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Design, Synthesis and In Vitro Evaluation of Acetylcholinesterase Inhibitory Activity Of Novel Thiadiazol Derivatives

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Supplementary Data:

Figure S1. HRMS of 3a:

Data File: C:\LabSolutions\Data\Analiz\derya\COMP-1_99.lcd

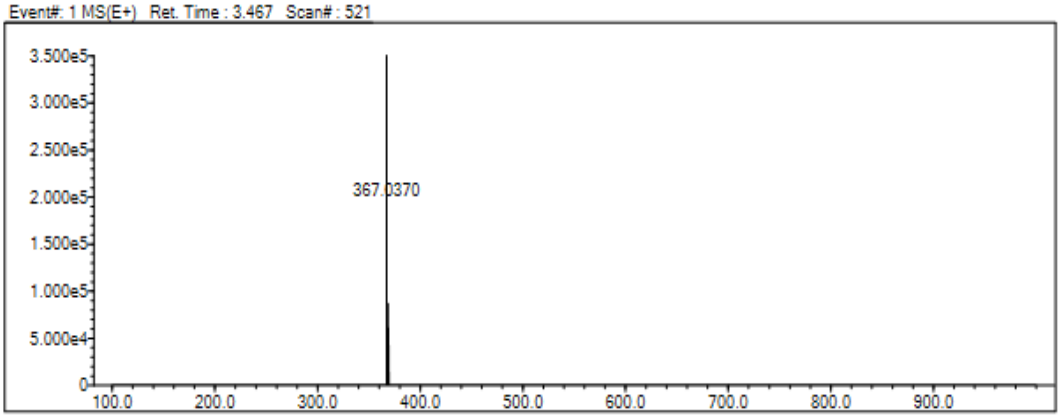
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N	3	2	7	P	3	0	0	Br	1	0	1	I	3	0	0	

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HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

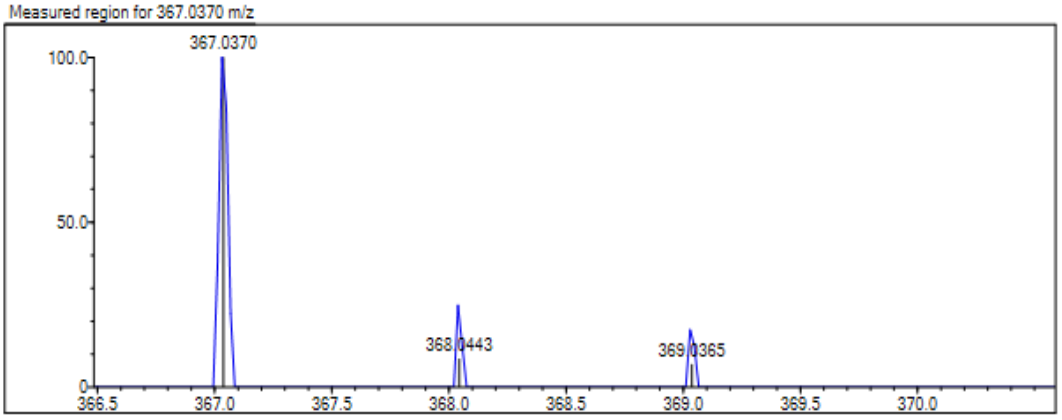
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MSn Logic Mode: AND

Electron Ions: both
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Max Results: 150

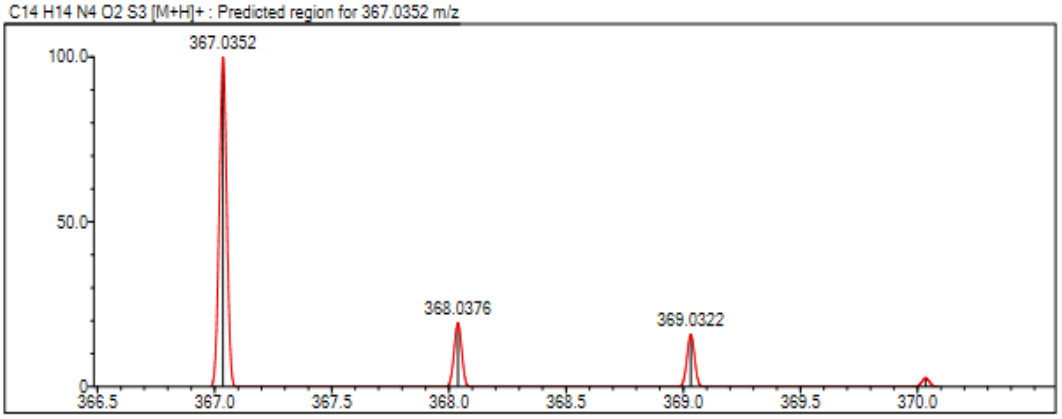
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Measured region for 367.0370 m/z



C14 H14 N4 O2 S3 [M+H]+ : Predicted region for 367.0352 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	58.68	C14 H14 N4 O2 S3	[M+H]+	367.0370	367.0352	1.8	4.90	65.02	10.0

Figure S2. HRMS of 3b:

Data File: C:\LabSolutions\Data\Analiz\derya\COMP-3_103.lcd

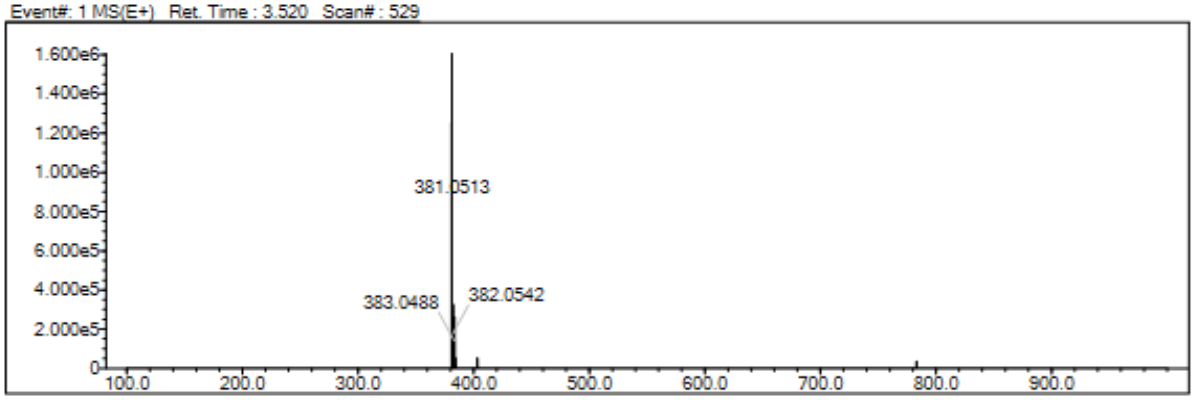
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C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	7	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

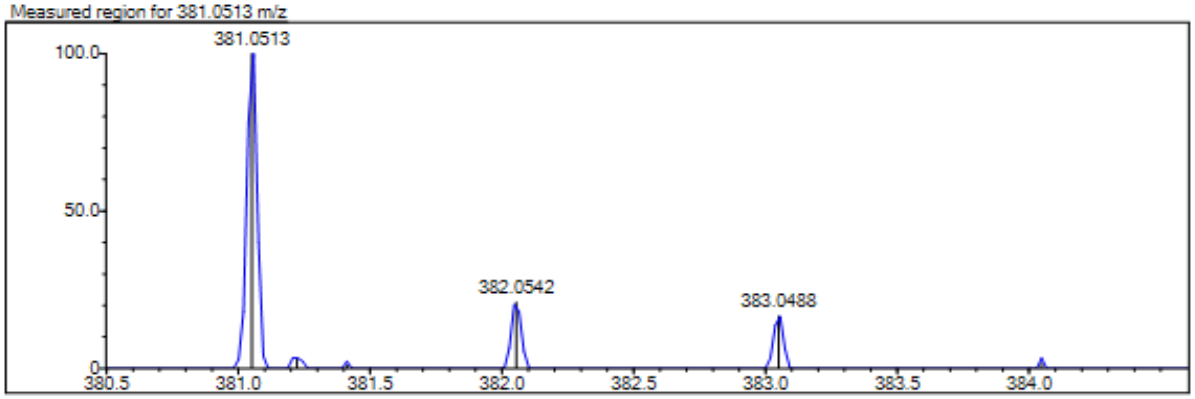
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MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 9000
Max Results: 150

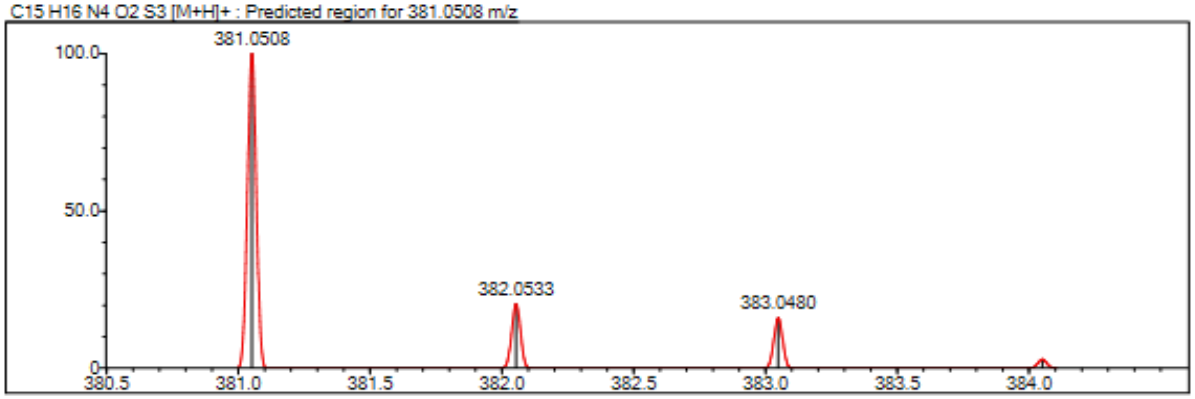
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Measured region for 381.0513 m/z



C15 H16 N4 O2 S3 [M+H]+ : Predicted region for 381.0508 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	88.22	C15 H16 N4 O2 S3	[M+H]+	381.0513	381.0508	0.5	1.31	88.91	10.0

Figure S3. HRMS of 3c:

Data File: C:\LabSolutions\Data\Analiz\derya\COMP-4_102.lcd

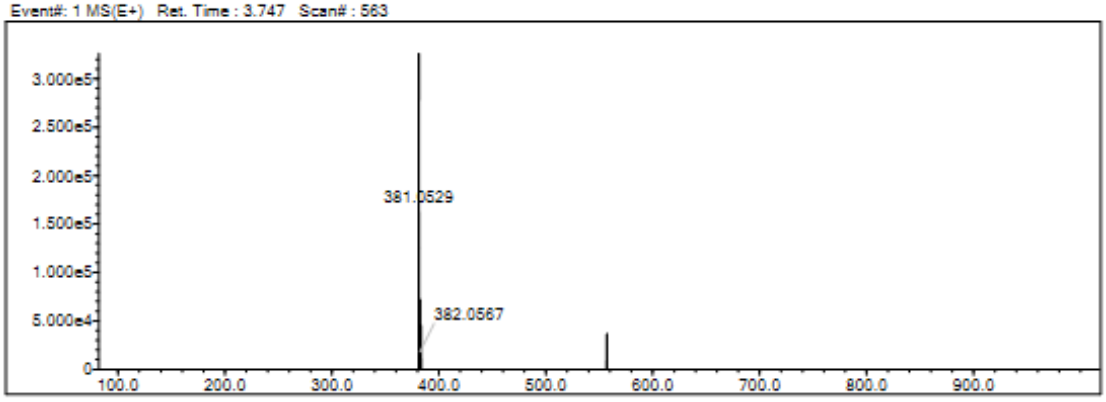
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C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	7	P	3	0	0	Br	1	0	1	I	3	0	0	

Error Margin (ppm): 10
HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

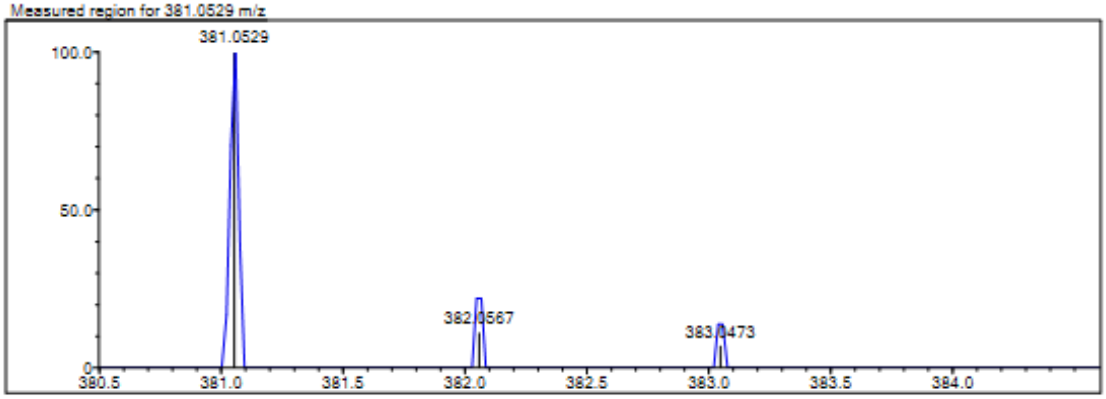
DBE Range: 10.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 9000
Max Results: 150

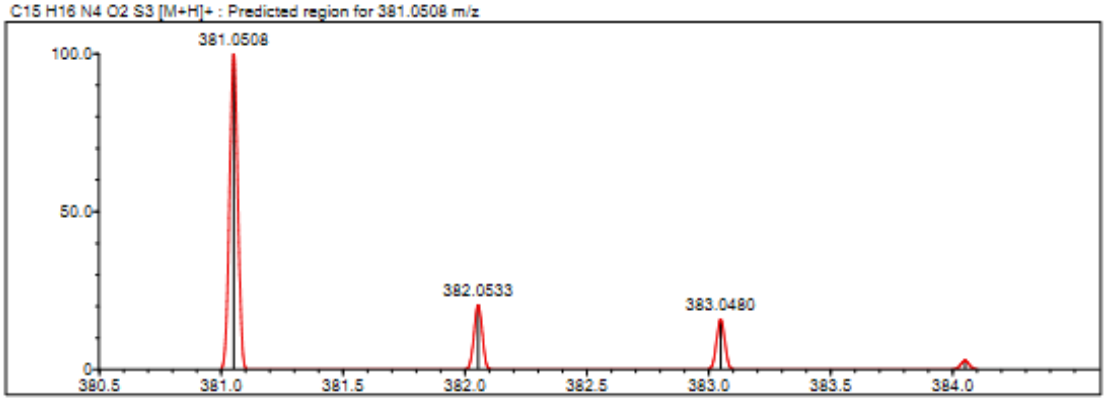
Event#: 1 MS(E+) Ret. Time : 3.747 Scan# : 563



Measured region for 381.0529 m/z



C15 H16 N4 O2 S3 [M+H]+ : Predicted region for 381.0508 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	52.99	C15 H16 N4 O2 S3	[M+H]+	381.0529	381.0508	2.1	5.51	62.42	10.0

Figure S4. HRMS of 3d:

Data File: C:\LabSolutions\Data\Analiz\derya\COMP-5_2_176.lcd

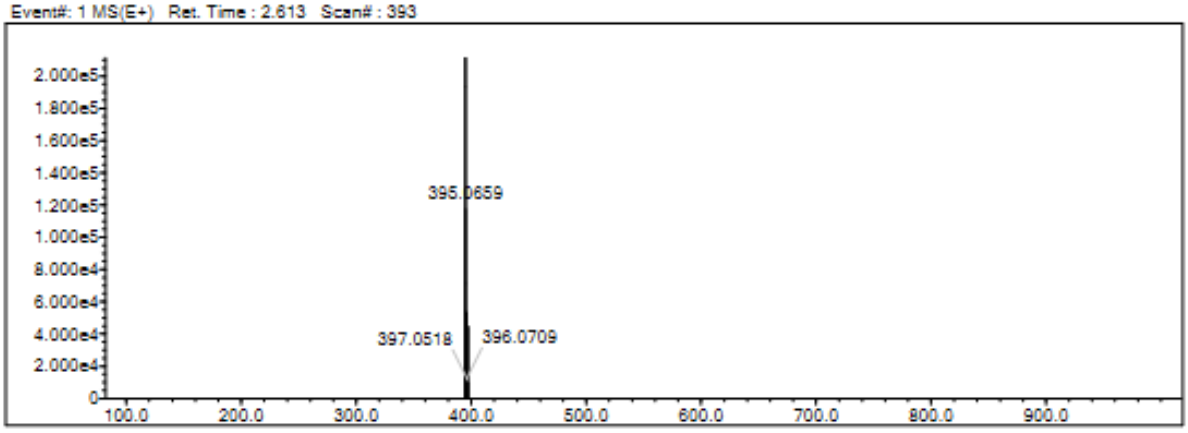
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C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	3	7	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

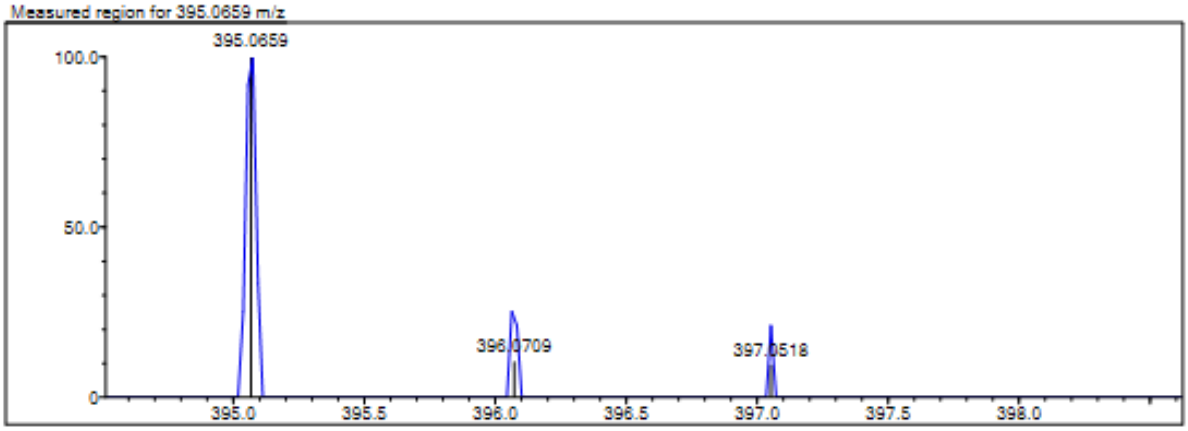
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Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 9000
Max Results: 150

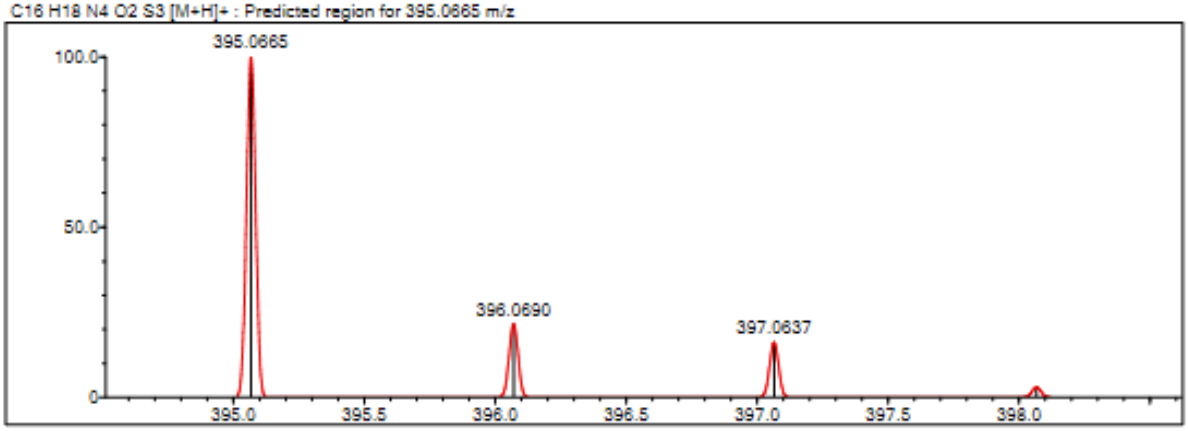
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Measured region for 395.0659 m/z



C16 H18 N4 O2 S3 [M+H]+ : Predicted region for 395.0665 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	46.37	C16 H18 N4 O2 S3	[M+H]+	395.0659	395.0665	-0.6	-1.52	46.98	10.0

Figure S5. HRMS of 3e:

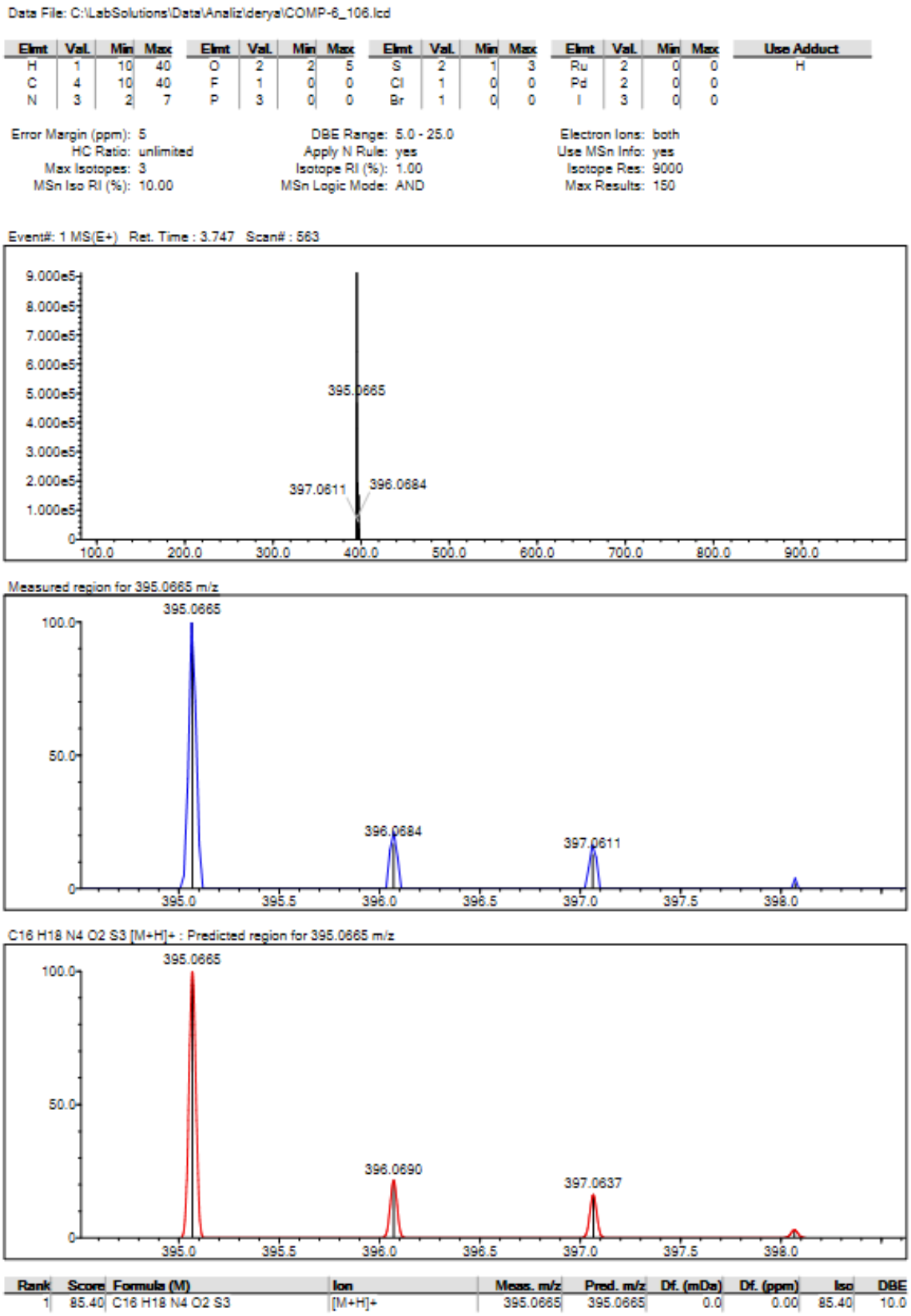


Figure S6. HRMS of 3f:

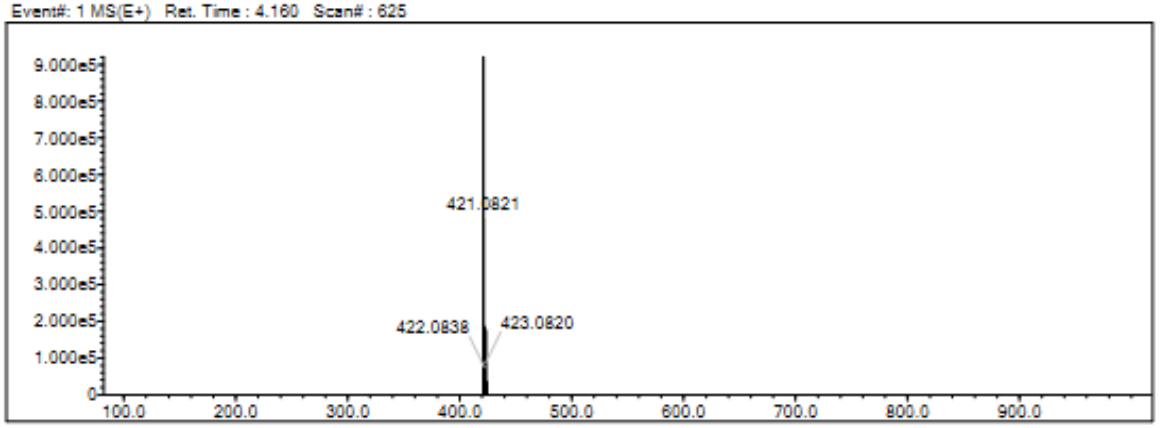
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C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	7	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

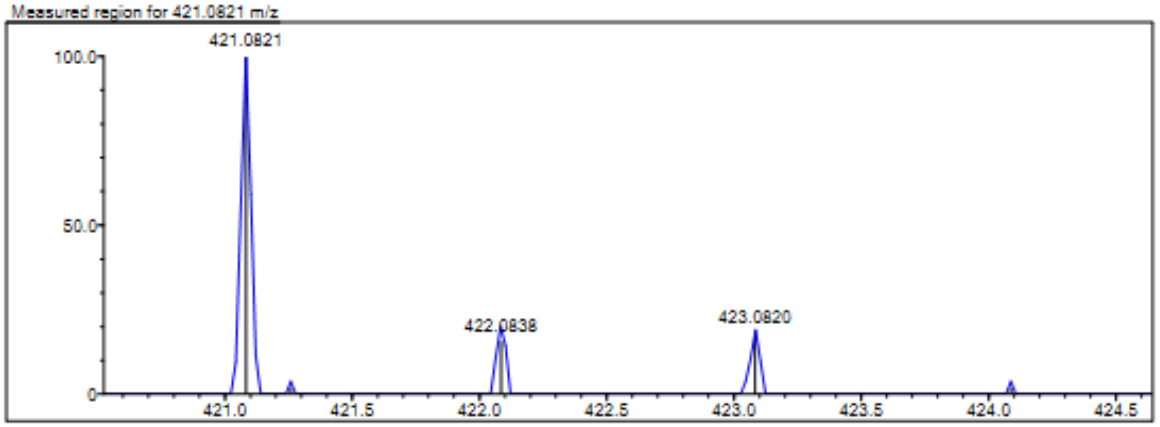
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Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 9000
Max Results: 150

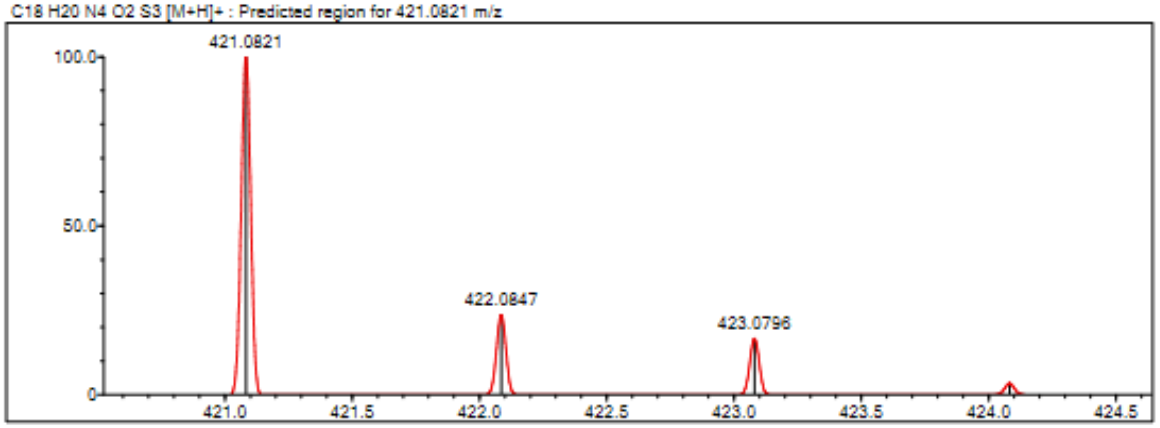
Event#: 1 MS(E+) Ret. Time : 4.160 Scan# : 625



Measured region for 421.0821 m/z



C18 H20 N4 O2 S3 [M+H]+ : Predicted region for 421.0821 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	87.90	C18 H20 N4 O2 S3	[M+H]+	421.0821	421.0821	-0.0	0.00	87.90	11.0

Figure S7. HRMS of 3g:

Data File: C:\LabSolutions\Data\Analiz\deryal\COMP-8_108.lcd

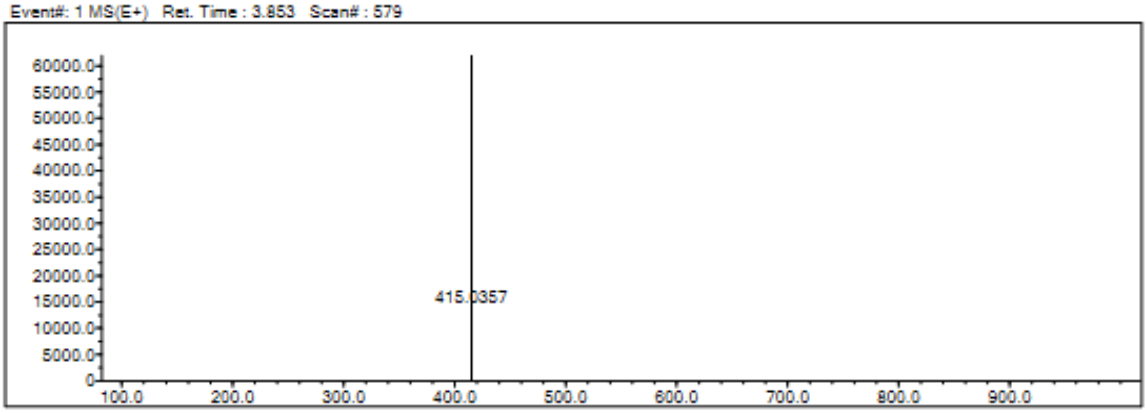
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C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	7	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

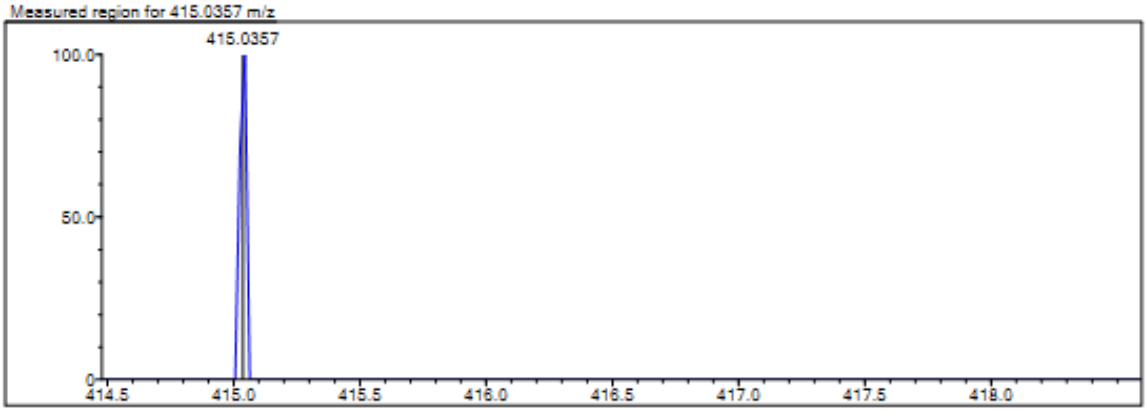
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 9000
Max Results: 150

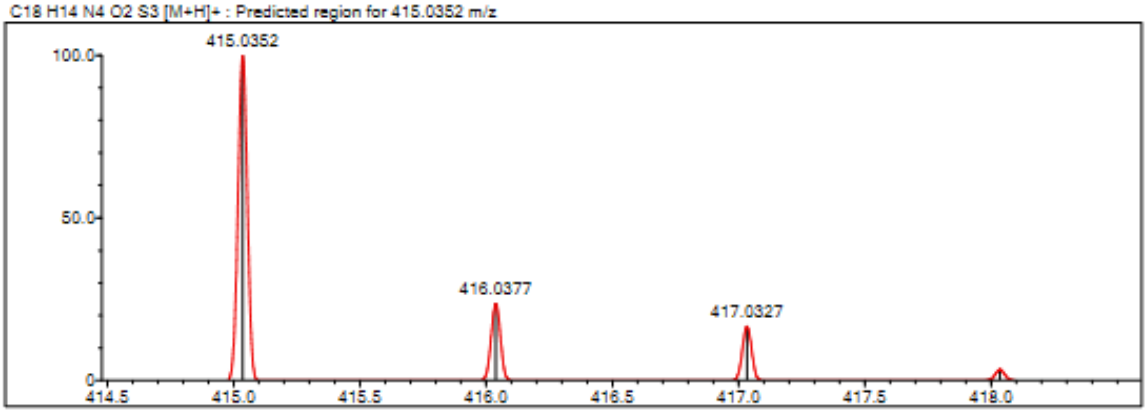
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Measured region for 415.0357 m/z



C18 H14 N4 O2 S3 [M+H]+ : Predicted region for 415.0352 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C18 H14 N4 O2 S3	[M+H]+	415.0357	415.0352	0.5	1.20	0.00	14.0

Figure S8. HRMS of 3h:

Data File: C:\LabSolutions\Data\Analiz\derya\COMP-9_109.lcd

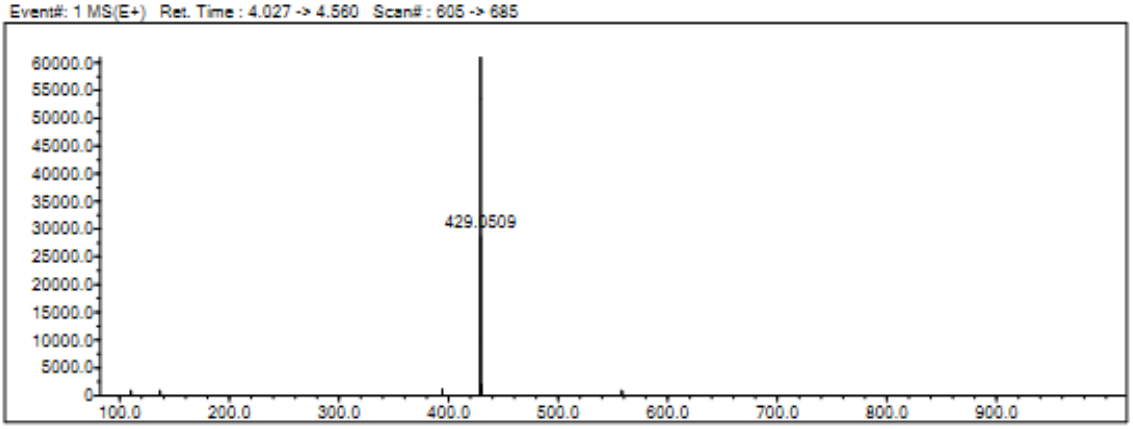
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C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	7	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

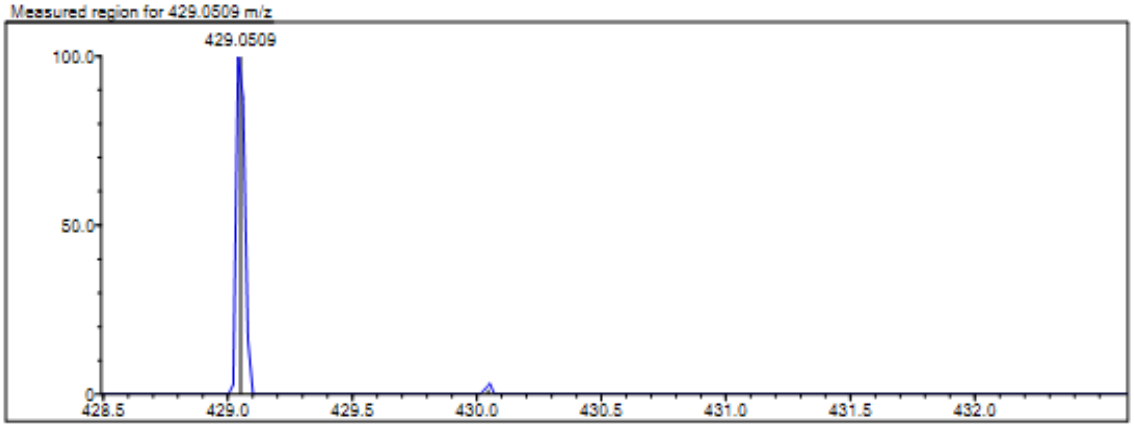
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MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 9000
Max Results: 150

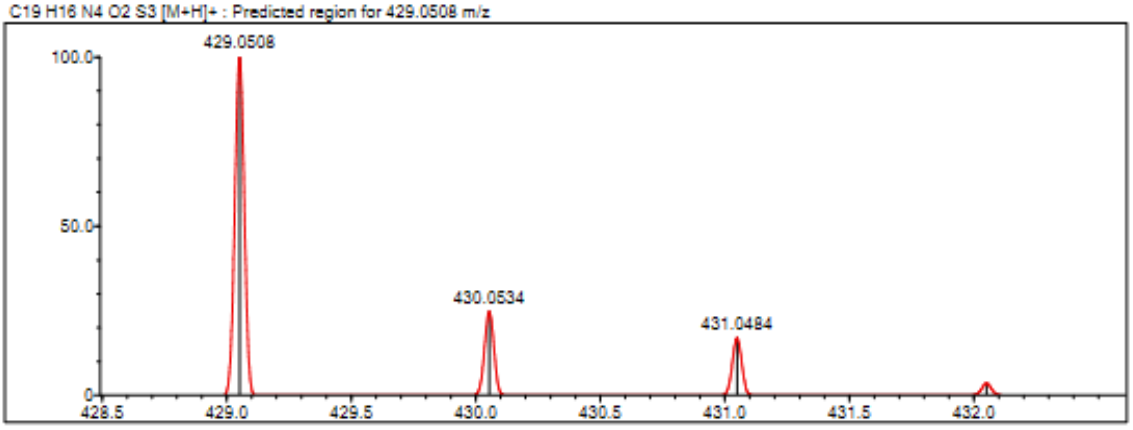
Event#: 1 MS(E+) Ret. Time : 4.027 -> 4.560 Scan# : 605 -> 685



Measured region for 429.0509 m/z



C19 H16 N4 O2 S3 [M+H]+ : Predicted region for 429.0508 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C19 H16 N4 O2 S3	[M+H]+	429.0509	429.0508	0.1	0.23	0.00	14.0

Figure S9. HRMS of 3i:

Data File: C:\LabSolutions\Data\Analiz\derya\COMP-10_111.lcd

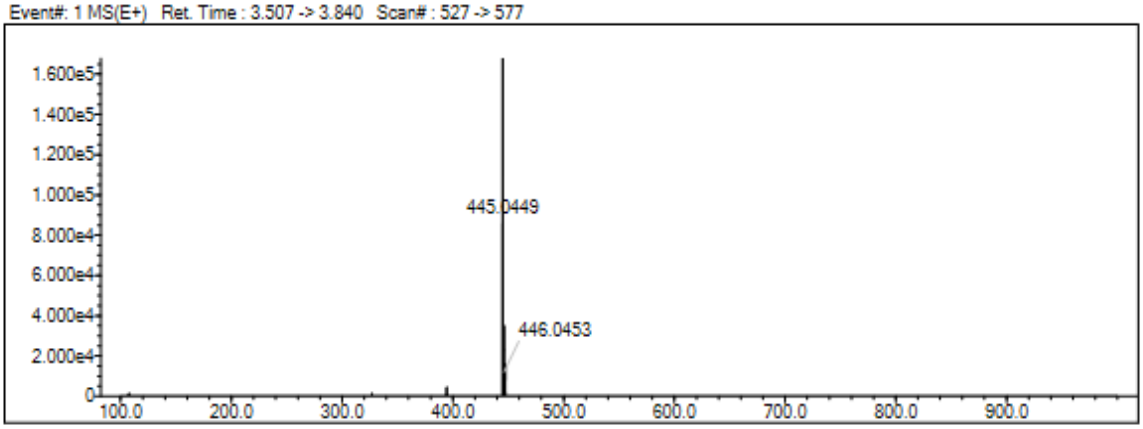
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	3	S	2	1	3	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	3	7	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

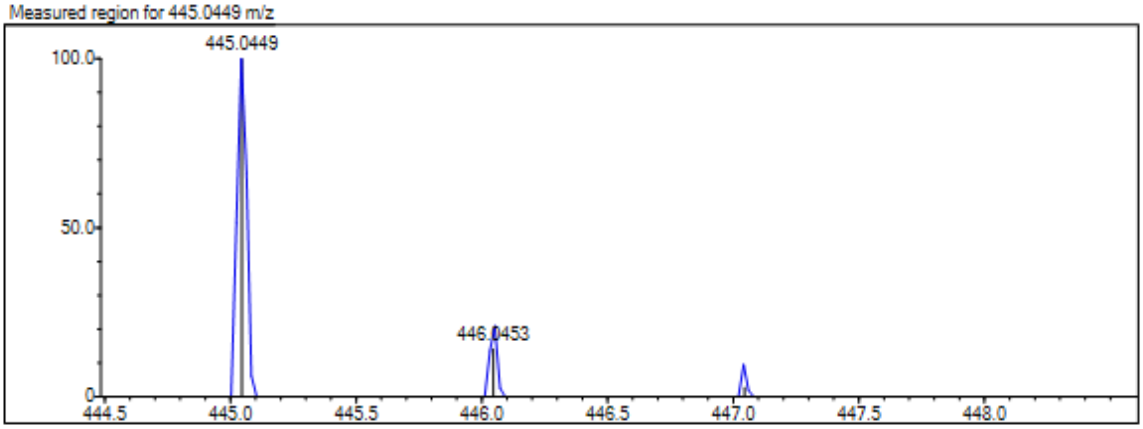
DBE Range: 5.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 9000
Max Results: 150

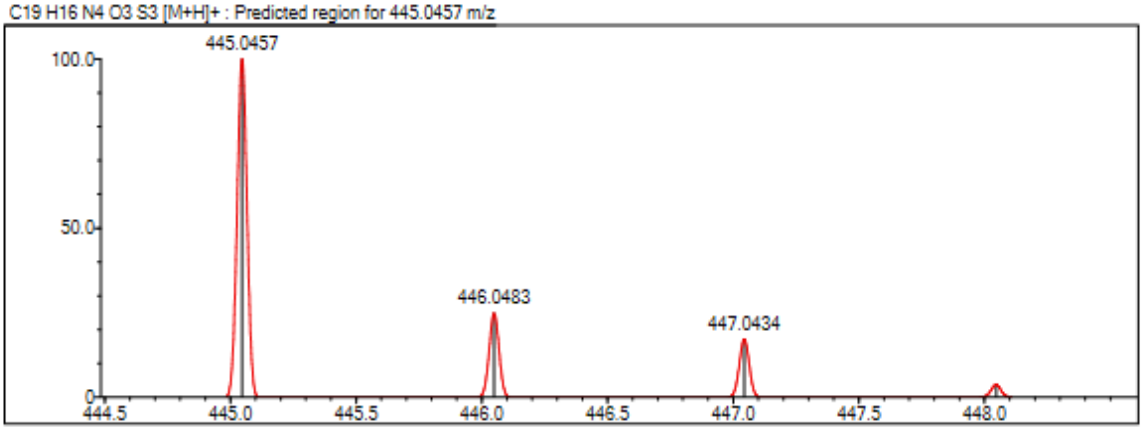
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Measured region for 445.0449 m/z

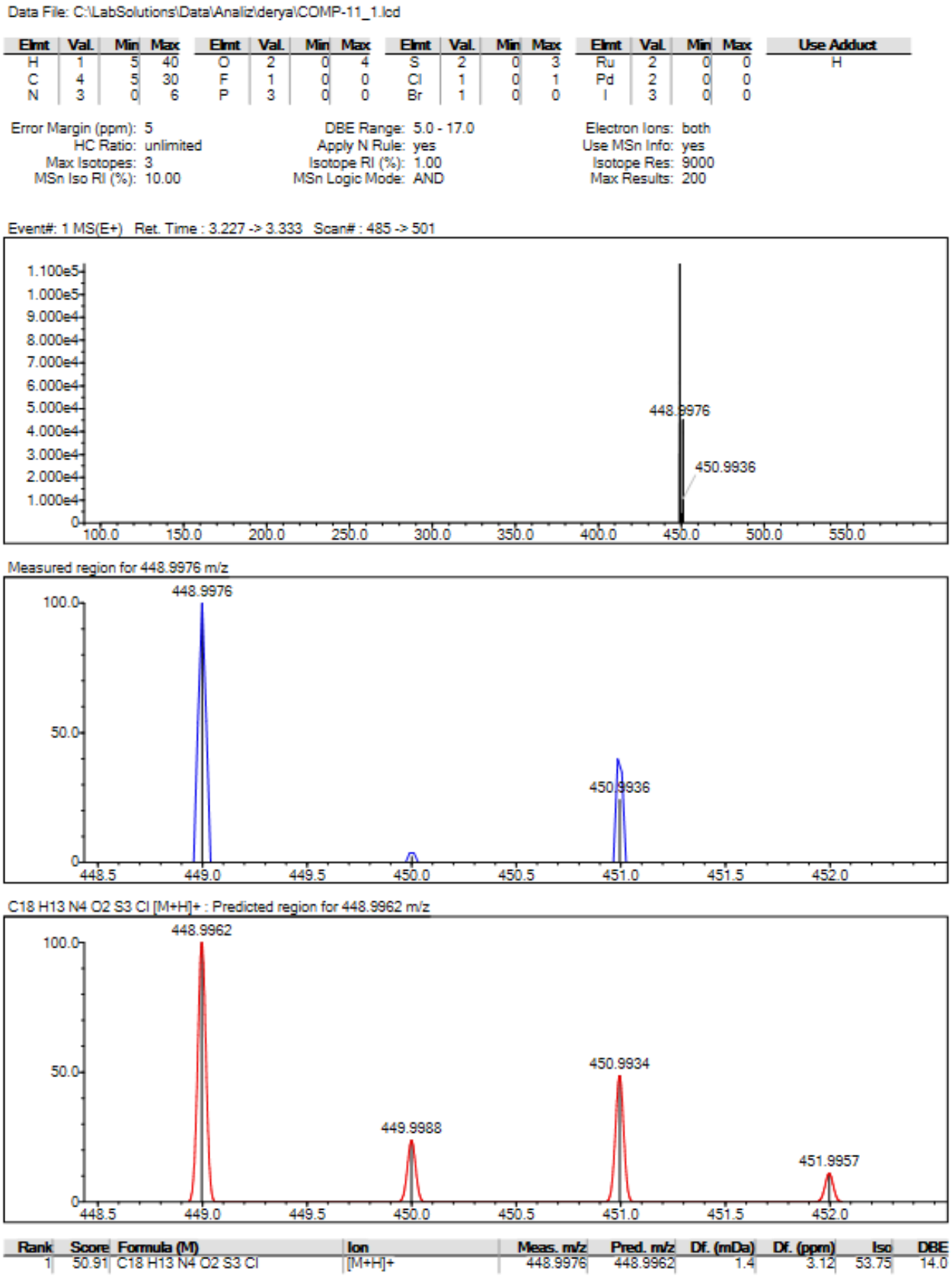


C19 H16 N4 O3 S3 [M+H]+ : Predicted region for 445.0457 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	67.37	C19 H16 N4 O3 S3	[M+H]+	445.0449	445.0457	-0.8	-1.80	68.75	14.0

Figure S10. HRMS of 3j:



[1]HNMR of Compound 3a-3j:

Figure S11. [1]HNMR 3a:

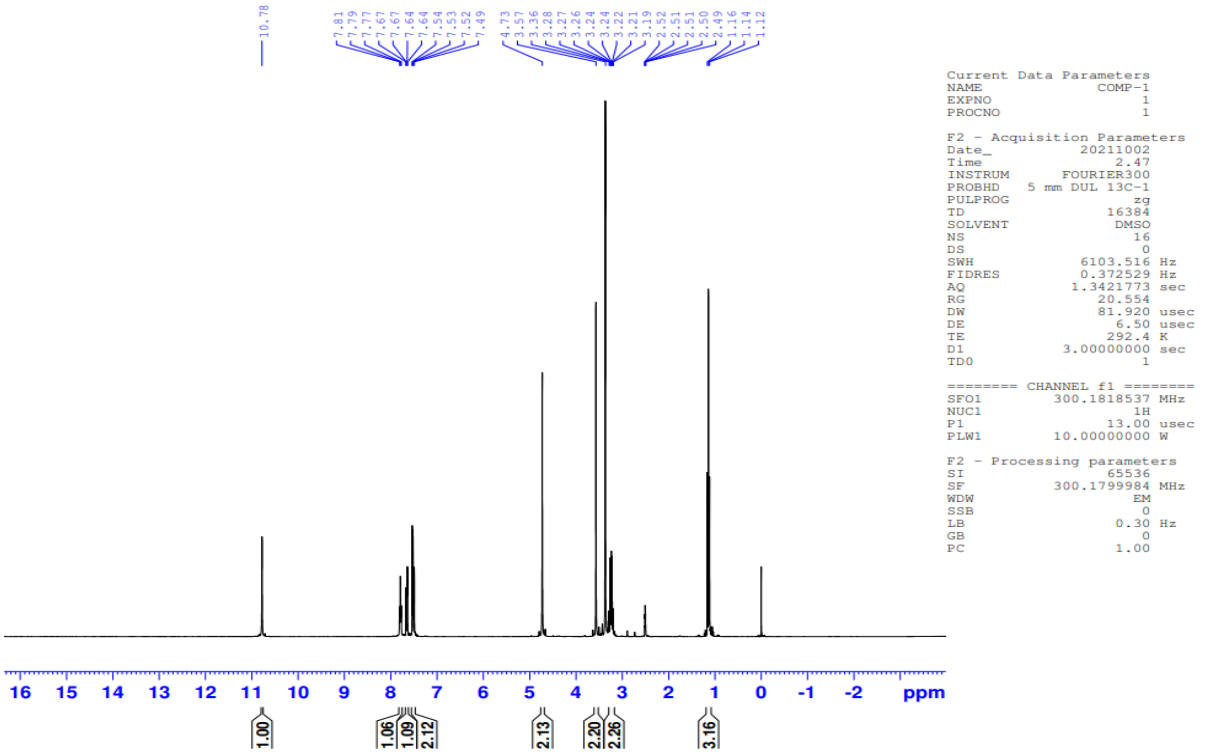


Figure S12. [1]HNMR 3b:

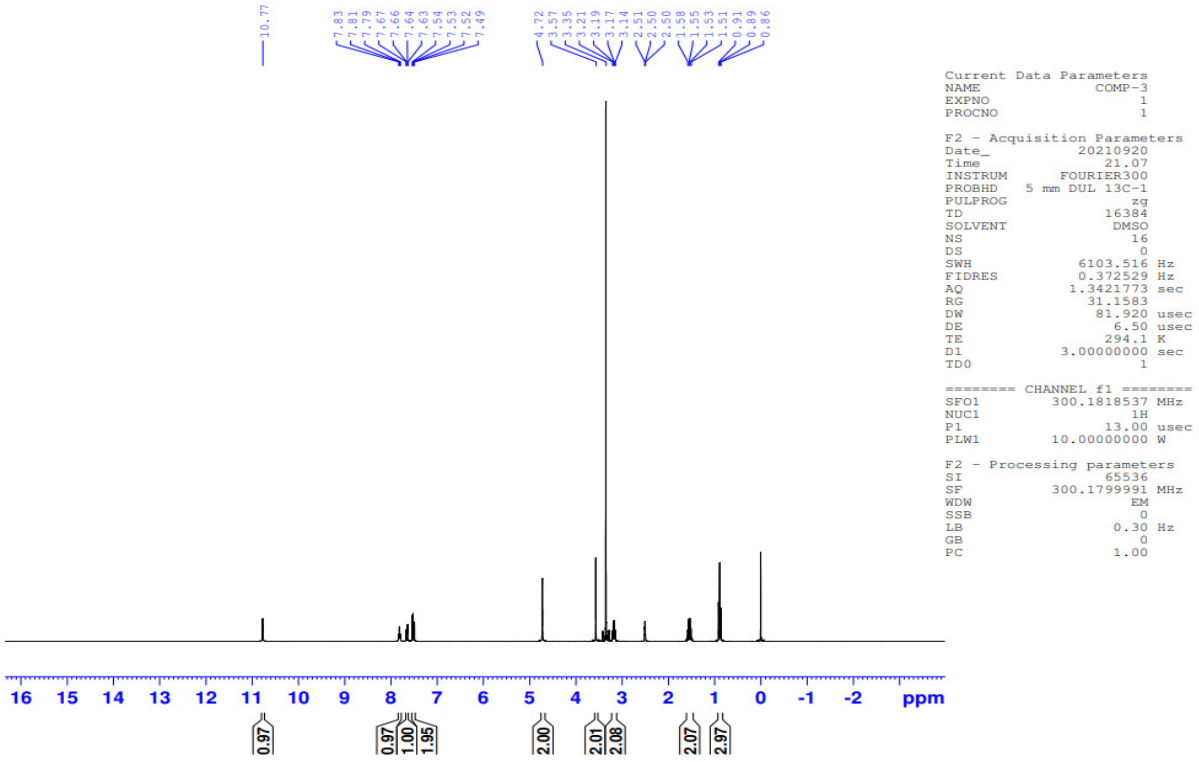


Figure S13. ^{1}HNMR 3c:

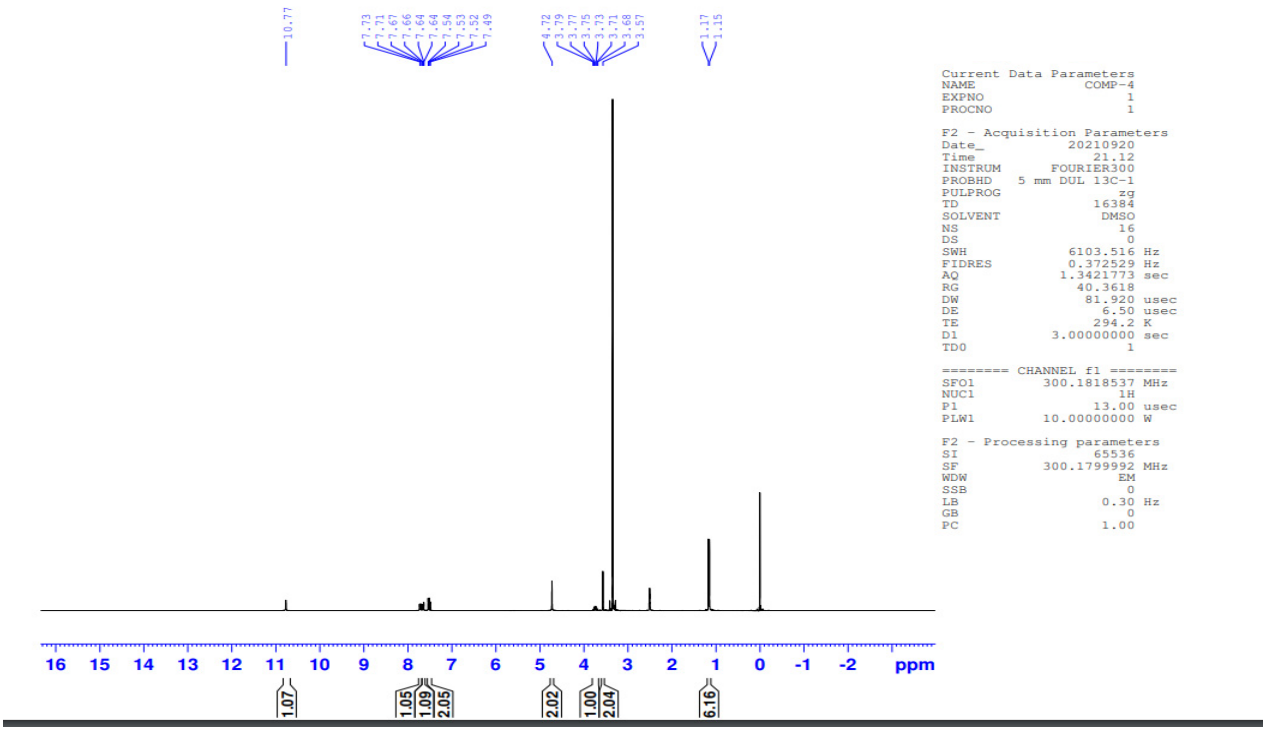


Figure S14. ^{1}HNMR 3d:

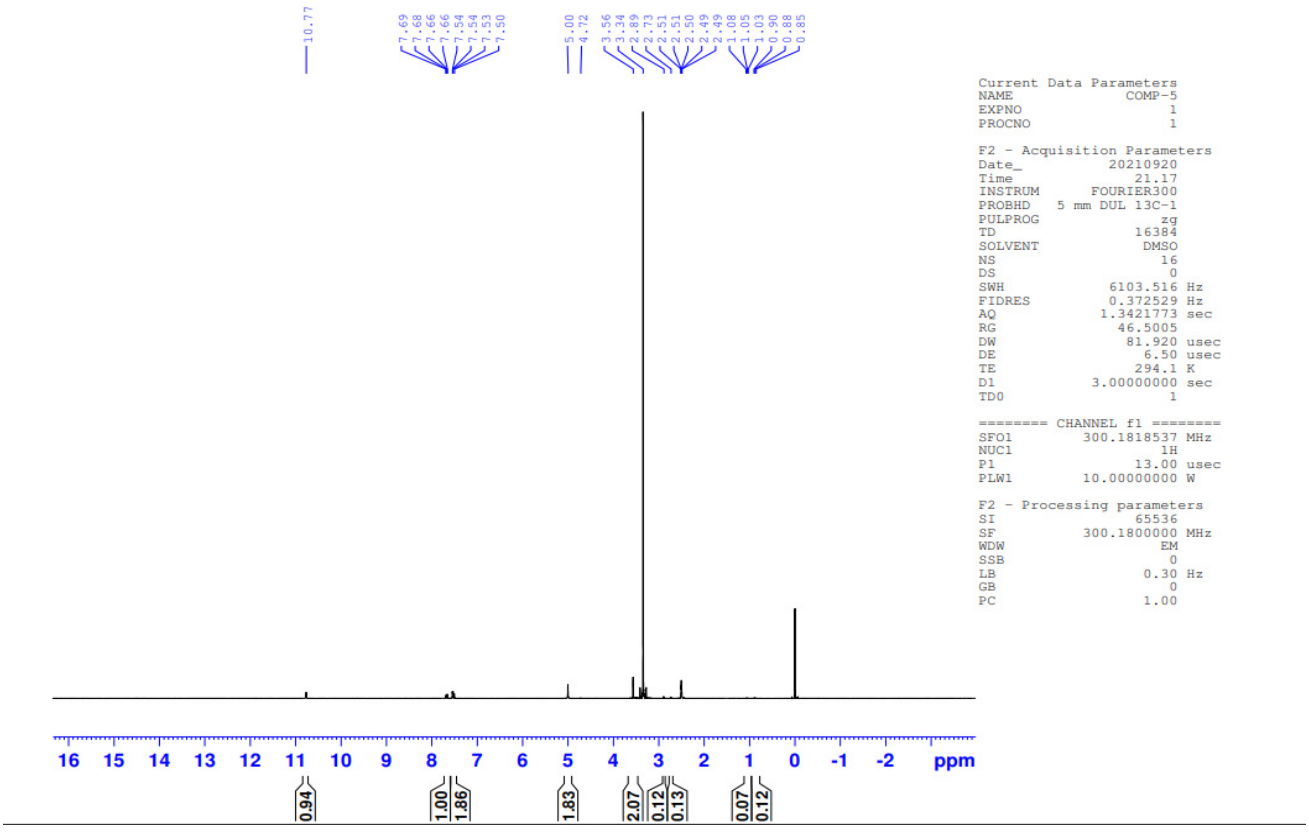


Figure S15. ^{1}HNMR 3e:

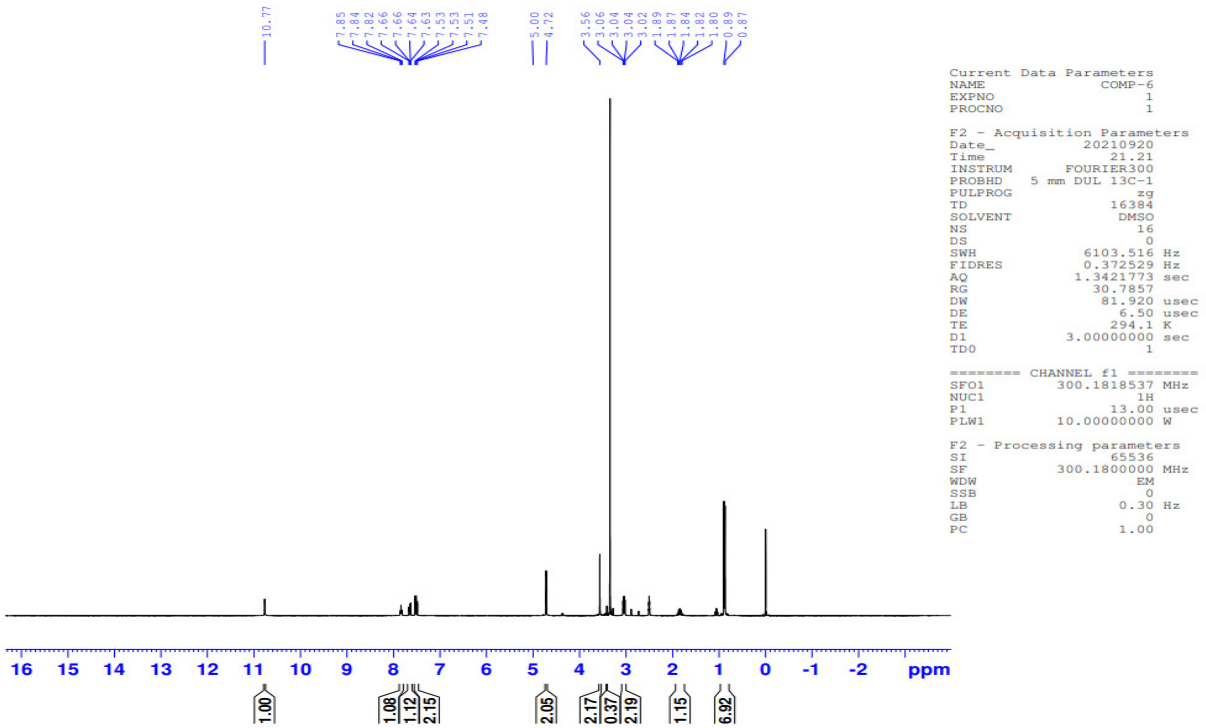


Figure S16. ^{1}HNMR 3f:

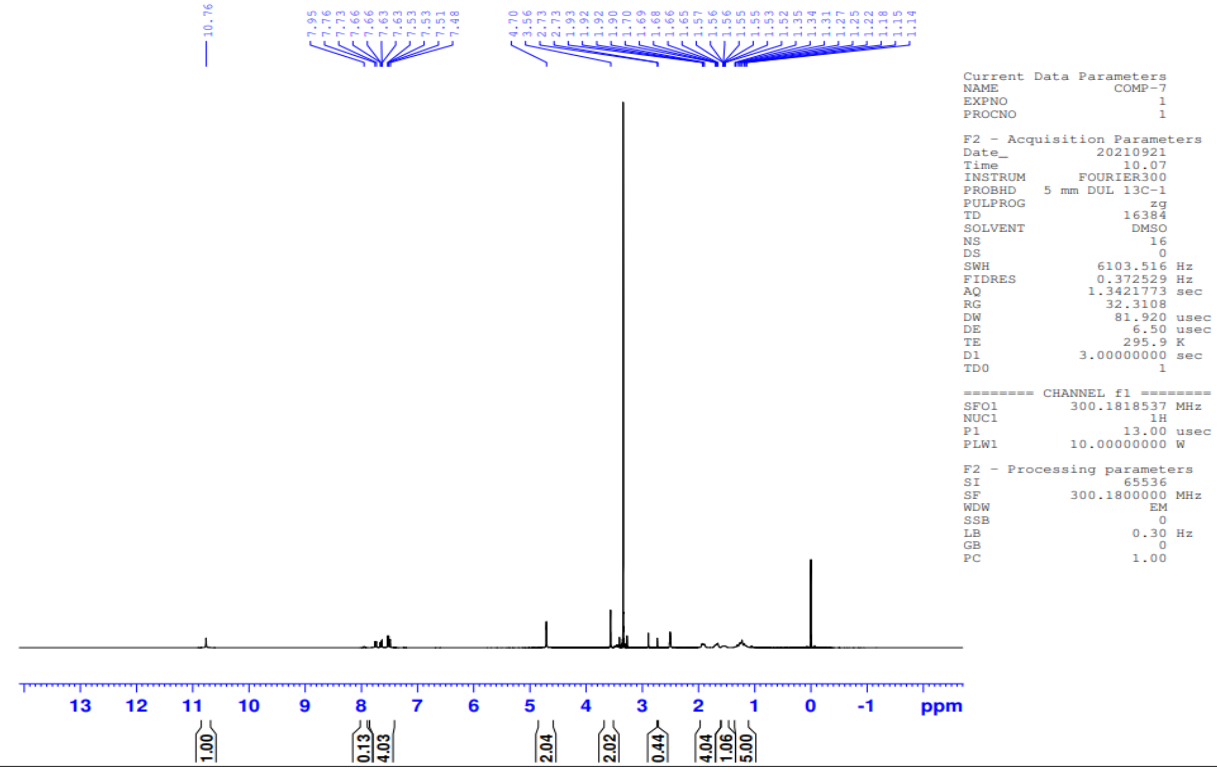


Figure S17. ^{1}HNMR 3g:

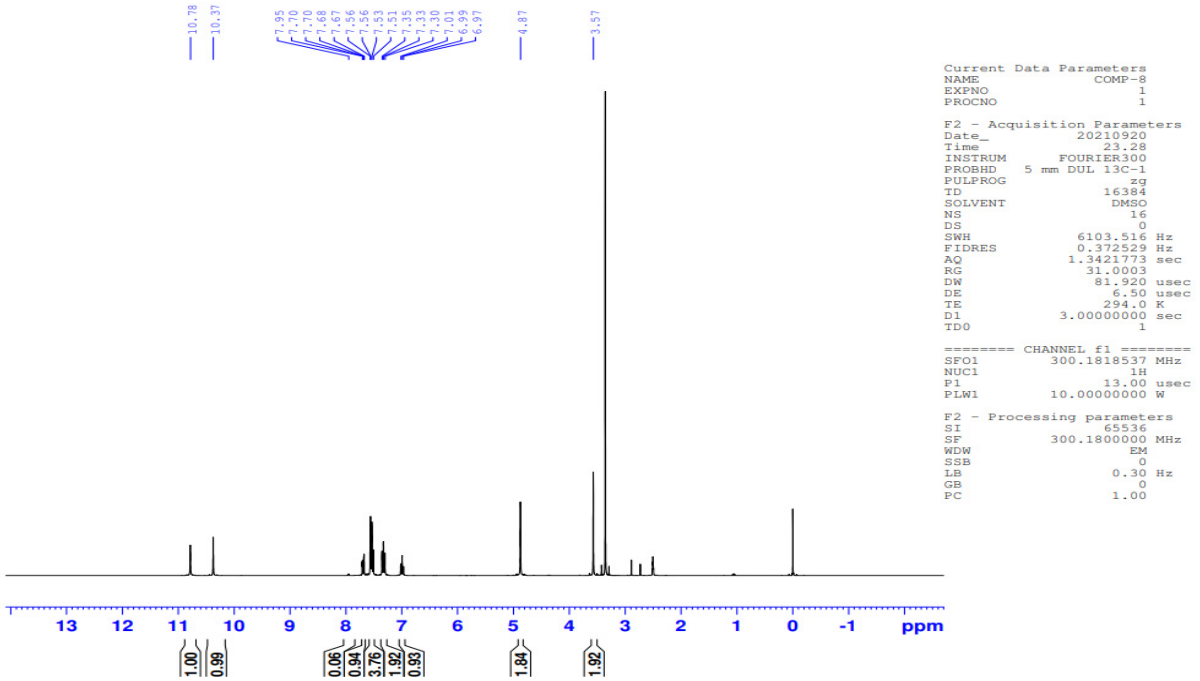


Figure S18. ^{1}HNMR 3h:

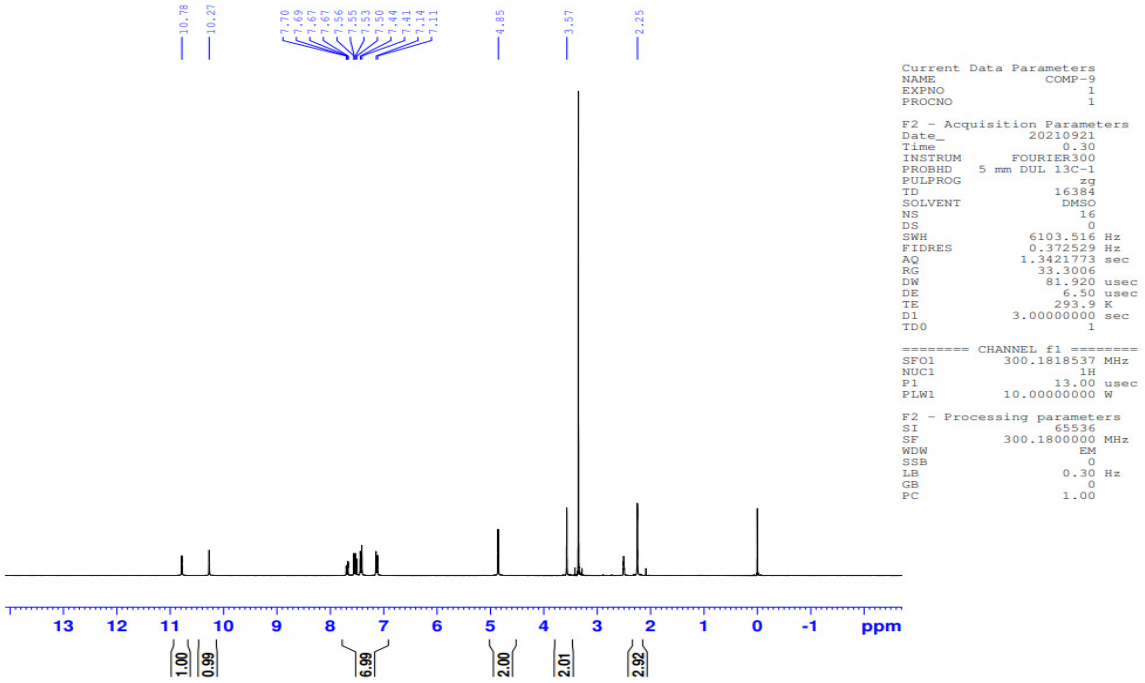


Figure S19. ^{1}HNMR 3i:

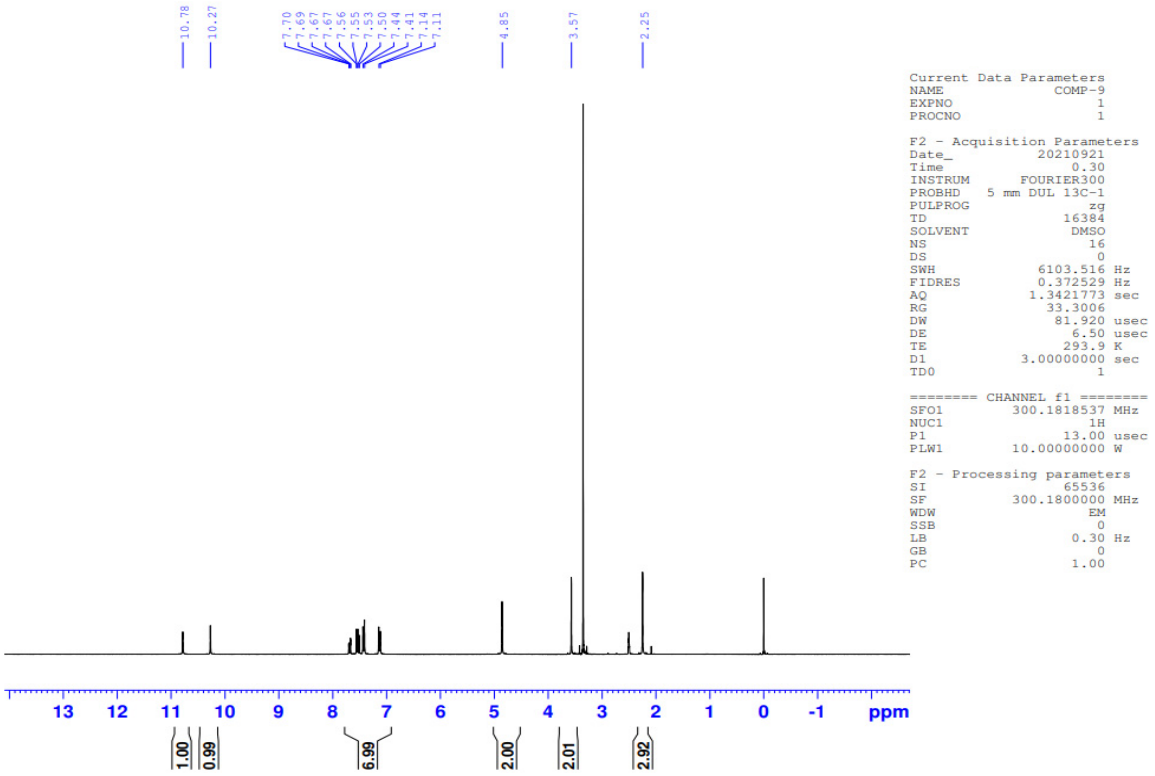


Figure S20. ^{1}HNMR 3j:

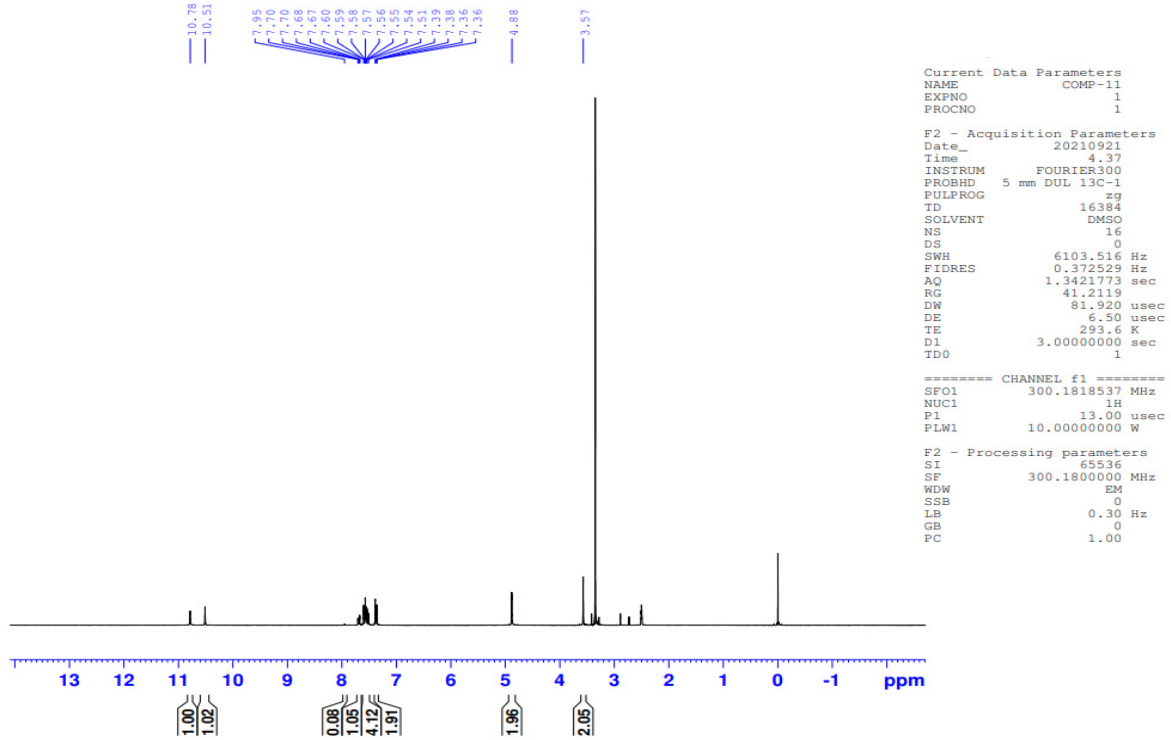


Figure S21. ^{13}CNMR-3a:

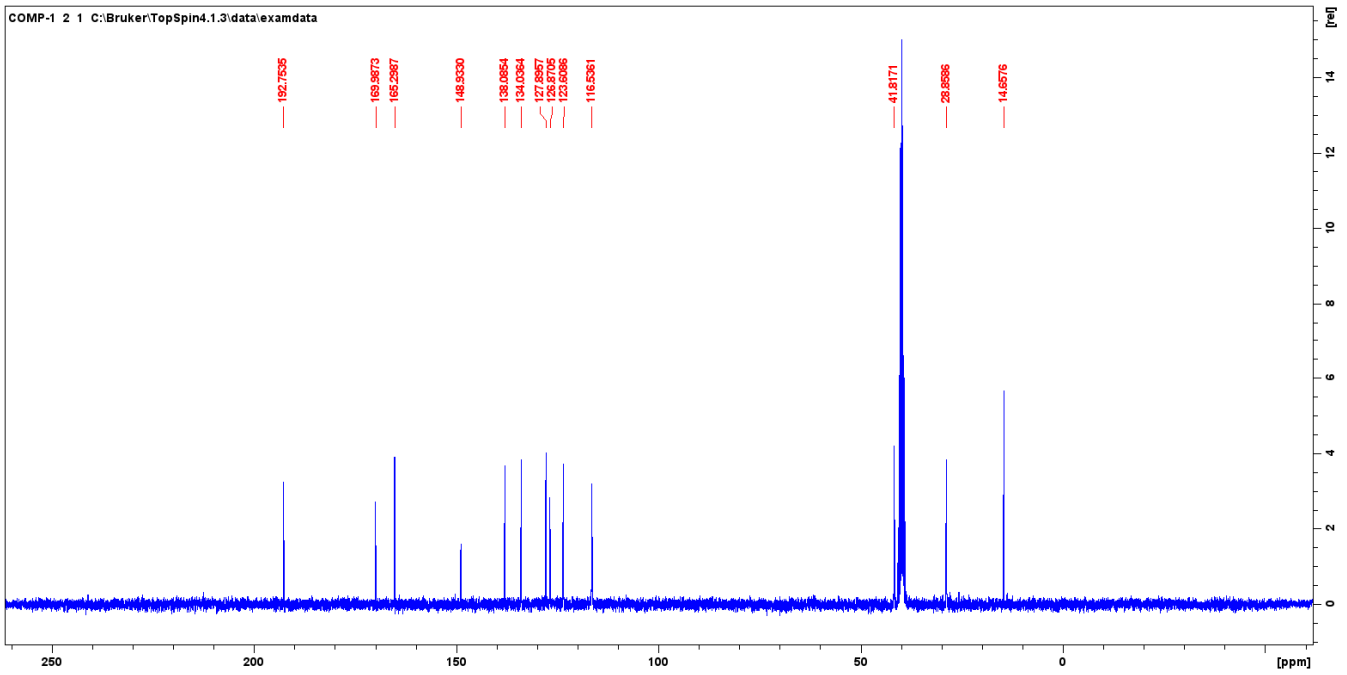


Figure S22. ^{13}CNMR-3b:

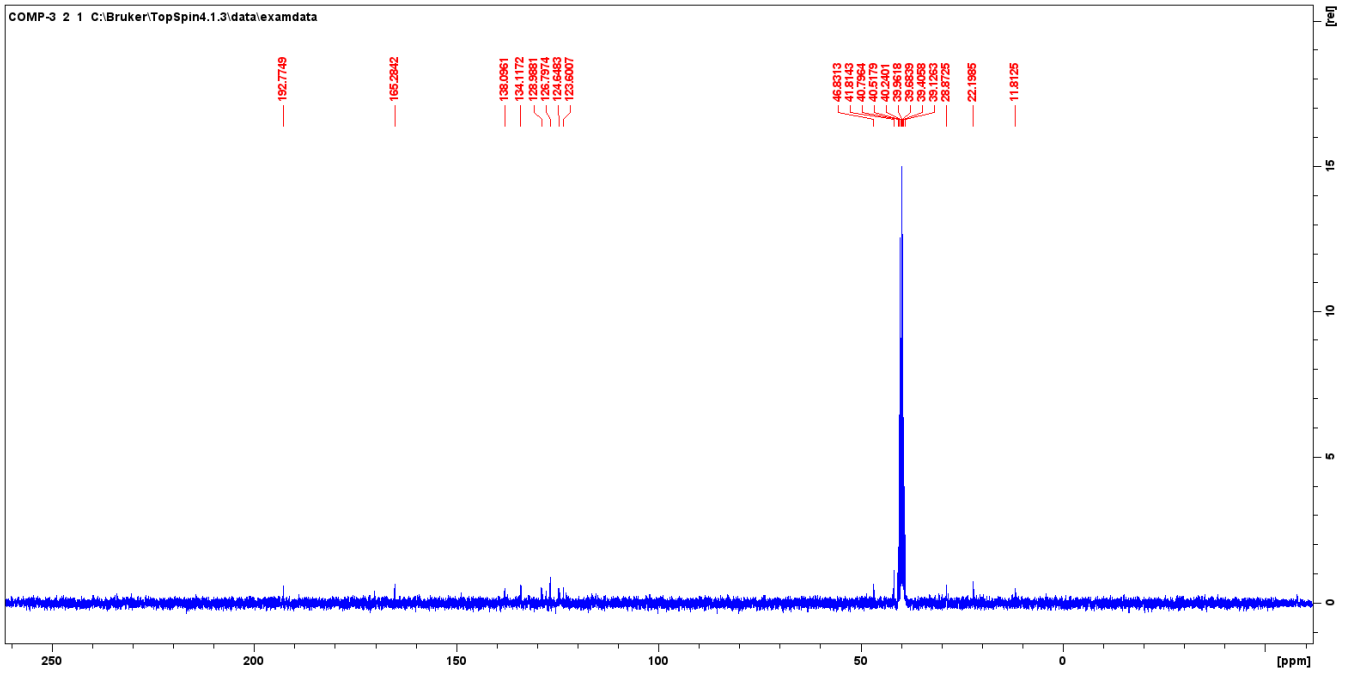


Figure S23. ^{13}CNMR-3c:

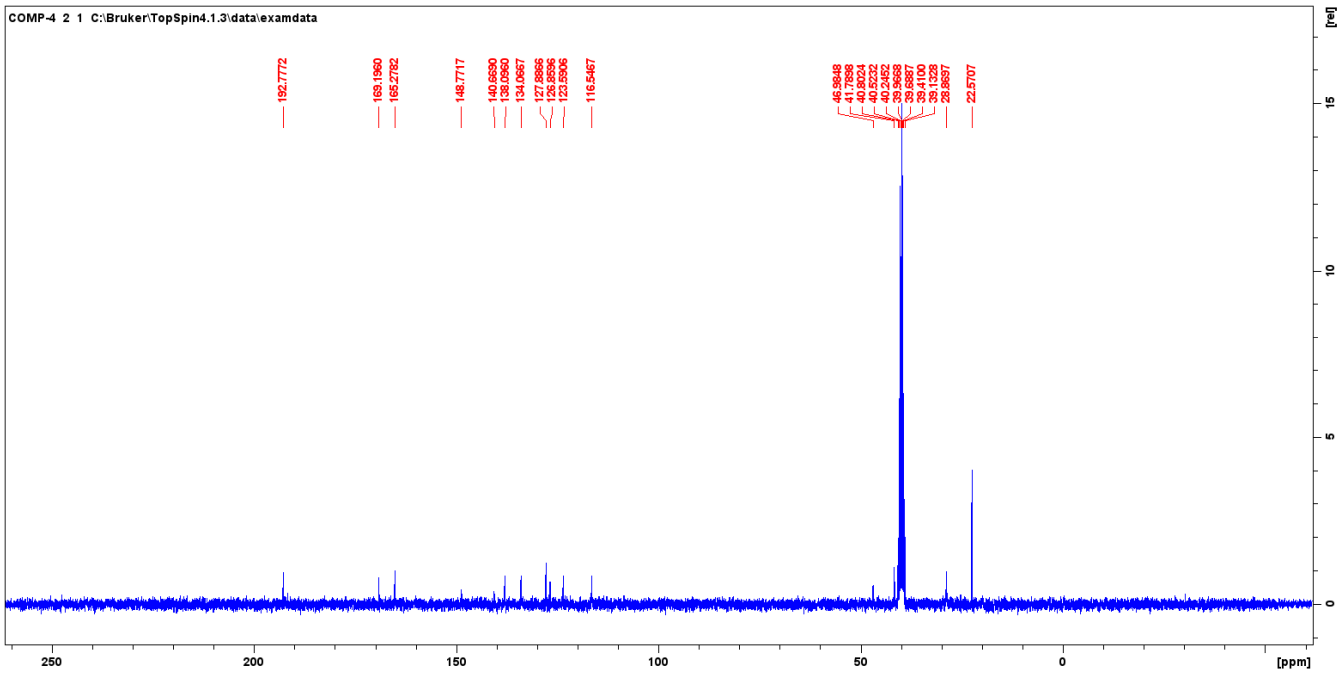


Figure S24. ^{13}CNMR-3e:

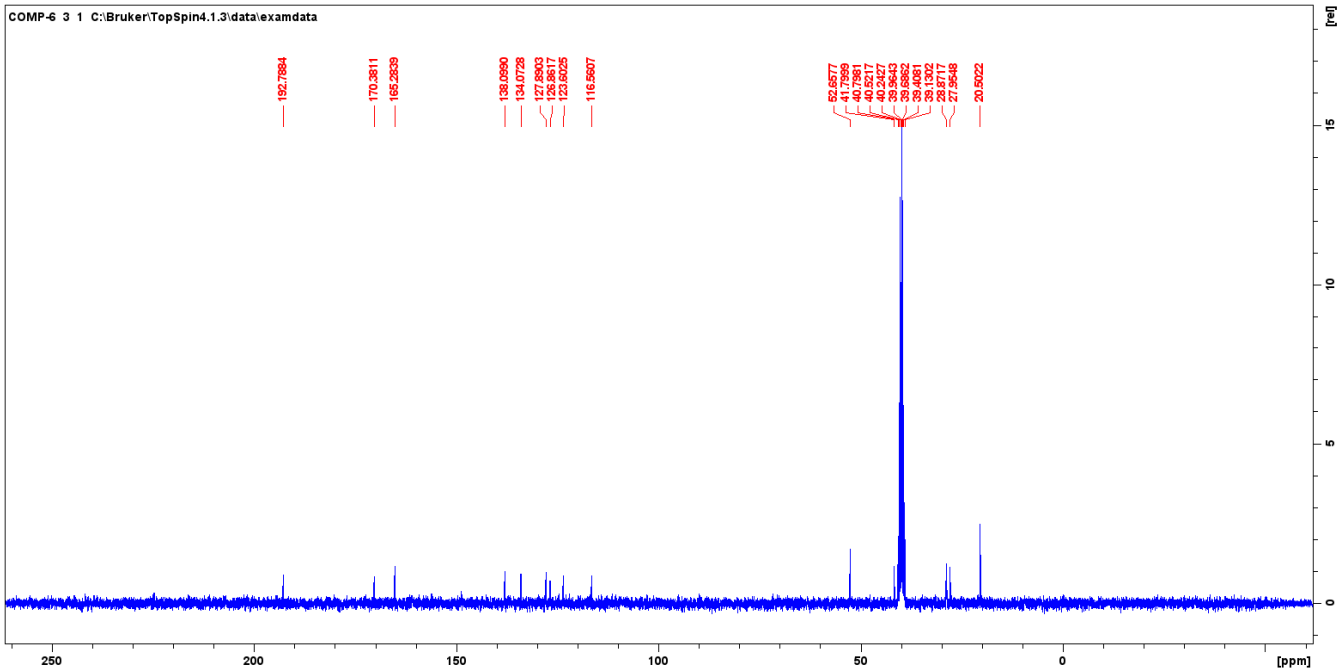


Figure S25. ^{13}CNMR-3f:

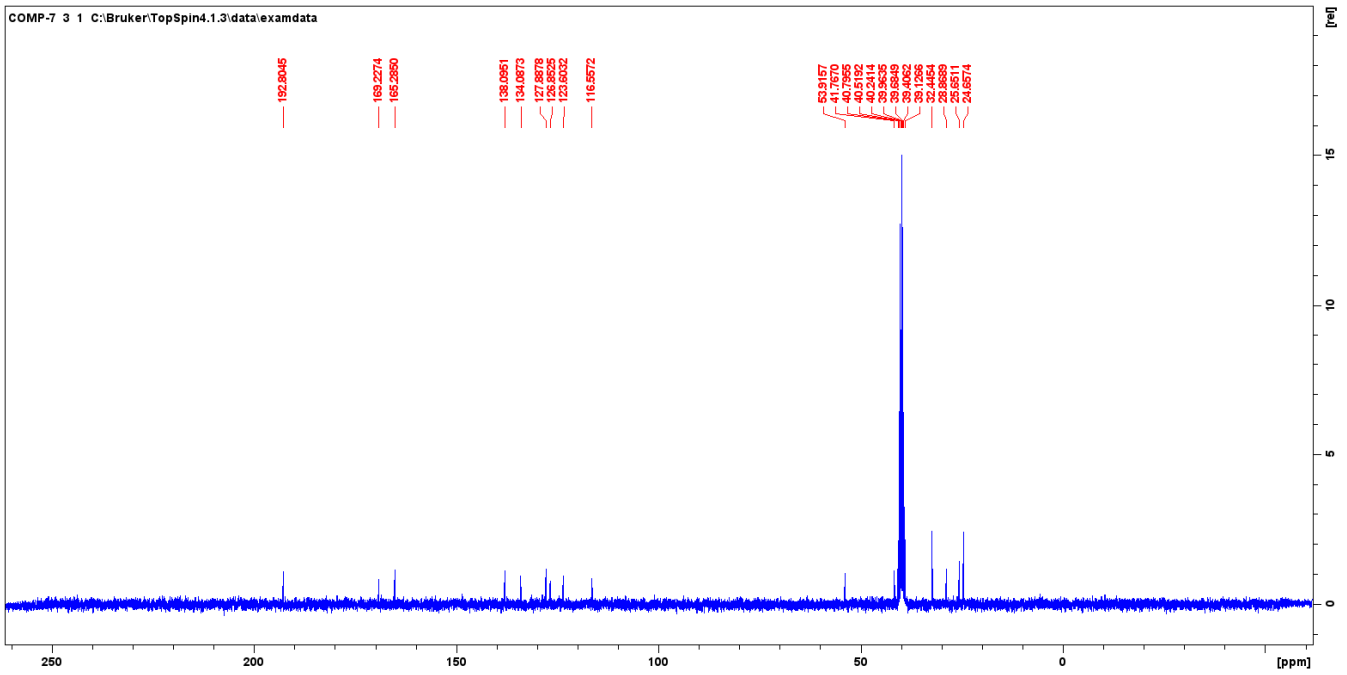


Figure S26. ^{13}CNMR-3g:

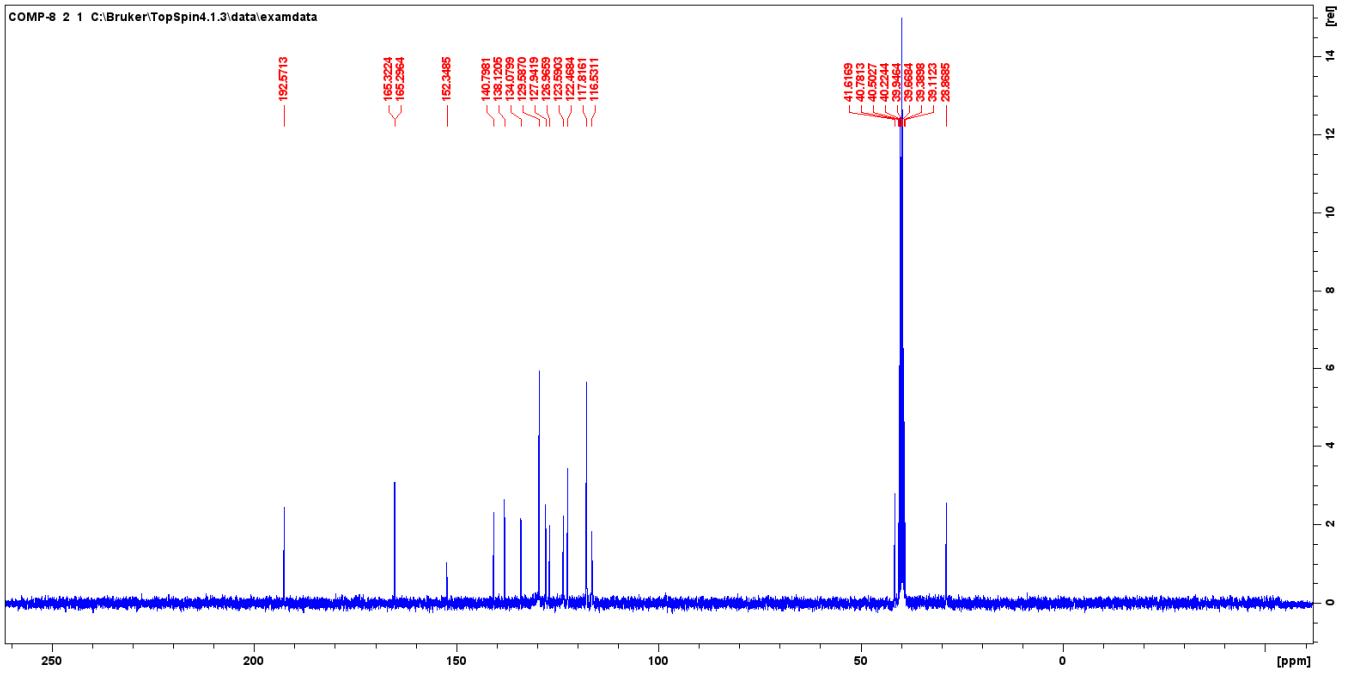


Figure S27. ^{13}CNMR-3h:

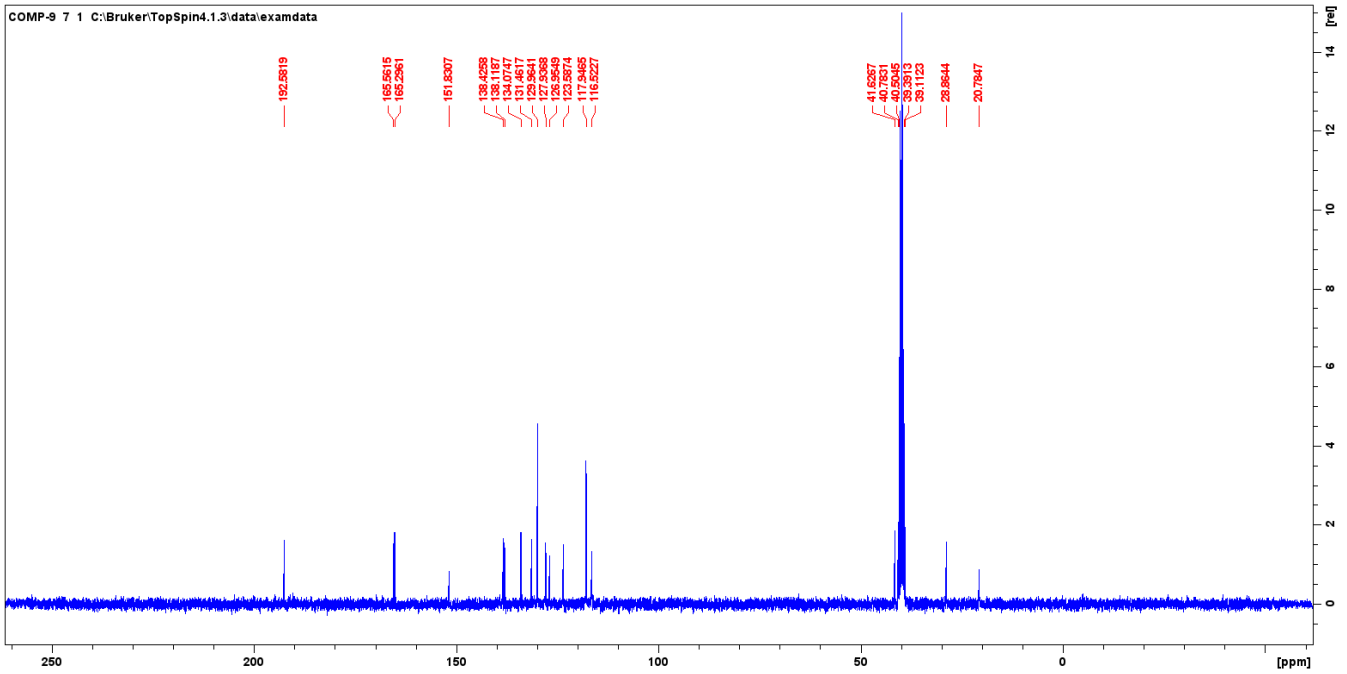


Figure S28. ^{13}CNMR-3i:

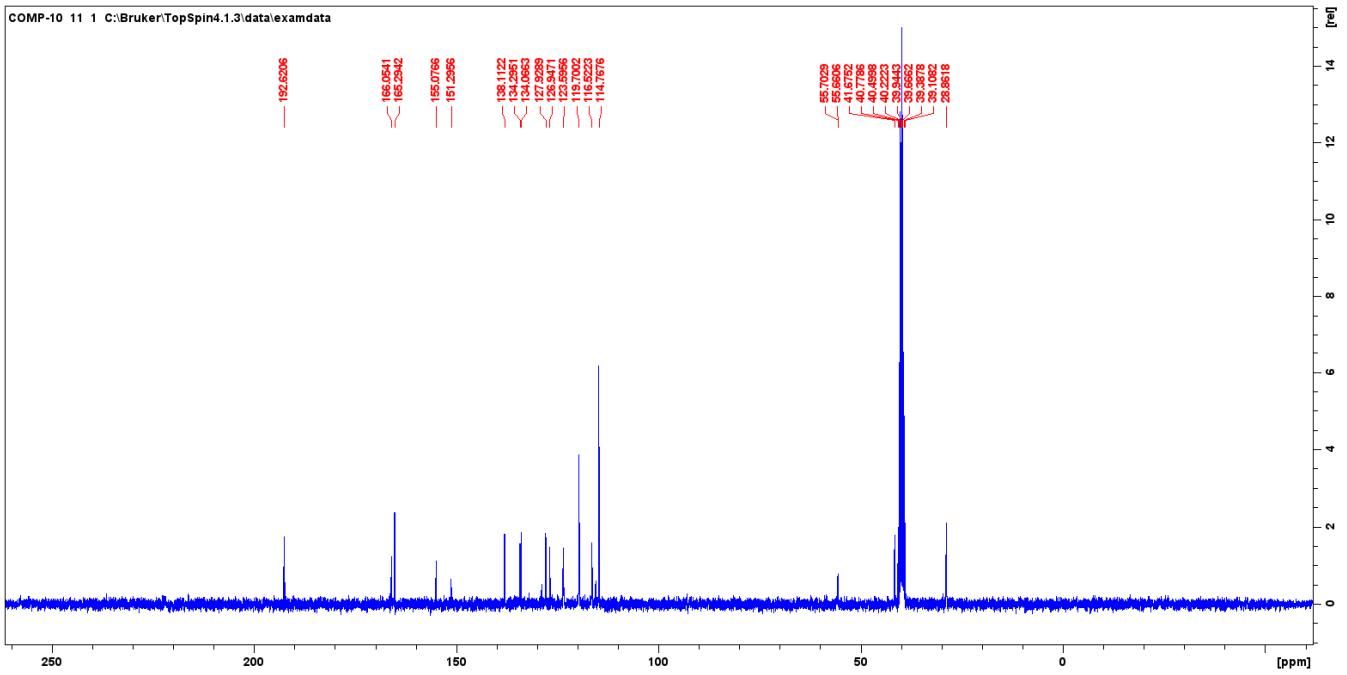


Figure S29. ^{13}CNMR-3j

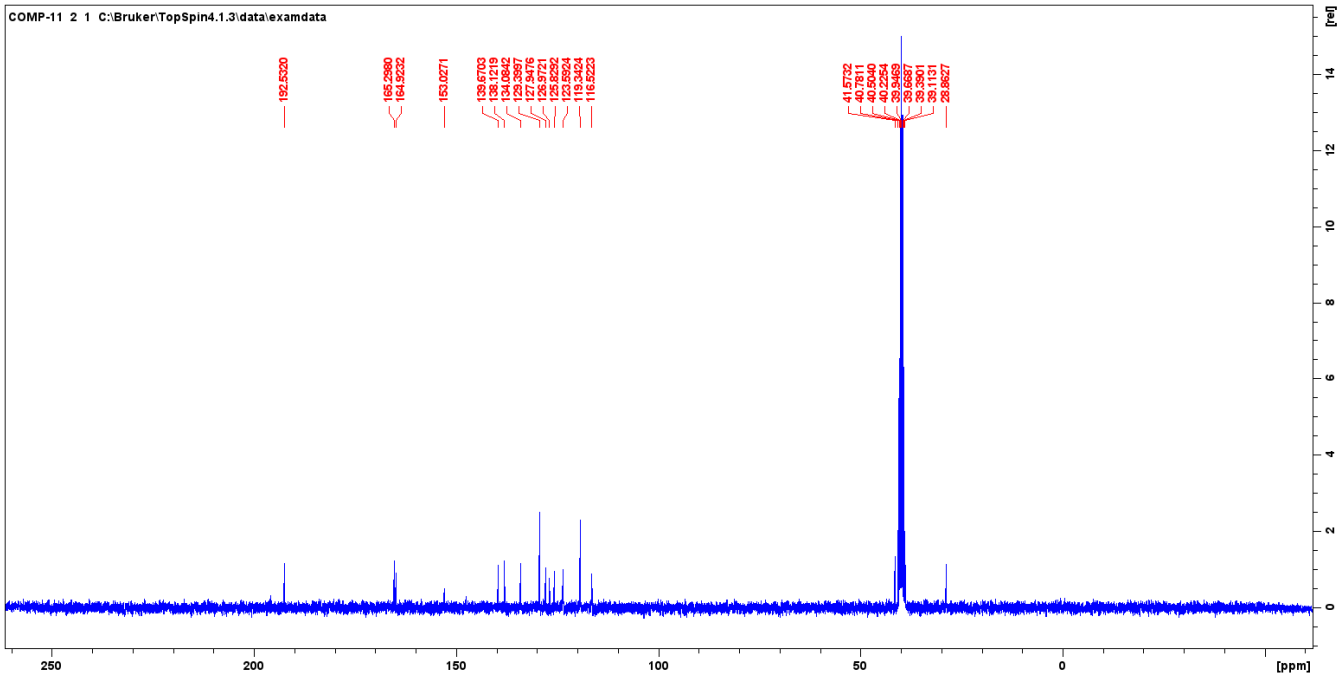


Figure S30. IR spectrum of 3a:

DOPNALAB

Item	Value
Acquired Date&Time	11.03.2022 15:25:51
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\sazan\comp-1.1.ispd
Spectrum name	comp-1.1
Sample name	comp-1
Sample ID	
Option	
Comment	
No. of Scans	15
Resolution	4 [cm-1]
Apodization	Happ-Genzel

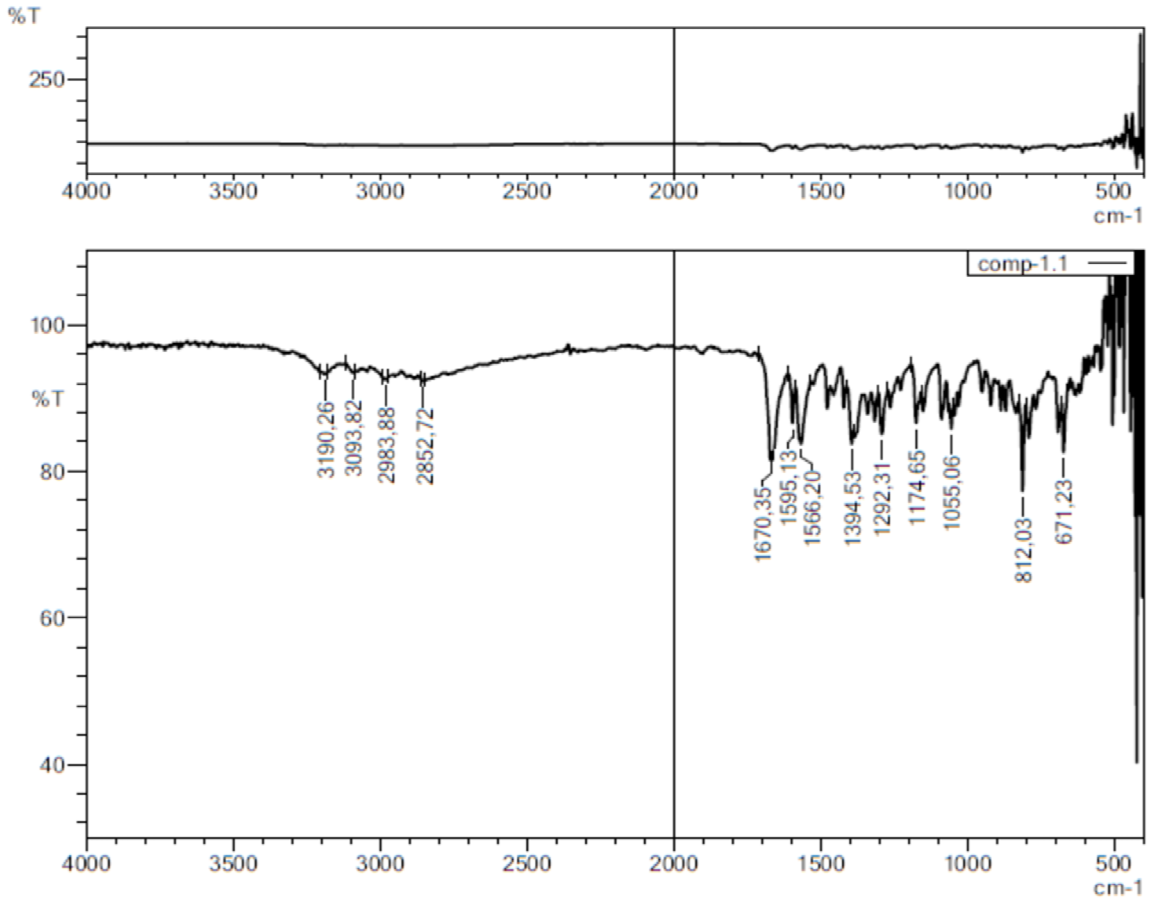


Figure S31. IR spectrum of 3b:

DOPNALAB

	Item	Value
	Acquired Date&Time	11.03.2022 15:36:20
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\sazan\3b.1.ispd
	Spectrum name	3b.1
	Sample name	3b
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

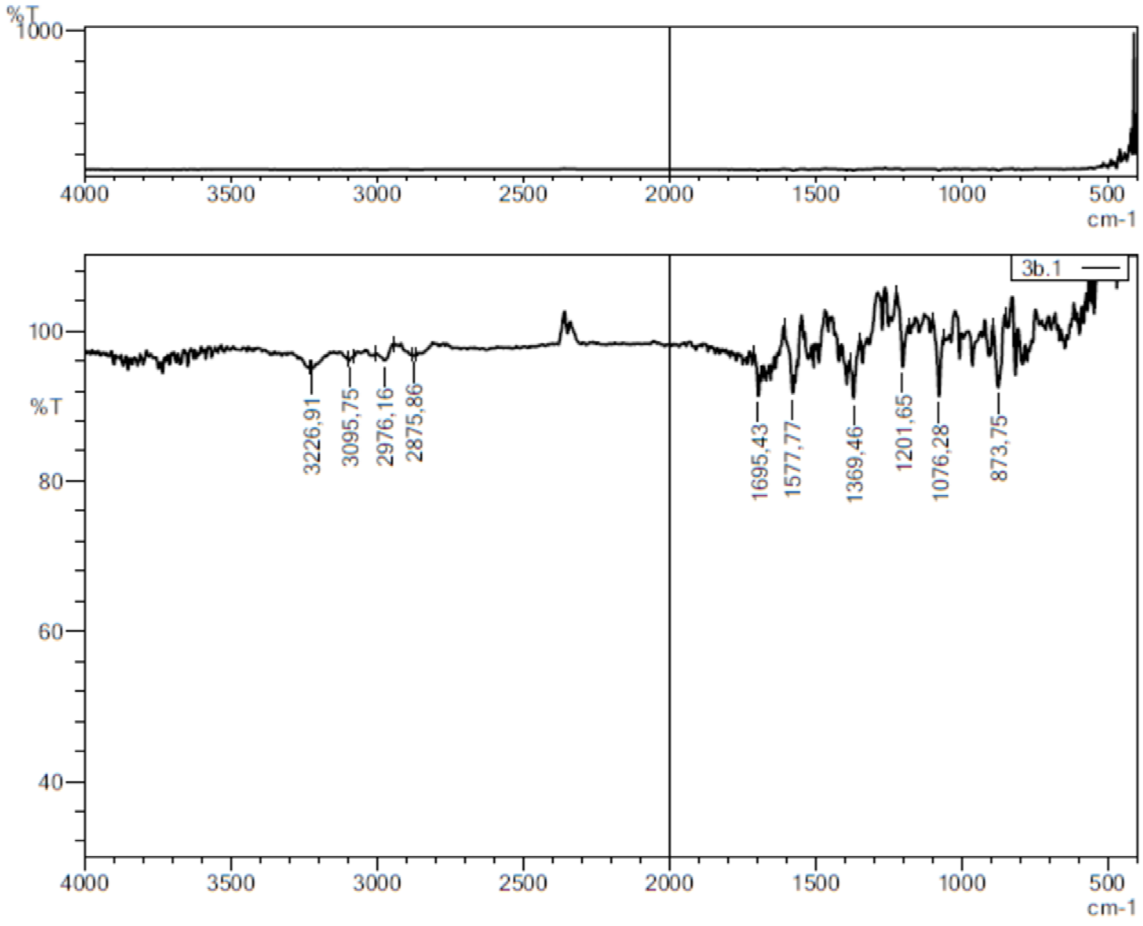


Figure S32. IR spectrum of 3c:

DOPNALAB

Item	Value
Acquired Date&Time	11.03.2022 15:45:04
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\sazan\3c.1.ispd
Spectrum name	3c.1
Sample name	3c
Sample ID	
Option	
Comment	
No. of Scans	15
Resolution	4 [cm-1]
Apodization	Happ-Genzel

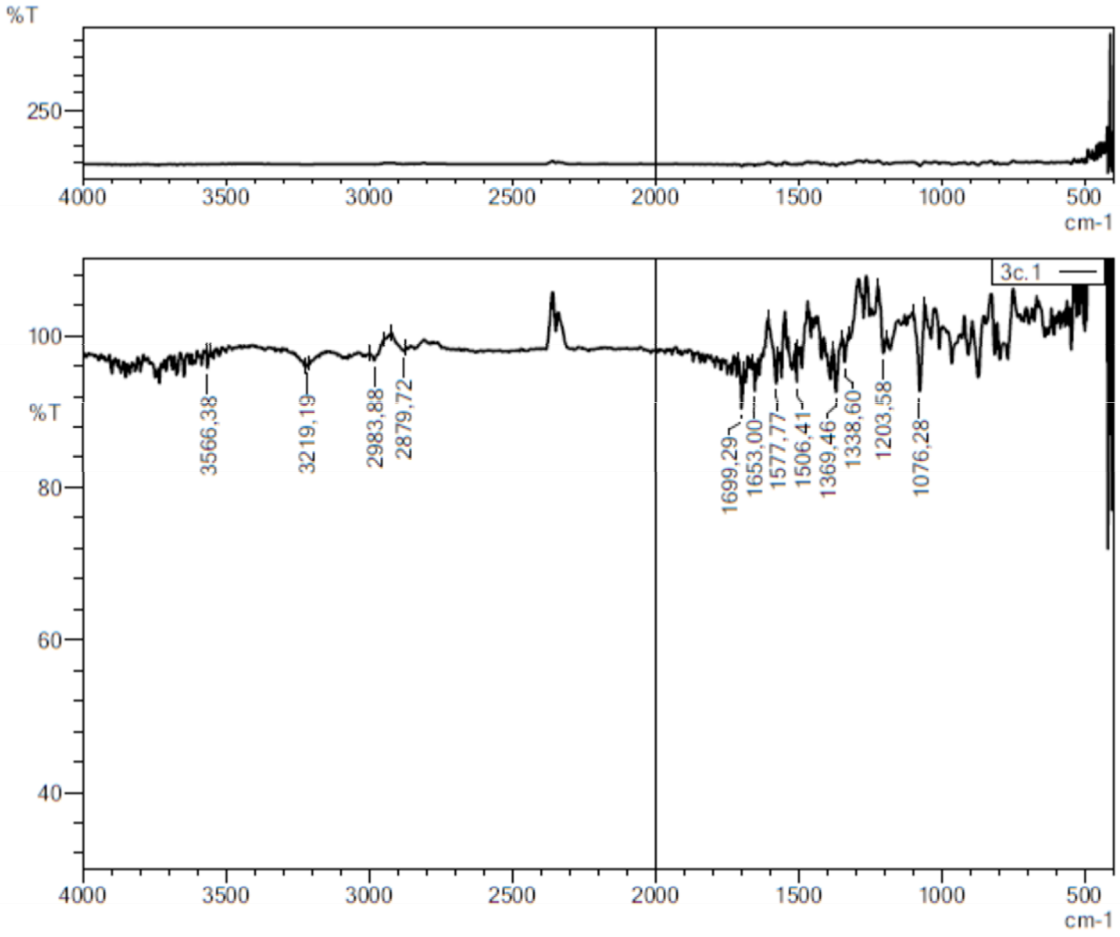


Figure S33. IR spectrum of 3d:

DOPNALAB

Item	Value
Acquired Date&Time	11.03.2022 15:55:10
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\sazan\3d.1.ispd
Spectrum name	3d.1
Sample name	3d
Sample ID	
Option	
Comment	
No. of Scans	15
Resolution	4 [cm-1]
Apodization	Happ-Genzel

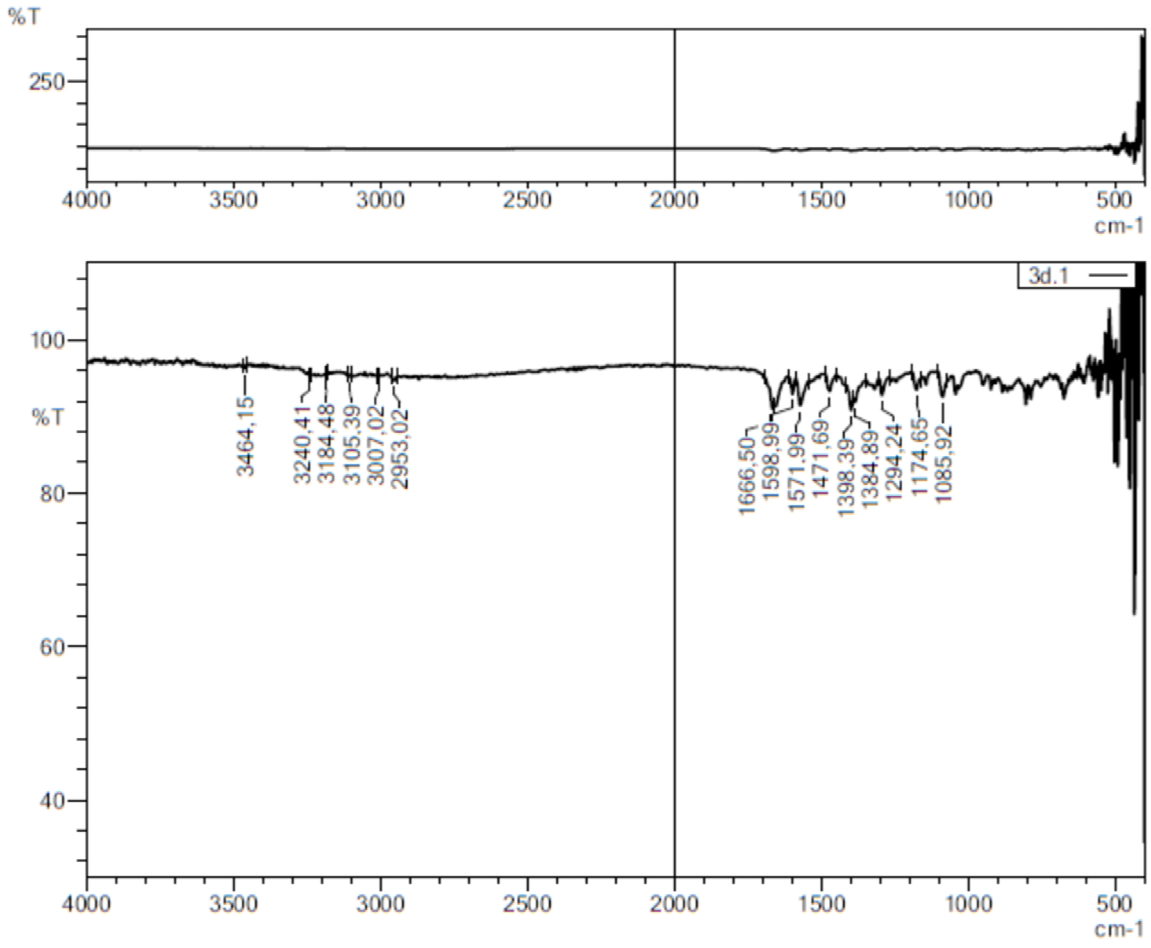


Figure S34. IR spectrum of 3e:

DOPNALAB

	Item	Value
	Acquired Date&Time	11.03.2022 16:02:59
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\sazan\3e.1.ispd
	Spectrum name	3e.1
	Sample name	3e
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

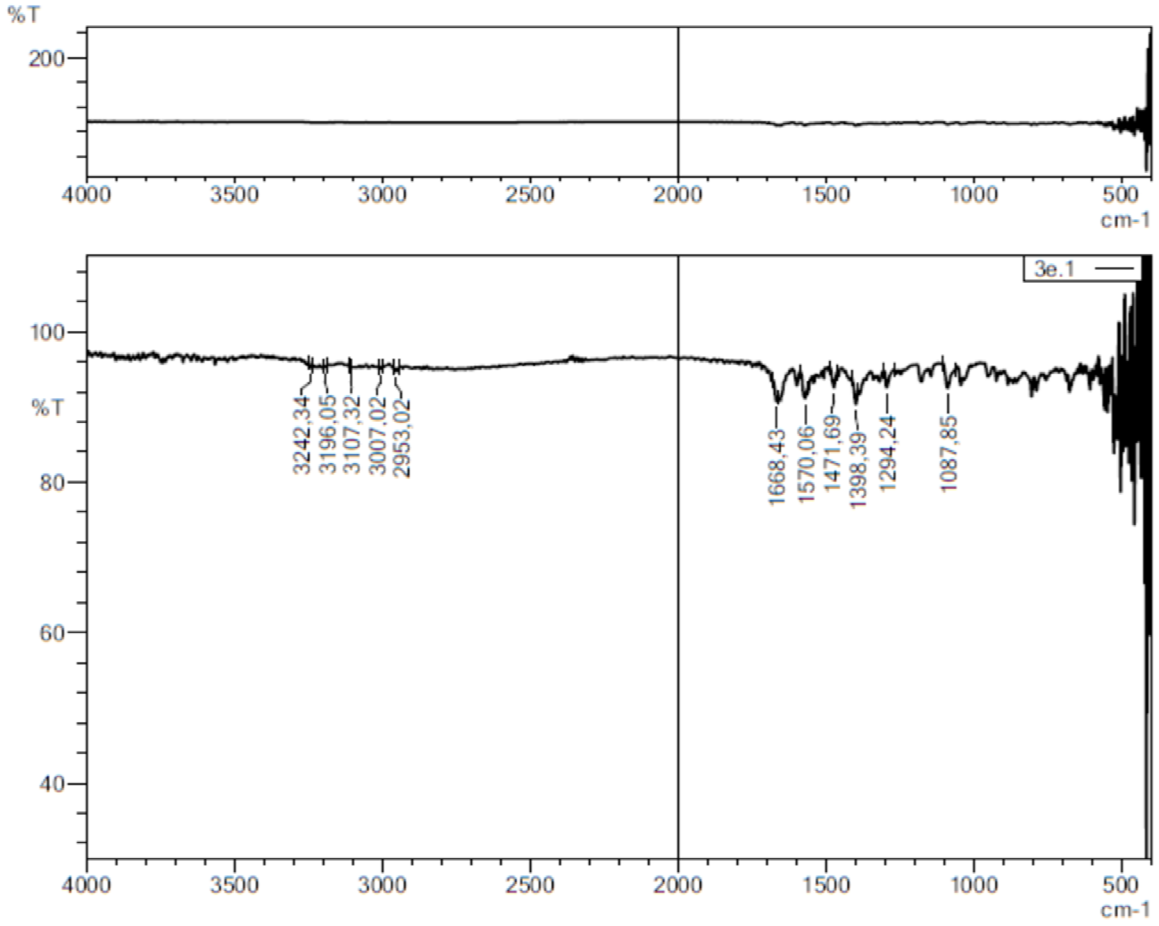


Figure S35. IR spectrum of 3f:

DOPNALAB

Item	Value
Acquired Date&Time	11.03.2022 16:10:03
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\sazan\3f.1.ispd
Spectrum name	3f.1
Sample name	3f
Sample ID	
Option	
Comment	
No. of Scans	15
Resolution	4 [cm-1]
Apodization	Happ-Genzel

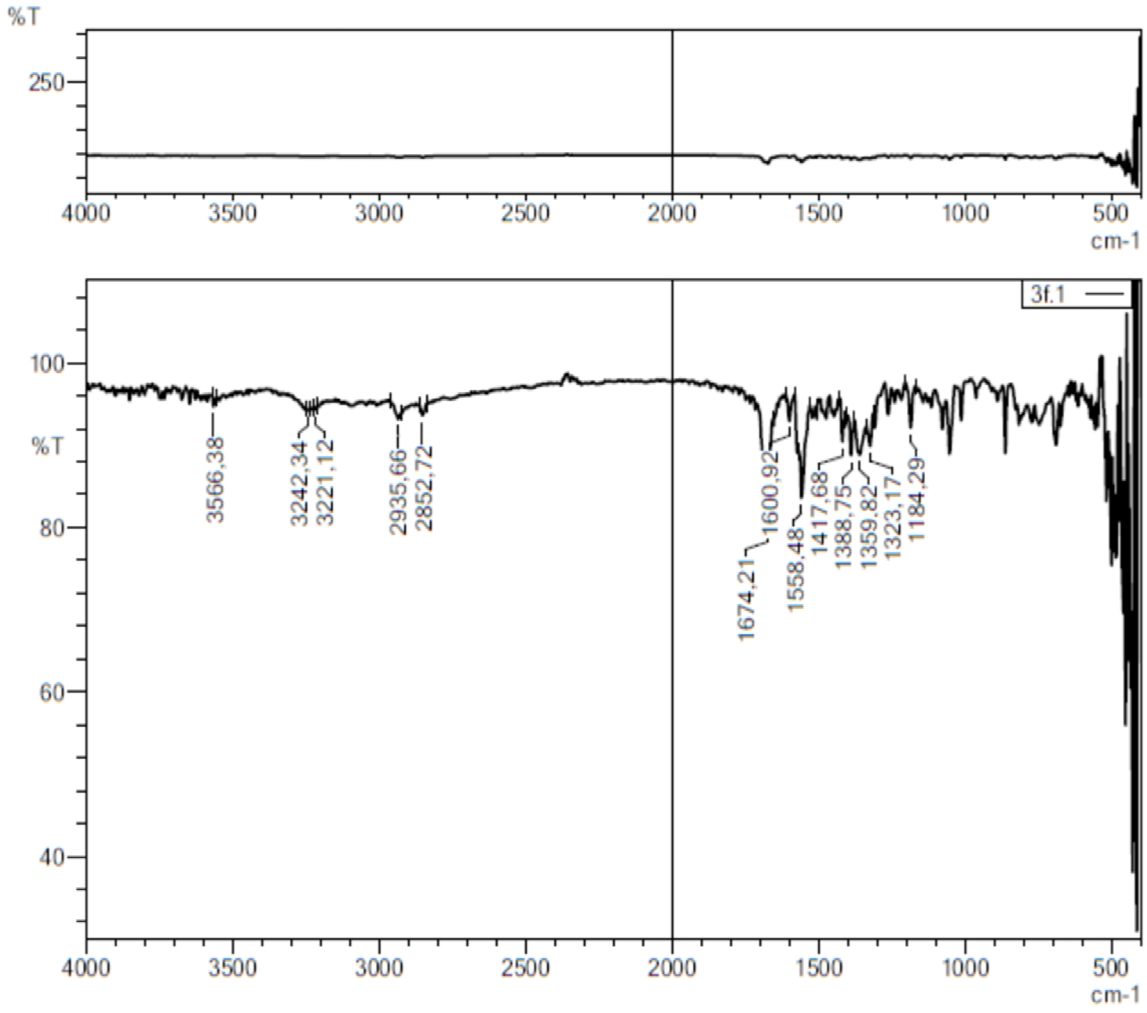


Figure S36. IR spectrum of 3g:

DOPNALAB

	Item	Value
	Acquired Date&Time	11.03.2022 16:20:17
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\sazan\3g.1.ispd
	Spectrum name	3g.1
	Sample name	3g
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

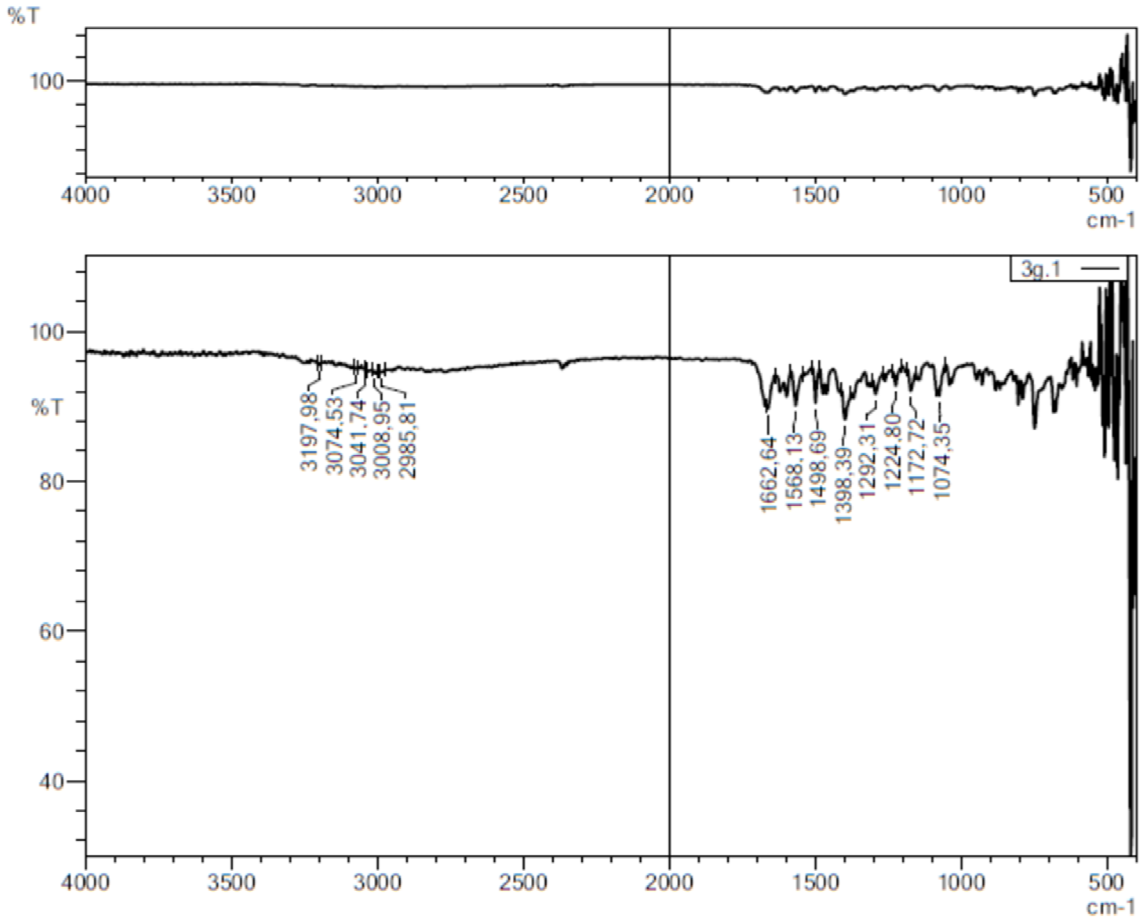


Figure S37. IR spectrum of 3h:

DOPNALAB

	Item	Value
	Acquired Date&Time	11.03.2022 16:28:45
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\sazan\3h.1.ispd
	Spectrum name	3h.1
	Sample name	3h
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

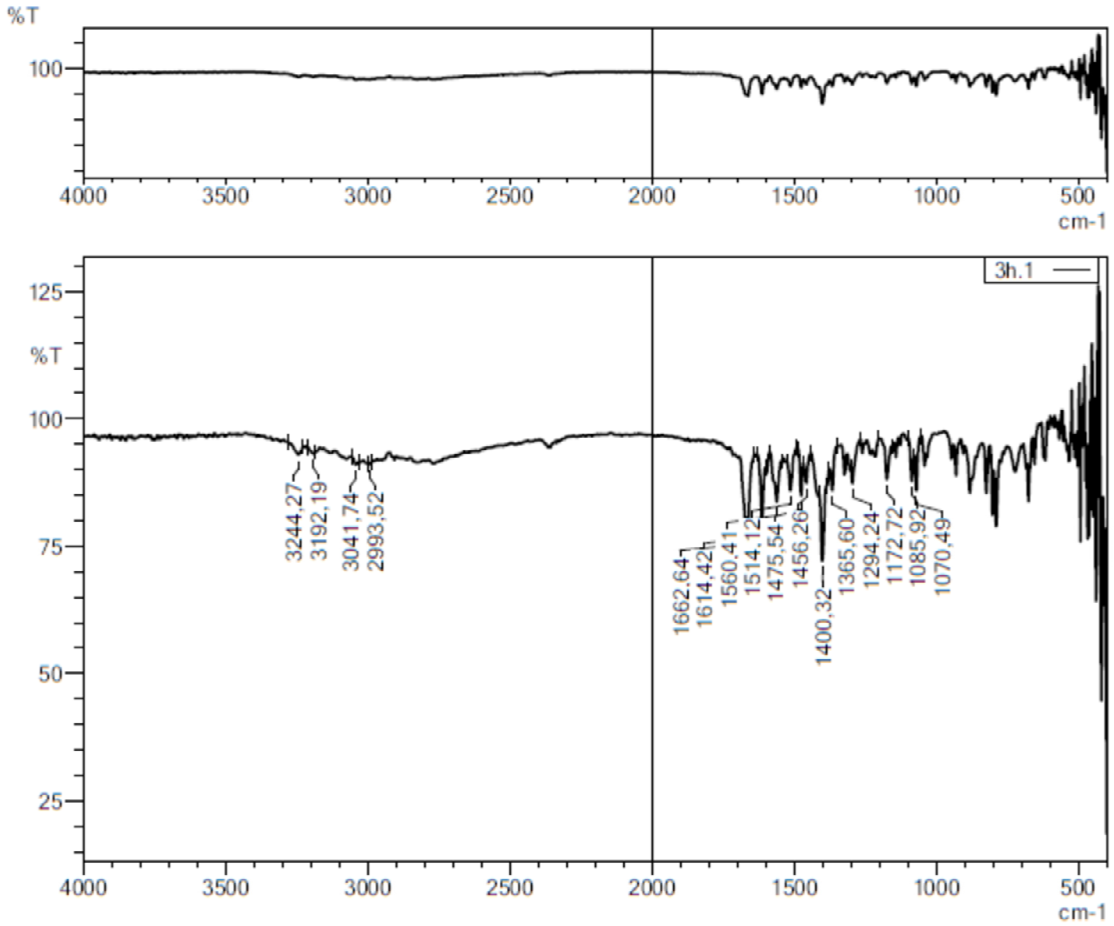


Figure S38. IR spectrum of 3i:

DOPNALAB

Item	Value
Acquired Date&Time	11.03.2022 16:34:51
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\sazan\3i.1.ispd
Spectrum name	3i.1
Sample name	3i
Sample ID	
Option	
Comment	
No. of Scans	15
Resolution	4 [cm-1]
Apodization	Happ-Genzel

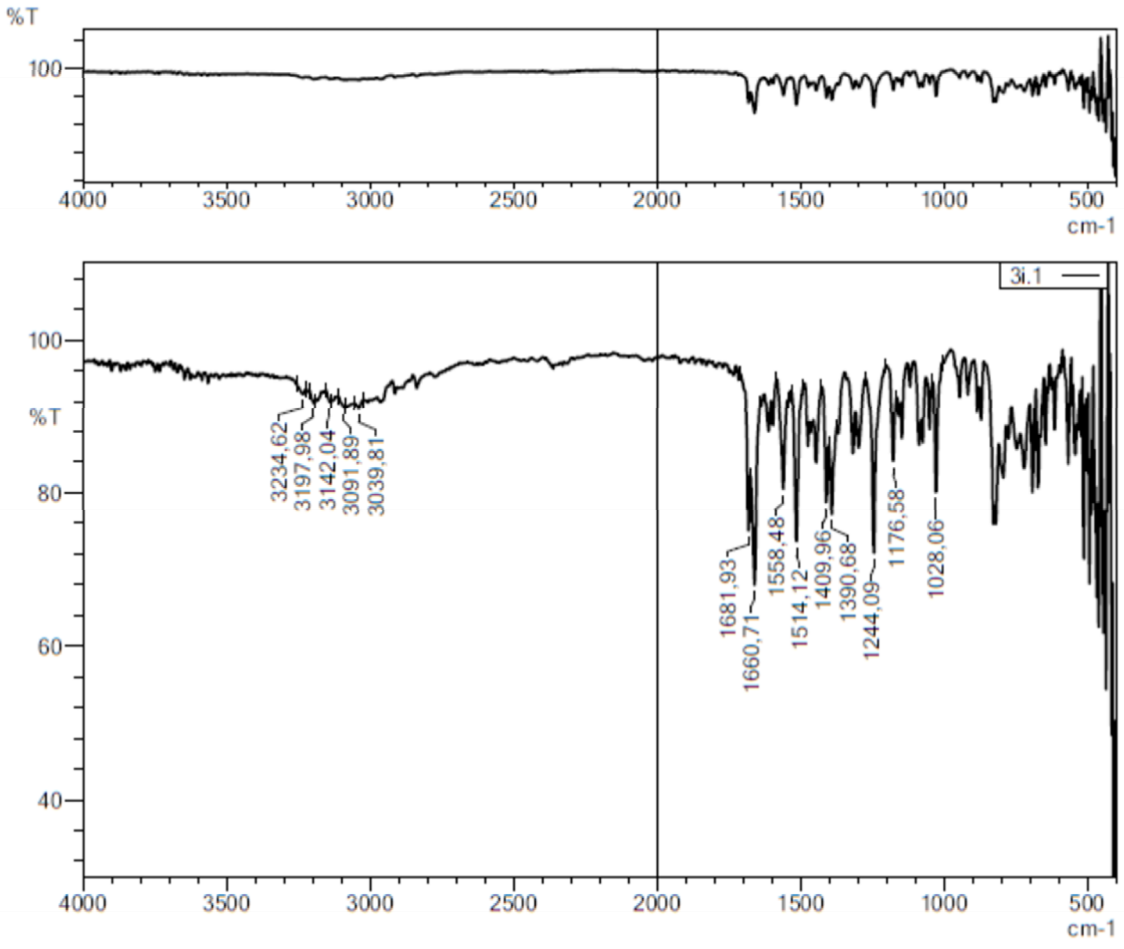


Figure S39. IR spectrum of 3j:

DOPNALAB

Item	Value
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Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\sazan\3j.1.ispd
Spectrum name	3j.1
Sample name	3j
Sample ID	
Option	
Comment	
No. of Scans	15
Resolution	4 [cm-1]
Apodization	Happ-Genzel

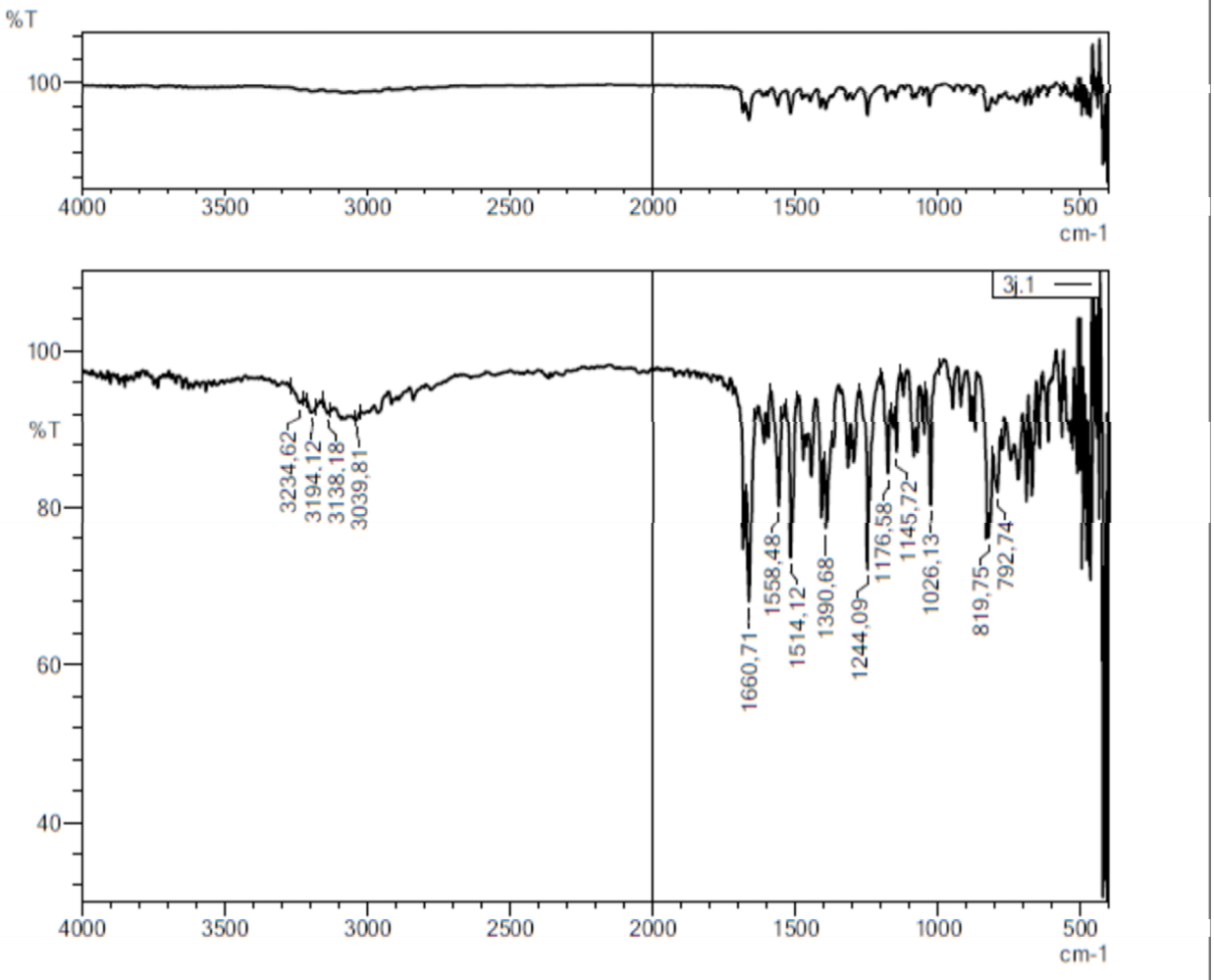


Figure S40. [1]HNMR of 2a:

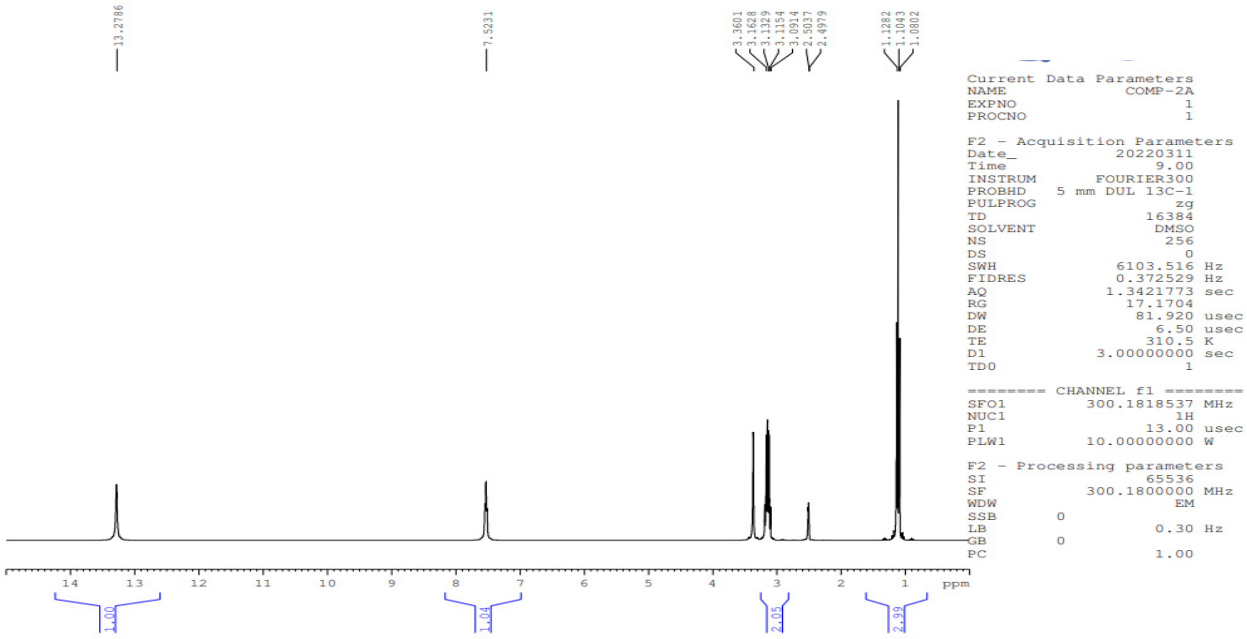


Figure S41. [1]HNMR of 2b:

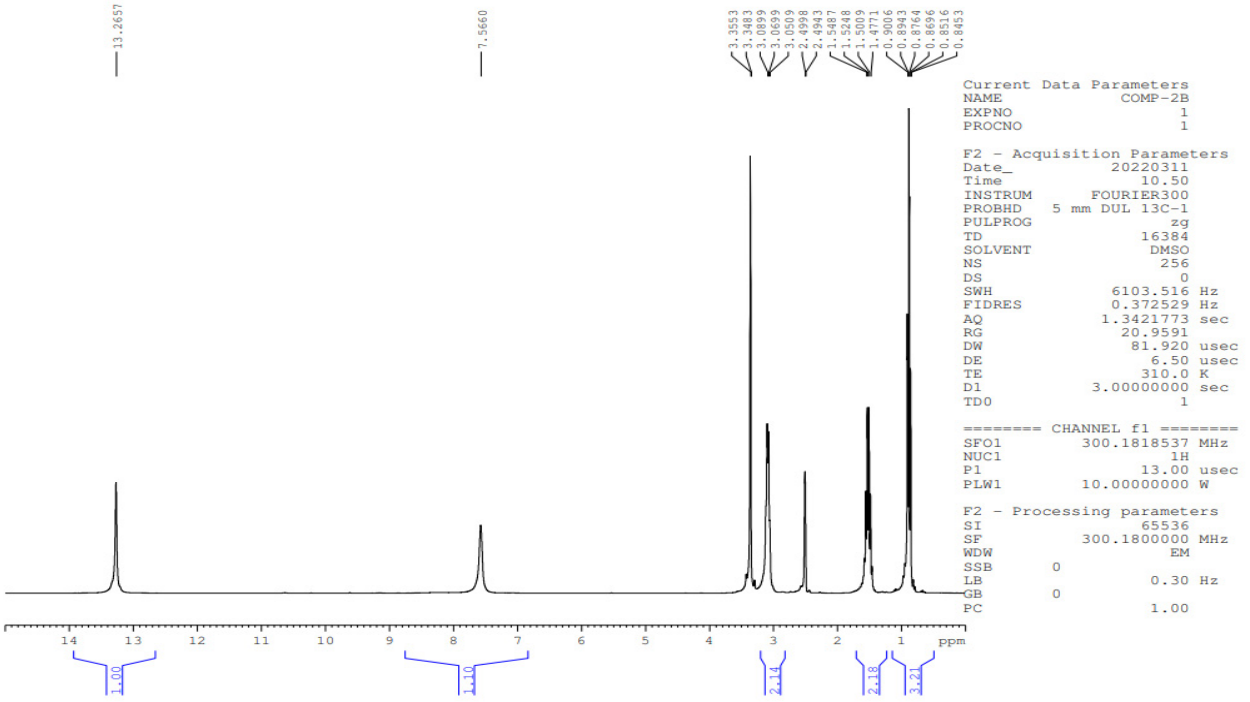


Figure S42. [1]HNMR of 2c:

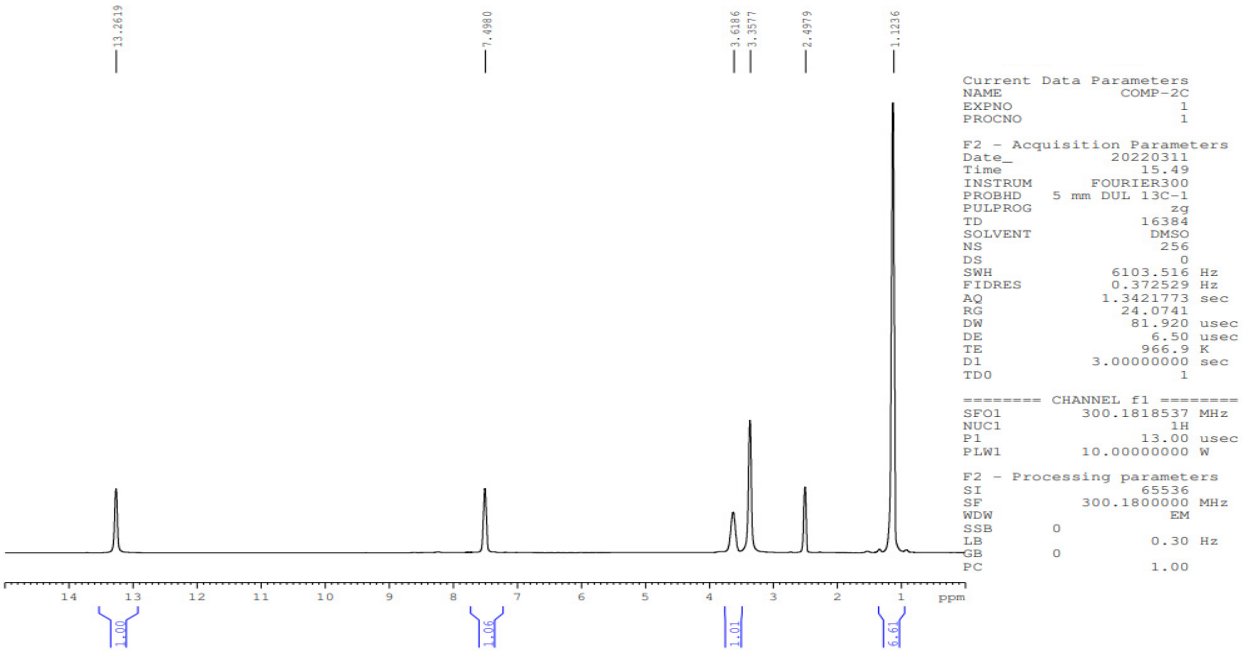


Figure S43. [1]HNMR of 2d:

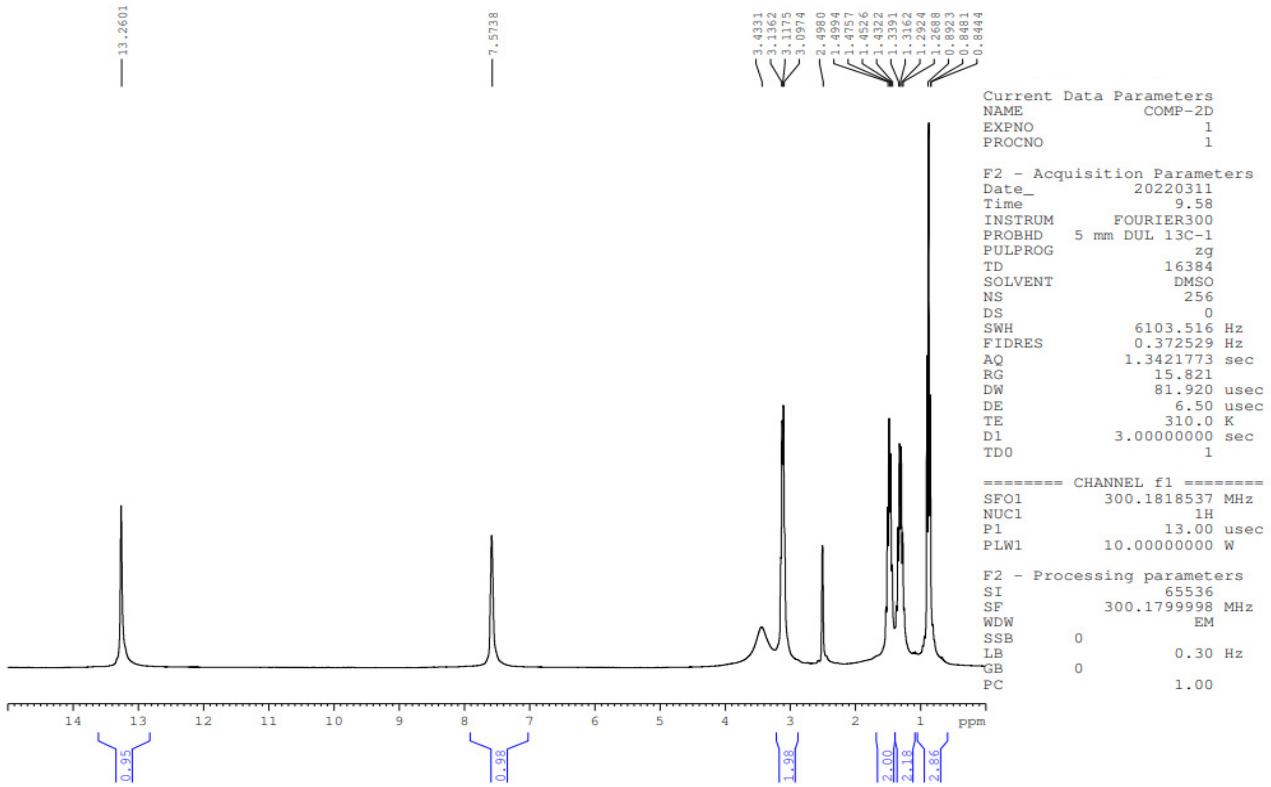


Figure S44. ^{1}HNMR of 2e:

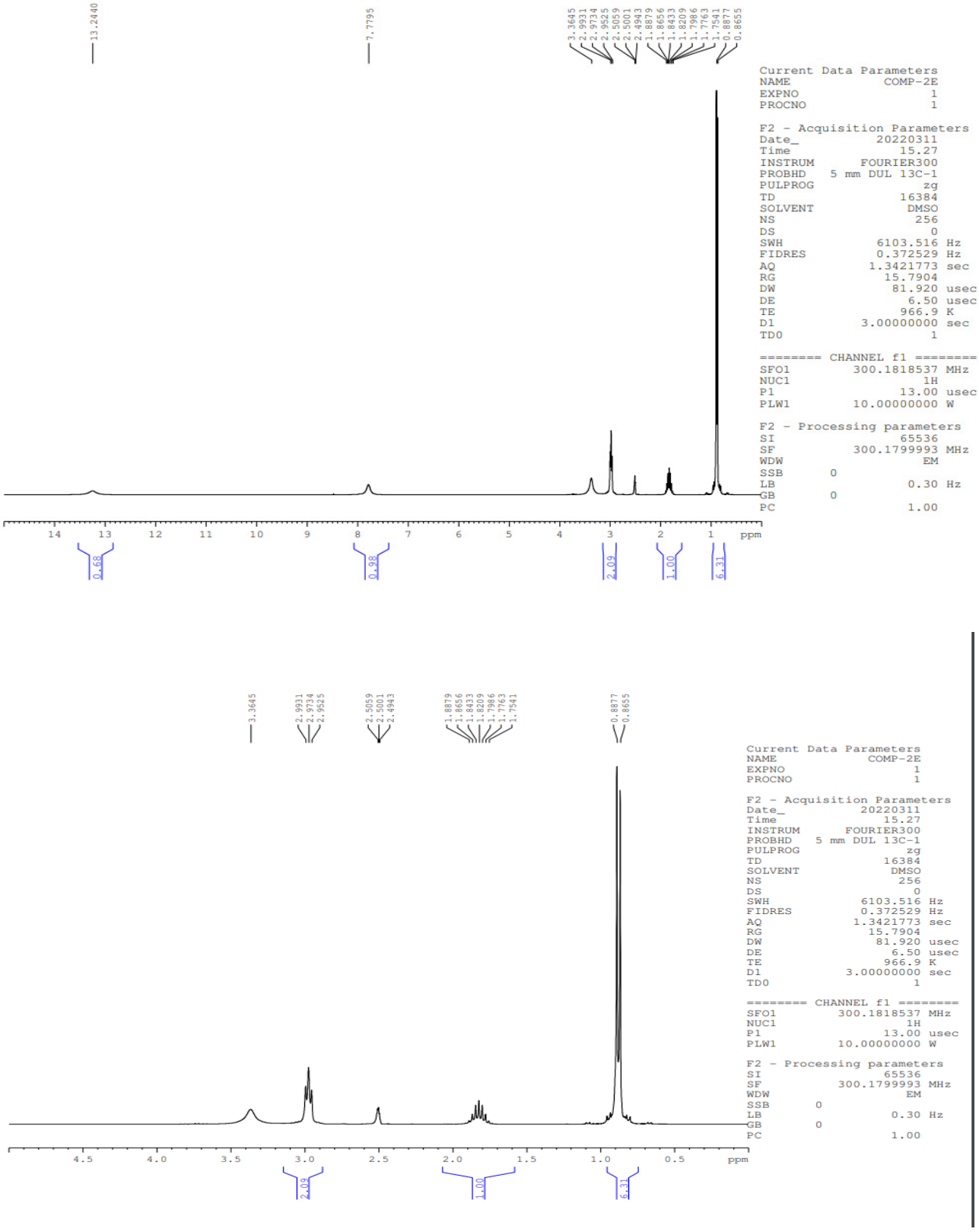


Figure S45. [1]HNMR of 2f:

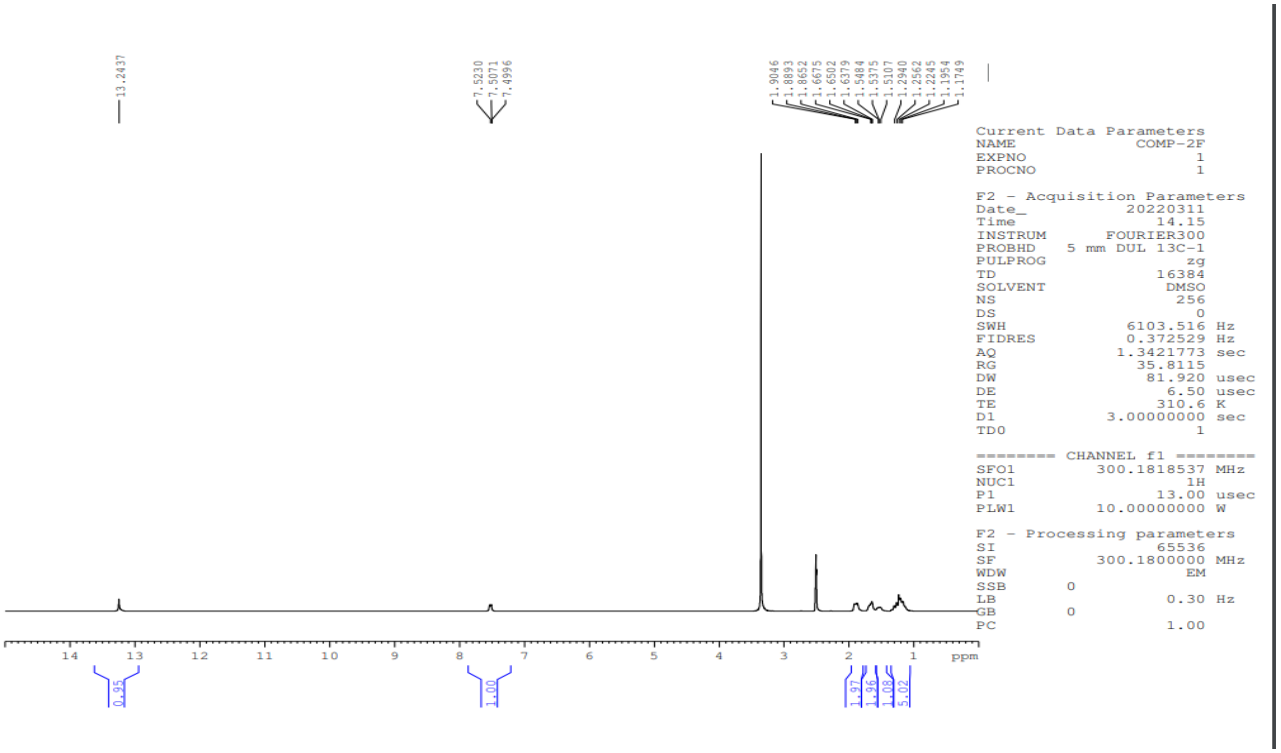


Figure S46. [1]HNMR of 2g:

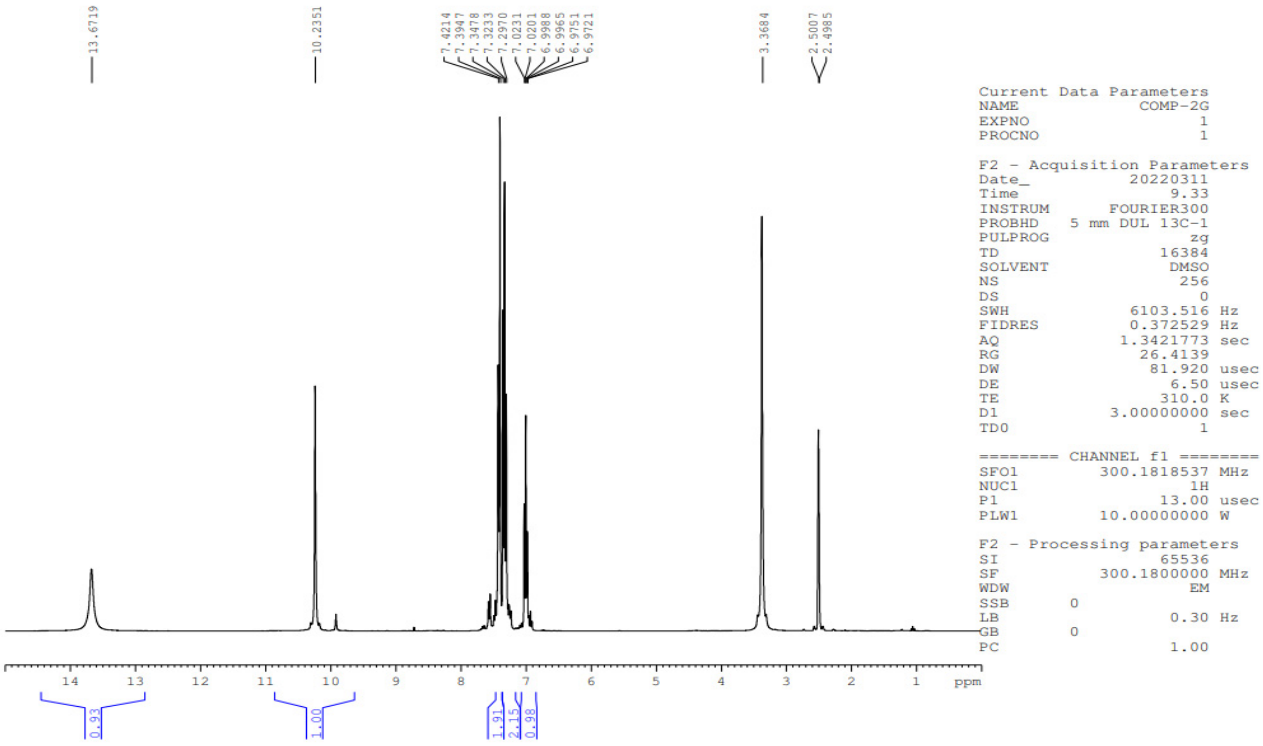


Figure S47. [1]HNMR of 2h:

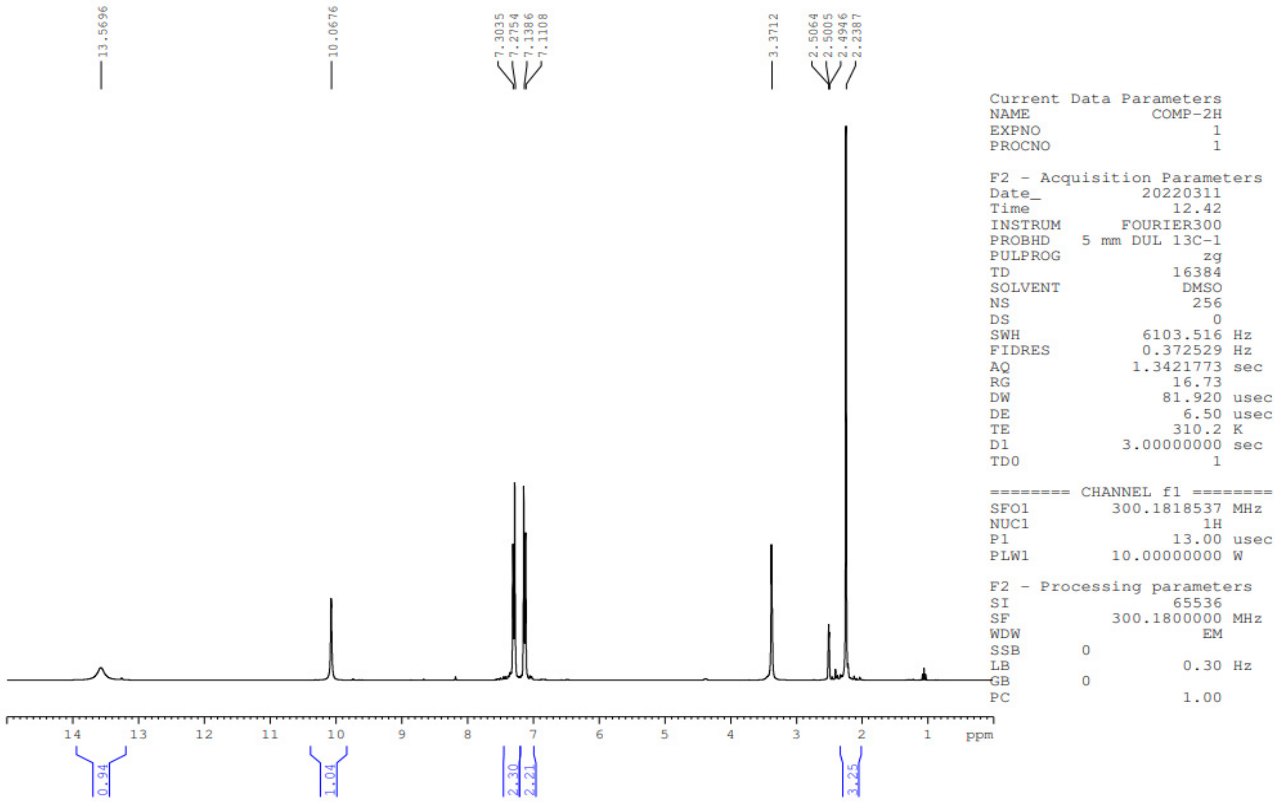


Figure S48. [1]HNMR of 2i:

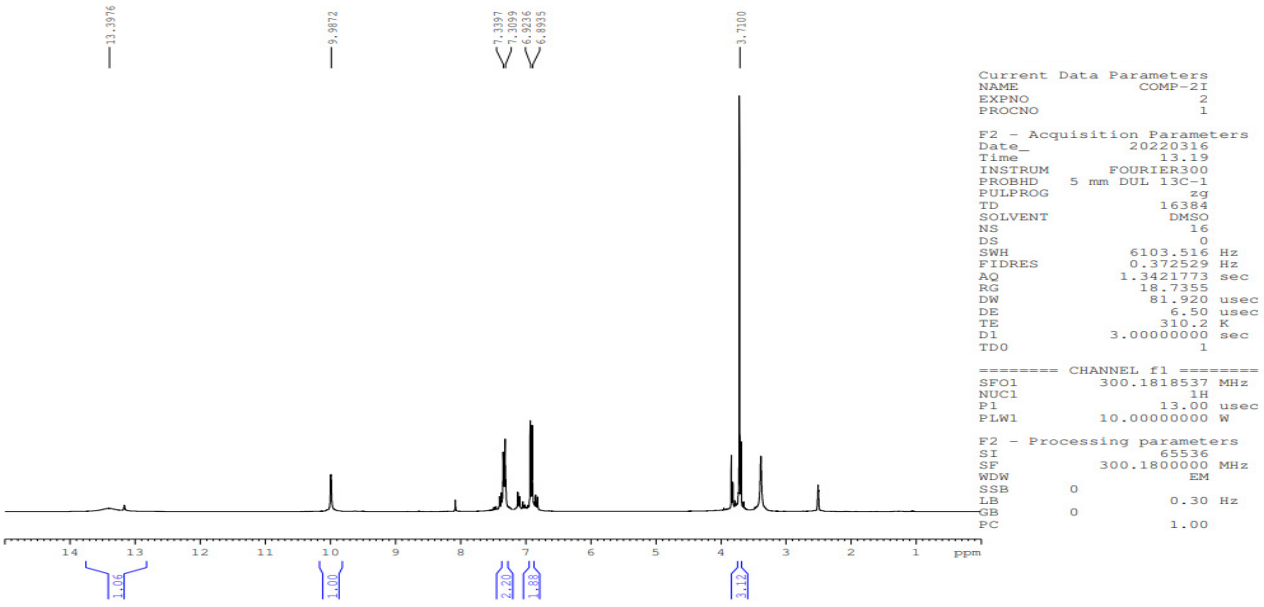


Figure S49. ^{1}HNMR of 2j:

