Supplementary Information

Structure-Based Design, Synthesis, and Biological Activity Evaluation of Chalcone-Piperazine DerivativeSaSDual AChE and MAO B Inhibitors

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Address: Anadolu University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, 26470, Eskişehir, Turkey.

DOPNALAB

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	Spectrum name	AL-11
	Sample name	AL-1
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
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	Apodization	Happ-Genzel

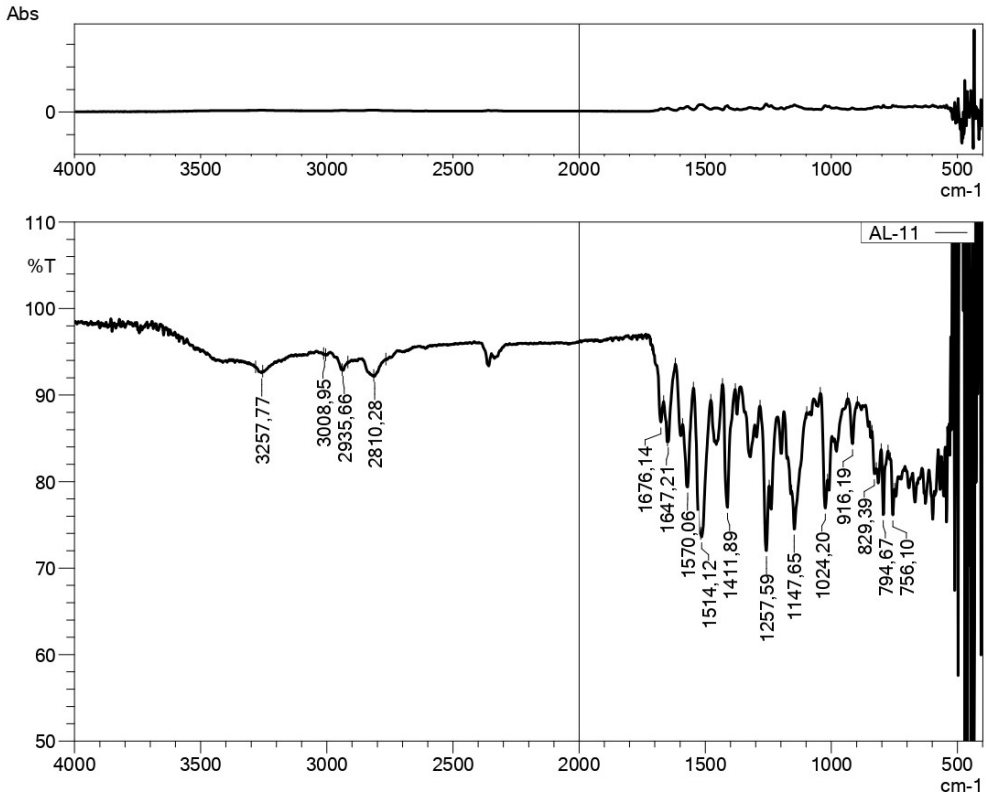


Figure S1. FTIR spectra of compound **4a**

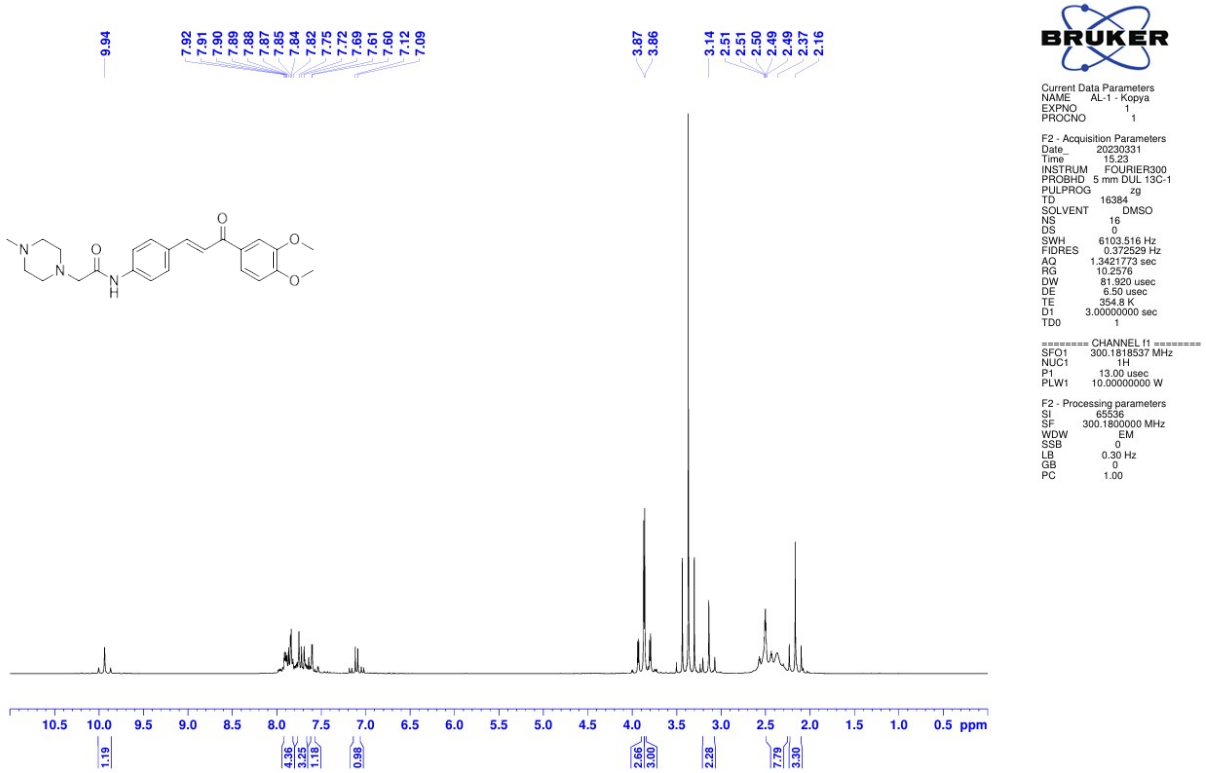


Figure S2. ^{1}H-NMR spectra of compound **4a**

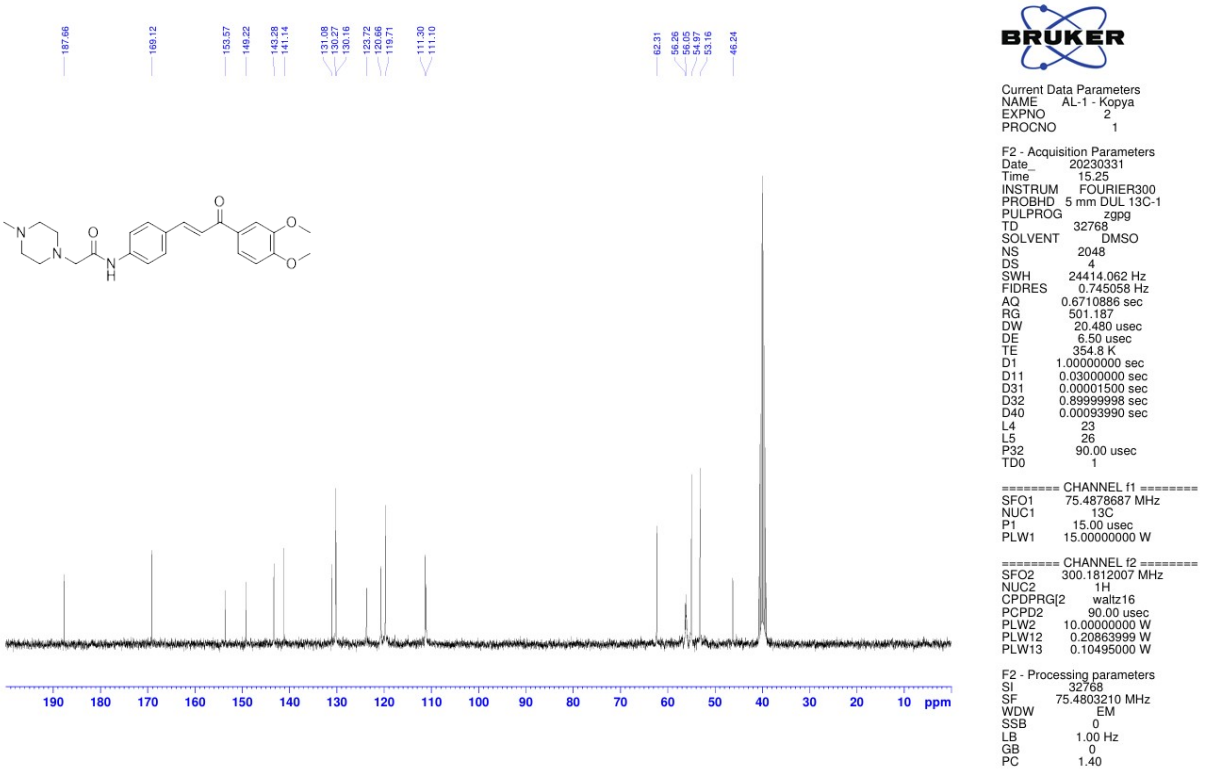


Figure S3. ^{13}C-NMR spectra of compound **4a**

Formula Predictor Report - AL-1_197.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-1_197.lcd

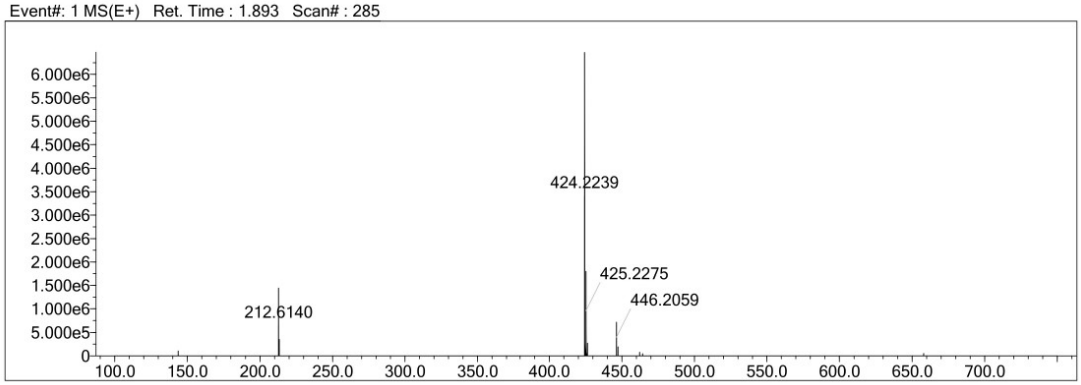
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

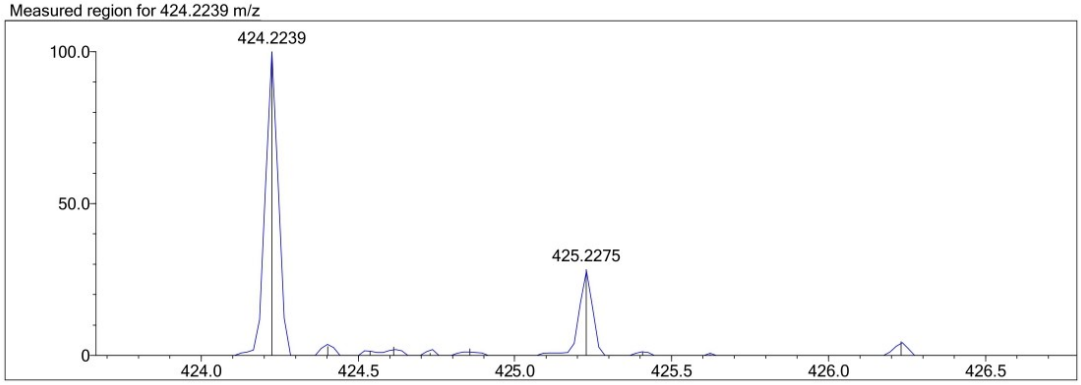
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

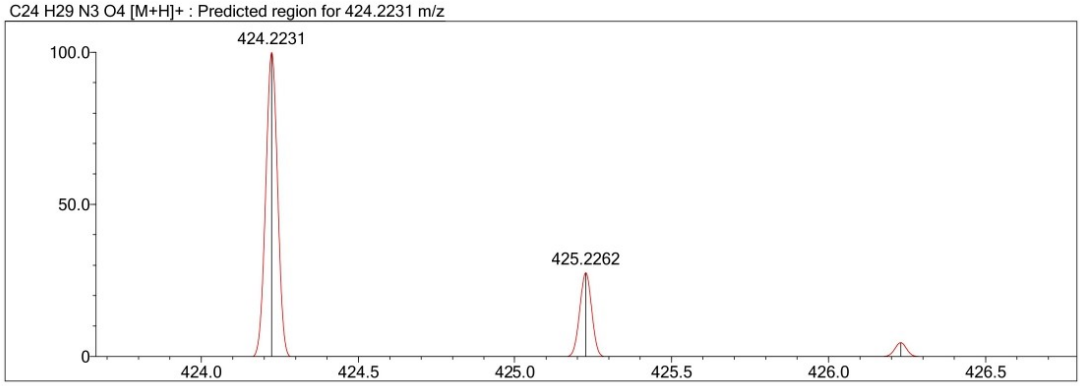
Event#: 1 MS(E+) Ret. Time : 1.893 Scan# : 285



Measured region for 424.2239 m/z



C24 H29 N3 O4 [M+H]+ : Predicted region for 424.2231 m/z



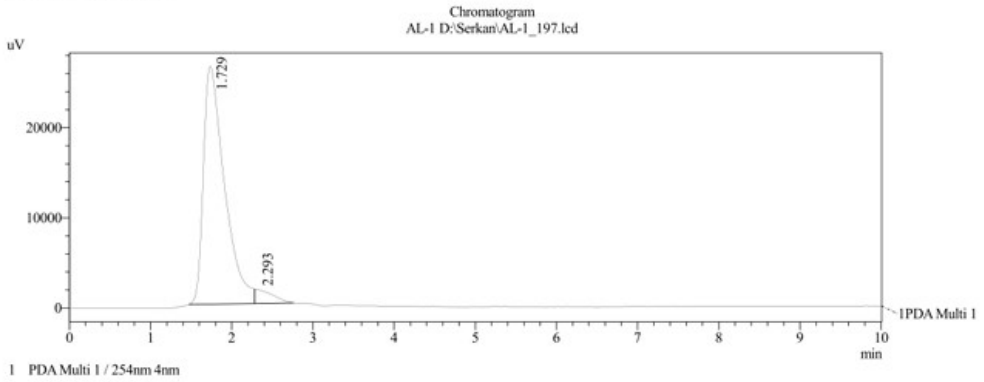
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	97.78	C24 H29 N3 O4	[M+H]+	424.2239	424.2231	0.8	1.89	100.00	12.0

Figure S4. HRMS spectra of compound **4a**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-1
Sample ID	:
Vail #	: 1
Injection Volume	: 0.5 uL
Data File Name	: AL-1_197.lcd
Method File Name	: isocratic_serkan.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 16:48:01
Data Processed	: 04.09.2025 10:33:36

<Chromatogram>



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	1.729	476869	26376	95.541
2	2.293	22255	1555	4.459
Total		499125	27932	100.000

Figure S5. HPLC chromatogram of compound **4a**

DOPNALAB

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	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-21.ispd
	Spectrum name	AL-21
	Sample name	AL-2
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

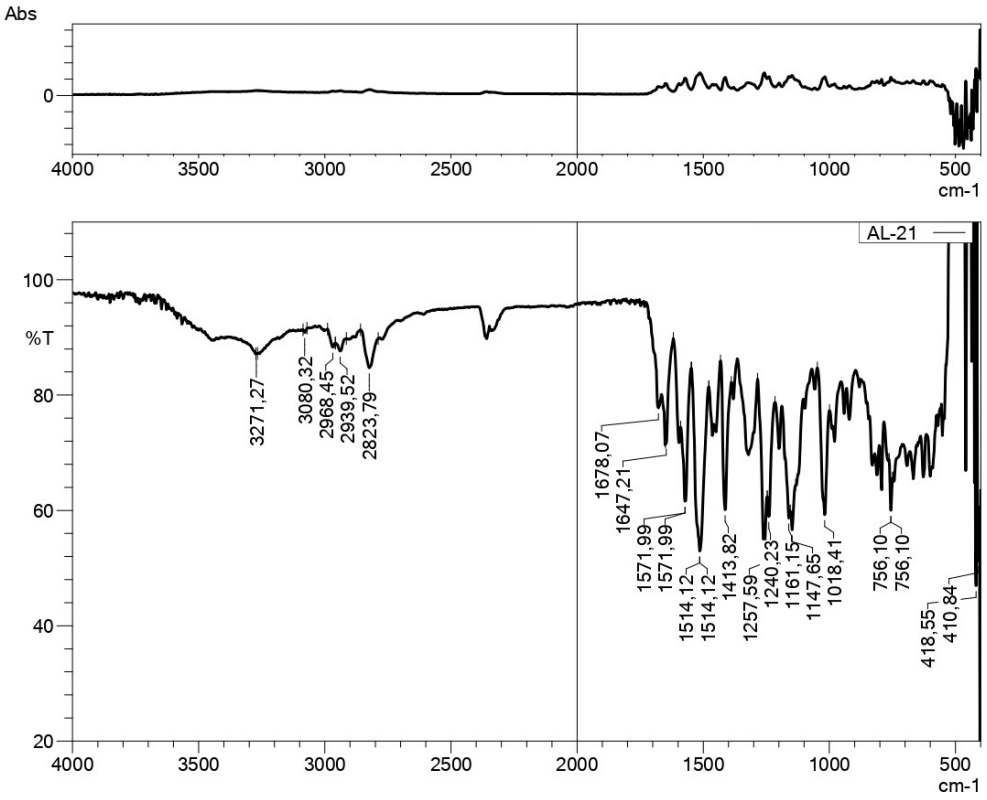


Figure S6. FTIR spectra of compound **4b**

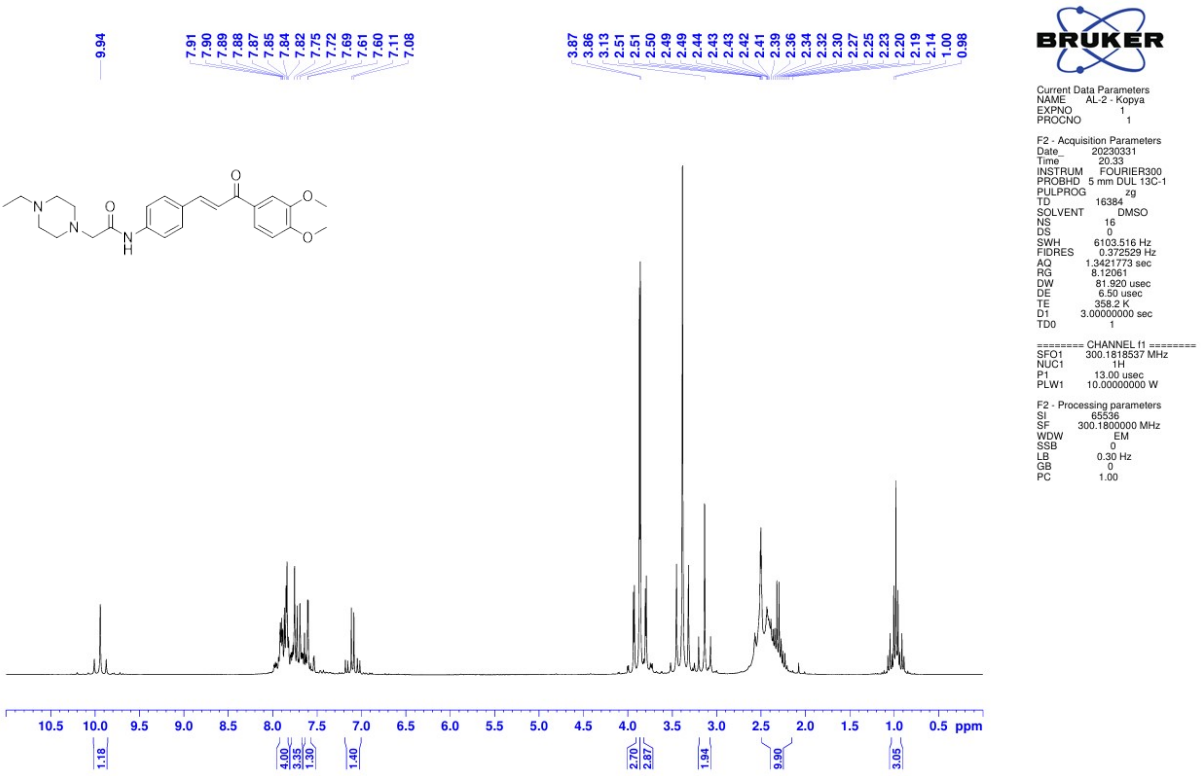


Figure S7. [1]H-NMR spectra of compound **4b**

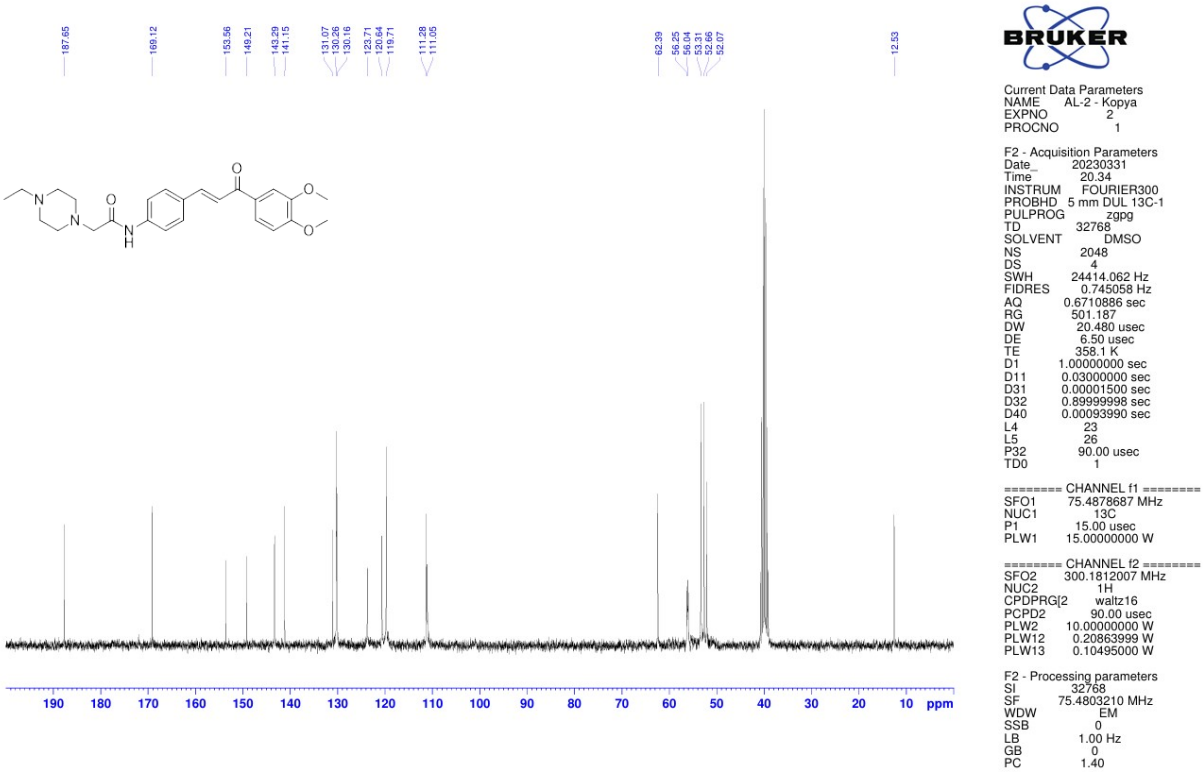


Figure S8. [13]C-NMR spectra of compound **4b**

Formula Predictor Report - AL-2_198.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-2_198.lcd

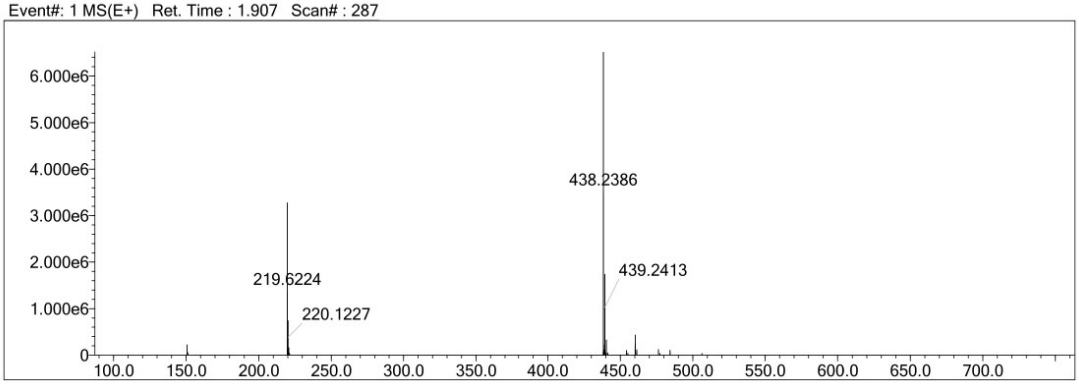
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	32	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

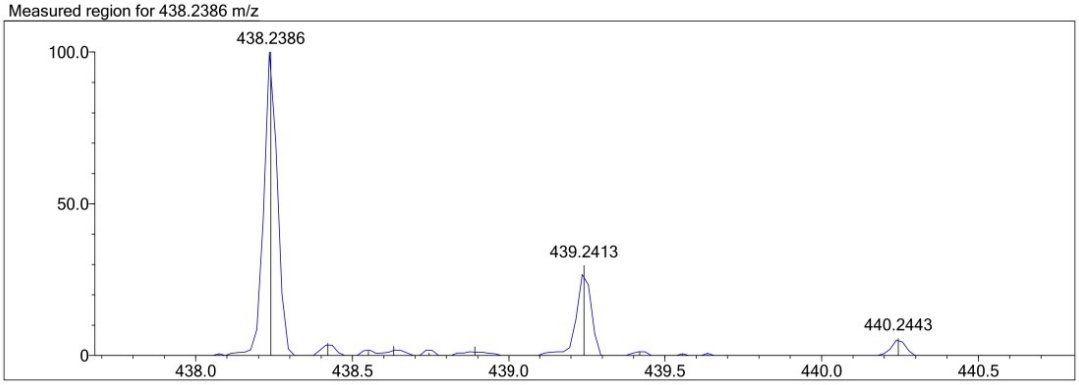
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

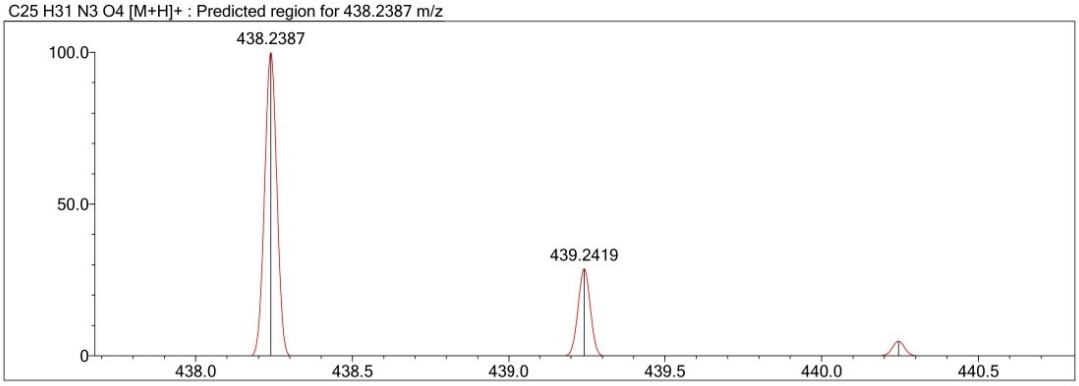
Event#: 1 MS(E+) Ret. Time : 1.907 Scan# : 287



Measured region for 438.2386 m/z



C25 H31 N3 O4 [M+H]+ : Predicted region for 438.2387 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	87.09	C25 H31 N3 O4	[M+H]+	438.2386	438.2387	-0.1	-0.23	87.09	12.0

Figure S9. HRMS spectra of compound **4b**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-2
Sample ID	:
Vail #	: 2
Injection Volume	: 0.5 uL
Data File Name	: AL-2_198.lcd
Method File Name	: isocratic_serkan.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 16:58:49
Data Processed	: 02.08.2022 17:08:52

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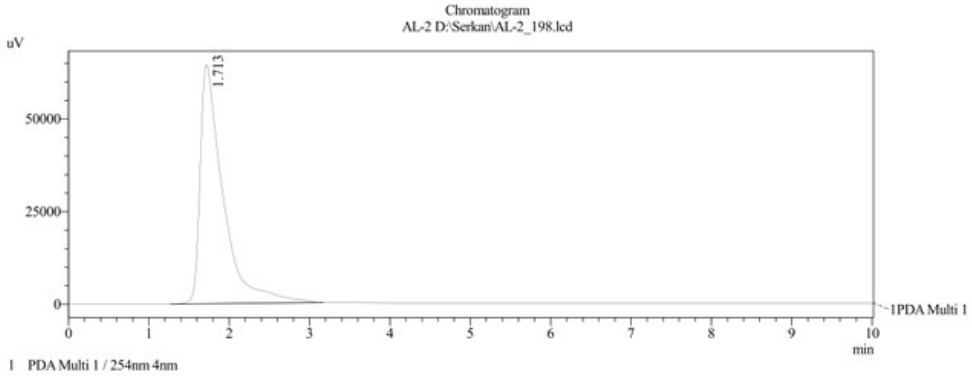

1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	1.713	1279956	64535	100.000
Total		1279956	64535	100.000

Figure S10. HPLC chromatogram of compound **4b**

DOPNALAB

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	Acquired by	System Administrator
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	Spectrum name	AL-31
	Sample name	AL-3
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

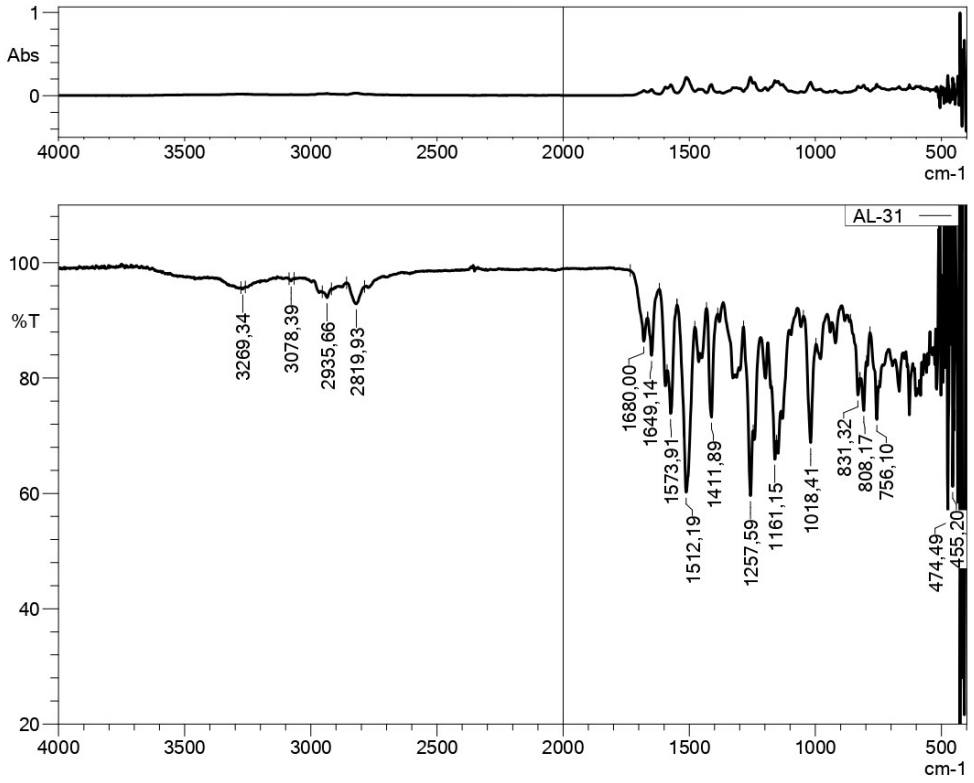


Figure S11. FTIR spectra of compound **4c.**

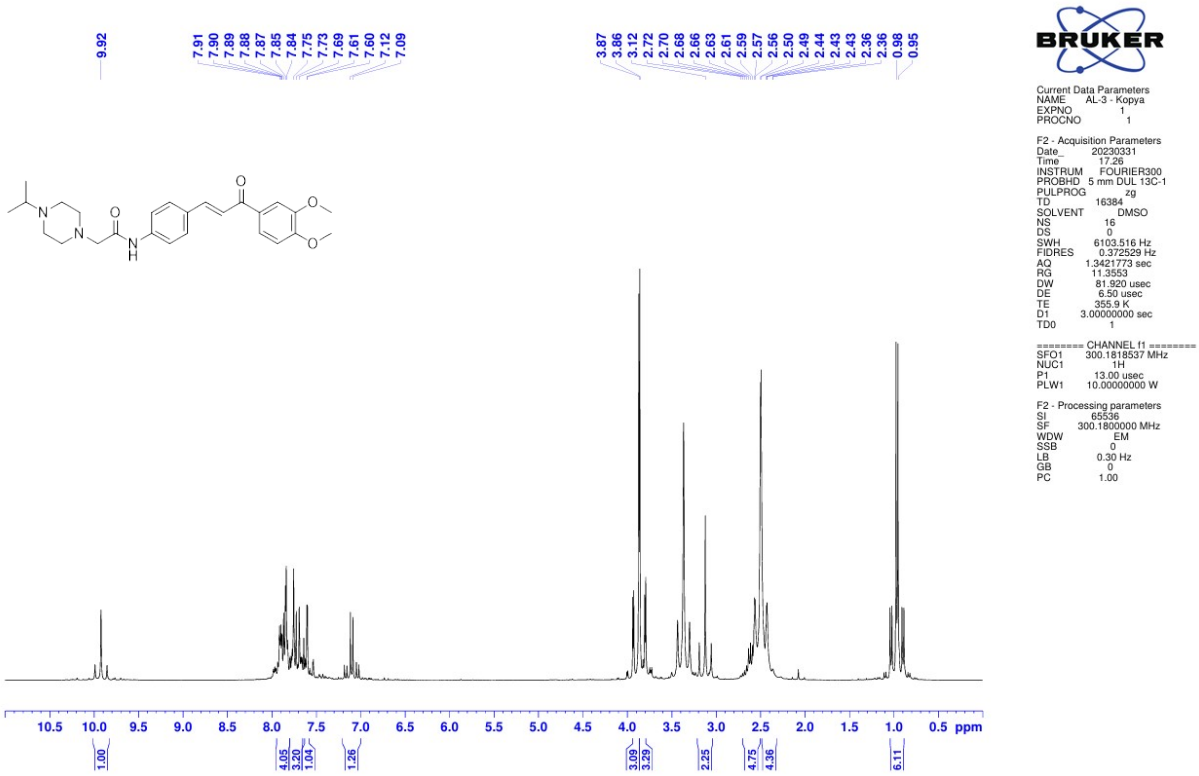


Figure S12. ^{1}H-NMR spectra of compound **4c**

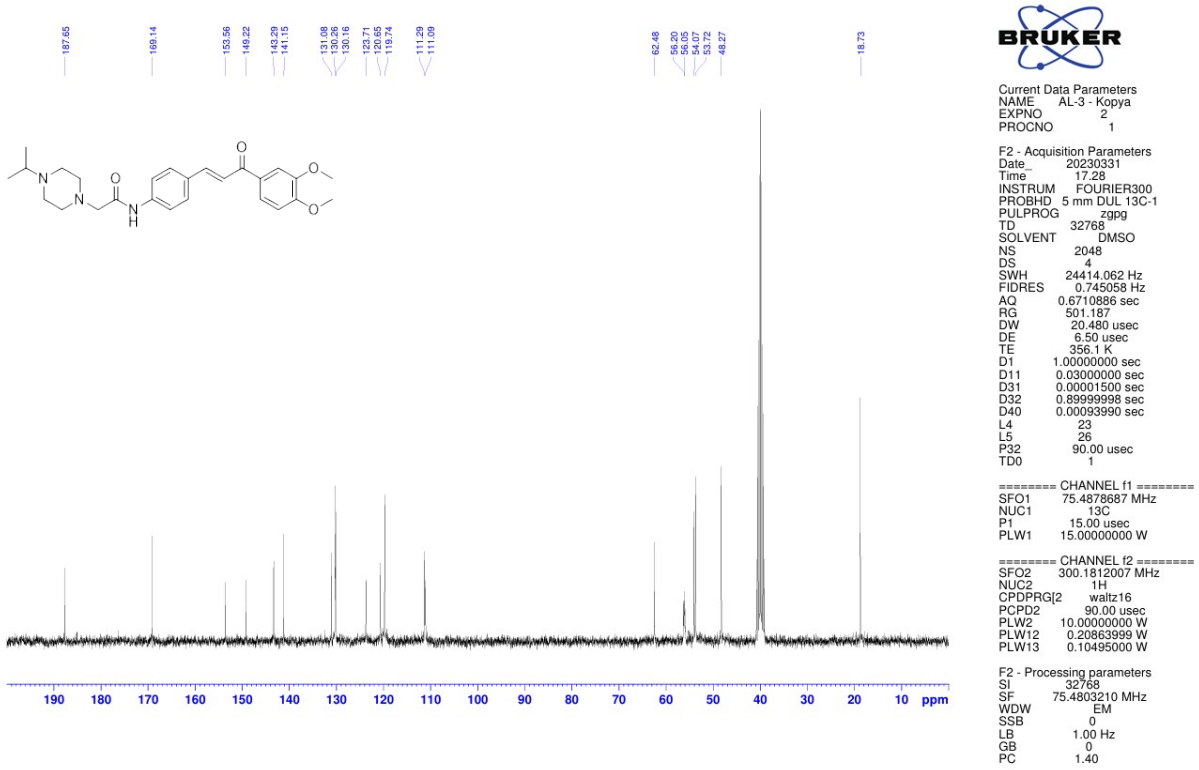


Figure S13. ^{13}C-NMR spectra of compound **4c**

Formula Predictor Report - AL-3_199.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-3_199.lcd

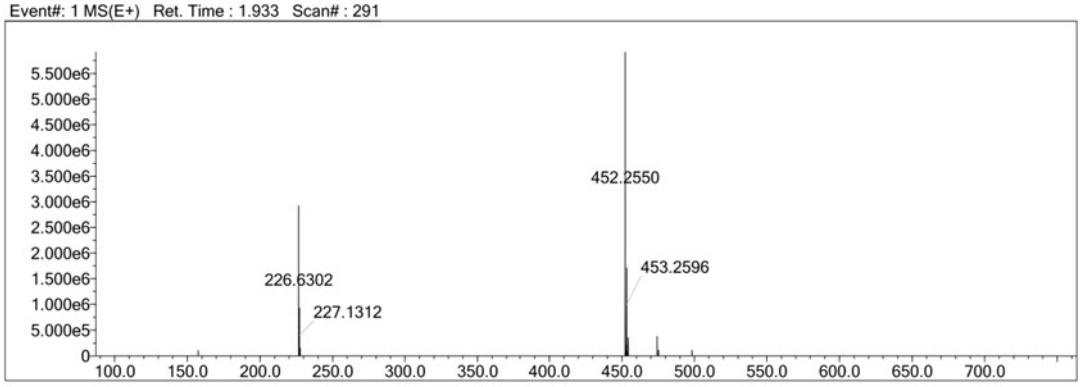
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	35	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

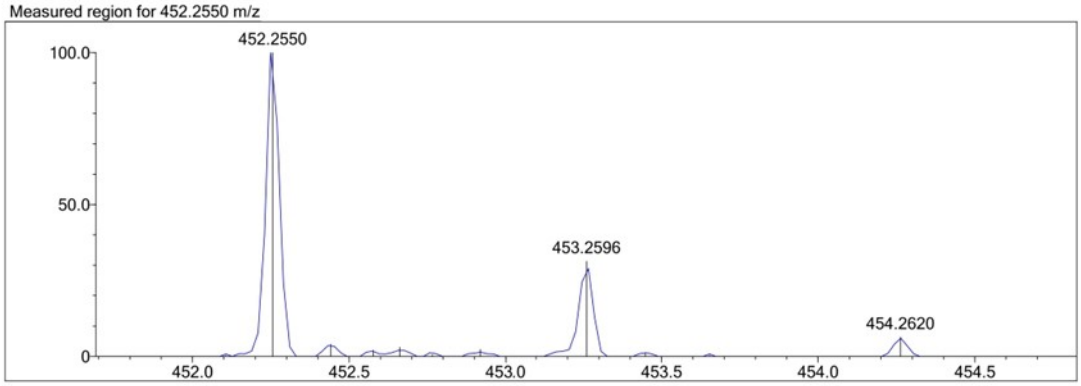
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

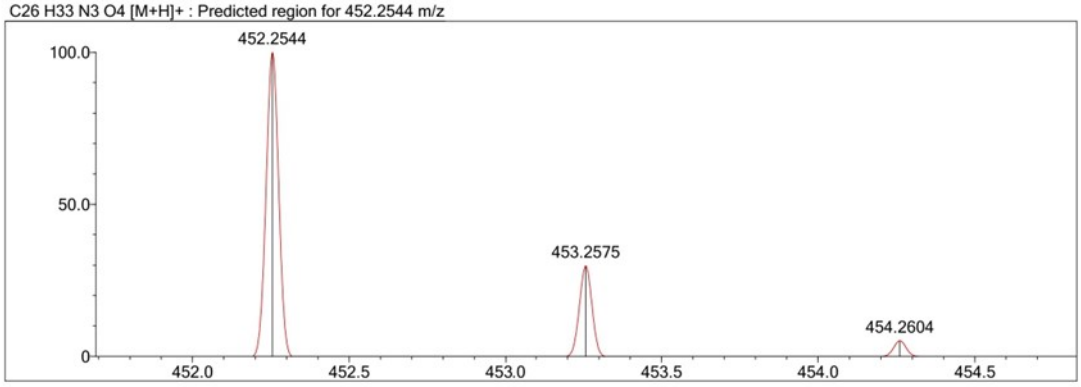
Event#: 1 MS(E+) Ret. Time : 1.933 Scan# : 291



Measured region for 452.2550 m/z



C26 H33 N3 O4 [M+H]+ : Predicted region for 452.2544 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	87.25	C26 H33 N3 O4	[M+H]+	452.2550	452.2544	0.6	1.33	87.98	12.0

Figure S14. HRMS spectra of compound **4c**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-3
Sample ID	:
Vail #	: 3
Injection Volume	: 0.5 uL
Data File Name	: AL-3_199.lcd
Method File Name	: isocratic_serkan.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 17:09:38
Data Processed	: 04.09.2025 10:37:24

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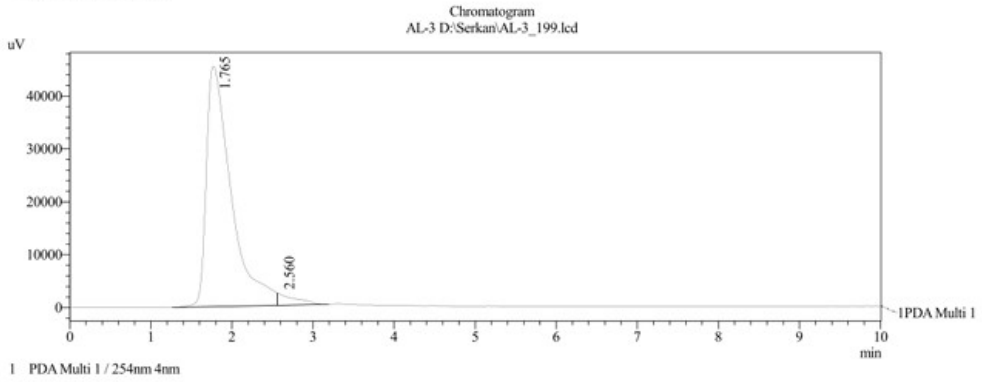

1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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1	1.765	968164	45508	96.637
2	2.560	33693	2338	3.363
Total		1001857	47847	100.000

Figure S15. HPLC chromatogram of compound **4c**

DOPNALAB

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	Spectrum name	AL-41
	Sample name	AL-4
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

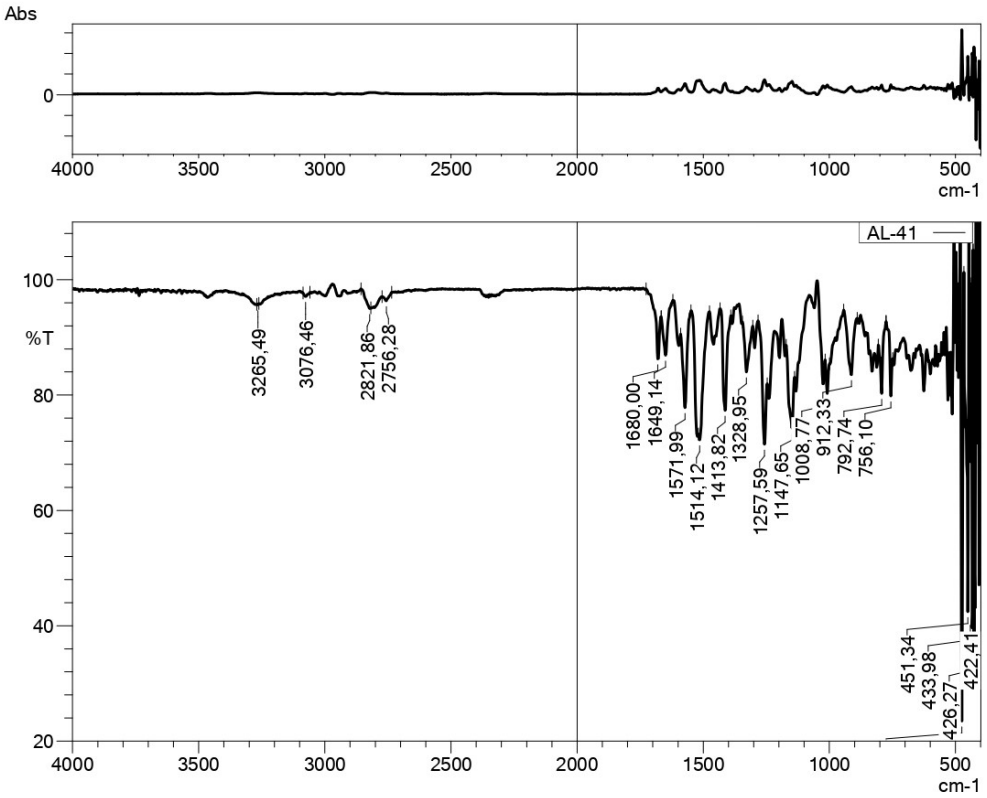


Figure S16. FTIR spectra of compund **4d**

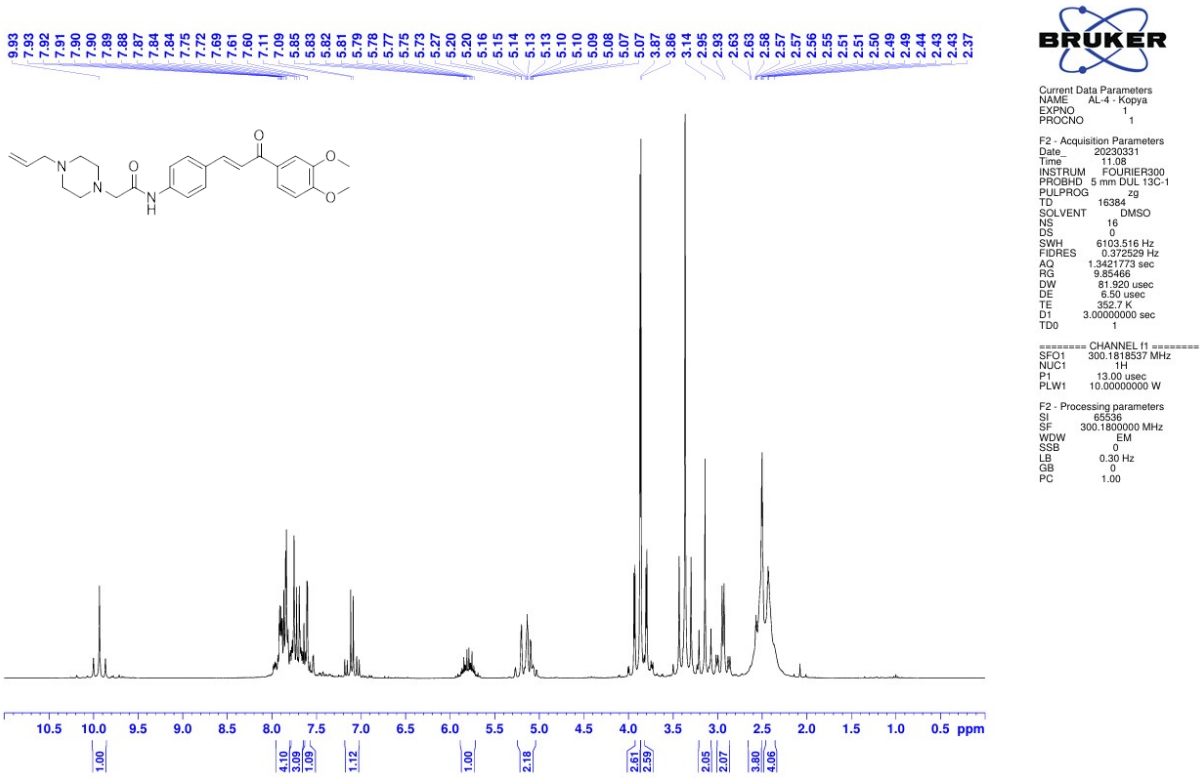


Figure S17. ^{1}H-NMR spectra of compound **4d**

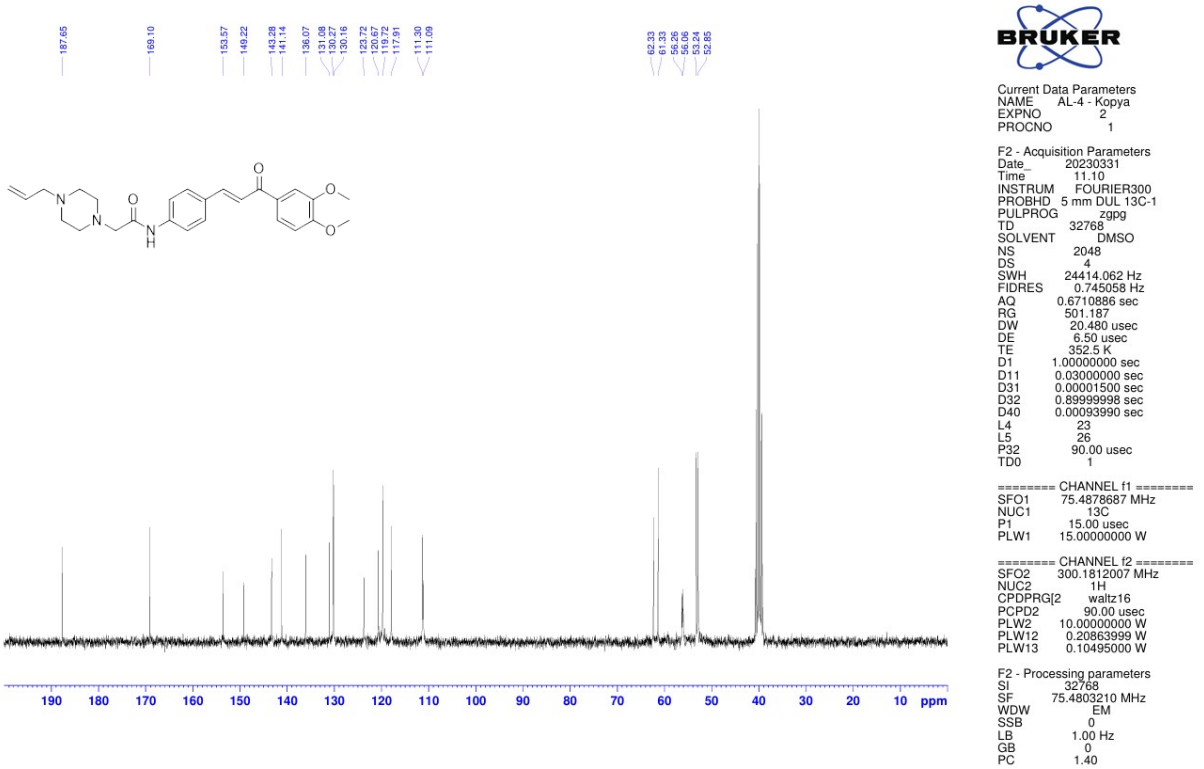


Figure S18. ^{13}C-NMR spectra of compound **4d**

Formula Predictor Report - AL-4_200.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-4_200.lcd

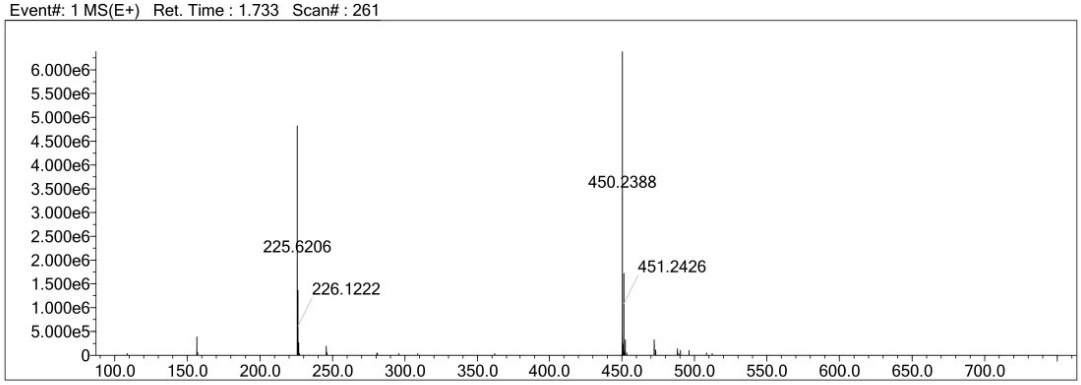
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	35	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

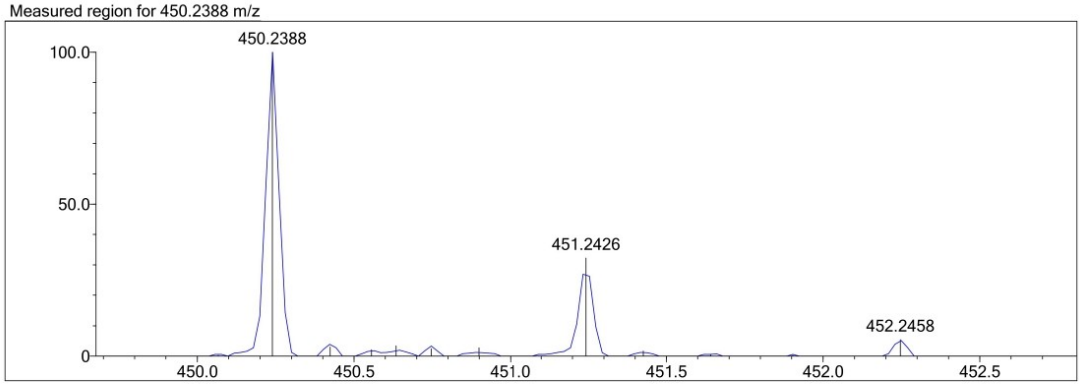
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

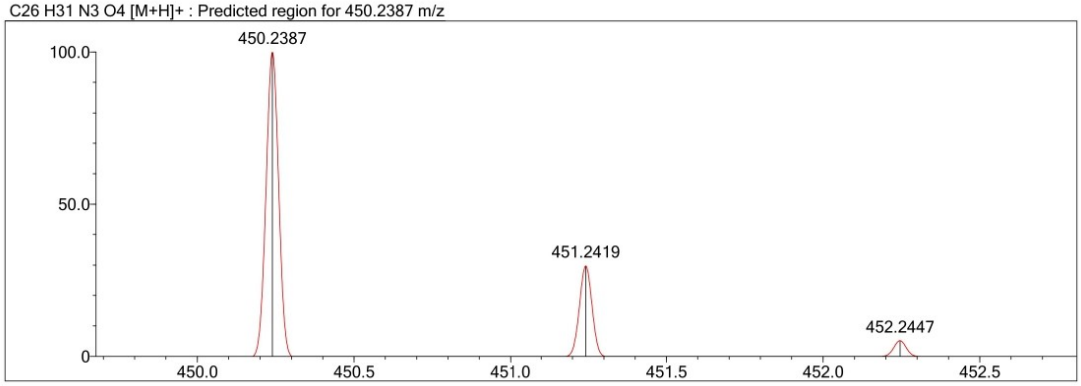
Event#: 1 MS(E+) Ret. Time : 1.733 Scan# : 261



Measured region for 450.2388 m/z



C26 H31 N3 O4 [M+H]+ : Predicted region for 450.2387 m/z



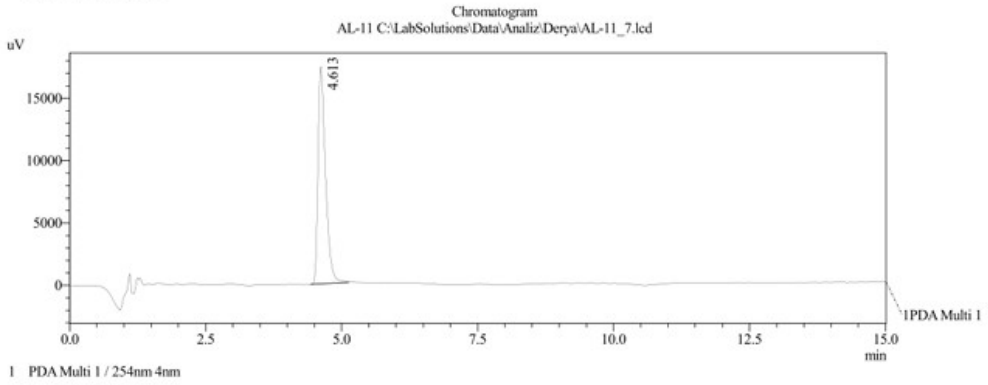
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	100.00	C26 H31 N3 O4	[M+H]+	450.2388	450.2387	0.1	0.22	100.00	13.0

Figure S19. HRMS spectra of compound **4d**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-11
Sample ID	:
Vail #	: 4
Injection Volume	: 1 uL
Data File Name	: AL-11_7.lcd
Method File Name	: isocratic_serkan-15DK.lcm
Batch File Name	: 1.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 18:36:08
Data Processed	: 08.09.2025 10:00:48

<Chromatogram>



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	4.613	167372	17415	100.000
Total		167372	17415	100.000

Figure S20. HPLC chromatogram of compound **4d**

DOPNALAB

	Item	Value
	Acquired Date&Time	17.05.2023 15:10:38
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-51.ispd
	Spectrum name	AL-51
	Sample name	AL-5
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

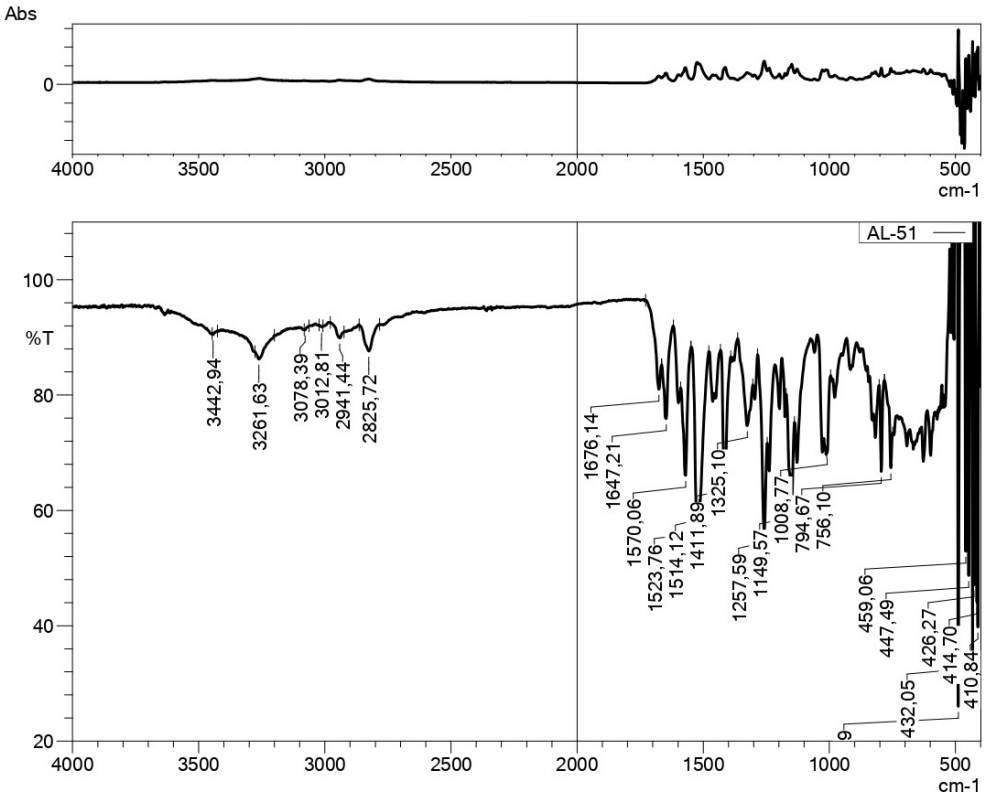


Figure S21. FTIR spectra of compound **4e**

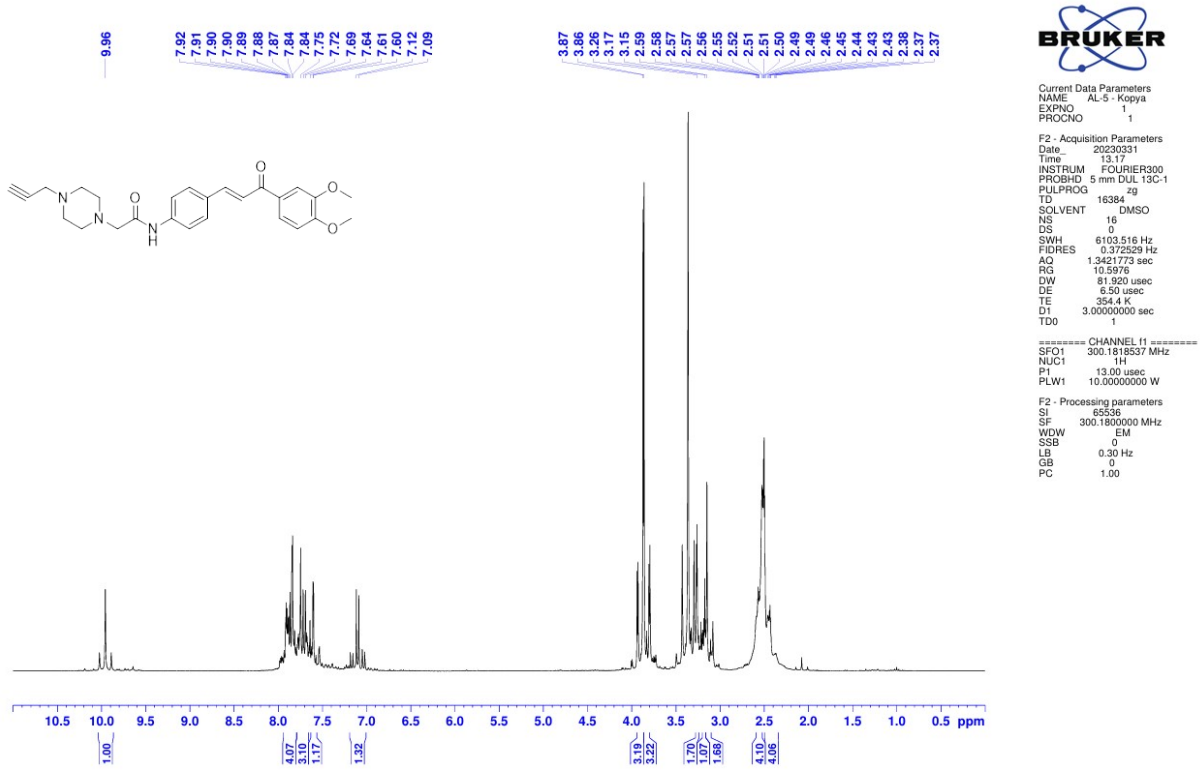


Figure S22. ^{1}H-NMR spectra of compound **4e**

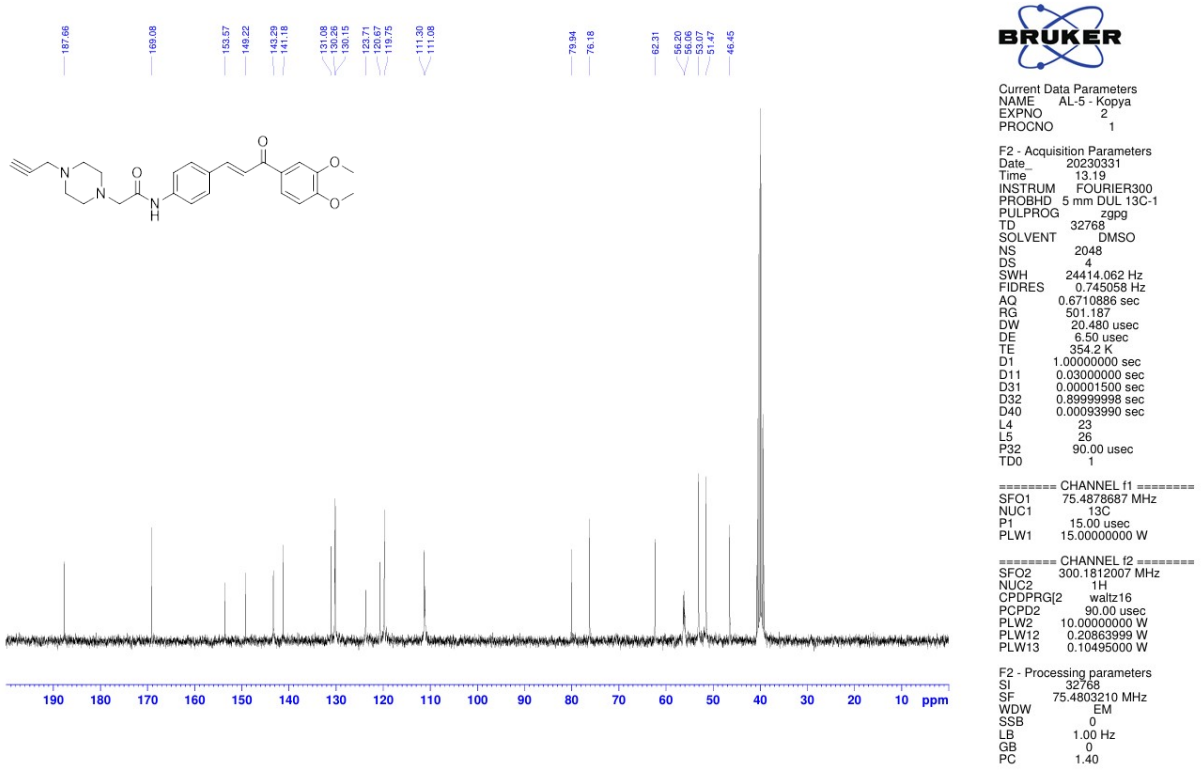


Figure S23. ^{13}C-NMR spectra of compound **4e**

Formula Predictor Report - AL-5_201.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-5_201.lcd

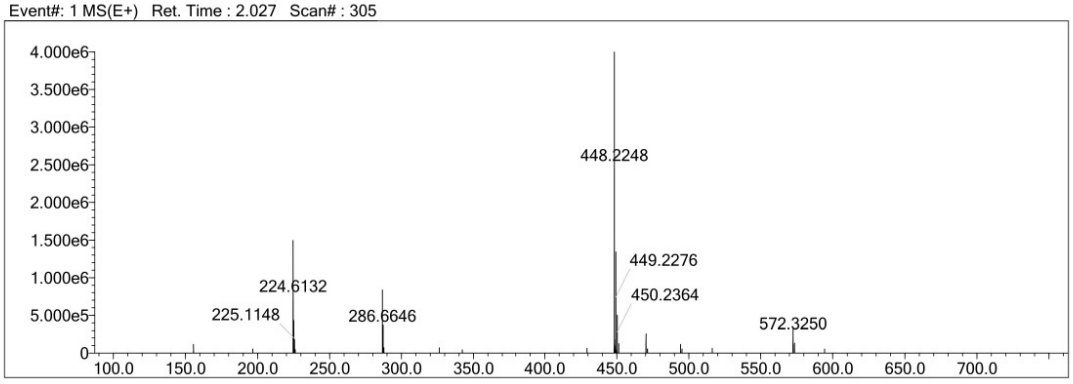
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	35	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

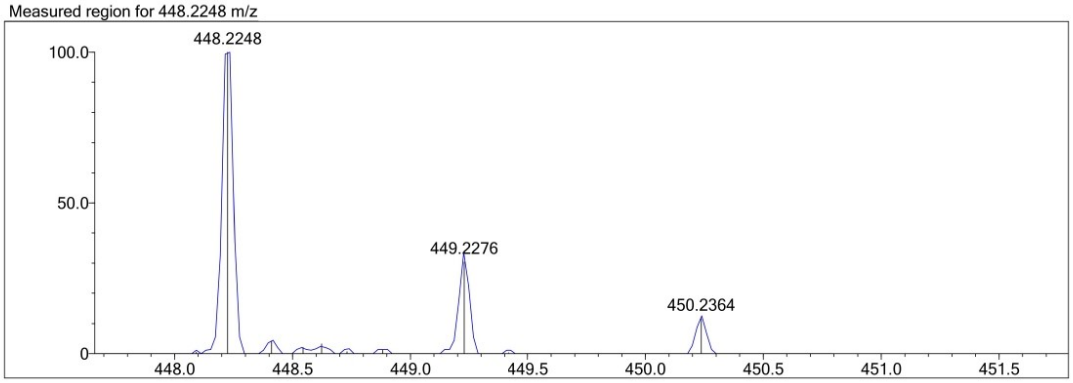
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

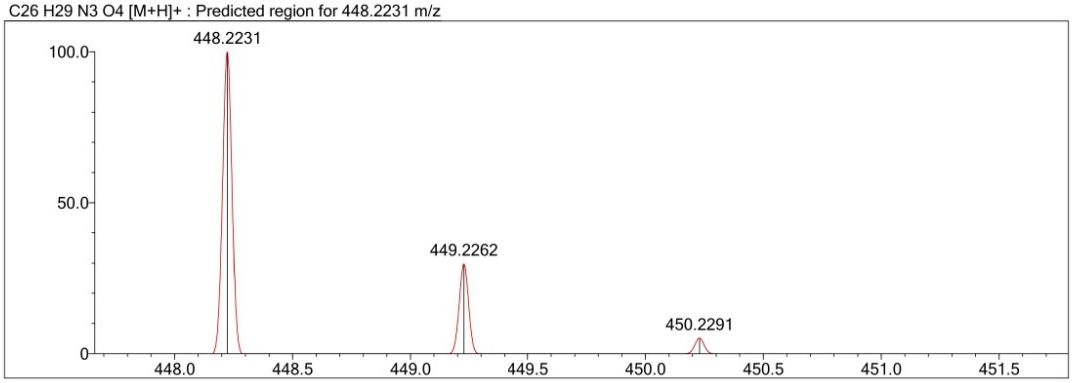
Event#: 1 MS(E+) Ret. Time : 2.027 Scan# : 305



Measured region for 448.2248 m/z



C26 H29 N3 O4 [M+H]+ : Predicted region for 448.2231 m/z



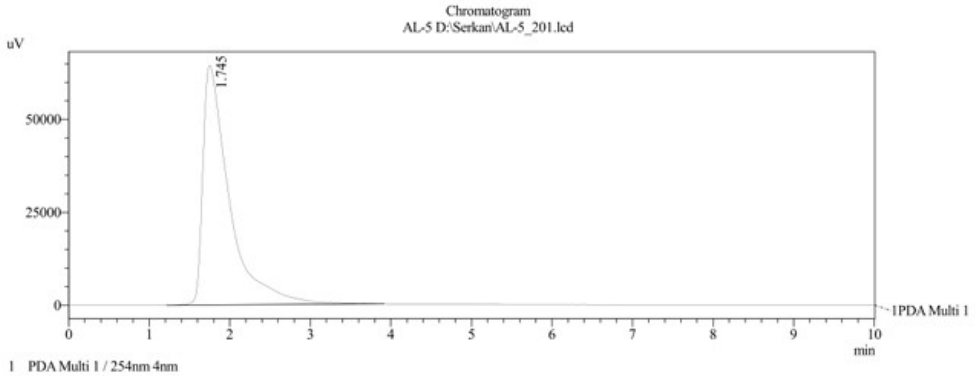
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	60.88	C26 H29 N3 O4	[M+H]+	448.2248	448.2231	1.7	3.79	65.44	14.0

Figure S24. HRMS spectra of compound **4e**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-5
Sample ID	:
Vail #	: 5
Injection Volume	: 0.5 uL
Data File Name	: AL-5_201.lcd
Method File Name	: isocratic_serkan.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 17:31:20
Data Processed	: 02.08.2022 17:41:22

<Chromatogram>



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	1.745	1480377	64508	100.000
Total		1480377	64508	100.000

Figure 25. HPLC chromatogram of compound **4e**

DOPNALAB

	Item	Value
	Acquired Date&Time	17.05.2023 15:25:31
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-61.ispd
	Spectrum name	AL-61
	Sample name	AL-6
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

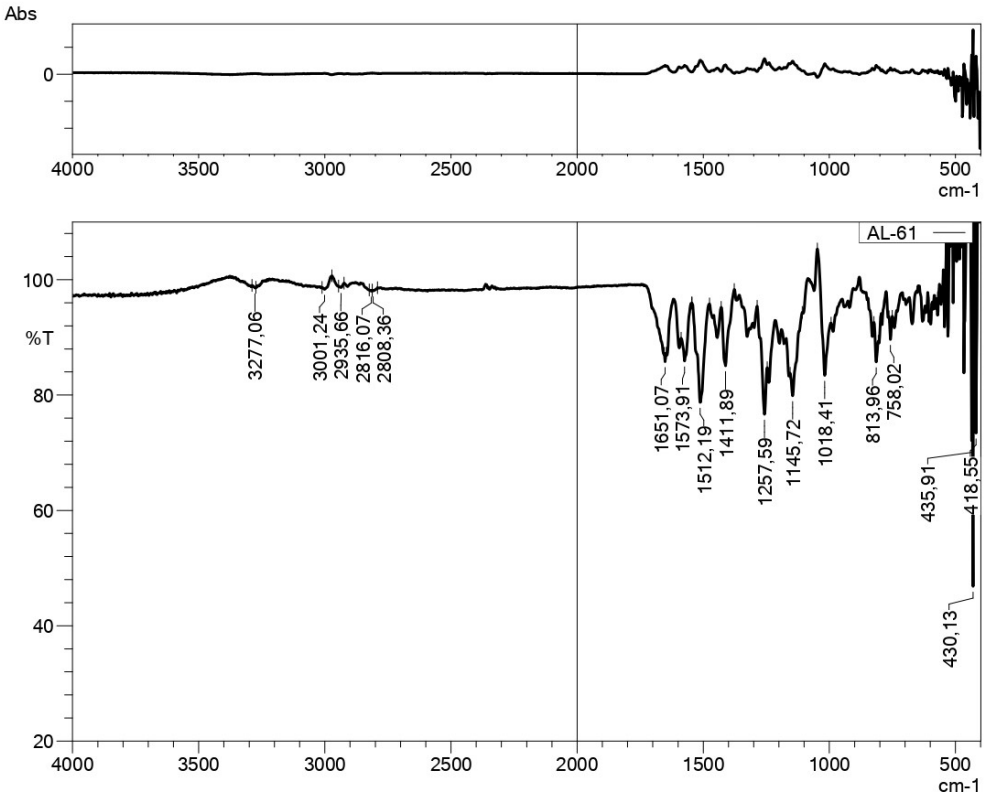


Figure S26. FTIR spectra of compound **4f**

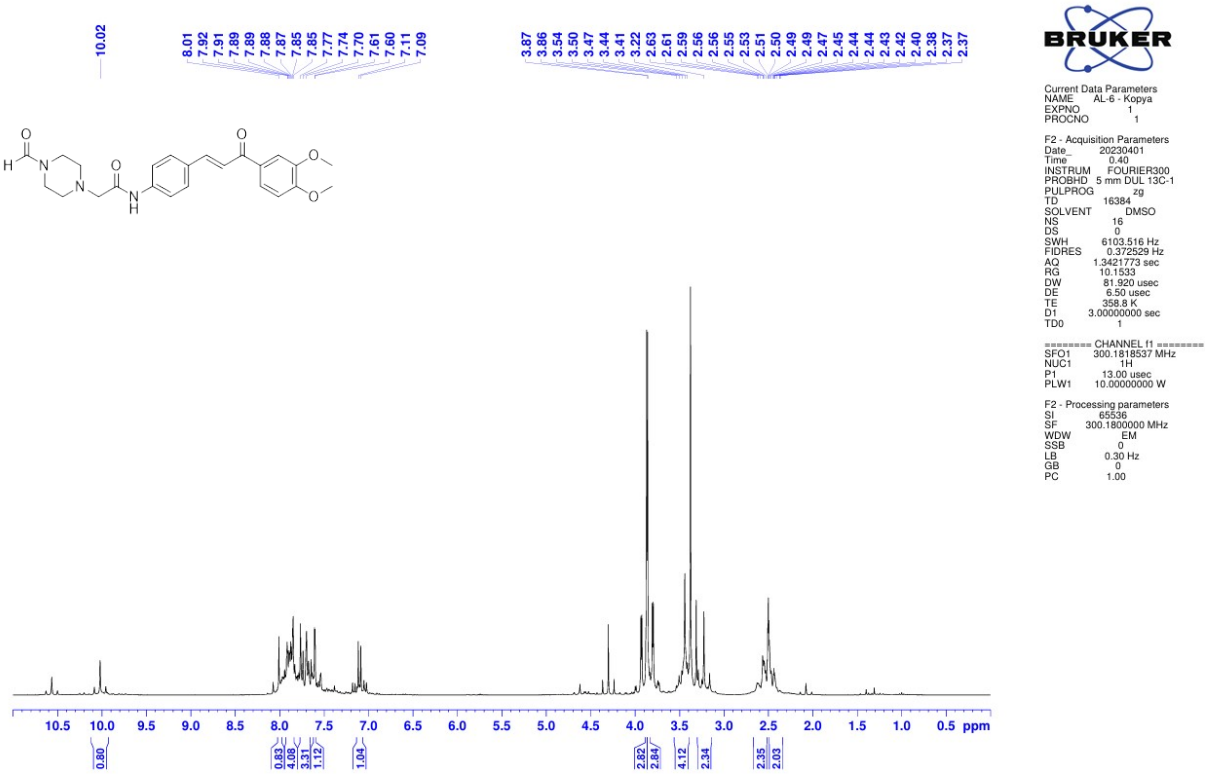


Figure S27. ^{1}H-NMR spectra of compound **4f**

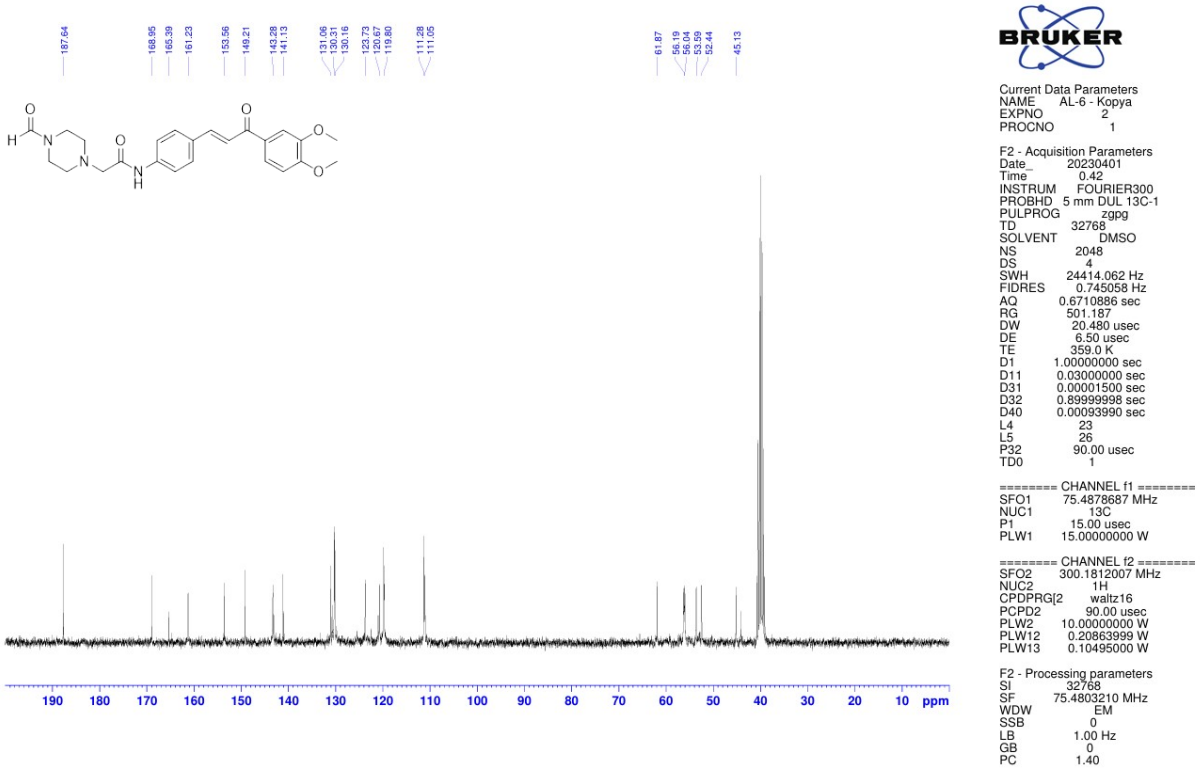


Figure S28. ^{13}C-NMR spectra of compound **4f**

Formula Predictor Report - AL-6_202.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-6_202.lcd

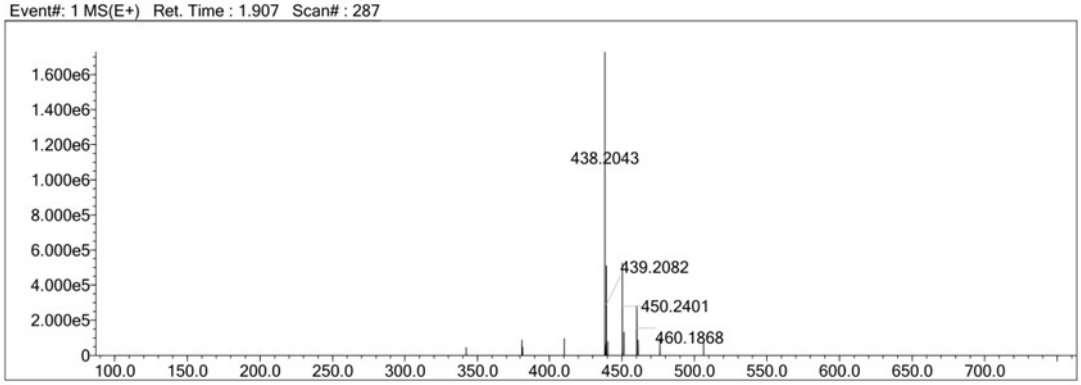
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

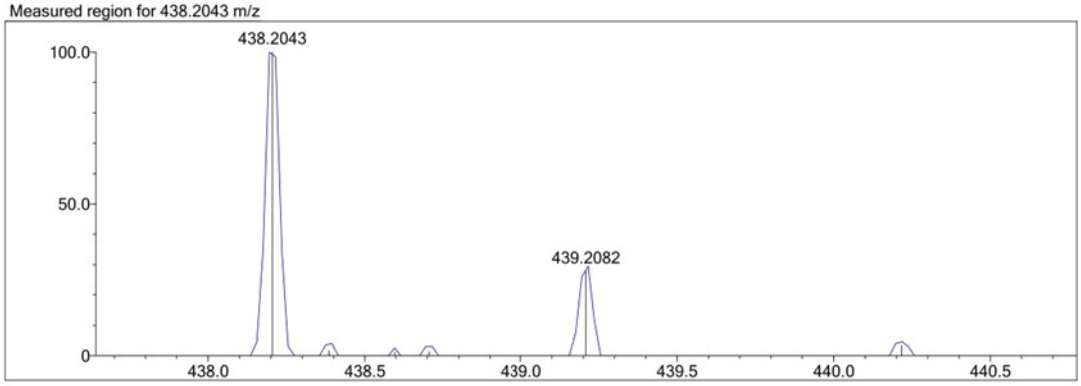
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

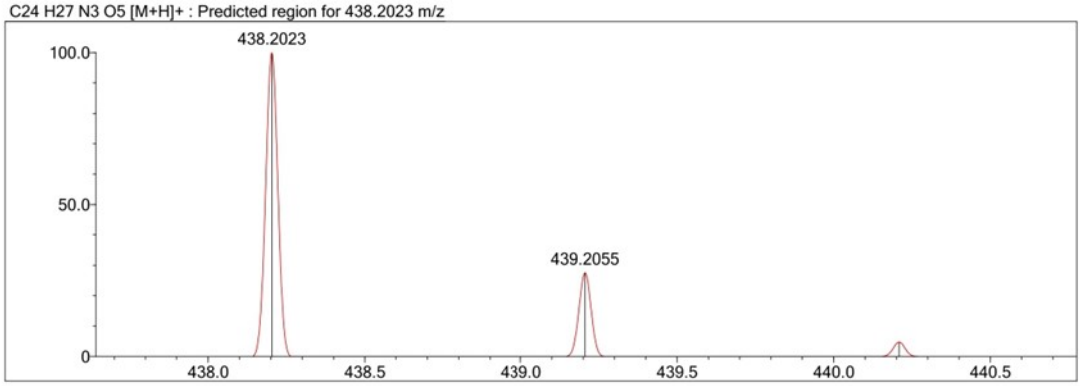
Event#: 1 MS(E+) Ret. Time : 1.907 Scan# : 287



Measured region for 438.2043 m/z



C24 H27 N3 O5 [M+H]+ : Predicted region for 438.2023 m/z



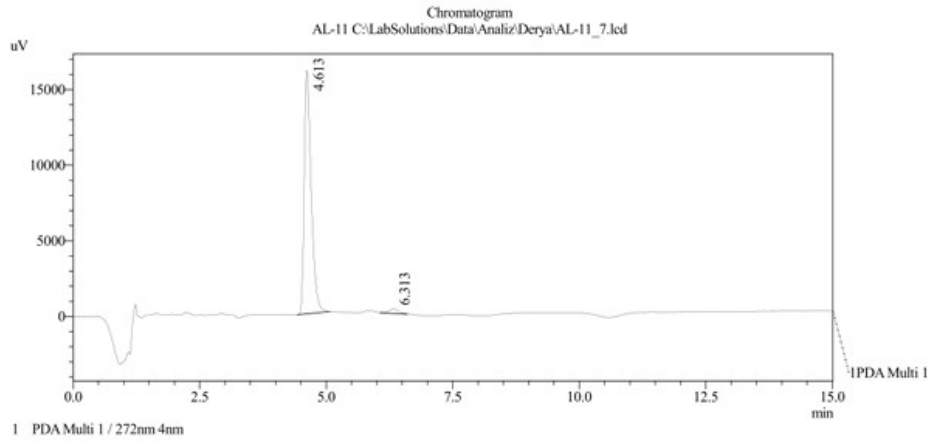
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	78.70	C24 H27 N3 O5	[M+H]+	438.2043	438.2023	2.0	4.56	86.39	13.0

Figure S29. HRMS spectra of compound **4f**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-6
Sample ID	:
Vail #	: 6
Injection Volume	: 1 uL
Data File Name	: AL-6_202.lcd
Method File Name	: isocratic_serkan-15DK.lcm
Batch File Name	: 1.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 17:42:05
Data Processed	: 08.09.2025 13:28:08

<Chromatogram>



1 PDA Multi 1 / 272nm 4nm

PeakTable

PDA Ch1 272nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	4.613	154083	16100	97.584
2	6.313	3815	289	2.416
Total		157898	16389	100.000

Figure S30. HPLC chromatogram of compound **4f**

DOPNALAB

	Item	Value
	Acquired Date&Time	17.05.2023 15:31:40
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-71.ispd
	Spectrum name	AL-71
	Sample name	AL-7
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

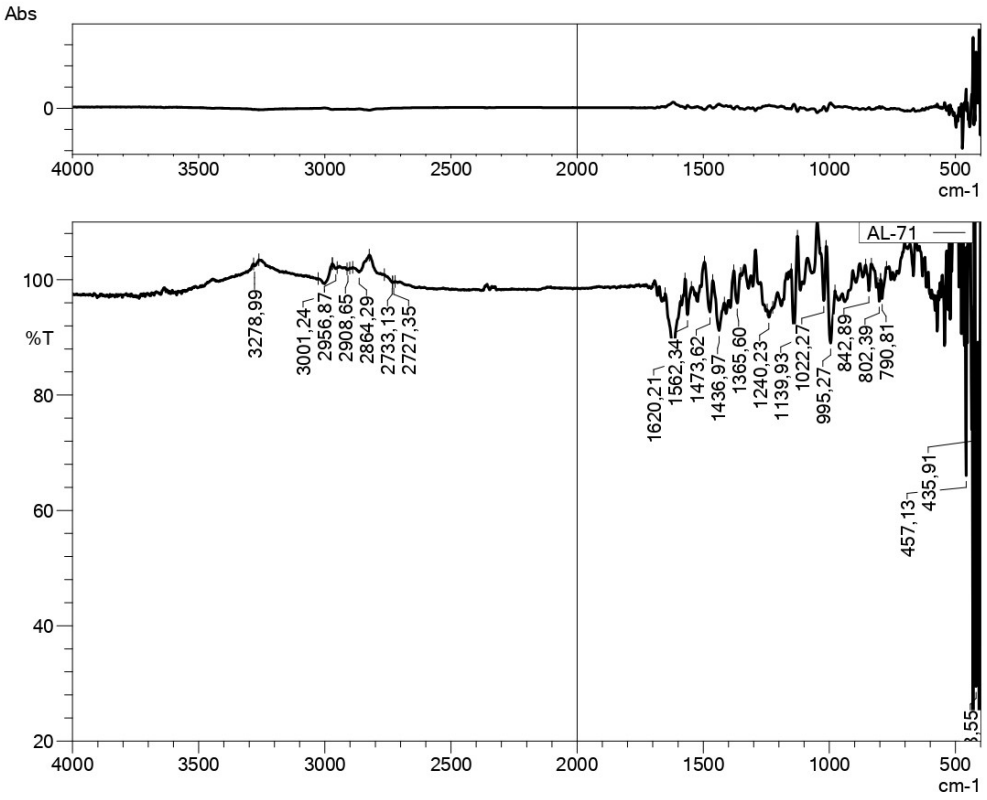
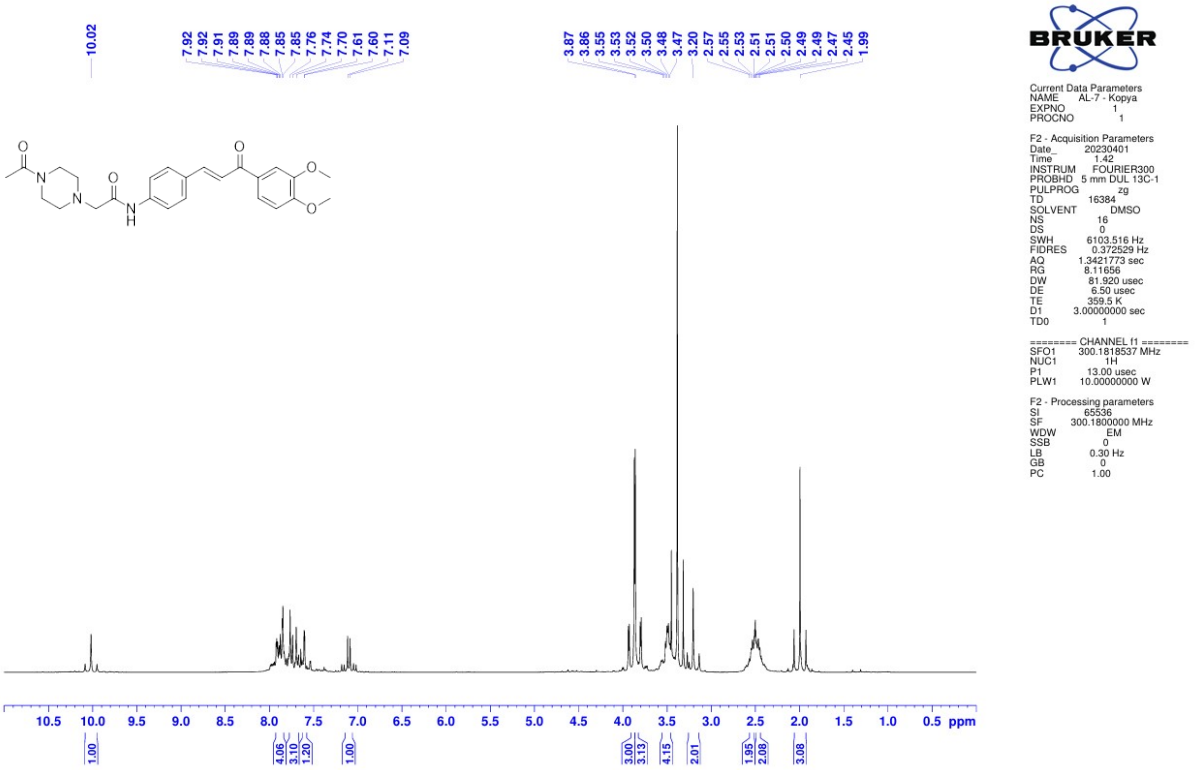


Figure S31. FTIR spectra of compound **4g**



BRUKER

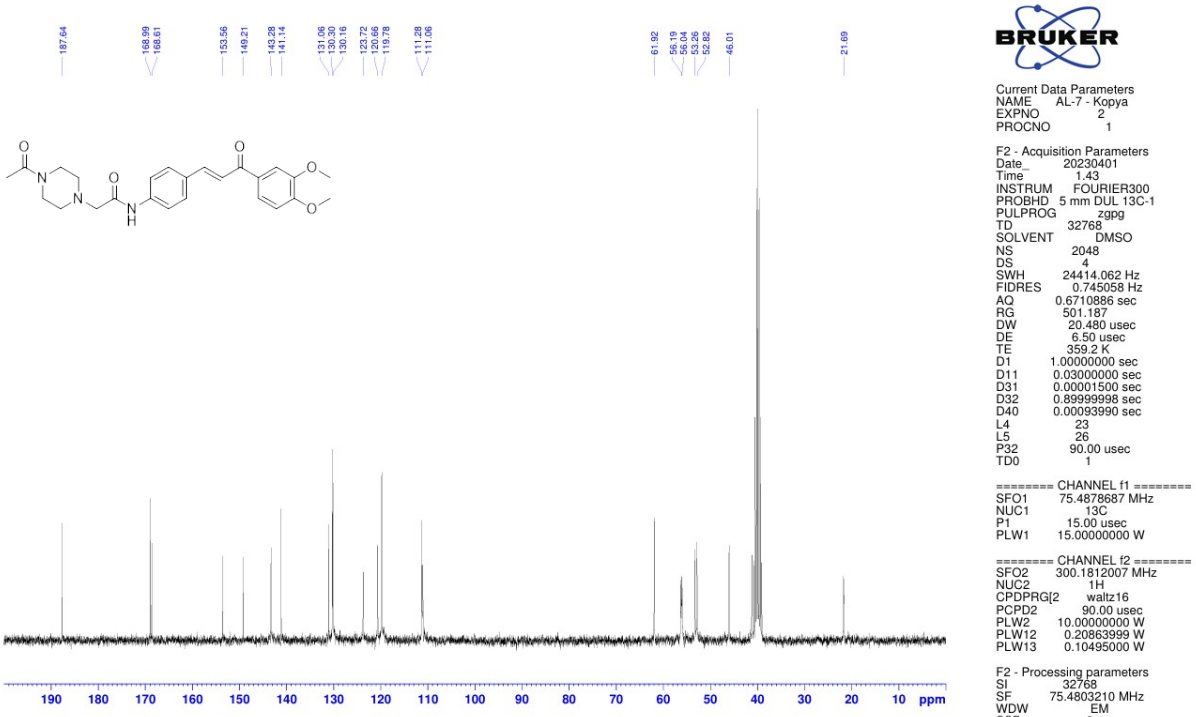
Current Data Parameters
NAME AL-7 - Kopya
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230401
Time 1.42
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6103.516 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 8.11656
DW 81.920 usec
DE 6.50 usec
TE 359.5 K
D1 3.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S32. ^{1}H-NMR spectra of compound **4g**



BRUKER

Current Data Parameters
NAME AL-7 - Kopya
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230401
Time 1.43
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 2048
DS 4
SWH 24414.062 Hz
FIDRES 0.745058 Hz
AQ 0.6710886 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 359.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D32 0.89999998 sec
D40 0.00093990 sec
L4 23
L5 26
P32 90.00 usec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.00000000 W

======== CHANNEL f2 ========
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.20863999 W
PLW13 0.10495000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S33. ^{13}C-NMR spectra of compound **4g**

Formula Predictor Report - AL-7_203.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-7_203.lcd

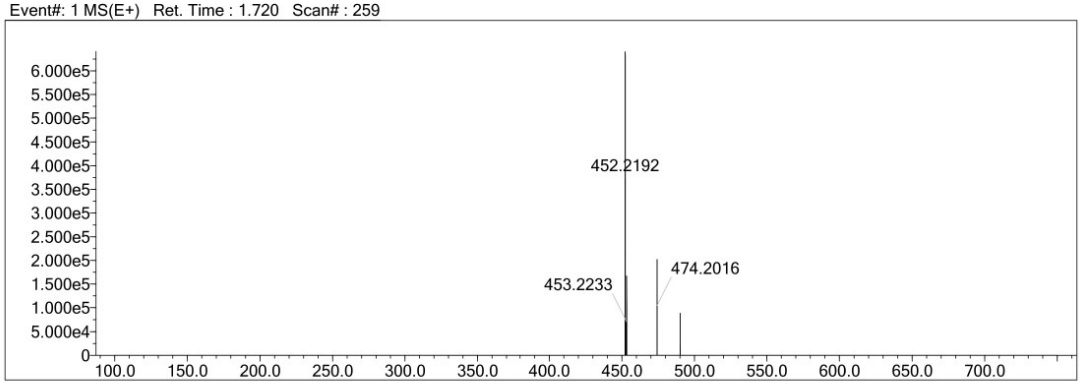
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

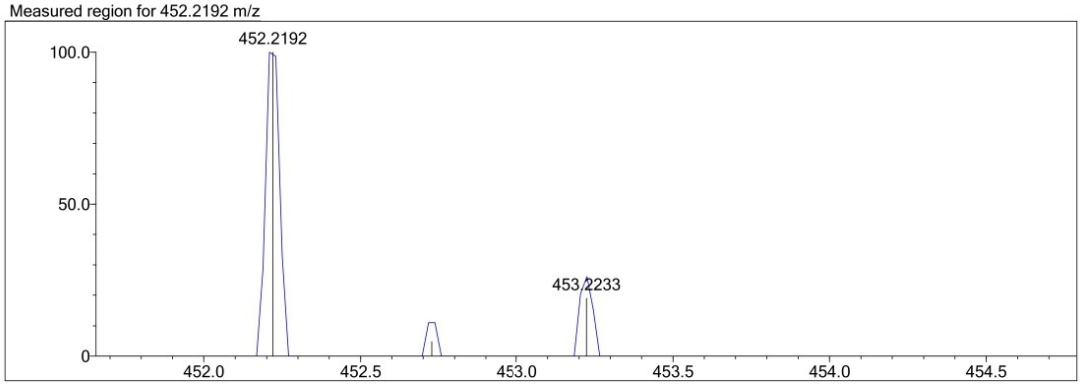
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

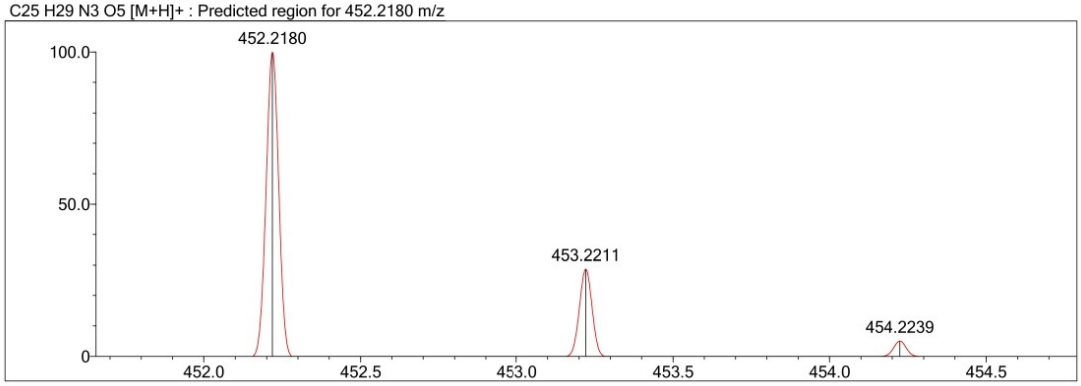
Event#: 1 MS(E+) Ret. Time : 1.720 Scan# : 259



Measured region for 452.2192 m/z



C25 H29 N3 O5 [M+H]+ : Predicted region for 452.2180 m/z



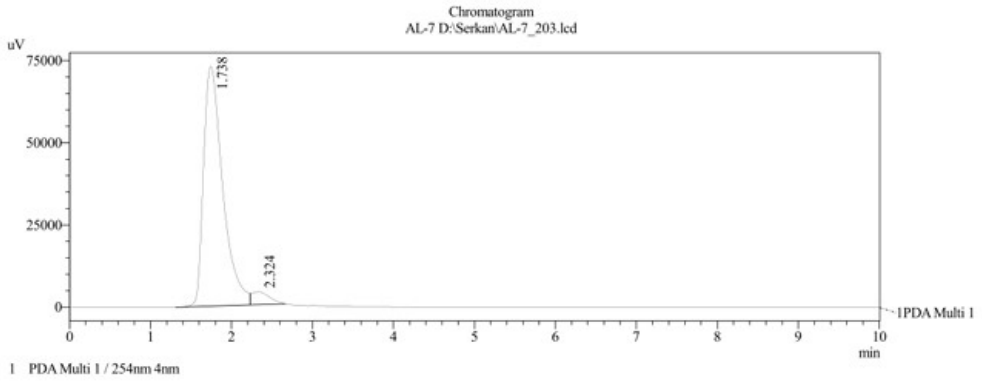
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	85.47	C25 H29 N3 O5	[M+H]+	452.2192	452.2180	1.2	2.65	89.15	13.0

Figure S34. HRMS spectra of compound **4g**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-7
Sample ID	:
Vail #	: 7
Injection Volume	: 0.5 uL
Data File Name	: AL-7_203.lcd
Method File Name	: isocratic_serkan.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 17:52:52
Data Processed	: 04.09.2025 10:55:36

<Chromatogram>



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	1.738	1202534	72994	95.322
2	2.324	59018	3885	4.678
Total		1261551	76879	100.000

Figure S35. HPLC chromatogram of compound **4g**

DOPNALAB

	Item	Value
	Acquired Date&Time	17.05.2023 15:37:31
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-81.ispd
	Spectrum name	AL-81
	Sample name	AL-8
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

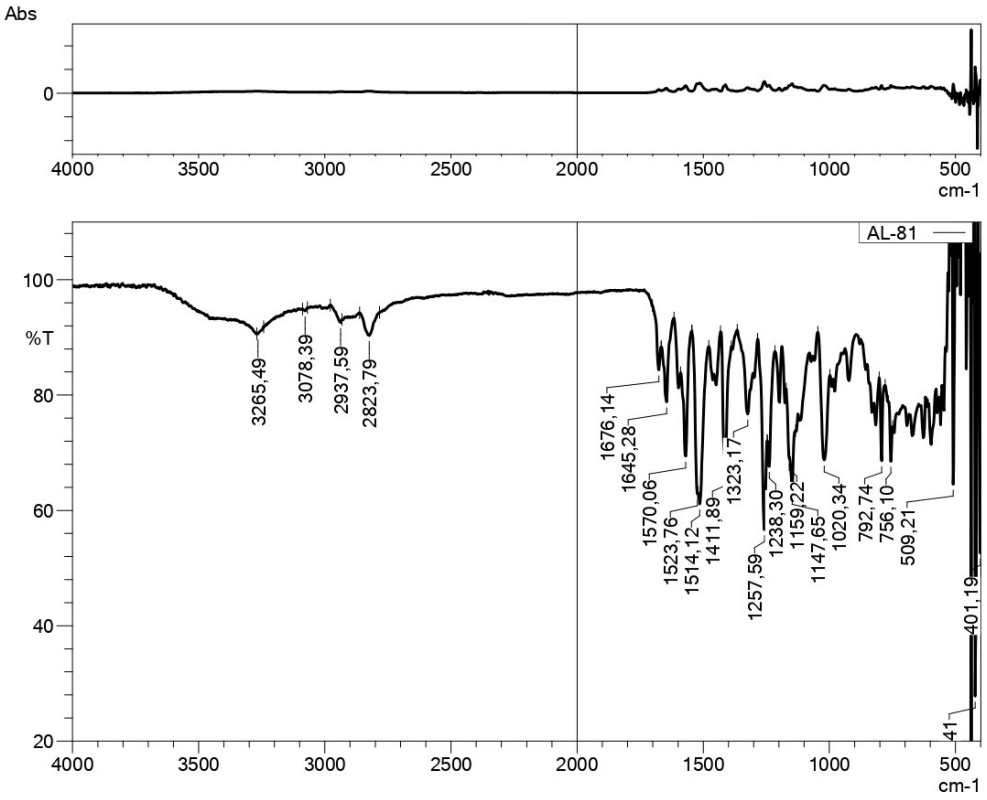
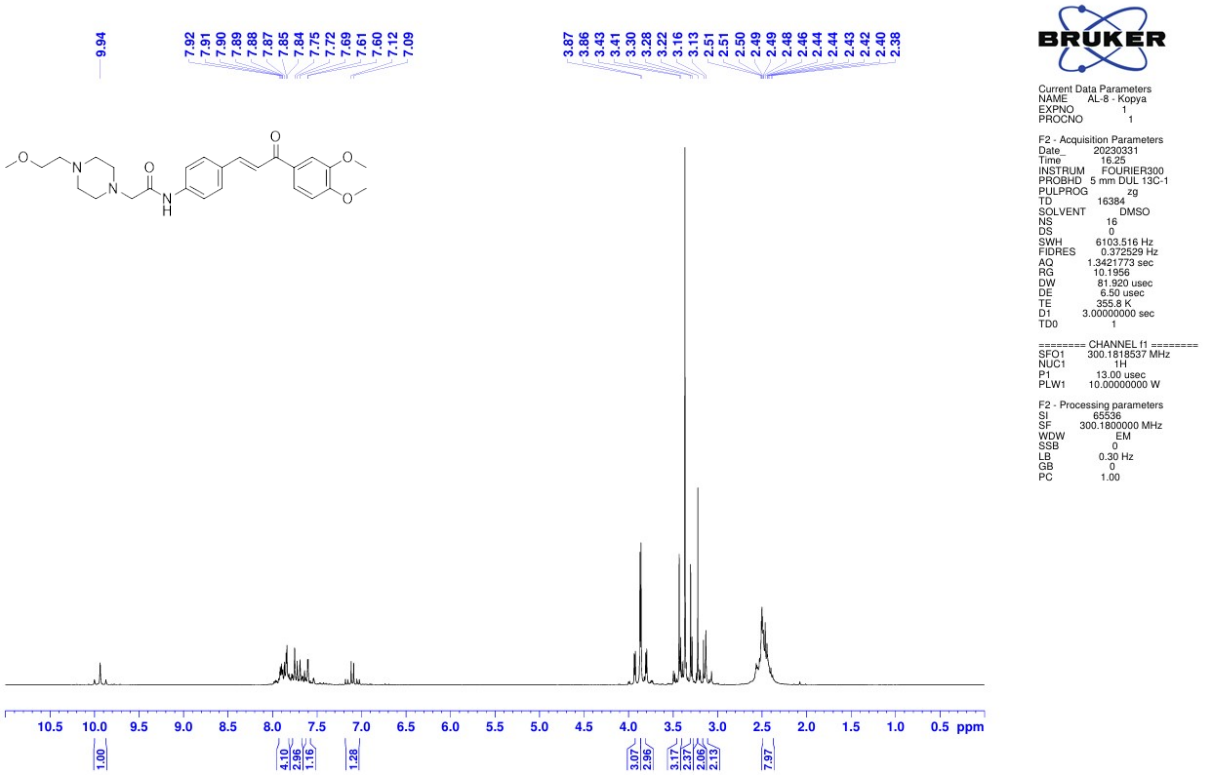


Figure 36. FTIR spectra of compound **4h**



BRUKER

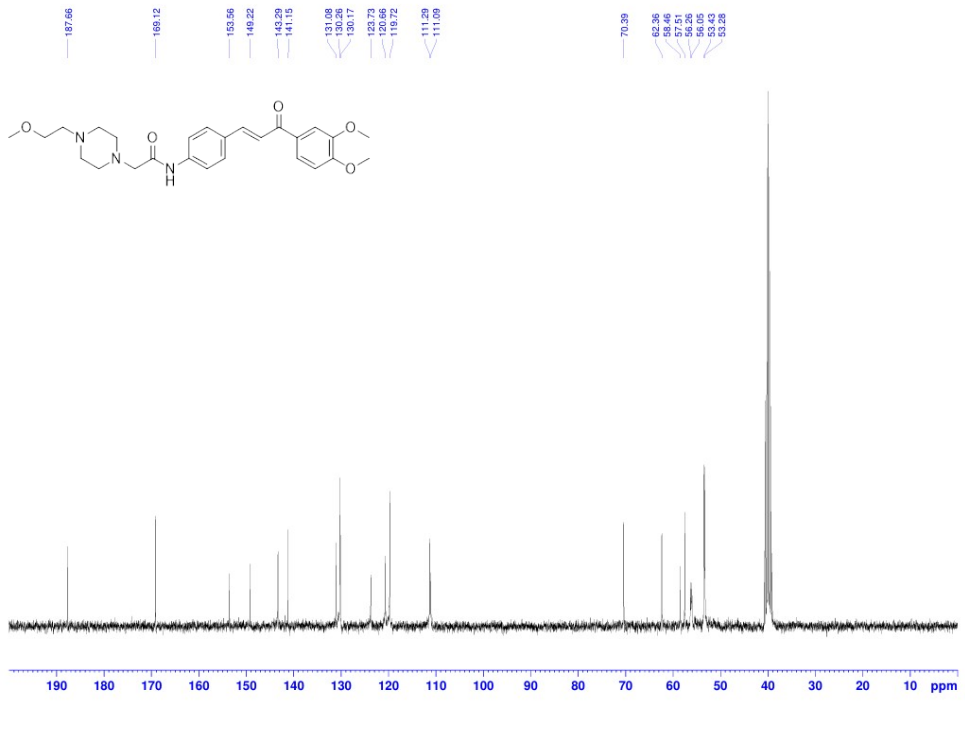
Current Data Parameters
NAME AL-8 - Kopya
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230331
Time 16.25
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6103.516 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 10.1956
DW 81.920 usec
DE 6.50 usec
TE 355.8 K
D1 3.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S37. ^{1}H-NMR spectra of compound **4h**



BRUKER

Current Data Parameters
NAME AL-8 - Kopya
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230331
Time 16.27
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 2048
DS 4
SWH 24414.062 Hz
FIDRES 0.745058 Hz
AQ 0.6710886 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 355.6 K
D1 1.00000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D32 0.89999998 sec
D40 0.00093990 sec
L4 23
L5 26
P32 90.00 usec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.00000000 W

======== CHANNEL f2 ========
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.20863999 W
PLW13 0.10495000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S38. ^{13}C-NMR spectra of compound **4h**

Formula Predictor Report - AL-8_204.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-8_204.lcd

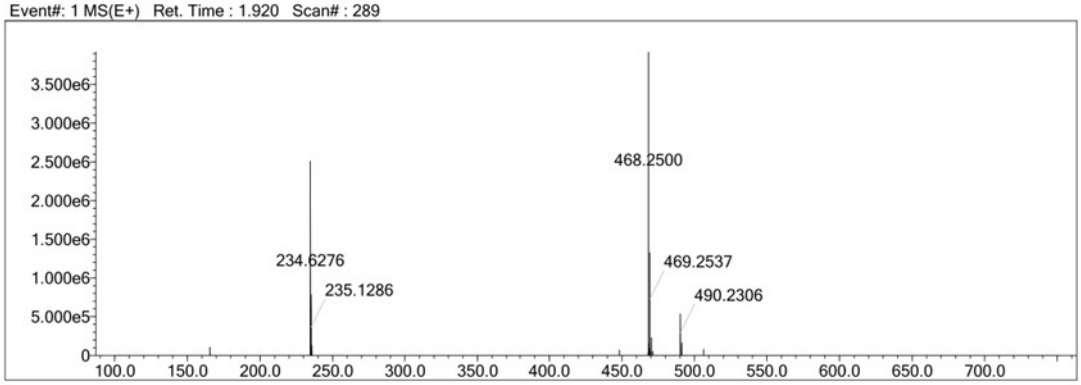
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	33	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

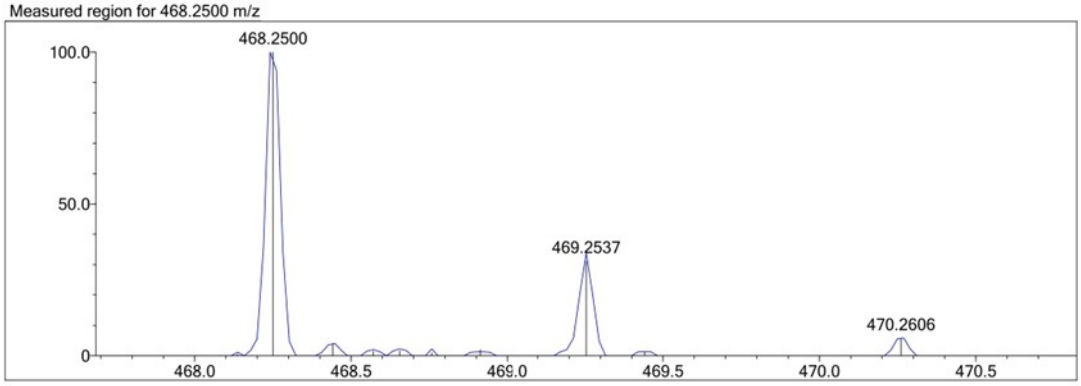
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

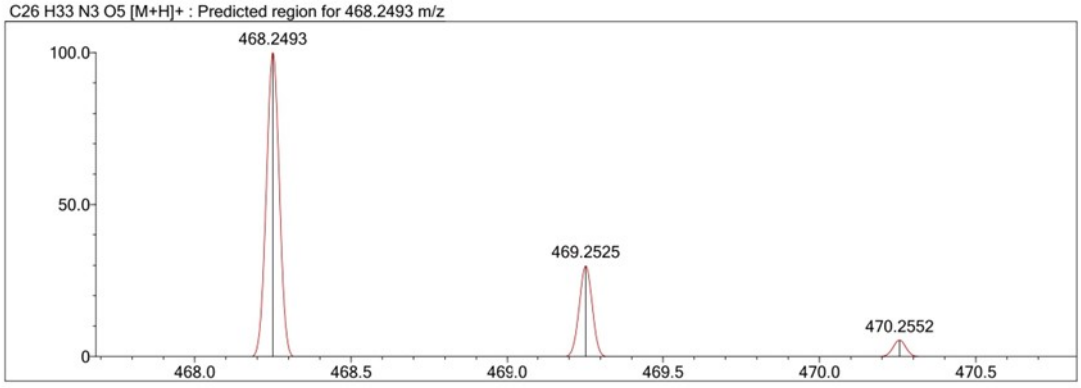
Event#: 1 MS(E+) Ret. Time : 1.920 Scan# : 289



Measured region for 468.2500 m/z



C26 H33 N3 O5 [M+H]+ : Predicted region for 468.2493 m/z



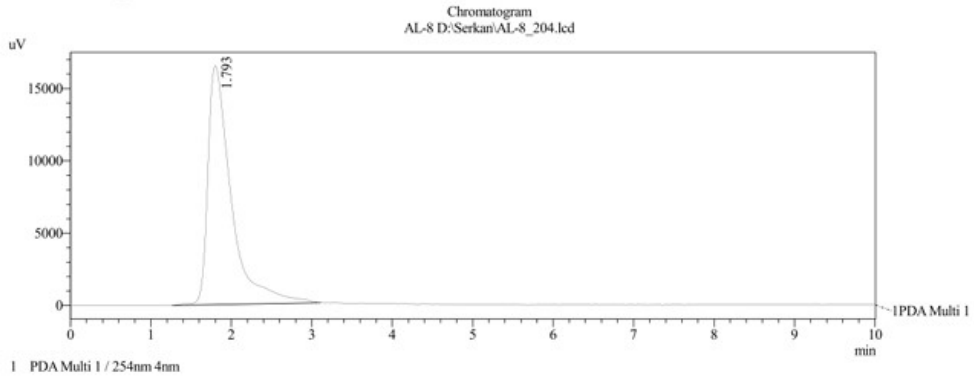
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	97.82	C26 H33 N3 O5	[M+H]+	468.2500	468.2493	0.7	1.49	99.03	12.0

Figure S39. HRMS spectra of compound **4h**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-8
Sample ID	:
Vail #	: 8
Injection Volume	: 0.5 uL
Data File Name	: AL-8_204.lcd
Method File Name	: isocratic_serkan.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 18:03:41
Data Processed	: 04.09.2025 10:44:17

<Chromatogram>



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	1.793	334610	16510	100.000
Total		334610	16510	100.000

Figure S40. HPLC chromatogram of compound **4h**

DOPNALAB

	Item	Value
	Acquired Date&Time	17.05.2023 15:42:32
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-91.ispd
	Spectrum name	AL-91
	Sample name	AL-9
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

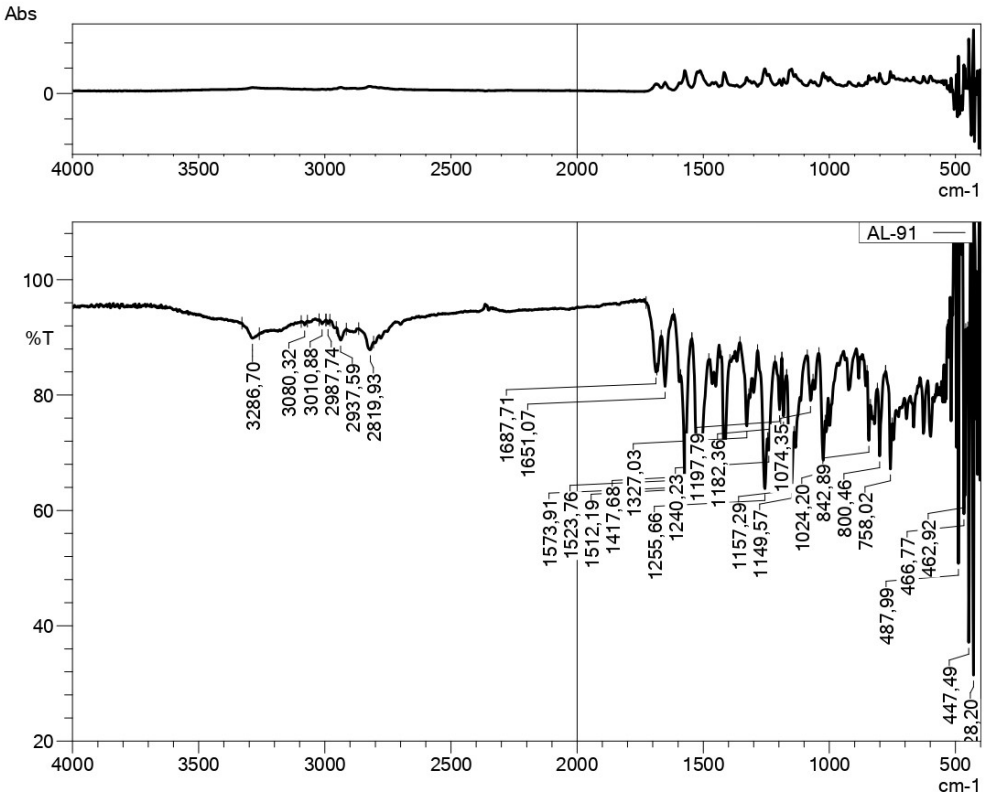


Figure S41. FTIR spectra of compound **4i**

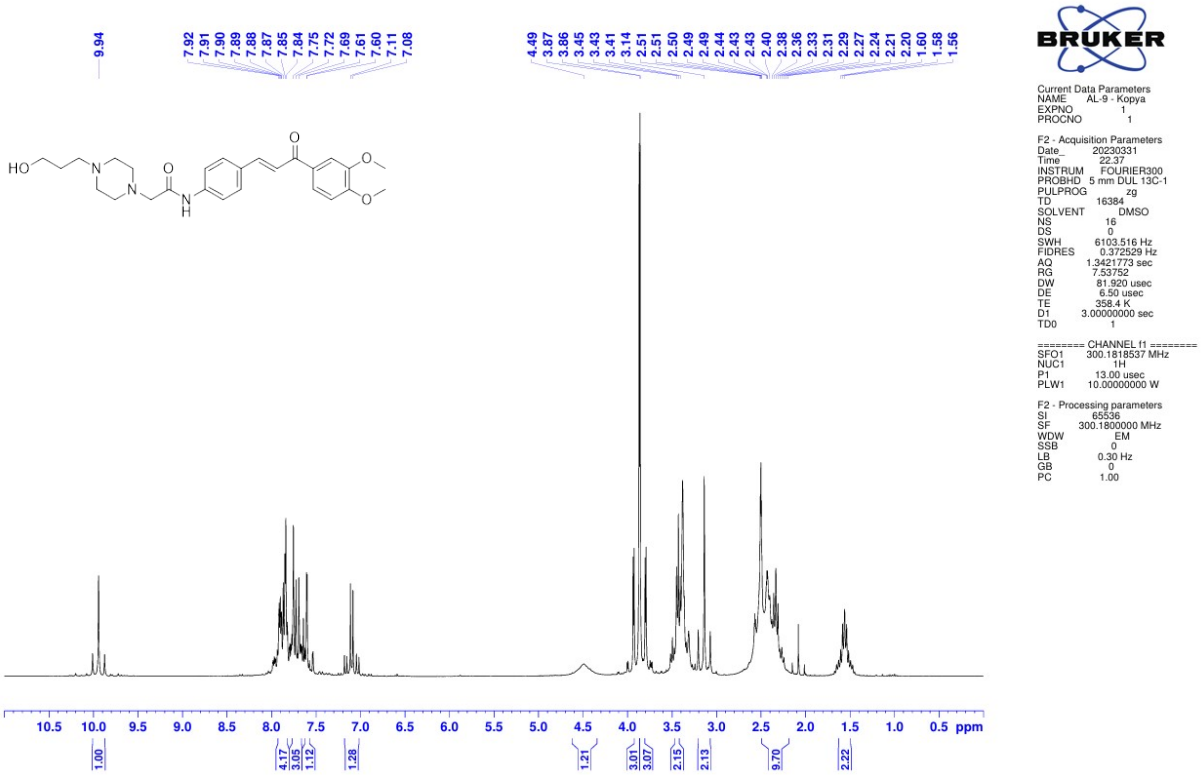


Figure S42. ^{1}H-NMR spectra of compound **4i**

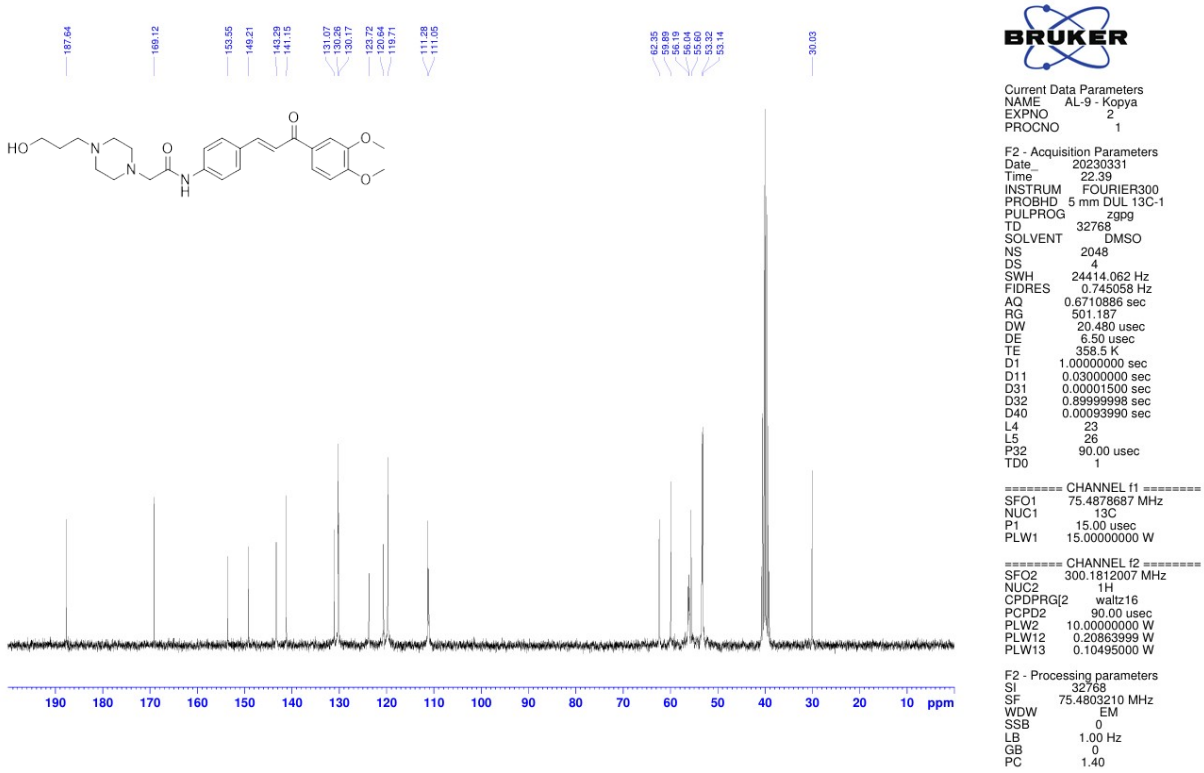


Figure S43. ^{13}C-NMR spectra of compound **4i**

Formula Predictor Report - AL-9_205.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-9_205.lcd

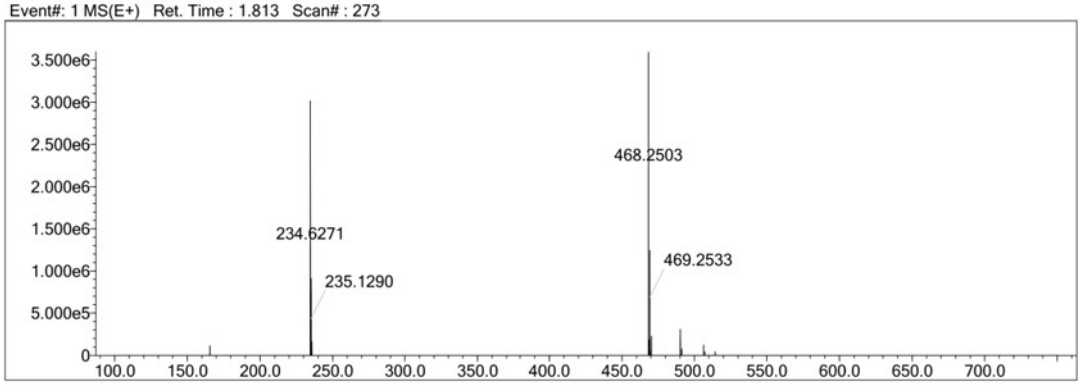
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	33	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

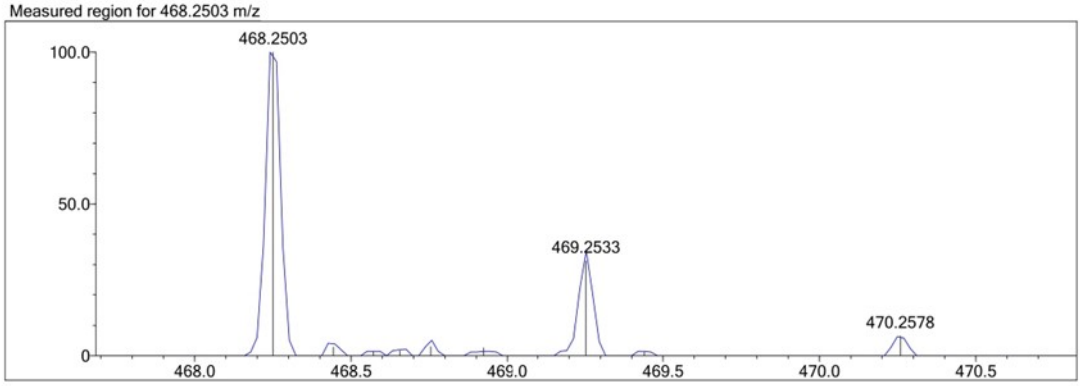
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

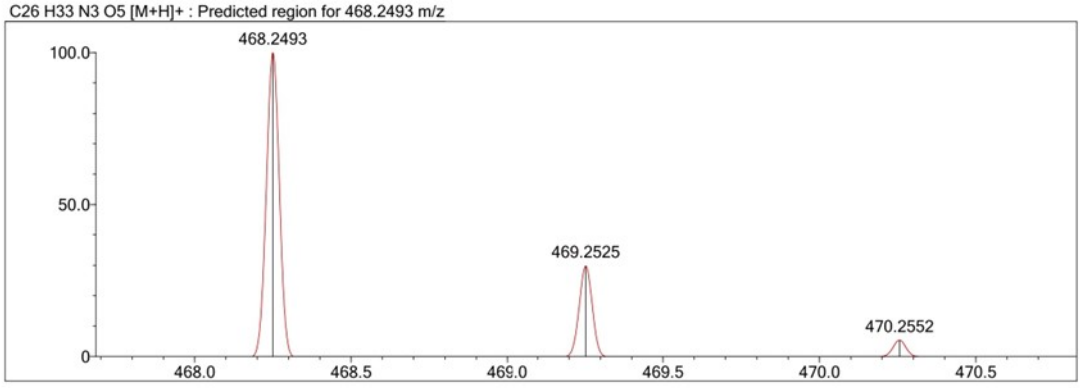
Event#: 1 MS(E+) Ret. Time : 1.813 Scan# : 273



Measured region for 468.2503 m/z



C26 H33 N3 O5 [M+H]+ : Predicted region for 468.2493 m/z



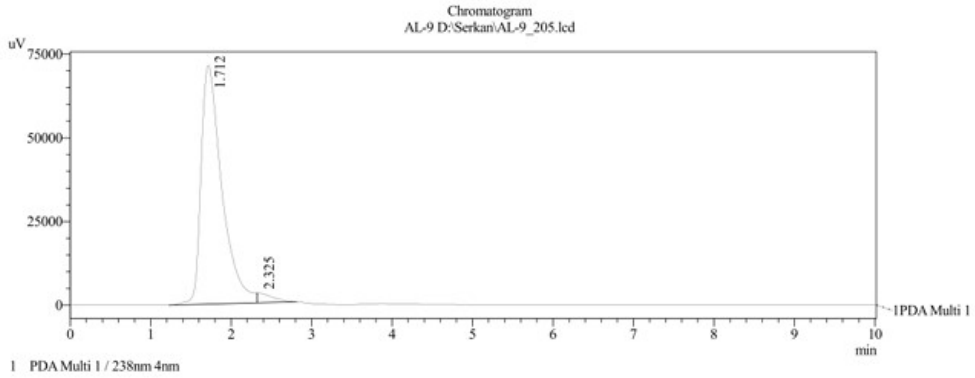
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	94.46	C26 H33 N3 O5	[M+H]+	468.2503	468.2493	1.0	2.14	97.23	12.0

Figure S44. HRMS spectra of compound **4i**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-9
Sample ID	:
Vail #	: 9
Injection Volume	: 0.5 uL
Data File Name	: AL-9_205.lcd
Method File Name	: isocratic_serkan.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 18:14:31
Data Processed	: 04.09.2025 10:45:40

<Chromatogram>



PeakTable

PDA Ch1 238nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	1.712	1285440	71375	97.133
2	2.325	37937	2954	2.867
Total		1323377	74329	100.000

Figure S45. HPLC chromatogram of compound **4i**

DOPNALAB

	Item	Value
	Acquired Date&Time	17.05.2023 15:46:43
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-101.ispd
	Spectrum name	AL-101
	Sample name	AL-10
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

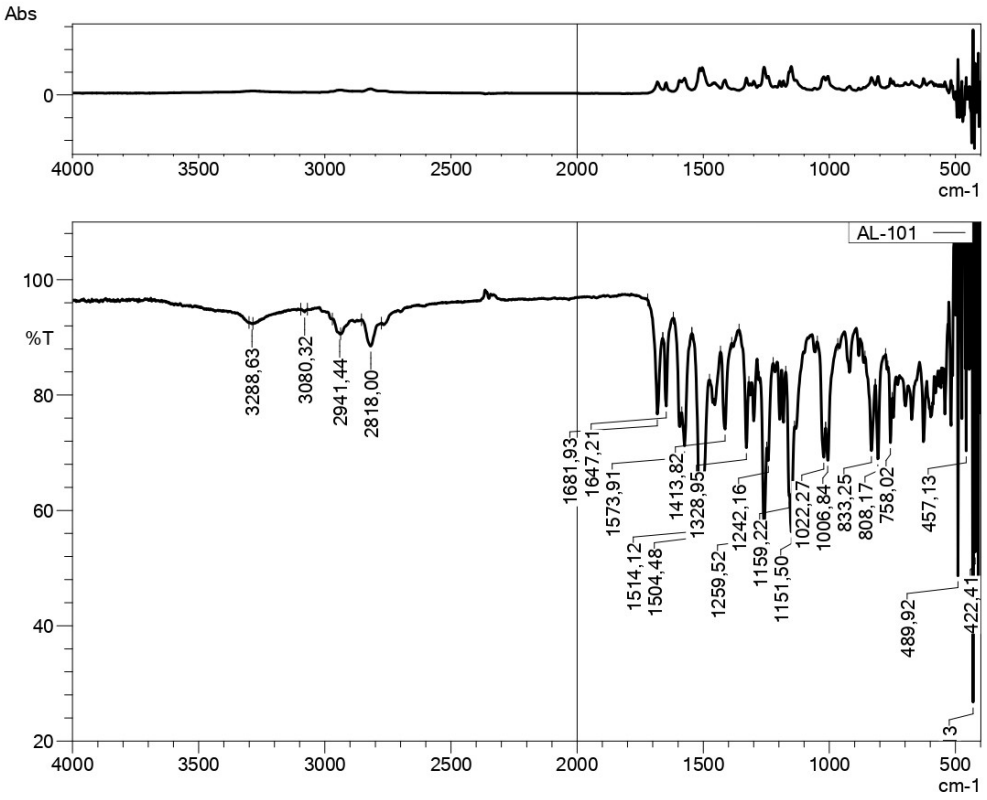
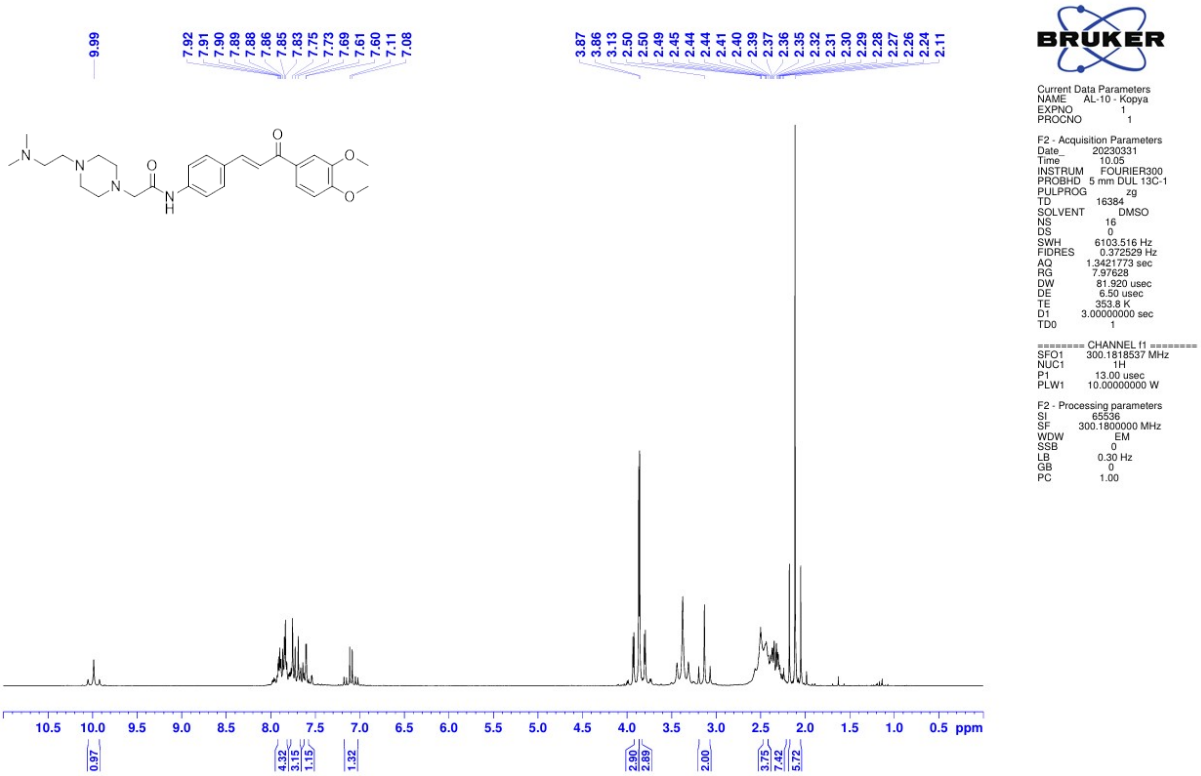


Figure S46. FTIR spectra of compound **4j**



BRUKER

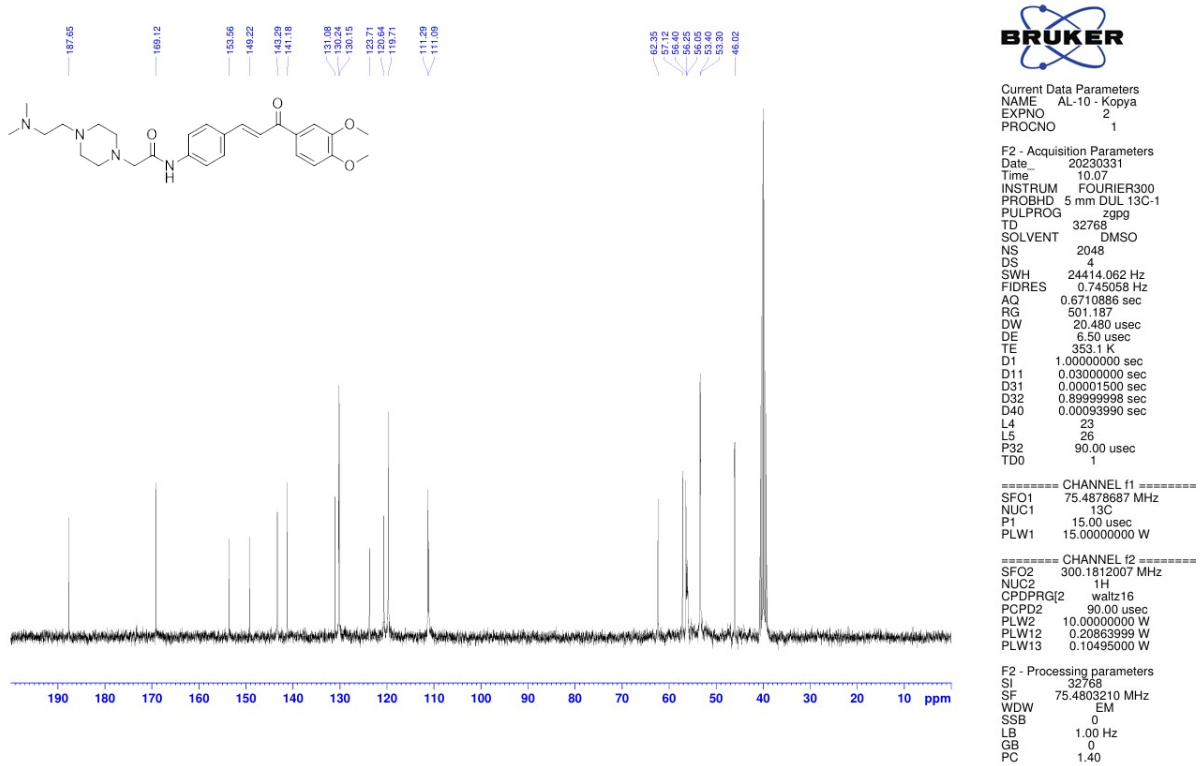
Current Data Parameters
NAME AL-10 - Kopya
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230331
Time 10.05
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6103.516 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 7.97628
DW 81.920 usec
DE 6.50 usec
TE 353.8 K
D1 3.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S47. ^{1}H-NMR spectra of compound **4j**



BRUKER

Current Data Parameters
NAME AL-10 - Kopya
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230331
Time 10.07
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 2048
DS 4
SWH 24414.062 Hz
FIDRES 0.745058 Hz
AQ 0.6710886 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 353.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D32 0.89999998 sec
D40 0.00093990 sec
L4 23
L5 26
P32 90.00 usec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.00000000 W

======== CHANNEL f2 ========
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.20863999 W
PLW13 0.10495000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S48. ^{13}C-NMR spectra of compound **4j**

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-10_206.lcd

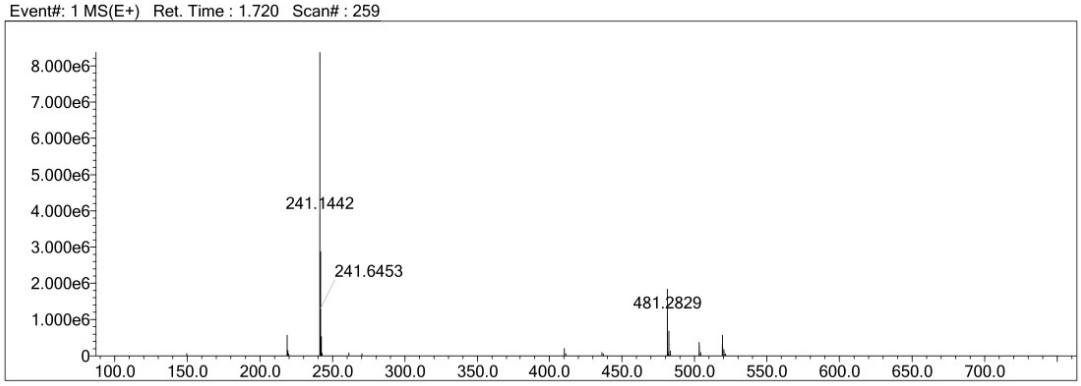
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	36	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

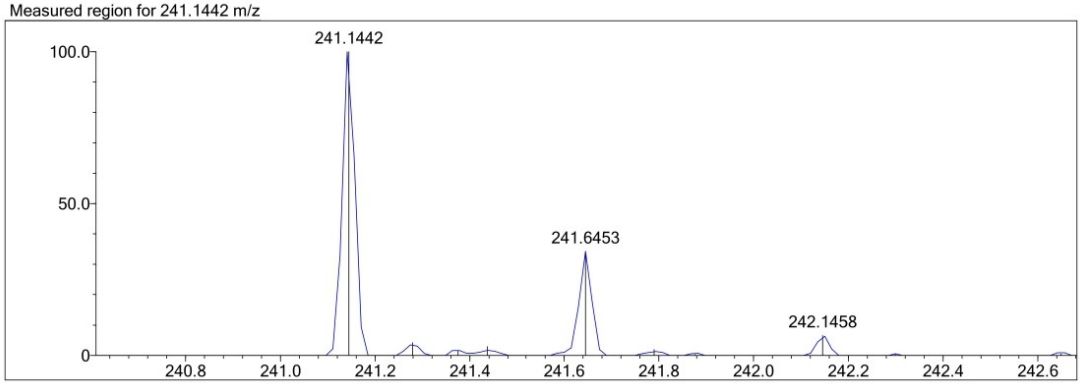
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

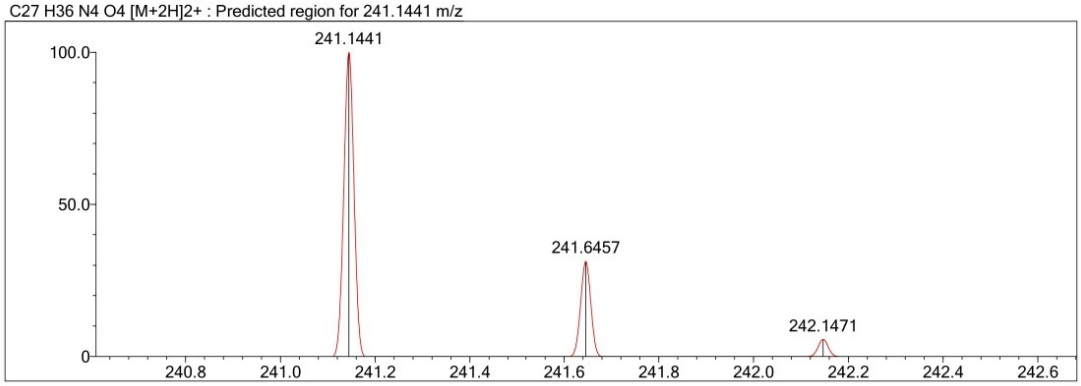
Event#: 1 MS(E+) Ret. Time : 1.720 Scan# : 259



Measured region for 241.1442 m/z



C27 H36 N4 O4 [M+2H]2+ : Predicted region for 241.1441 m/z



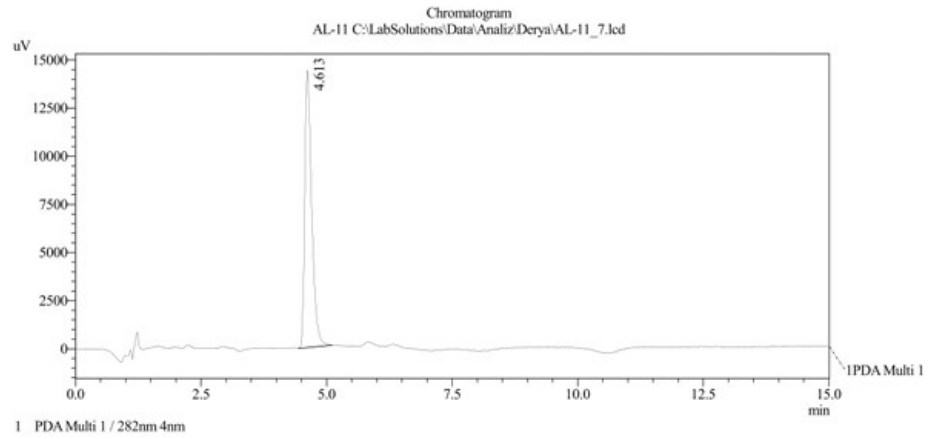
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	80.57	C27 H36 N4 O4	[M+2H]2+	241.1442	241.1441	0.1	0.41	80.57	12.0

Figure S49. HRMS spectra of compound **4j**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-10
Sample ID	:
Vail #	: 10
Injection Volume	: 1 uL
Data File Name	: AL-10_206.lcd
Method File Name	: isocratic_serkan-15DK.lcm
Batch File Name	: 1.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 18:25:18
Data Processed	: 09.09.2025 10:09:17

<Chromatogram>



PeakTable

PDA Ch1 282nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	4.613	138184	14404	100.000
Total		138184	14404	100.000

Figure S50. HPLC chromatogram of compound **4j**

DOPNALAB

	Item	Value
	Acquired Date&Time	17.05.2023 15:50:52
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-111.ispd
	Spectrum name	AL-111
	Sample name	AL-11
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

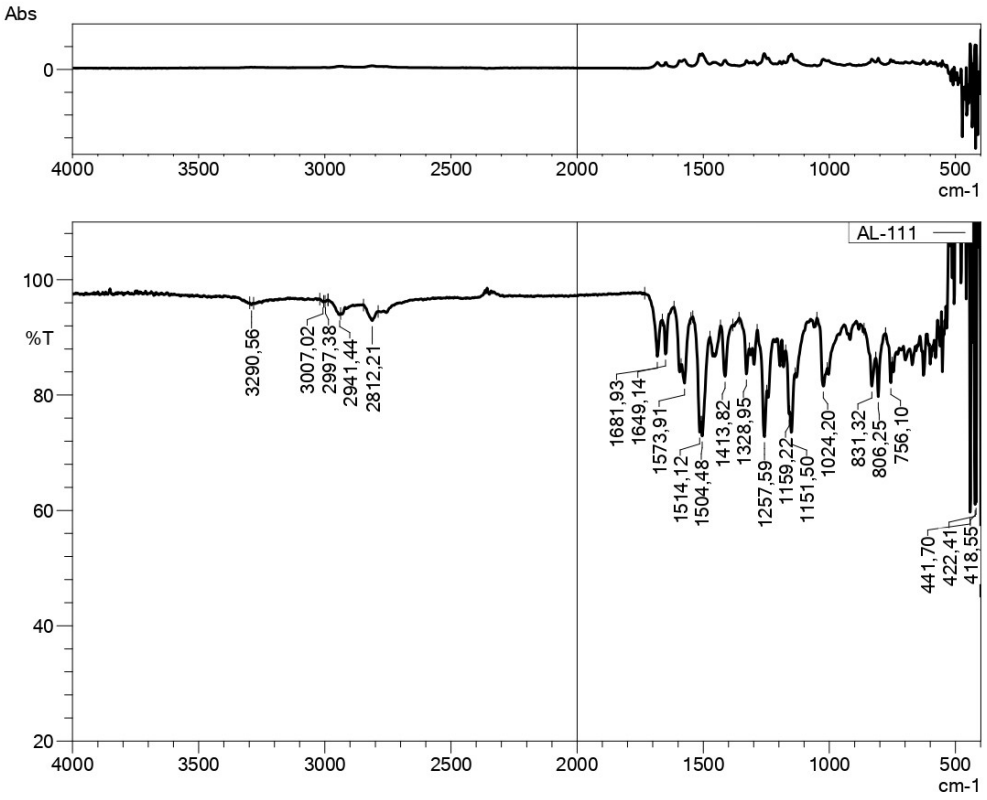
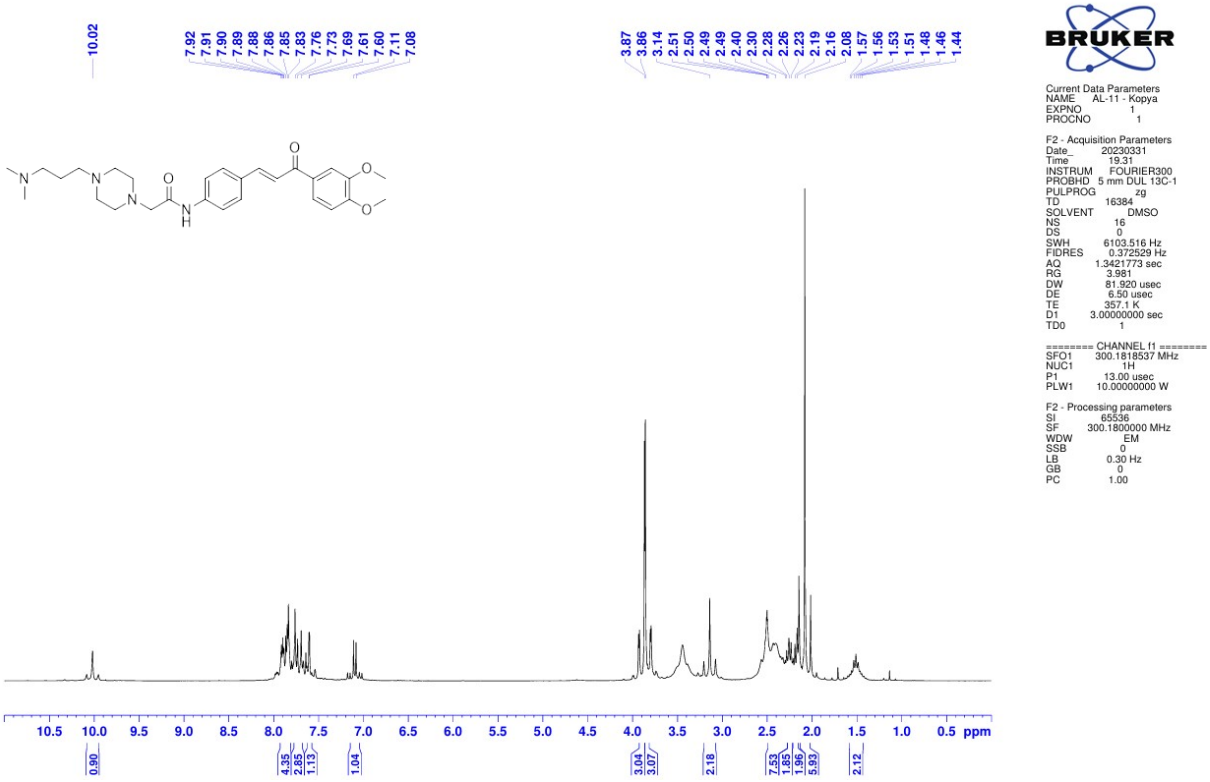


Figure S51. FTIR spectra of compound **4k**



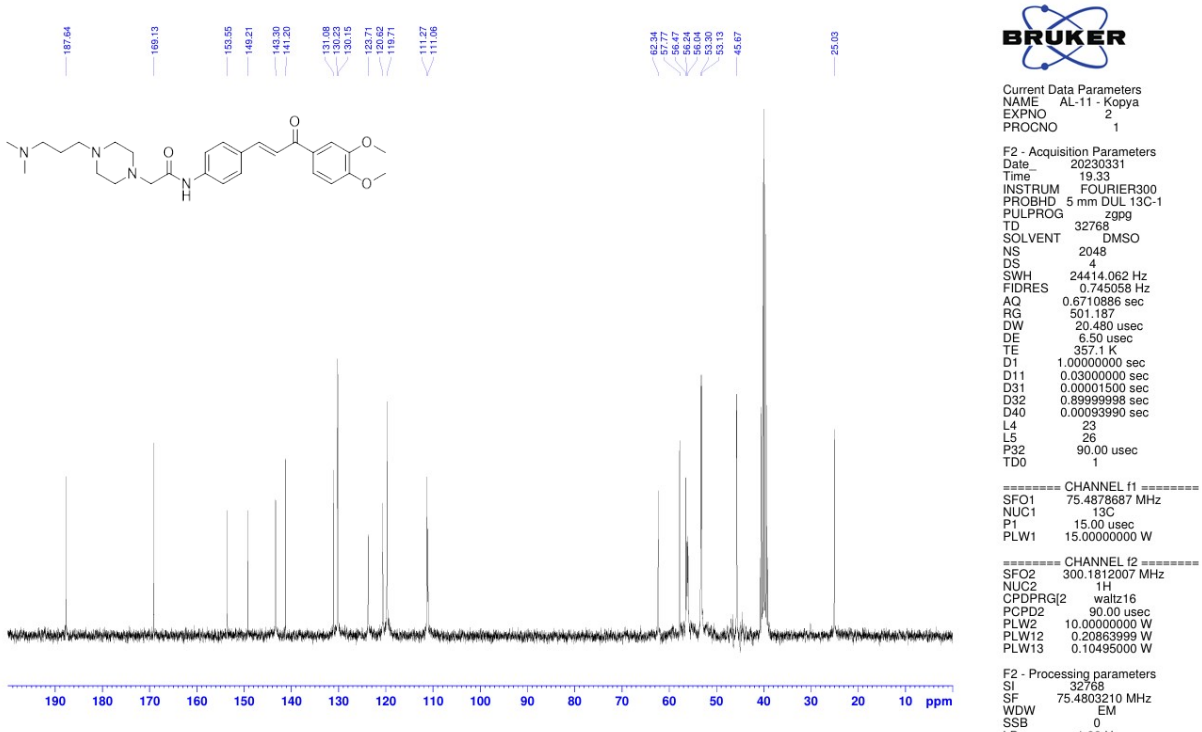

```
Current Data Parameters
NAME      AL-11 - Kopya
EXPNO             1
PROCNO            1

F2 - Acquisition Parameters
Date_       20230331
Time          19.31
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG           zg
TD             16384
SOLVENT         DMSO
NS                16
DS                 0
SWH          6103.516 Hz
FIDRES       0.372529 Hz
AQ           1.3421773 sec
RG                3.981
DW            81.920 usec
DE             6.50 usec
TE             357.1 K
D1          3.00000000 sec
TD0               1

======== CHANNEL f1 ========
SFO1       300.1818537 MHz
NUC1               1H
P1           13.00 usec
PLW1       10.00000000 W

F2 - Processing parameters
SI             65536
SF        300.1800000 MHz
WDW              EM
SSB               0
LB             0.30 Hz
GB                0
PC             1.00
```

Figure S52. ^{1}H-NMR spectra of compound **4k**




```
Current Data Parameters
NAME      AL-11 - Kopya
EXPNO             2
PROCNO            1

F2 - Acquisition Parameters
Date_       20230331
Time          19.33
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG         zgpg
TD             32768
SOLVENT         DMSO
NS              2048
DS                 4
SWH         24414.062 Hz
FIDRES       0.745058 Hz
AQ           0.6710886 sec
RG              501.187
DW            20.480 usec
DE             6.50 usec
TE             357.1 K
D1          1.00000000 sec
D11         0.03000000 sec
D31         0.00001500 sec
D32         0.89999998 sec
D40         0.00093990 sec
L4                23
L5                26
P32           90.00 usec
TD0               1

======== CHANNEL f1 ========
SFO1       75.4878687 MHz
NUC1              13C
P1           15.00 usec
PLW1       15.00000000 W

======== CHANNEL f2 ========
SFO2      300.1812007 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2         90.00 usec
PLW2       10.00000000 W
PLW12       0.20863999 W
PLW13       0.10495000 W

F2 - Processing parameters
SI             32768
SF         75.4803210 MHz
WDW              EM
SSB               0
LB             1.00 Hz
GB                0
PC             1.40
```

Figure S53. ^{13}C-NMR spectra of compound **4k**

Formula Predictor Report - AL-11_207.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-11_207.lcd

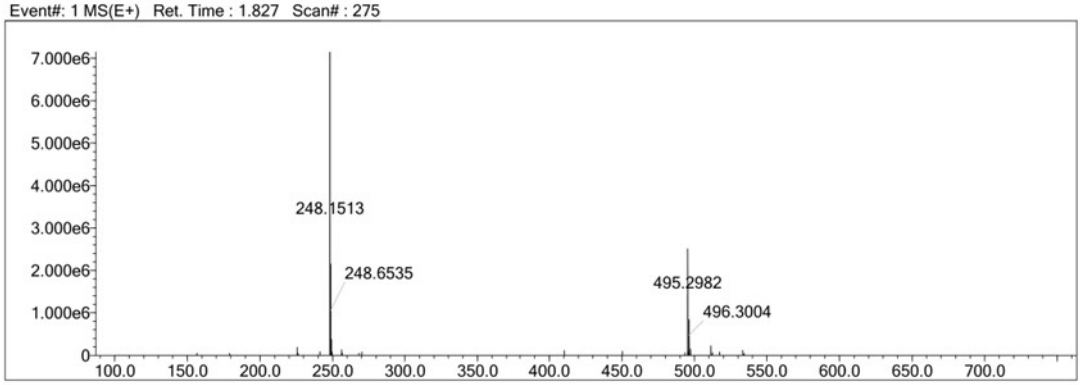
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	38	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

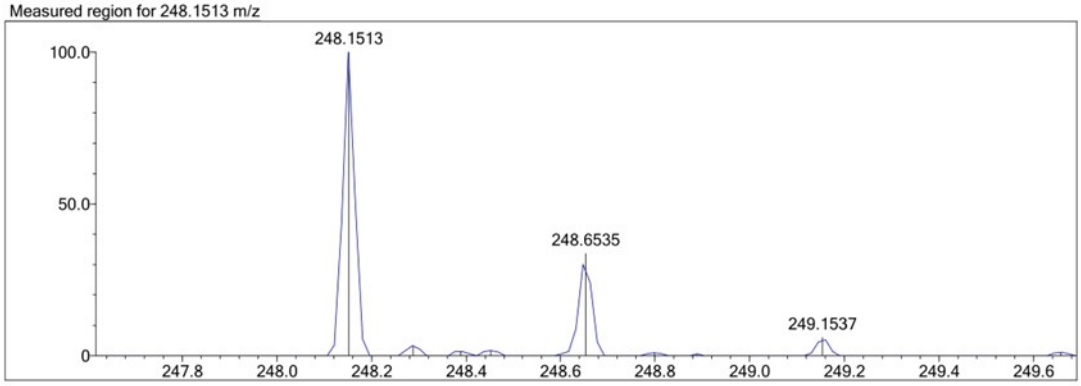
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

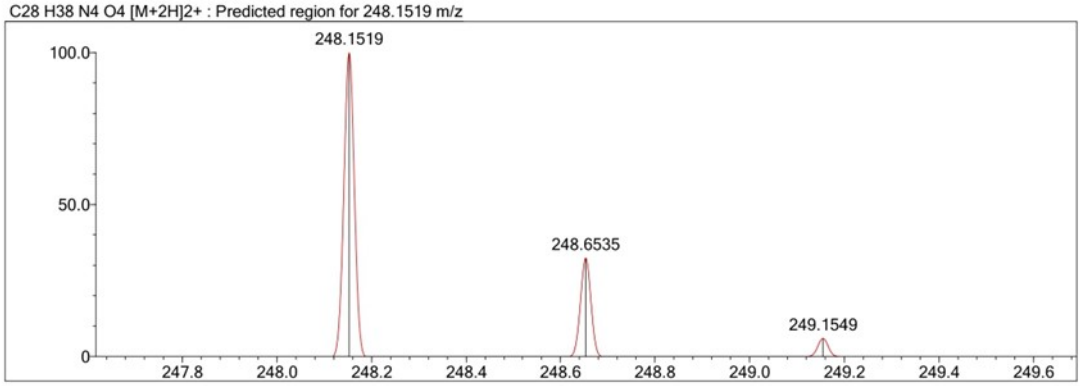
Event#: 1 MS(E+) Ret. Time : 1.827 Scan# : 275



Measured region for 248.1513 m/z



C28 H38 N4 O4 [M+2H]2+ : Predicted region for 248.1519 m/z



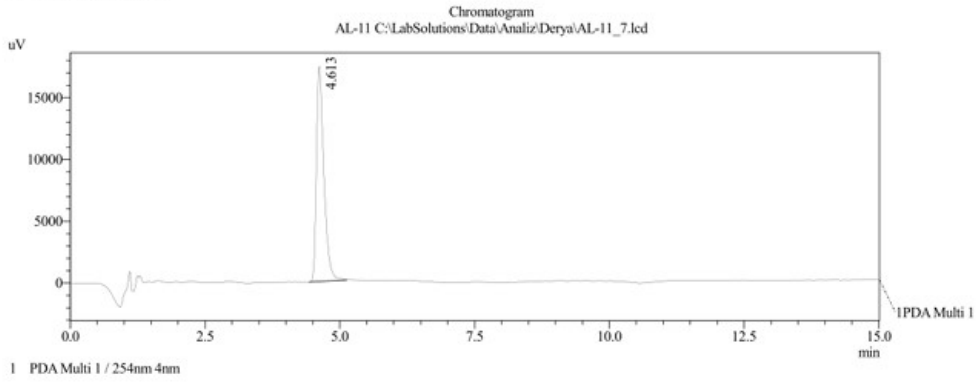
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	77.68	C28 H38 N4 O4	[M+2H]2+	248.1513	248.1519	-0.6	-2.42	80.54	12.0

Figure S54. HRMS spectra of compound **4k**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-11
Sample ID	:
Vail #	: 4
Injection Volume	: 1 uL
Data File Name	: AL-11_7.lcd
Method File Name	: isocratic_serkan-15DK.lcm
Batch File Name	: 1.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 18:36:08
Data Processed	: 08.09.2025 10:00:48

<Chromatogram>



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	4.613	167372	17415	100.000
Total		167372	17415	100.000

Figure S55. HPLC chromatogram of compound **4k**

DOPNALAB

	Item	Value
	Acquired Date&Time	17.05.2023 15:56:06
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-121.ispd
	Spectrum name	AL-121
	Sample name	AL-12
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

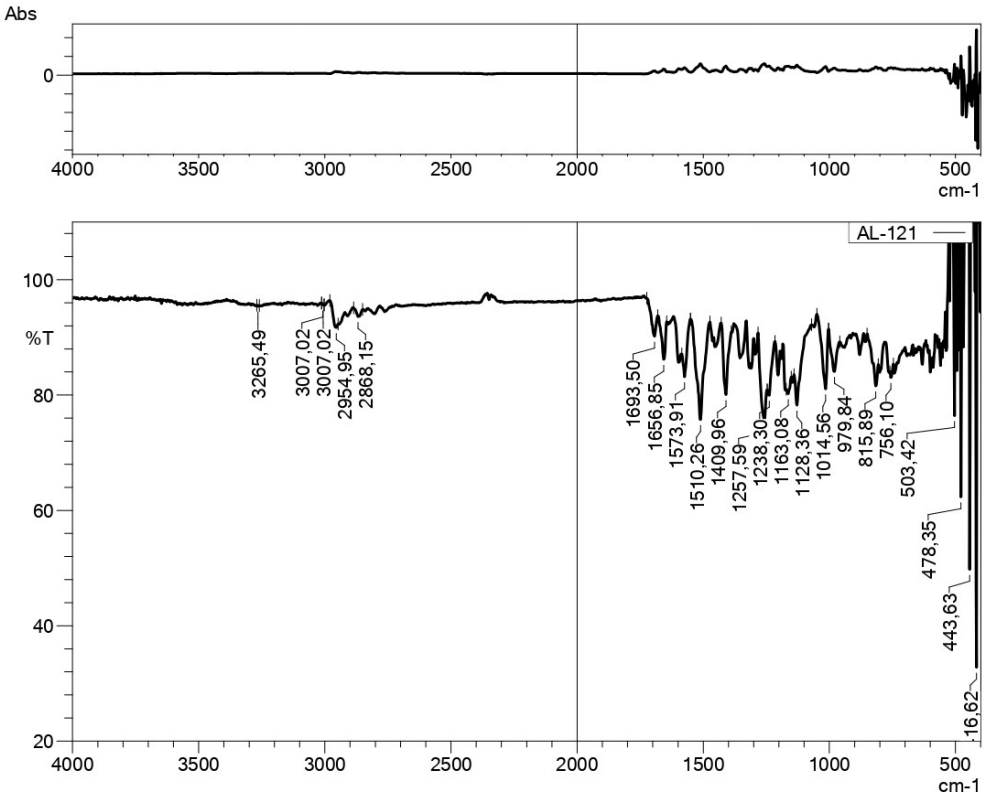


Figure S56. FTIR spectra of compound **4l**

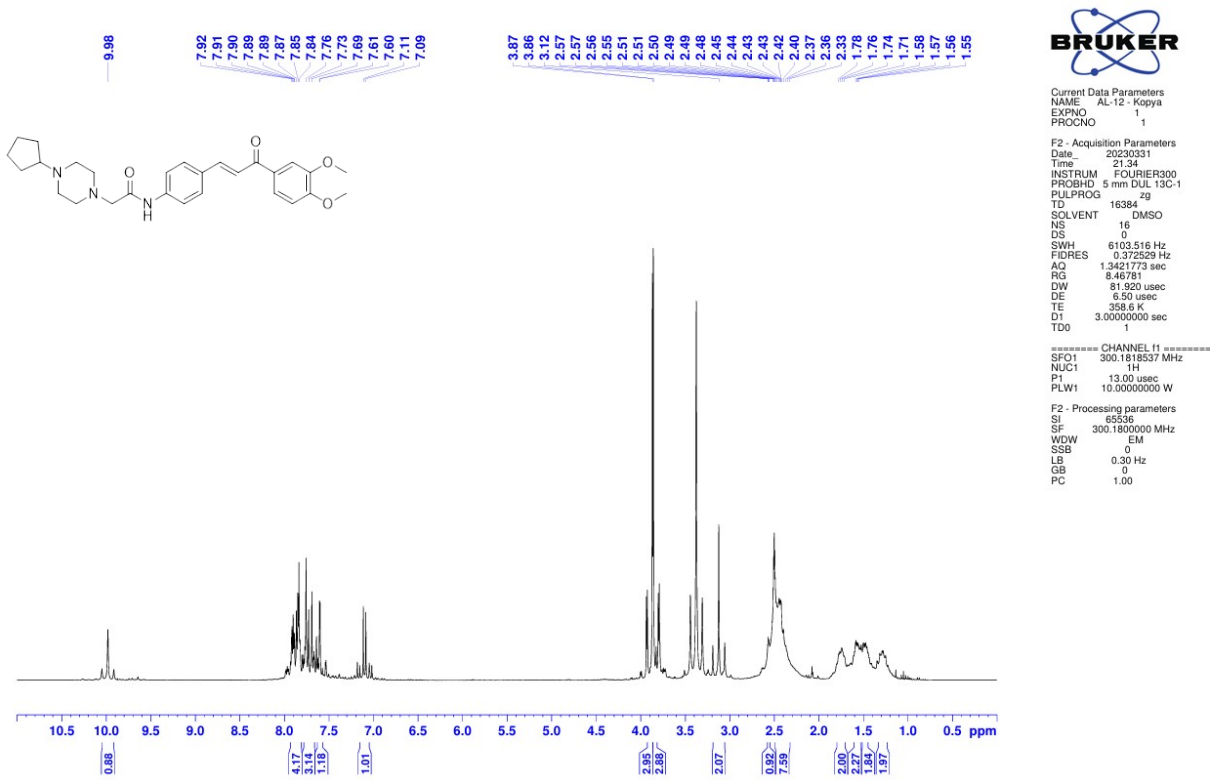


Figure S57. ^{1}H-NMR spectra of compound **4l**

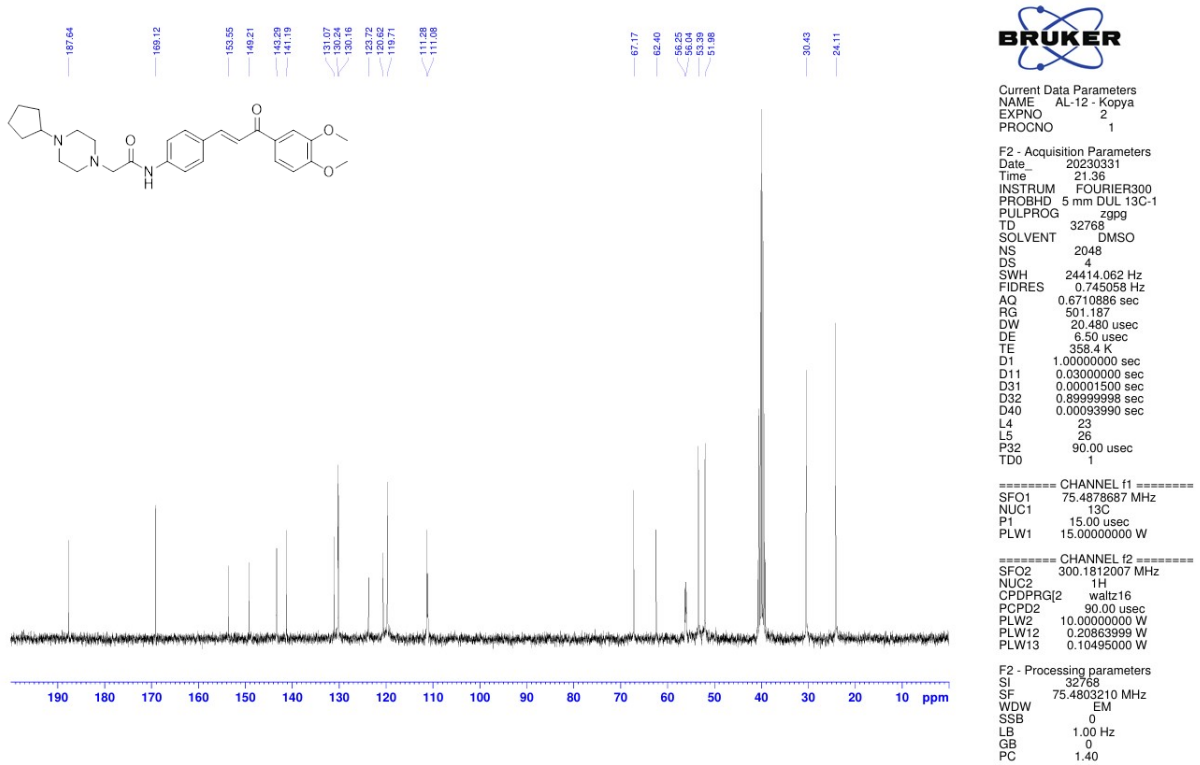


Figure S58. ^{13}C-NMR spectra of compound **4l**

Formula Predictor Report - AL-12_208.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-12_208.lcd

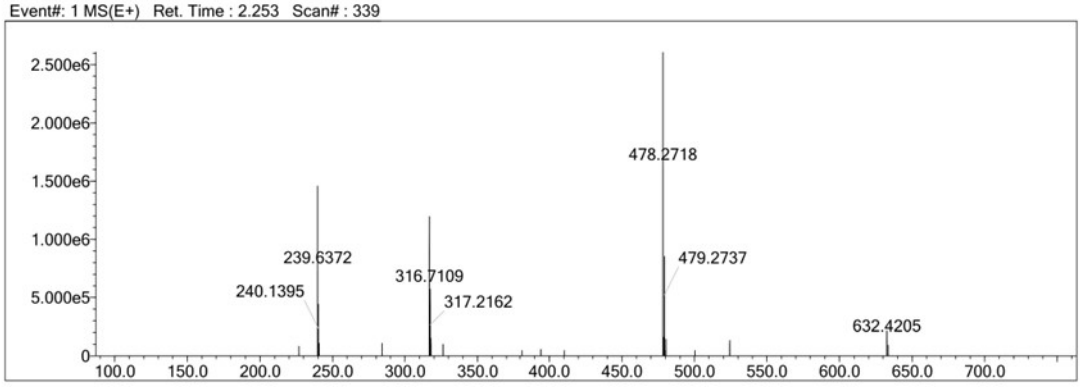
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	38	O	2	0	5	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

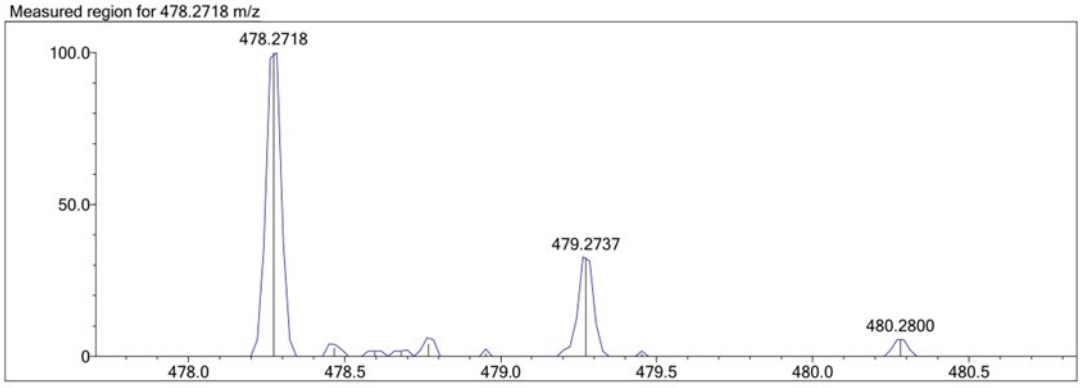
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

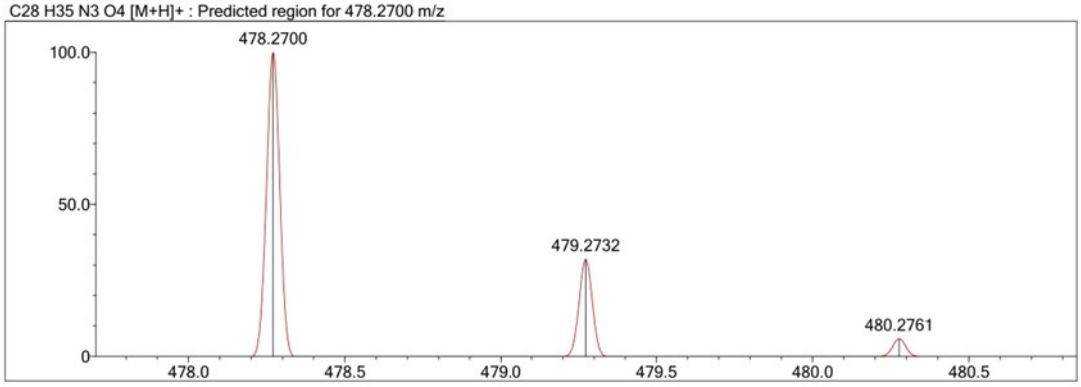
Event#: 1 MS(E+) Ret. Time : 2.253 Scan# : 339



Measured region for 478.2718 m/z



C28 H35 N3 O4 [M+H]+ : Predicted region for 478.2700 m/z



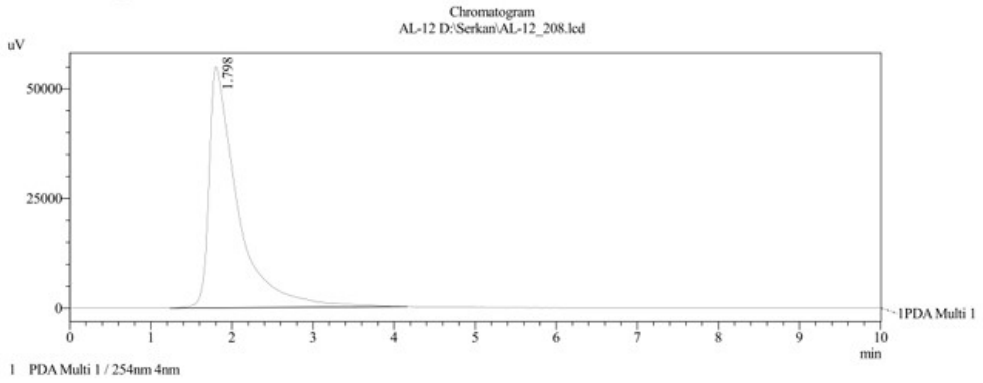
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	93.10	C28 H35 N3 O4	[M+H]+	478.2718	478.2700	1.8	3.76	100.00	13.0

Figure S59. HRMS spectra of compound **4l**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-12
Sample ID	:
Vail #	: 12
Injection Volume	: 0.5 uL
Data File Name	: AL-12_208.lcd
Method File Name	: isocratic_serkan.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 18:46:56
Data Processed	: 02.08.2022 18:56:59

<Chromatogram>



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	1.798	1355435	55035	100.000
Total		1355435	55035	100.000

Figure S60. HPLC chromatogram of compound **4l**

DOPNALAB

	Item	Value
	Acquired Date&Time	17.05.2023 16:01:29
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-131.ispd
	Spectrum name	AL-131
	Sample name	AL-13
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

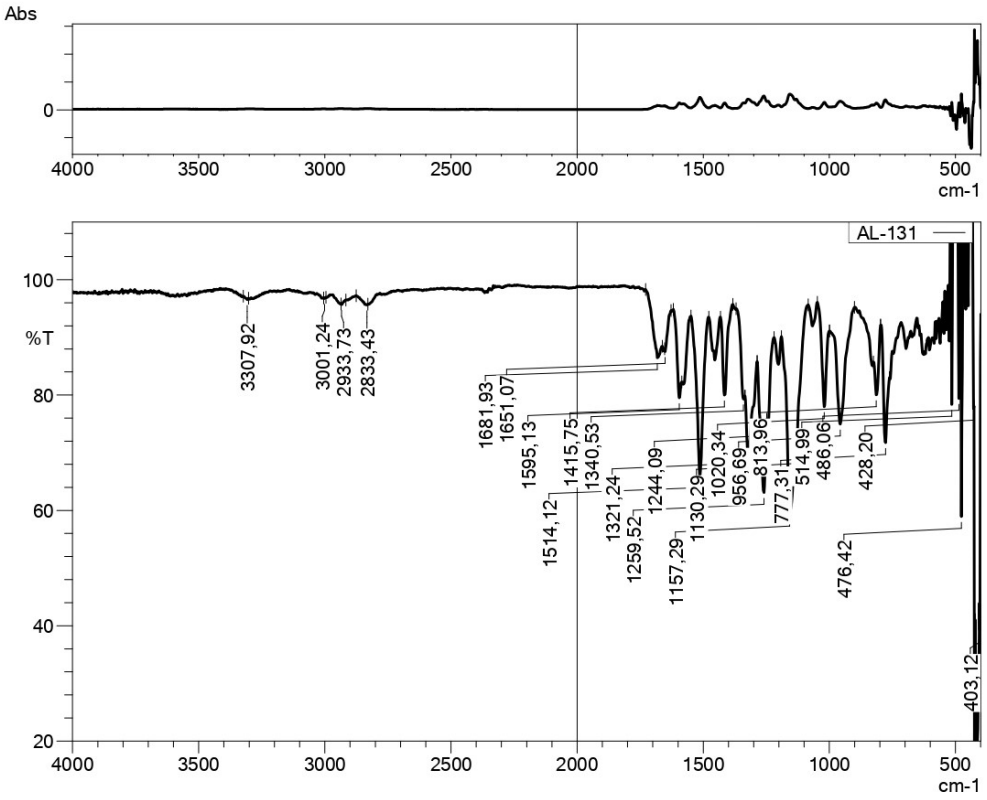
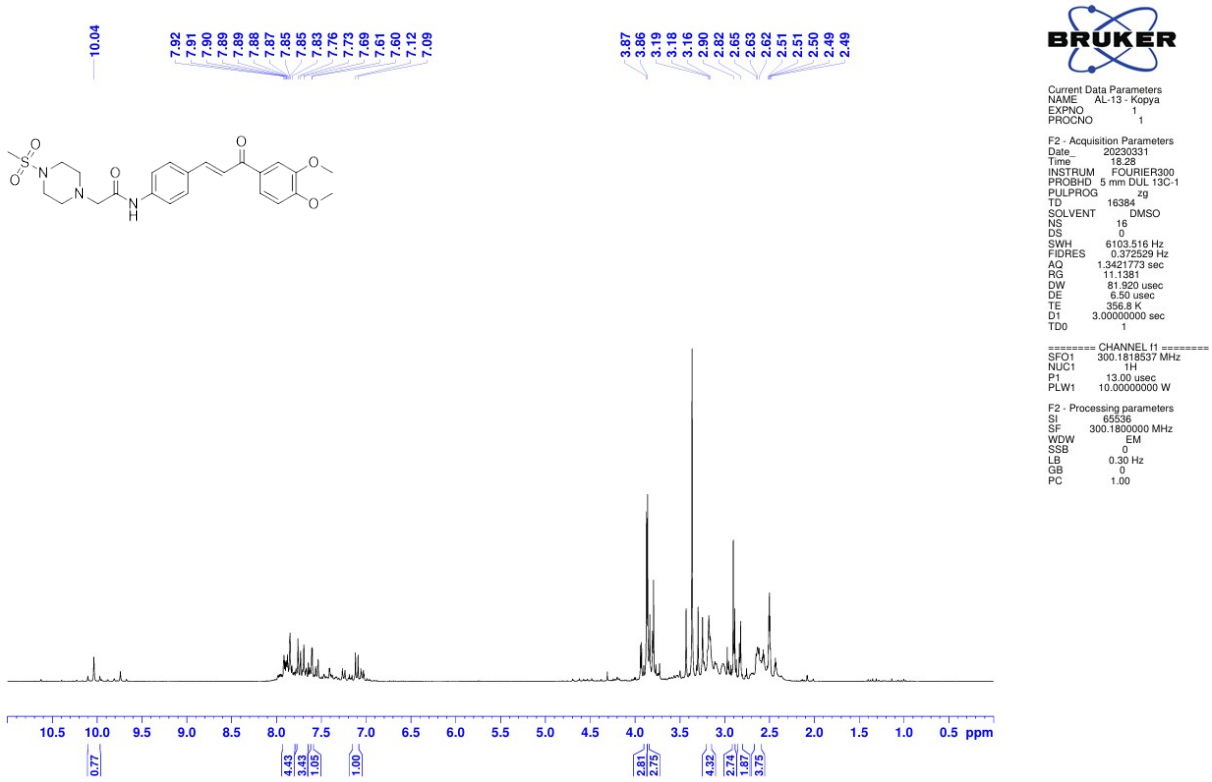


Figure S61. FTIR spectra of compound **4m**



BRUKER

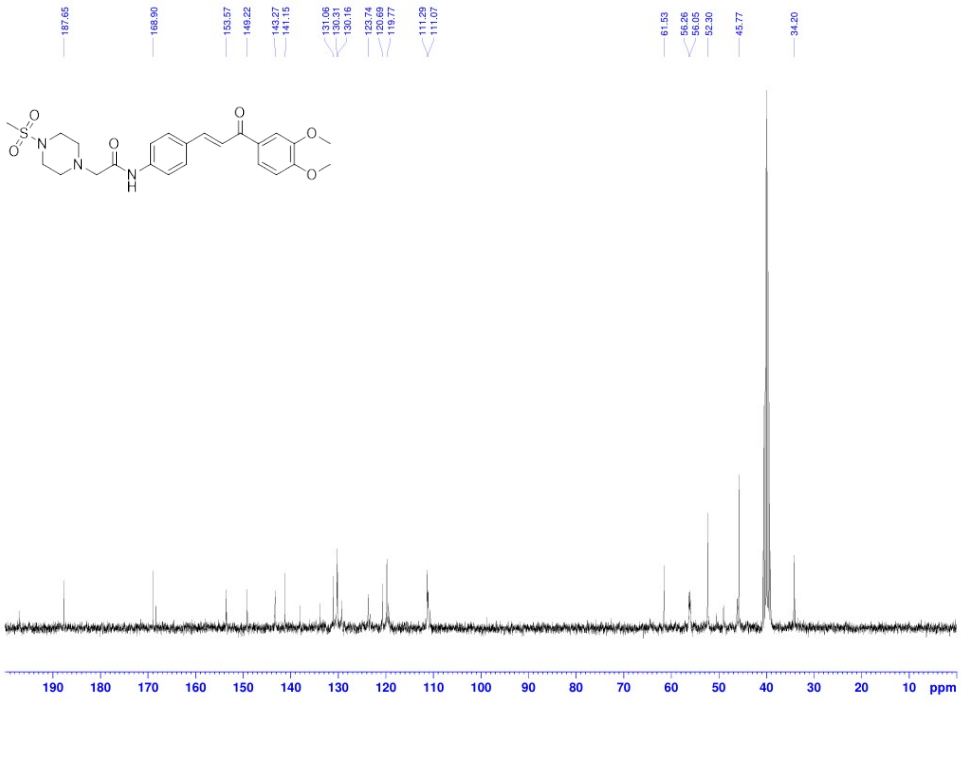
Current Data Parameters
NAME AL-13 - Kopya
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230331
Time 18.28
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6103.516 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 11.1381
DW 81.920 usec
DE 6.50 usec
TE 356.8 K
D1 3.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S62. ^{1}H-NMR spectra of compound **4m**



BRUKER

Current Data Parameters
NAME AL-13 - Kopya
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230331
Time 18.30
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 2048
DS 4
SWH 24414.062 Hz
FIDRES 0.745058 Hz
AQ 0.6710886 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 356.4 K
D1 1.00000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D32 0.89999998 sec
D40 0.00093990 sec
L4 23
L5 26
P32 90.00 usec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.00000000 W

======== CHANNEL f2 ========
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.20863999 W
PLW13 0.10495000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S63. ^{13}C-NMR spectra of compound **4m**

Formula Predictor Report - AL-13_209.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-13_209.lcd

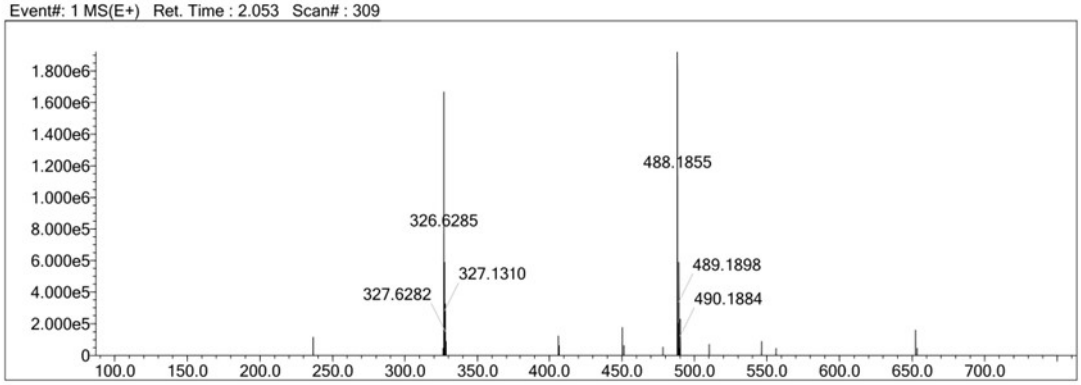
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	38	O	2	0	6	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

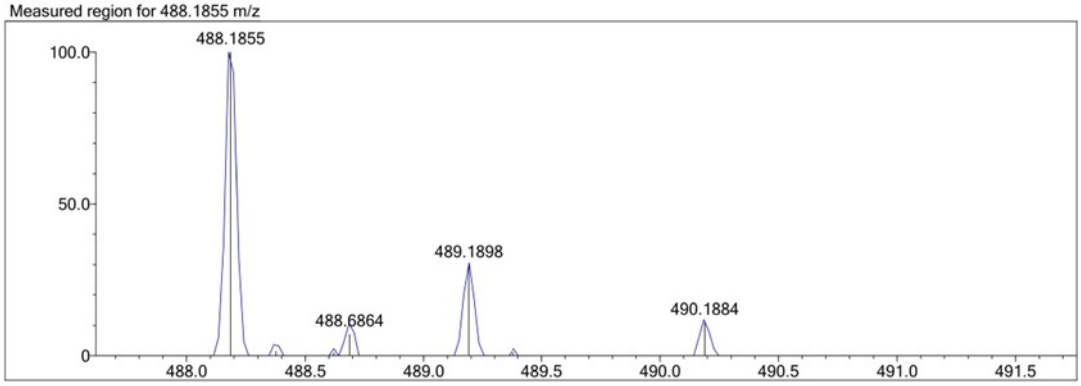
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

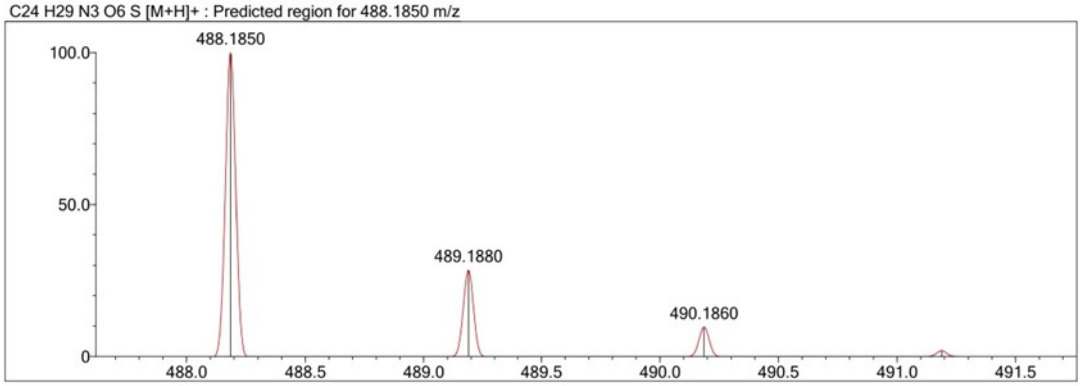
Event#: 1 MS(E+) Ret. Time : 2.053 Scan# : 309



Measured region for 488.1855 m/z



C24 H29 N3 O6 S [M+H]+ : Predicted region for 488.1850 m/z



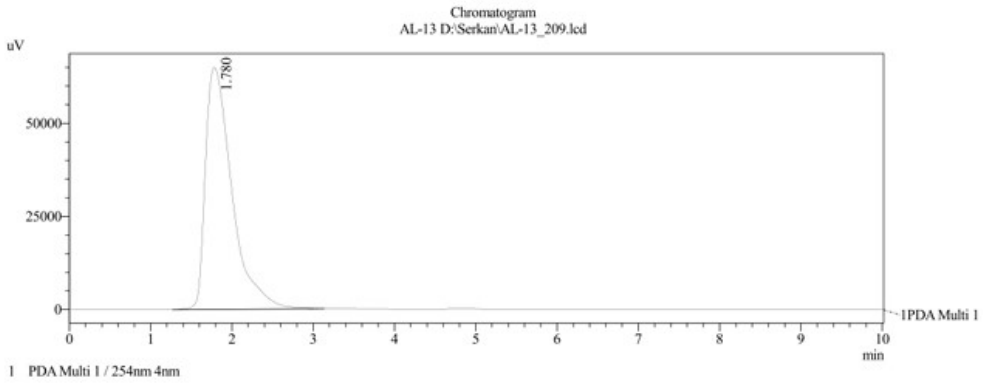
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	94.60	C24 H29 N3 O6 S	[M+H]+	488.1855	488.1850	0.5	1.02	94.65	12.0

Figure S64. HRMS spectra of compound **4m**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-13
Sample ID	:
Vail #	: 13
Injection Volume	: 0.5 uL
Data File Name	: AL-13_209.lcd
Method File Name	: isocratic_serkan.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 18:57:45
Data Processed	: 04.09.2025 11:01:09

<Chromatogram>



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	1.780	1480249	65016	100.000
Total		1480249	65016	100.000

Figure S65. HPLC chromatogram of compound **4m**

DOPNALAB

	Item	Value
	Acquired Date&Time	17.05.2023 16:05:08
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\MASAÜSTÜ\derya\berkant\AL serisi\AL-141.ispd
	Spectrum name	AL-141
	Sample name	AL-14
	Sample ID	
	Option	
	Comment	
	No. of Scans	15
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

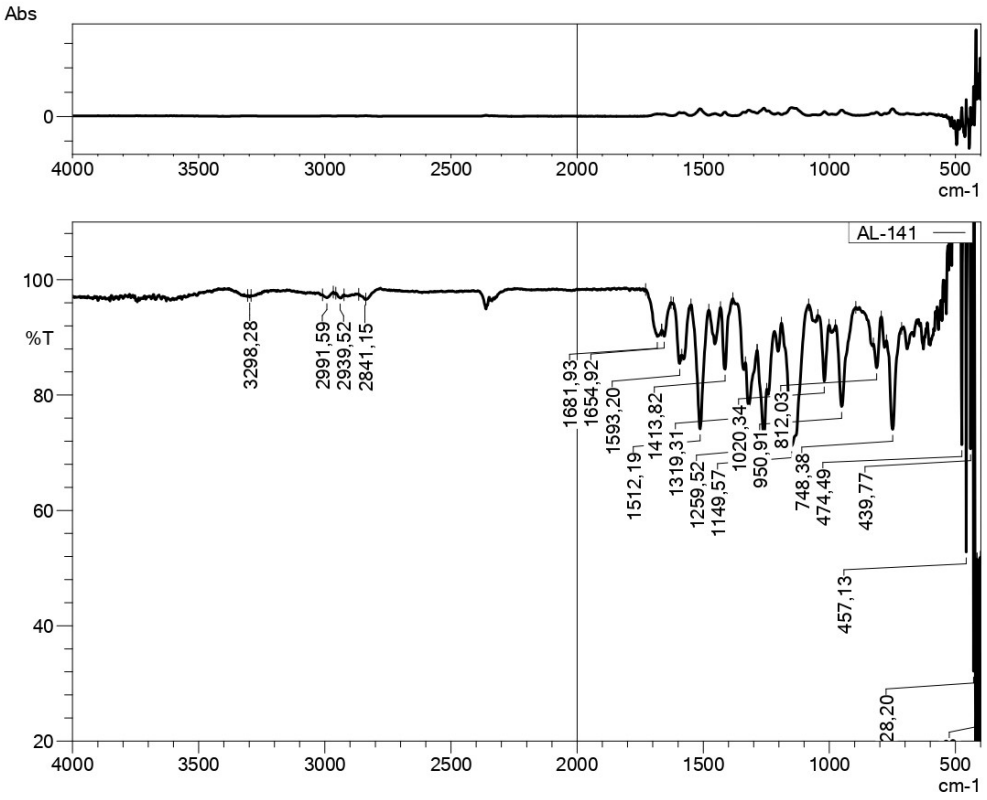


Figure S66. FTIR spectra of compound **4n**

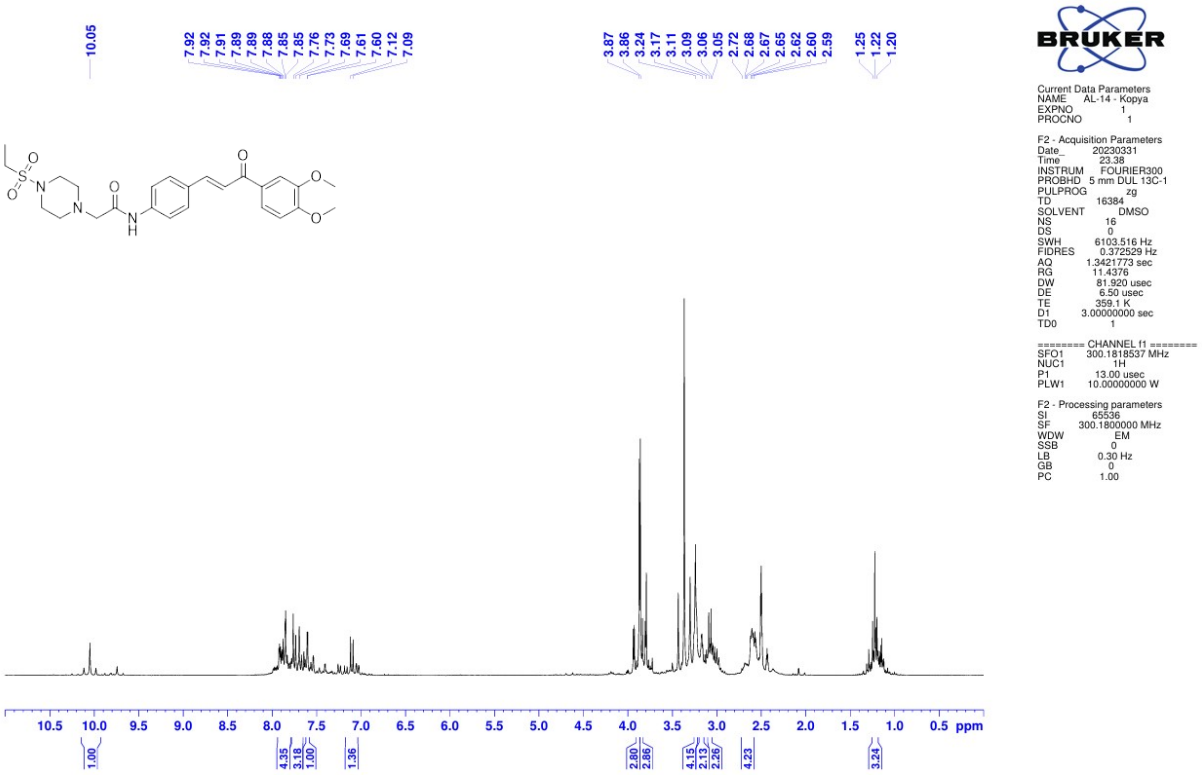


Figure S67. ^{1}H-NMR spectra of compound **4n**

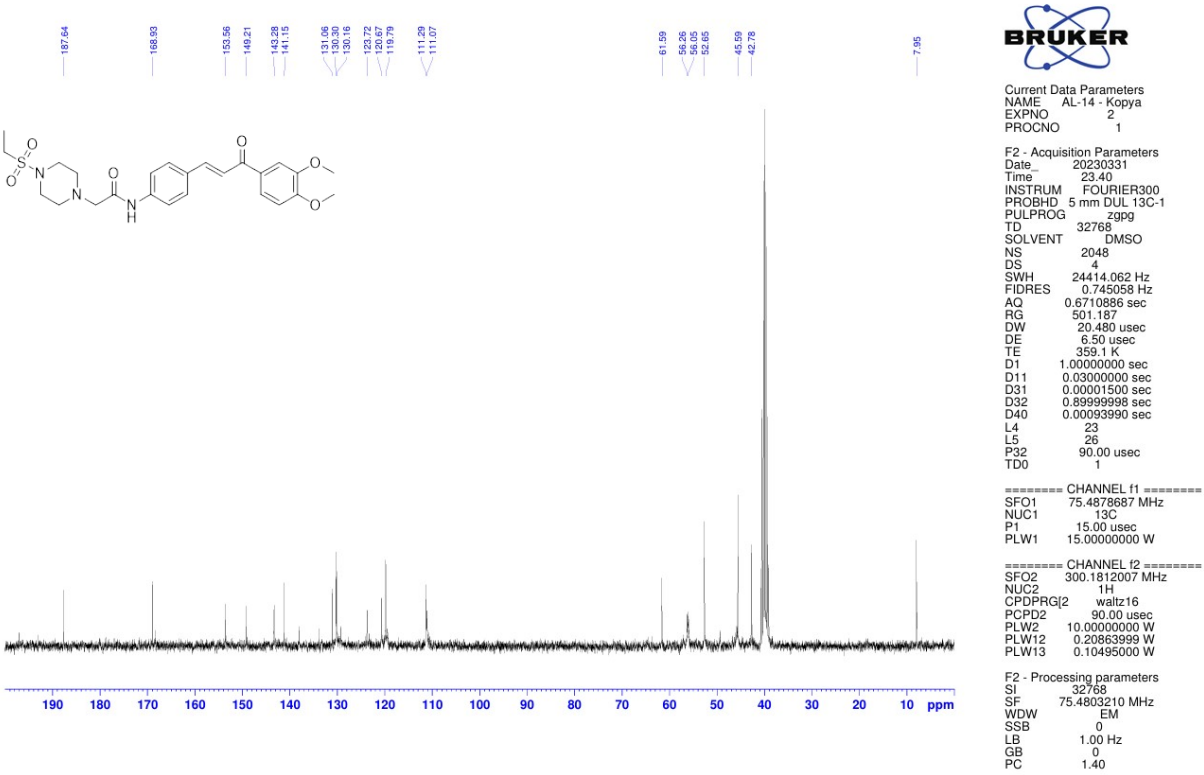


Figure S68. ^{13}C-NMR spectra of compound **4n**

Formula Predictor Report - AL-14_210.lcd

Data File: C:\LabSolutions\Data\Analiz\Serkan\AL-14_210.lcd

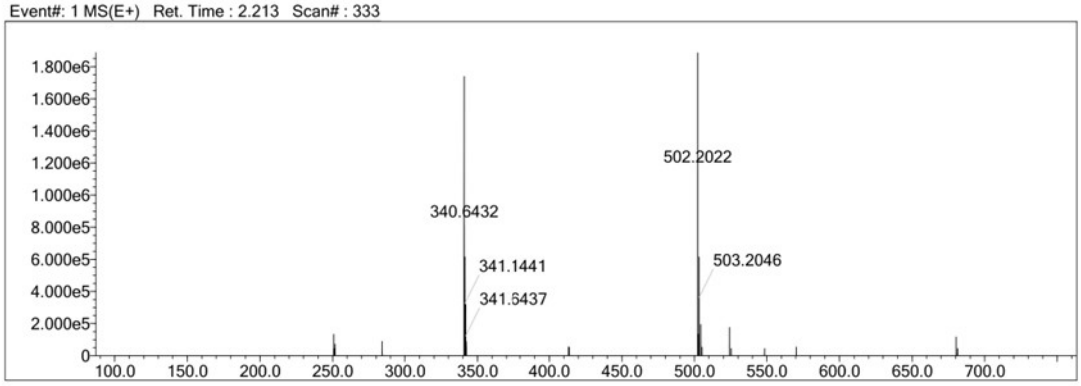
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	38	O	2	0	6	Cl	1	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Br	1	0	0					
C	4	0	32	P	3	0	0	Ru	2	0	0					
N	3	0	5	S	2	0	2	Pd	2	0	0					

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

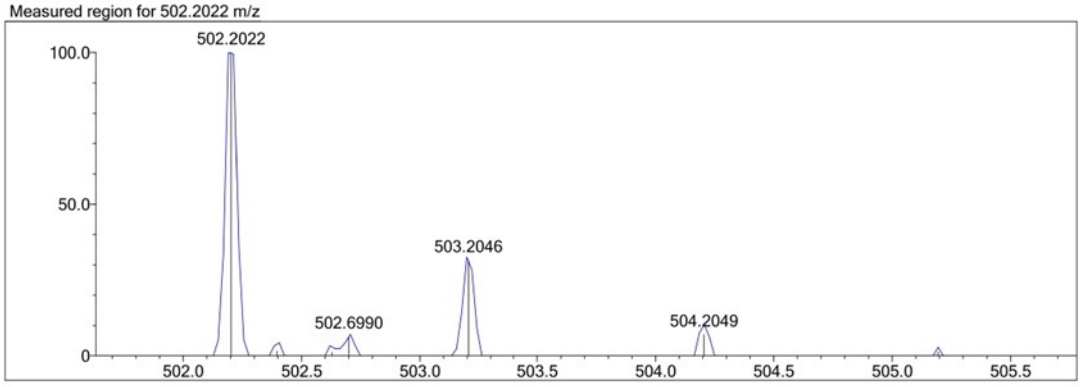
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: odd
Use MSn Info: yes
Isotope Res: 9000
Max Results: 50

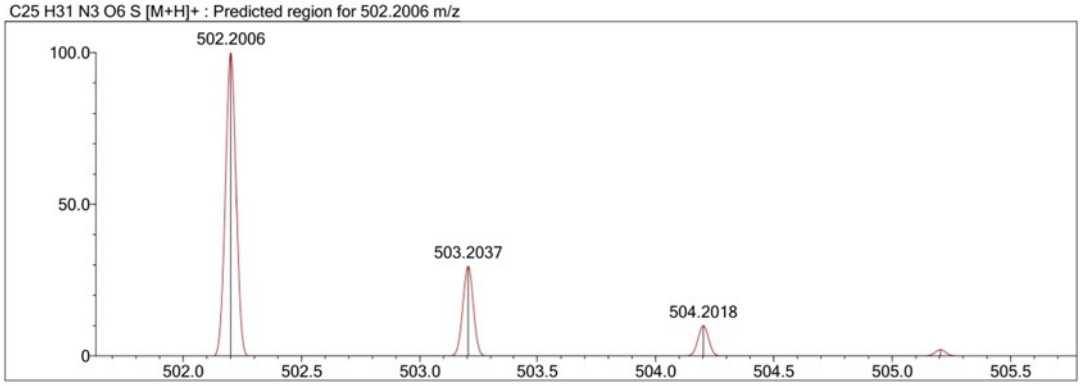
Event#: 1 MS(E+) Ret. Time : 2.213 Scan# : 333



Measured region for 502.2022 m/z



C25 H31 N3 O6 S [M+H]+ : Predicted region for 502.2006 m/z



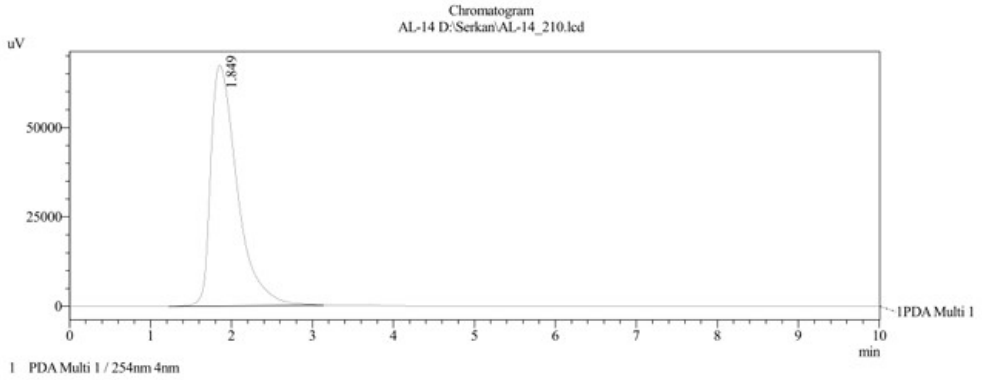
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	81.27	C25 H31 N3 O6 S	[M+H]+	502.2022	502.2006	1.6	3.19	85.98	12.0

Figure S69. HRMS spectra of compound **4n**

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: AL-14
Sample ID	:
Vail #	: 14
Injection Volume	: 0.5 uL
Data File Name	: AL-14_210.lcd
Method File Name	: isocratic_serkan.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 02.08.2022 19:08:33
Data Processed	: 02.08.2022 19:18:35

<Chromatogram>



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	1.849	1542887	67392	100.000
Total		1542887	67392	100.000

Figure S70. HPLC chromatogram of compound **4n**