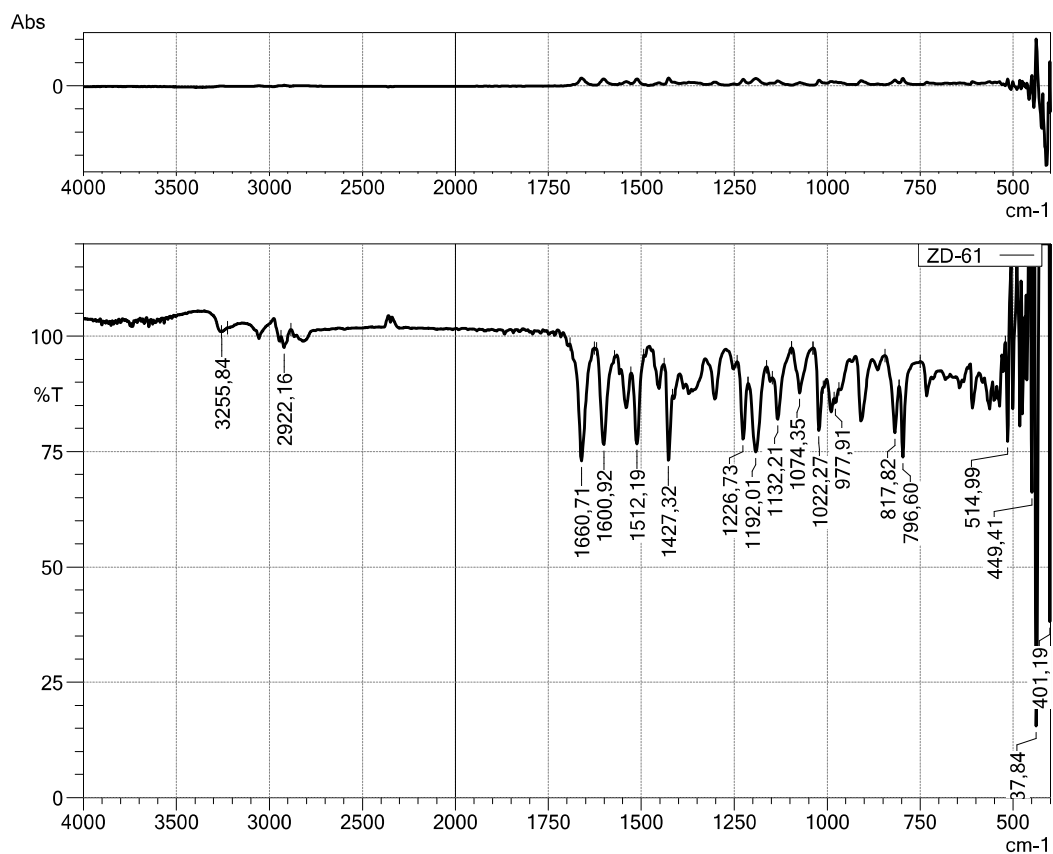


## DOPNALAB

Item	Value
Acquired Date&Time	23.12.2016 15:53:23
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\ZD seri\ZD-61.ispd
Spectrum name	ZD-61
Sample name	ZD-6
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel



**Spectra 1.** Compound **4d** IR spectra.

Data File: C:\LabSolutions\Data\Analiz\derya\ZD-6\_33.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	4	30	O	2	1	3	S	2	0	3	Ru	2	0	0	H
C	4	5	33	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0					

Error Margin (ppm): 15

DBE Range: 10.0 - 15.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: no

Max Isotopes: 3

Isotope RI (%): 1.00

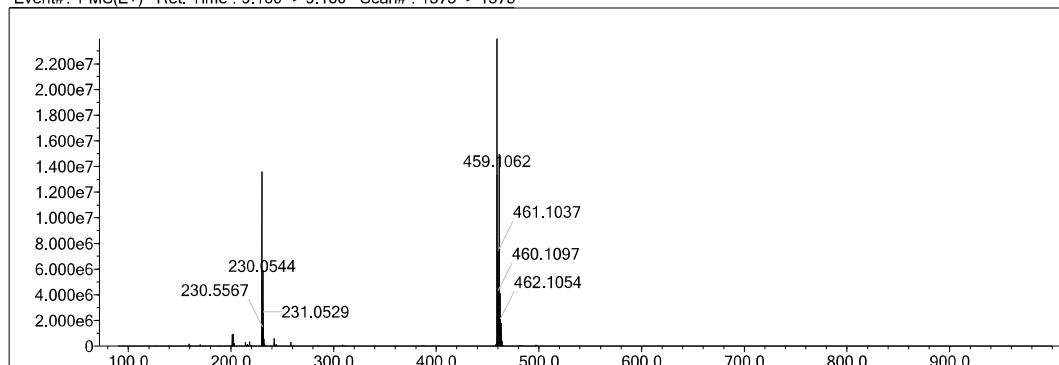
Isotope Res: 10000

MSn Iso RI (%): 10.00

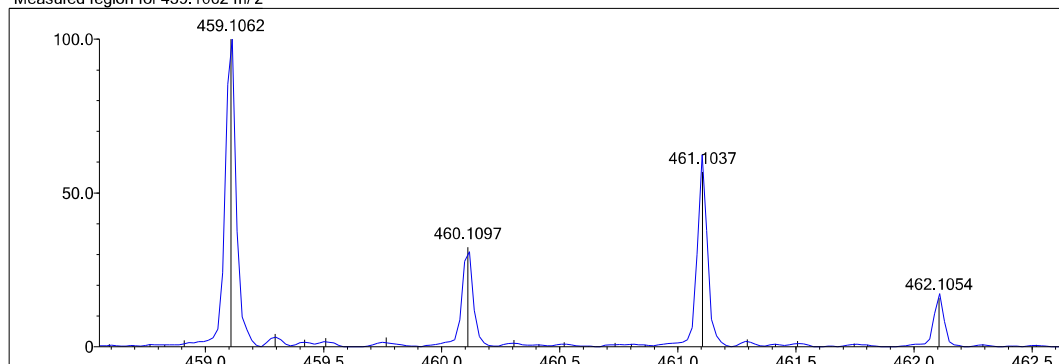
MSn Logic Mode: AND

Max Results: 500

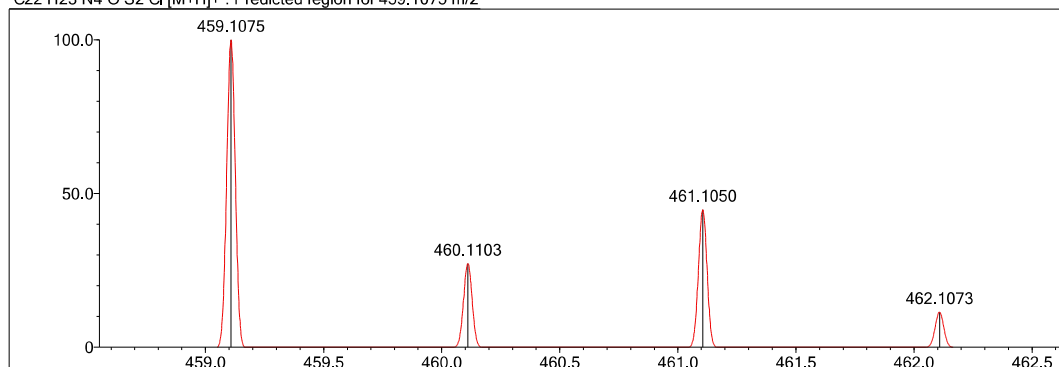
Event#: 1 MS(E+) Ret. Time : 9.160 -&gt; 9.160 Scan#: 1375 -&gt; 1375



Measured region for 459.1062 m/z

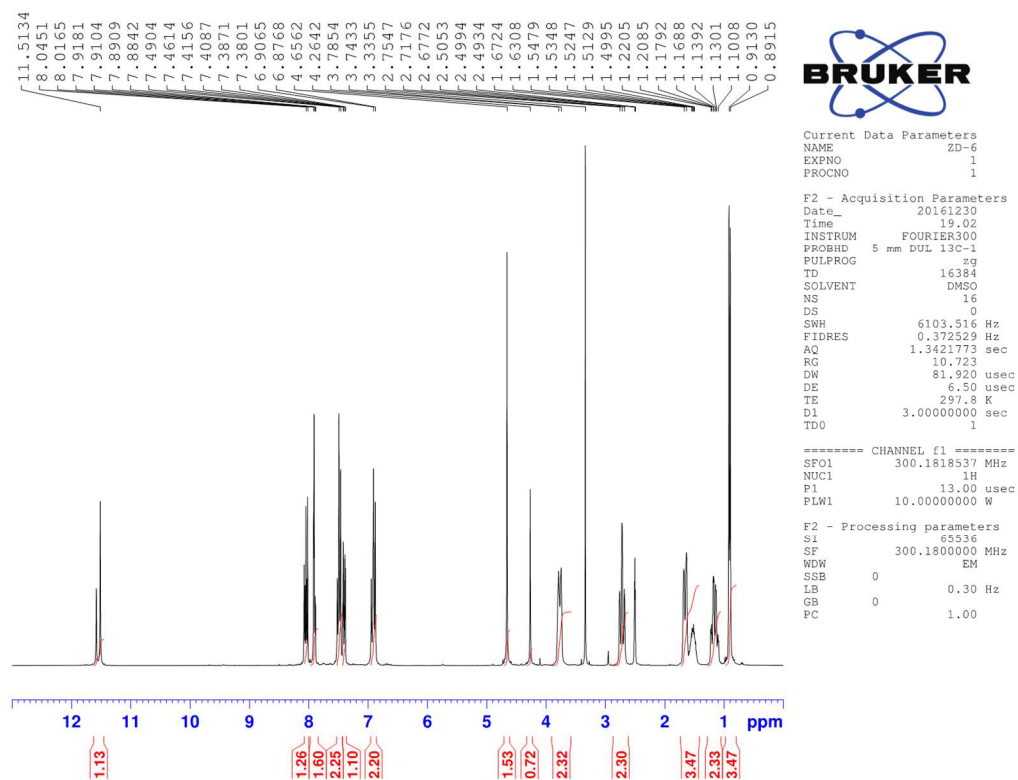


C22 H23 N4 O S2 Cl [M+H]+ : Predicted region for 459.1075 m/z

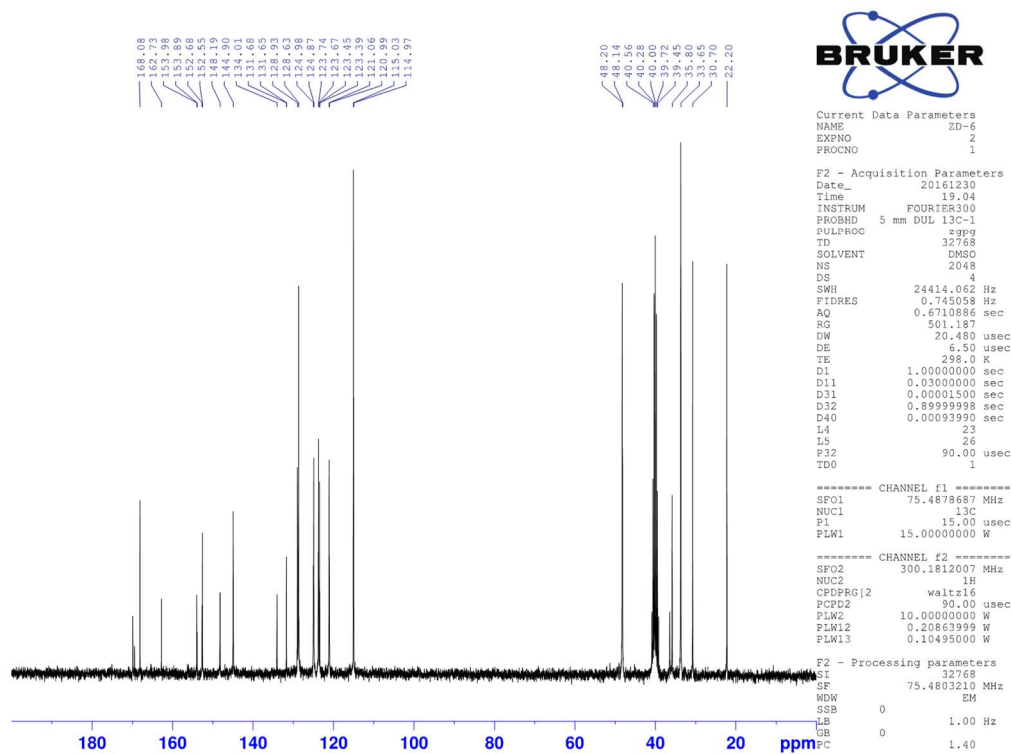


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	64.71	C22 H23 N4 O S2 Cl	[M+H]+	459.1062	459.1075	-1.3	-2.83	67.81	13.0

## Spectra 2. Compound 4d HRMS spectra.



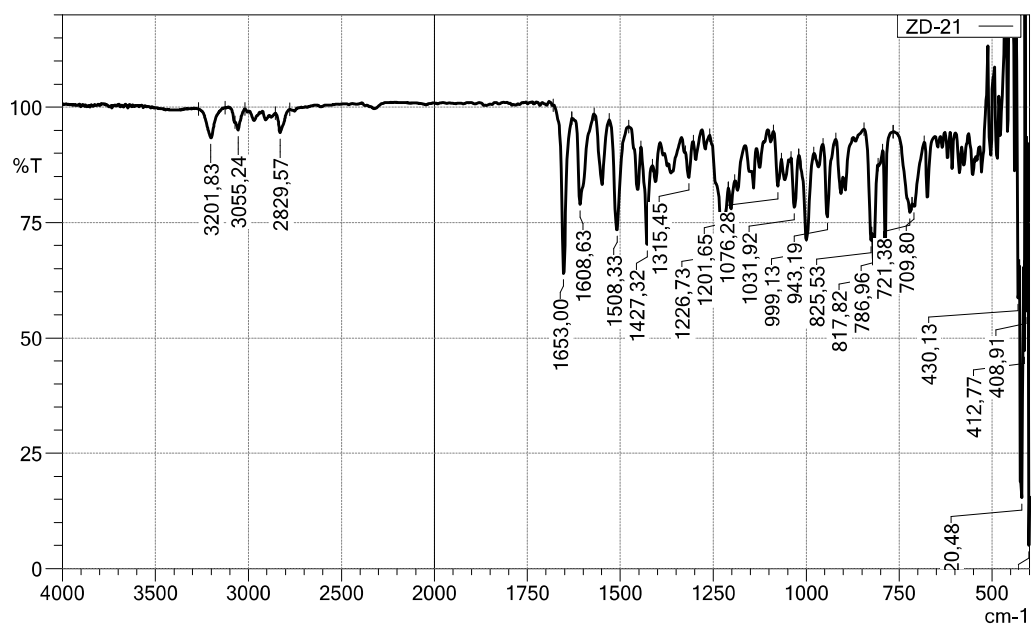
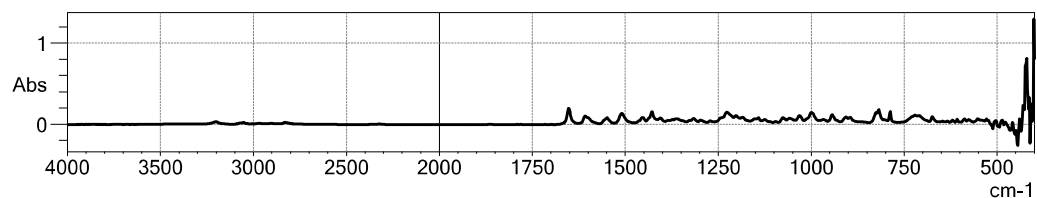
**Spectra 3.** Compound **4d**  $^1\text{H}$ -NMR spectra.



**Spectra 4.** Compound **4d**  $^{13}\text{C}$ -NMR spectra.

## DOPNALAB

Item	Value
Acquired Date&Time	23.12.2016 15:03:05
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\ZD seri\ZD-21.ispd
Spectrum name	ZD-21
Sample name	ZD-2
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel



**Spectra 5.** Compound **4e** IR spectra.

Data File: C:\LabSolutions\Data\Analiziderya\ZD-2\_29.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	4	30	O	2	1	3	S	2	0	3	Ru	2	0	0	H
C	4	5	33	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	2	6	P	3	0	0	Br	1	0	0					

Error Margin (ppm): 15

DBE Range: 15.0 - 18.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: no

Max Isotopes: 3

Isotope RI (%): 1.00

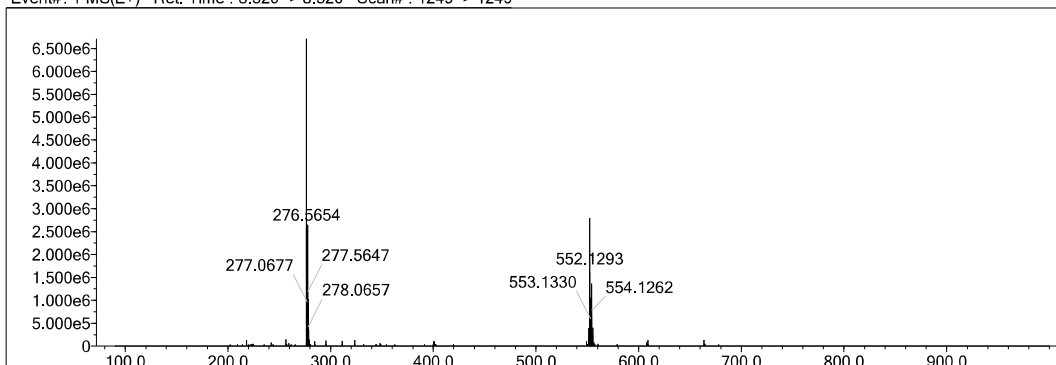
Isotope Res: 10000

MSn Iso RI (%): 10.00

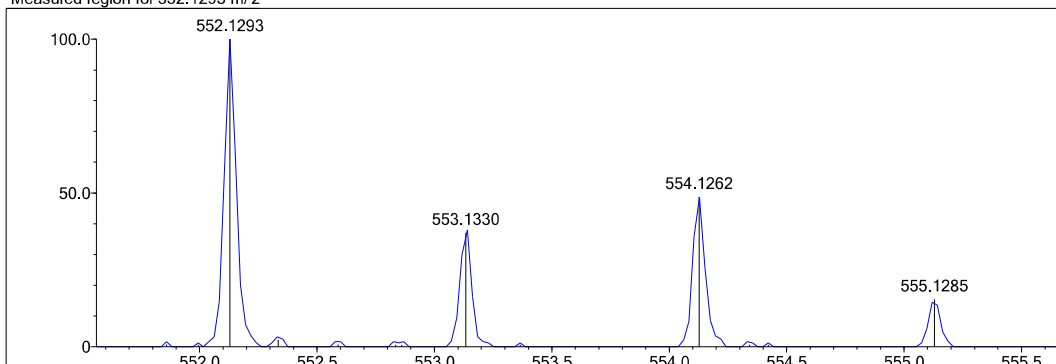
MSn Logic Mode: AND

Max Results: 500

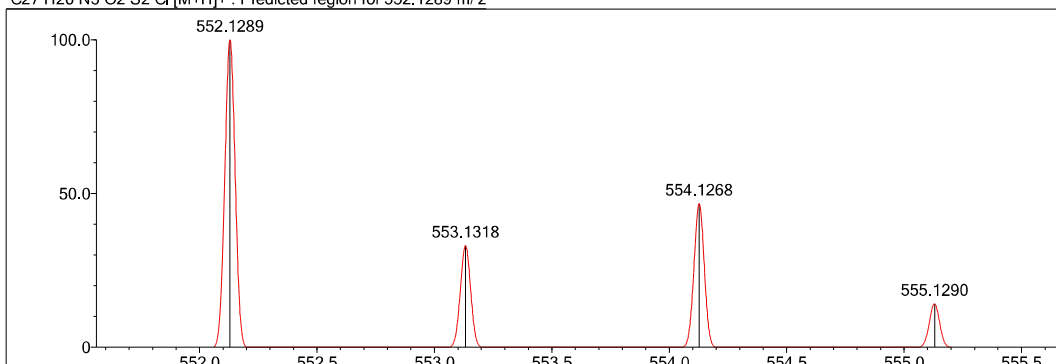
Event#: 1 MS(E+) Ret. Time : 8.320 -&gt; 8.320 Scan#: 1249 -&gt; 1249



Measured region for 552.1293 m/z

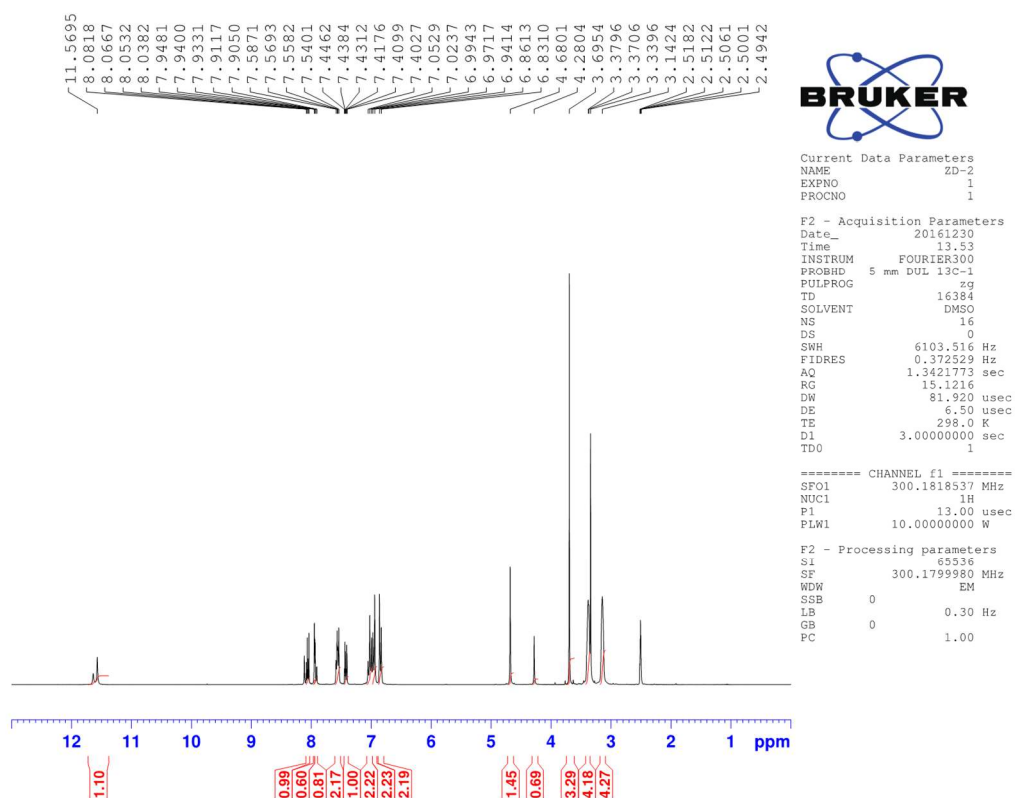


C27 H26 N5 O2 S2 Cl [M+H]+ : Predicted region for 552.1289 m/z

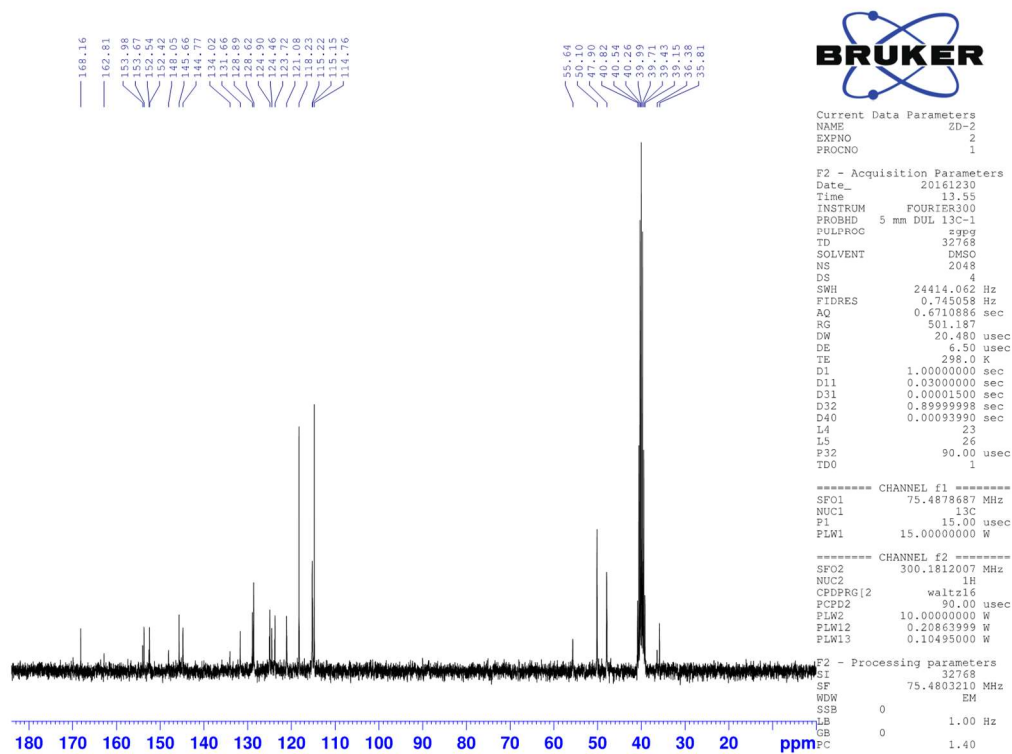


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	100.00	C27 H26 N5 O2 S2 Cl	[M+H] <sup>+</sup>	552.1293	552.1289	0.4	0.72	100.00	17.0

Spectra 6. Compound 4e HRMS spectra.



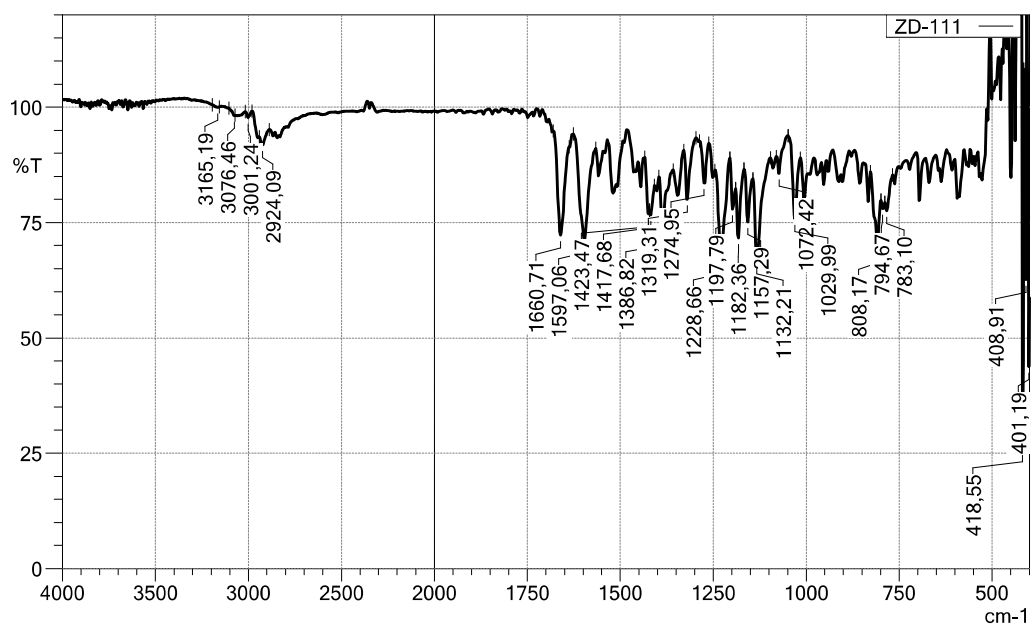
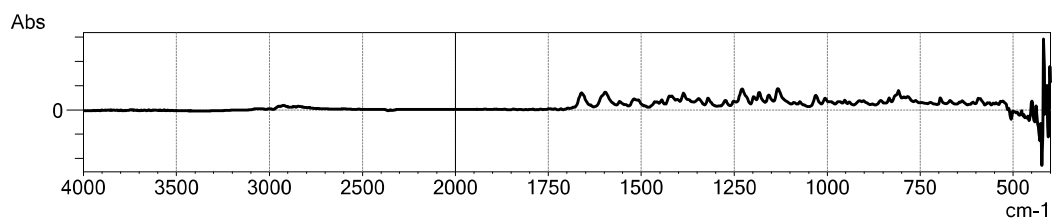
Spectra 7. Compound **4e**  $^1\text{H}$ -NMR spectra.



Spectra 8. Compound **4e**  $^{13}\text{C}$ -NMR spectra.

## DOPNALAB

Item	Value
Acquired Date&Time	23.12.2016 16:04:09
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\ZD seri\ZD-111.ispd
Spectrum name	ZD-111
Sample name	ZD-11
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel



**Spectra 9.** Compound **4h** IR spectra.

Data File: C:\LabSolutions\Data\Analiziderya\ZD-11\_38.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	4	30	O	2	1	3	S	2	0	3	Ru	2	0	0	H
C	4	5	33	F	1	0	0	Cl	1	0	0	I	3	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0					

Error Margin (ppm): 10

DBE Range: 10.0 - 15.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: no

Max Isotopes: 3

Isotope RI (%): 1.00

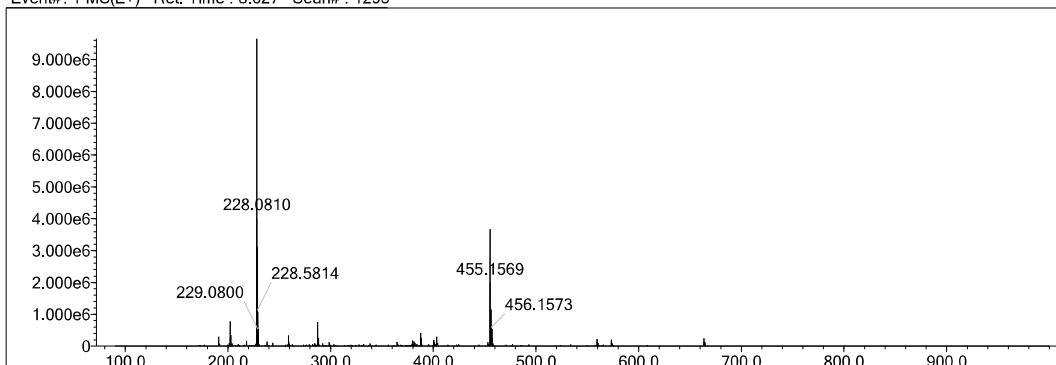
Isotope Res: 10000

MSn Iso RI (%): 10.00

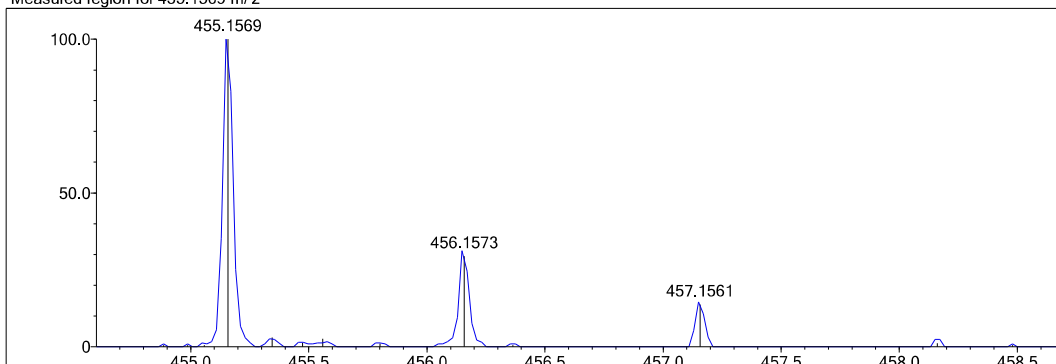
MSn Logic Mode: AND

Max Results: 500

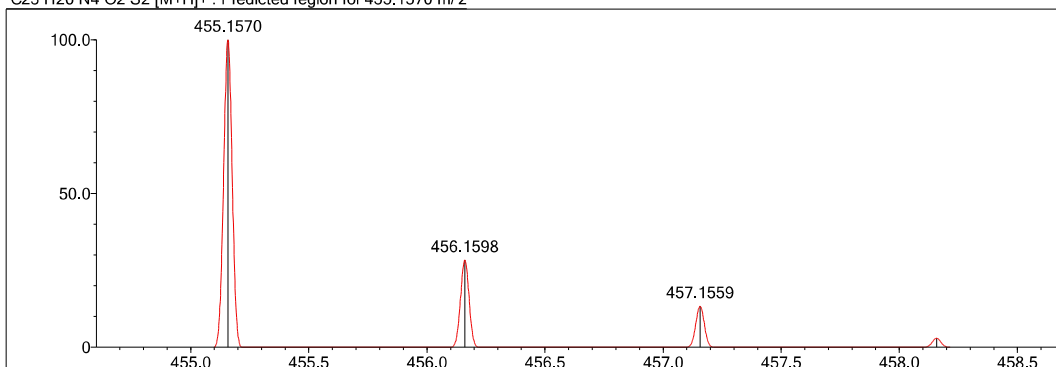
Event#: 1 MS(E+) Ret. Time : 8.627 Scan#: 1295



Measured region for 455.1569 m/z



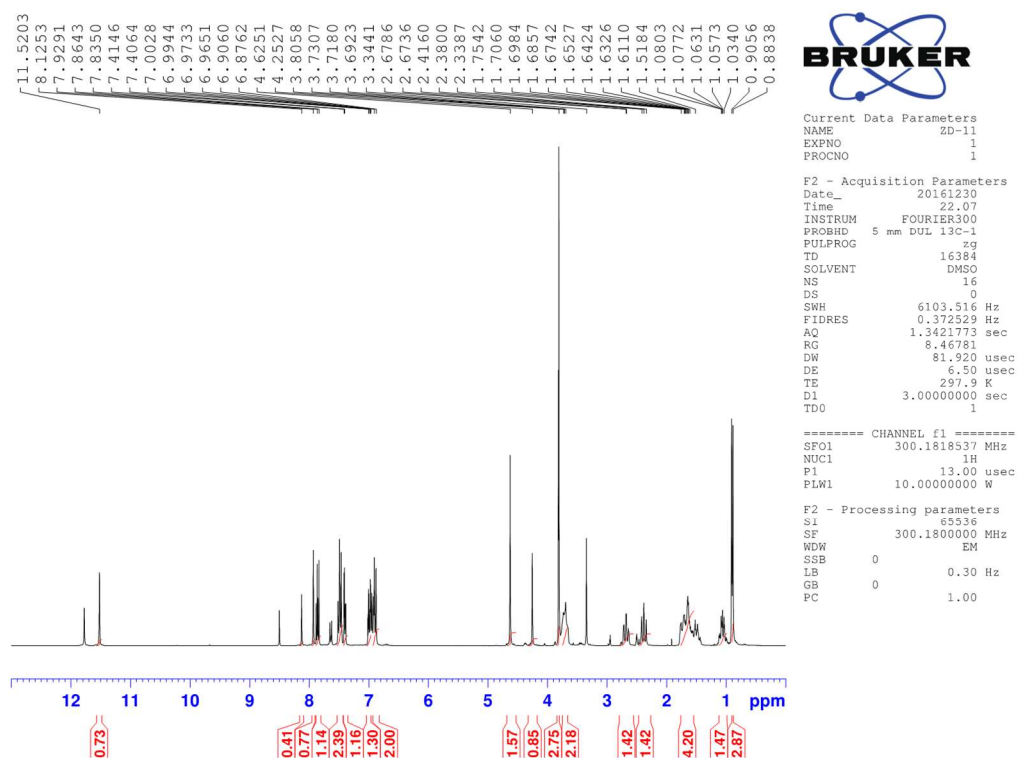
C23 H26 N4 O2 S2 [M+H]+ : Predicted region for 455.1570 m/z



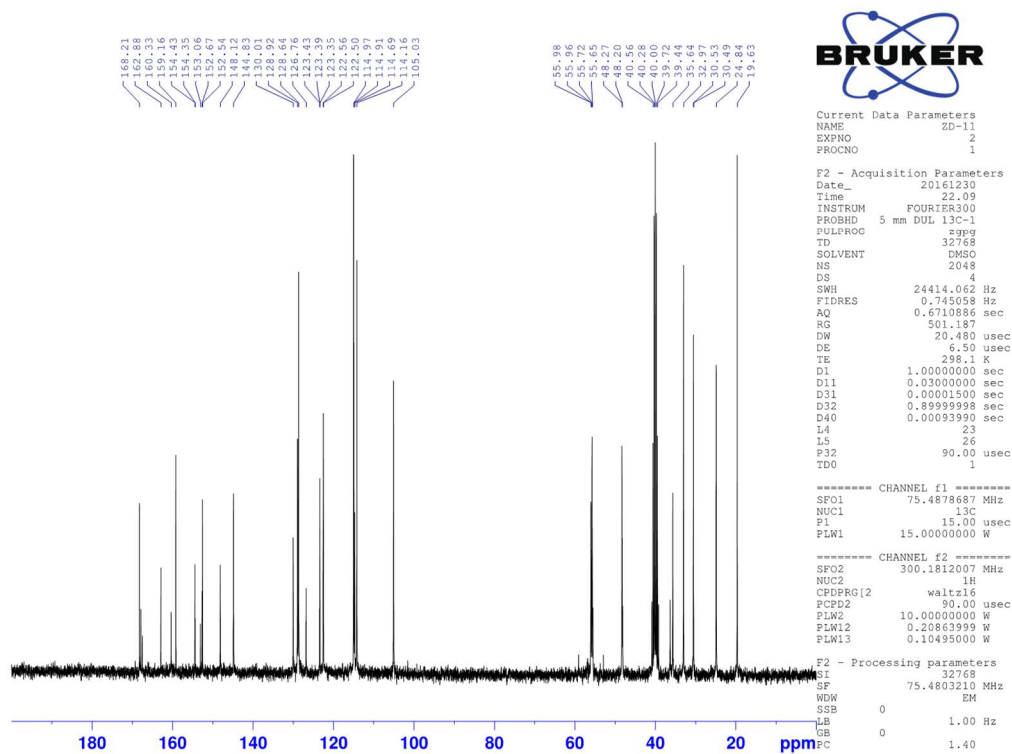
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.68	C23 H26 N4 O2 S2	[M+H] <sup>+</sup>	455.1569	455.1570	-0.1	-0.22	83.68	13.0

Spectra 10. Compound **4h** HRMS spectra.





Spectra 11. Compound **4h**  $^1\text{H}$ -NMR spectra.



Spectra 12. Compound **4h**  $^{13}\text{C}$ -NMR spectra.