Supplementary Information (SI) for RSC Advances.
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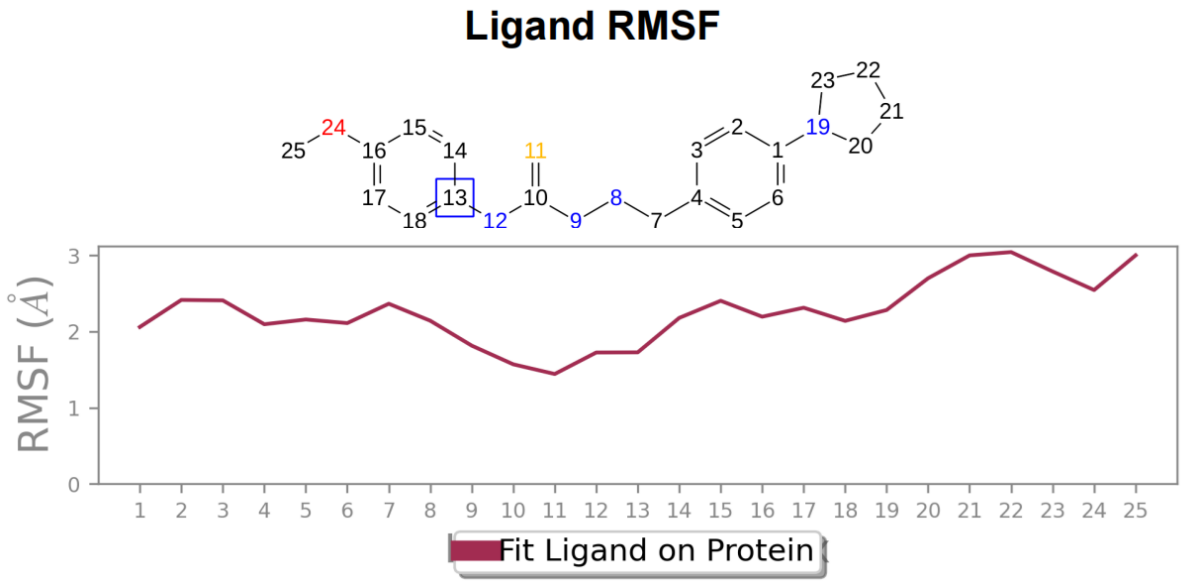
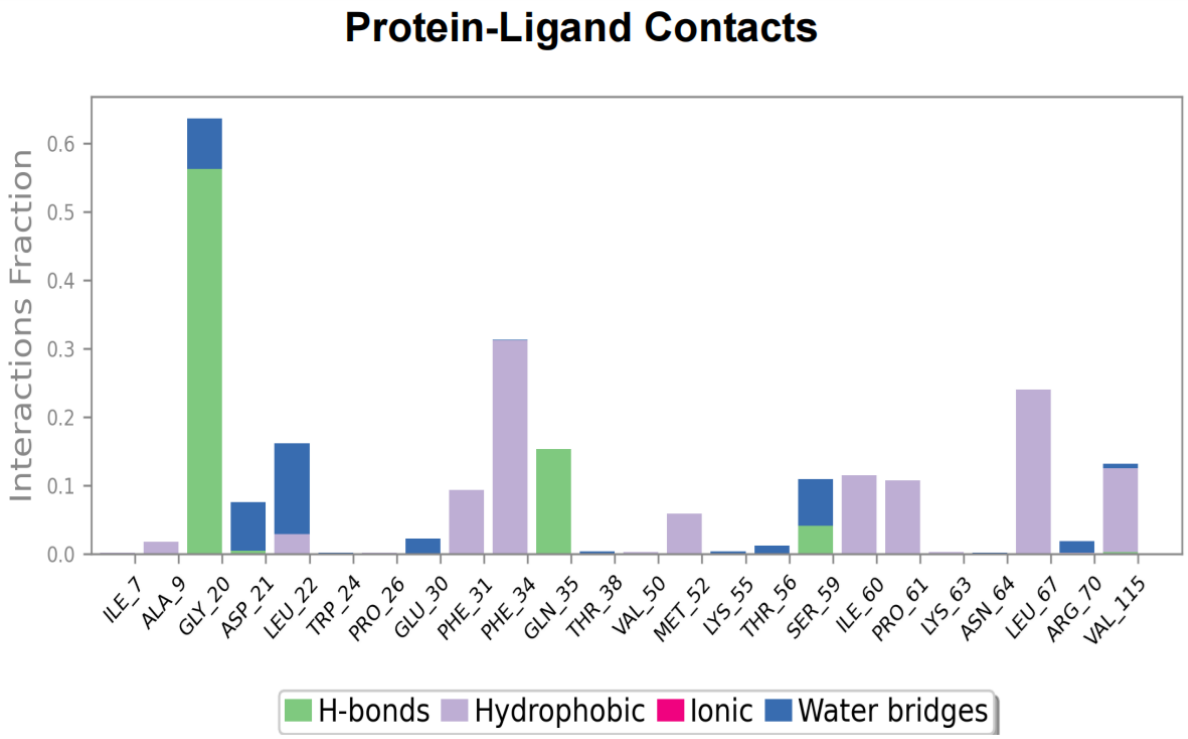
Molecular Docking Molecular Dynaimcs Simulation Studies

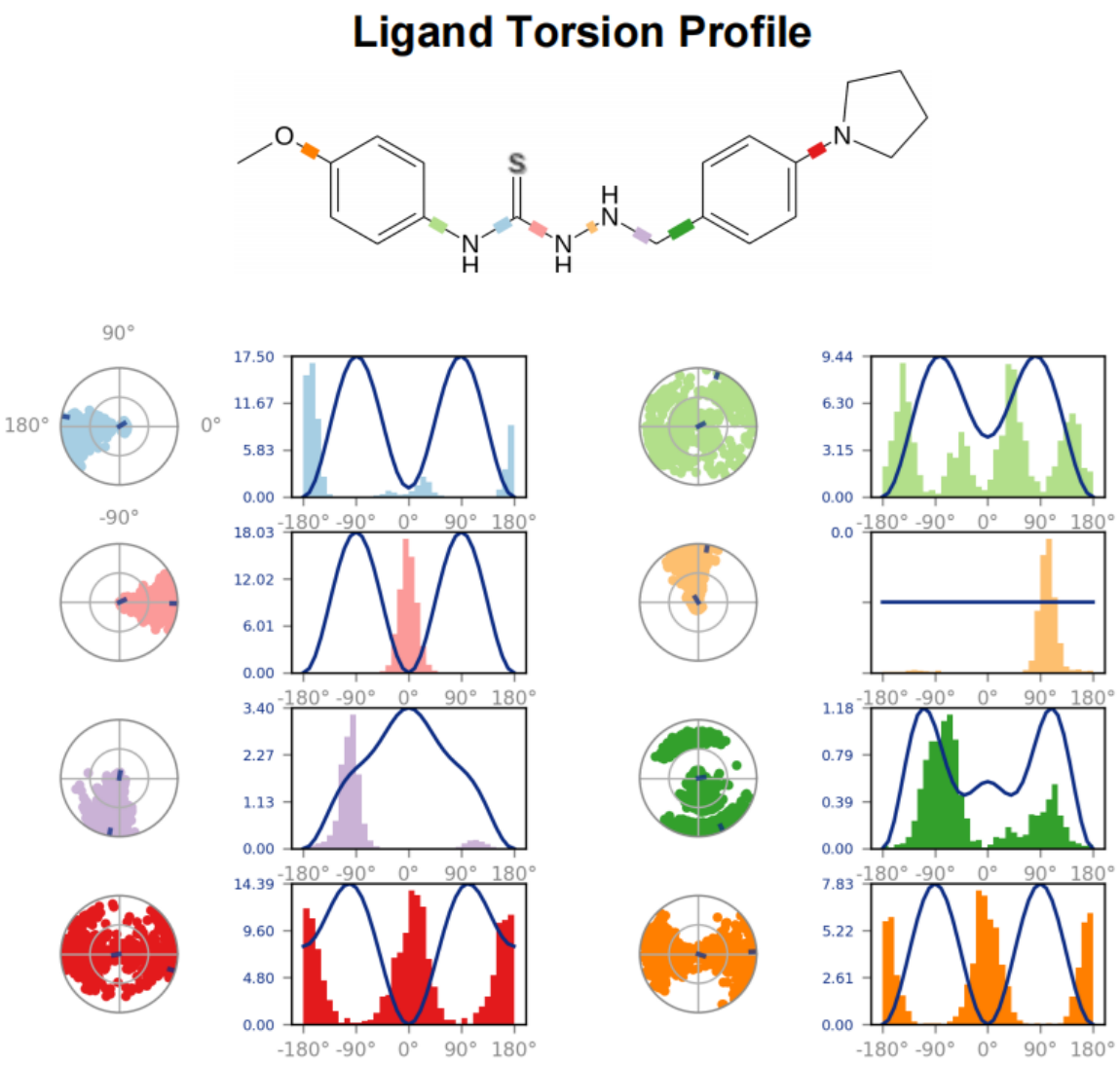
For molecular docking studies BioSolveIT's LeadIT software was used www.biosolveit.de/LeadIT. For visualization of docked conformations, Desmond Molecular Dynamics (D.E. Shaw Research) on Schrödinger Maestro 2023.4 software was opted to perform Molecular Dynamic Simulations study[1]. In Molecular Dynamics Simulations the complex of **5d** with hDHFR was first prepared with Protein Preparation Workflow by options opting for replacing hydrogens, assigning bond orders, using CCD database, creating zero-order bonds to metals and disulfide bonds, and deleting waters beyond 0 Å from het groups. In the refine tab, sample water orientations, use PROPKA pH 7.4 option was opted and the structure was optimized. In system builder panel, TIP3P solvent model was used for solvation in the orthorhombic box using buffer settings with 10 Å x 10 Å x 10 Å and minimized volume option was used, then Ions placement (default-recalculated) with salt addition (0.15M NaCl) was carried out. Complex of **5d** with hDHFR after solvation resulted in 23599 atoms. In molecular dynamics panel, 100ns (nanoseconds) simulation time was entered, while recording interval was set to 100ps (picoseconds), with energy option at 1.2, it resulted in approximation for 1000 frames. For final run, NPT ensemble class was opted at 300.0 Kelvin with Nosé-Hoover chain temperature coupling and 1.01325 bar pressure with Martyna-Tobias-Klein pressure coupling. The system followed the default relaxation protocol before the simulation, which included small simulations, using NVT and NPT ensembles with different restraints parameters.



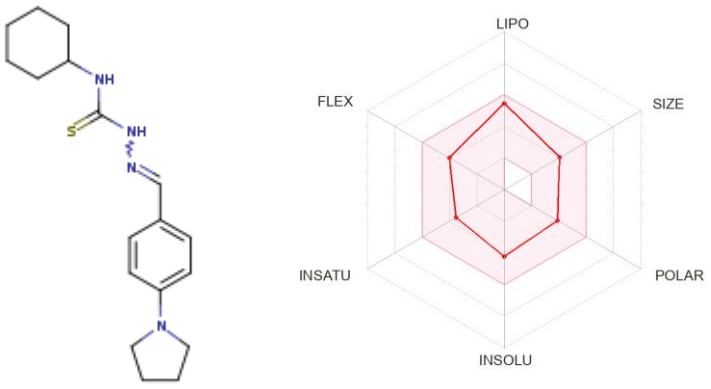
SI Figure 1. Ligand RMSF.



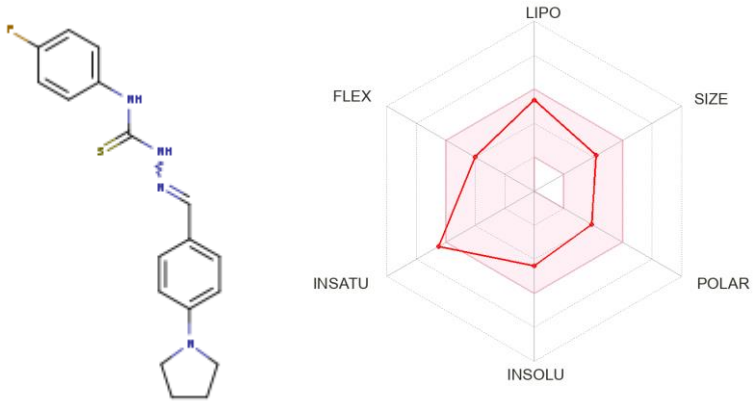
SI Figure 2. Protein-Ligand interaction fraction graph of 5d-hDHFR complex.



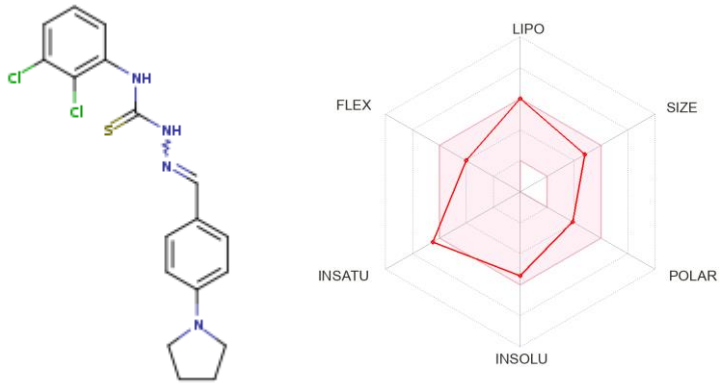
SI Figure 3. Torsion profile of ligand 5d.



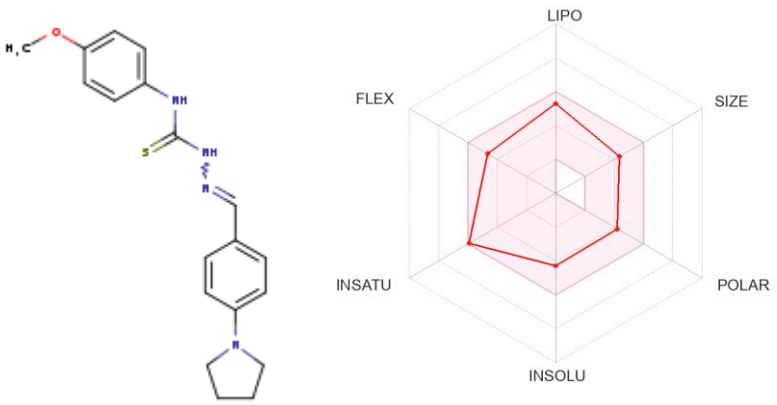
Bioavailability radar diagram for compound 5a.



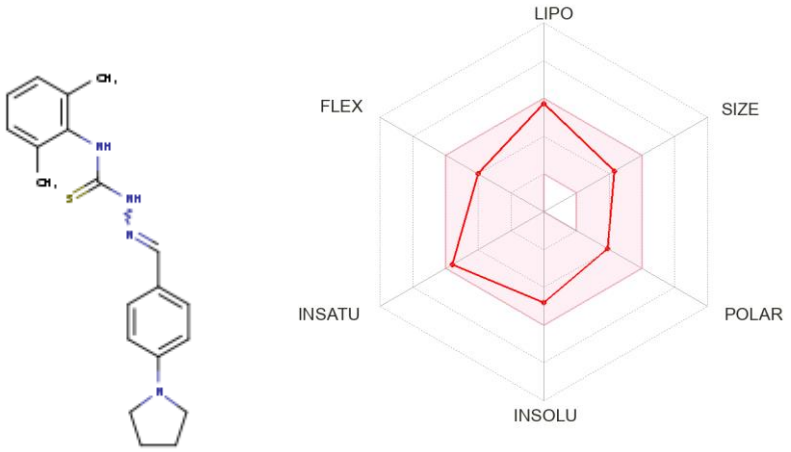
Bioavailability radar diagram for compound 5b.



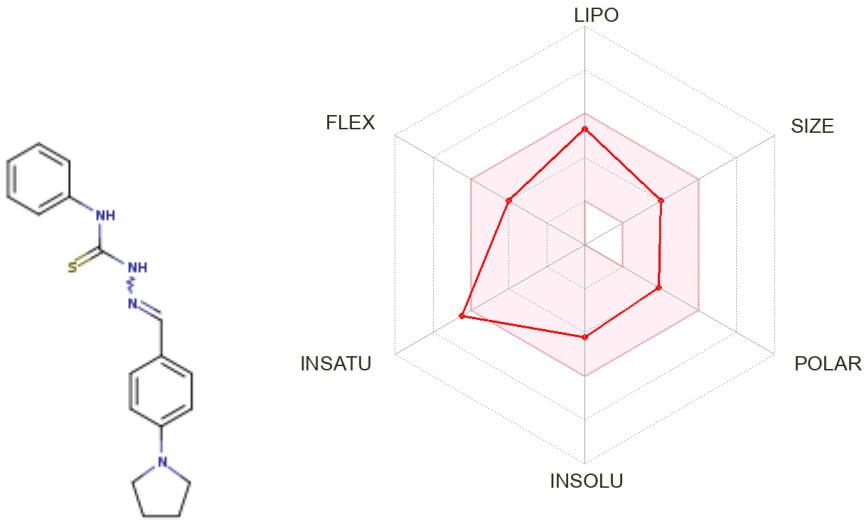
Bioavailability radar diagram for compound 5c.



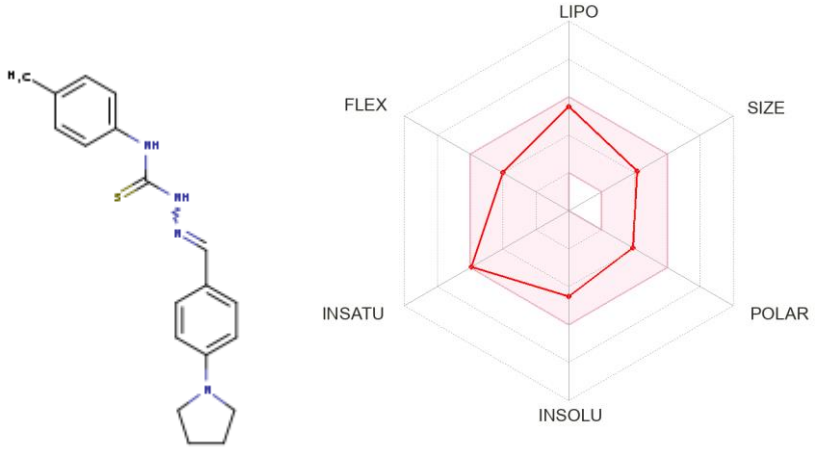
Bioavailability radar diagram for compound 5d.



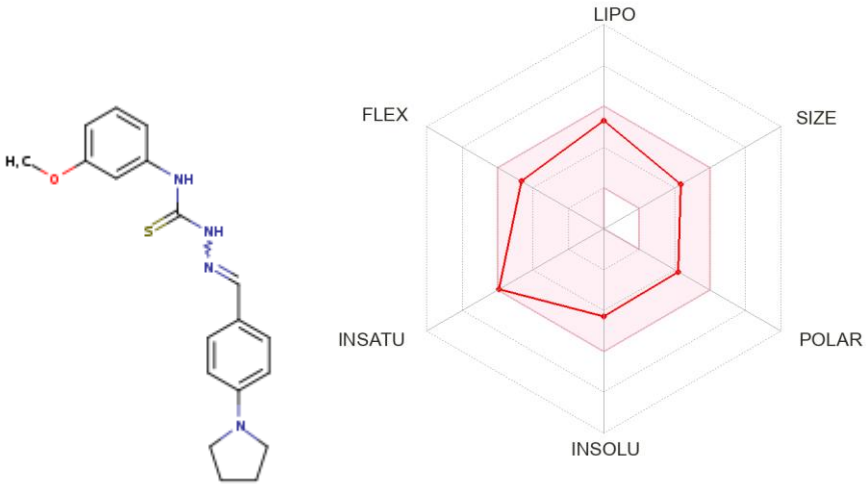
Bioavailability radar diagram for compound 5e.



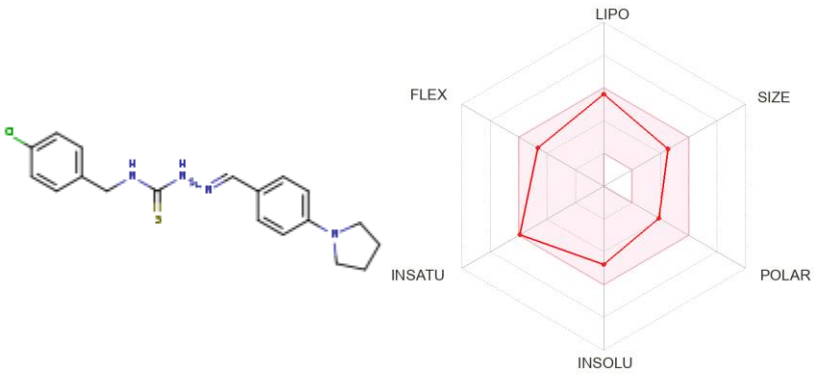
Bioavailability radar diagram for compound 5f.



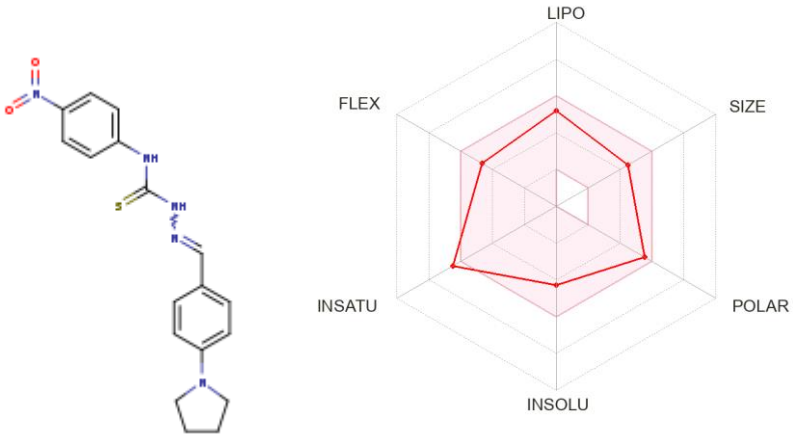
Bioavailability radar diagram for compound 5g.



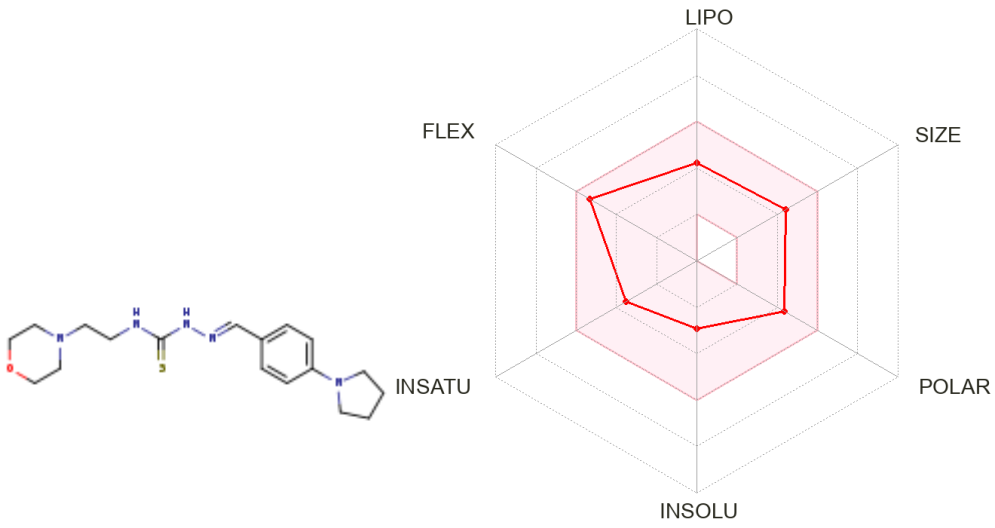
Bioavailability radar diagram for compound 5h.



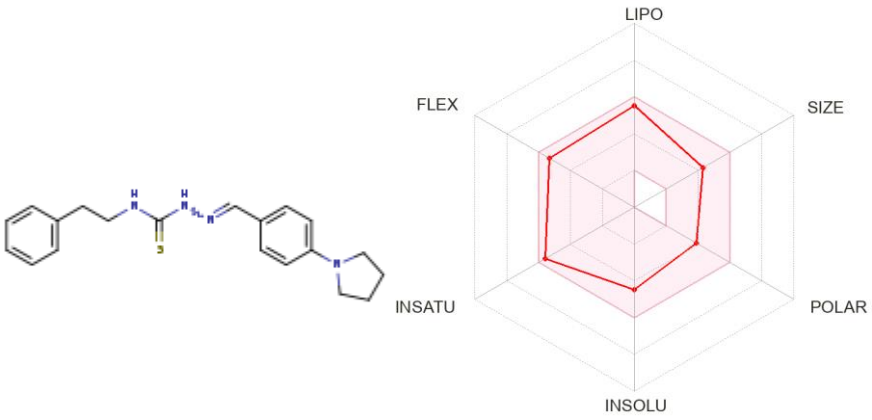
Bioavailability radar diagram for compound 5i.



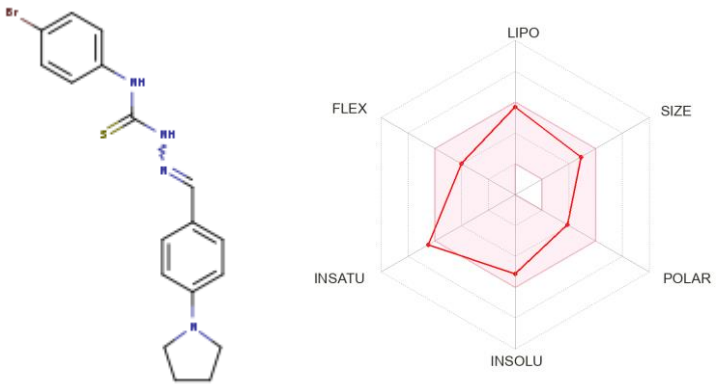
Bioavailability radar diagram for compound 5j.



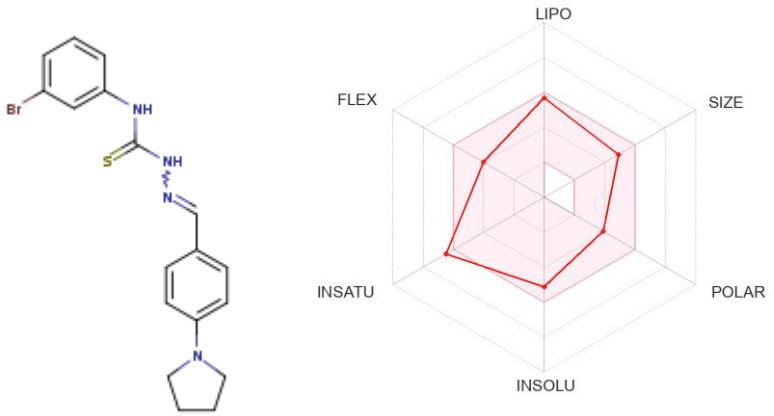
Bioavailability radar diagram for compound 5k.



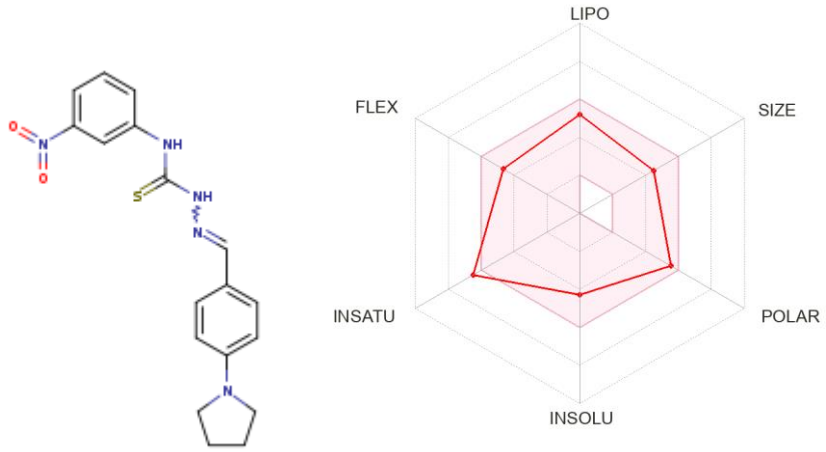
Bioavailability radar diagram for compound 5l.



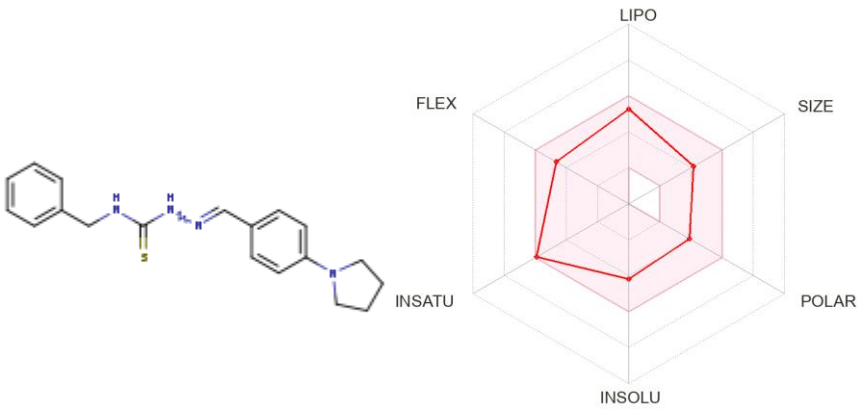
Bioavailability radar diagram for compound 5m.



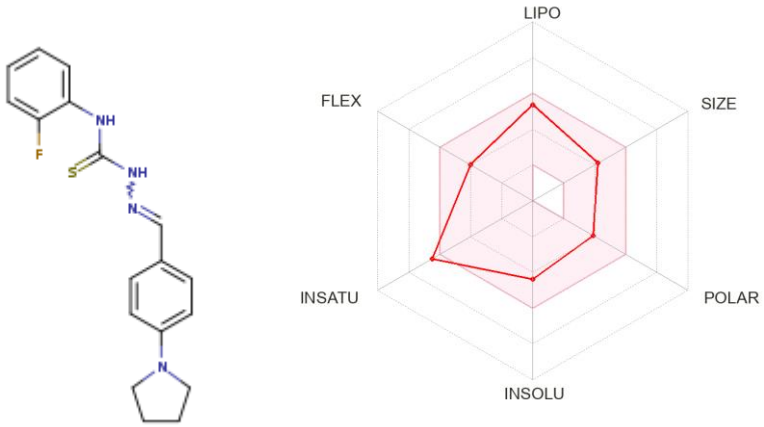
Bioavailability radar diagram for compound 5n.



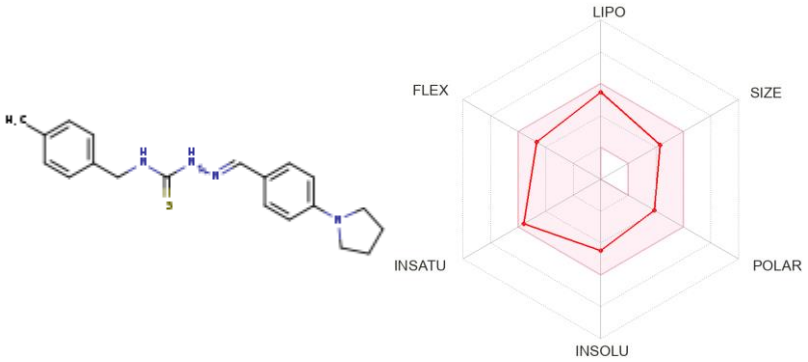
Bioavailability radar diagram for compound 5o.



Bioavailability radar diagram for compound 5p.



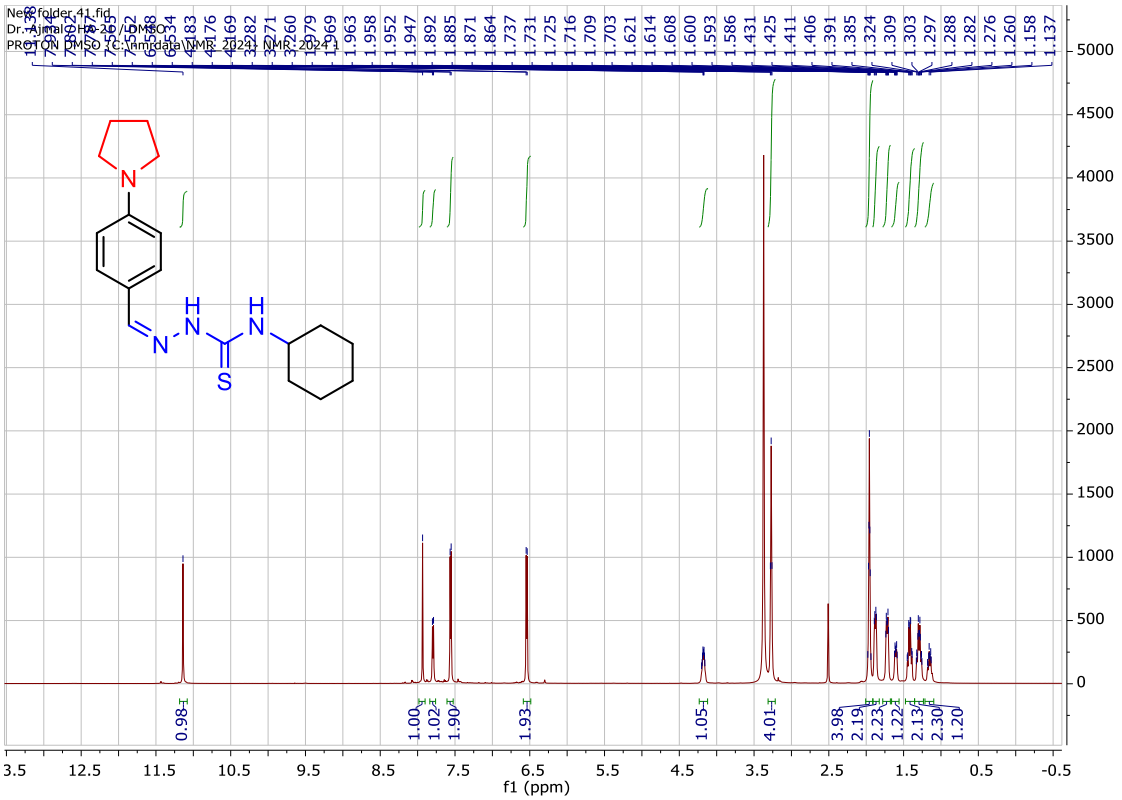
Bioavailability radar diagram for compound 5q.



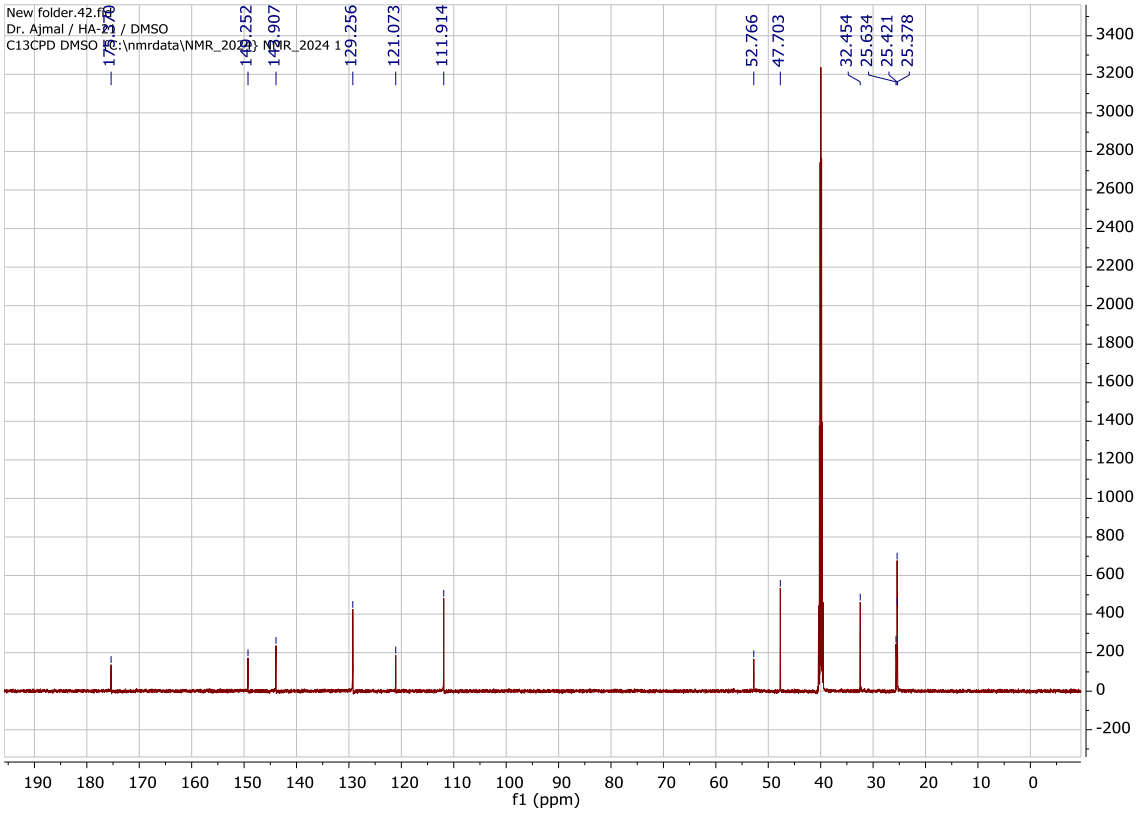
Bioavailability radar diagram for compound 5r.

1H-NMR and 13C-NMR of Synthesized compounds 5(a-r)

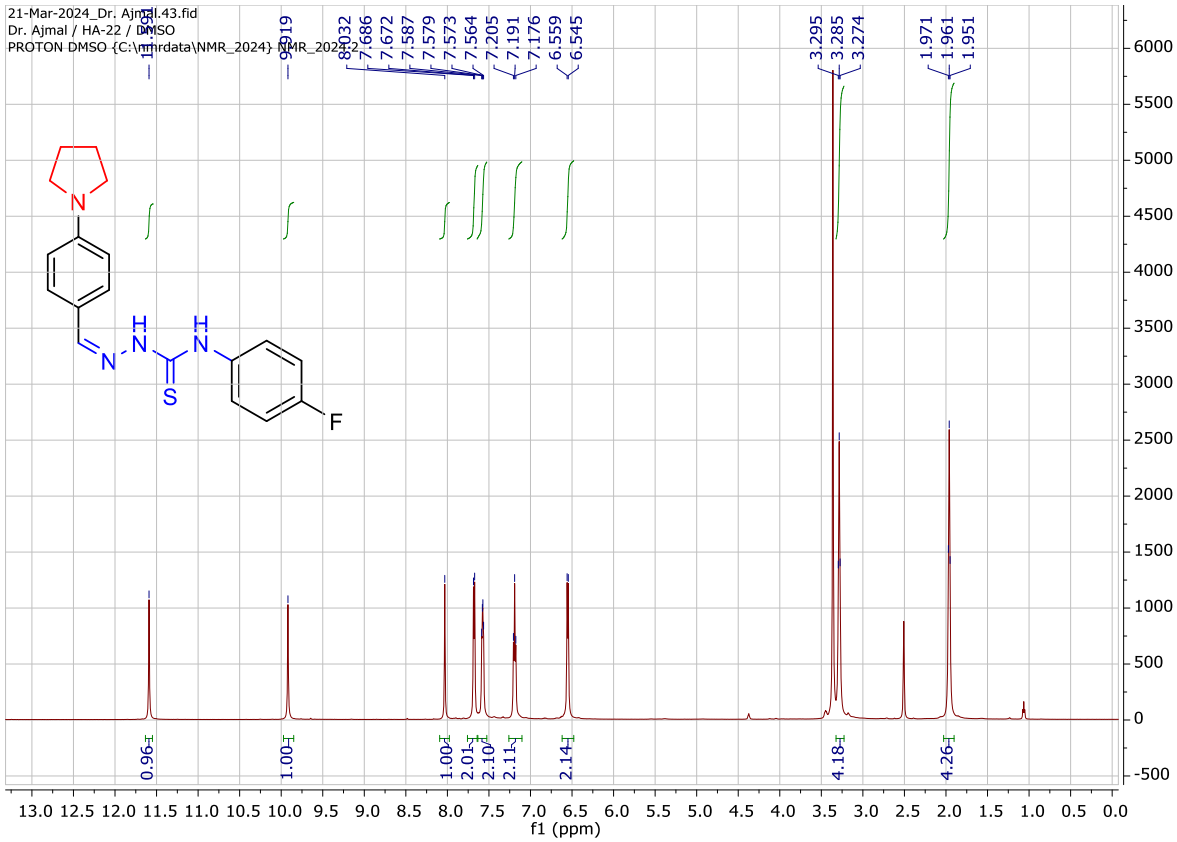
1HNMR, 600 MHz, DMSO-d6 of 5a



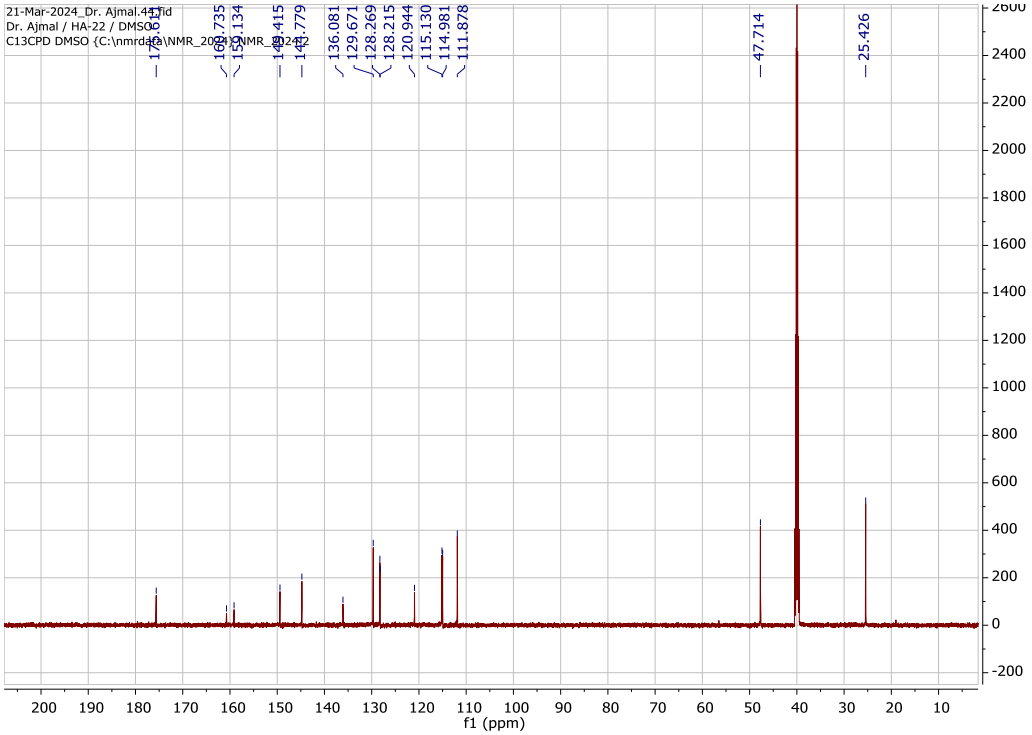
13CNMR, 100 MHz, DMSO-d6 of 5a



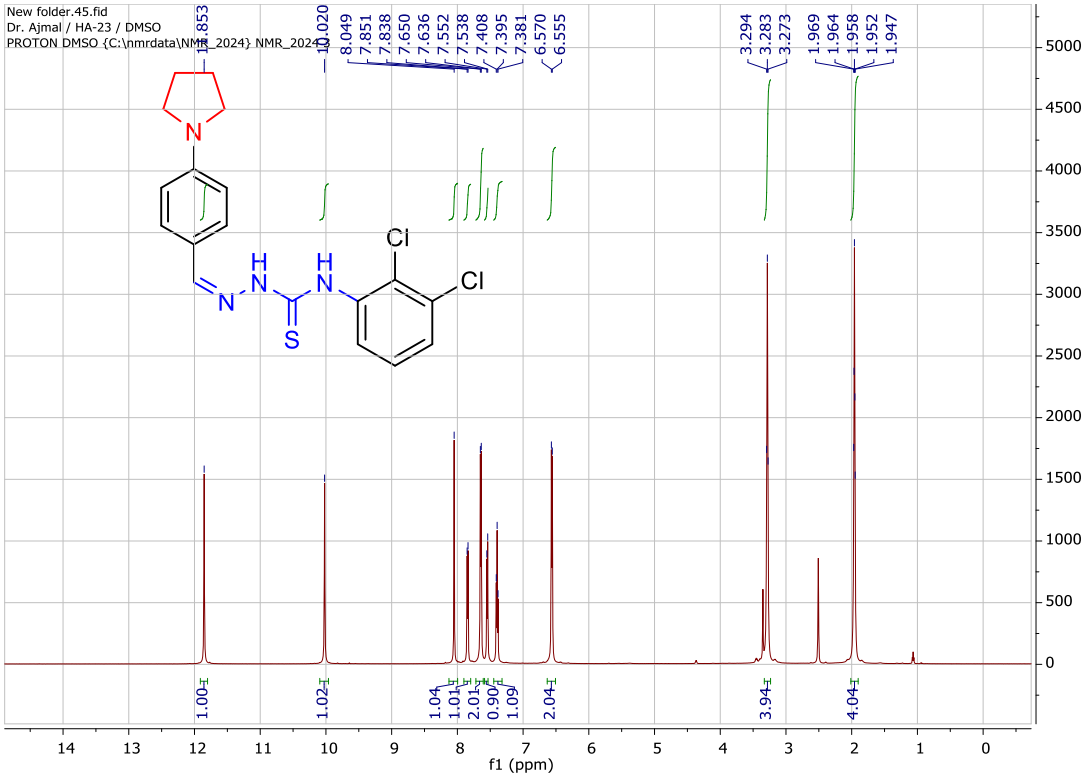
1HNMR, 600 MHz, DMSO-d6 of 5b



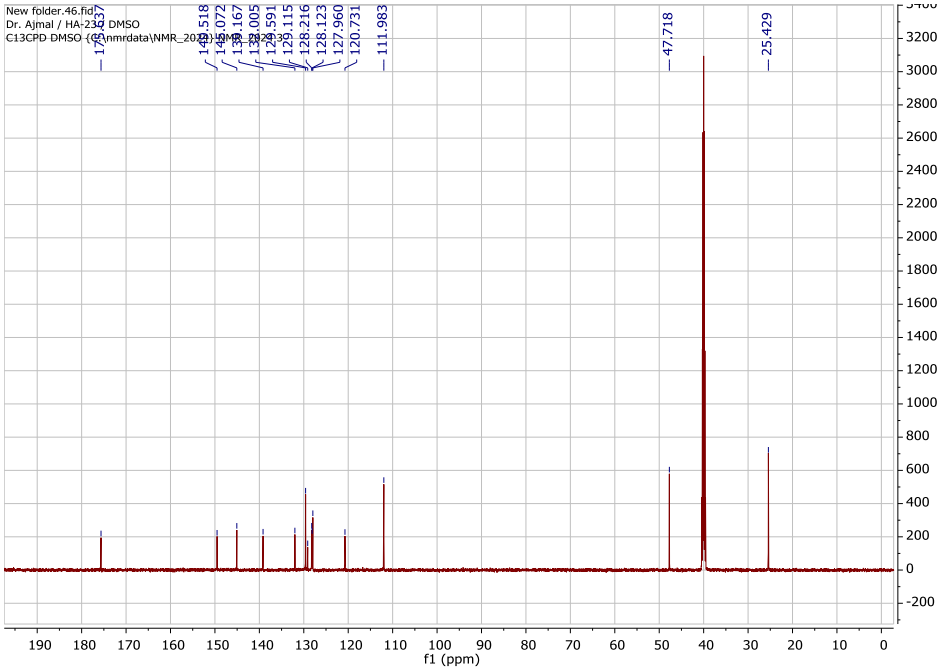
13CNMR, 151 MHz, DMSO-d6 of 5b



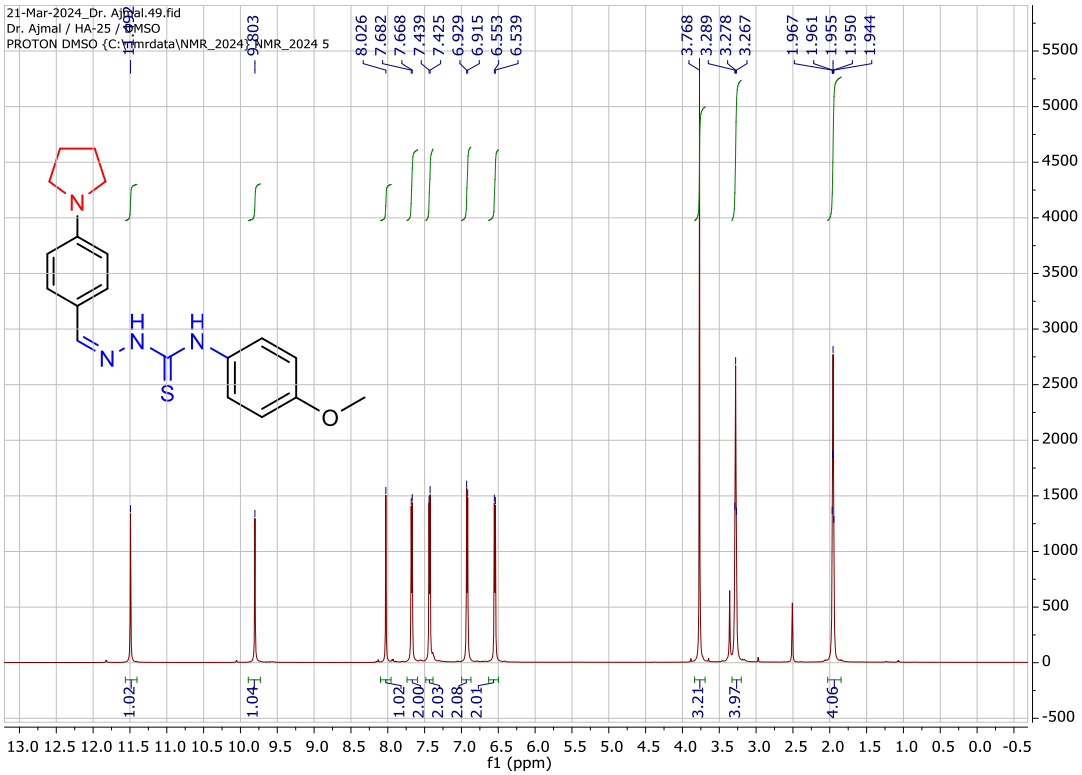
1HNMR, 600 MHz, DMSO-d6 of 5c



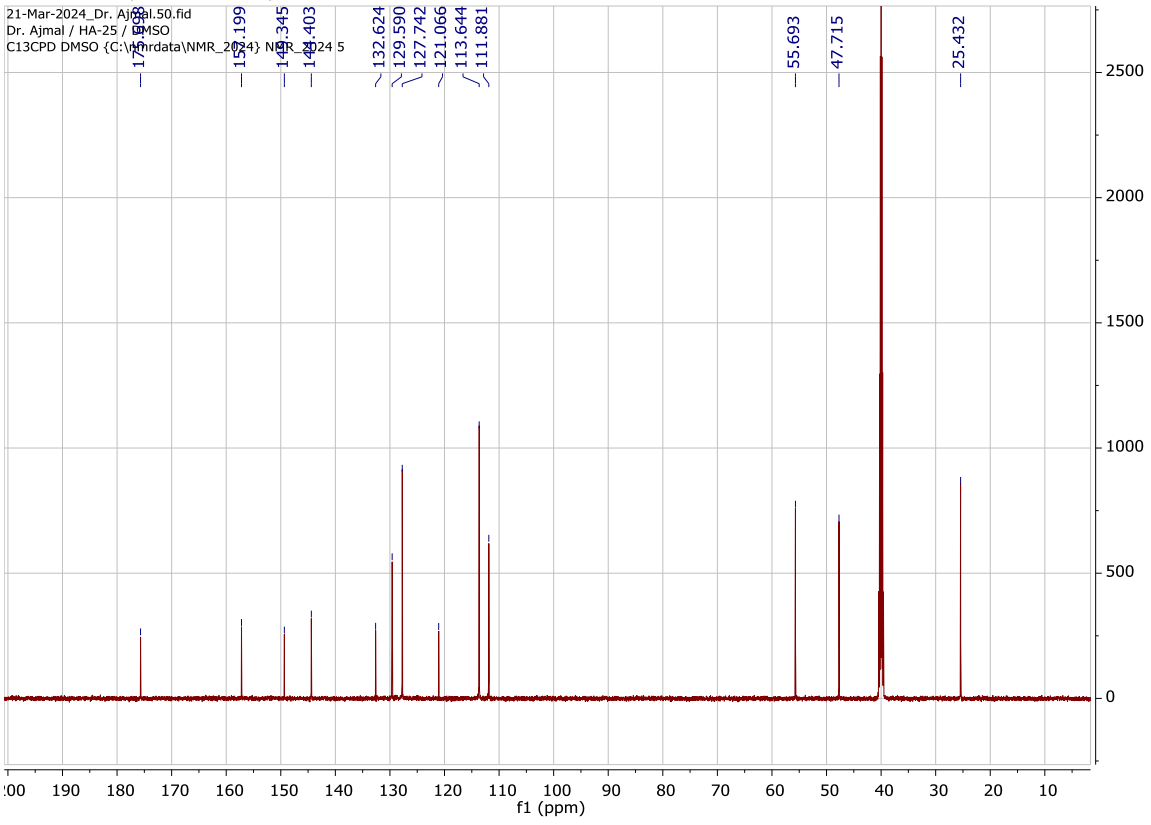
13CNMR, 151 MHz, DMSO-d6 of 5c



1HNMR, 600 MHz, DMSO-d6 of 5d



13CNMR, 151 MHz, DMSO-d6 of 5d



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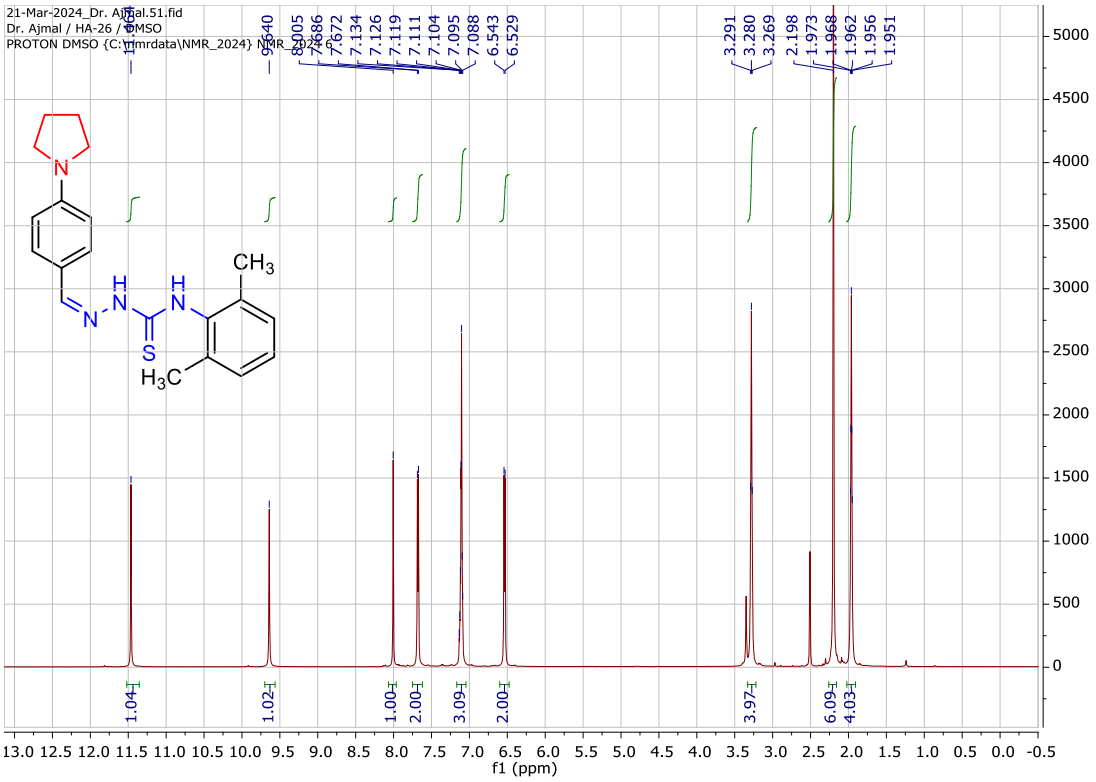
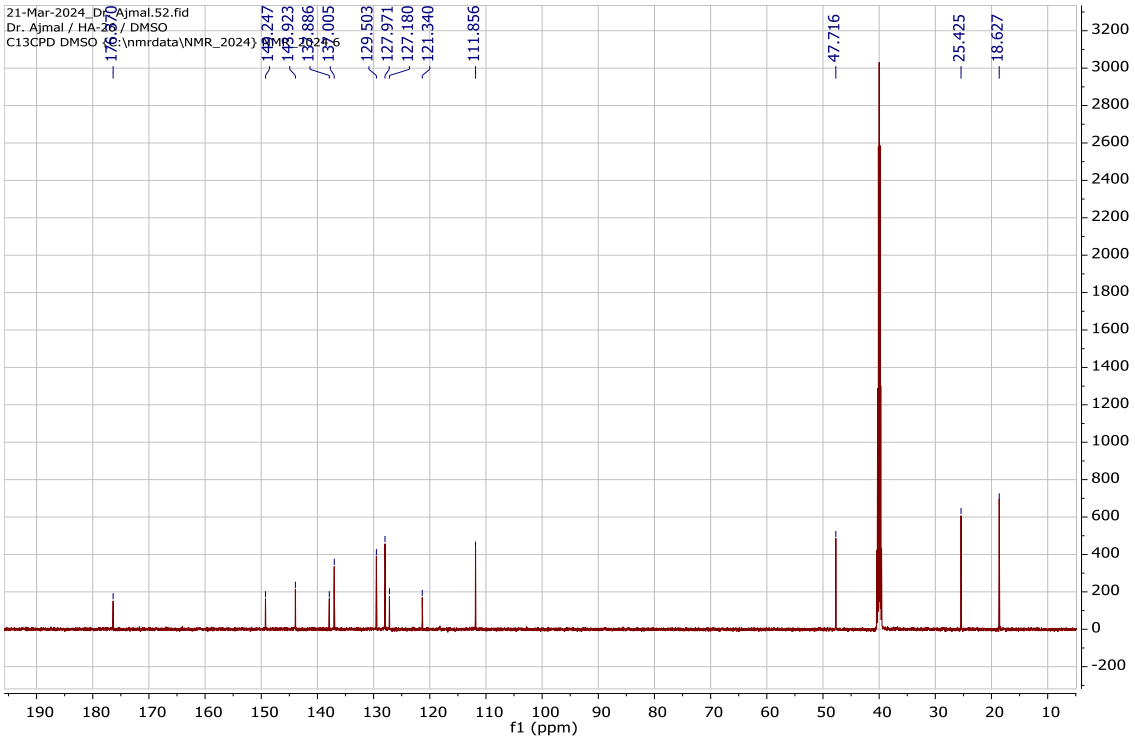
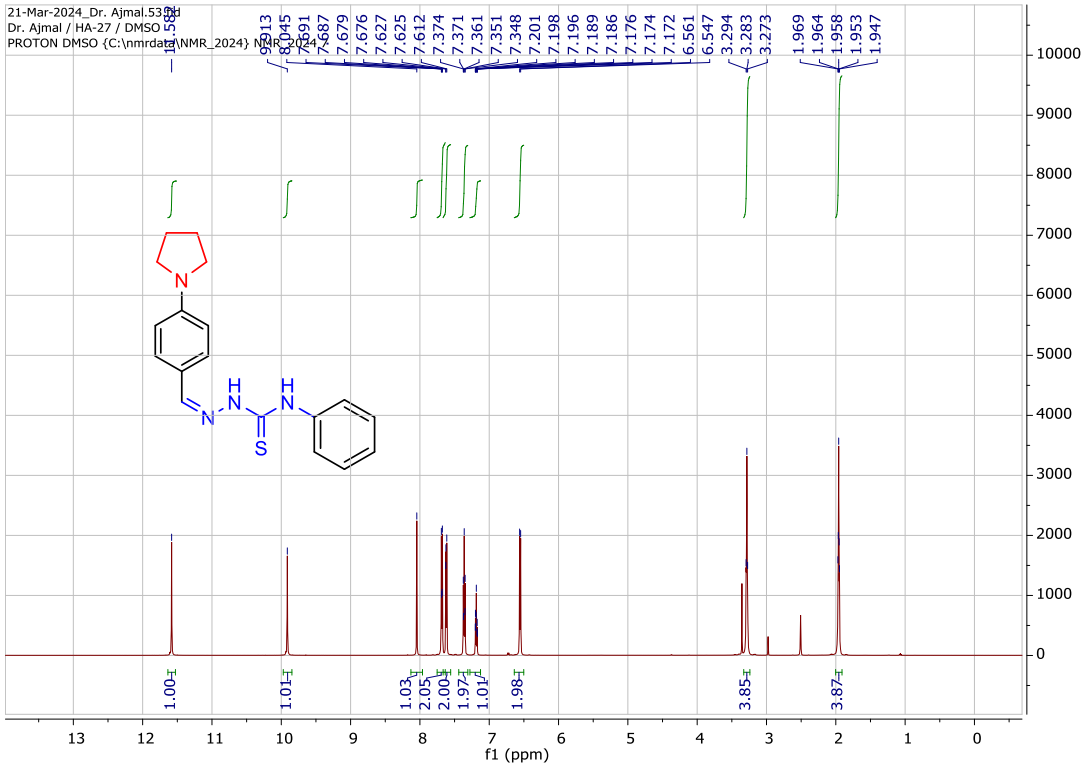


13CNMR, 151 MHz, DMSO-d6 of 5e



1HNMR, 600 MHz, DMSO-d6 of 5f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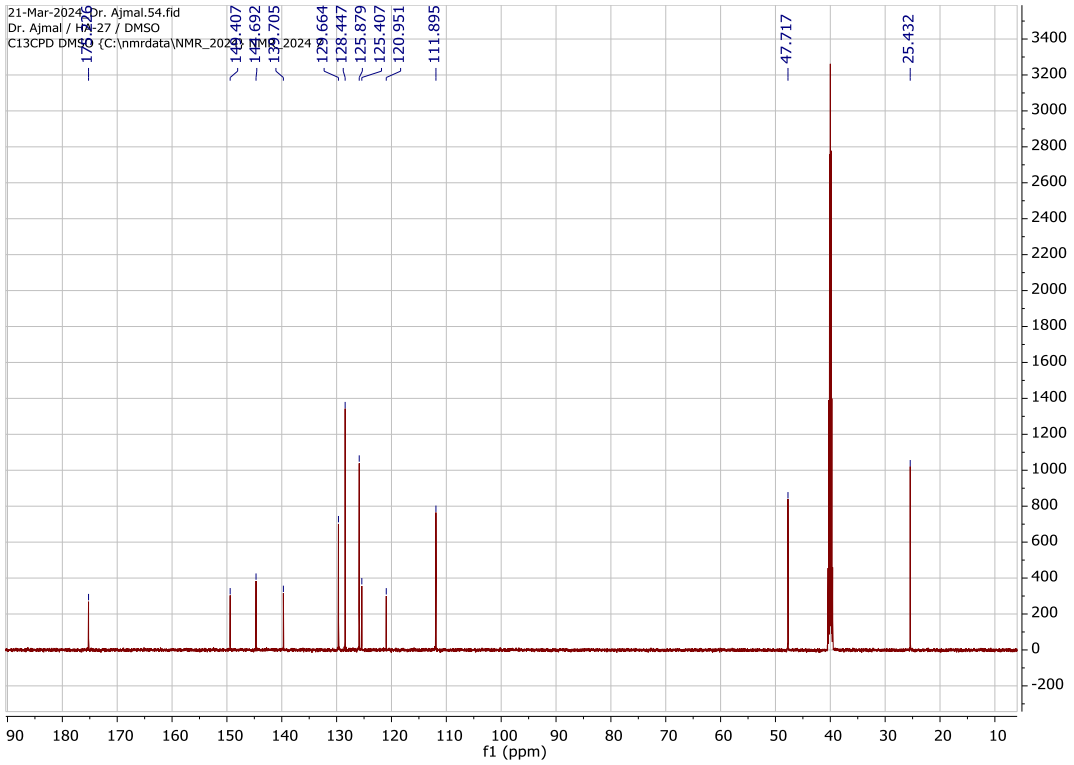
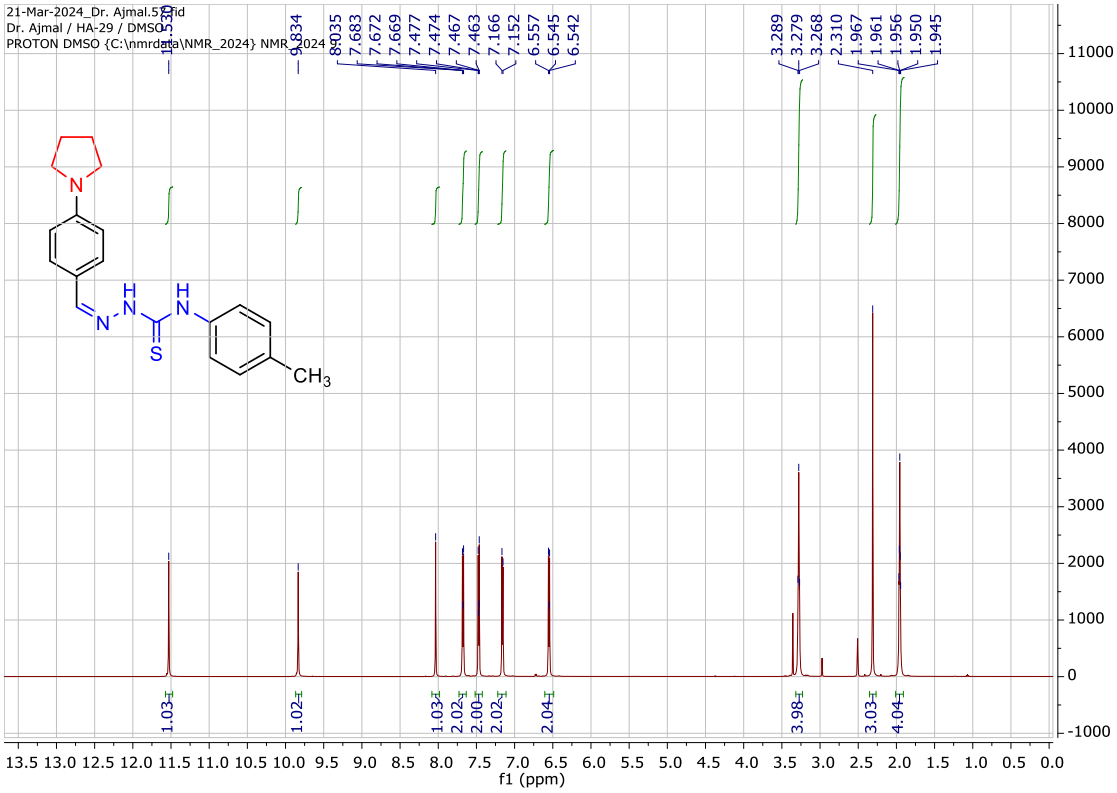
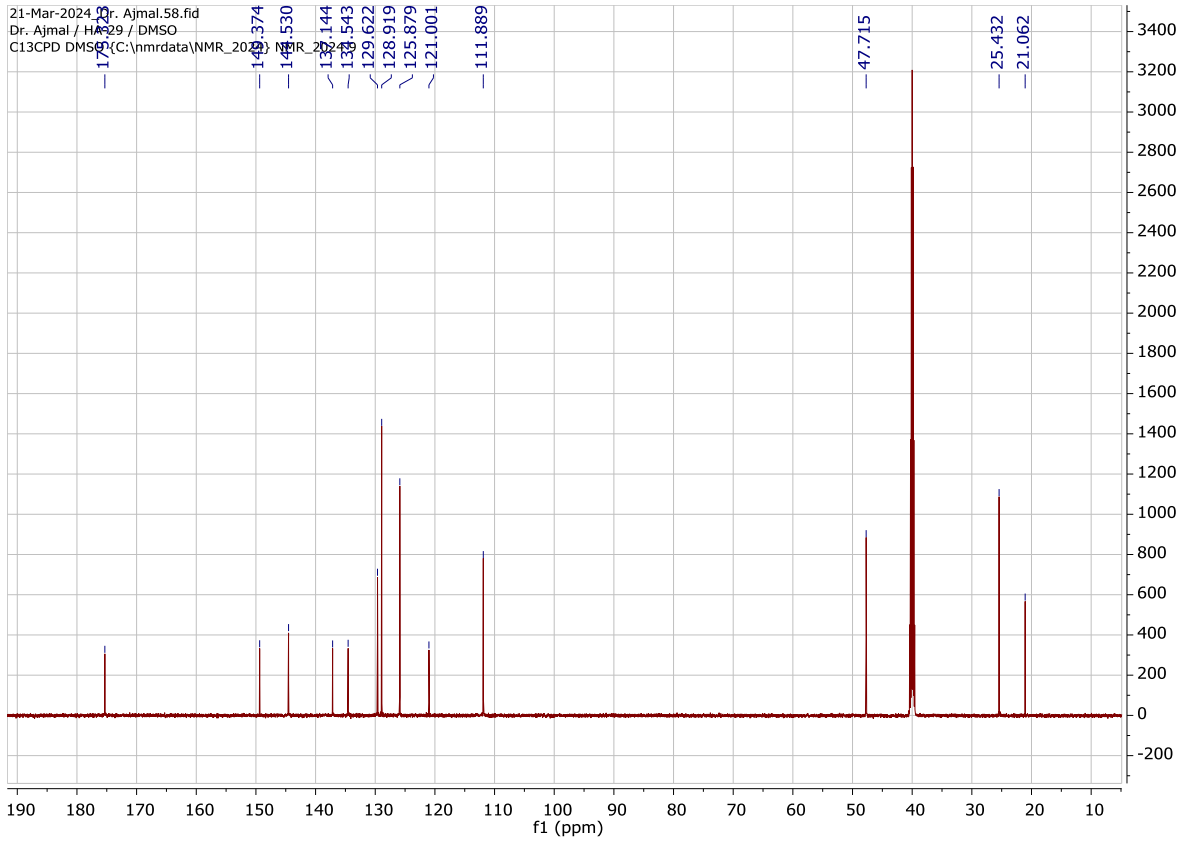
13CNMR, 151 MHz, DMSO-d6 of 5f



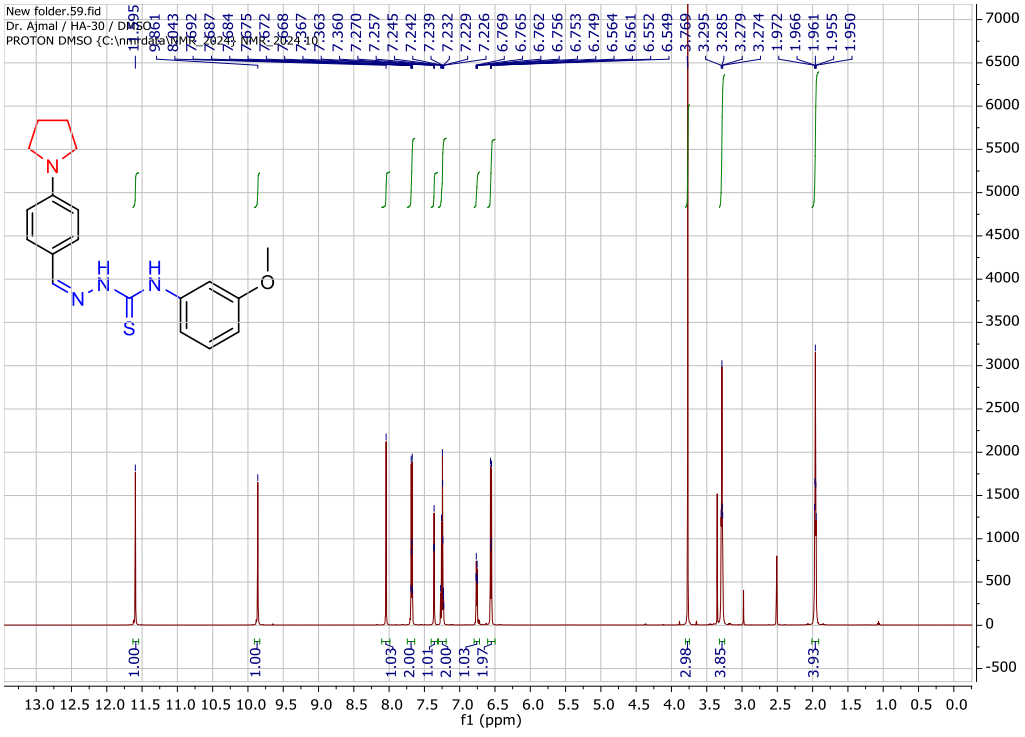
1HNMR, 600 MHz, DMSO-d6 of 5g



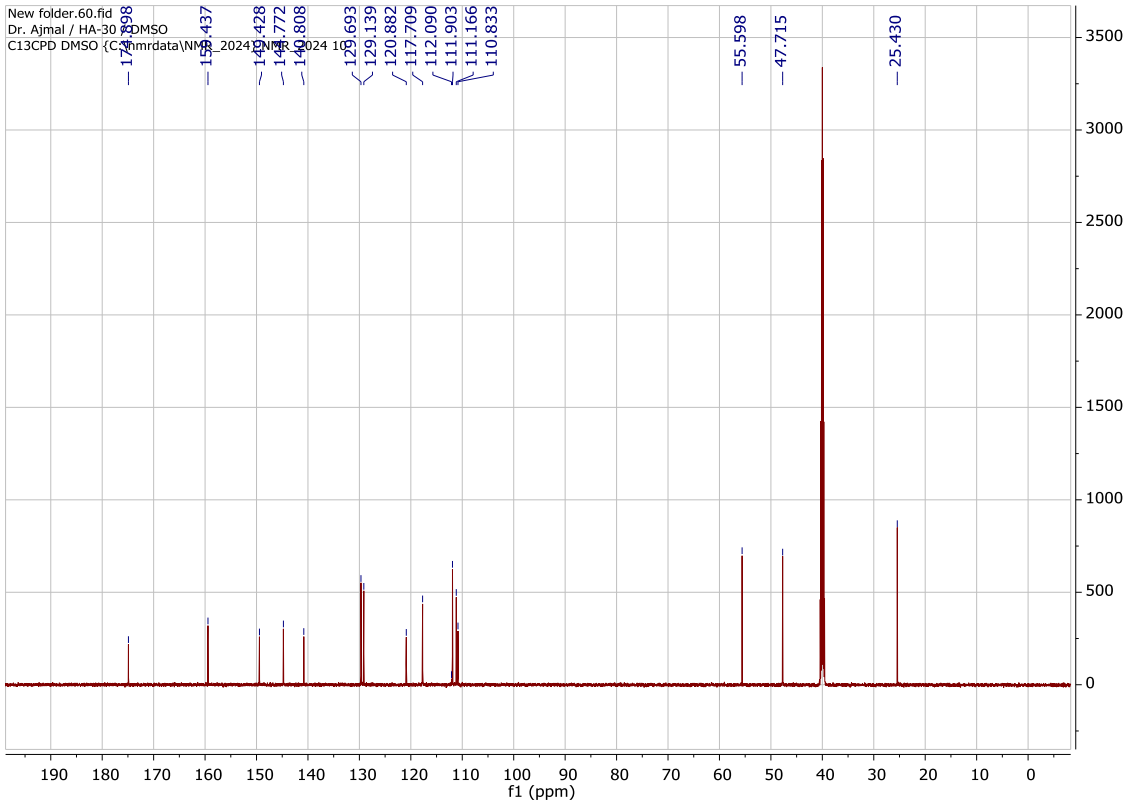
13CNMR,151 MHz, DMSO-d6 of 5g



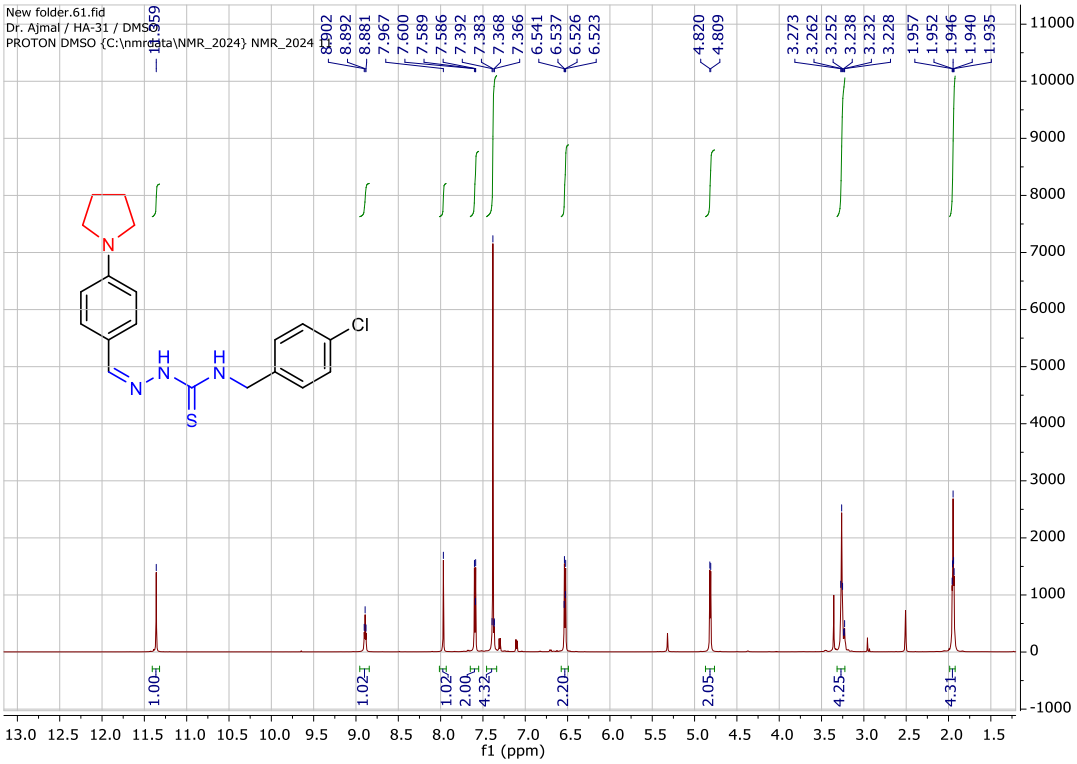
1HNMR, 600 MHz, DMSO-d6 of 5h



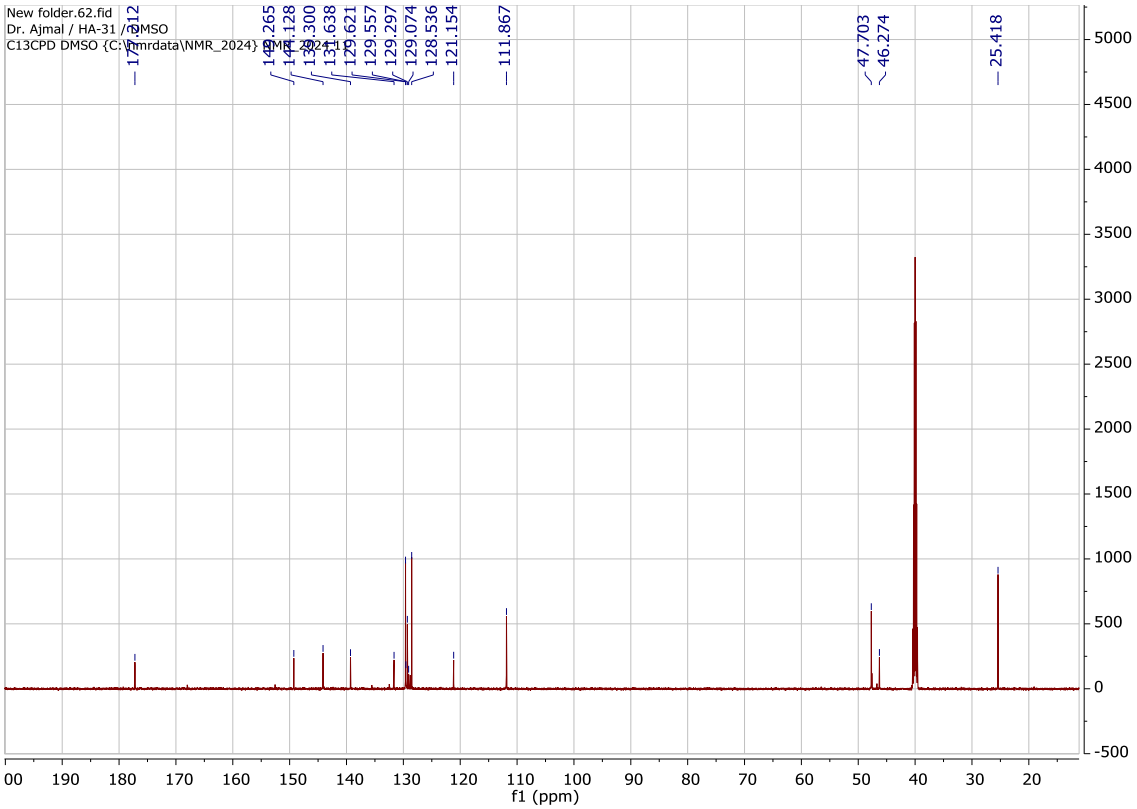
13CNMR, 151 MHz, DMSO-d6 of 5h



1HNMR, 600 MHz, DMSO-d6 of 5i



13CNMR, 151 MHz, DMSO-d6 of 5i



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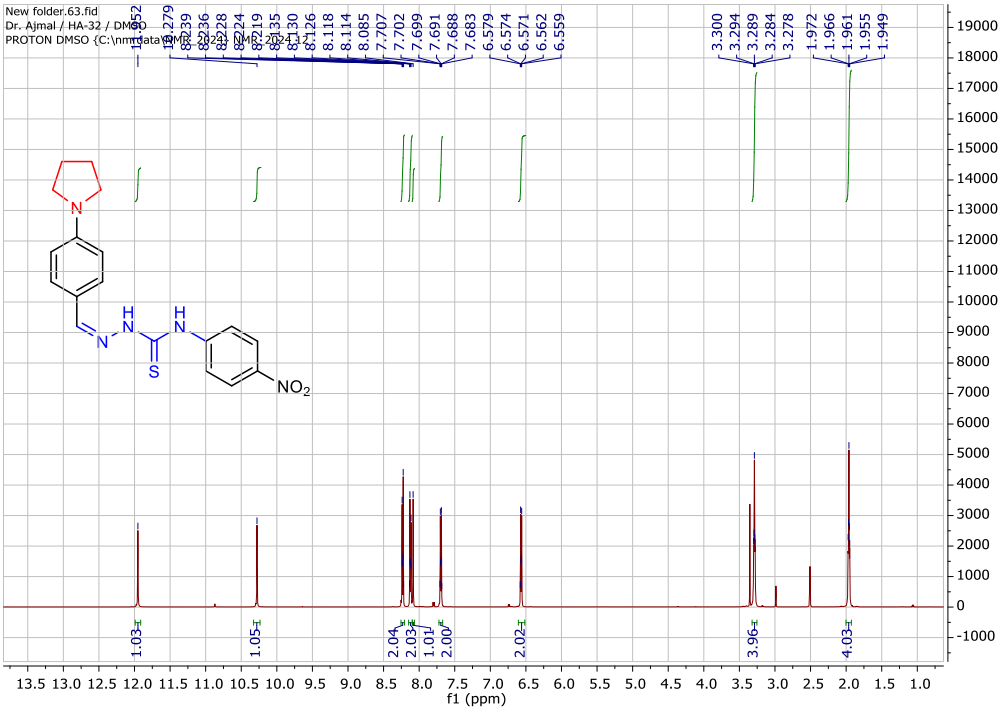
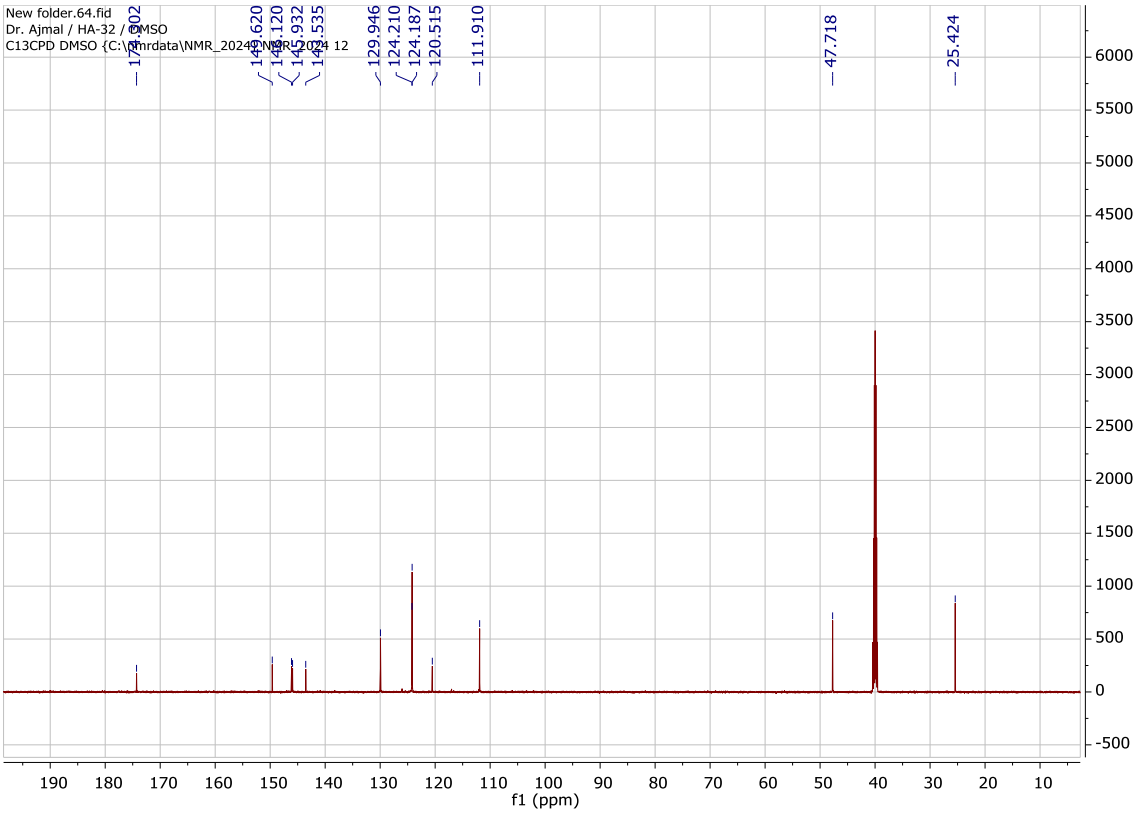
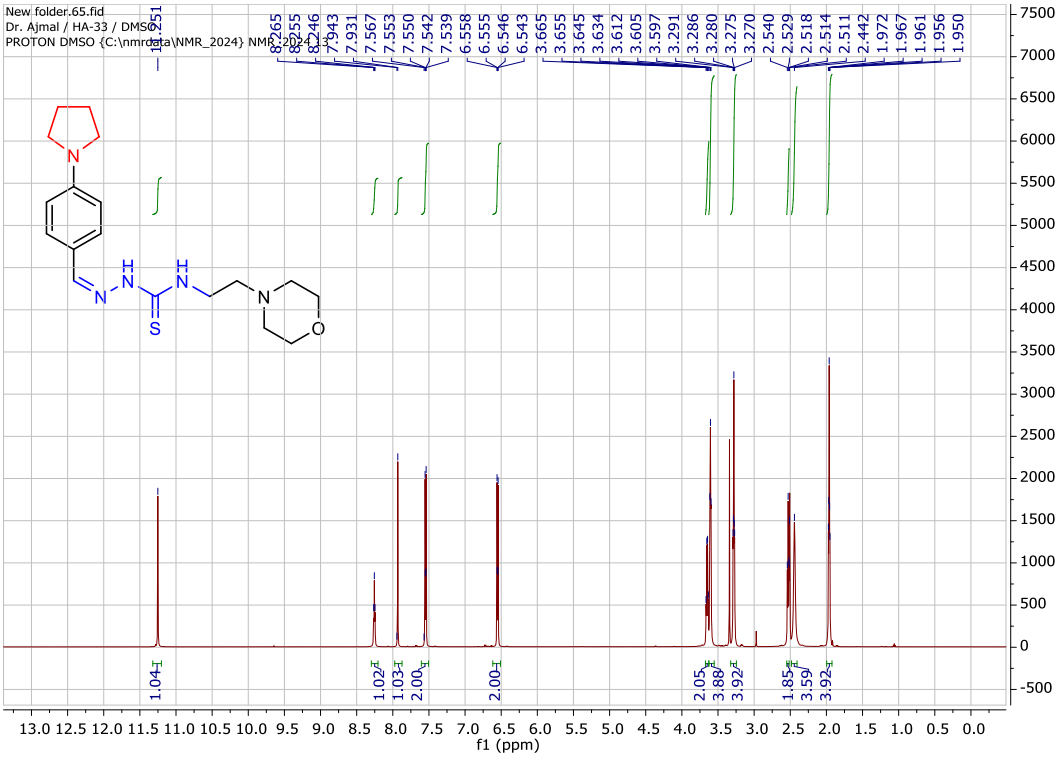


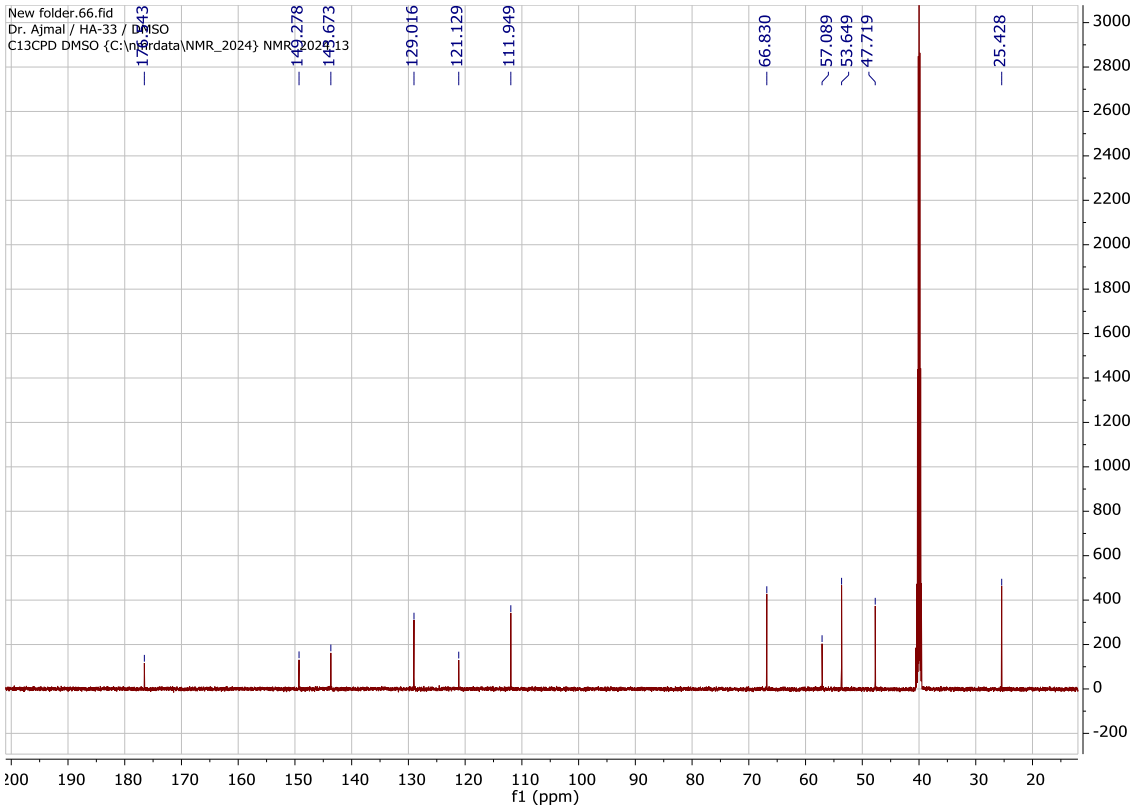
13CNMR, 151 MHz, DMSO-d6 of 5j



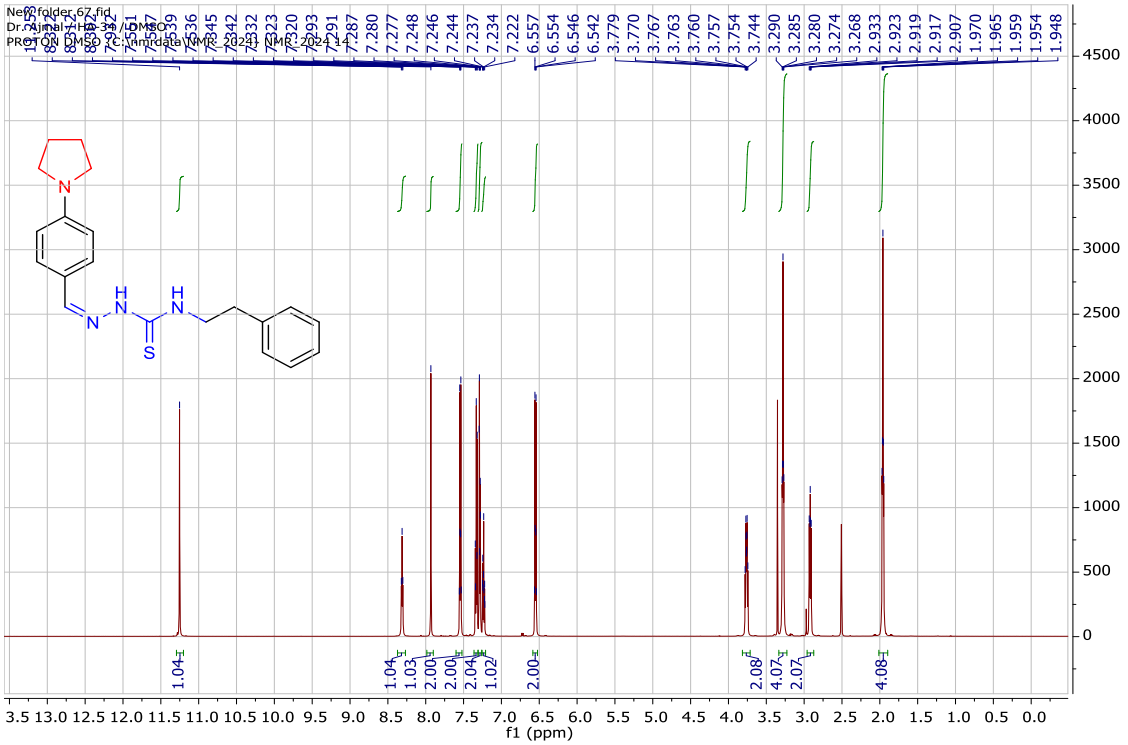
1HNMR, 600 MHz, DMSO-d6 of 5k



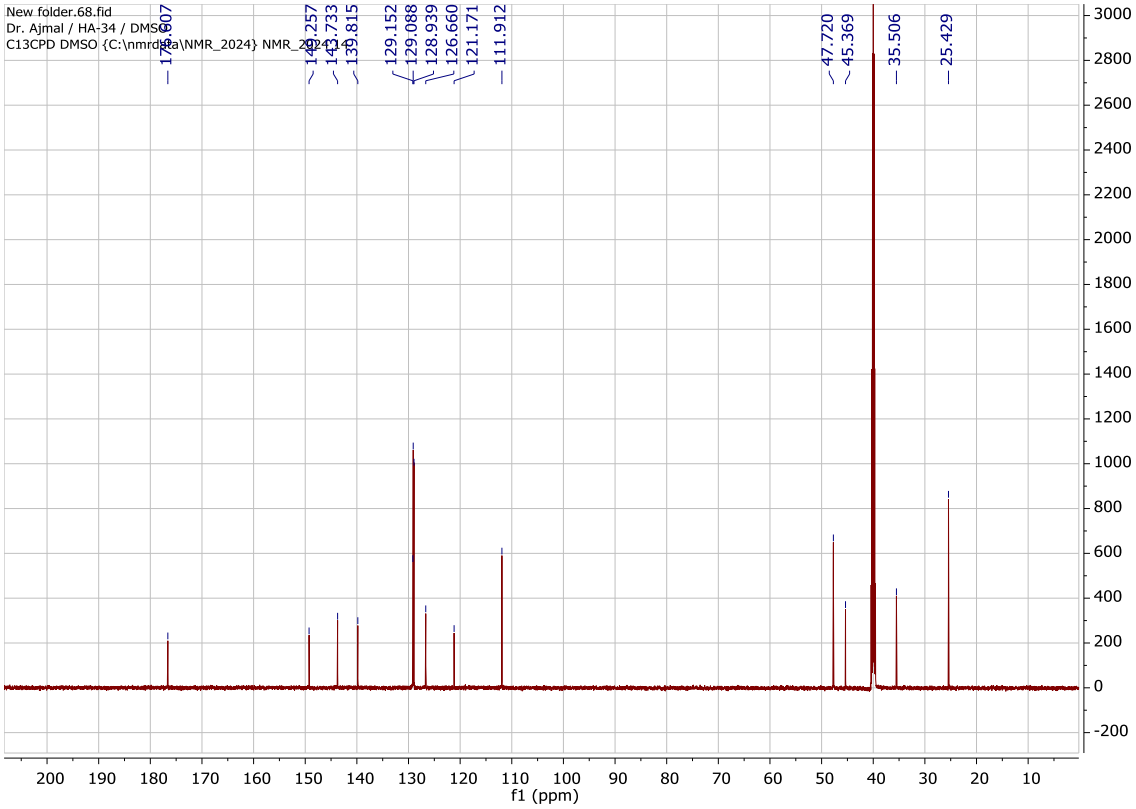
13CNMR, 151 MHz, DMSO-d6 of 5k



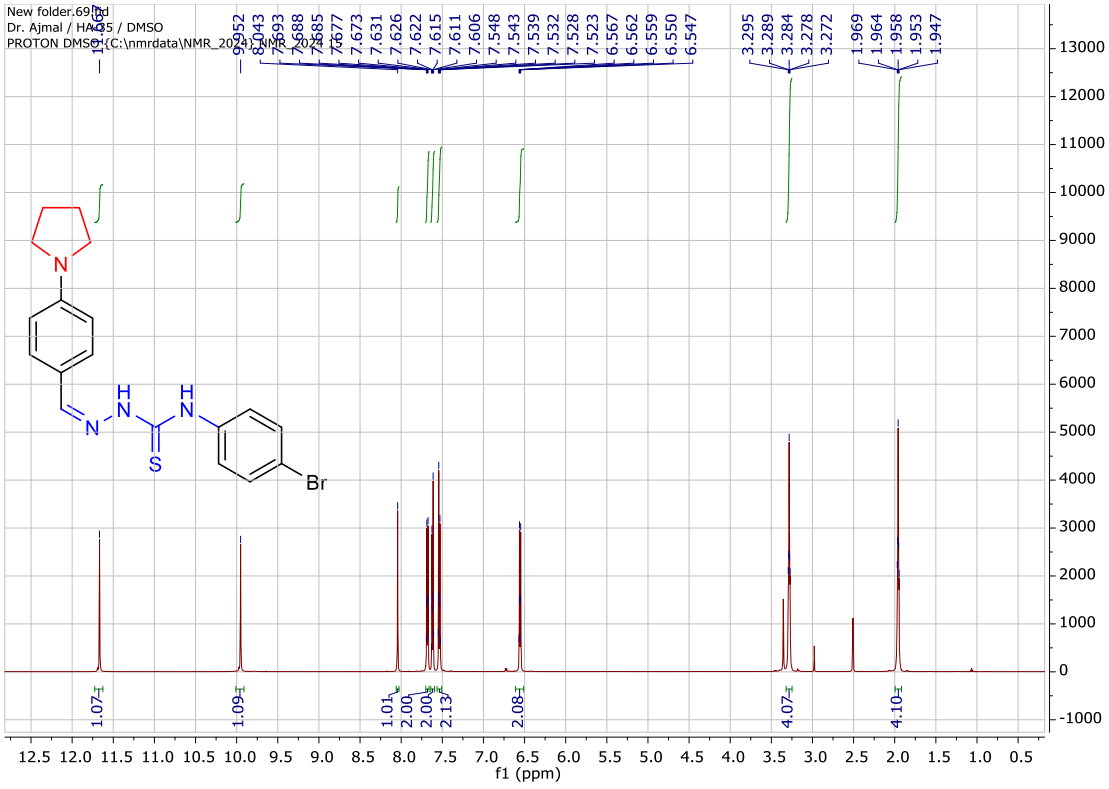
1HNMR, 600 MHz, DMSO-d6 of 5l



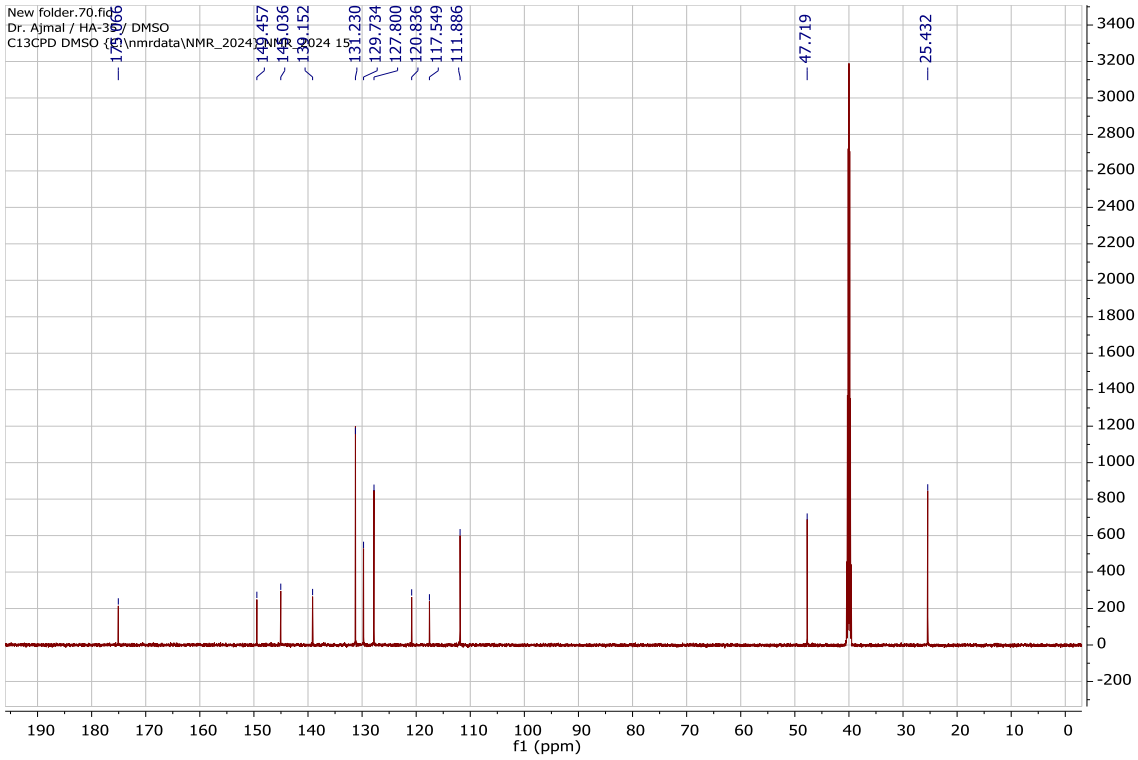
13CNMR, 151 MHz, DMSO-d6 of 5l



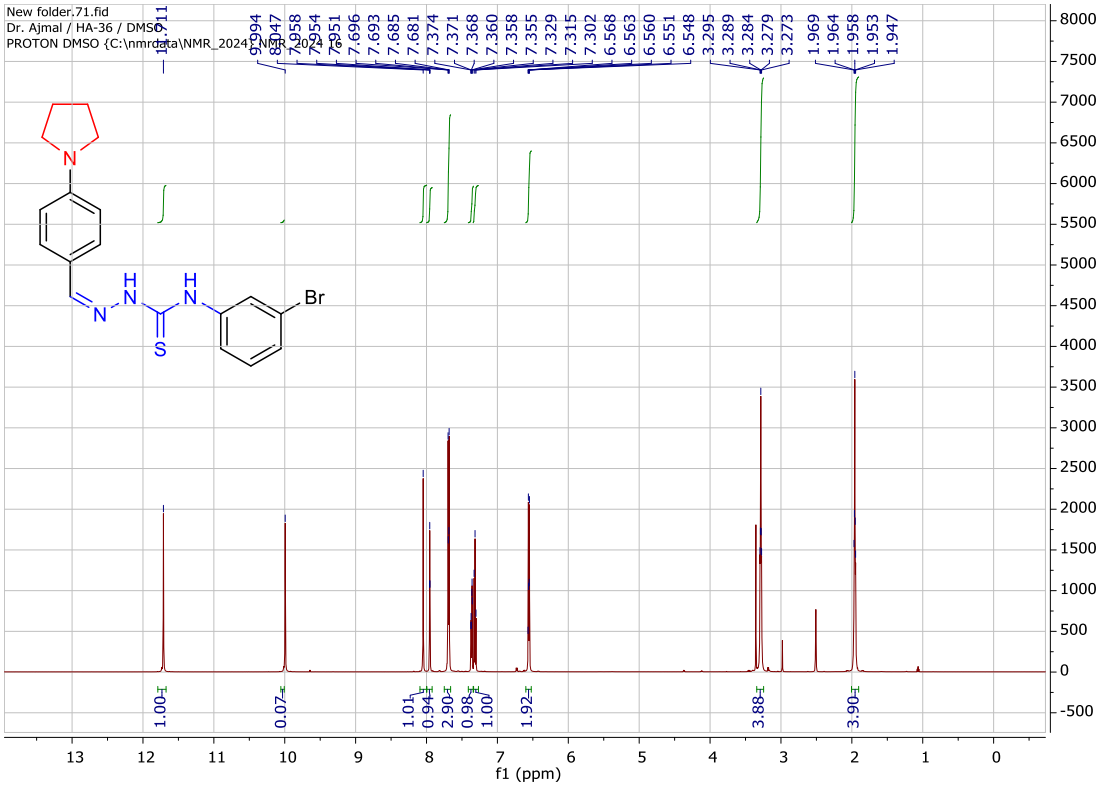
1HNMR, 600 MHz, DMSO-d6 of 5m



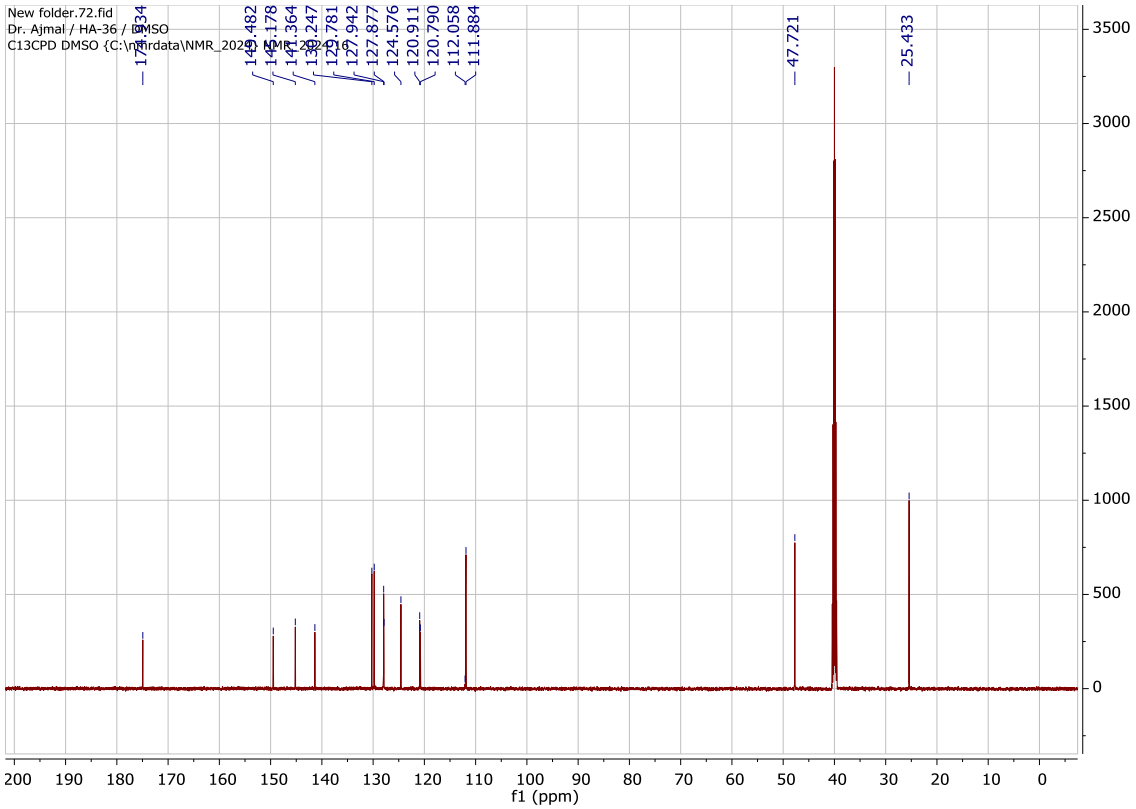
13CNMR, 151 MHz, DMSO-d6 of 5m



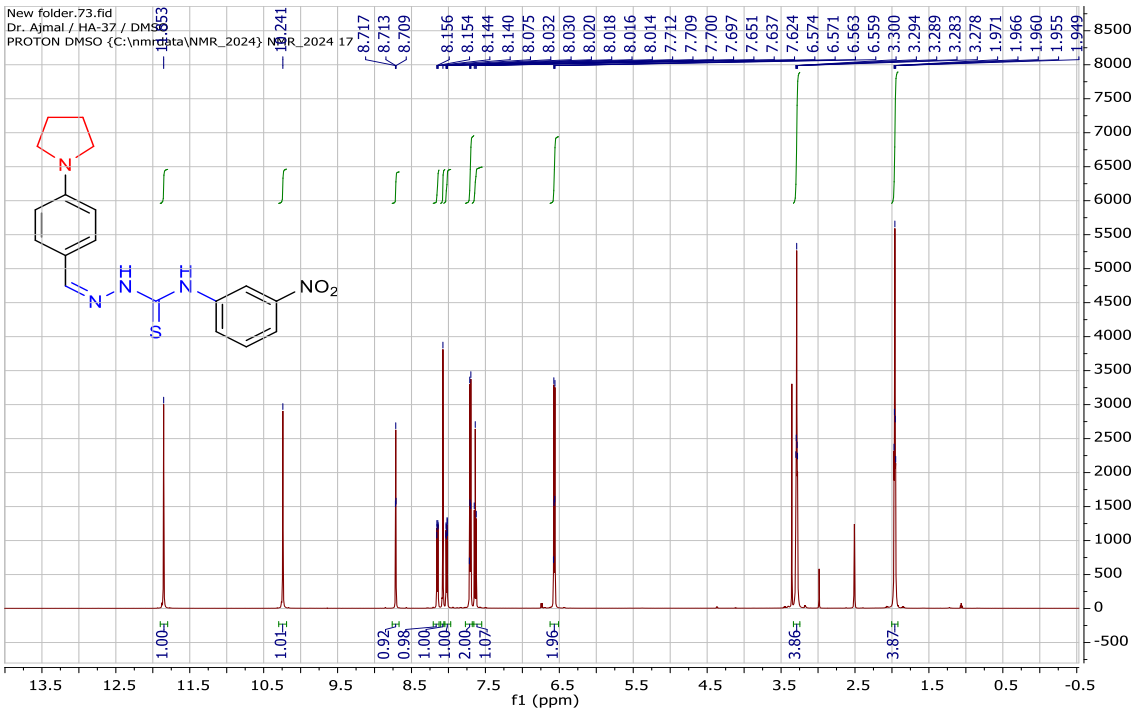
1HNMR, 600 MHz, DMSO-d6 of 5n



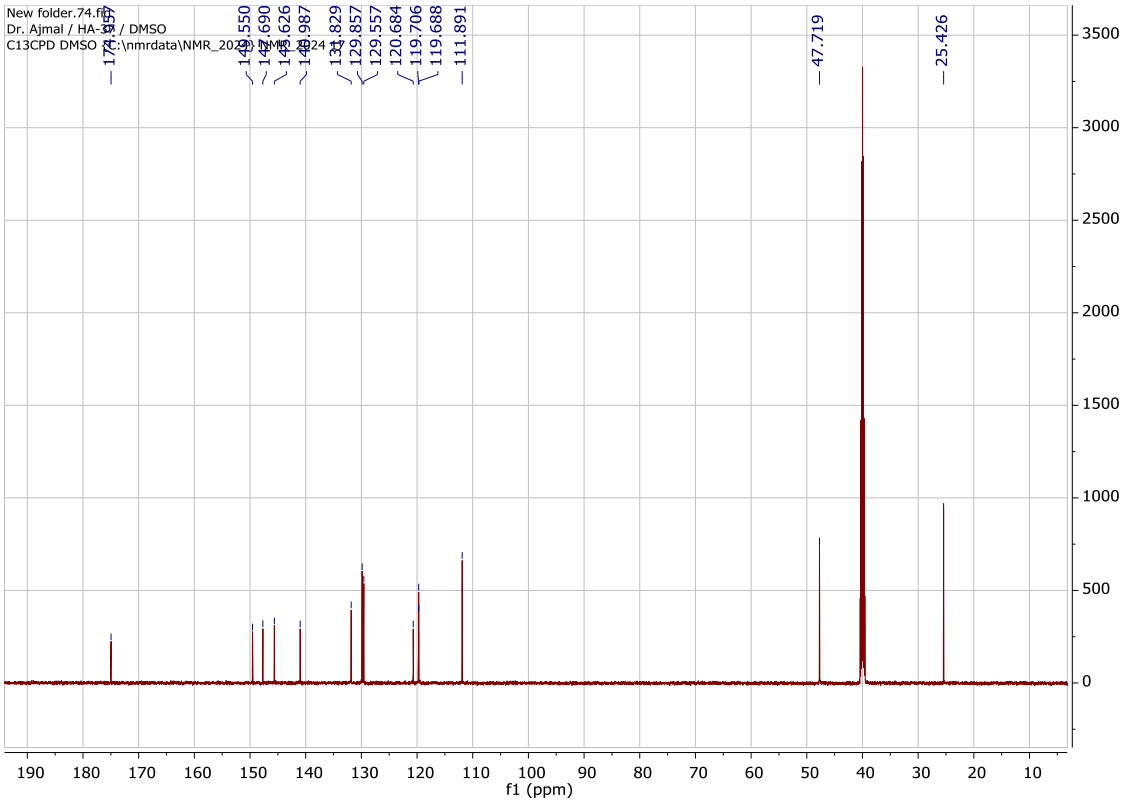
13CNMR, 151 MHz, DMSO-d6 of 5n



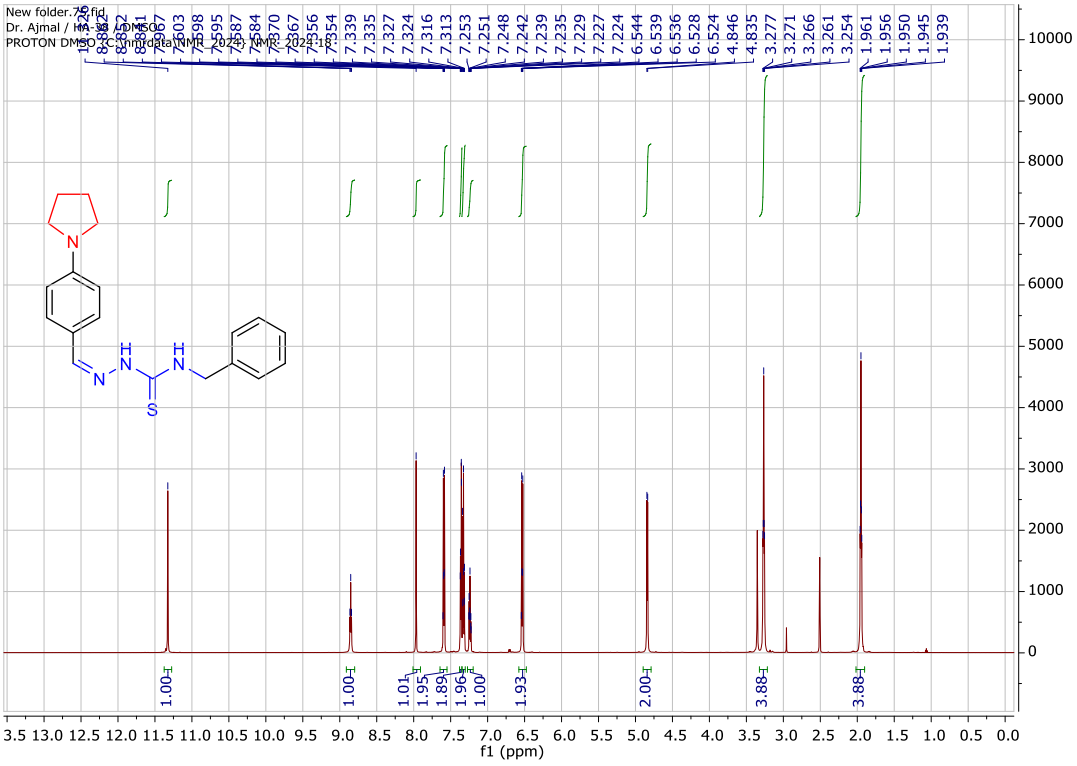
1HNMR, 600 MHz, DMSO-d6 of 5o



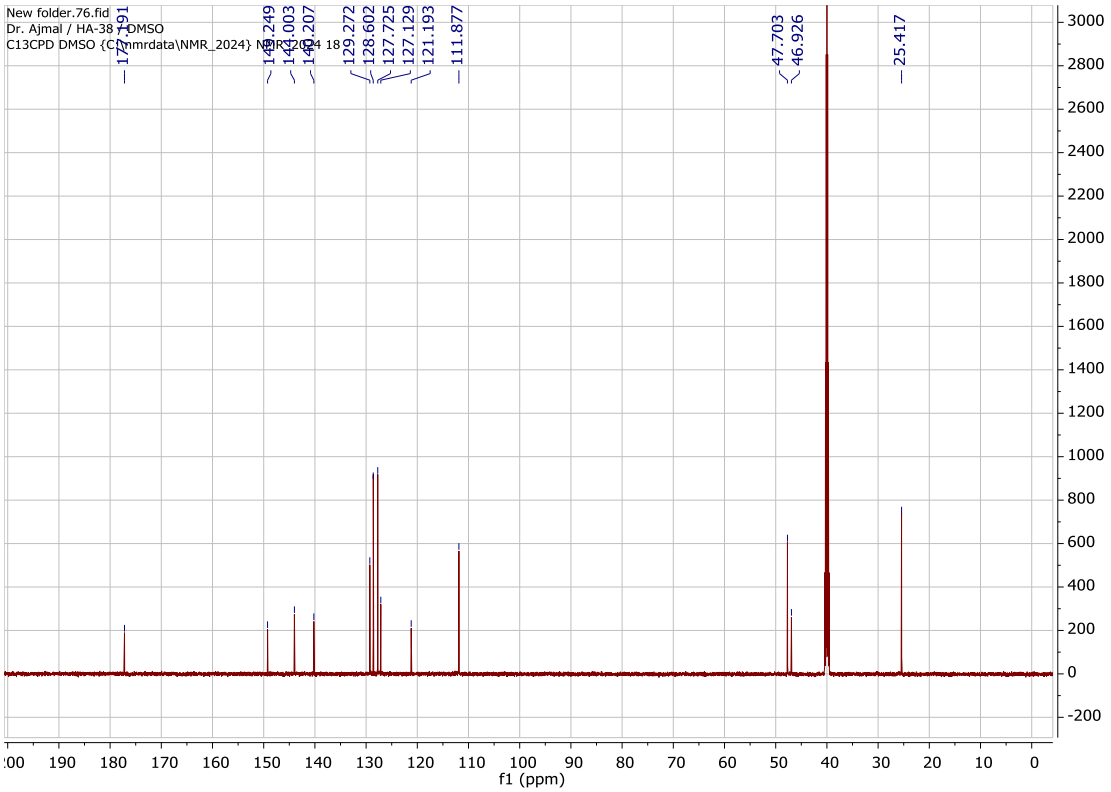
13CNMR, 151 MHz, DMSO-d6 of 5o



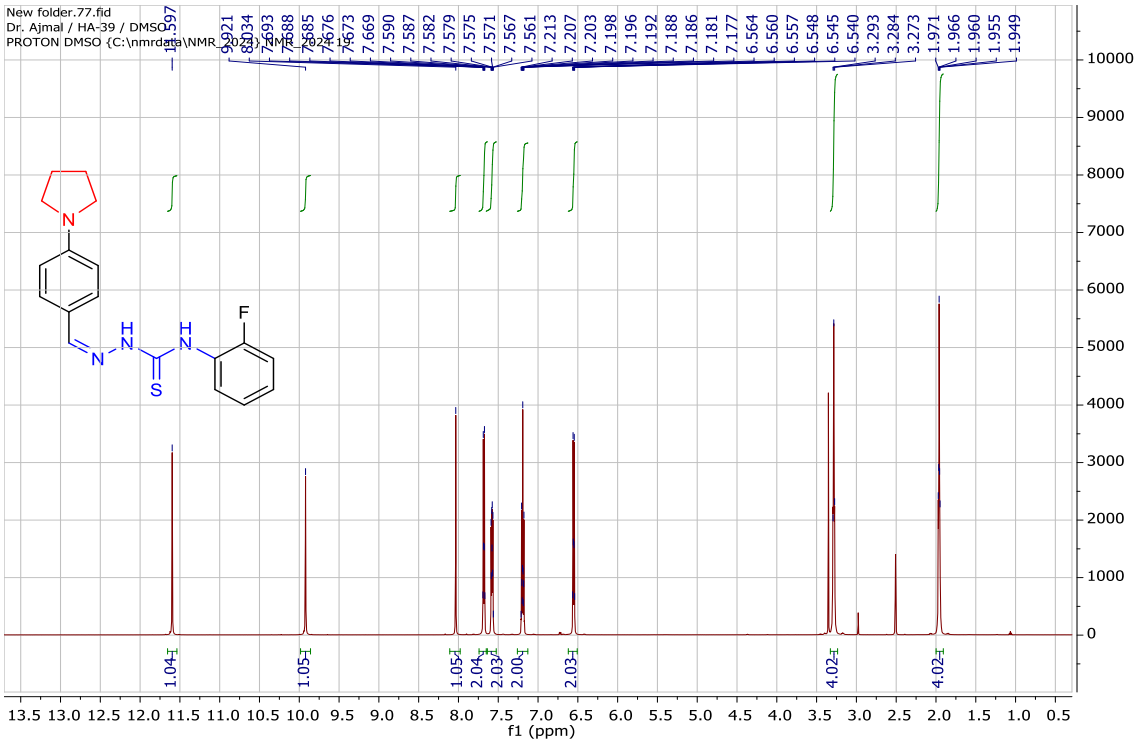
1HNMR, 600 MHz, DMSO-d6 of 5p



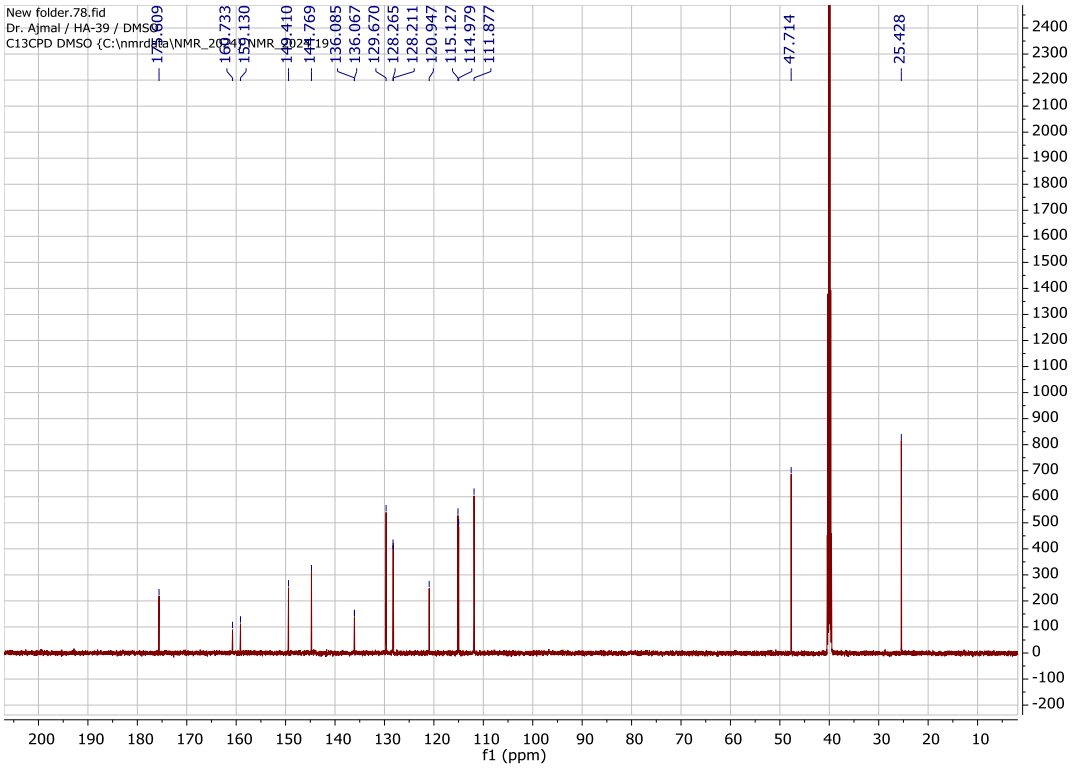
13CNMR, 151 MHz, DMSO-d6 of 5p



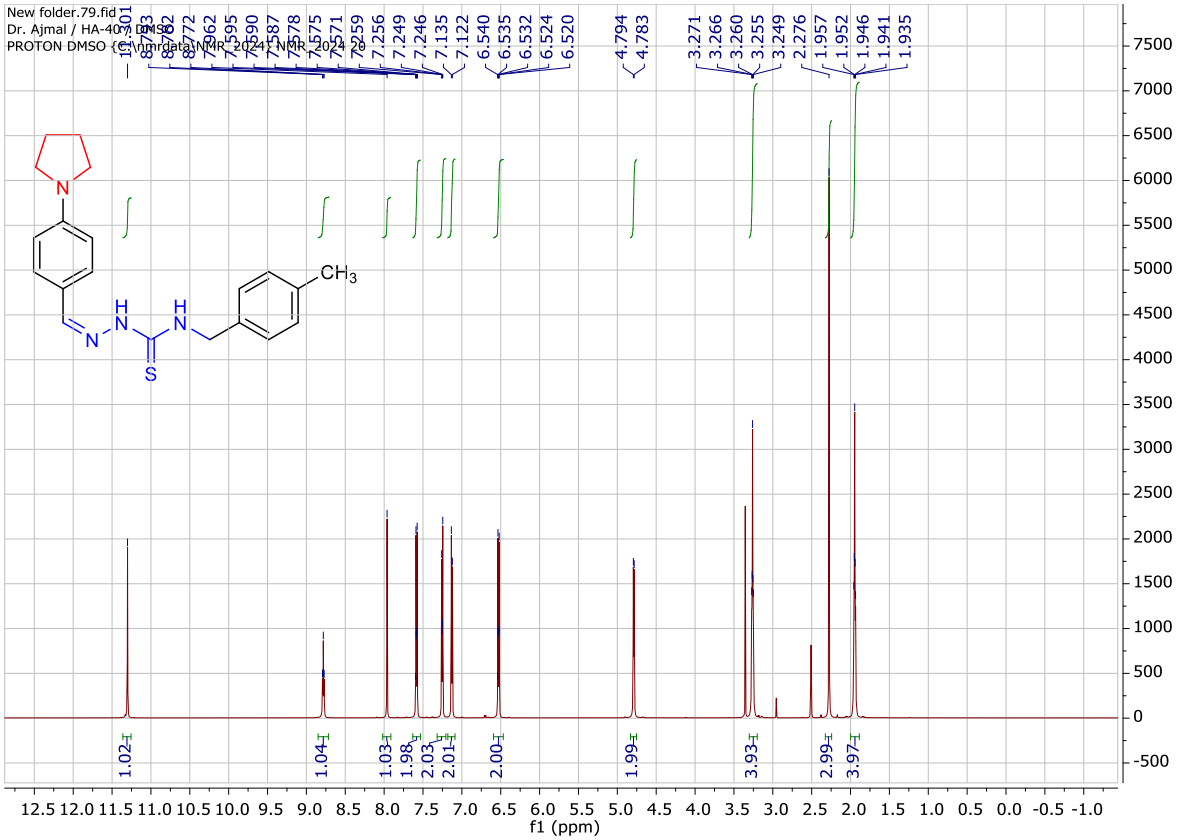
1HNMR, 600 MHz, DMSO-d6 of 5q



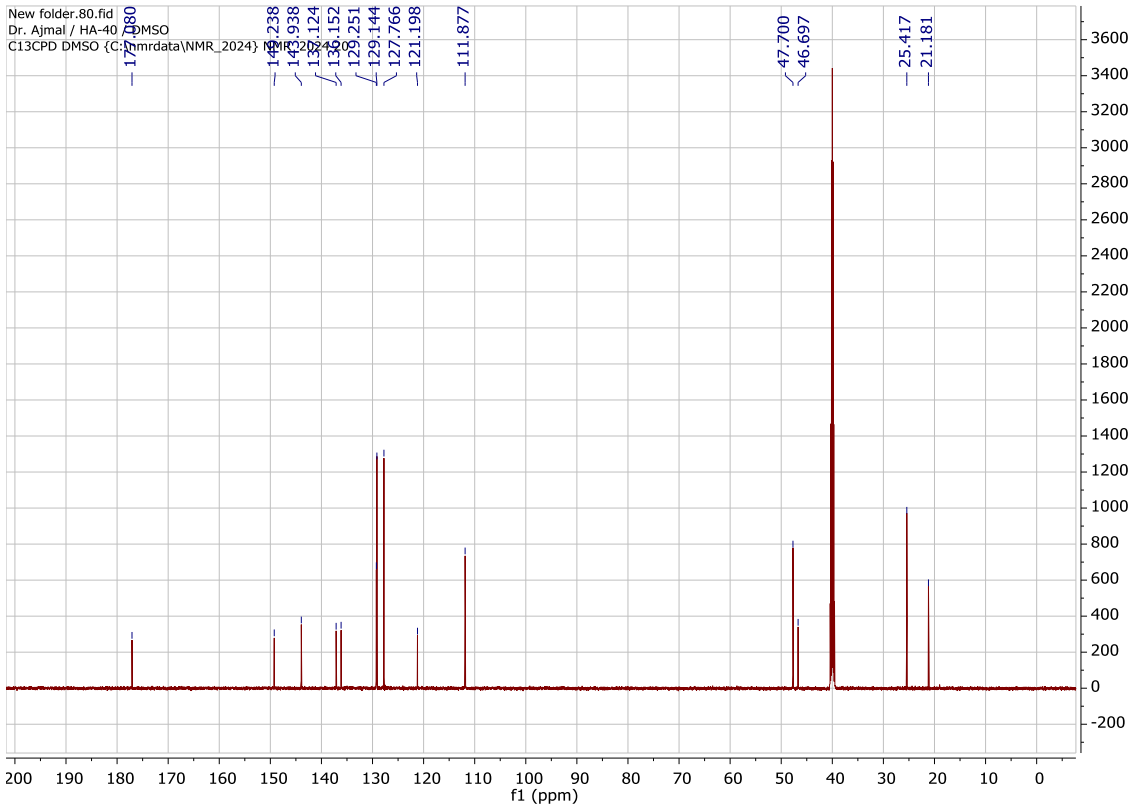
13CNMR, 151 MHz, DMSO-d6 of 5q



1HNMR, 600 MHz, DMSO-d6 of 5r

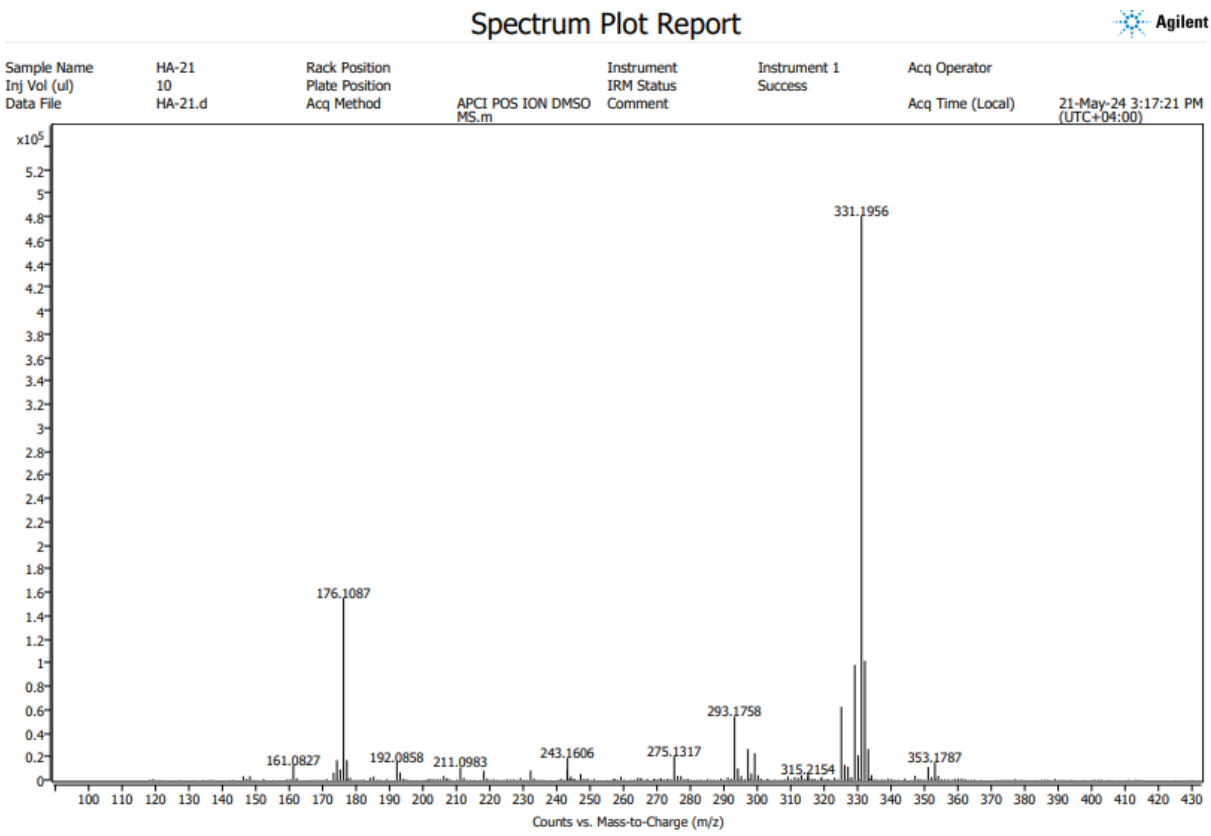


13CNMR, 151 MHz, DMSO-d6 of 5r

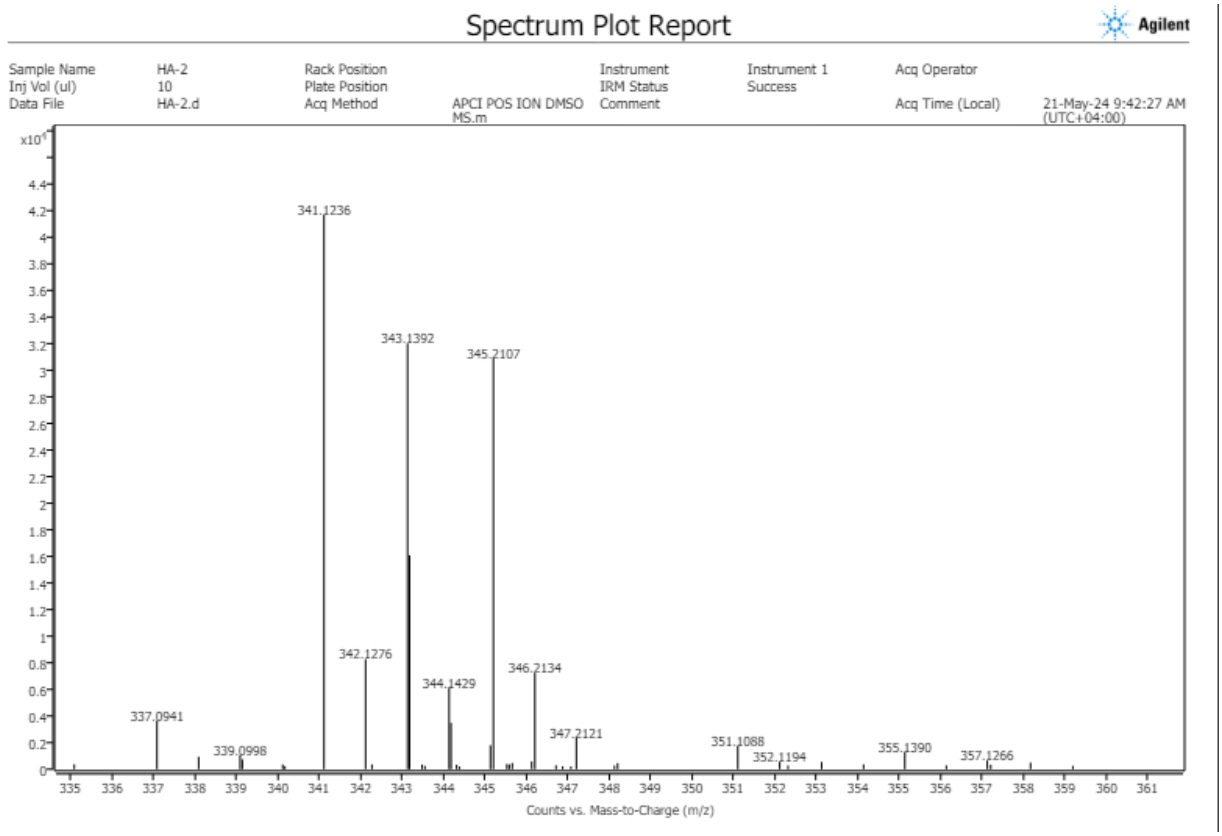


HRMS of synthesized compounds 5(a-r)

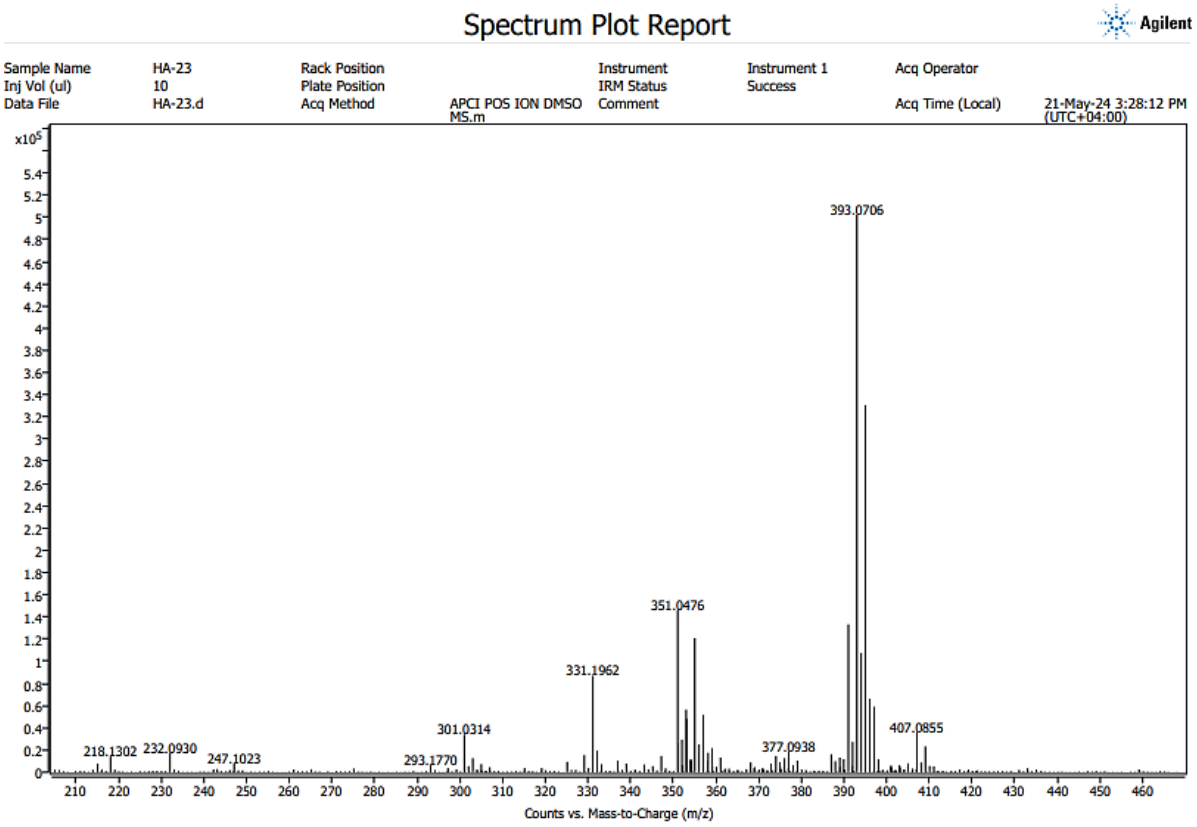
5a


Spectrum Plot Report
Agilent
Sample Name HA-21
Inj Vol (ul) 10
Data File HA-21.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 3:17:21 PM (UTC+04:00)
x10^5
331.1956
176.1087
293.1758
161.0827
192.0858
211.0983
243.1606
275.1317
315.2154
353.1787
Counts vs. Mass-to-Charge (m/z)

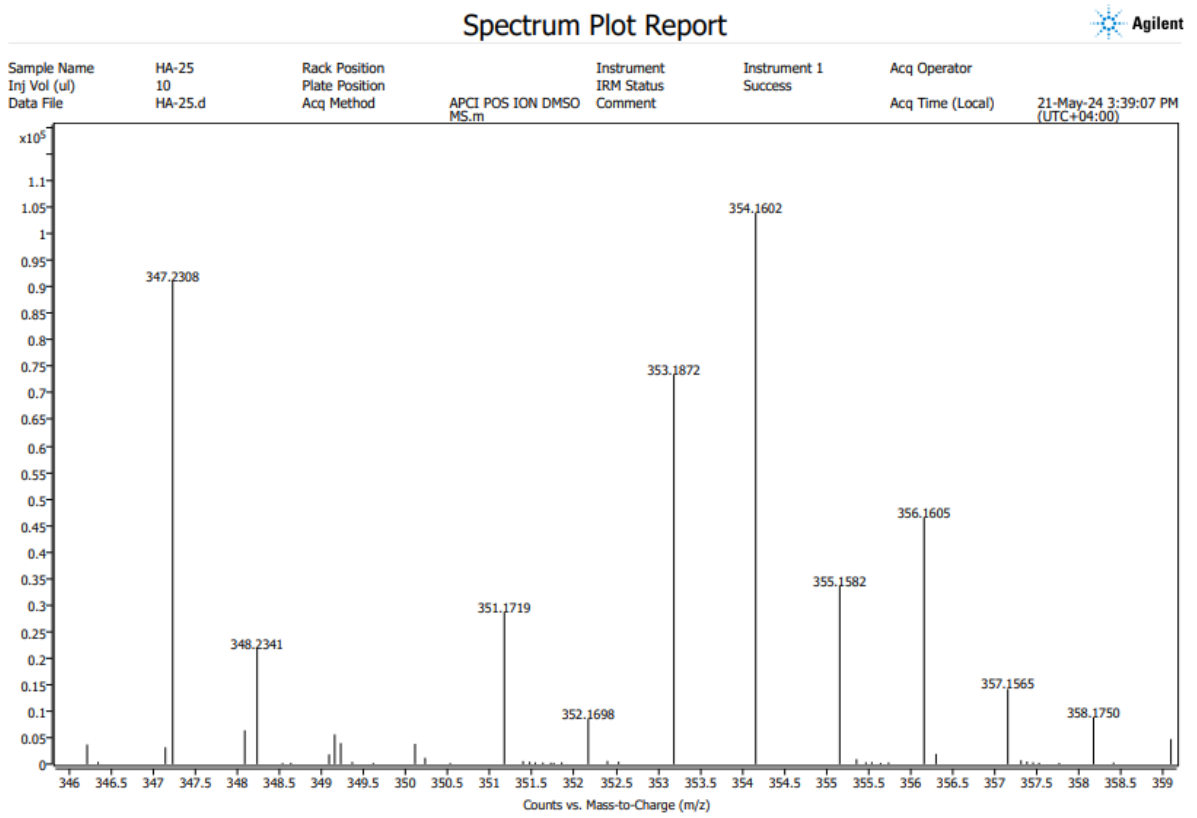
5b


Spectrum Plot Report
Agilent
Sample Name HA-2
Inj Vol (ul) 10
Data File HA-2.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 9:42:27 AM (UTC+04:00)
x10^4
341.1236
343.1392
345.2107
342.1276
344.1429
346.2134
337.0941
339.0998
347.2121
351.1088
352.1194
355.1390
357.1266
Counts vs. Mass-to-Charge (m/z)

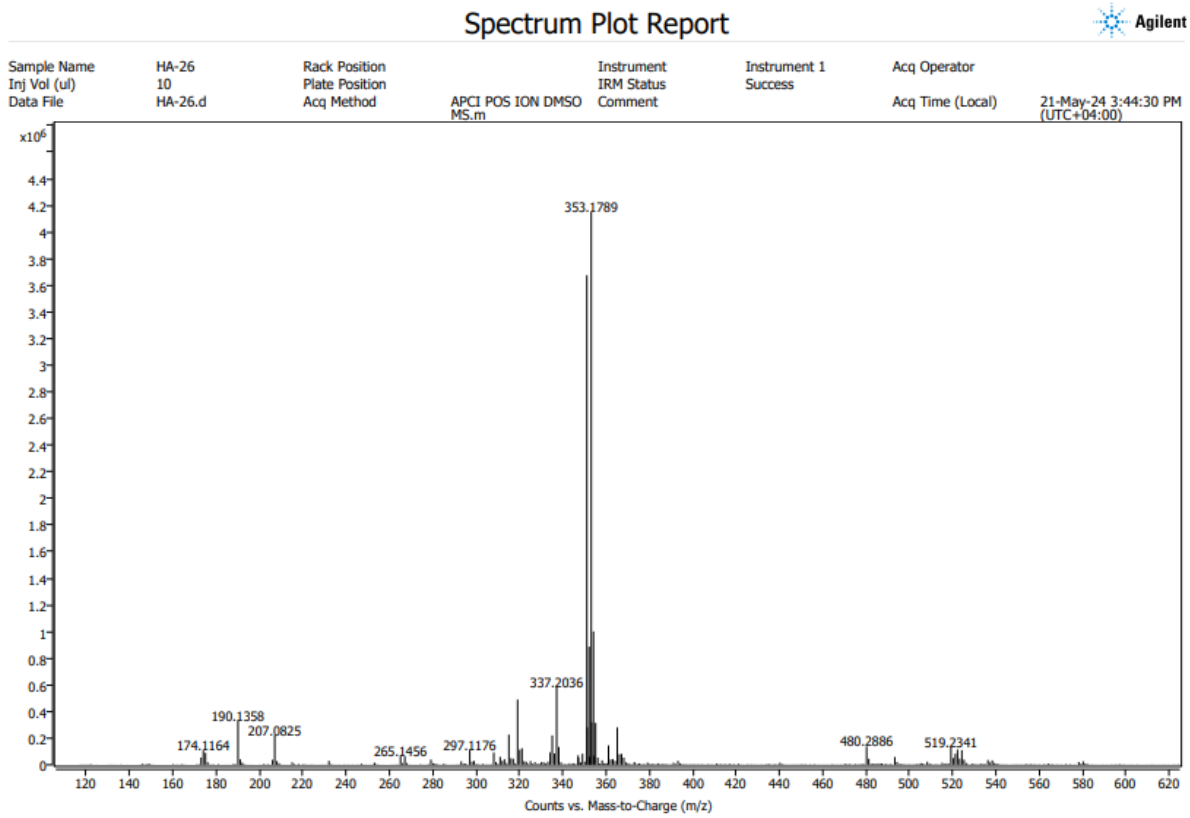
5c


Spectrum Plot Report
Agilent
Sample Name HA-23
Inj Vol (ul) 10
Data File HA-23.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 3:28:12 PM (UTC+04:00)
x10^5
393.0706
351.0476
331.1962
301.0314
407.0855
377.0938
218.1302
232.0930
247.1023
293.1770
Counts vs. Mass-to-Charge (m/z)

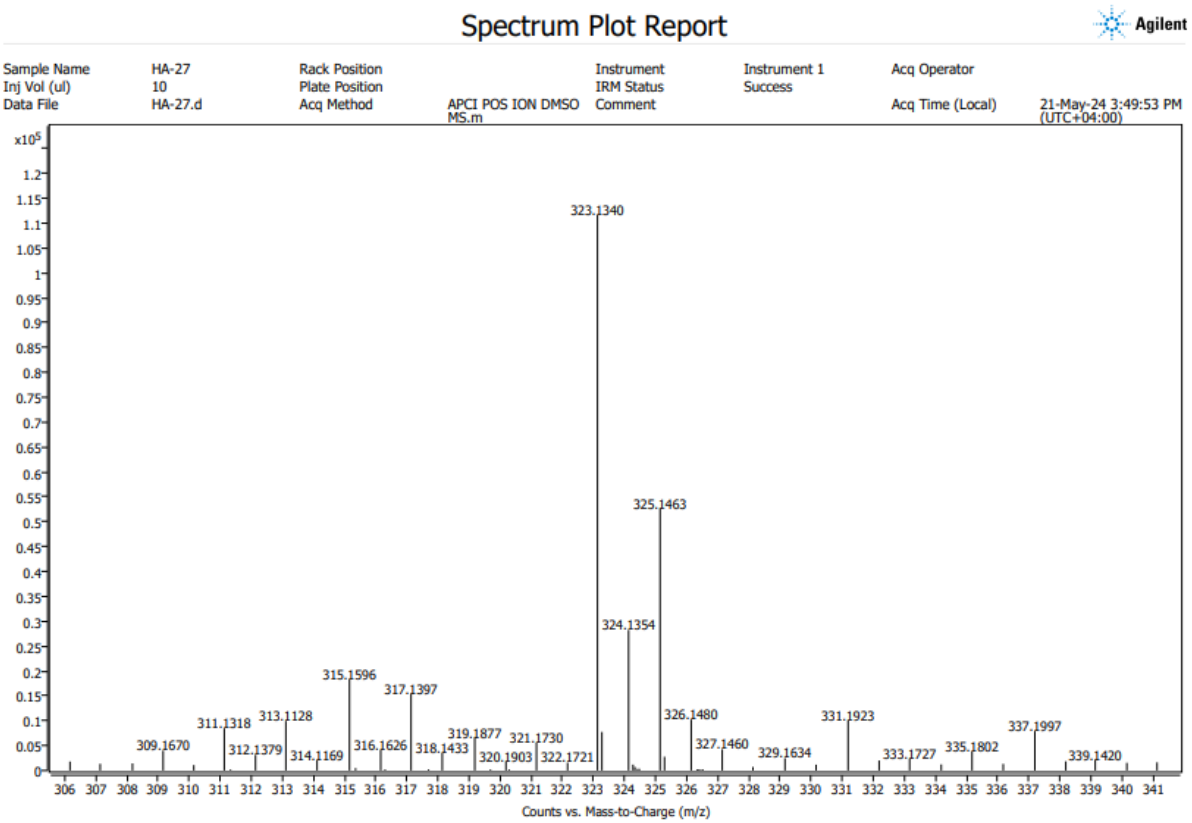
5d


Spectrum Plot Report
Agilent
Sample Name HA-25
Inj Vol (ul) 10
Data File HA-25.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 3:39:07 PM (UTC+04:00)
x10^5
354.1602
347.2308
353.1872
356.1605
355.1582
351.1719
348.2341
357.1565
358.1750
352.1698
Counts vs. Mass-to-Charge (m/z)

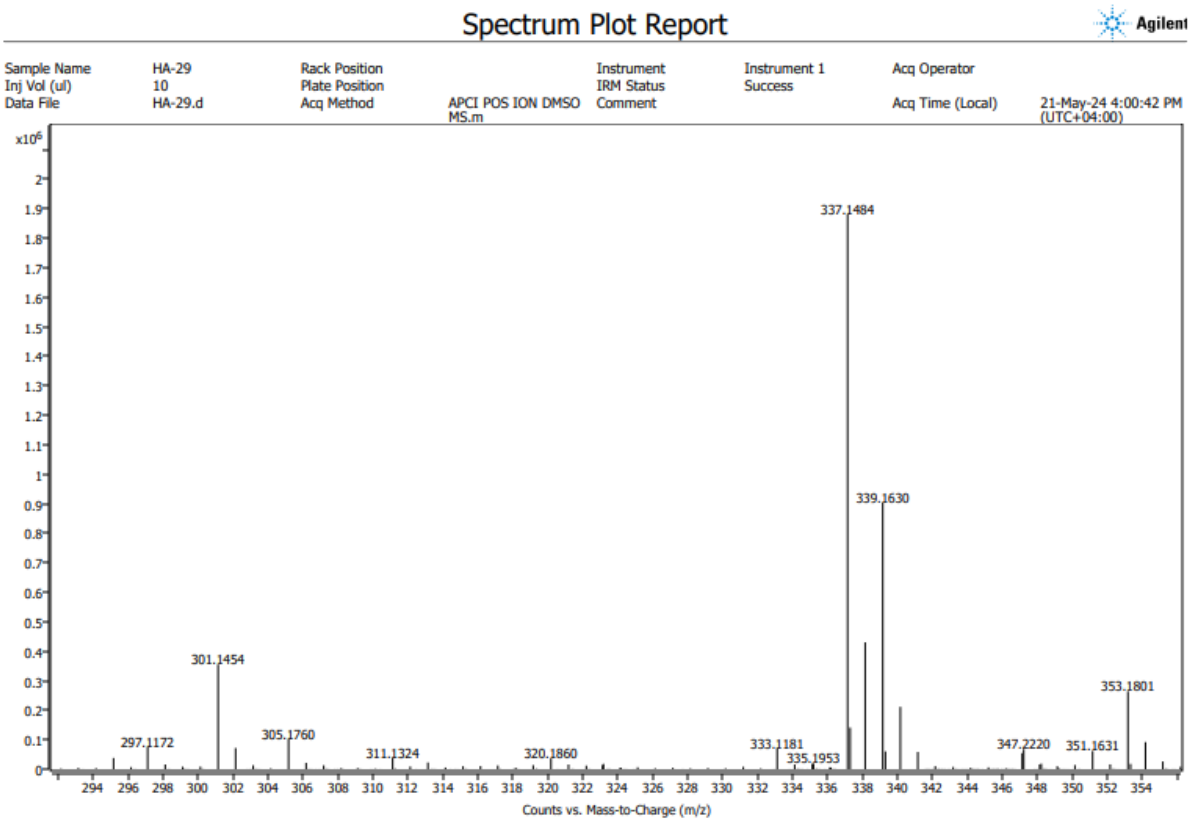
5e


Spectrum Plot Report
Agilent
Sample Name HA-26
Inj Vol (ul) 10
Data File HA-26.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 3:44:30 PM (UTC+04:00)
x10^6
353.1789
337.2036
190.1358
207.0825
174.1164
265.1456
297.1176
480.2886
519.2341
Counts vs. Mass-to-Charge (m/z)

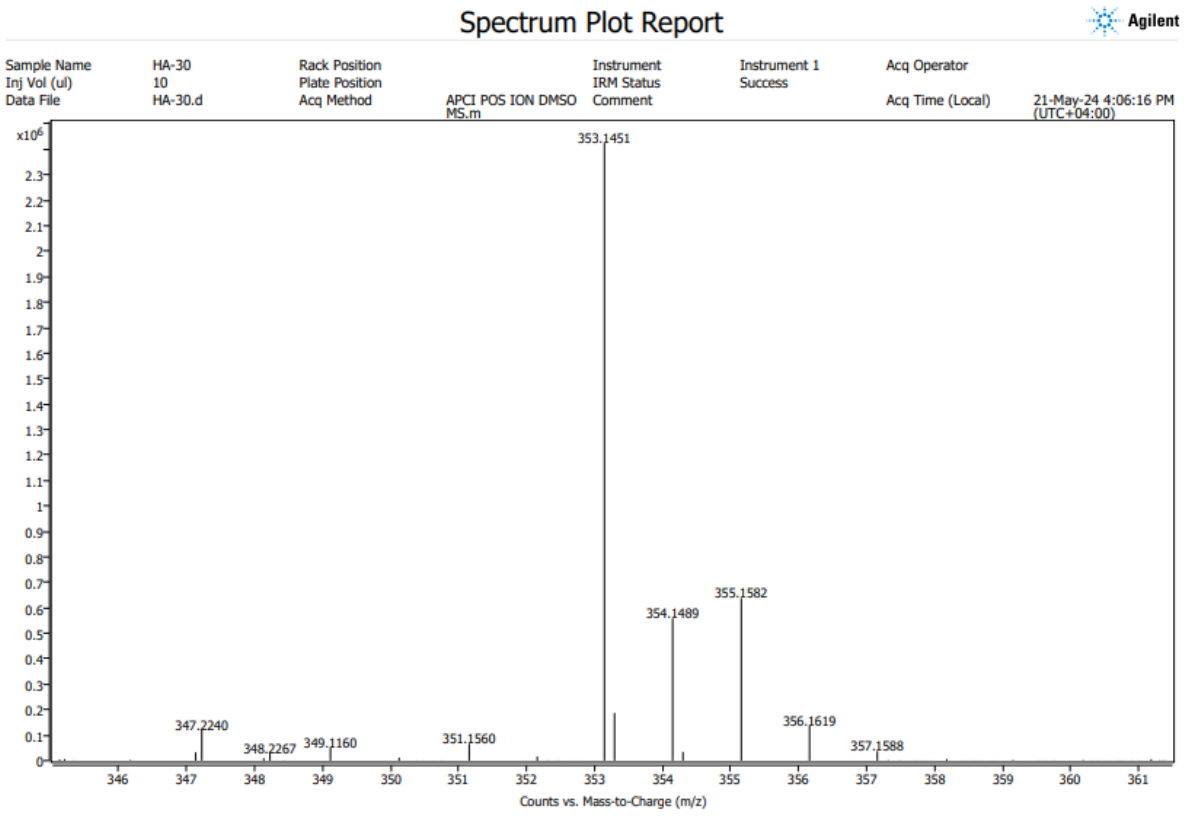
5f


Spectrum Plot Report
Agilent
Sample Name HA-27
Inj Vol (ul) 10
Data File HA-27.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 3:49:53 PM (UTC+04:00)
x10^5
323.1340
325.1463
324.1354
315.1596
317.1397
326.1480
331.1923
337.1997
311.1318
313.1128
319.1877
321.1730
309.1670
312.1379
314.1169
316.1626
318.1433
320.1903
322.1721
327.1460
329.1634
333.1727
335.1802
339.1420
Counts vs. Mass-to-Charge (m/z)

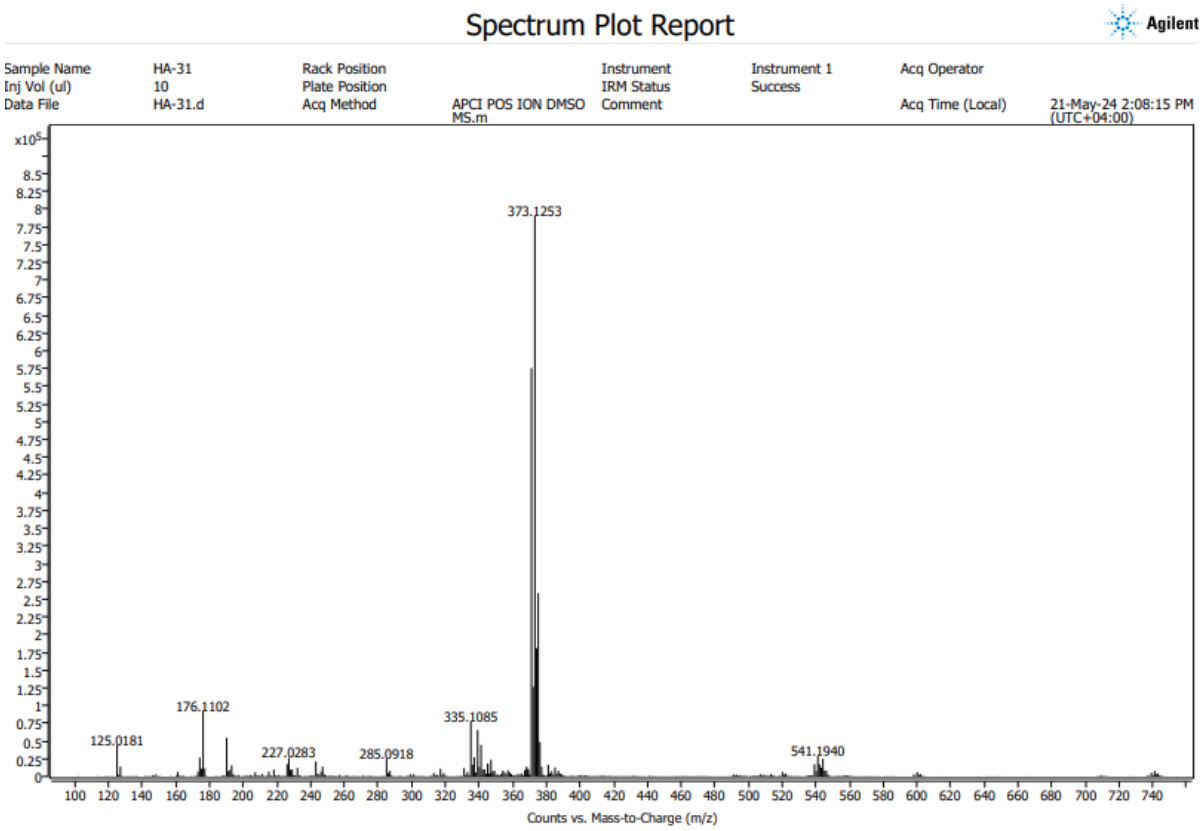
5g


Spectrum Plot Report
Agilent
Sample Name HA-29
Inj Vol (ul) 10
Data File HA-29.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 4:00:42 PM (UTC+04:00)
x10^6
337.1484
339.1630
301.1454
353.1801
297.1172
305.1760
311.1324
320.1860
333.1181
335.1953
347.2220
351.1631
Counts vs. Mass-to-Charge (m/z)

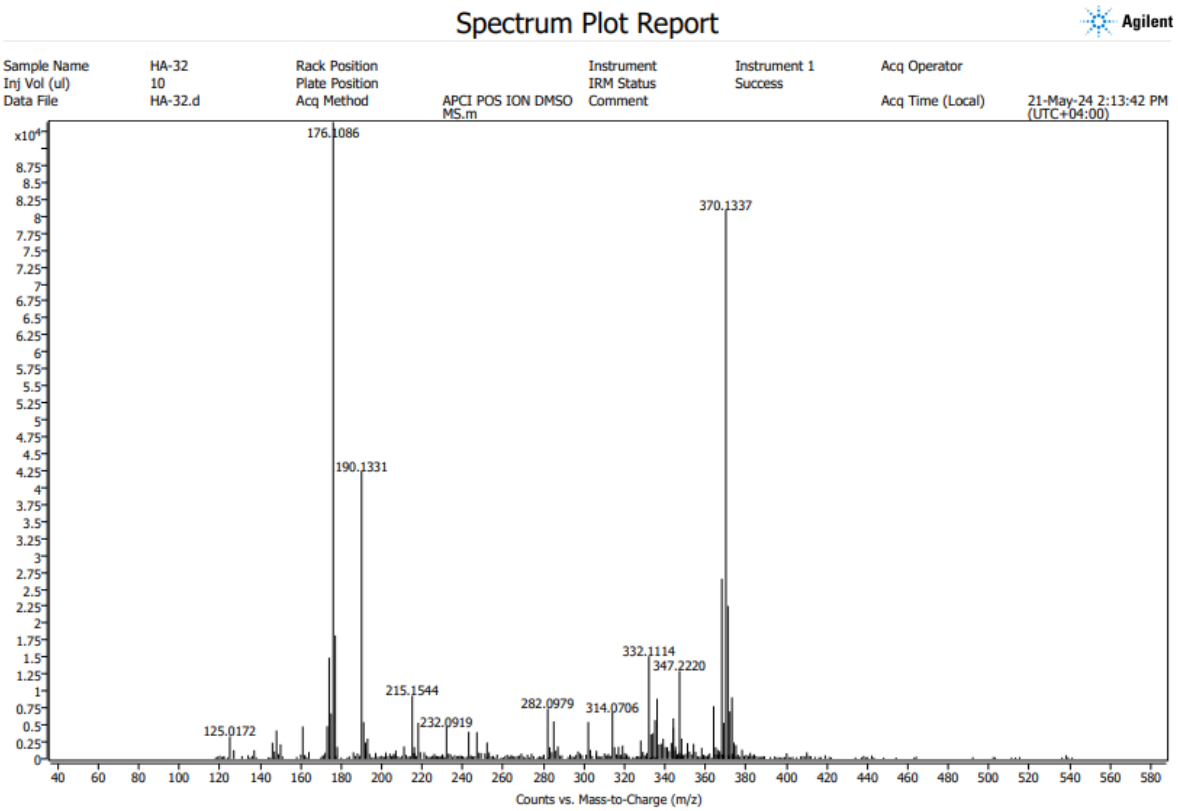
5h


Spectrum Plot Report
Agilent
Sample Name HA-30
Inj Vol (ul) 10
Data File HA-30.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 4:06:16 PM (UTC+04:00)
x10^6
353.1451
355.1582
354.1489
347.2240
348.2267
349.1160
351.1560
356.1619
357.1588
Counts vs. Mass-to-Charge (m/z)

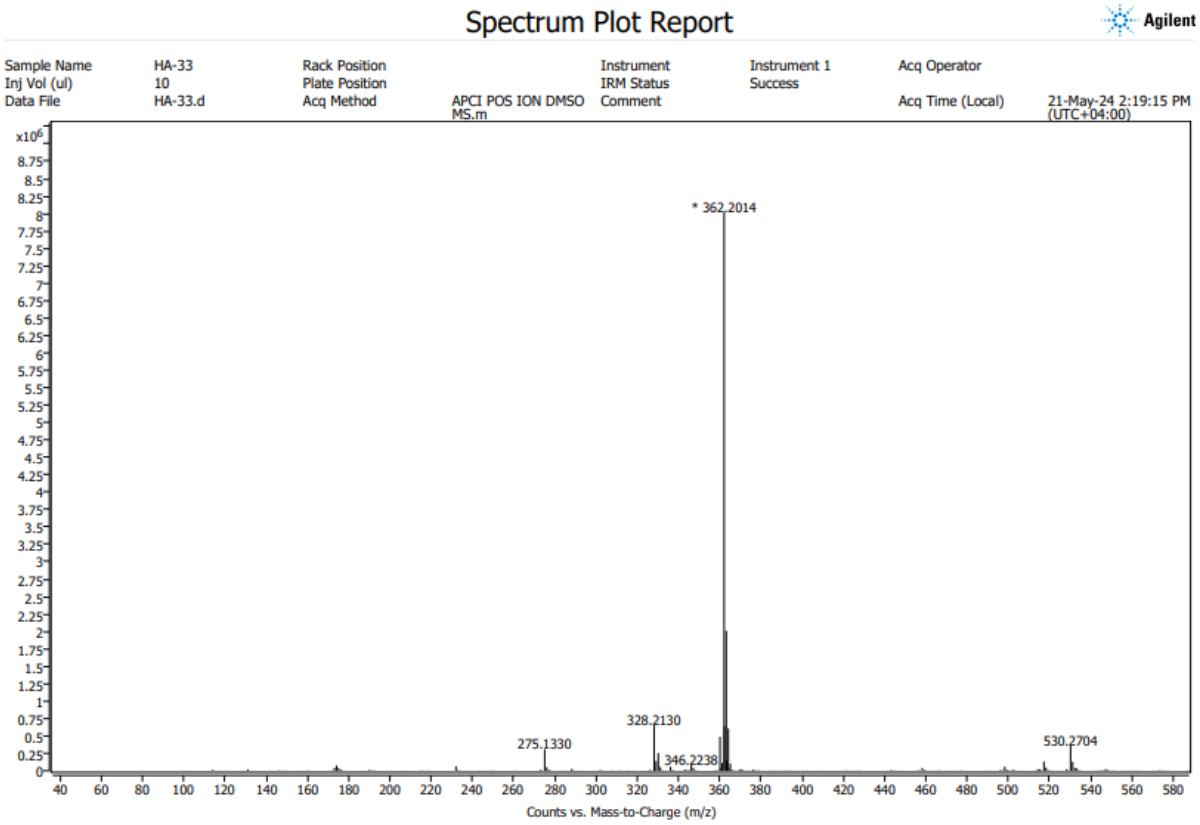
5i


Spectrum Plot Report
Agilent
Sample Name HA-31
Inj Vol (ul) 10
Data File HA-31.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 2:08:15 PM (UTC+04:00)
x10^5
373.1253
176.1102
335.1085
125.0181
227.0283
285.0918
541.1940
Counts vs. Mass-to-Charge (m/z)

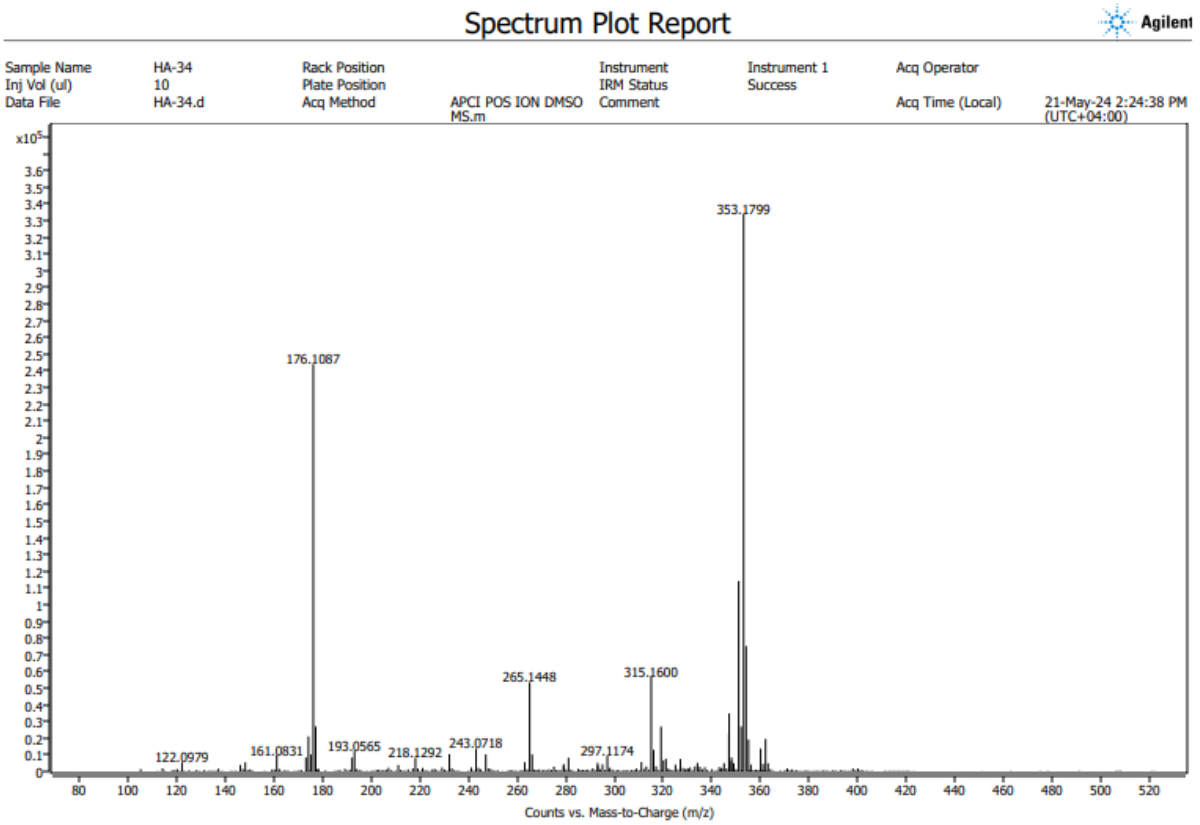
5j


Spectrum Plot Report
Agilent
Sample Name HA-32
Inj Vol (ul) 10
Data File HA-32.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 2:13:42 PM (UTC+04:00)
x10^4
176.1086
370.1337
190.1331
332.1114
347.2220
215.1544
282.0979
314.0706
232.0919
125.0172
Counts vs. Mass-to-Charge (m/z)

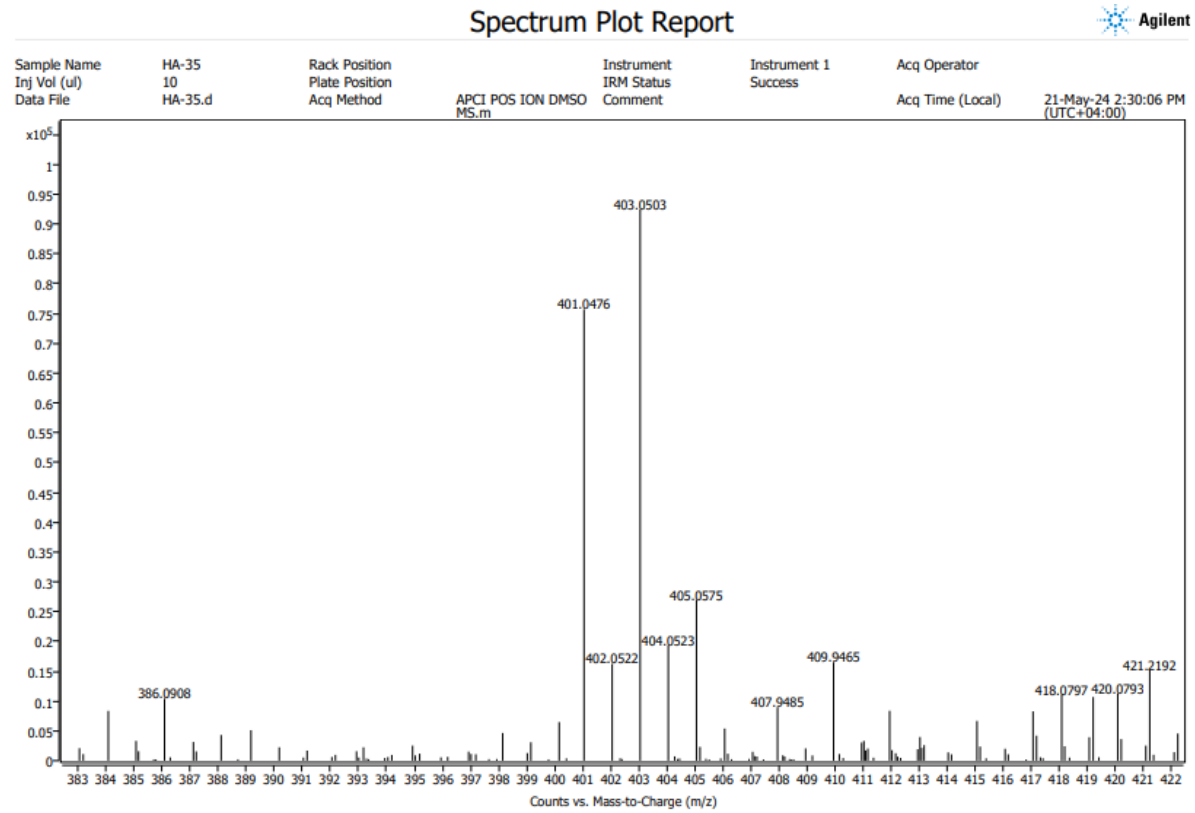
5k


Spectrum Plot Report
Agilent
Sample Name HA-33
Inj Vol (ul) 10
Data File HA-33.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 2:19:15 PM (UTC+04:00)
x10^6
* 362.2014
328.2130
275.1330
346.2238
530.2704
Counts vs. Mass-to-Charge (m/z)

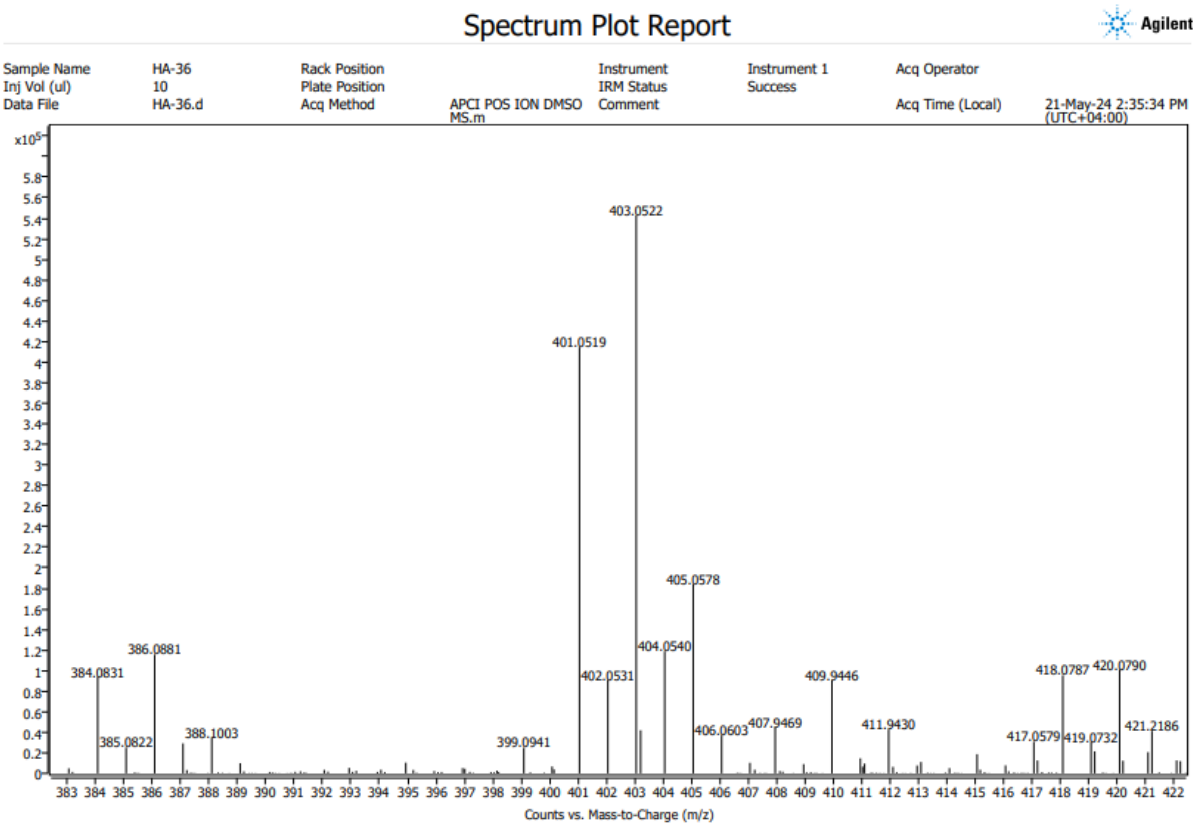
5l


Spectrum Plot Report
Agilent
Sample Name HA-34
Inj Vol (ul) 10
Data File HA-34.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 2:24:38 PM (UTC+04:00)
x10^5
353.1799
176.1087
265.1448
315.1600
122.0979
161.0831
193.0565
218.1292
243.0718
297.1174
Counts vs. Mass-to-Charge (m/z)

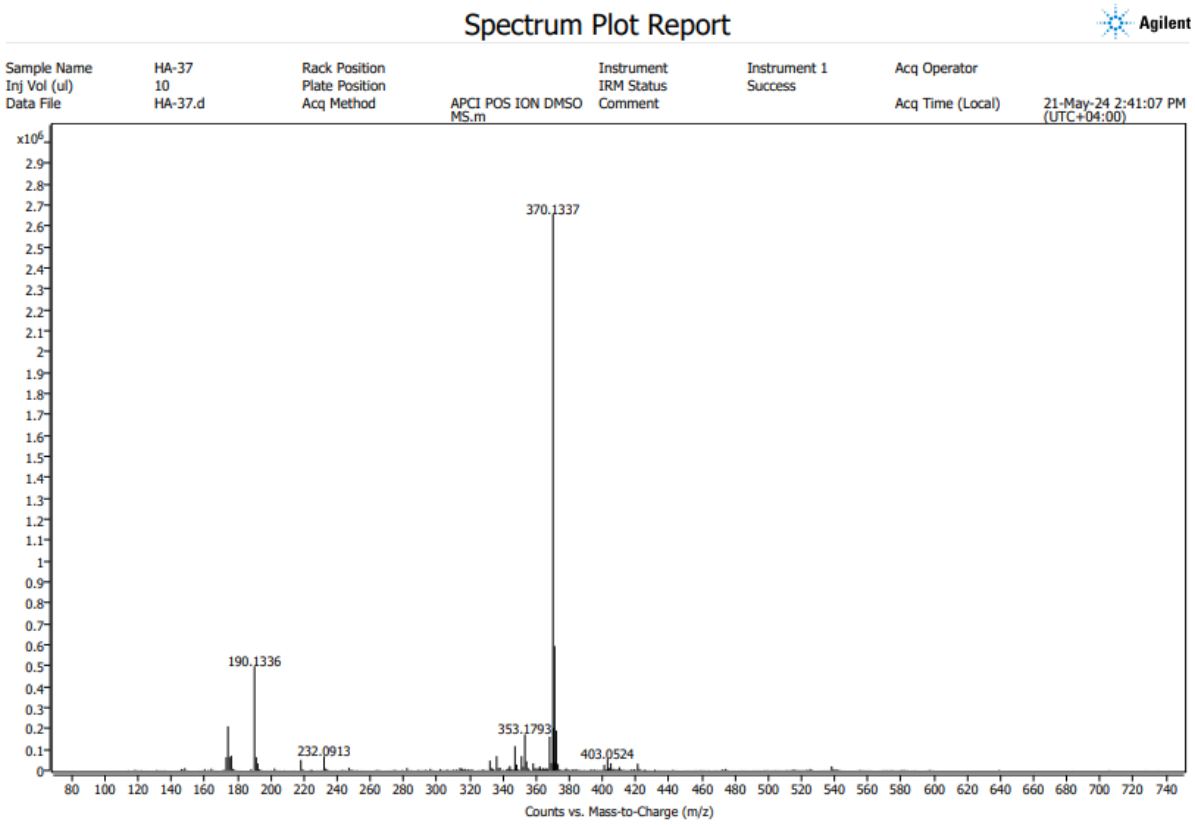
5m


Spectrum Plot Report
Agilent
Sample Name HA-35
Inj Vol (ul) 10
Data File HA-35.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 2:30:06 PM (UTC+04:00)
x10^5
403.0503
401.0476
405.0575
404.0523
402.0522
409.9465
421.2192
386.0908
418.0797
420.0793
407.9485
Counts vs. Mass-to-Charge (m/z)

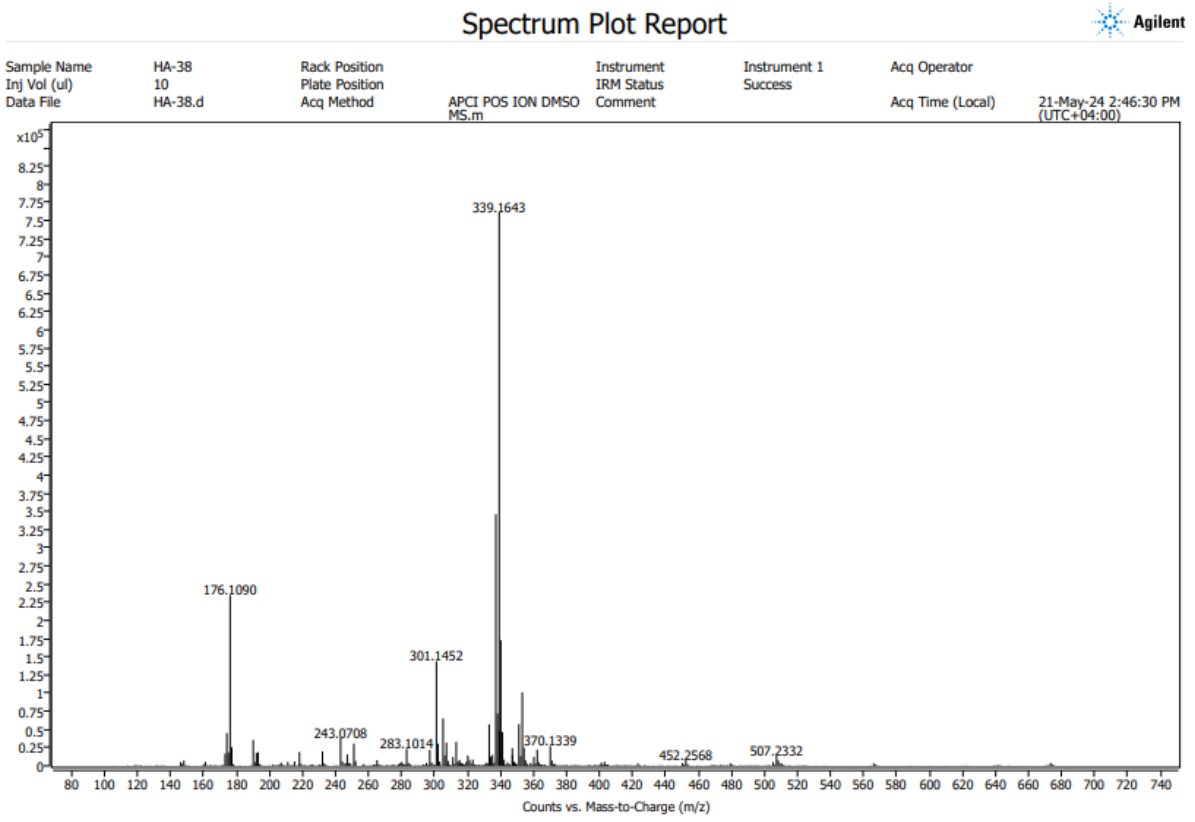
5n


Spectrum Plot Report
Agilent
Sample Name HA-36
Inj Vol (ul) 10
Data File HA-36.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 2:35:34 PM (UTC+04:00)
x10^5
403.0522
401.0519
405.0578
386.0881
384.0831
404.0540
402.0531
409.9446
418.0787
420.0790
385.0822
388.1003
399.0941
406.0603
407.9469
411.9430
417.0579
419.0732
421.2186
Counts vs. Mass-to-Charge (m/z)

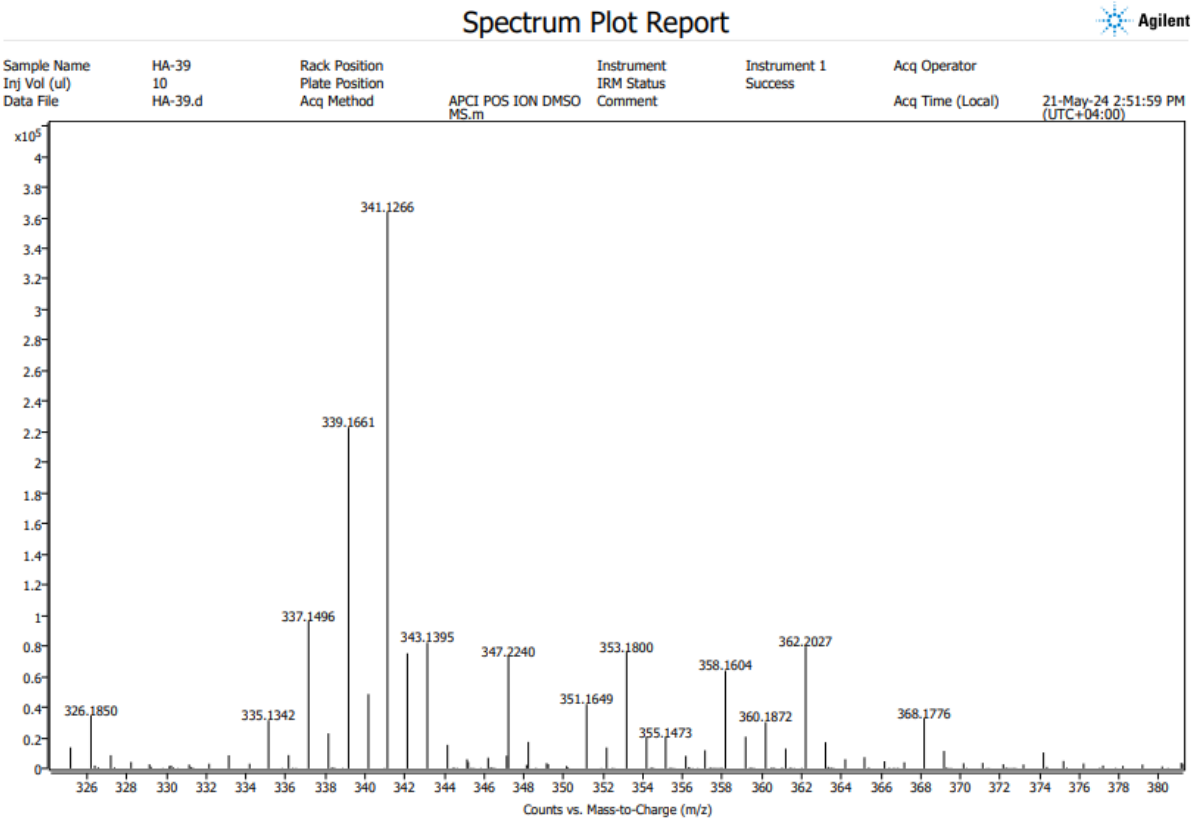
5o


Spectrum Plot Report
Agilent
Sample Name HA-37
Inj Vol (ul) 10
Data File HA-37.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 2:41:07 PM (UTC+04:00)
x10^6
370.1337
190.1336
232.0913
353.1793
403.0524
Counts vs. Mass-to-Charge (m/z)

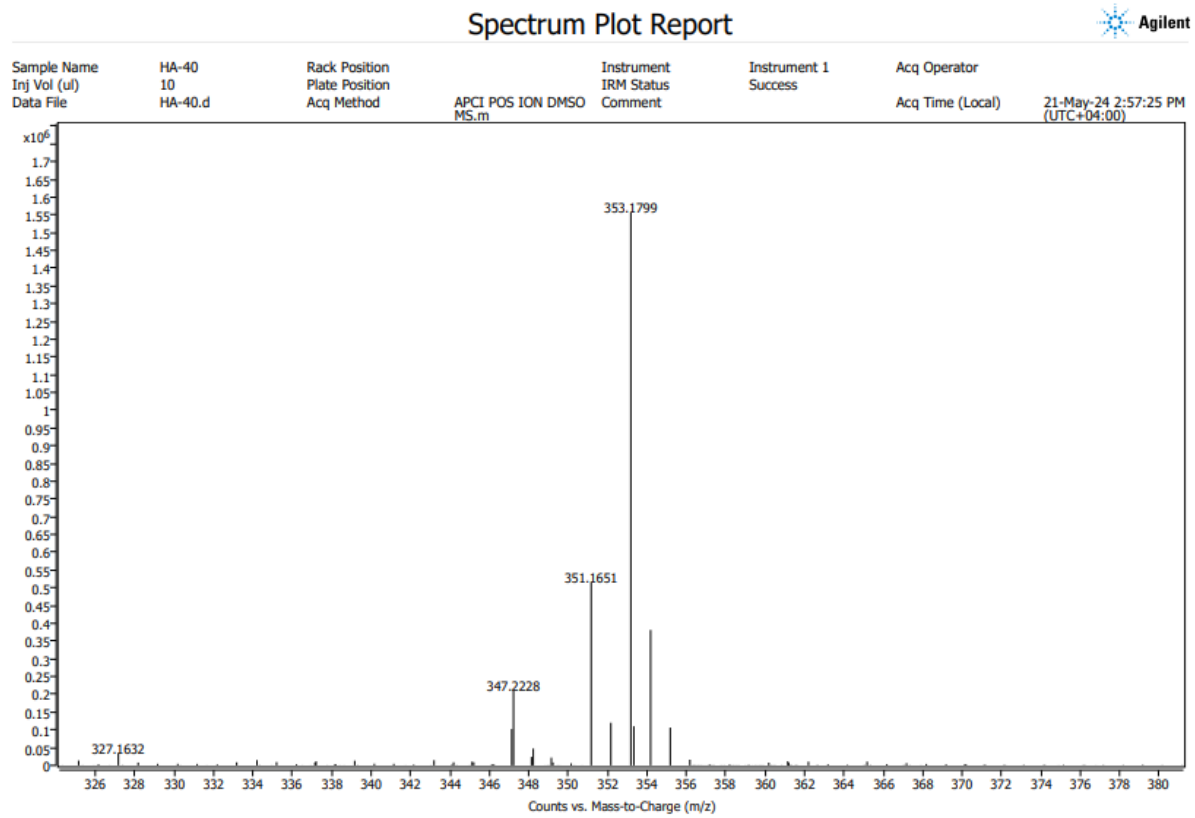
5p


Spectrum Plot Report
Agilent
Sample Name HA-38
Inj Vol (ul) 10
Data File HA-38.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 2:46:30 PM (UTC+04:00)
x10^5
339.1643
176.1090
301.1452
243.0708
283.1014
370.1339
452.2568
507.2332
Counts vs. Mass-to-Charge (m/z)

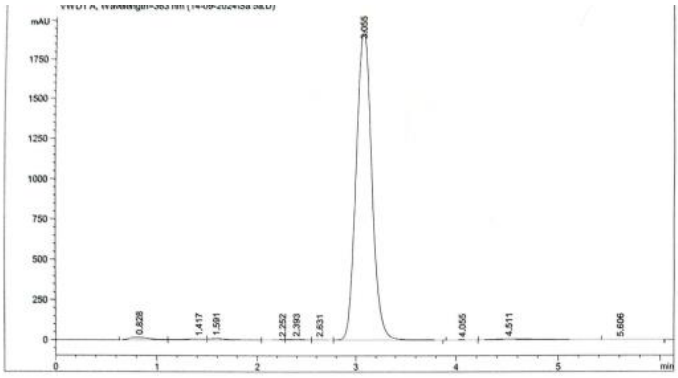
5q


Spectrum Plot Report
Agilent
Sample Name HA-39
Inj Vol (ul) 10
Data File HA-39.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 2:51:59 PM (UTC+04:00)
x10^5
341.1266
339.1661
337.1496
343.1395
347.2240
353.1800
362.2027
358.1604
351.1649
326.1850
335.1342
355.1473
360.1872
368.1776
Counts vs. Mass-to-Charge (m/z)

5r


Spectrum Plot Report
Agilent
Sample Name HA-40
Inj Vol (ul) 10
Data File HA-40.d
Rack Position
Plate Position
Acq Method APCI POS ION DMSO MS.m
Instrument
IRM Status
Comment
Instrument 1
Success
Acq Operator
Acq Time (Local) 21-May-24 2:57:25 PM (UTC+04:00)
x10^6
353.1799
351.1651
347.2228
327.1632
Counts vs. Mass-to-Charge (m/z)

HPLC chromatogram of 5a



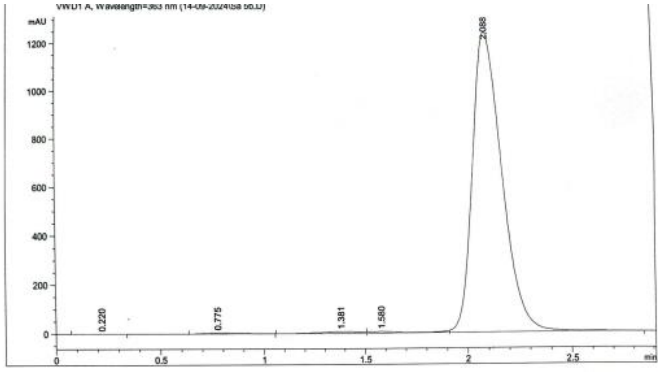
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.828	BV	0.2247	220.97006	15.08996	1.0111
2	1.417	VV	0.2112	118.47029	7.65351	0.5421
3	1.591	VB	0.1769	114.48515	9.31631	0.5239
4	2.252	BV	0.1063	19.22764	2.79957	0.0880
5	2.393	VV	0.1583	52.85017	4.99728	0.2418
6	2.631	VB	0.1396	13.79169	1.55979	0.0631
7	3.055	BB	0.1699	2.11048e4	1928.44250	96.5745
8	4.055	BB	0.1540	4.33859	4.52895e-1	0.0199
9	4.511	BV R	0.4419	199.41382	6.56117	0.9125
10	5.606	VBAE	0.2348	5.03643	2.94047e-1	0.0230

HPLC chromatogram of 5b



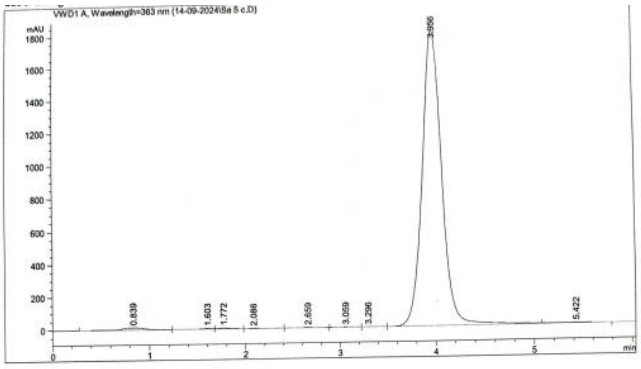
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.220	BV	0.1044	2.91614e-1	3.66915e-2	2.318e-3
2	0.775	BB	0.1677	47.14600	4.48620	0.3748
3	1.381	BV E	0.2049	104.36163	7.48348	0.8295
4	1.580	VV E	0.1740	80.38326	6.47262	0.6389
5	2.088	VB R	0.1528	1.23485e4	1253.52112	98.1544

HPLC chromatogram of 5c



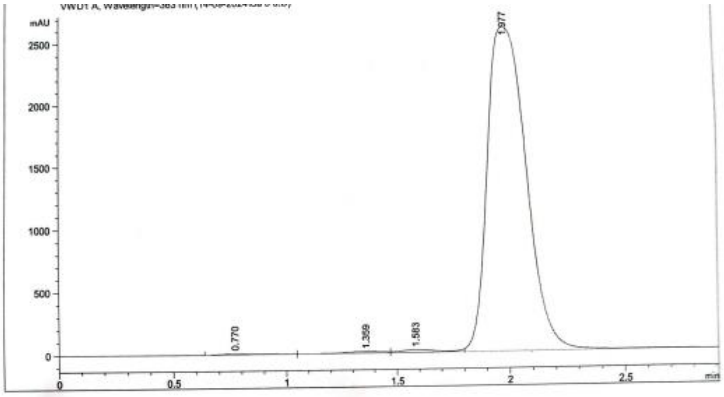
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.839	BB	0.2622	223.03247	13.43007	0.8706
2	1.603	BV	0.1376	47.98867	5.15921	0.1873
3	1.772	VV	0.1577	70.17262	6.59256	0.2739
4	2.086	VB	0.1593	23.48802	2.20387	0.0917
5	2.659	BB	0.1885	22.90609	1.90270	0.0894
6	3.059	BV	0.1705	19.77284	1.79870	0.0772
7	3.296	VB	0.1617	7.72665	7.54708e-1	0.0302
8	3.956	BV R	0.2124	2.51757e4	1802.65649	98.2749
9	5.422	VBAE	0.2680	26.83294	1.45233	0.1047

HPLC chromatogram of 5d



Area Percent Report

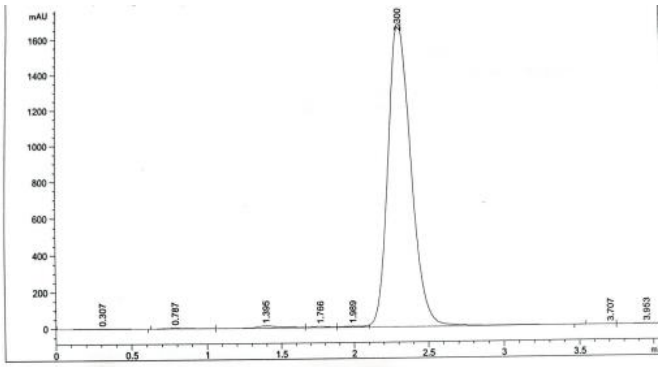
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.770	BB	0.1510	107.91707	10.45714	0.3462
2	1.359	BV E	0.1920	163.36404	13.37330	0.5241
3	1.583	VV E	0.1576	241.43596	22.69774	0.7745
4	1.977	VBAR	0.1857	3.06596e4	2598.65601	98.3552

Totals : 3.11724e4 2645.18419

HPLC chromatogram of 5e



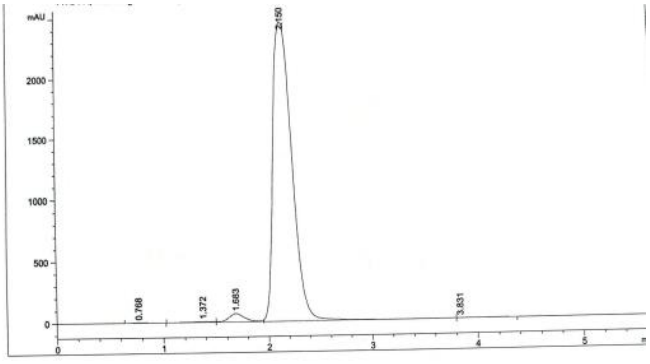
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.307	BB	0.2078	20.26543	1.50706	0.1099
2	0.787	BB	0.1637	56.14553	5.32858	0.3046
3	1.395	BV E	0.1927	170.49765	12.49250	0.9250
4	1.766	VV E	0.1500	68.69591	6.79330	0.3727
5	1.989	VV E	0.1393	59.01897	6.17034	0.3202
6	2.300	VB R	0.1660	1.80546e4	1682.05115	97.9513
7	3.707	BV	0.1080	7.24892e-1	9.34527e-2	3.933e-3
8	3.953	VBA	0.1275	2.26344	2.46534e-1	0.0123

HPLC chromatogram of 5f



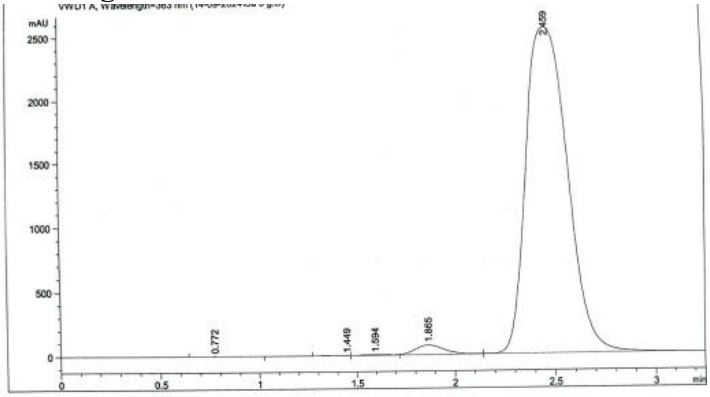
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.768	BB	0.1425	7.32521	7.94550e-1	0.0232
2	1.372	BV E	0.1607	66.46423	6.23718	0.2104
3	1.683	VV E	0.1558	709.17096	69.32246	2.2452
4	2.150	VB R	0.1991	3.08026e4	2449.22681	97.5187
5	3.831	BB	0.3047	8.01374e-1	3.19033e-2	2.537e-3

HPLC chromatogram of 5g



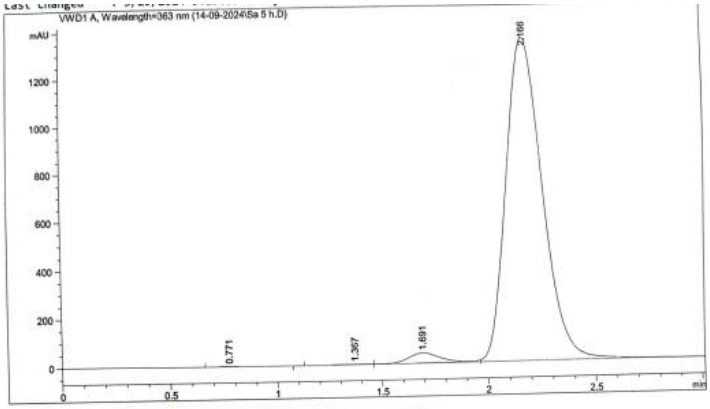
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.772	BB	0.1490	4.73922	4.90860e-1	0.0127
2	1.449	BV E	0.0994	10.66048	1.69837	0.0286
3	1.594	VV E	0.1364	38.11235	4.26230	0.1023
4	1.865	VV R	0.1597	790.89423	76.62309	2.1229
5	2.459	VBA	0.2296	3.64106e4	2543.97217	97.7334

HPLC chromatogram of 5h



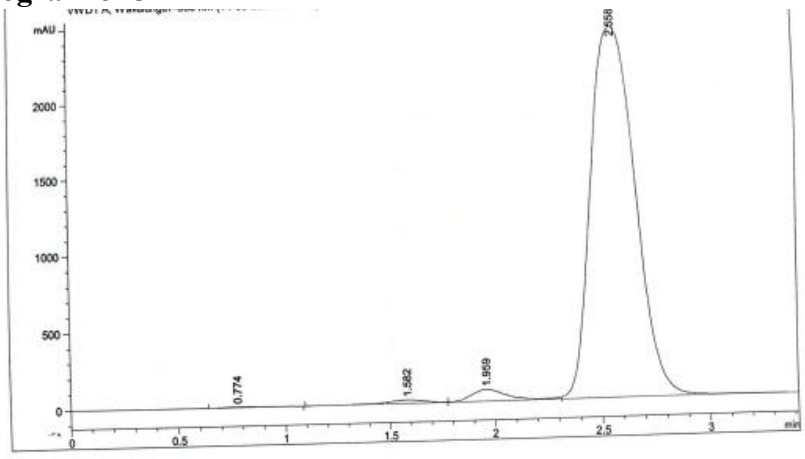
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.771	BB	0.1591	2.83867	2.69833e-1	0.0175
2	1.367	BV E	0.1471	7.49101	7.68937e-1	0.0462
3	1.691	VV E	0.1589	449.61575	43.32738	2.7737
4	2.166	VBAR	0.1822	1.57502e4	1355.52893	97.1626

HPLC chromatogram of 5i



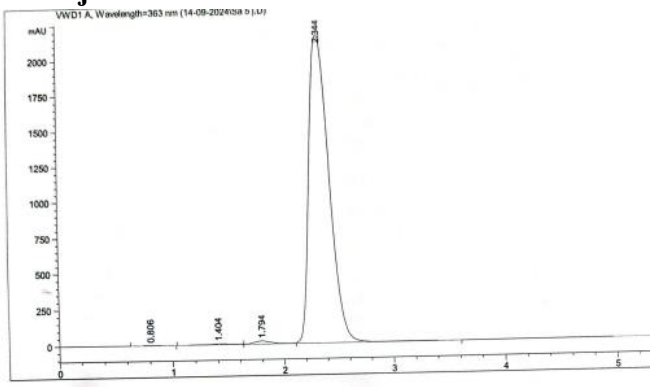
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.774	BB	0.1670	46.44295	4.39282	0.1294
2	1.582	BV E	0.2004	329.60278	24.53732	0.9181
3	1.959	VV E	0.1804	936.61987	79.07034	2.6090
4	2.558	VBAR	0.2283	3.45876e4	2434.81543	96.3436

HPLC chromatogram of 5j



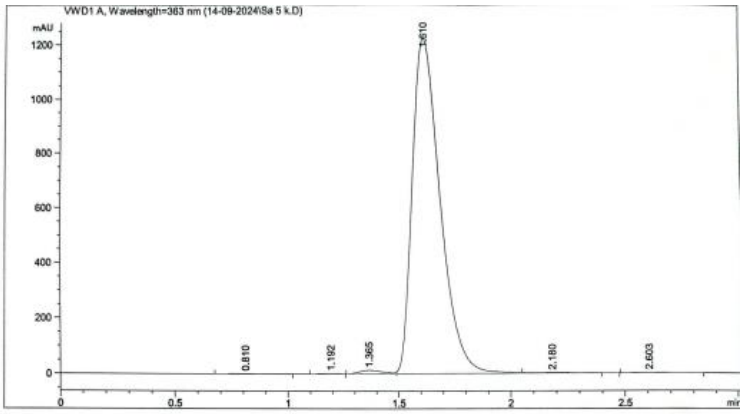
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.806	BB	0.1375	7.79837	8.50758e-1	0.0282
2	1.404	BV E	0.1821	82.34154	6.46454	0.2974
3	1.794	VV E	0.1694	231.76300	21.02710	0.8372
4	2.344	VB R	0.2021	2.73620e4	2153.67236	98.8372

HPLC chromatogram of 5k

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================================================================================
                            Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=363 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  0.810 BB    0.1434    5.51140 5.62803e-1   0.0514
   2  1.192 BB    0.0927    8.20703    1.50632   0.0766
   3  1.365 BV E  0.1116   84.40572   11.93555   0.7877
   4  1.610 VV R  0.1333 1.05932e4  1220.40430  98.8621
   5  2.180 VB E  0.1447   10.35813    1.05932   0.0967
   6  2.603 BB    0.1443   13.44899    1.45368   0.1255

Totals :                  1.07151e4  1236.92198
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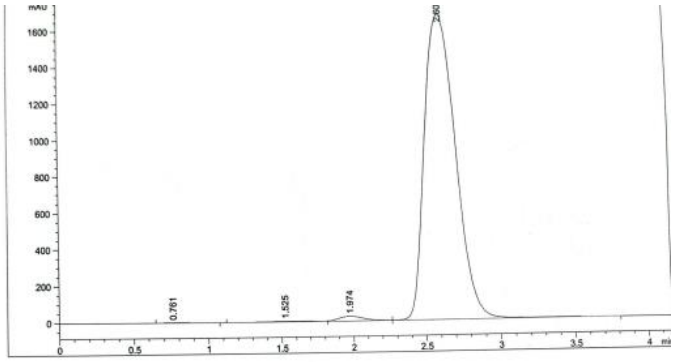
HPLC chromatogram of 5l

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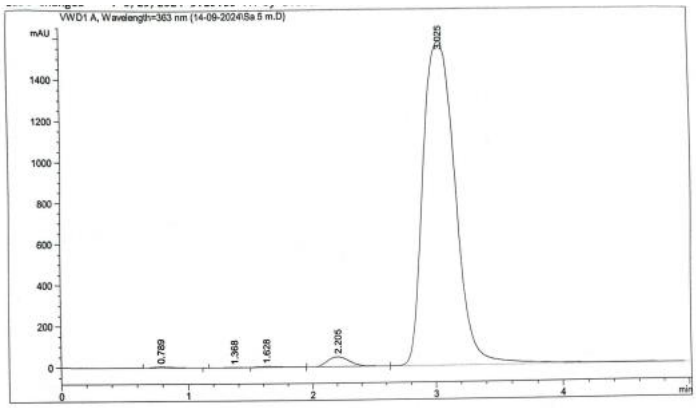
================================================================================
                            Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=363 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  0.761 BB    0.1521    8.26315 8.22819e-1   0.0331
   2  1.525 BV E  0.2273   59.29700    3.65220   0.2372
   3  1.974 VV R  0.1882  325.96219   26.85067   1.3041
   4  2.608 VB    0.2356 2.46018e4  1688.04285  98.4256
```

HPLC chromatogram of 5m



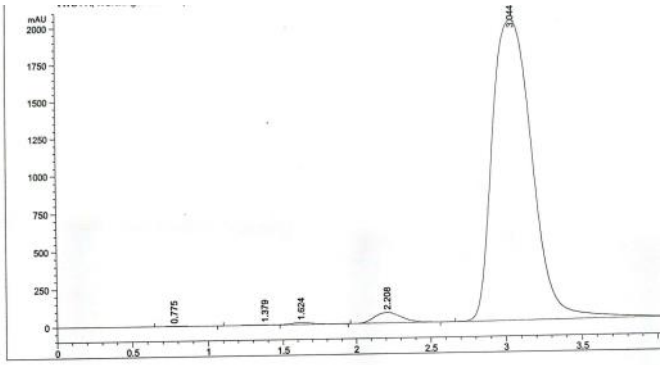
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.789	BB	0.1356	44.72926	5.11155	0.1559
2	1.368	BV E	0.1553	3.35077	3.45758e-1	0.0117
3	1.628	VB R	0.1688	53.31473	4.91221	0.1858
4	2.205	BV	0.2055	631.26990	49.05482	2.2005
5	3.025	VBA	0.2842	2.79544e4	1575.01587	97.4460

HPLC chromatogram of 5n



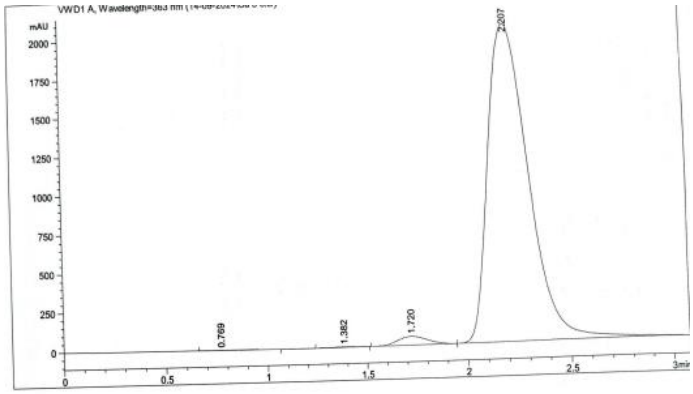
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.775	BB	0.1587	7.60358	7.33850e-1	0.0204
2	1.379	BV E	0.1539	9.15810	8.76571e-1	0.0245
3	1.624	VB R	0.1616	129.77696	12.38212	0.3475
4	2.208	BB	0.2025	907.47040	71.91394	2.4297
5	3.044	BBA	0.2920	3.62953e4	1998.35449	97.1780

HPLC chromatogram of 5o



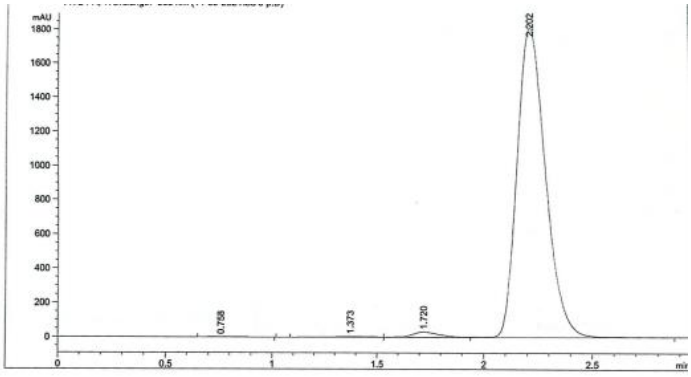
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.769	BB	0.1796	7.29650	6.06951e-1	0.0258
2	1.382	BB	0.1329	15.90338	1.98306	0.0562
3	1.720	BB	0.1625	575.58179	55.83282	2.0327
4	2.207	BBA	0.2149	2.77167e4	2045.55811	97.8853

HPLC chromatogram of 5p



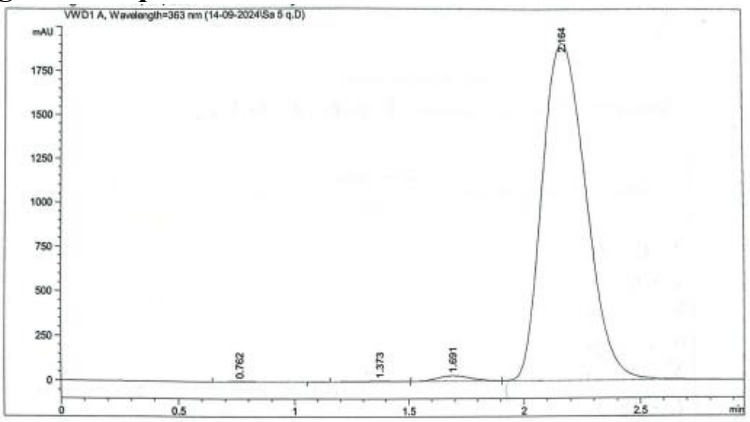
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.758	BB	0.1267	13.17538	1.59848	0.0784
2	1.373	BV E	0.1453	45.15085	4.59325	0.2688
3	1.720	VV E	0.1306	254.05200	30.06845	1.5122
4	2.202	VB R	0.1413	1.64875e4	1808.41406	98.1406

HPLC chromatogram of 5q



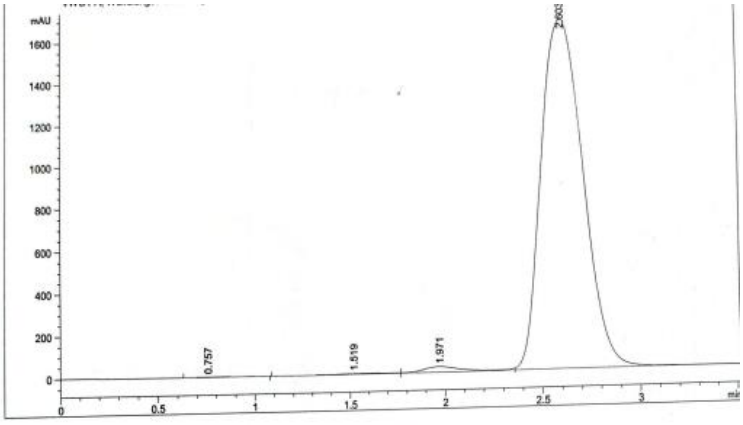
Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.762	BB	0.1510	4.99847	5.21913e-1	0.0199
2	1.373	BB	0.1423	15.47462	1.75311	0.0617
3	1.691	BV	0.1621	309.19778	30.07982	1.2318
4	2.164	VBA	0.2084	2.47707e4	1905.47839	98.6866

HPLC chromatogram of 5r



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=363 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.757	BB	0.1495	8.33536	8.48565e-1	0.0333
2	1.519	BV E	0.2140	53.85298	3.65853	0.2149
3	1.971	VV E	0.2027	353.25421	26.39203	1.4098
4	2.603	VBAR	0.2398	2.46416e4	1663.11511	98.3420
Totals :				2.50571e4	1694.01424	