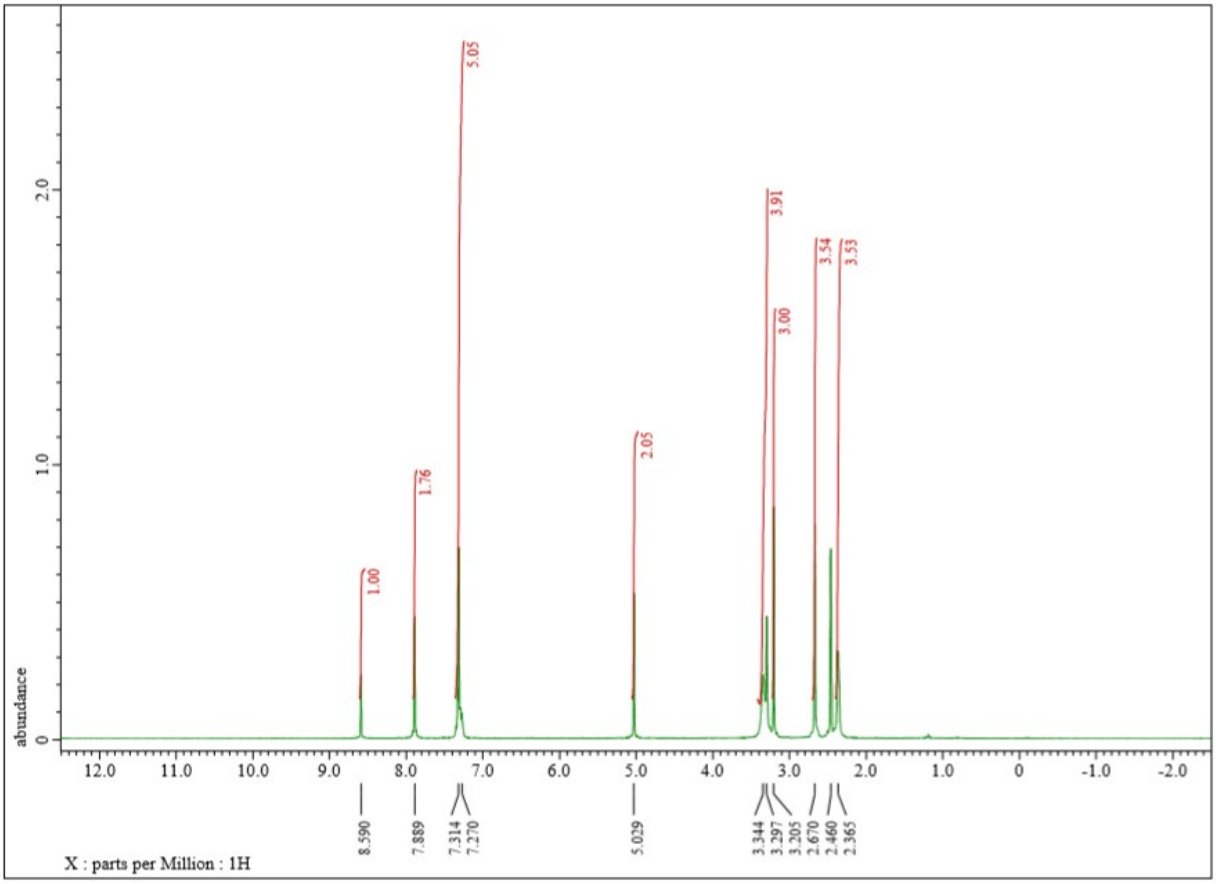


MFE MS Zoomed Spectrum



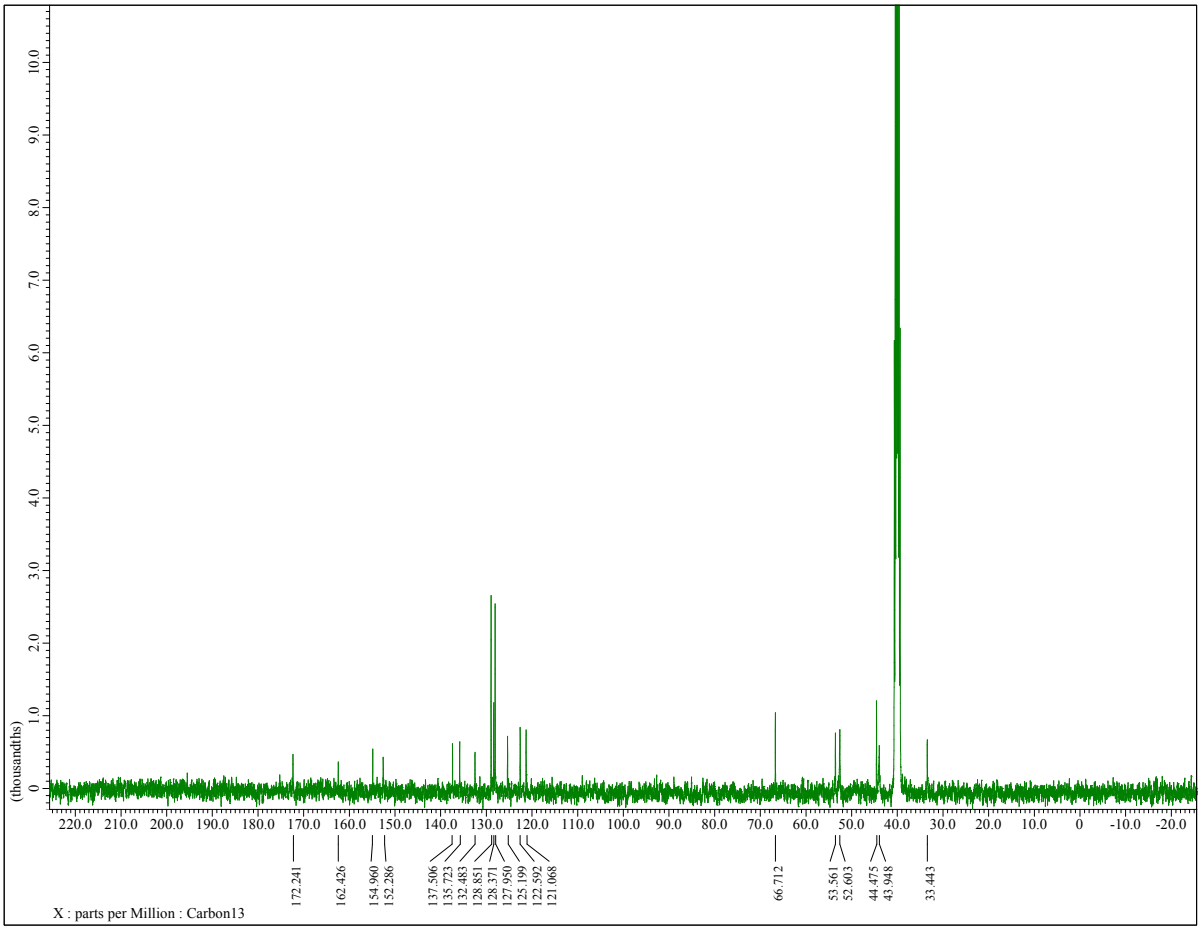
Supplementary Data

^{1}H NMR of Compound 15



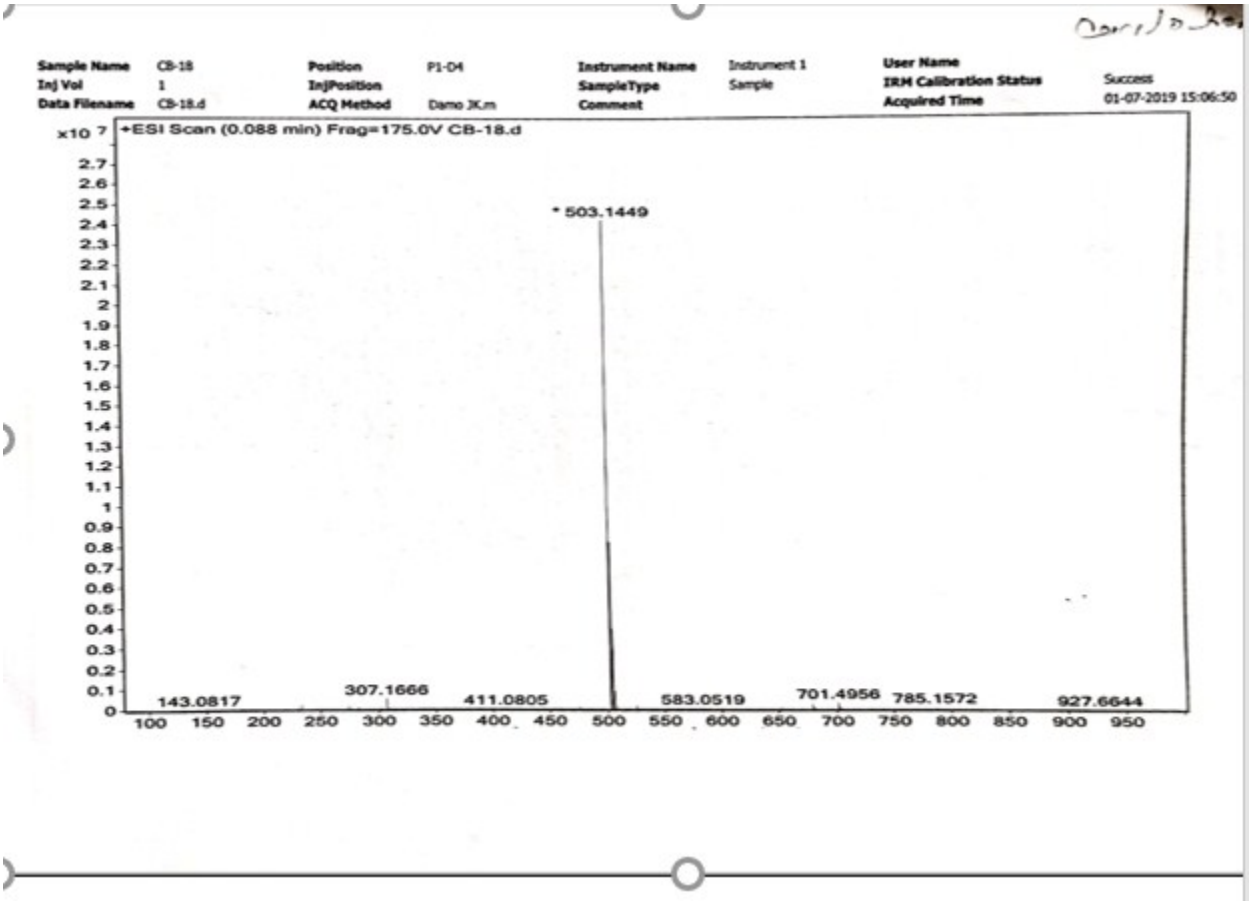
Supplementary Data

^{13}C spectra of Compound 15



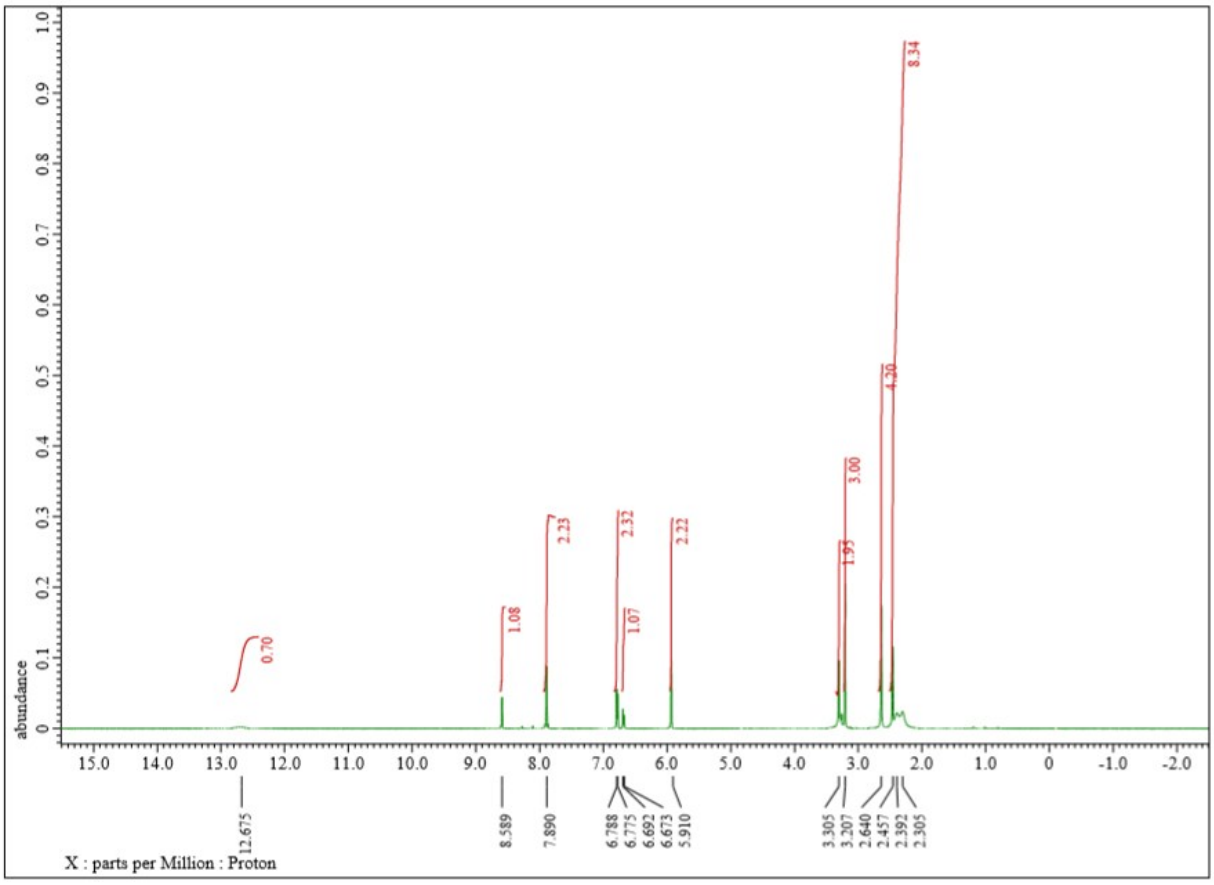
Supplementary Data

Mass spectra of Compound 15



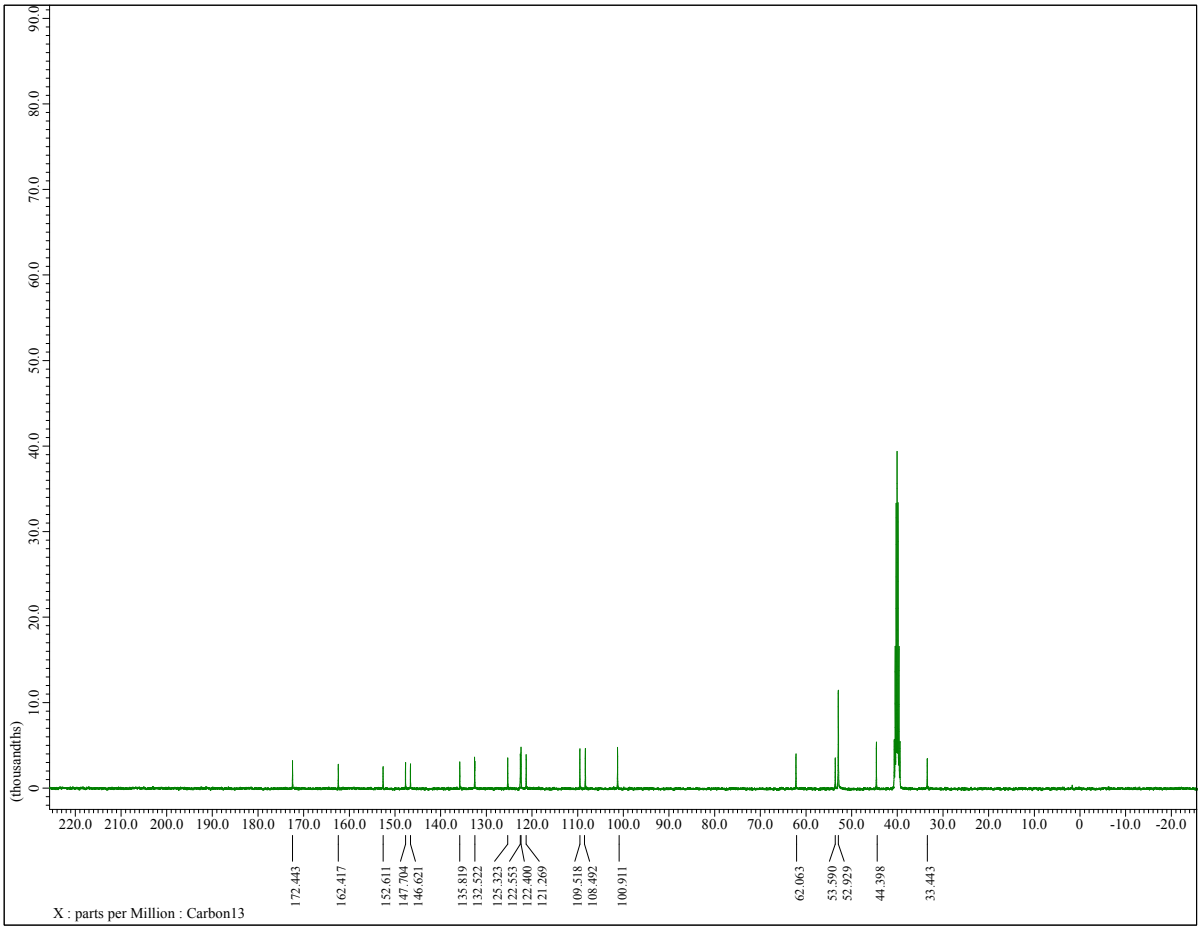
Supplementary Data

^{1}H NMR of Compound 16



Supplementary Data

^{13}C NMR of Compound 16



Supplementary Data

Mass spectra of Compound 16

Data File	CBM-25.d	**Sample Name**	CBM-25
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Demo JK.m	**Acquired Time**	01-04-2019 15:50:49
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

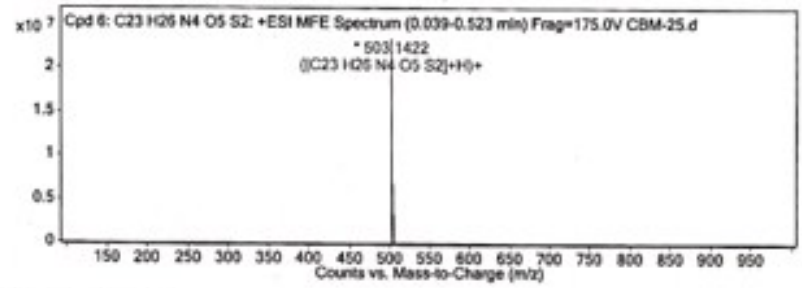
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

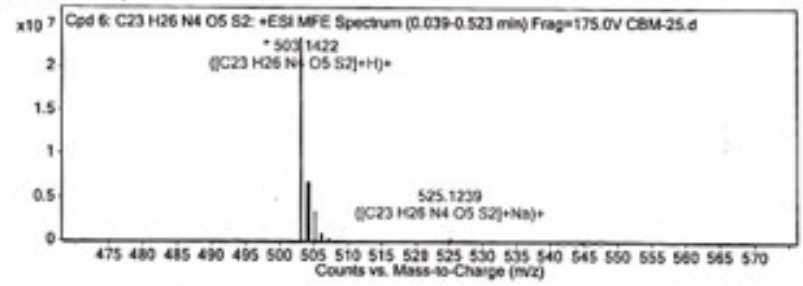
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C23 H26 N4 O5 S2	0.108	502.135	C23 H26 N4 O5 S2	C23 H26 N4 O5 S2	-1.14	C23 H26 N4 O5 S2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C23 H26 N4 O5 S2	503.1422	0.108	Find by Molecular Feature	502.135

MFE MS Spectrum

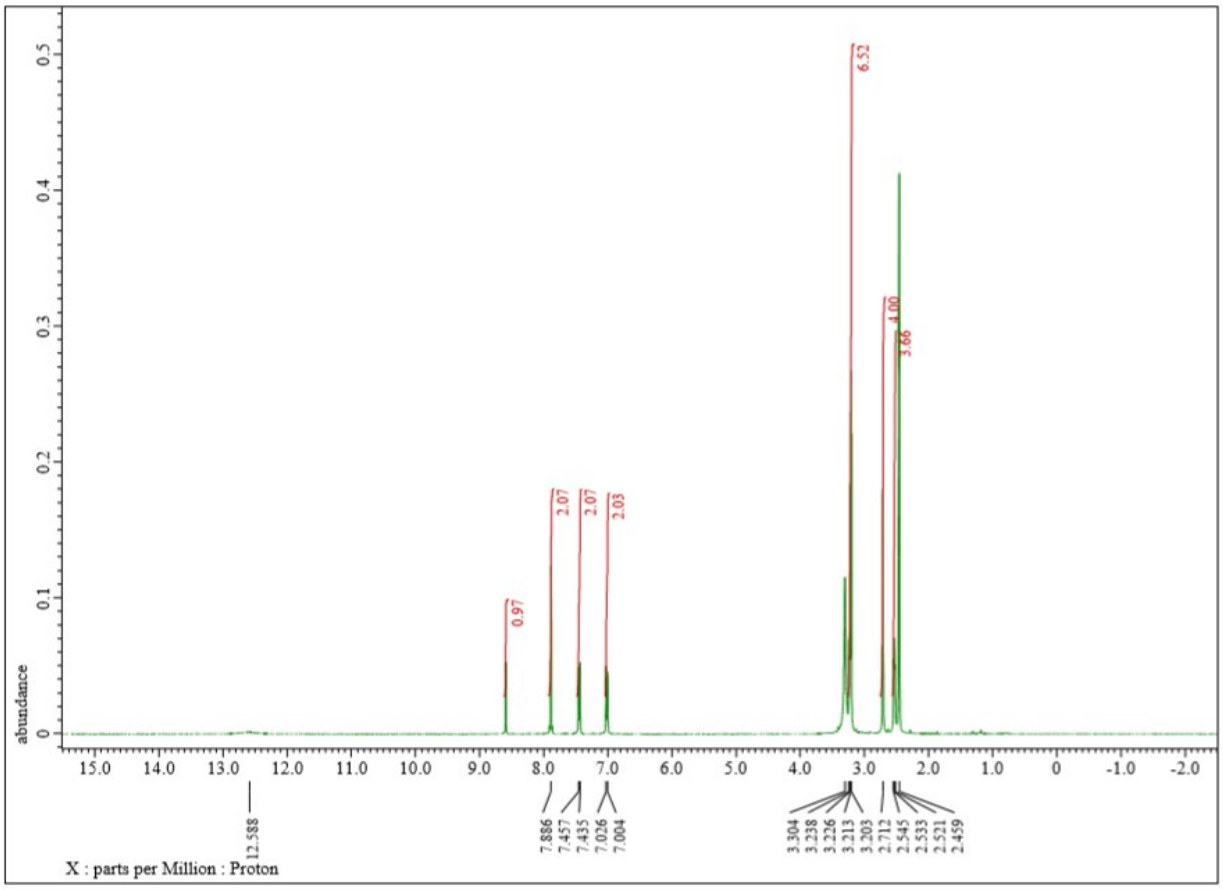


MFE MS Zoomed Spectrum



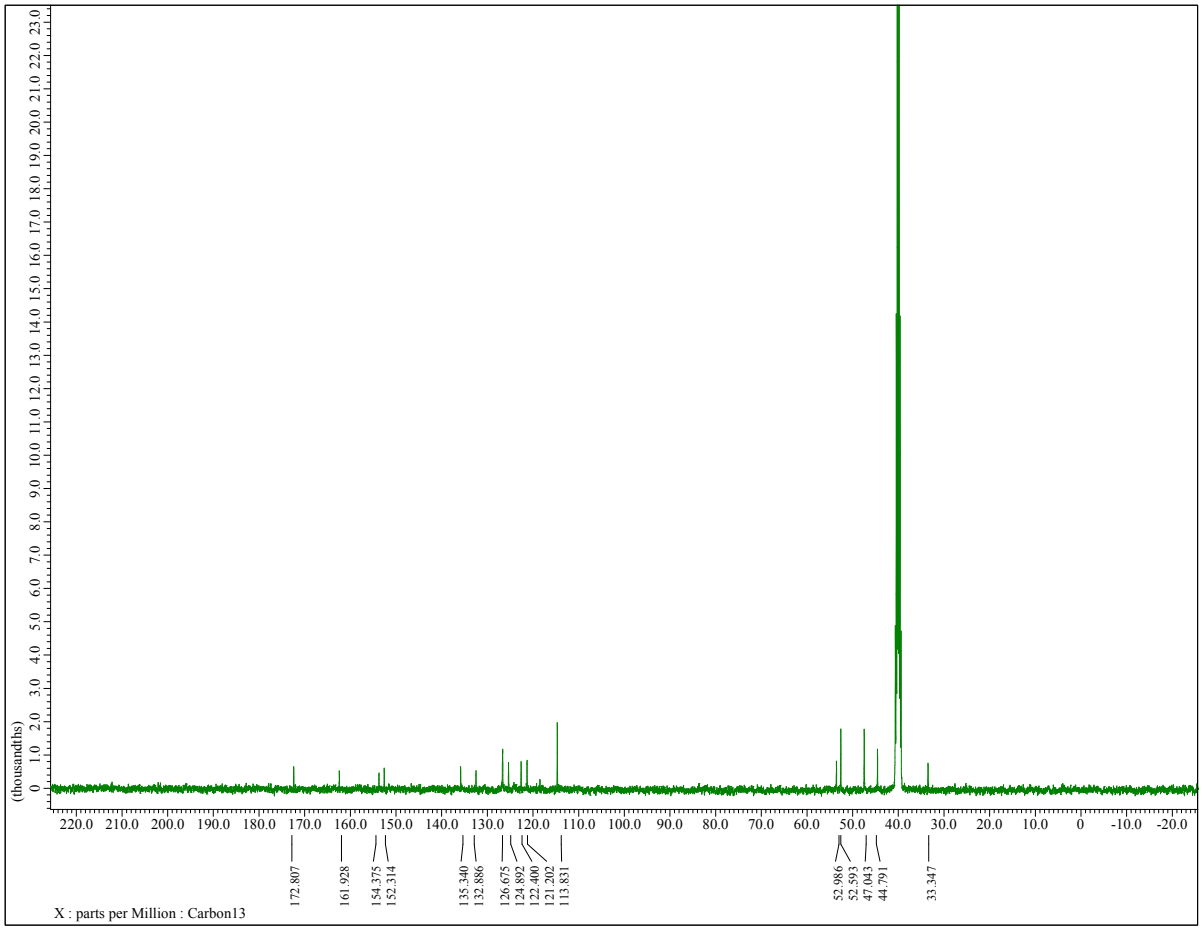
Supplementary Data

^{1}H NMR of Compound 17



Supplementary Data

^{13}C NMR of Compound 17



Supplementary Data

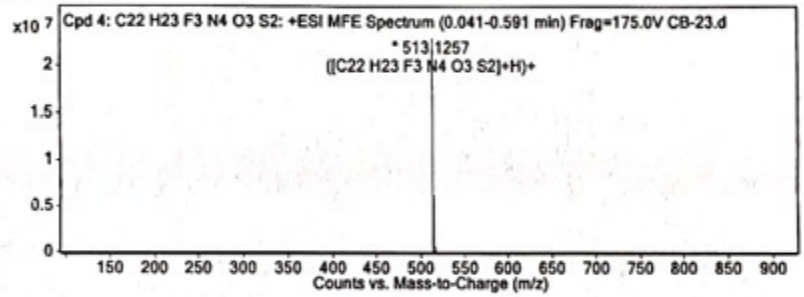
Mass spectra of Compound 17

Compound Table

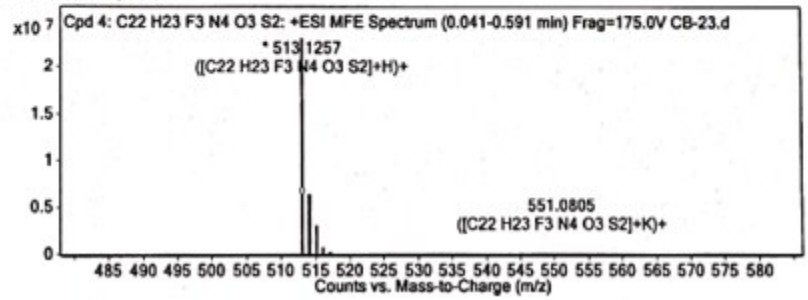
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C22 H23 F3 N4 O3 S2	0.089	512.1182	C22 H23 F3 N4 O3 S2	C22 H23 F3 N4 O3 S2	-3.66	C22 H23 F3 N4 O3 S2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C22 H23 F3 N4 O3 S2	513.1257	0.089	Find by Molecular Feature	512.1182

MFE MS Spectrum



MFE MS Zoomed Spectrum



Supplementary Data