

Antitubercular evaluation of dihydropyridine-triazole conjugates: Design, synthesis, in vitro screening, SAR and in silico ADME predictions

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^e Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, U.P., India.

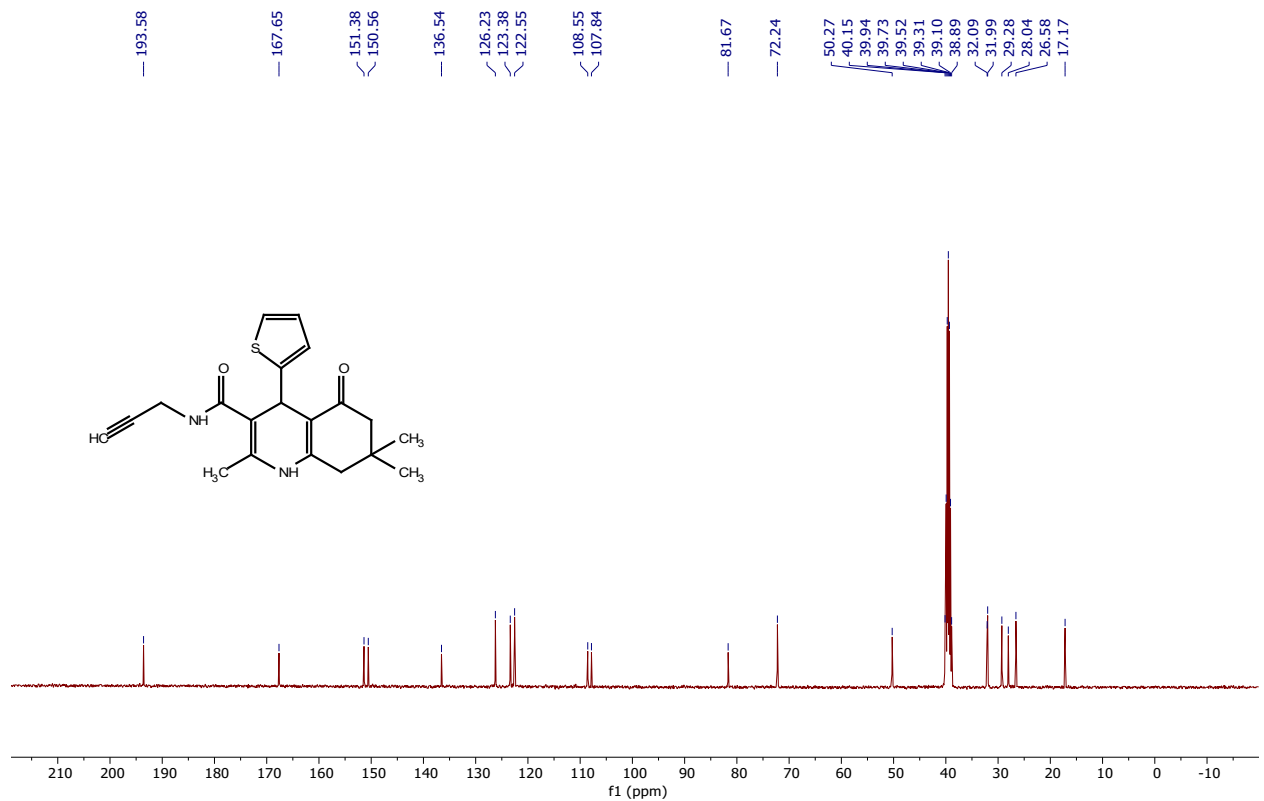
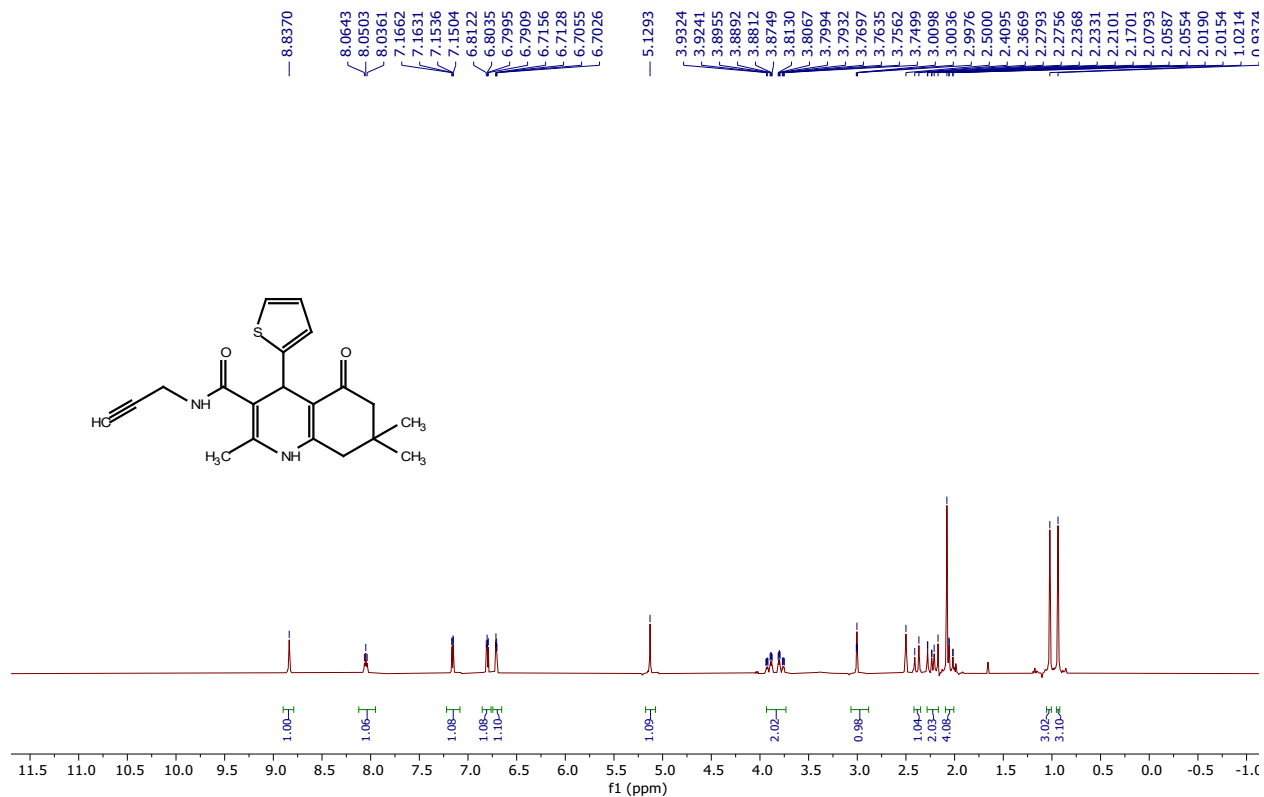
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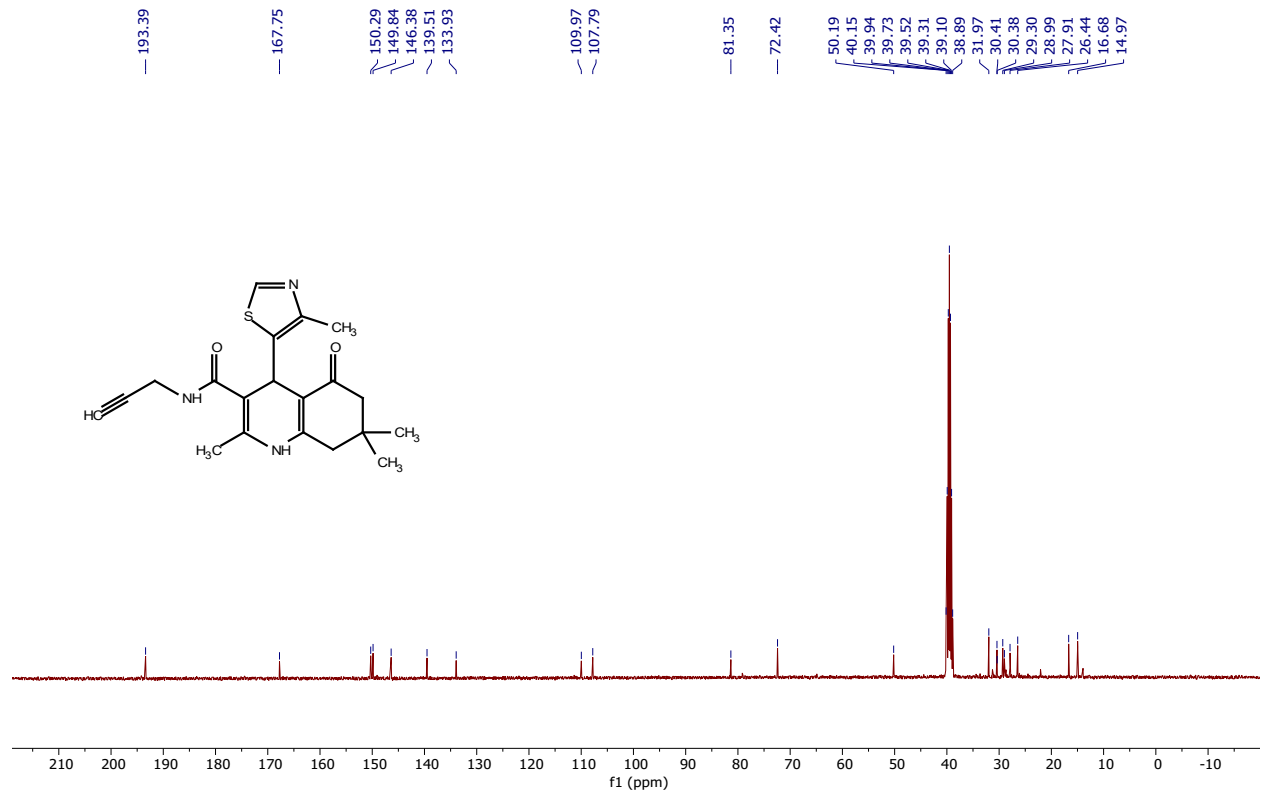
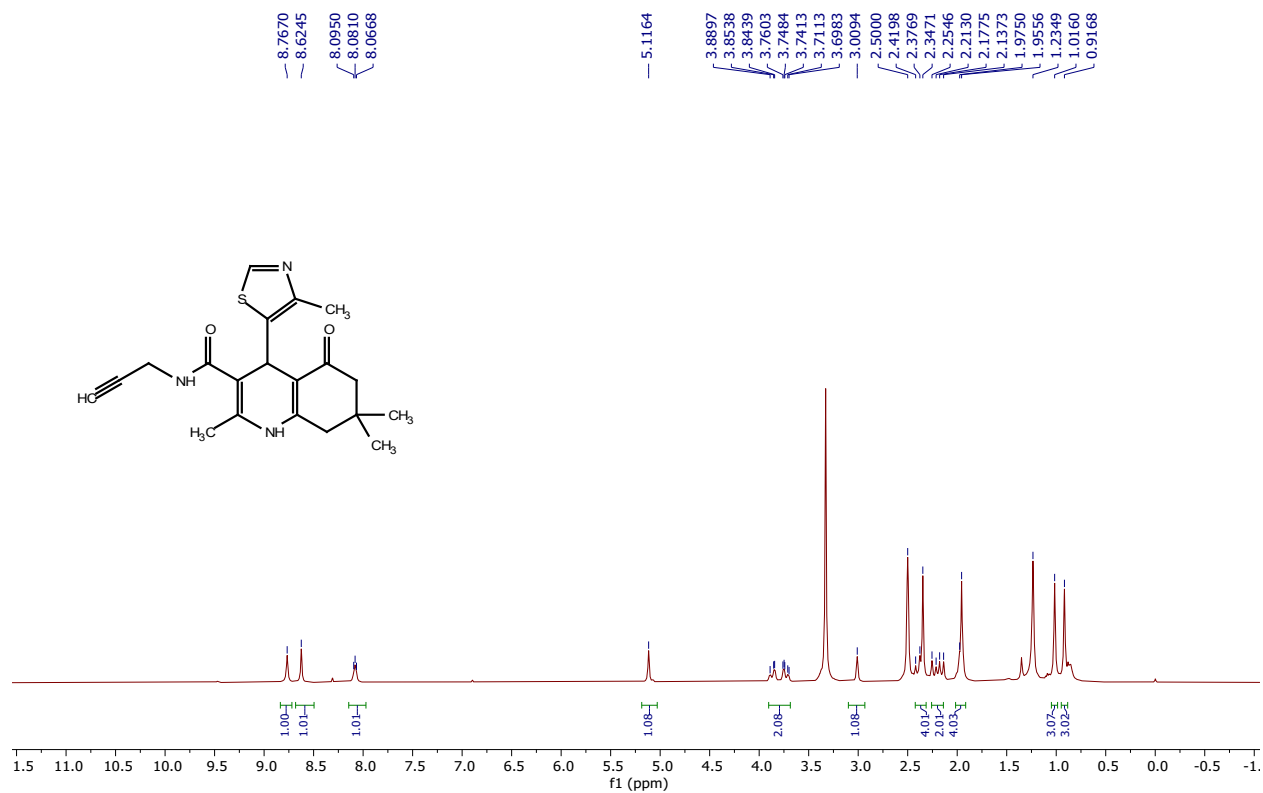
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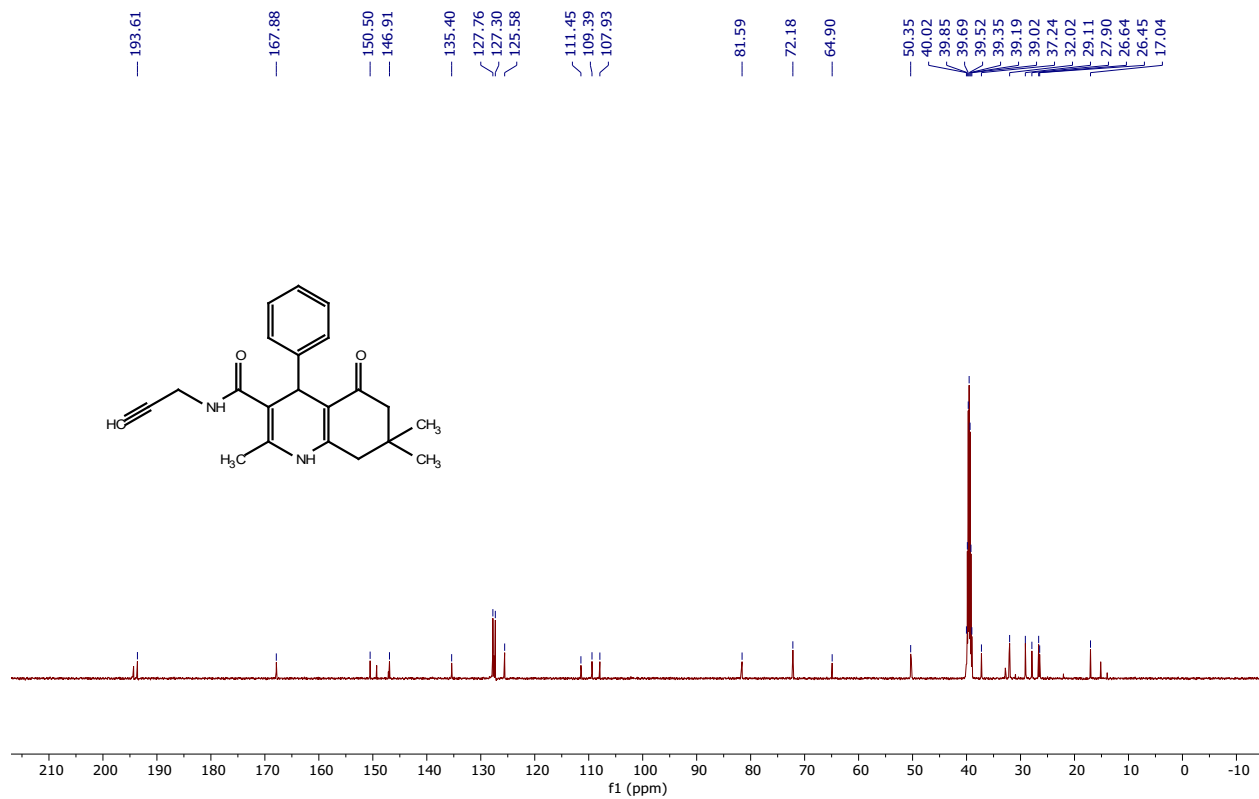
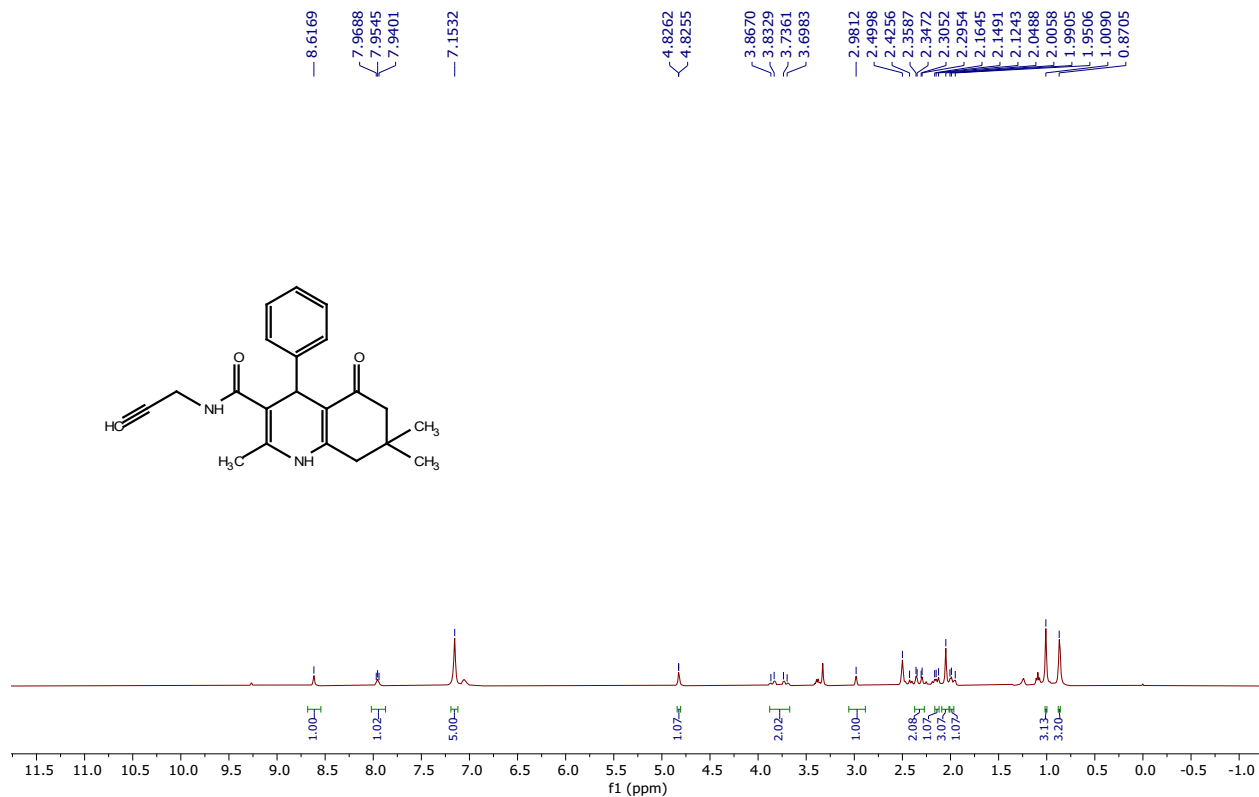
NMR spectrum of compound H1



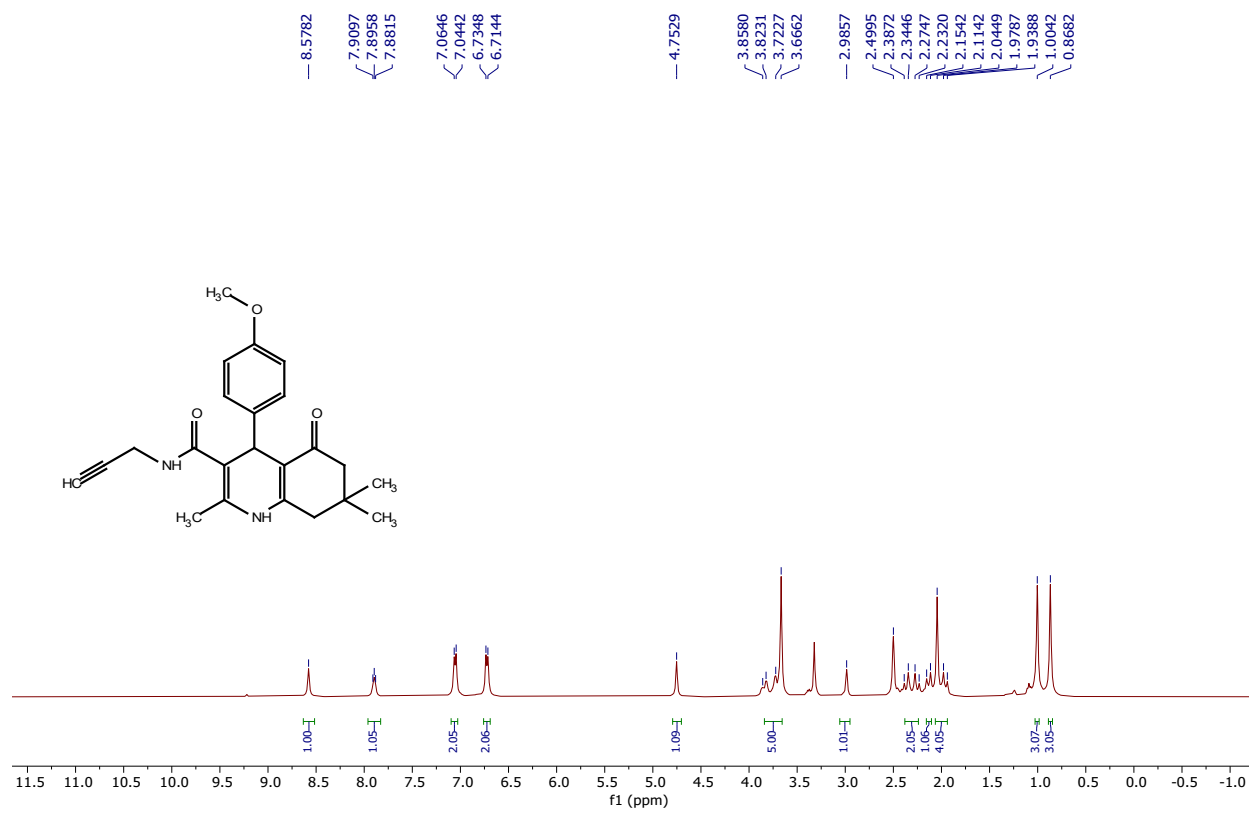
NMR spectrum of compound H2

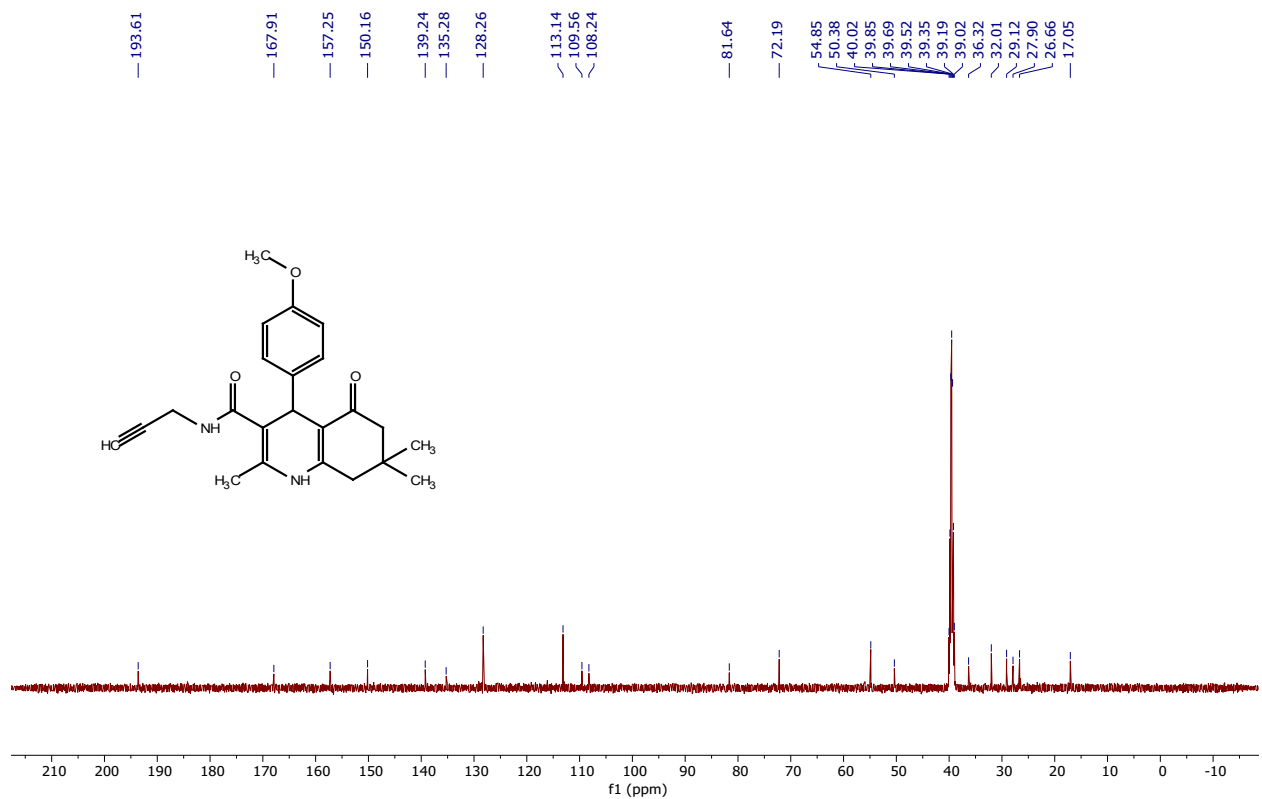


NMR spectrum of compound I1

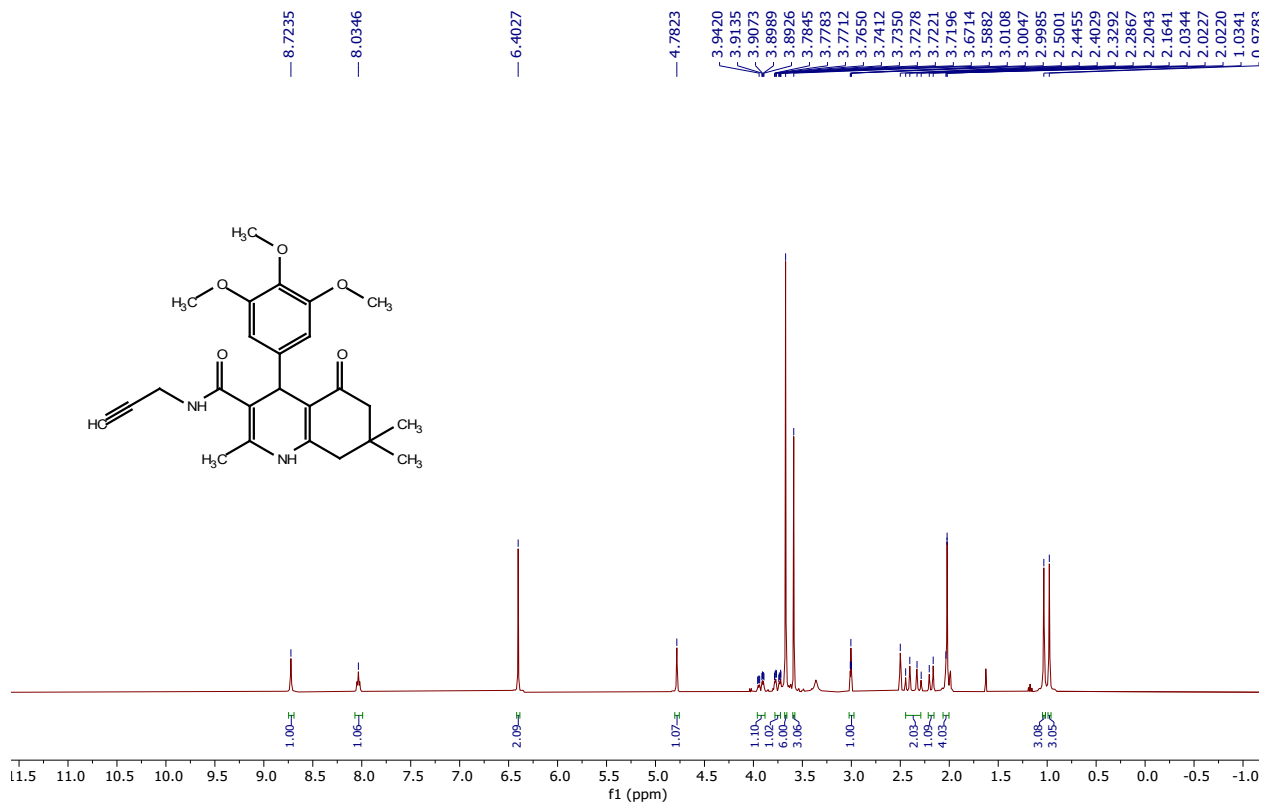


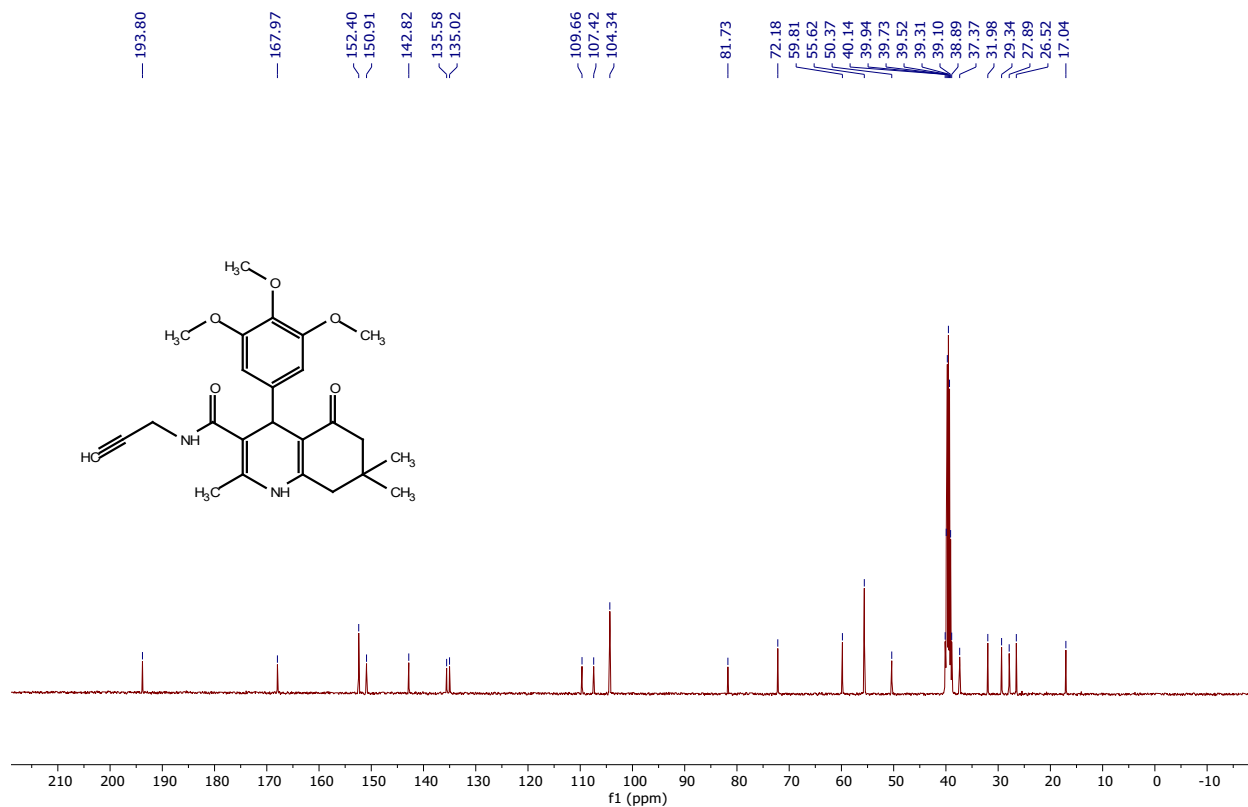
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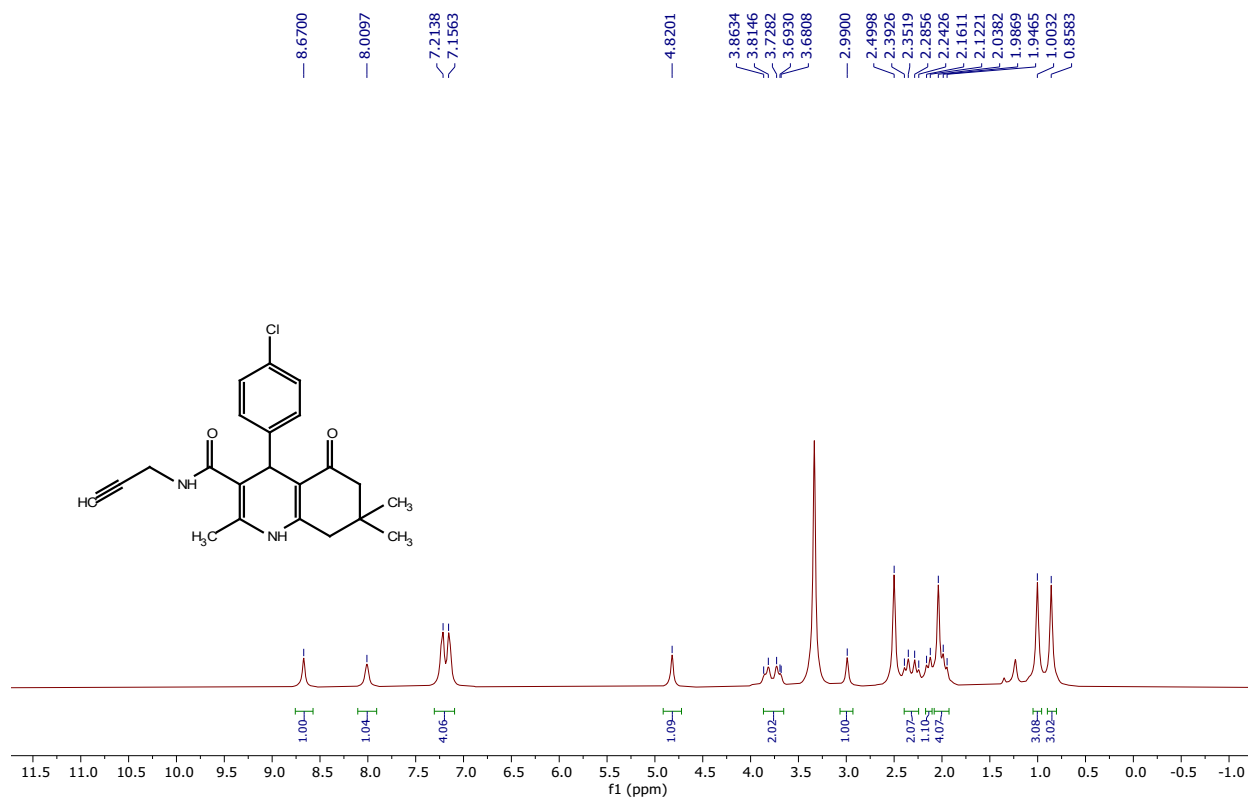


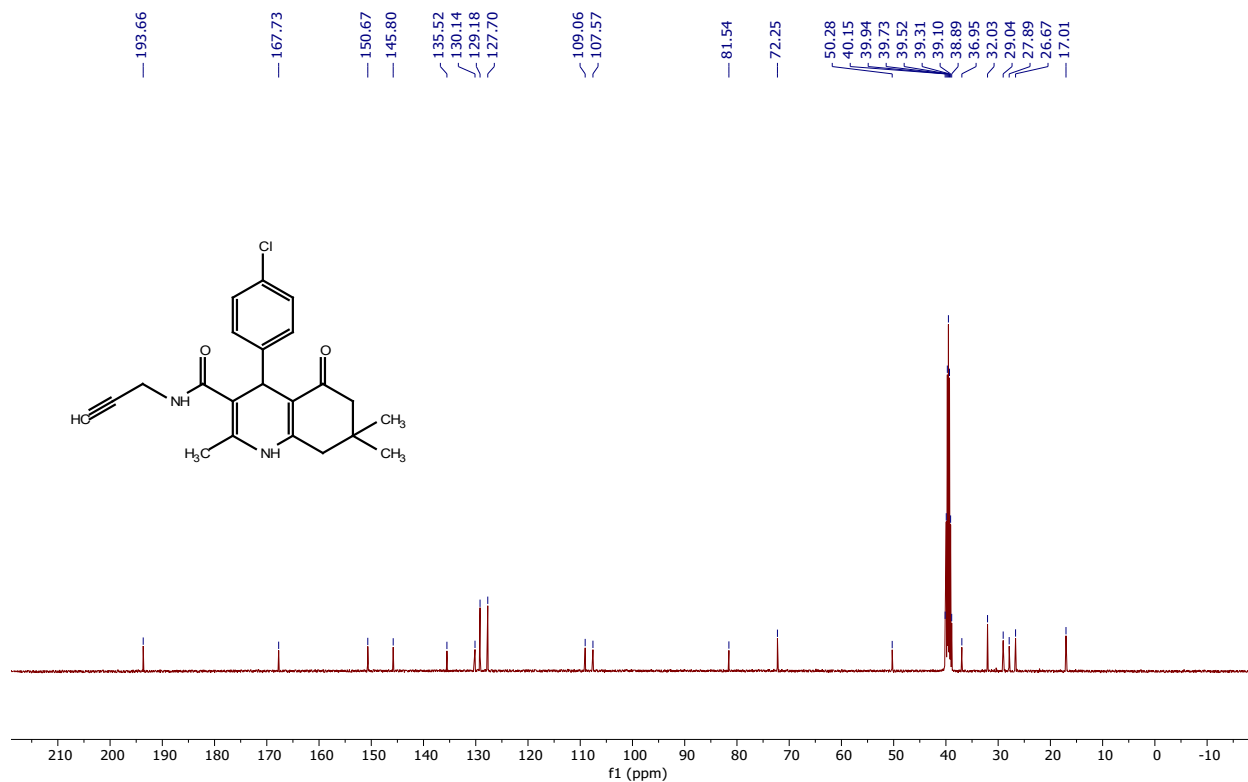
NMR spectrum of compound I3



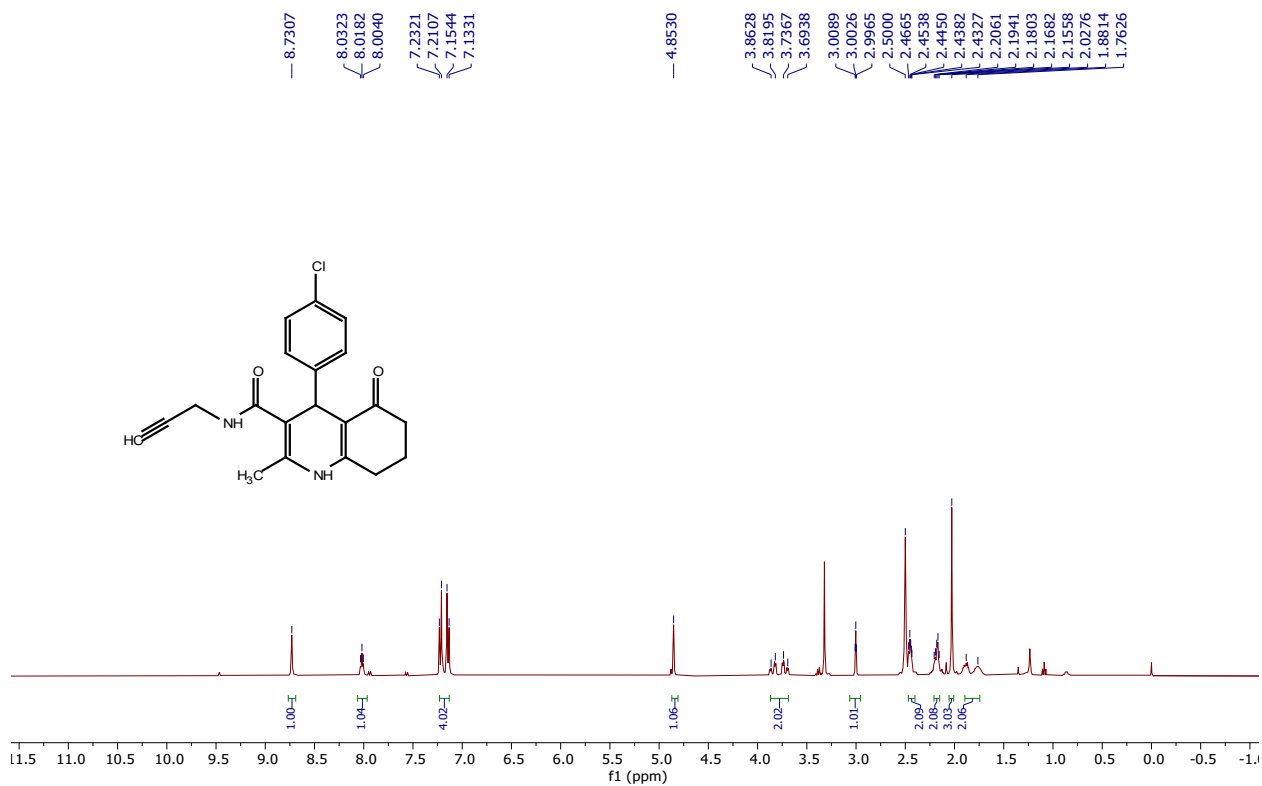


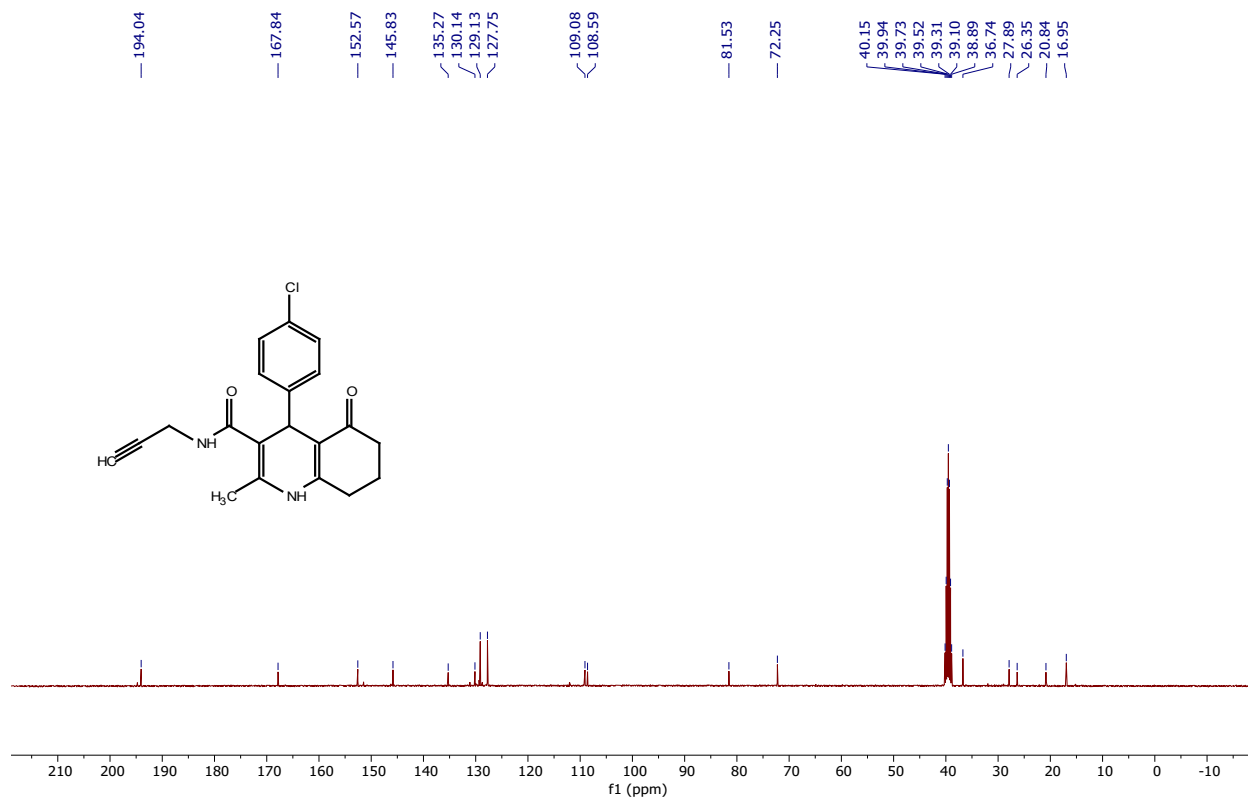
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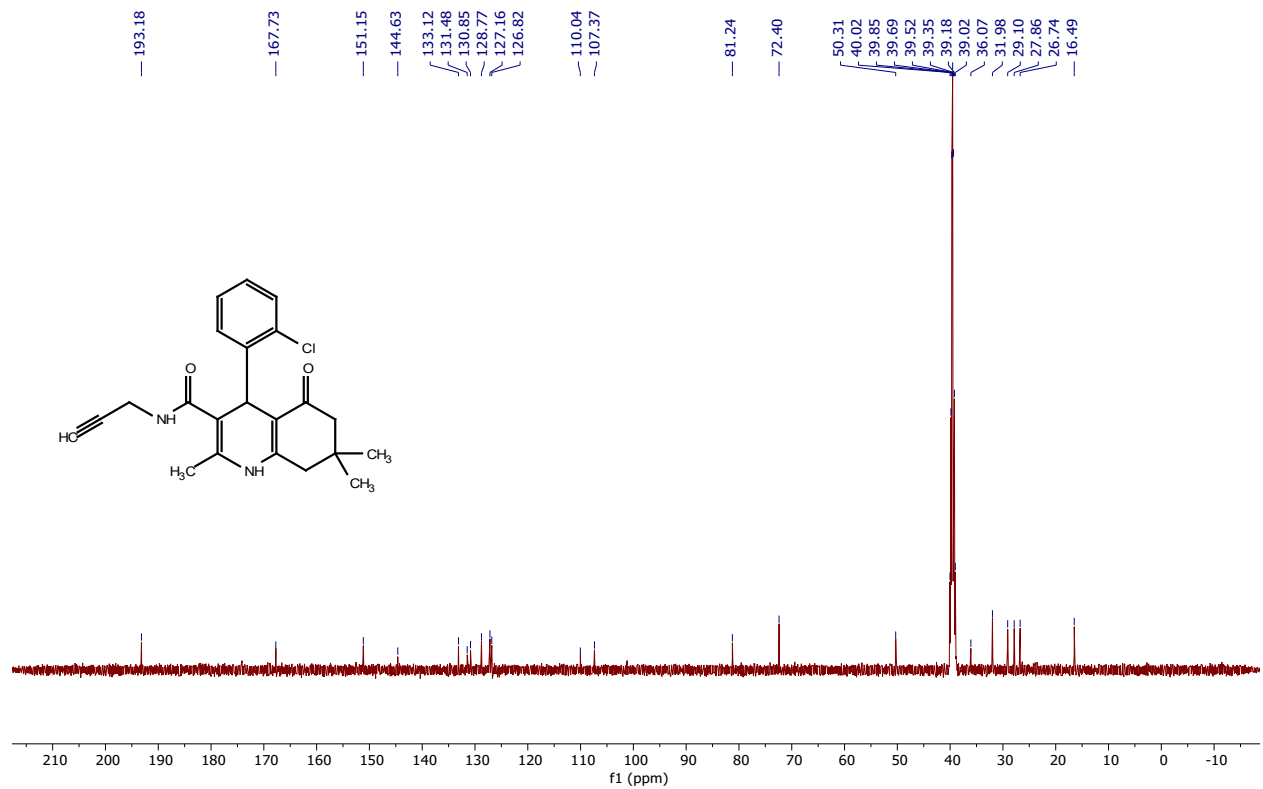
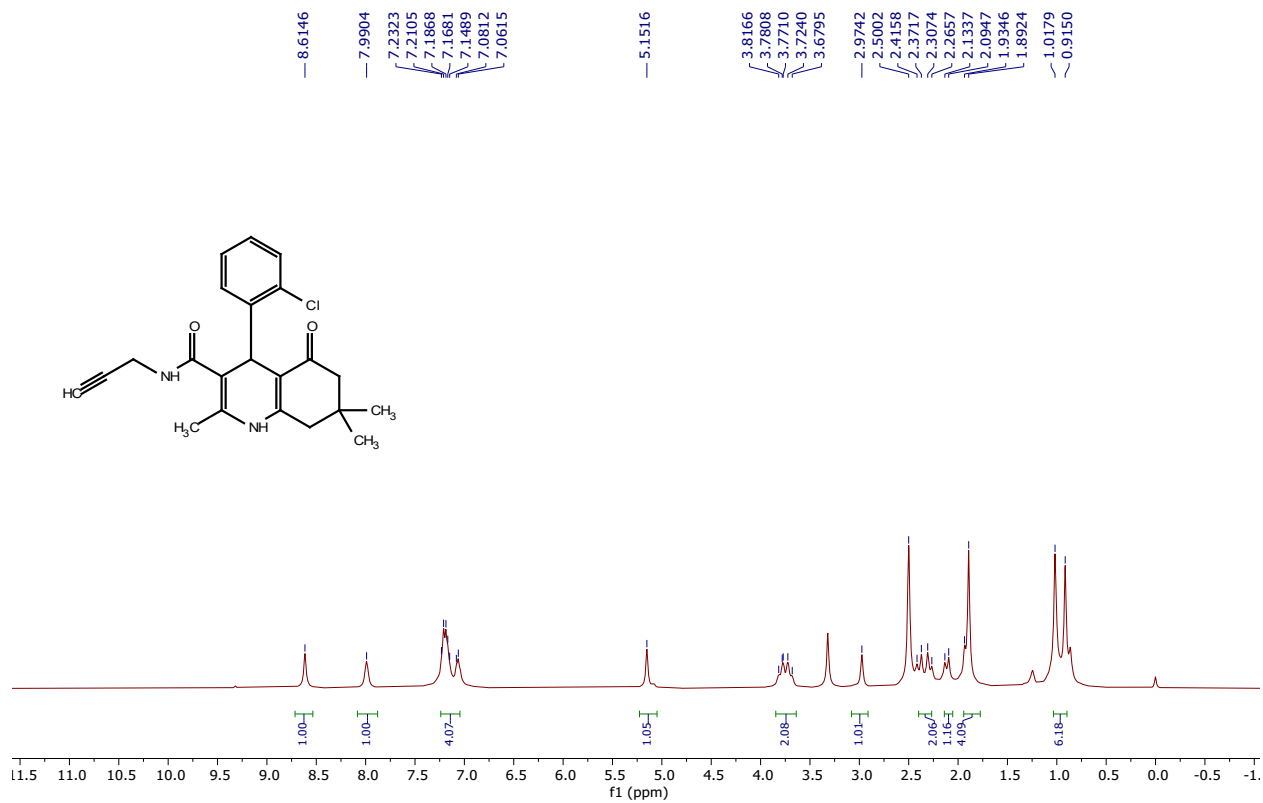


NMR spectrum of compound I5

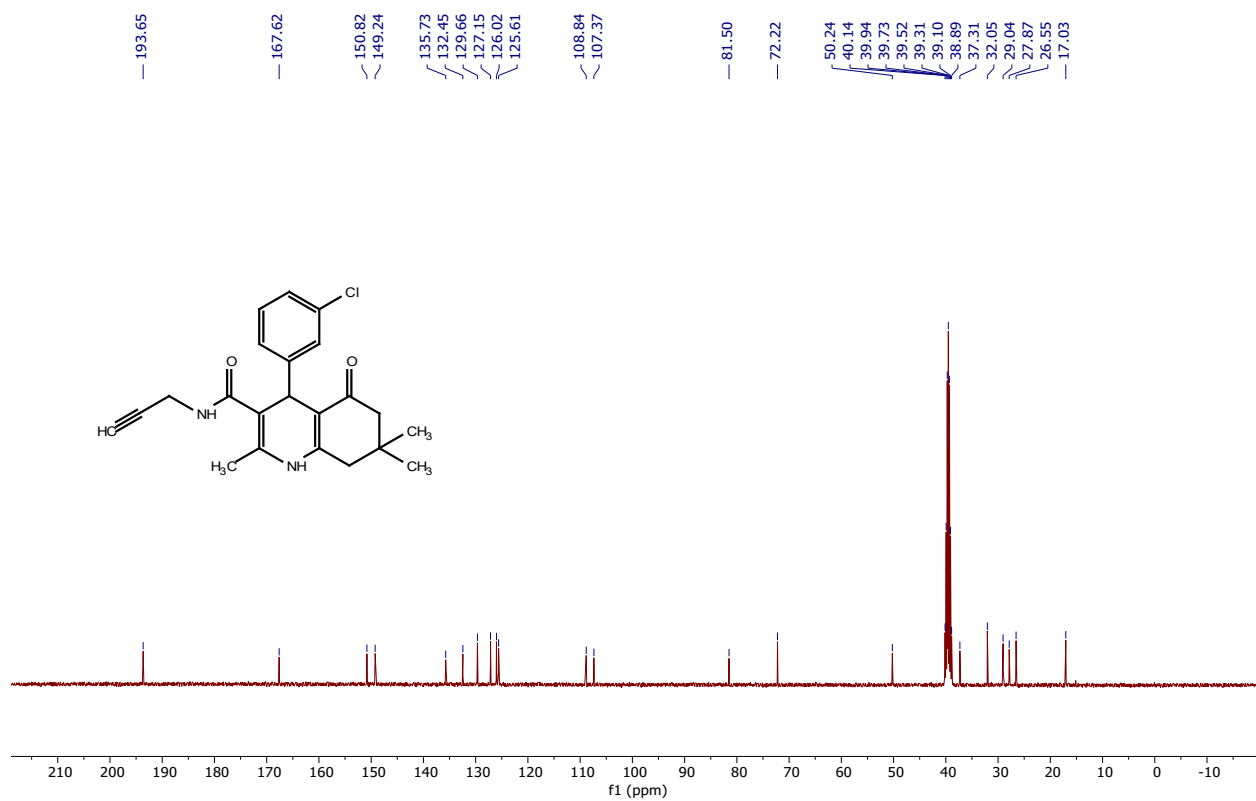
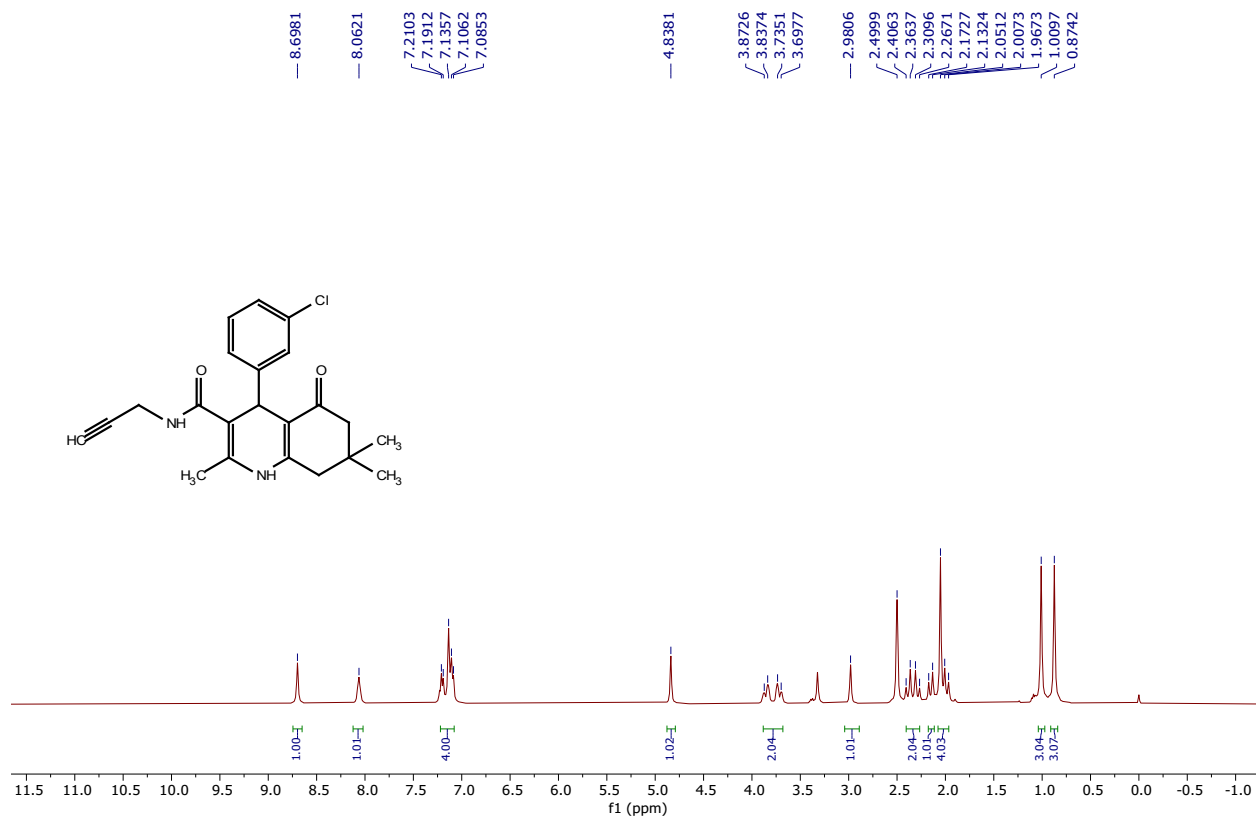




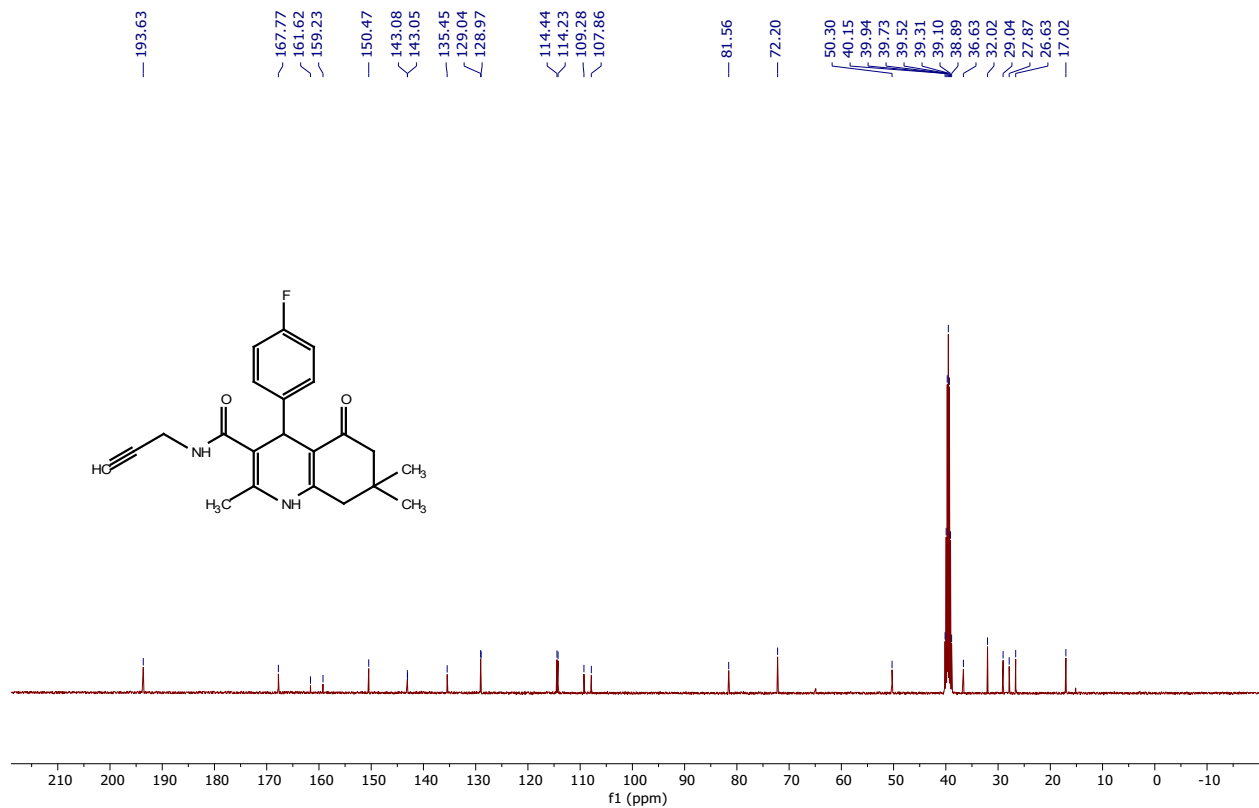
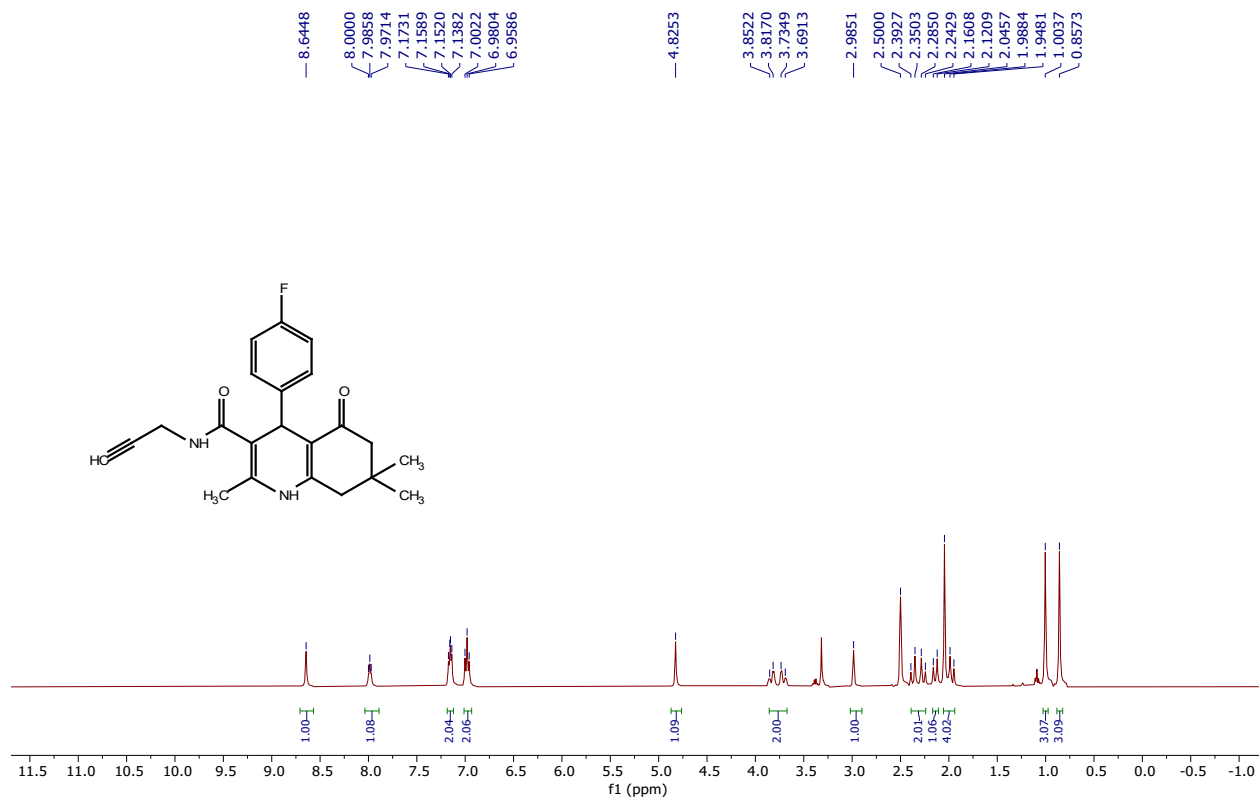
NMR spectrum of compound I6



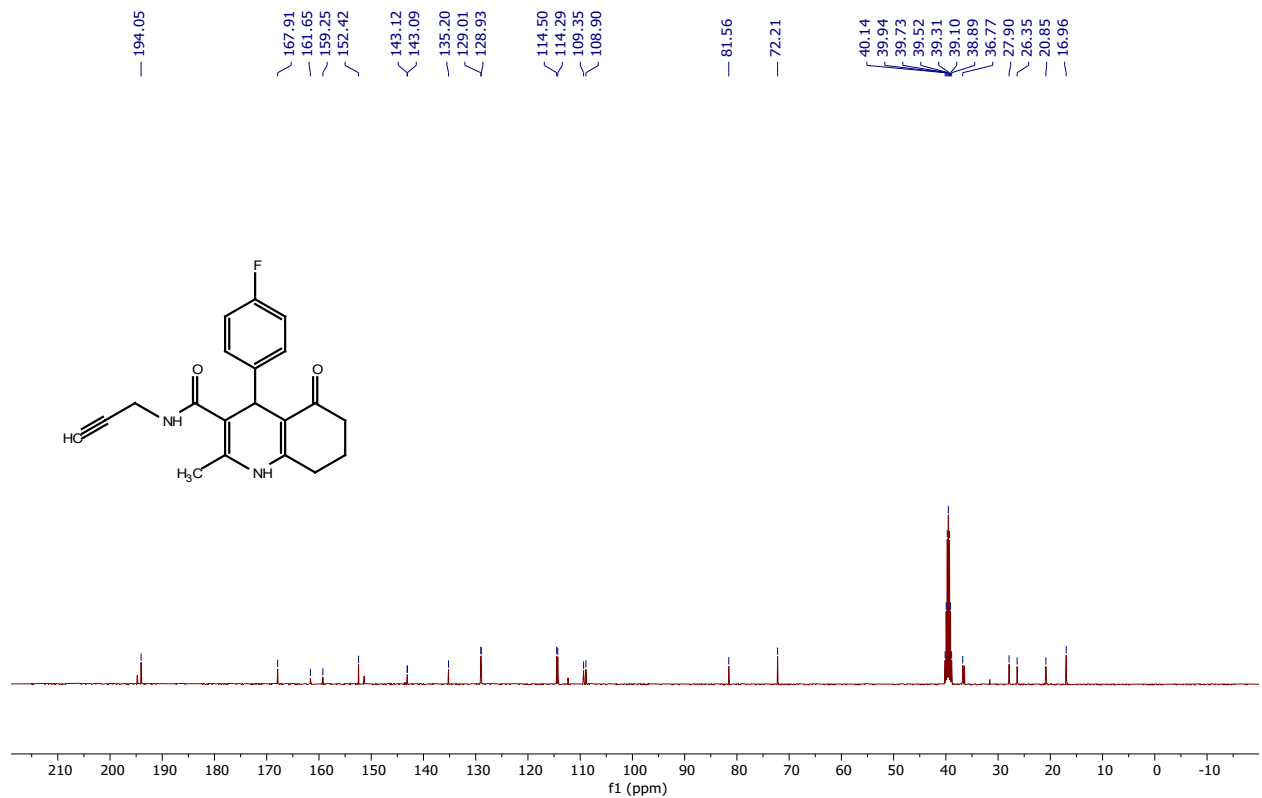
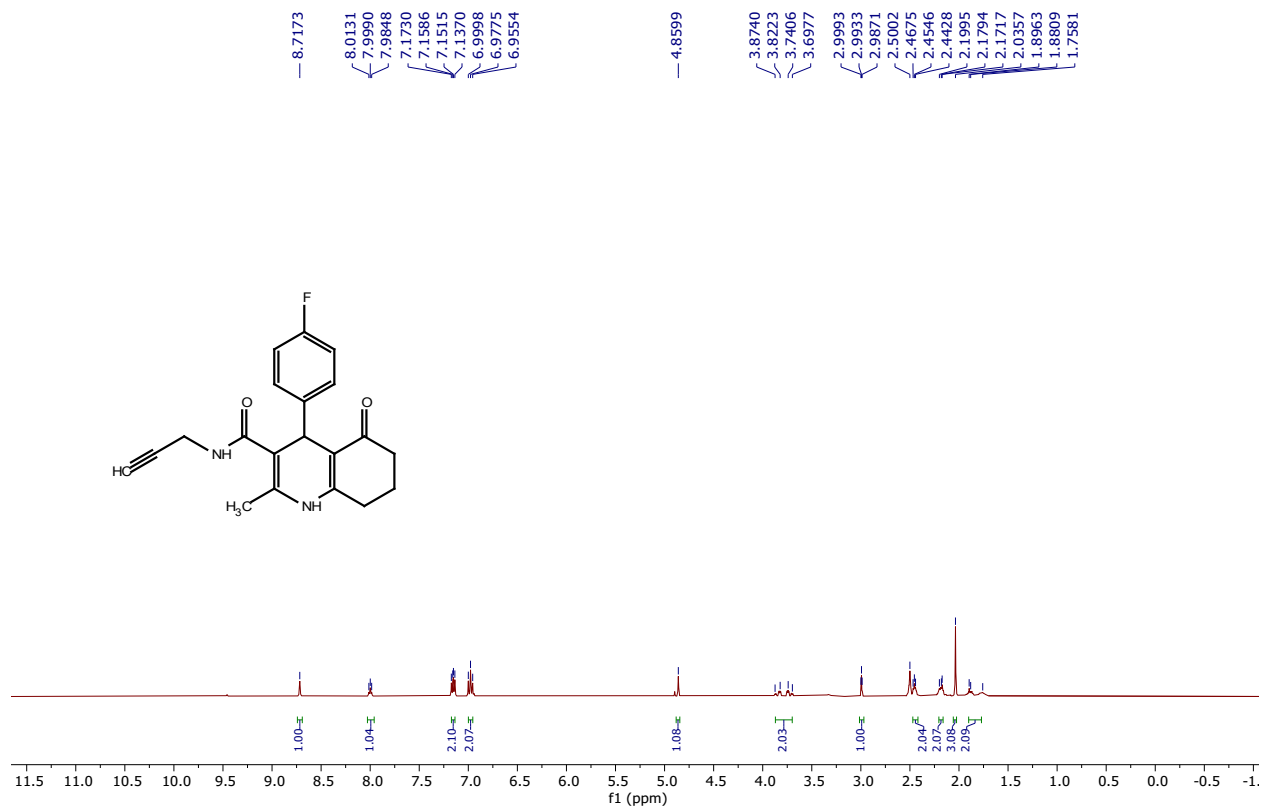
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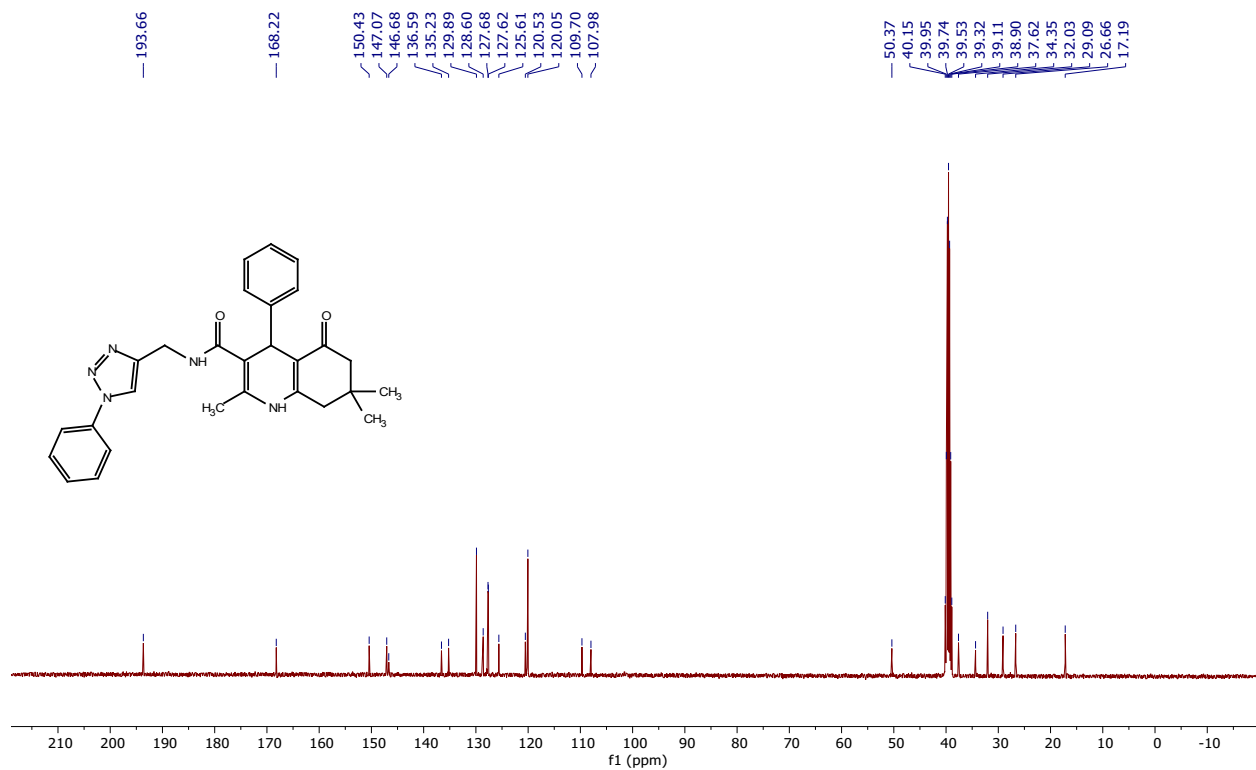
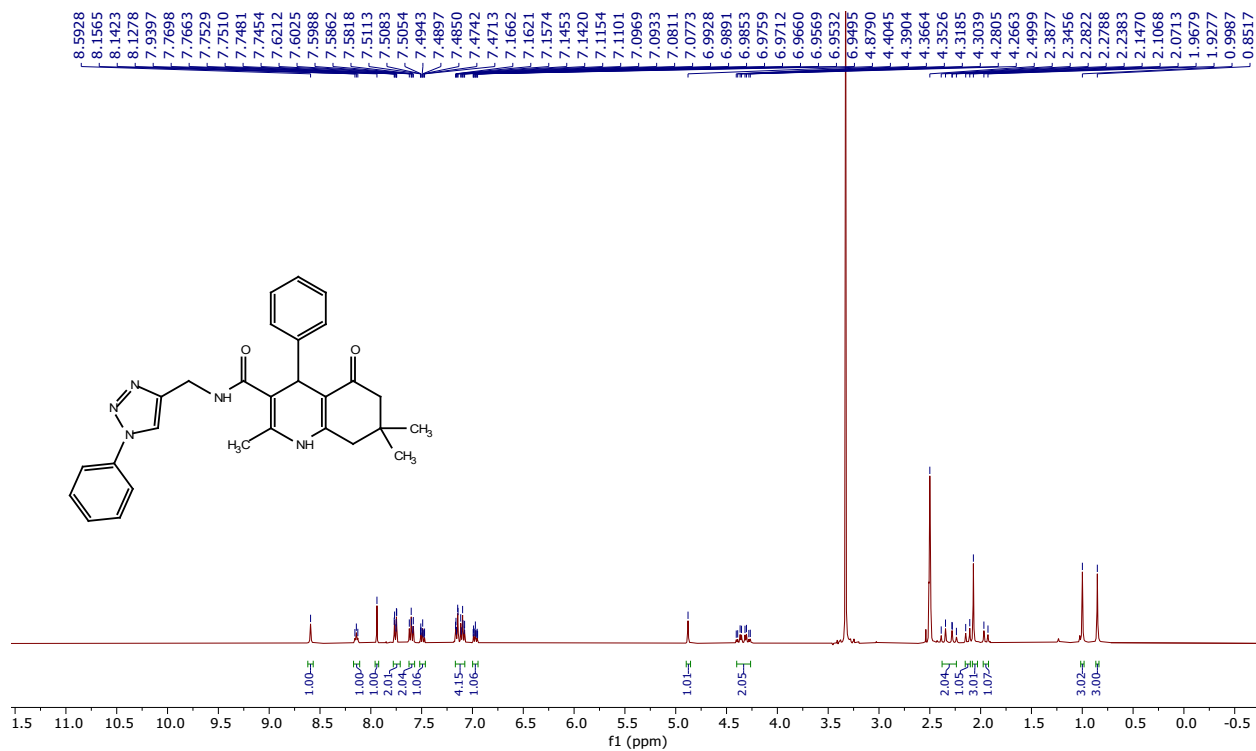
NMR spectrum of compound I8



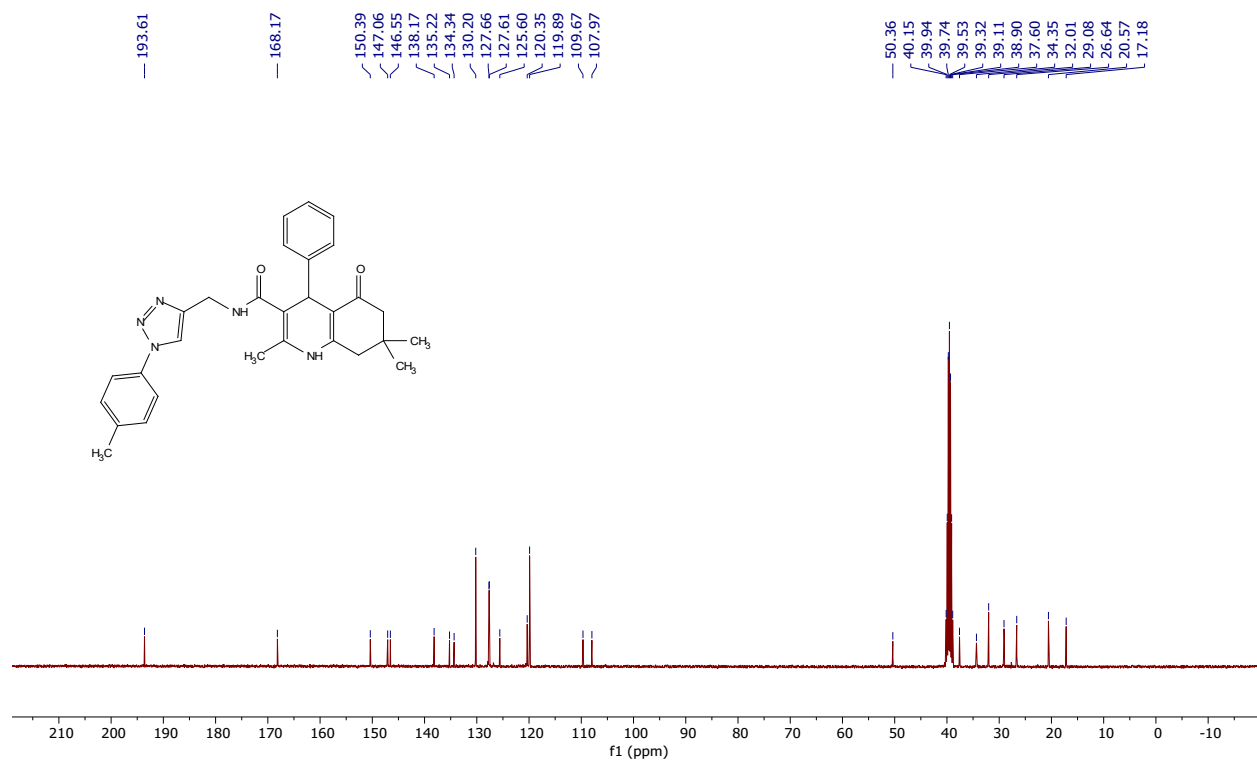
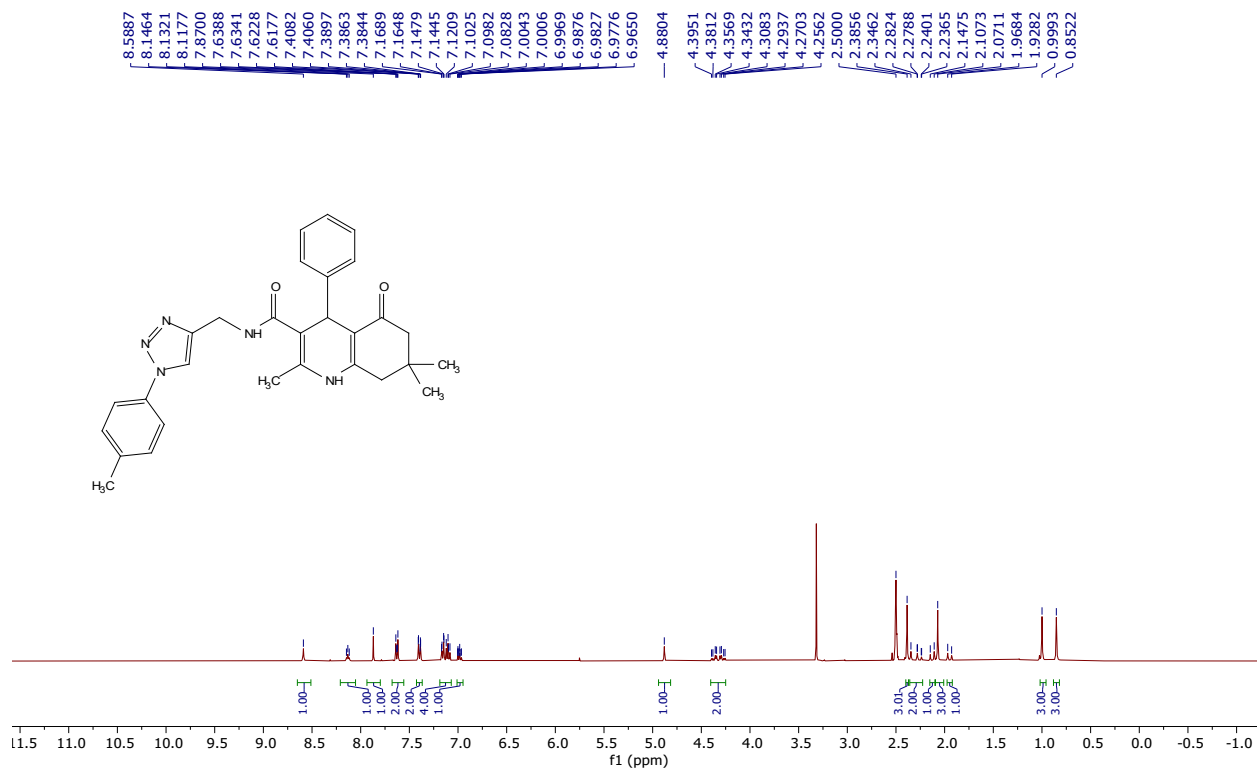
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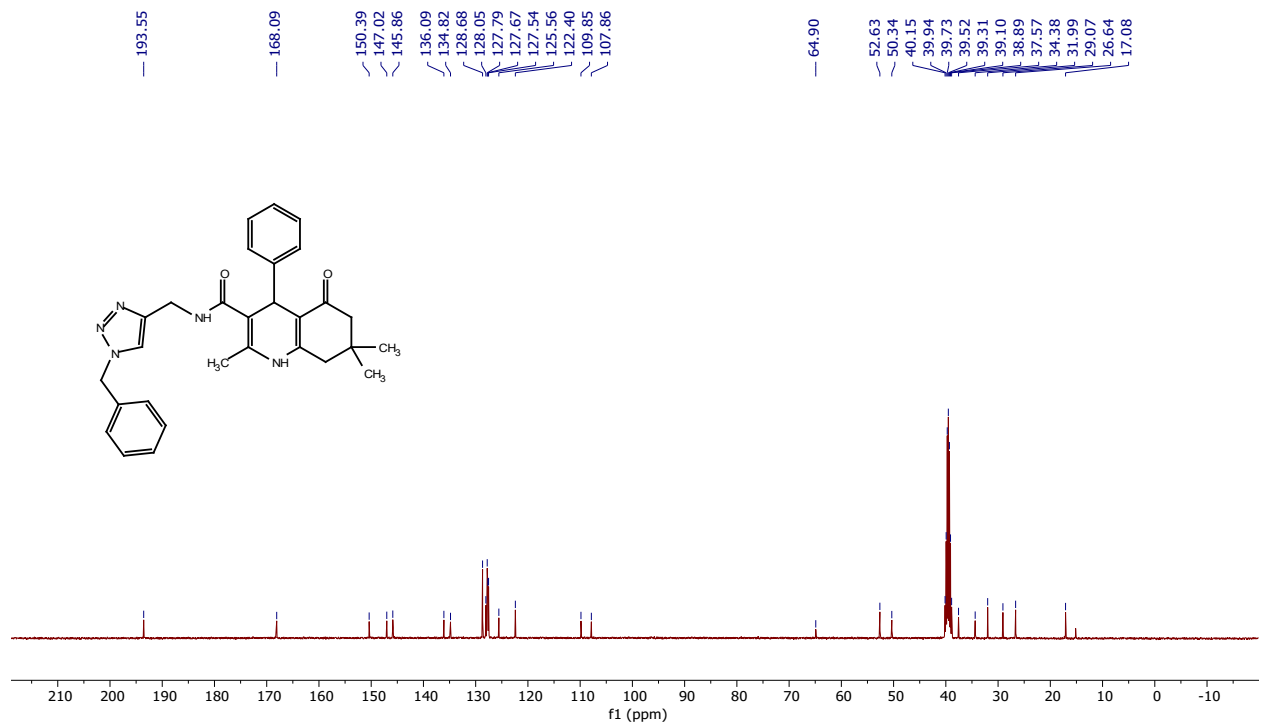
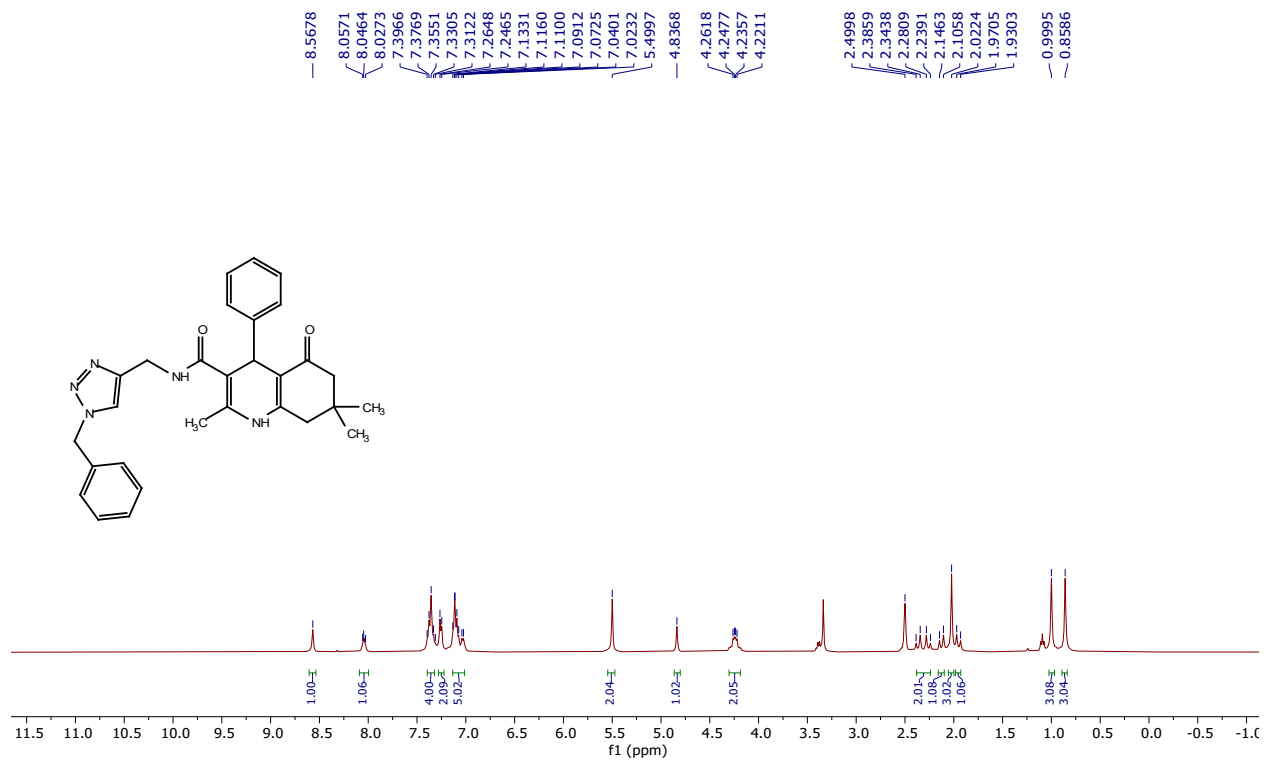
NMR spectrum of compound I10



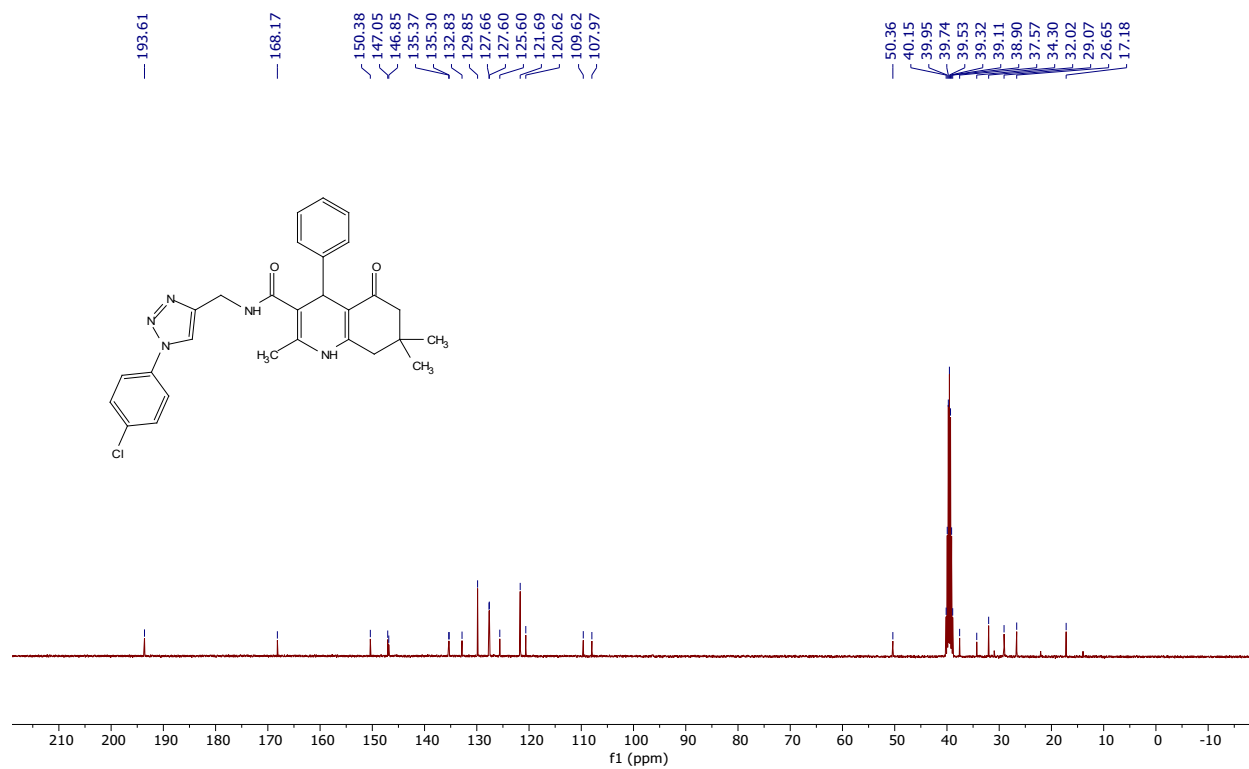
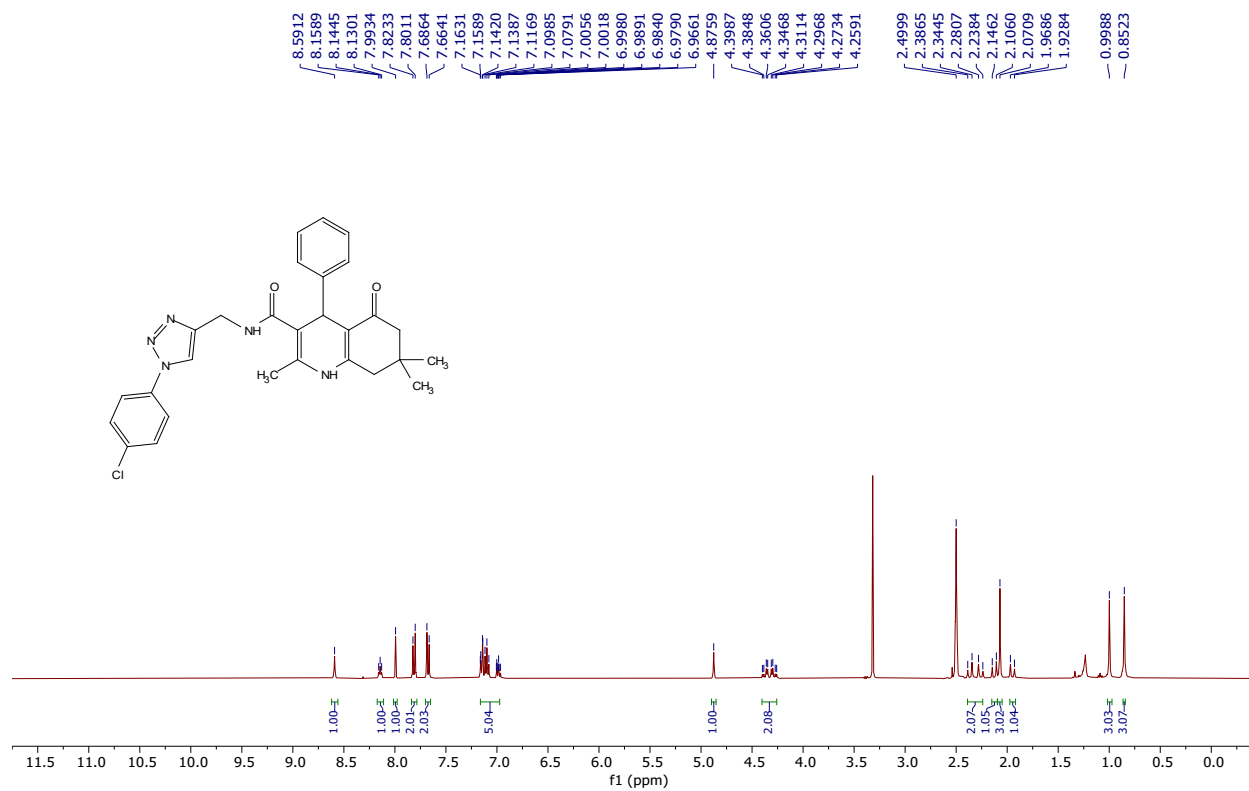
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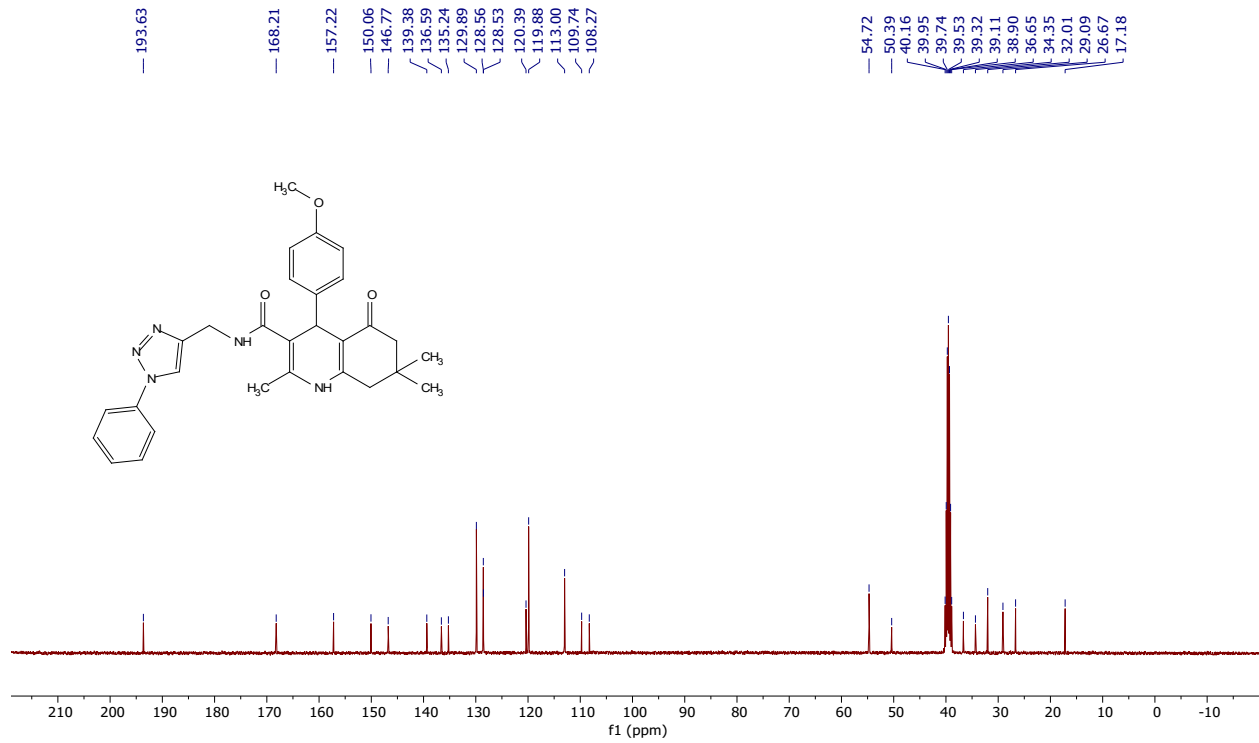
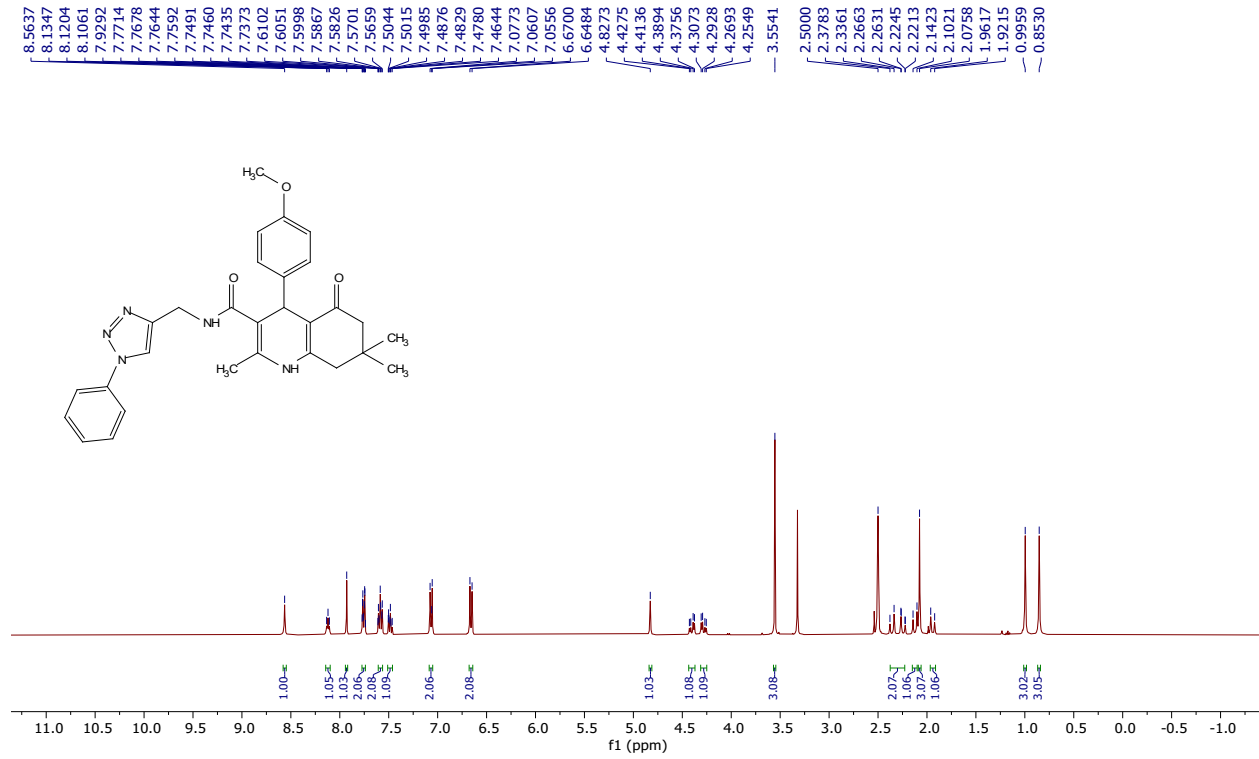
NMR spectrum of compound J3



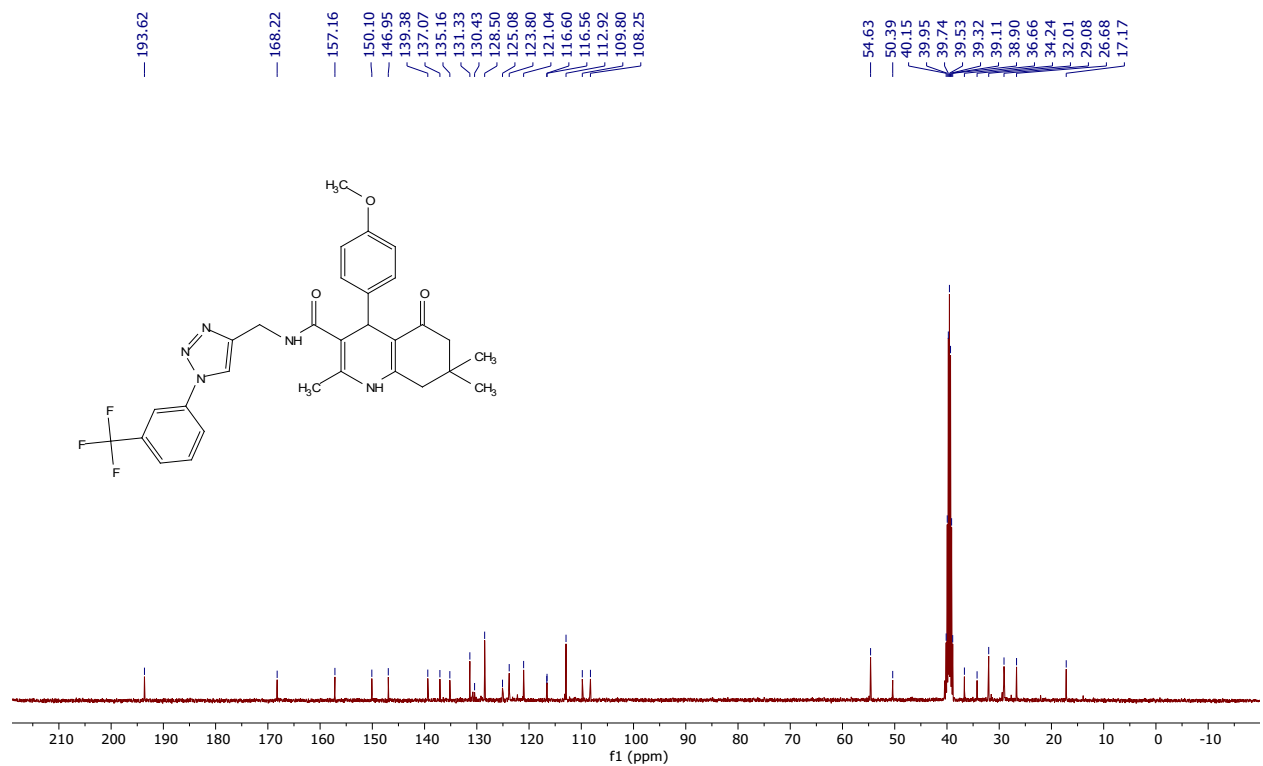
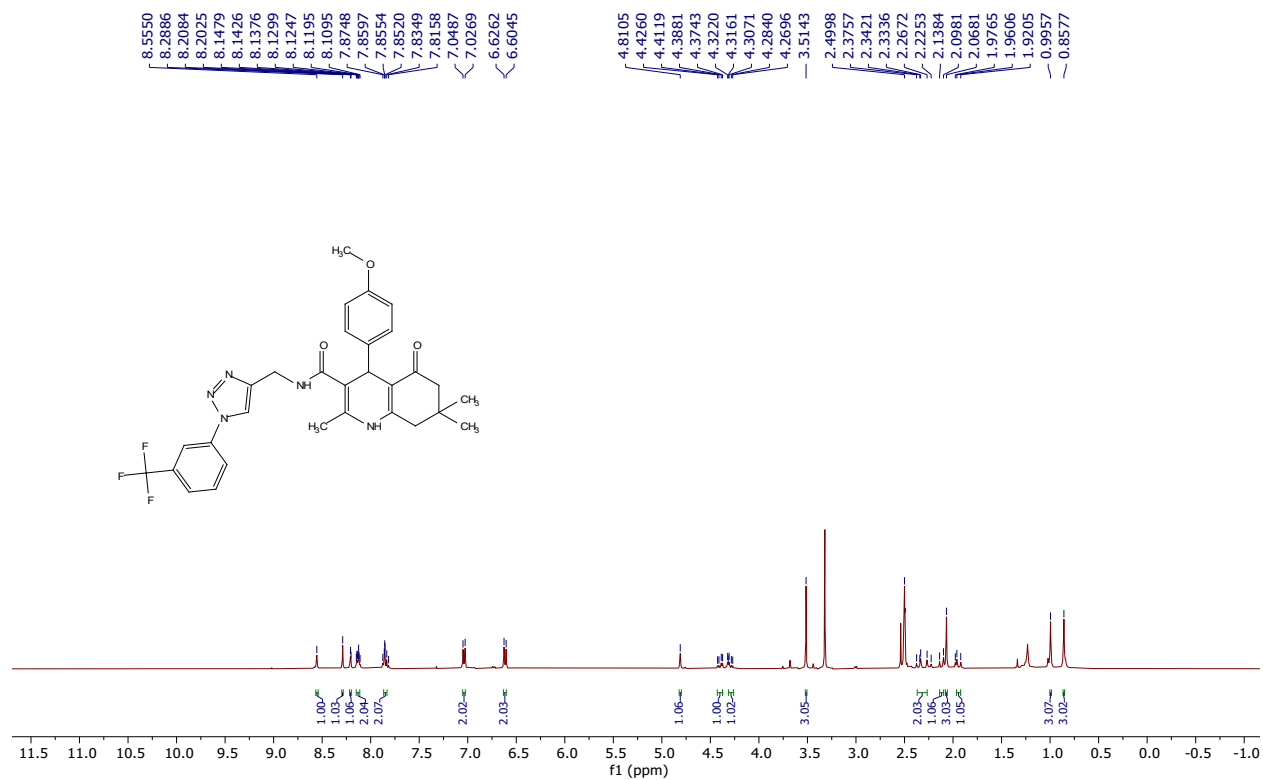
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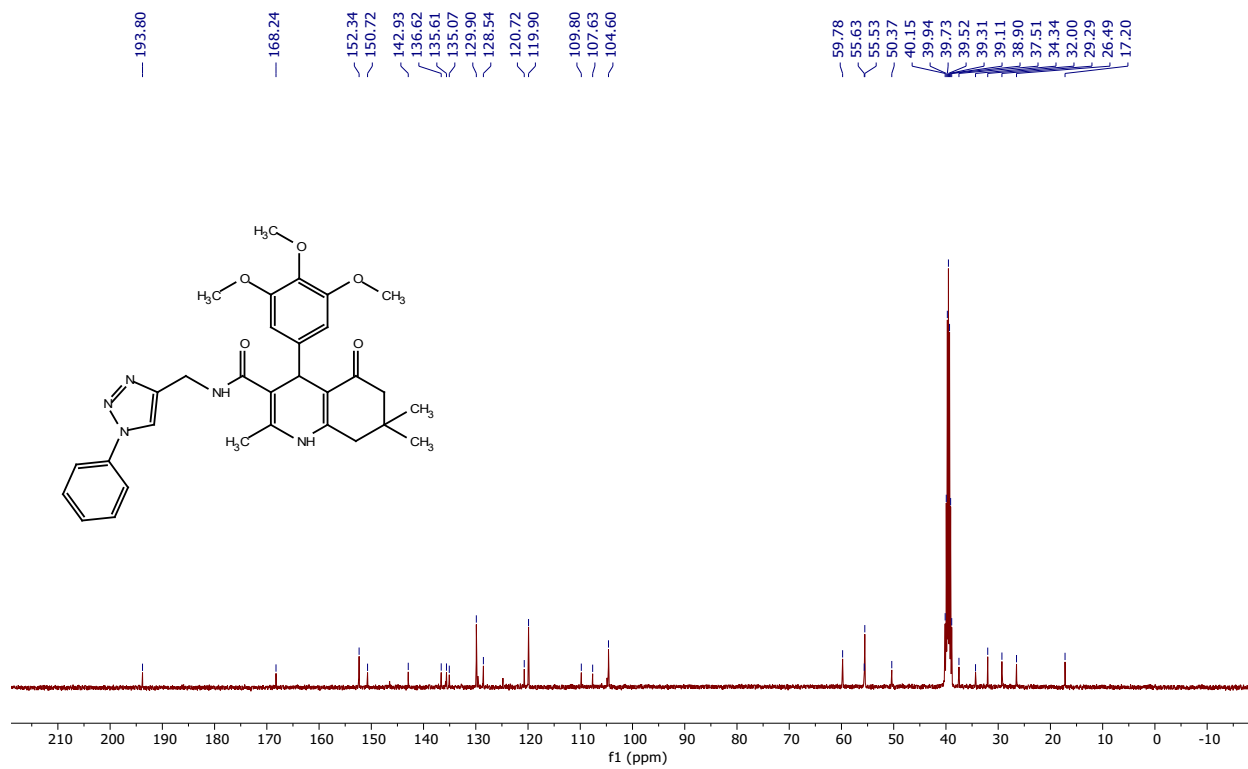
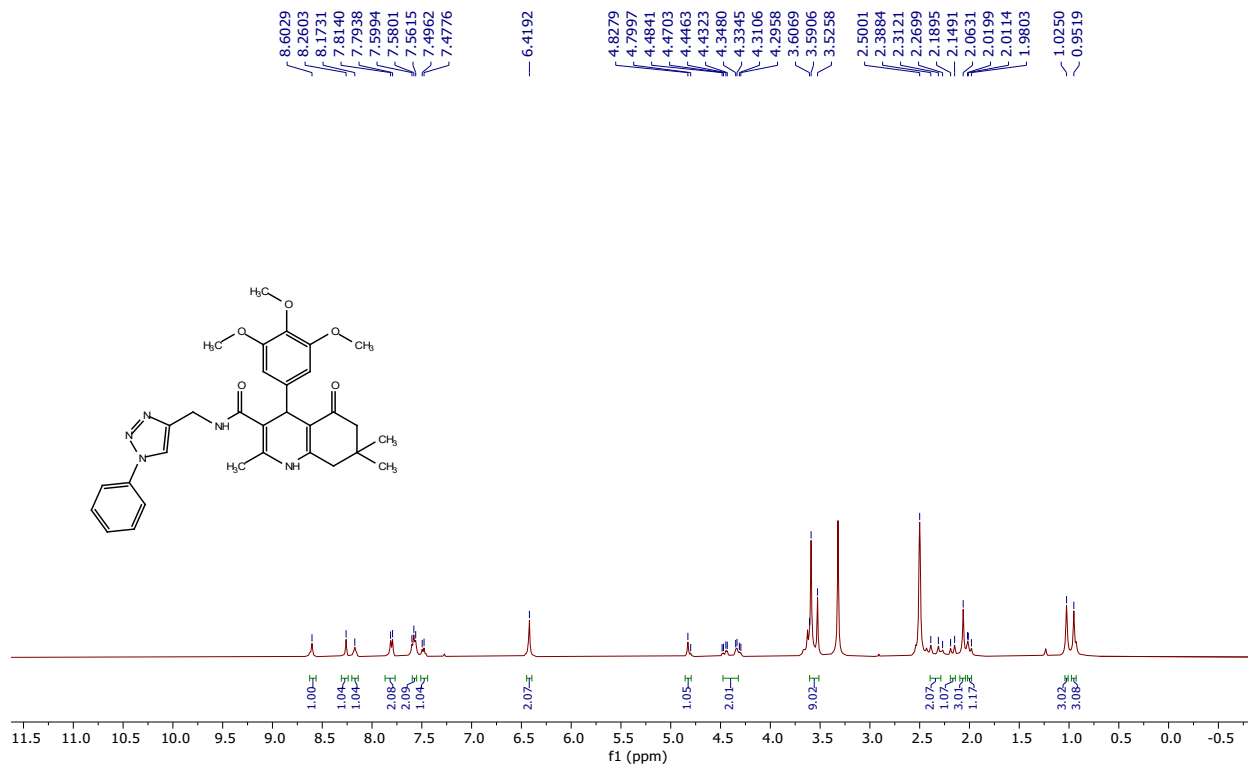
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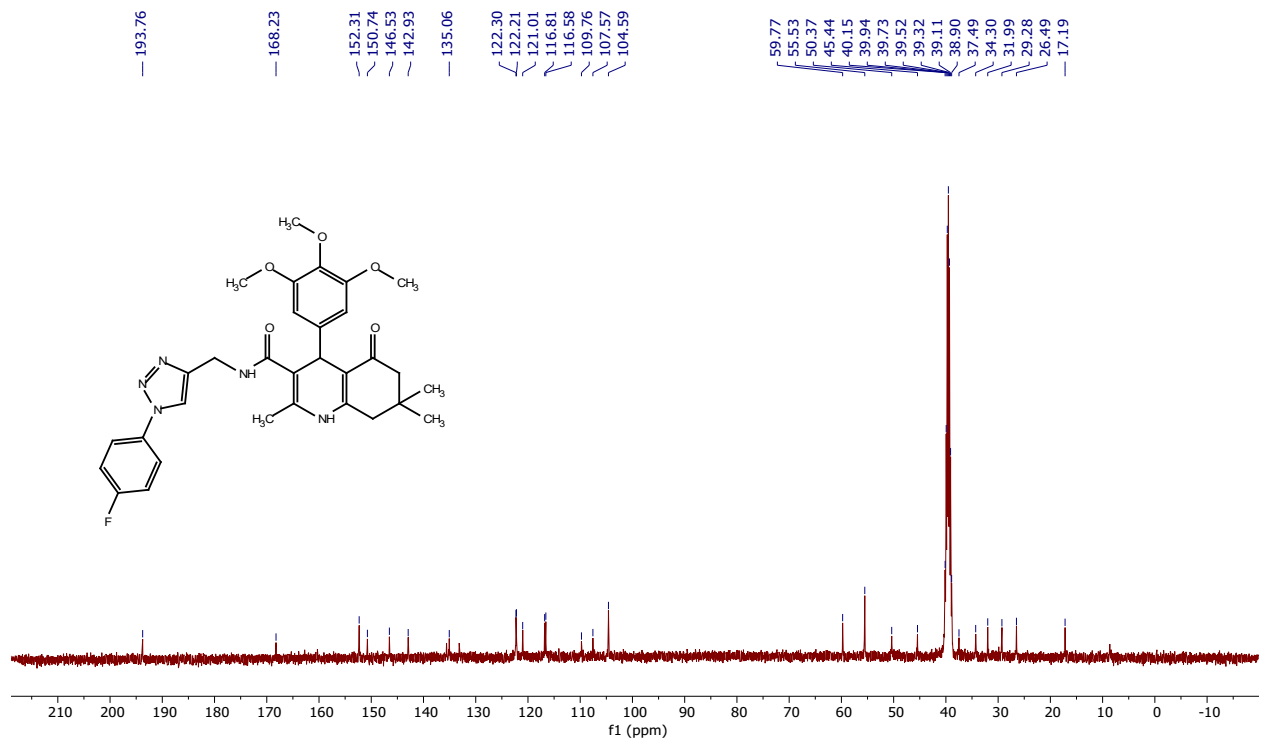
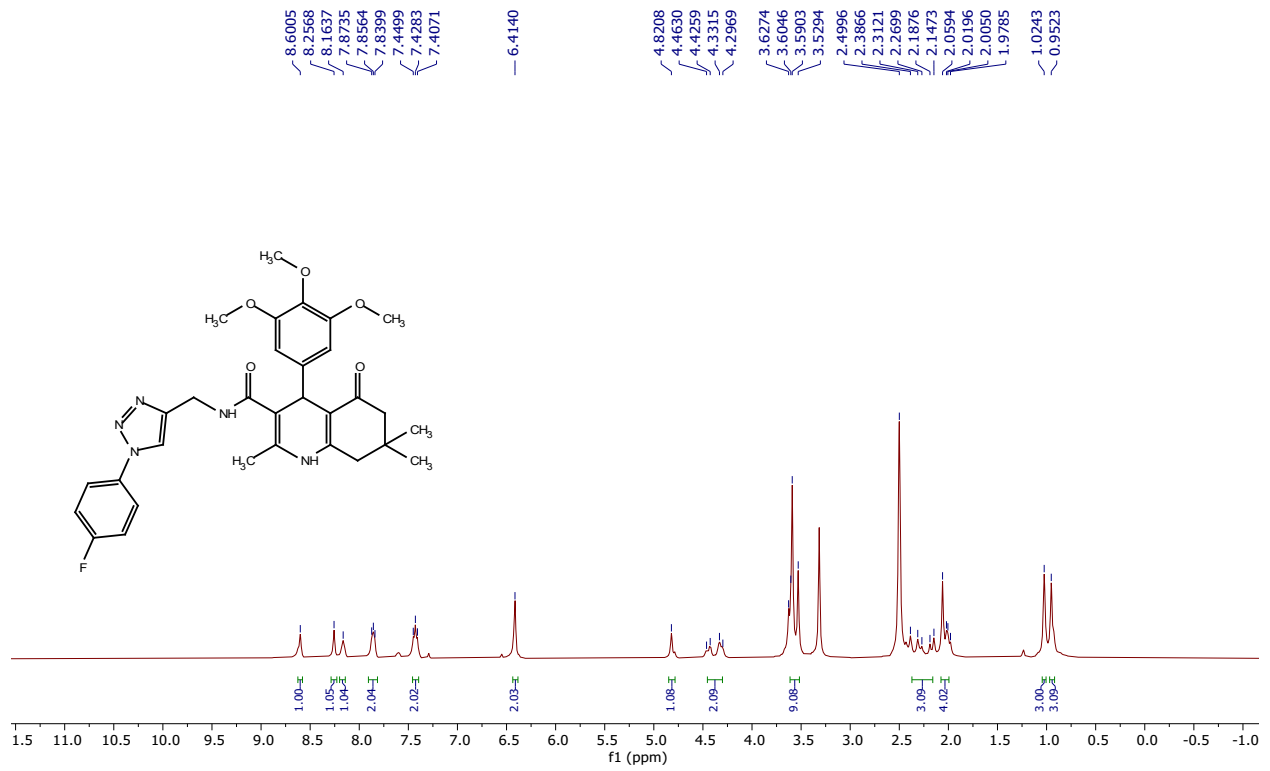
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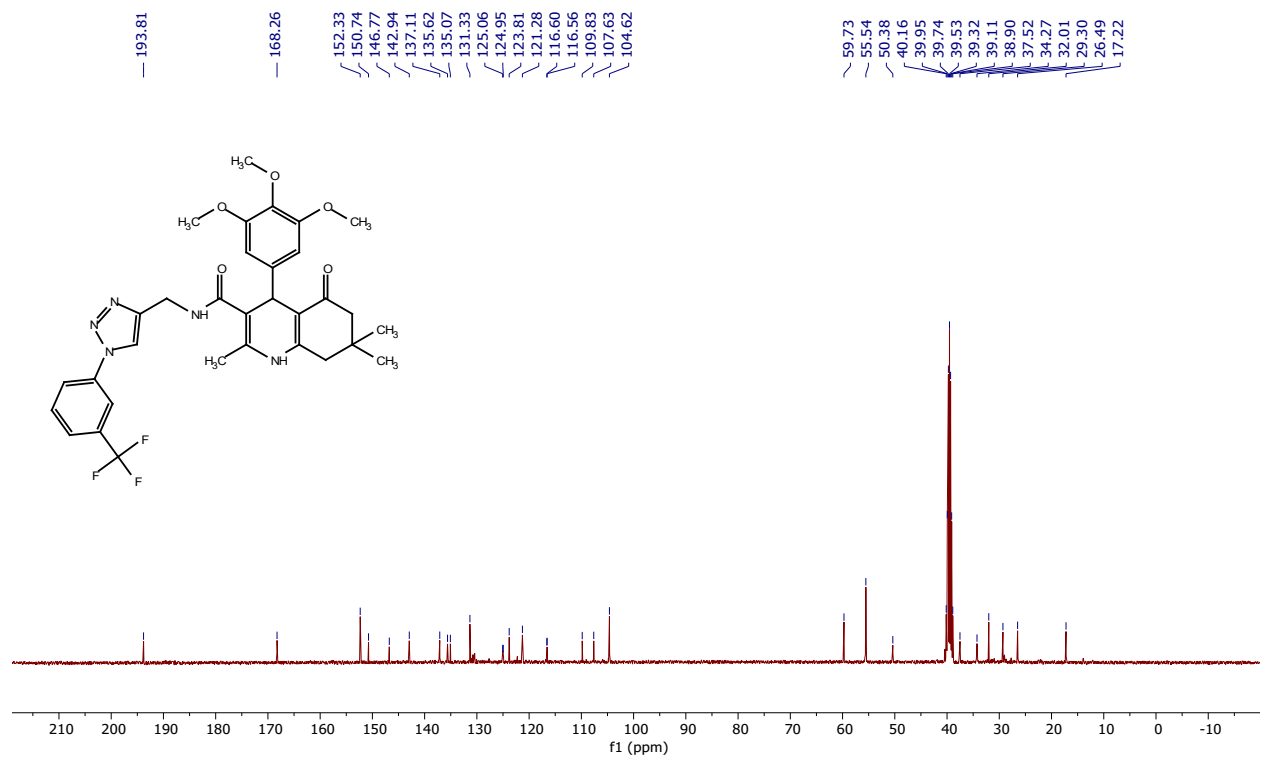
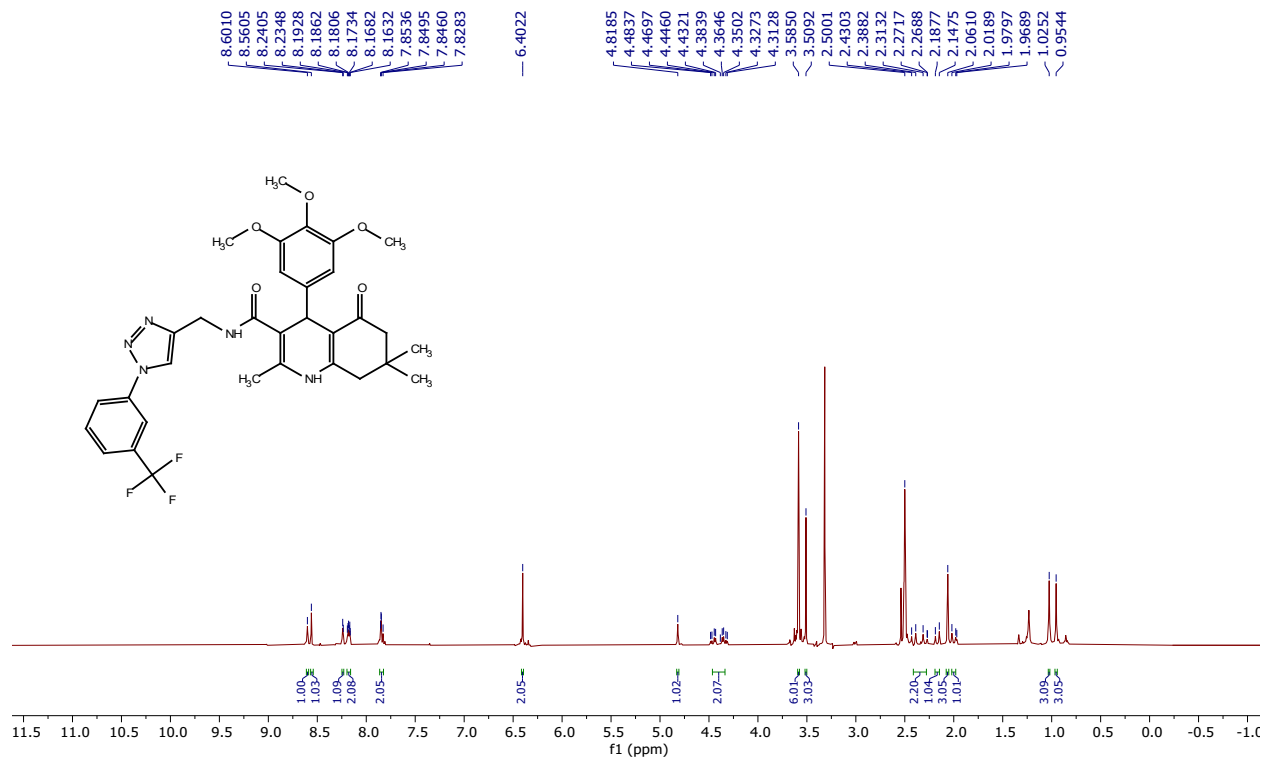
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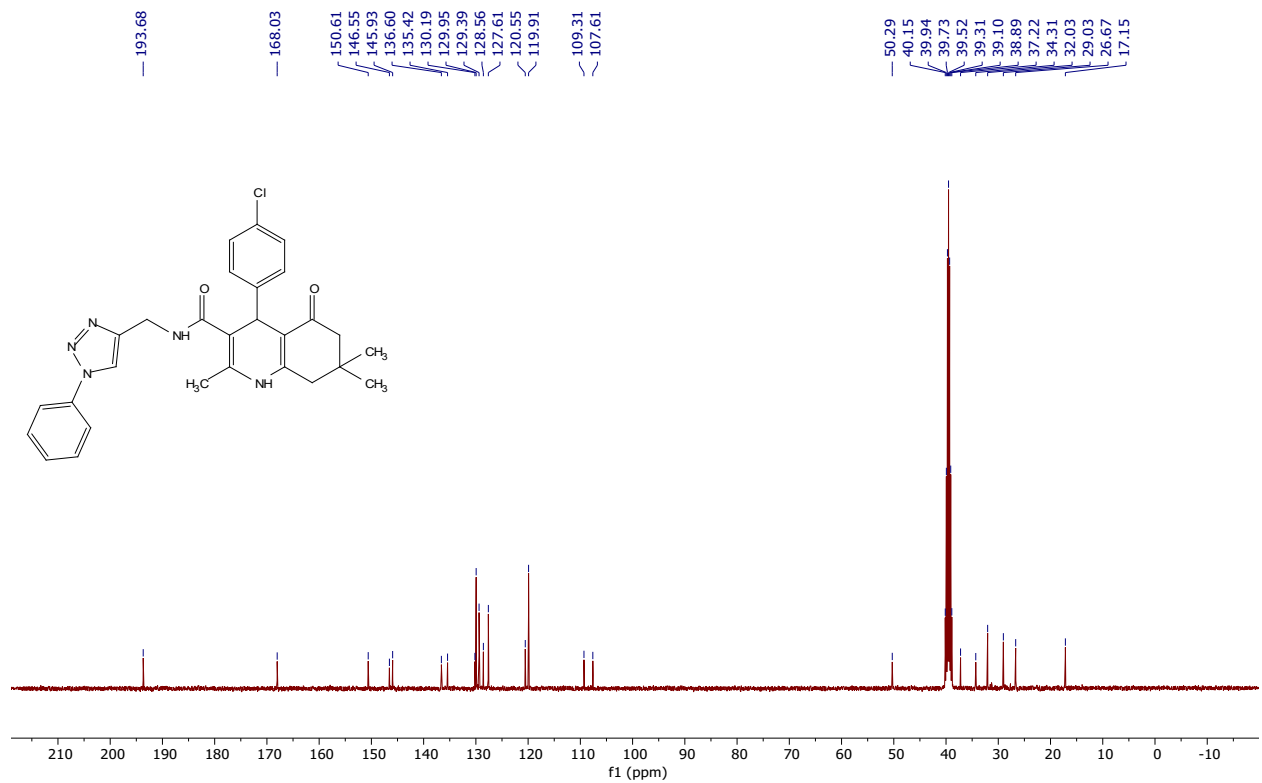
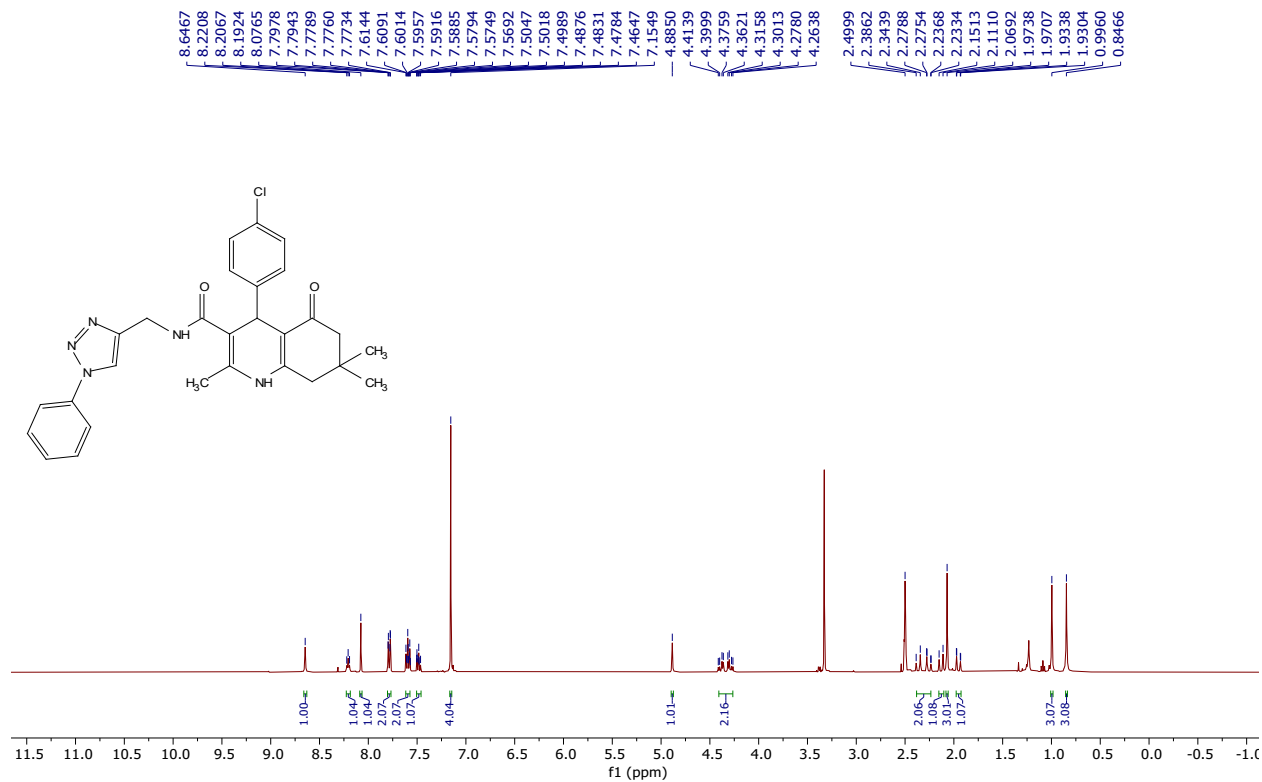
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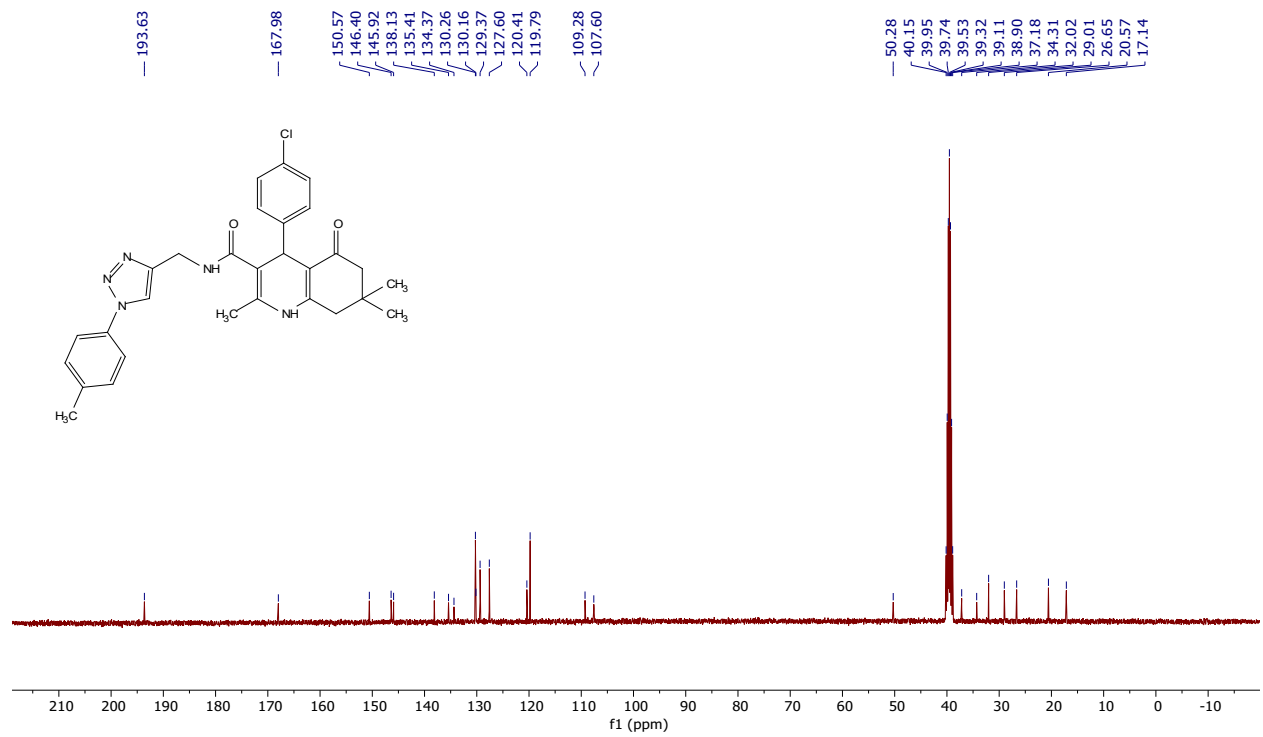
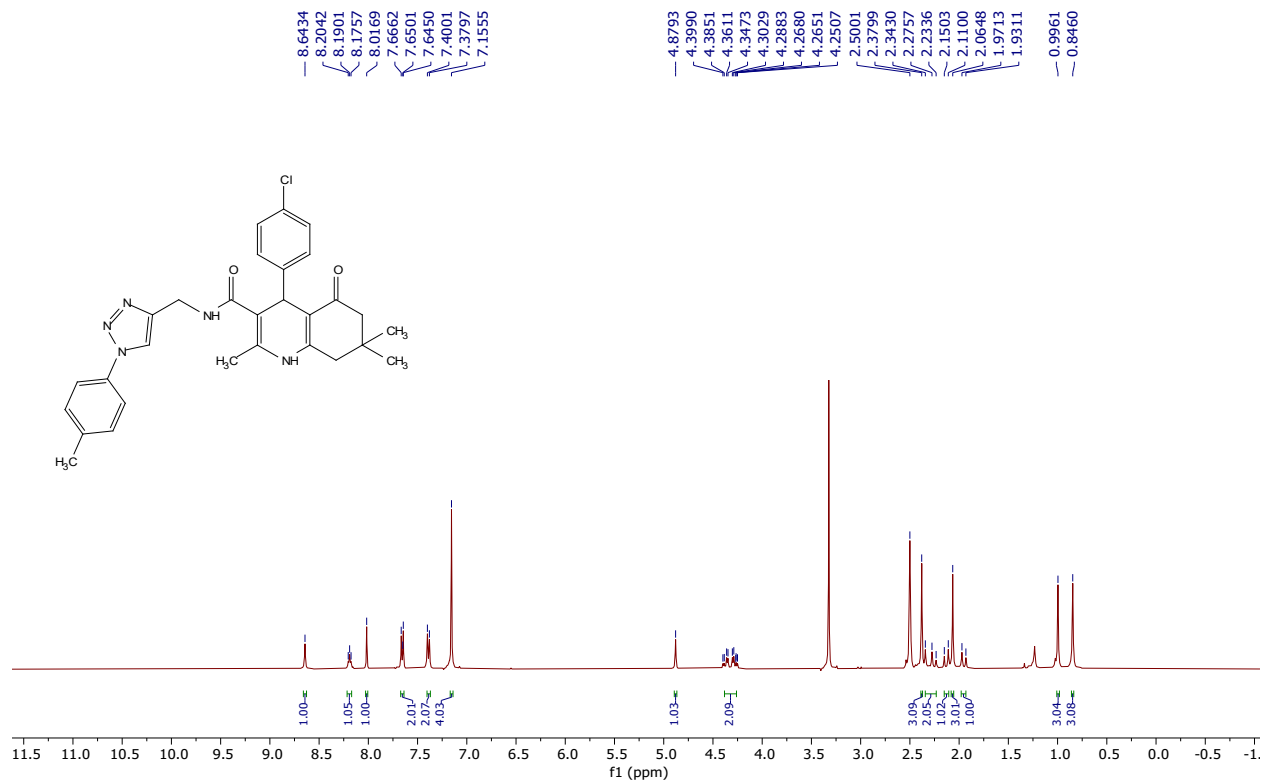
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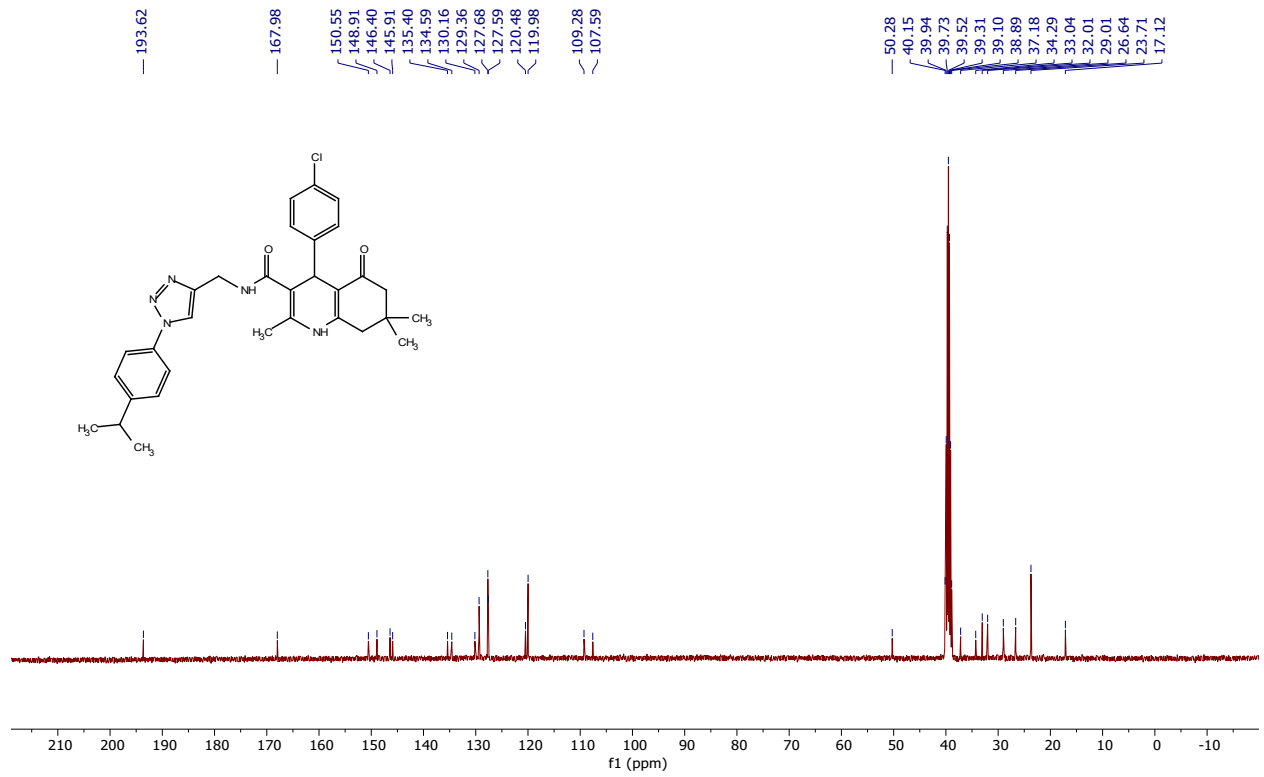
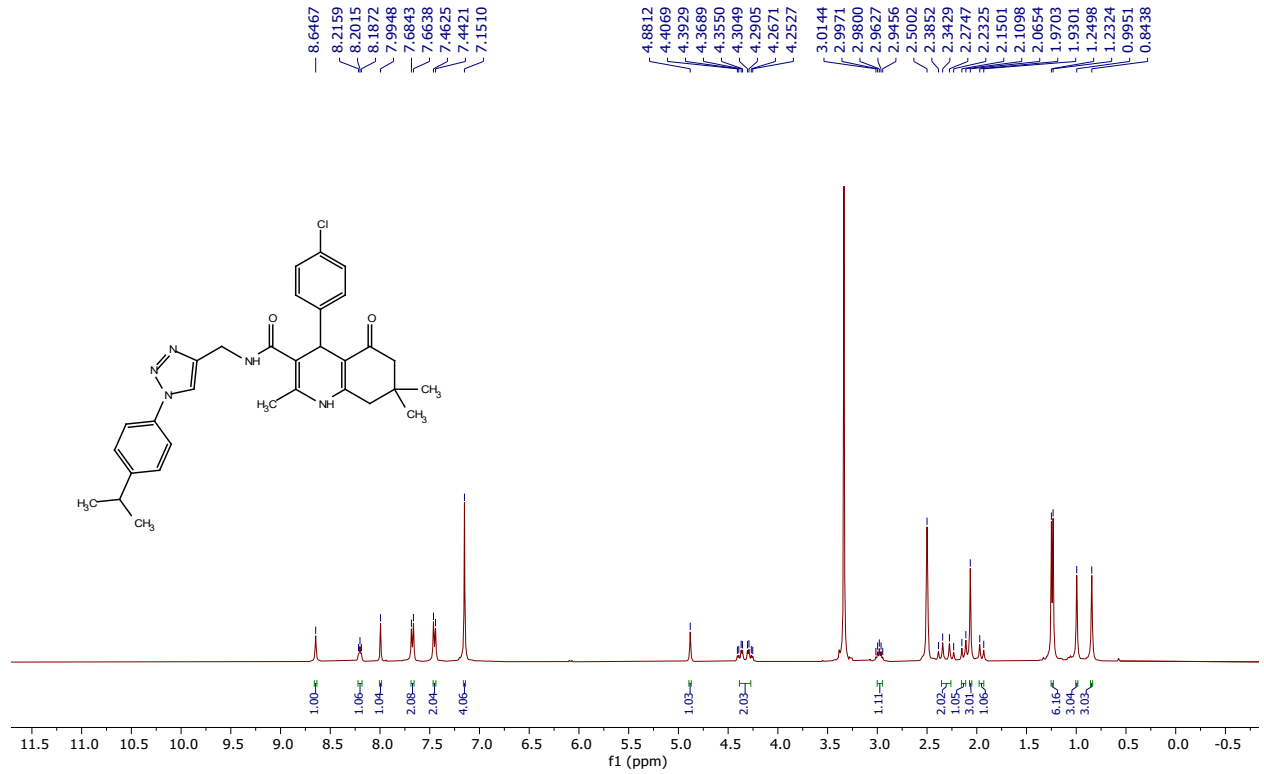
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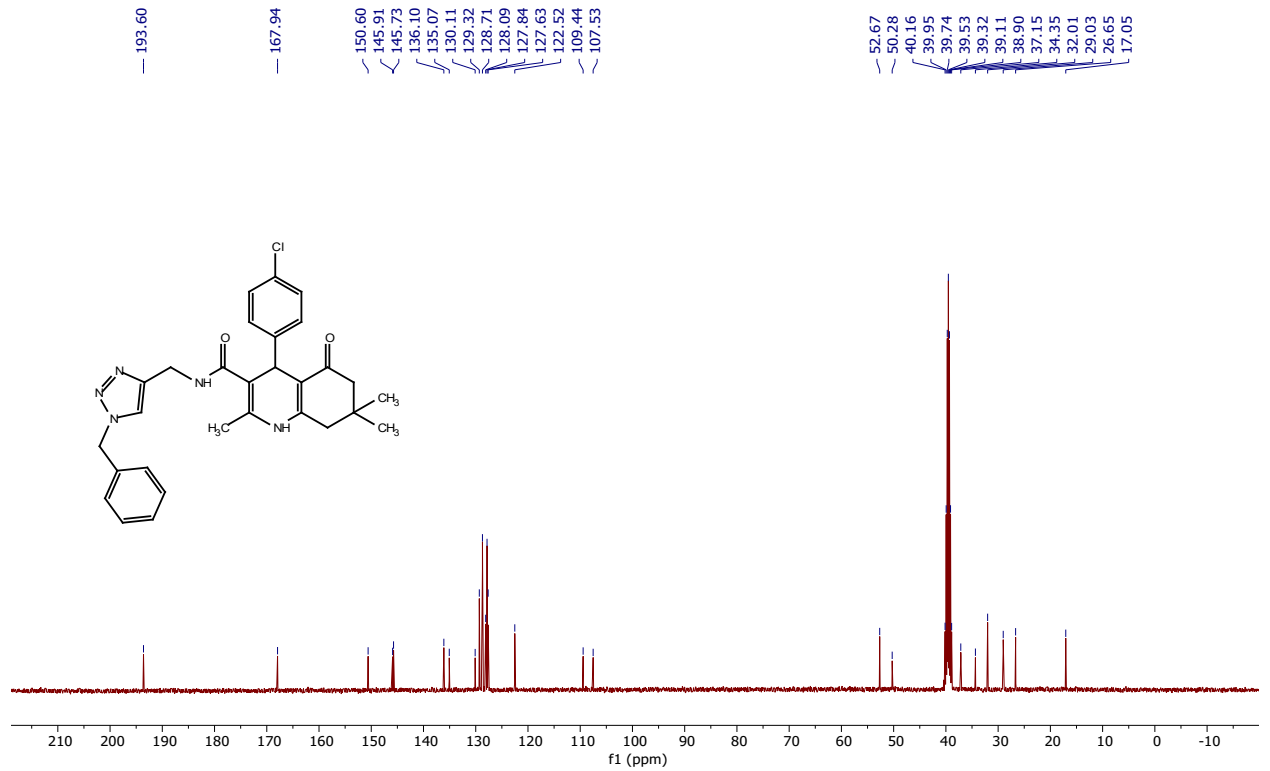
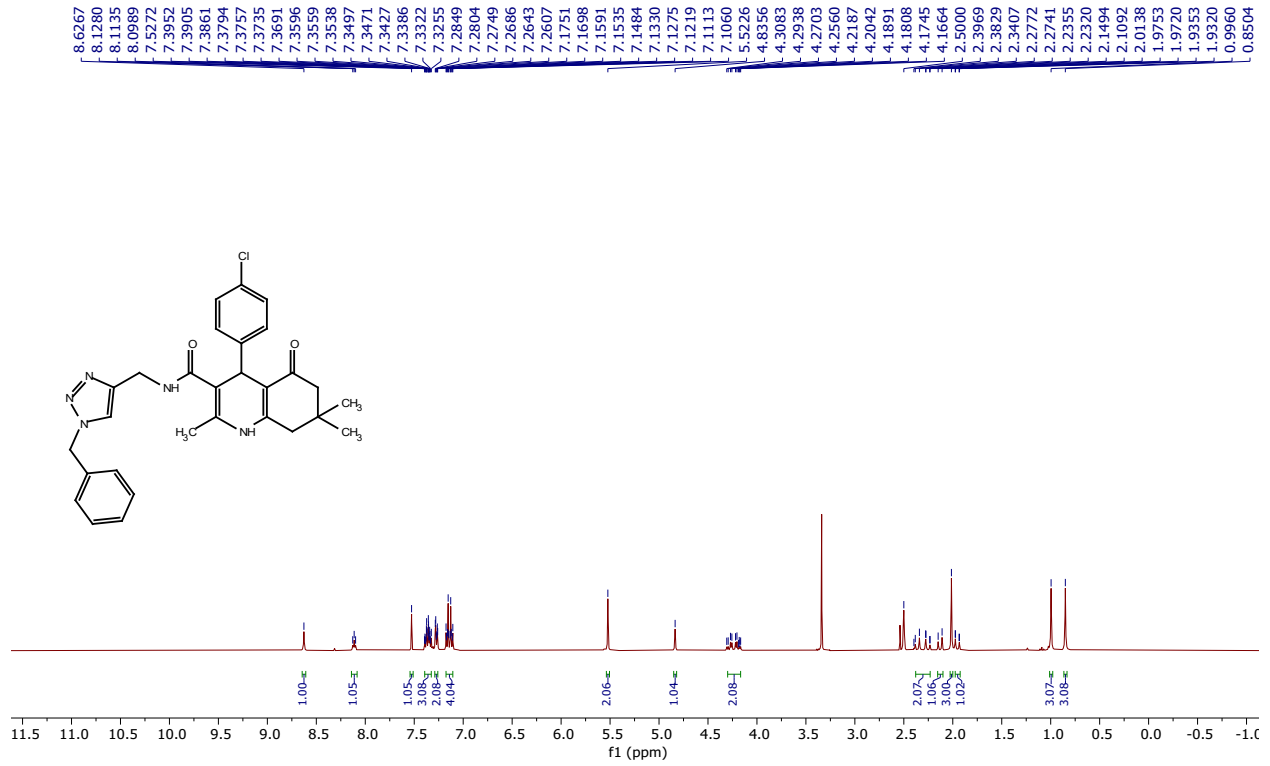
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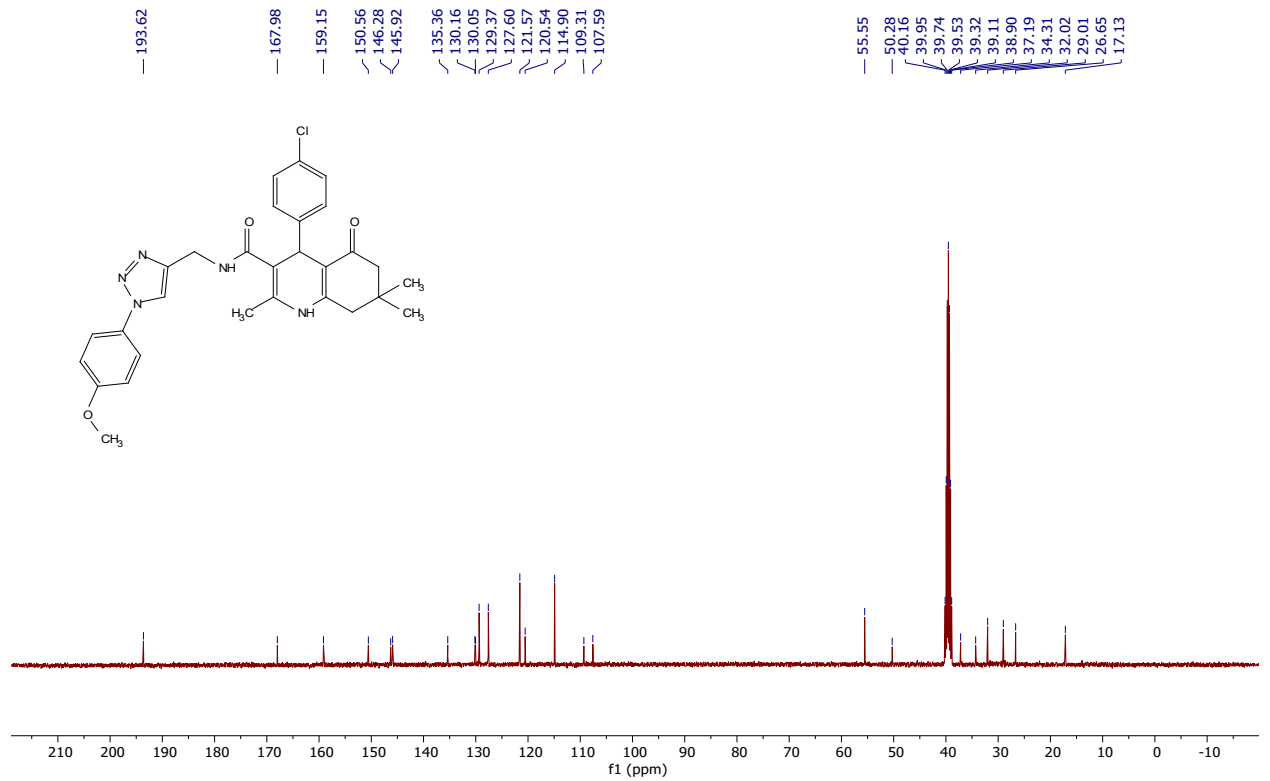
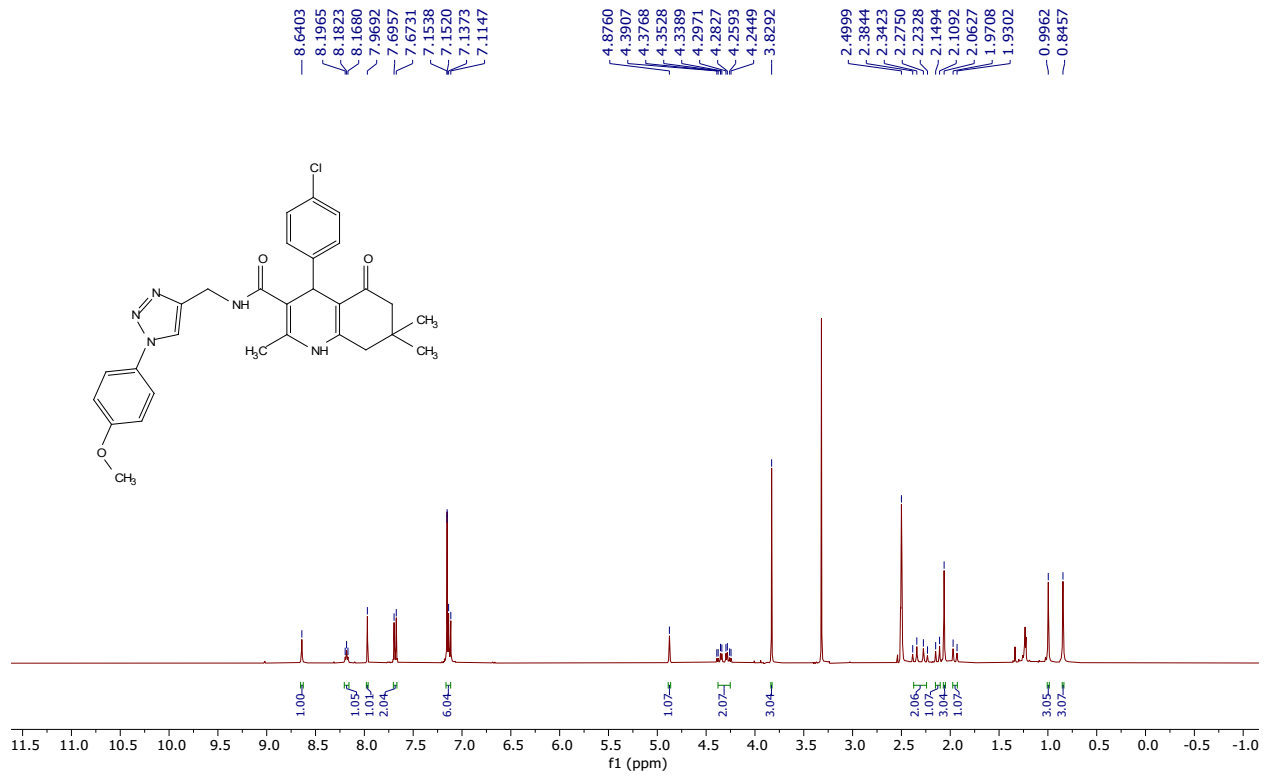
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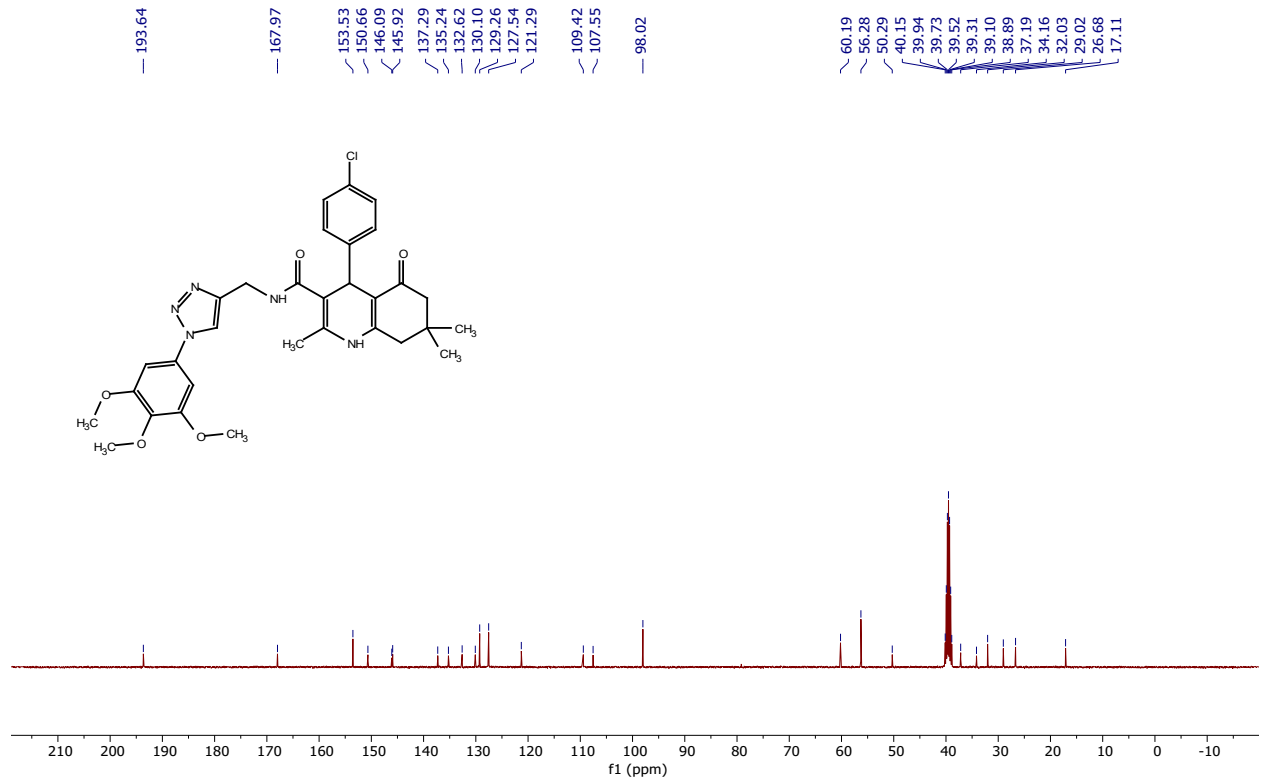
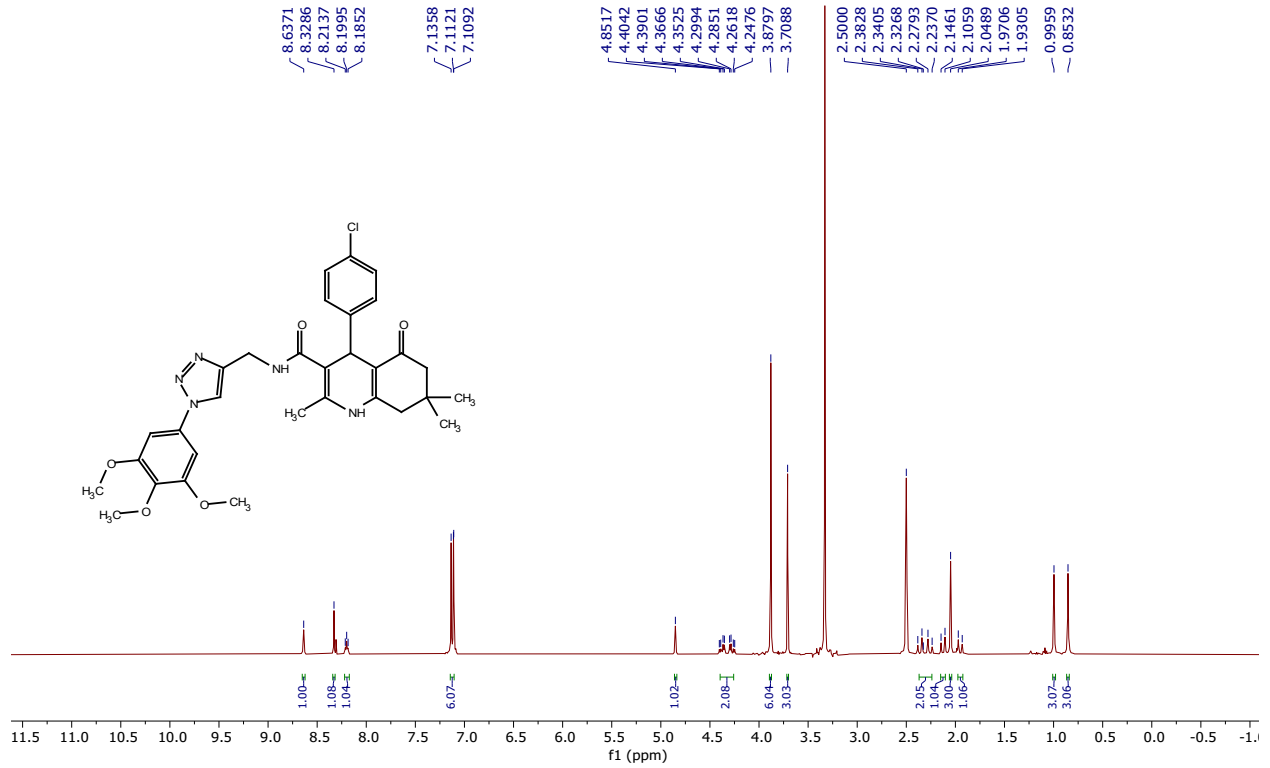
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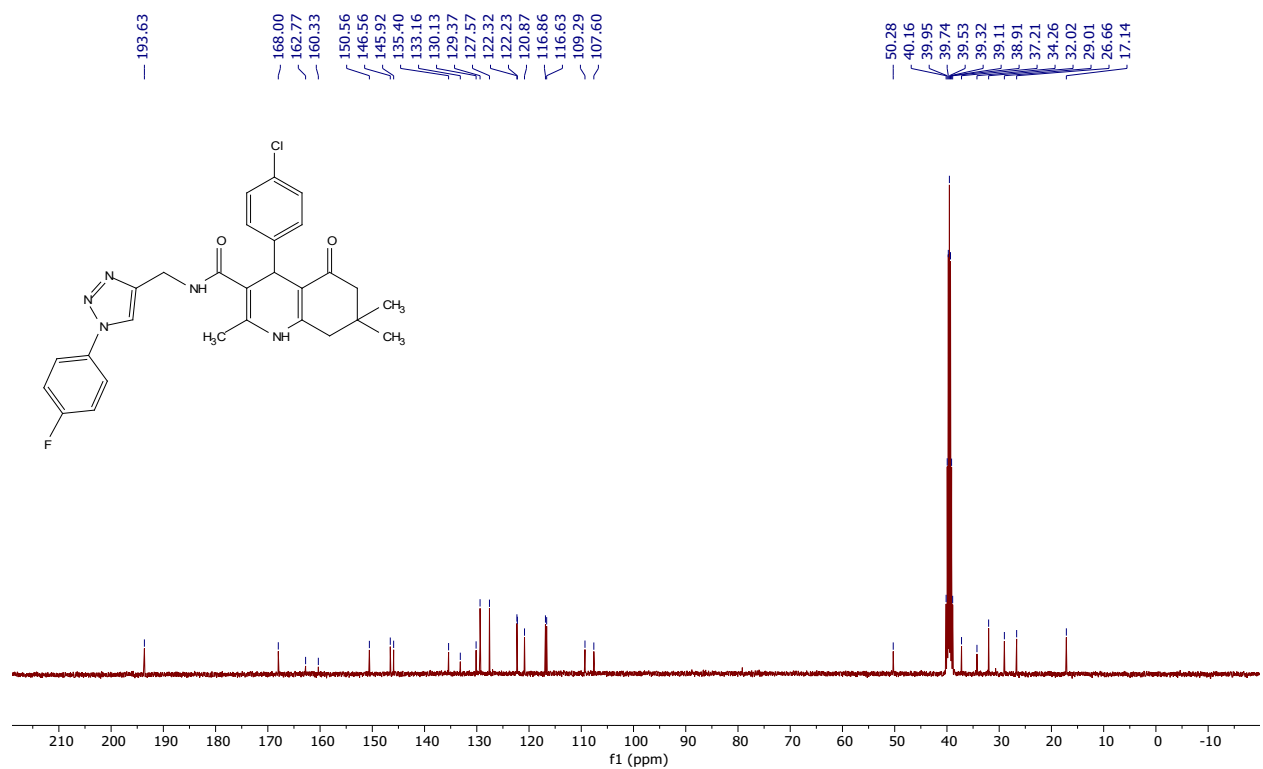
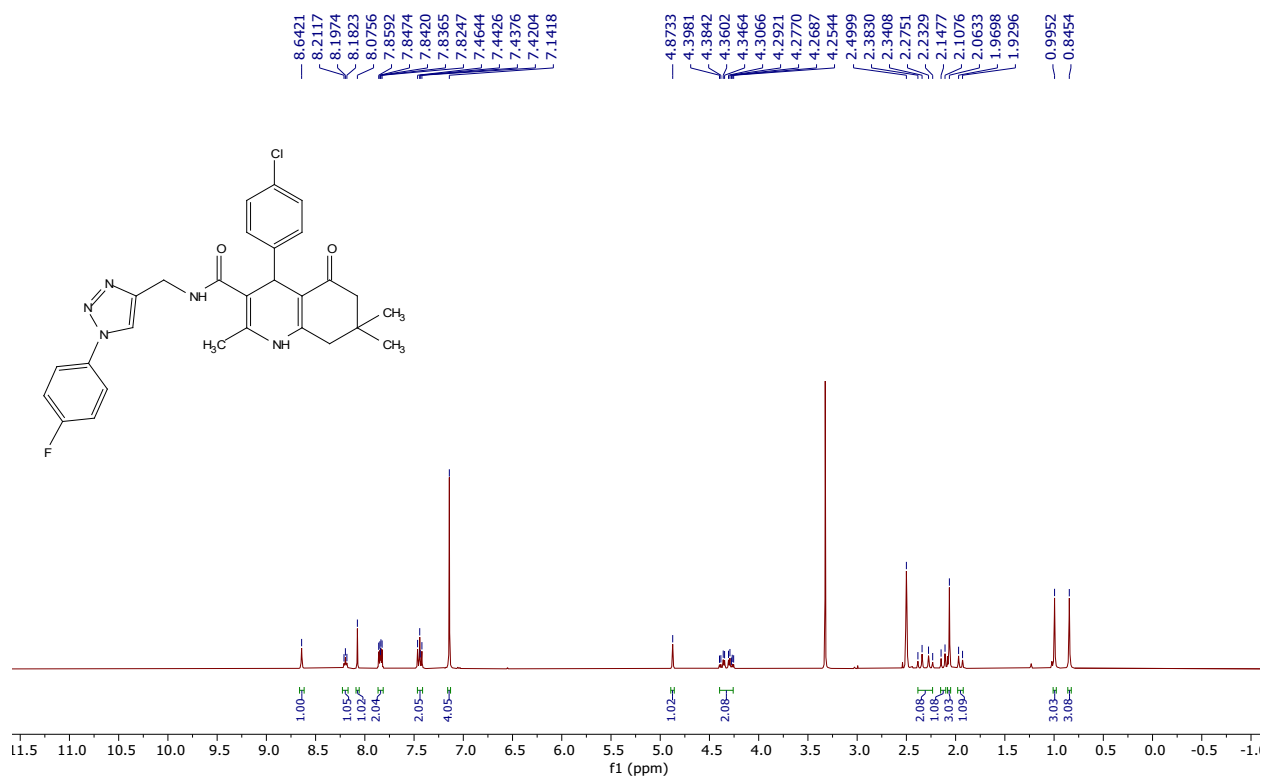
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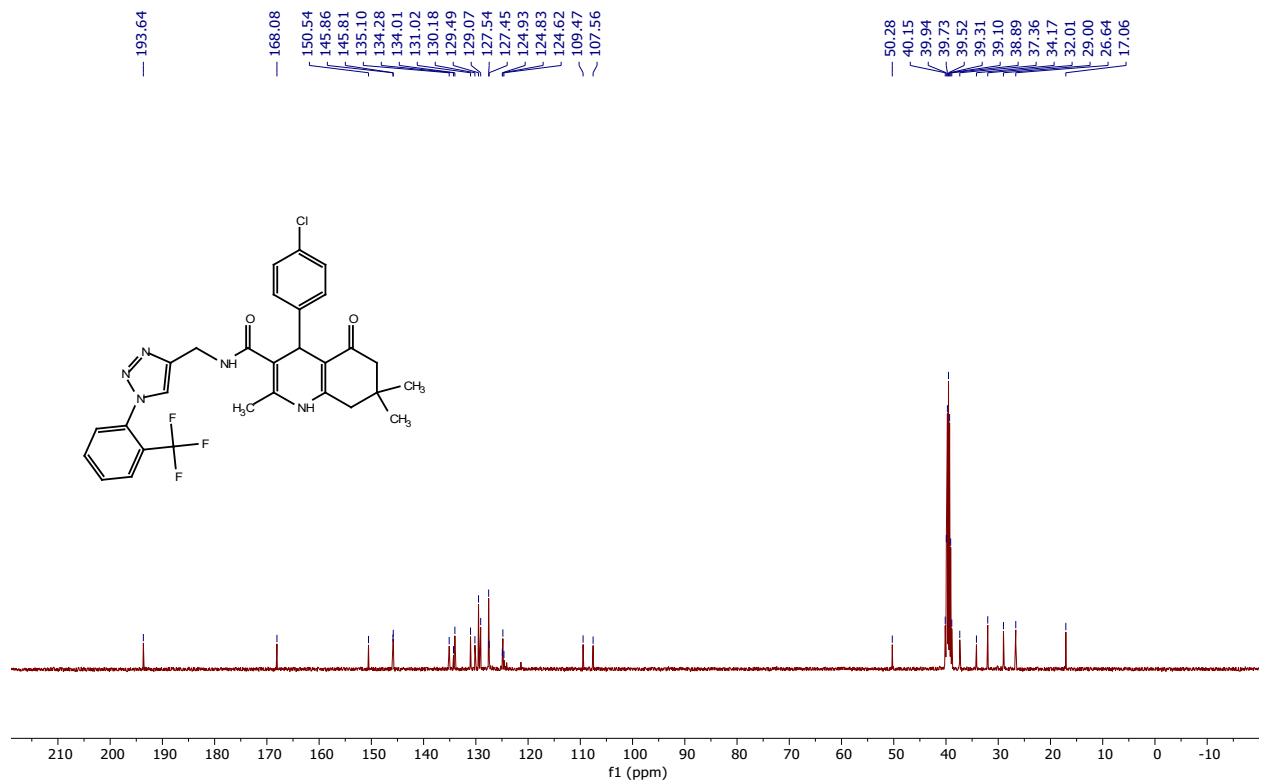
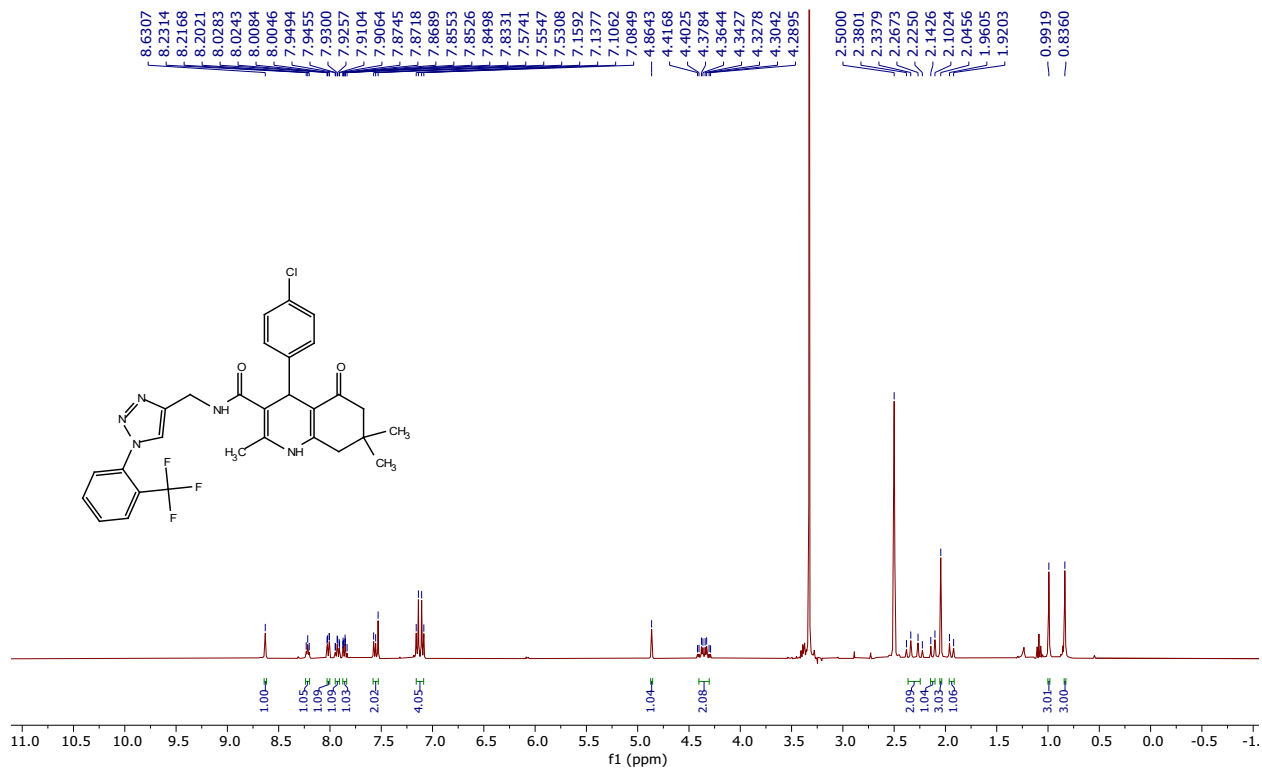
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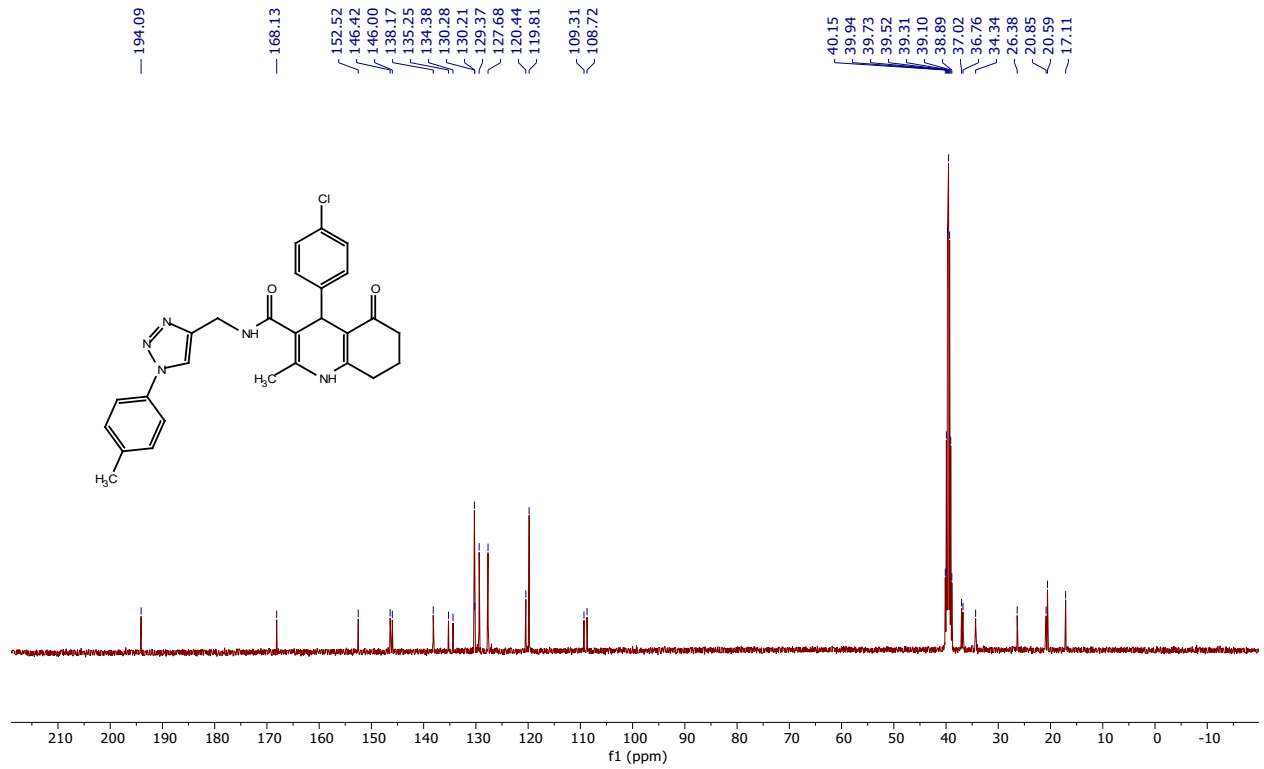
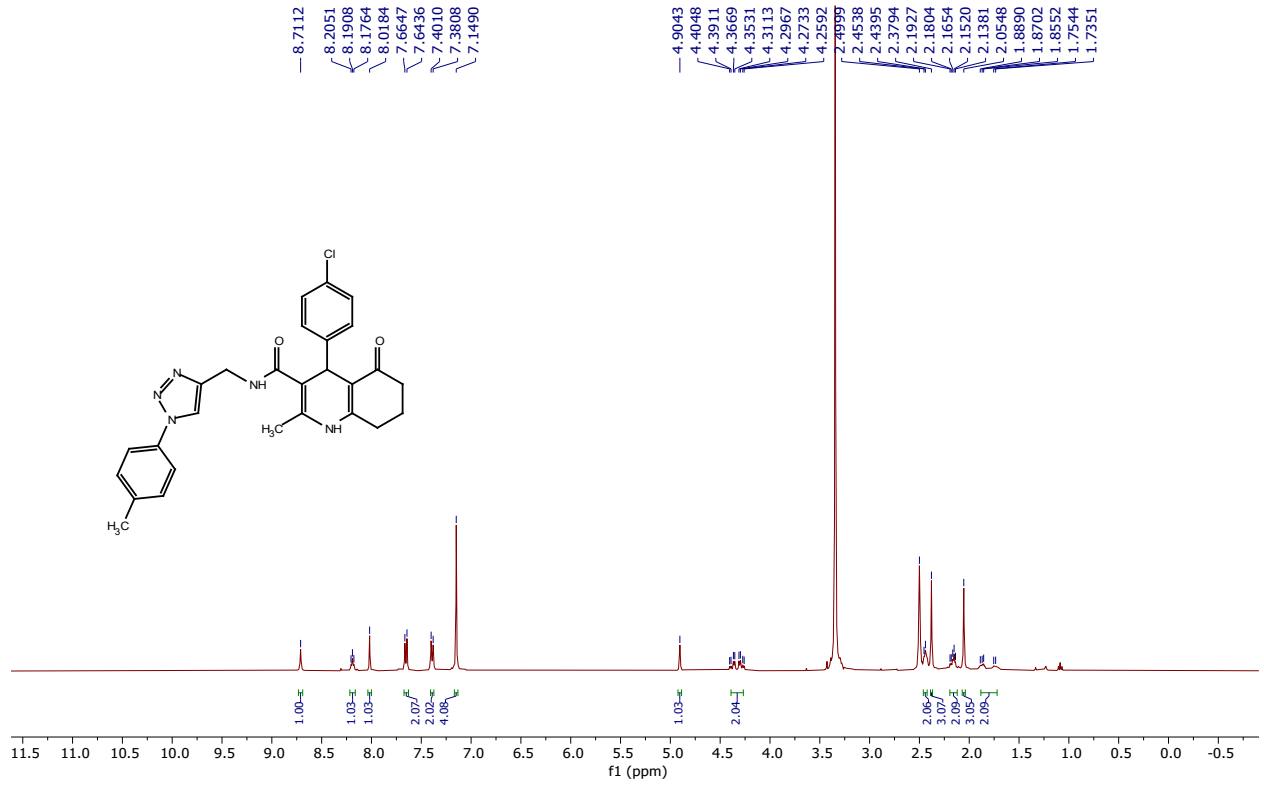
NMR spectrum of compound J16



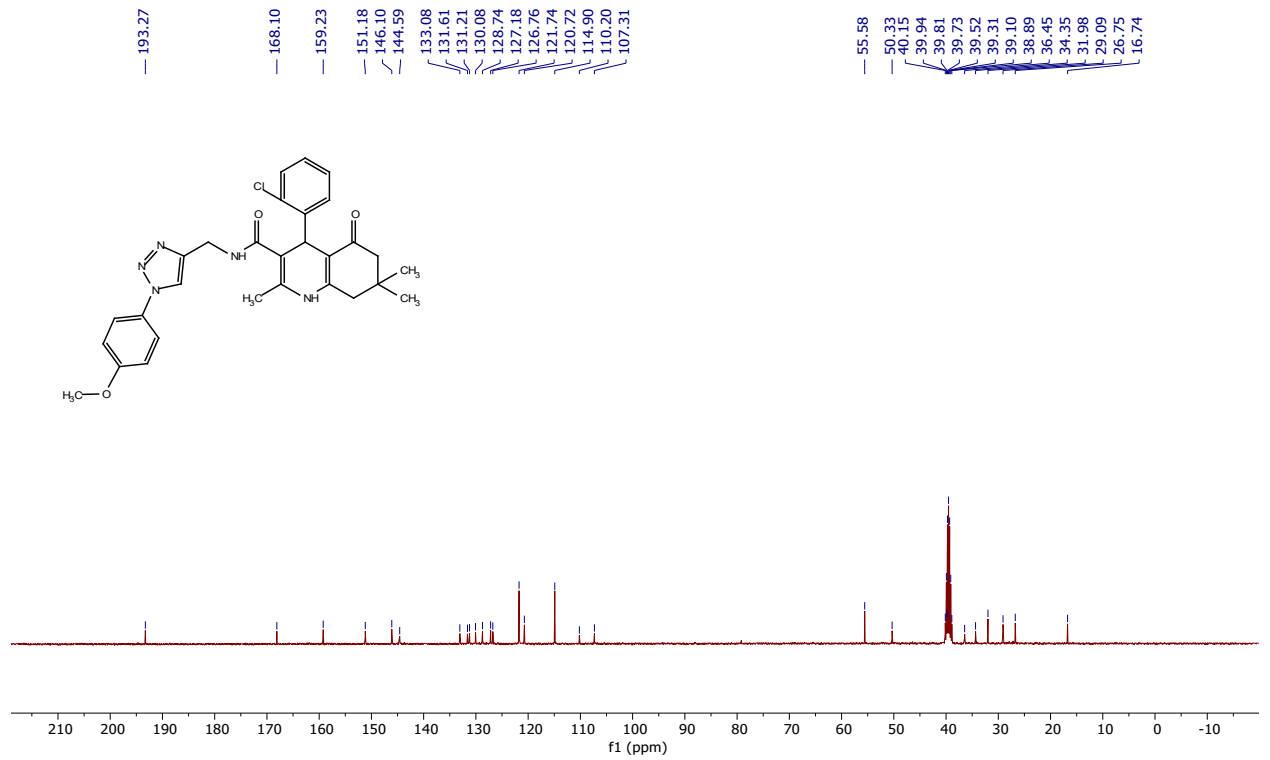
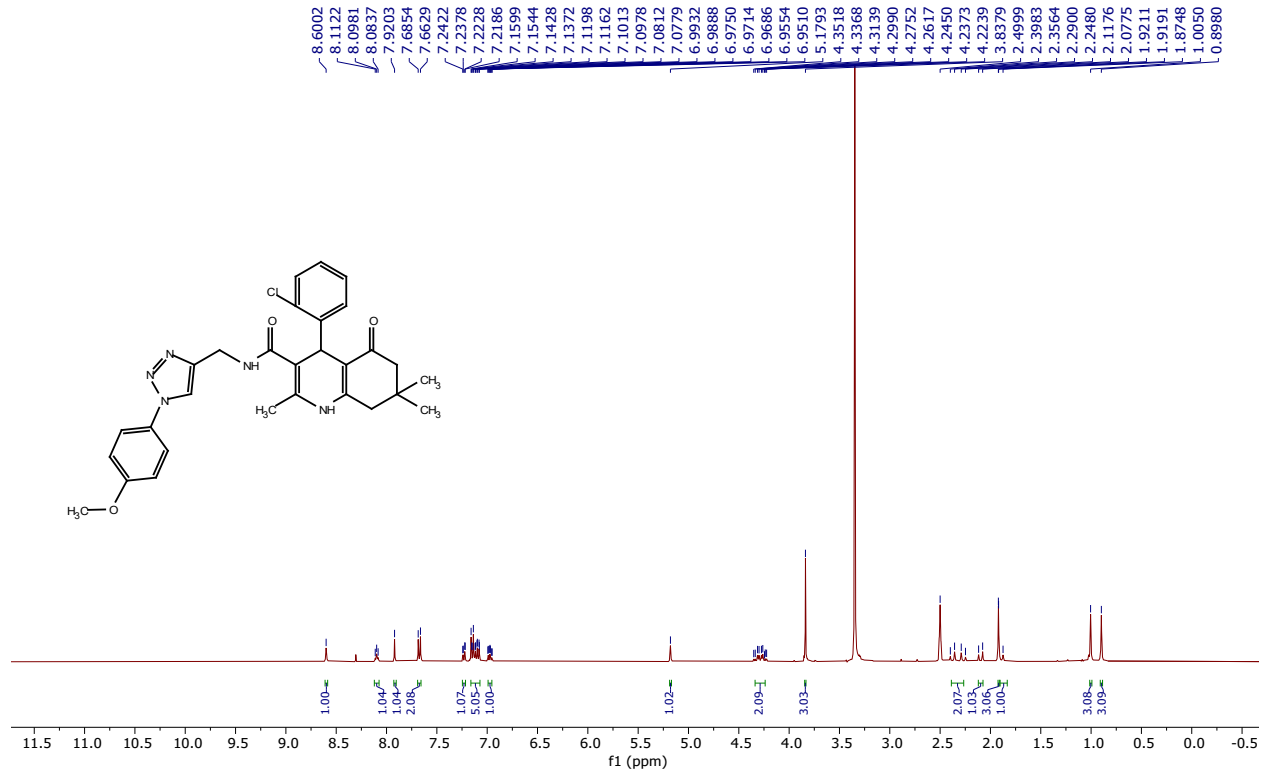
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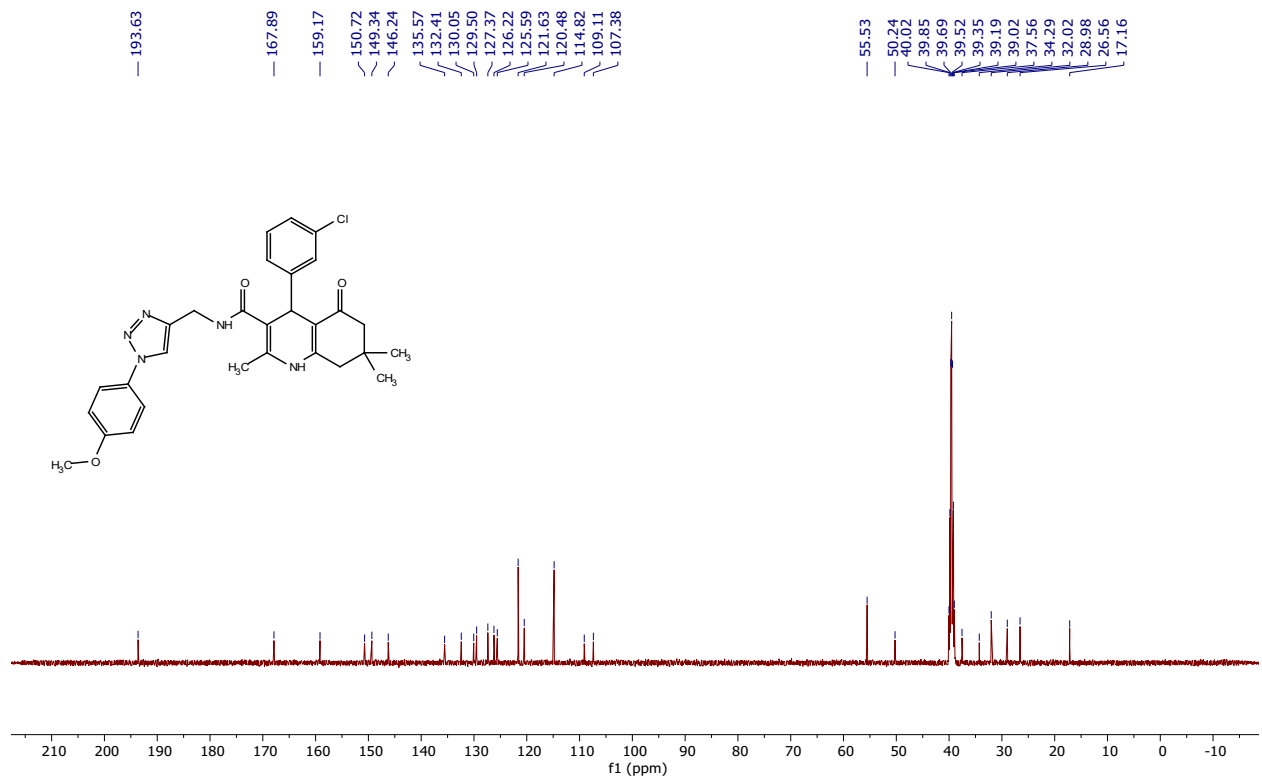
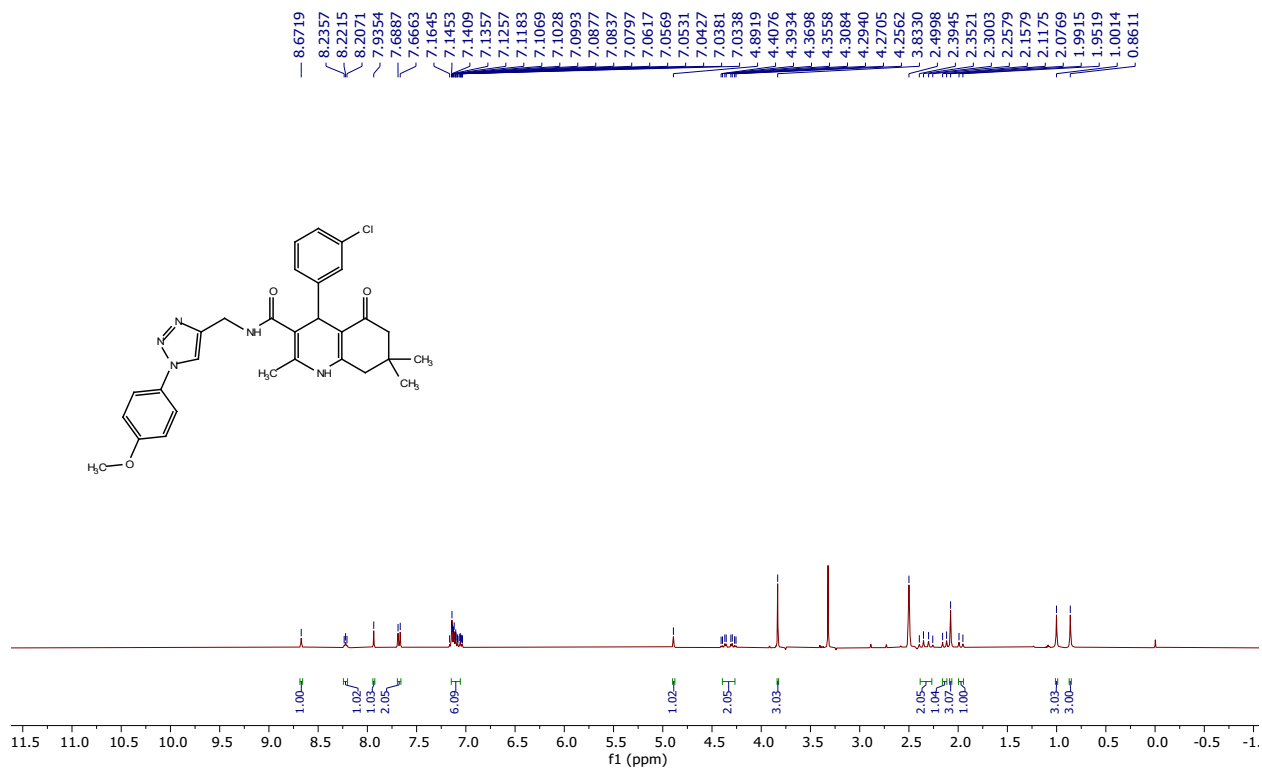
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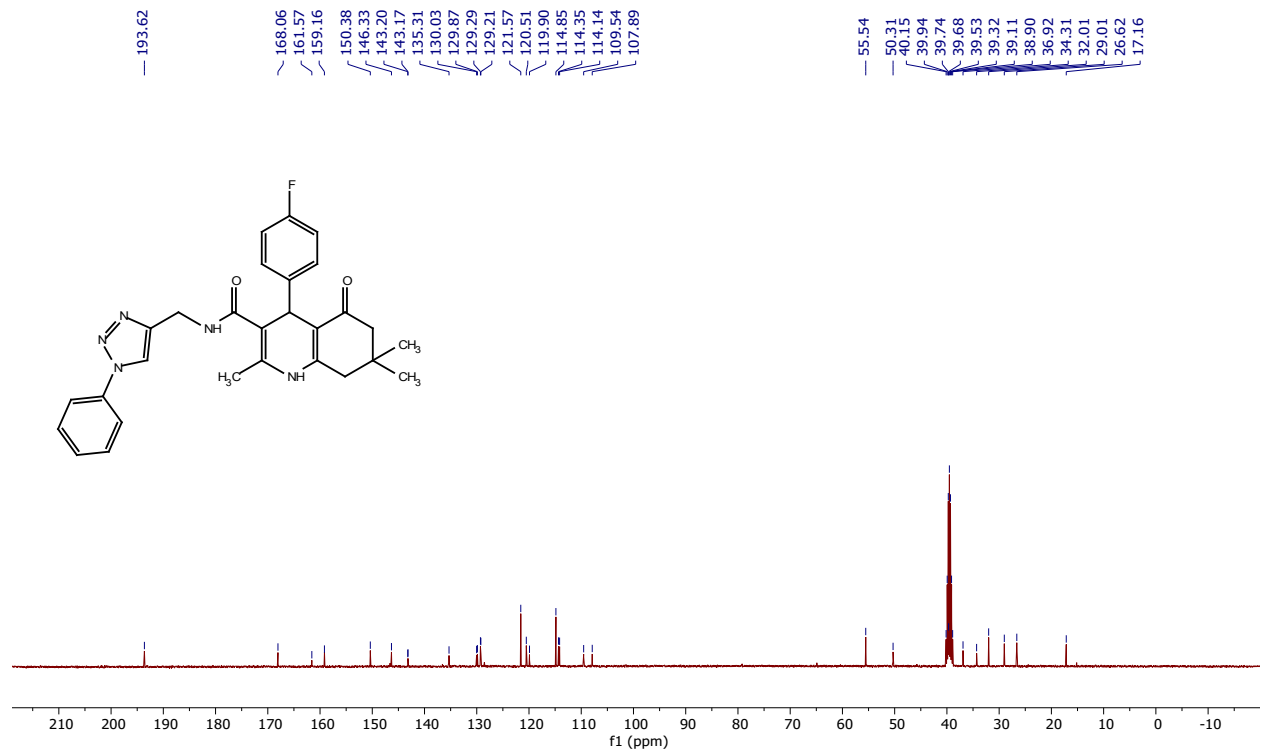
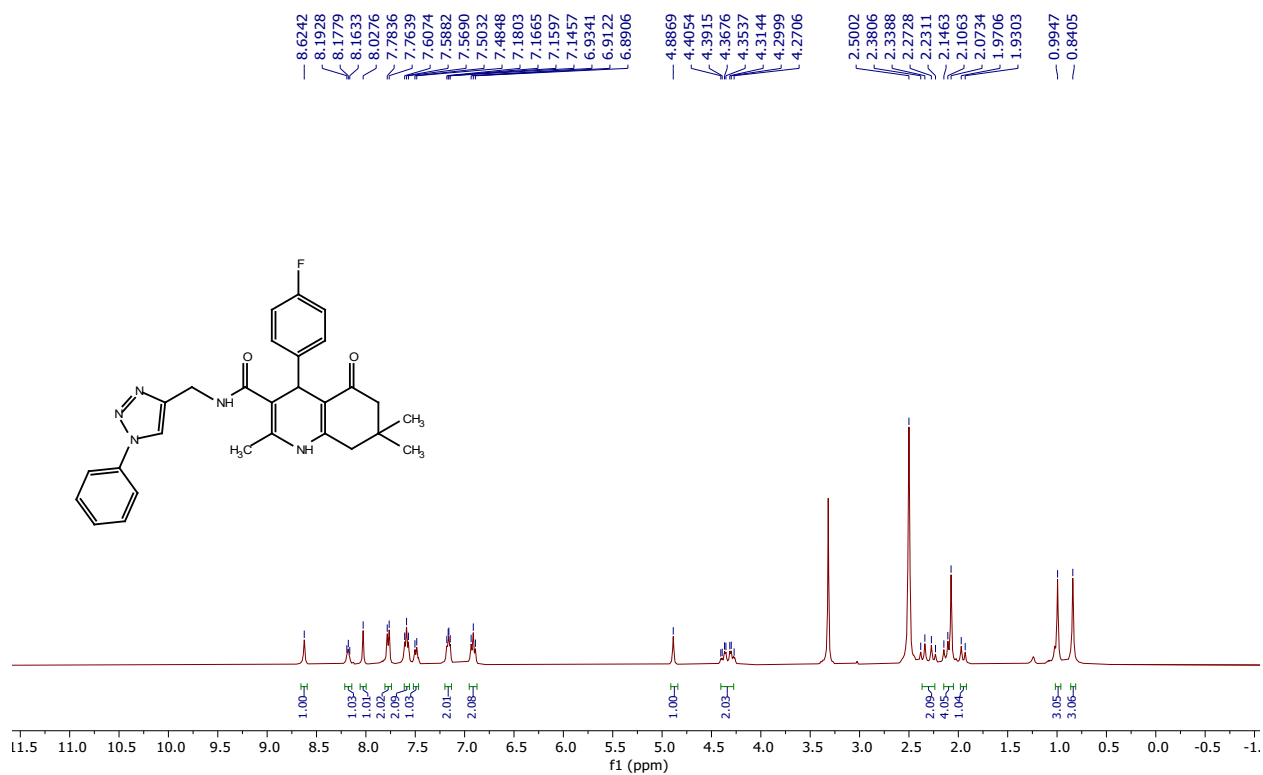
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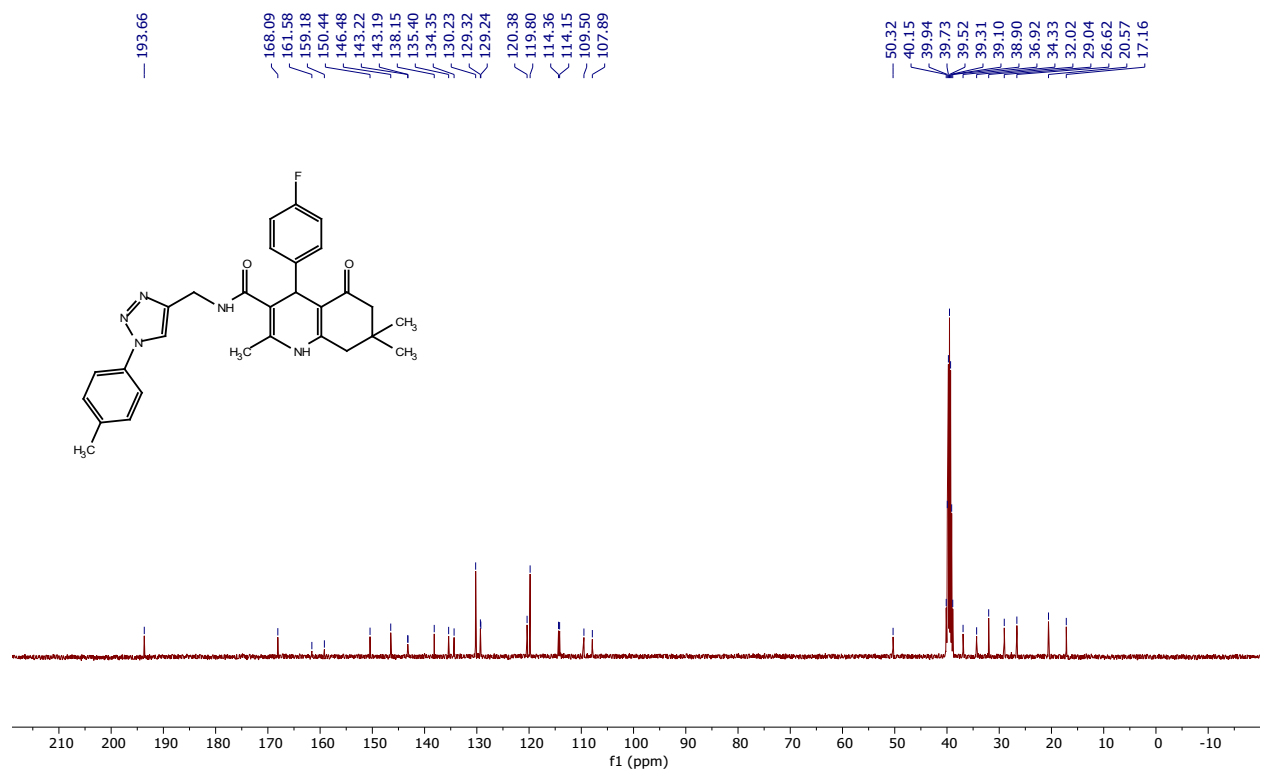
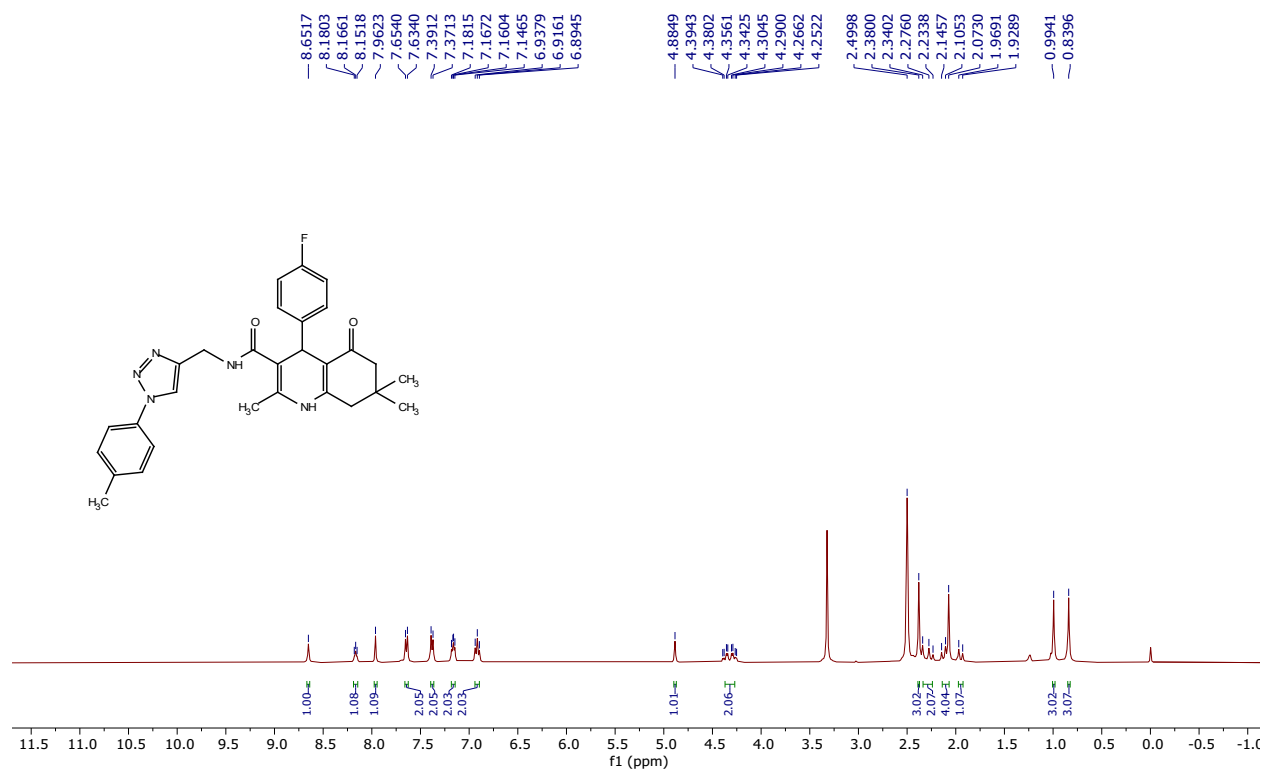
NMR spectrum of compound J20



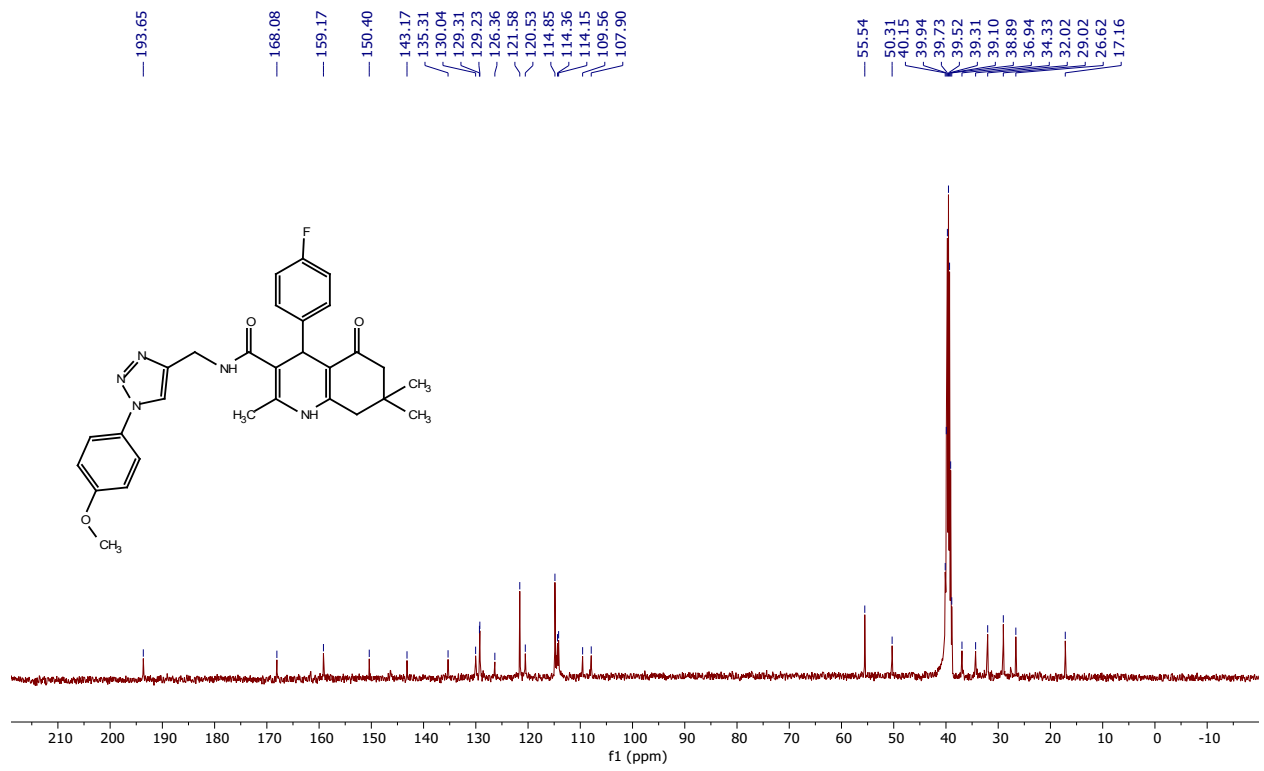
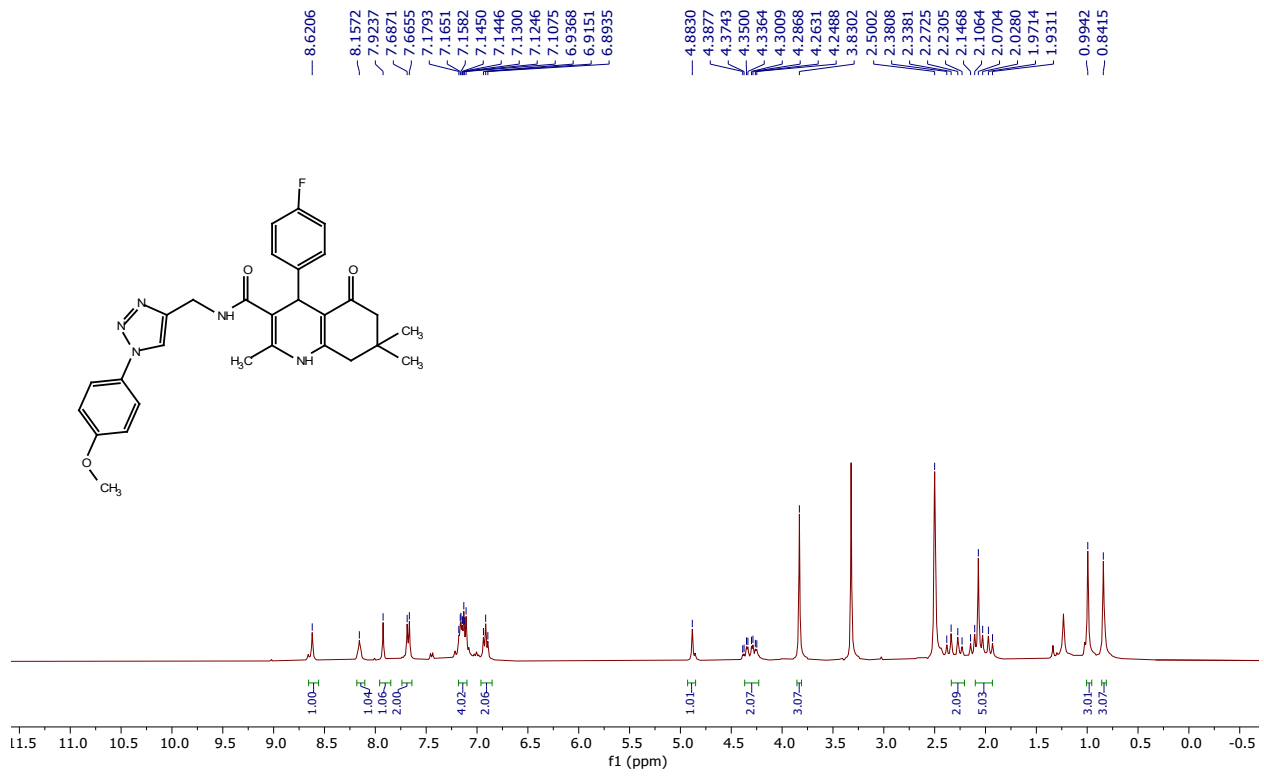
NMR spectrum of compound J21



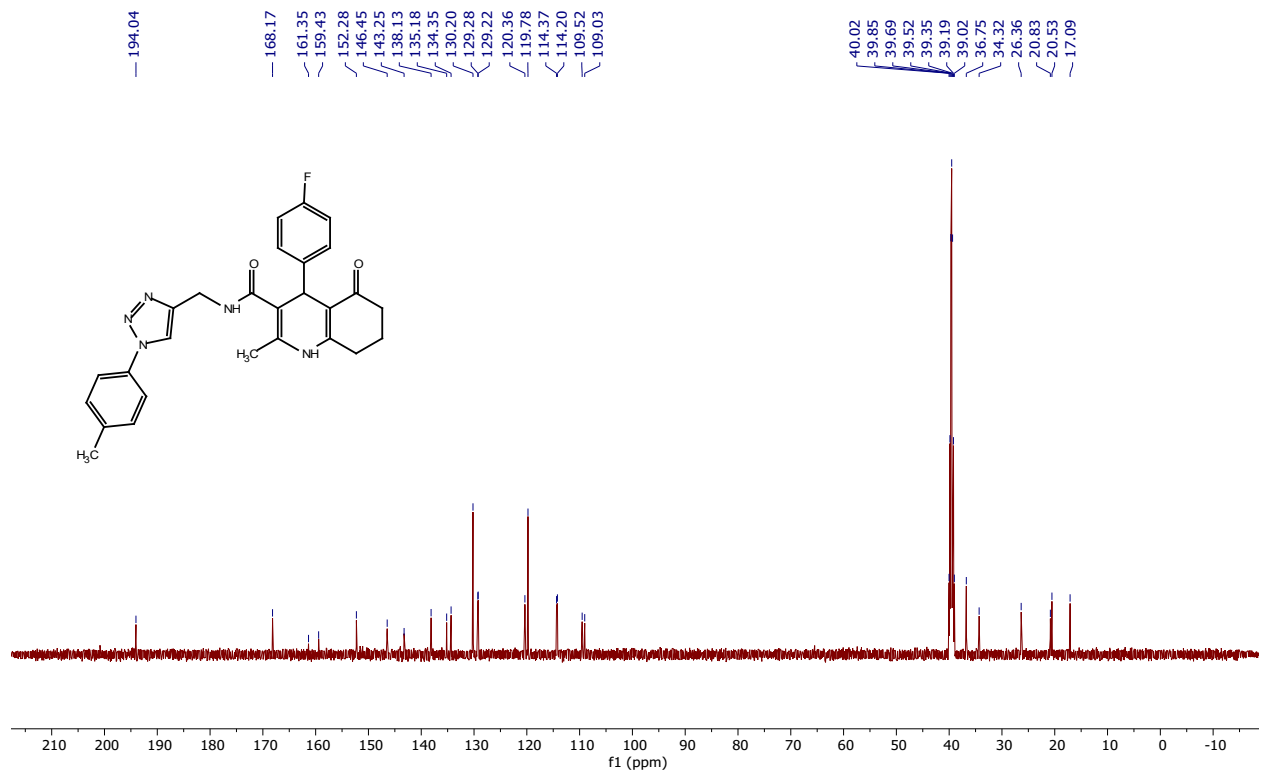
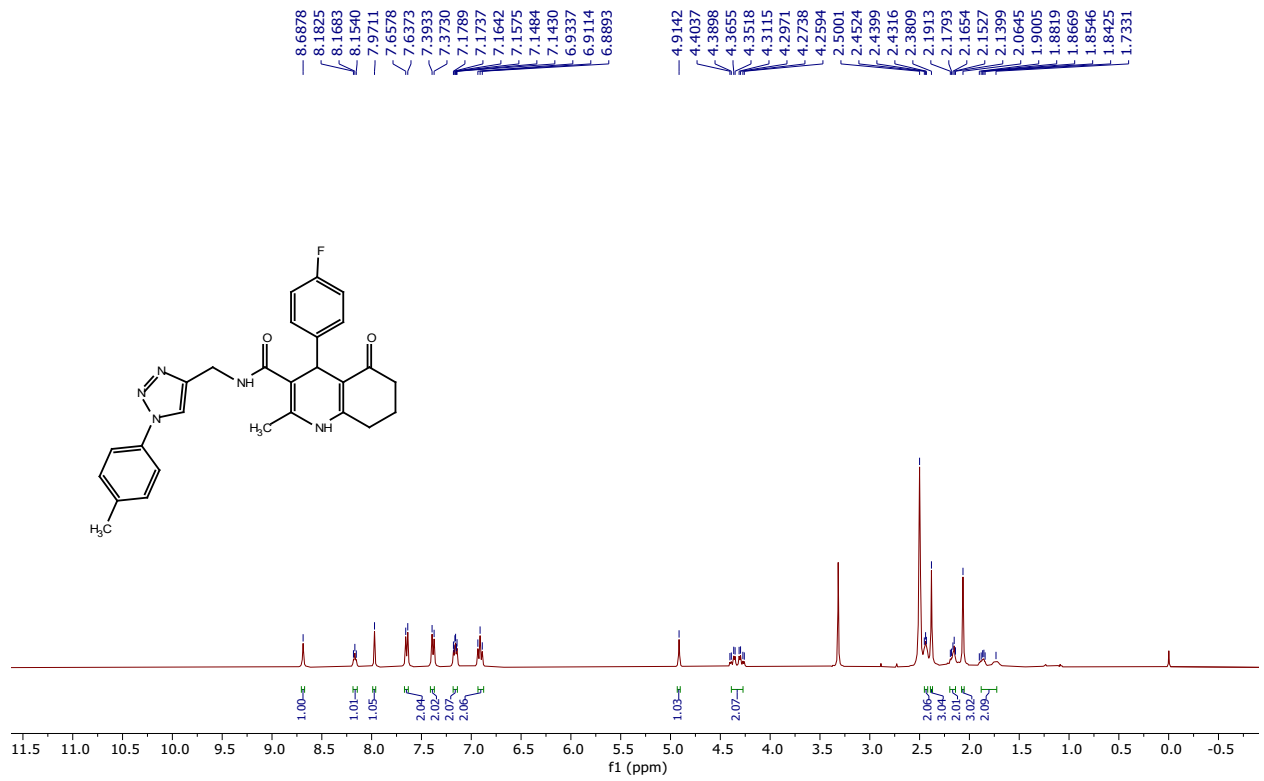
NMR spectrum of compound J22



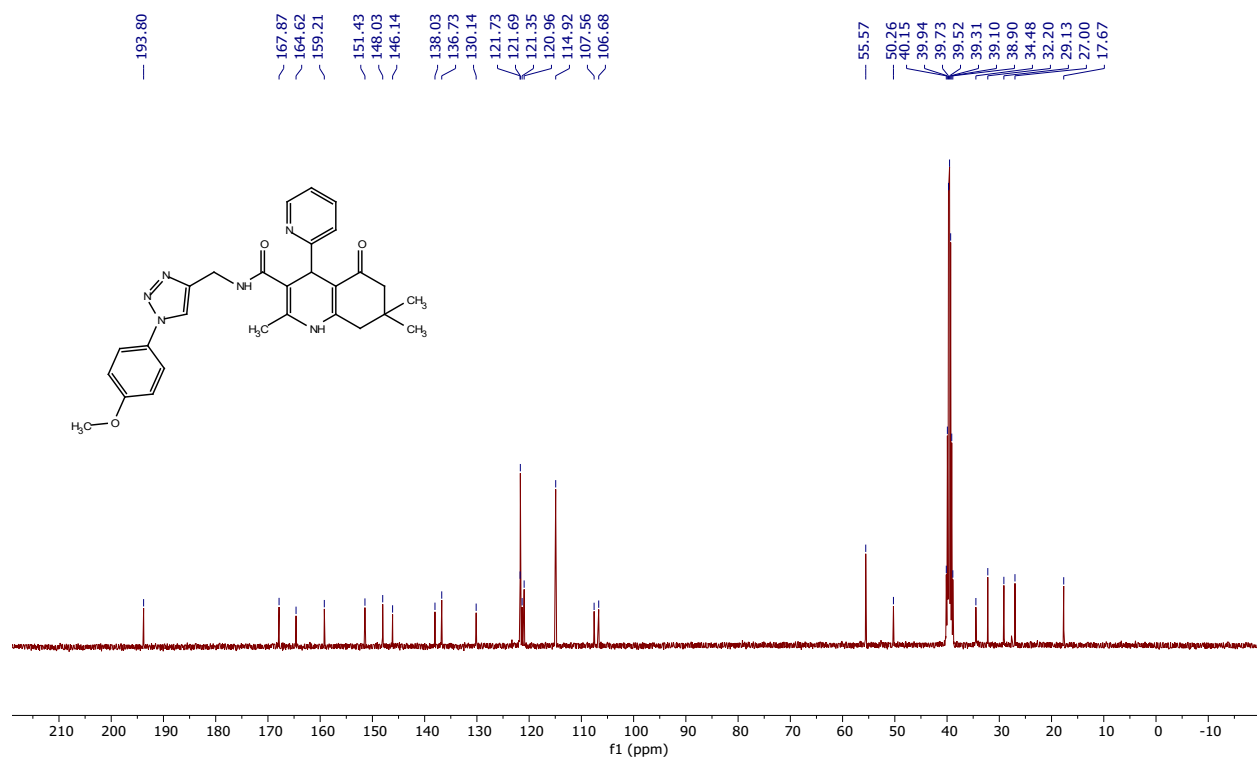
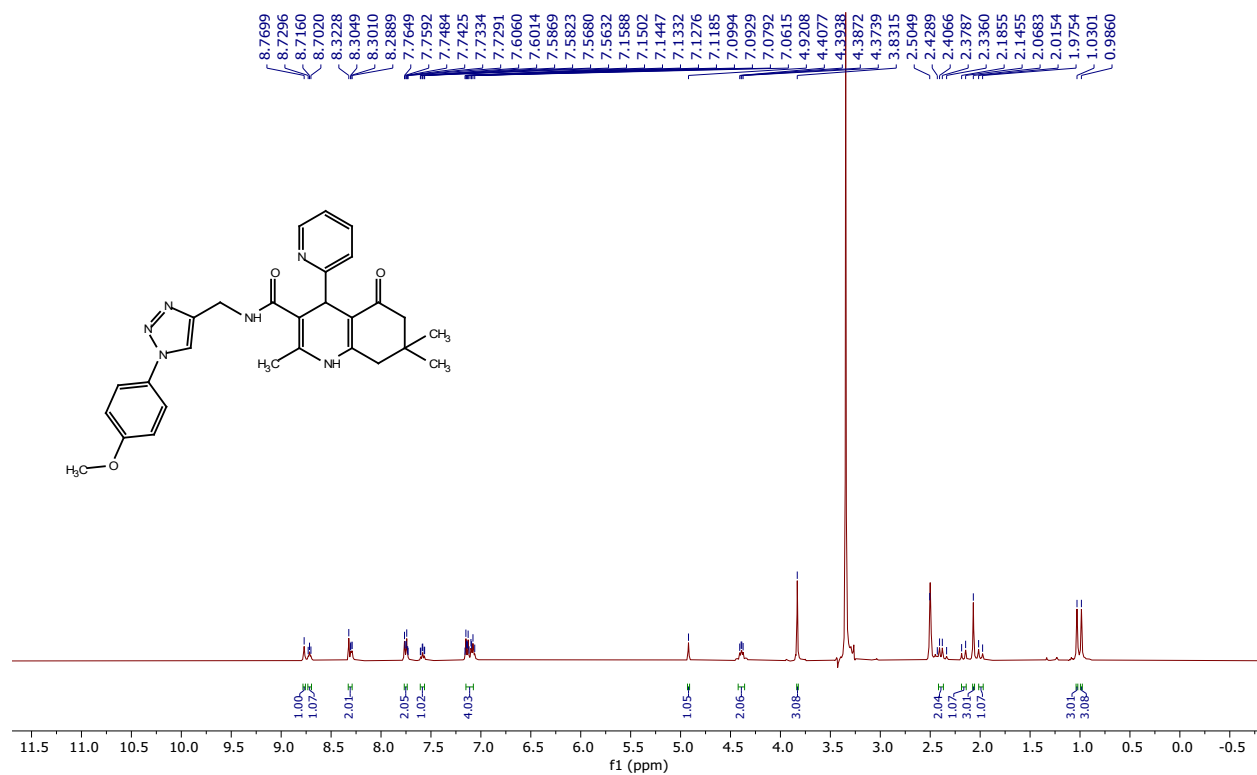
NMR spectrum of compound J23



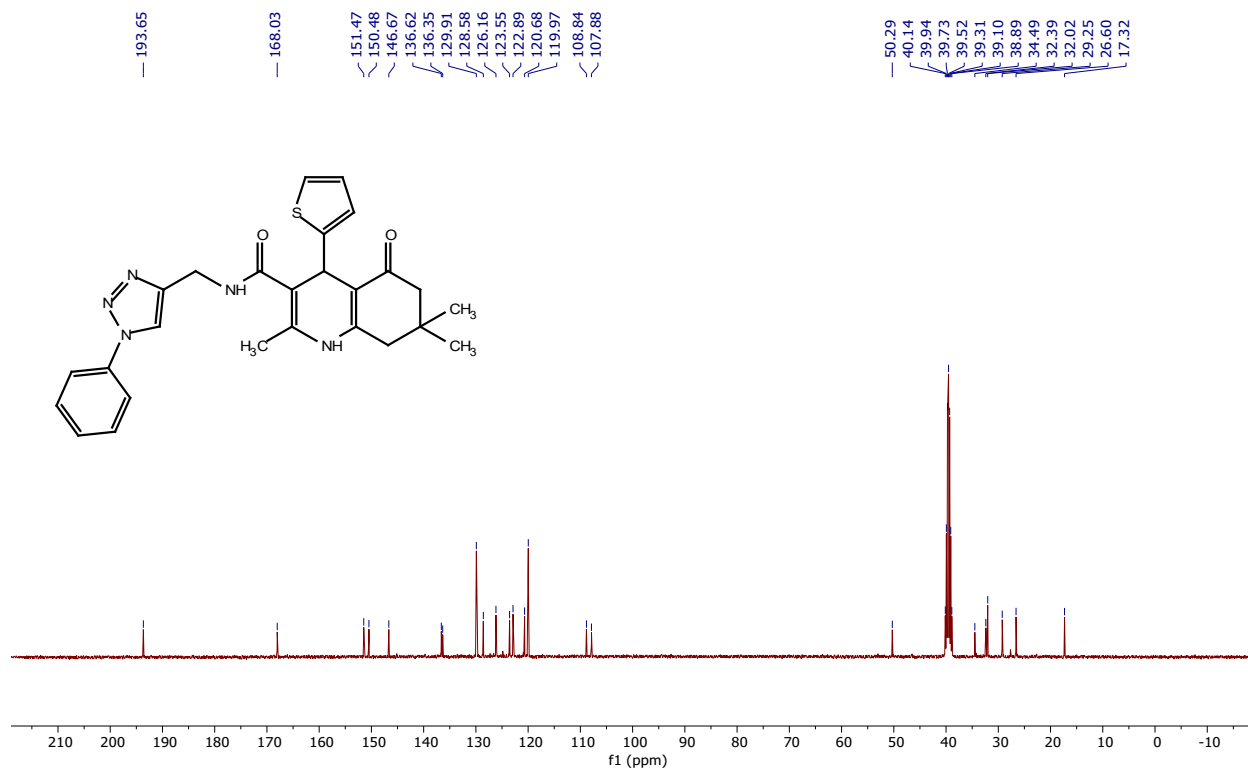
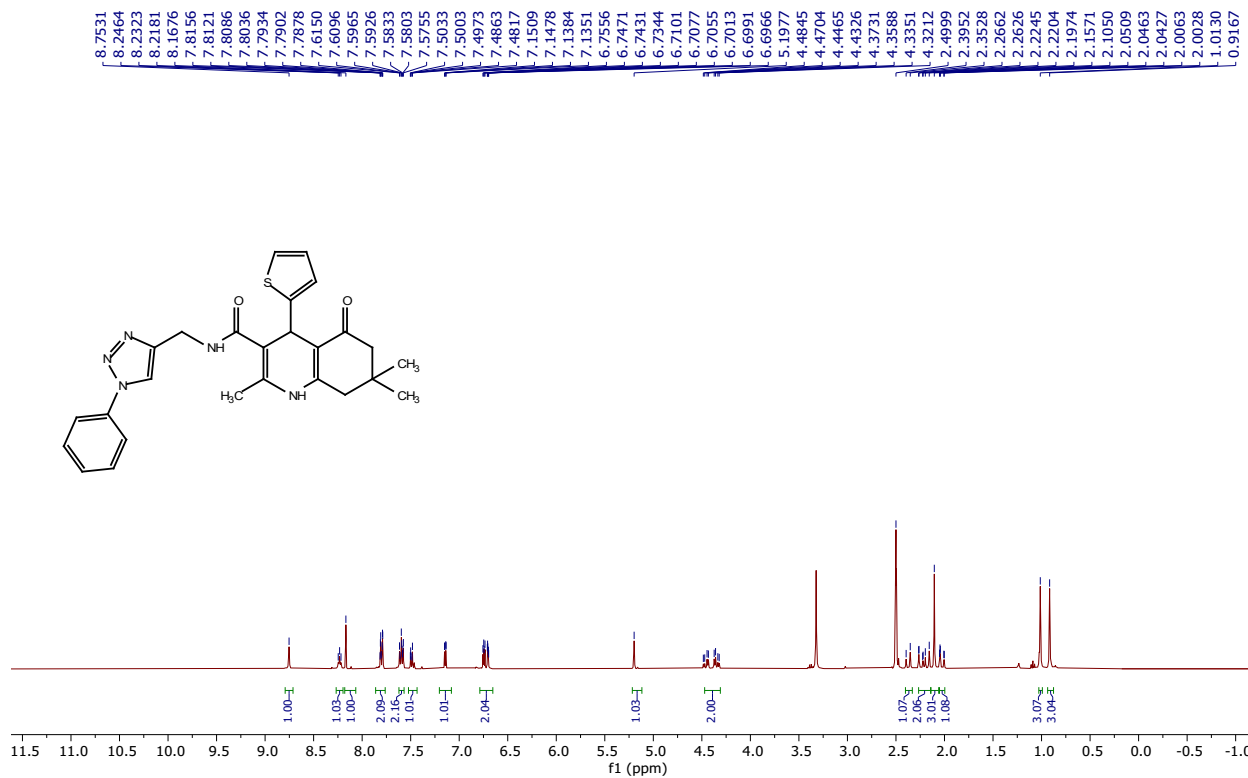
NMR spectrum of compound J24



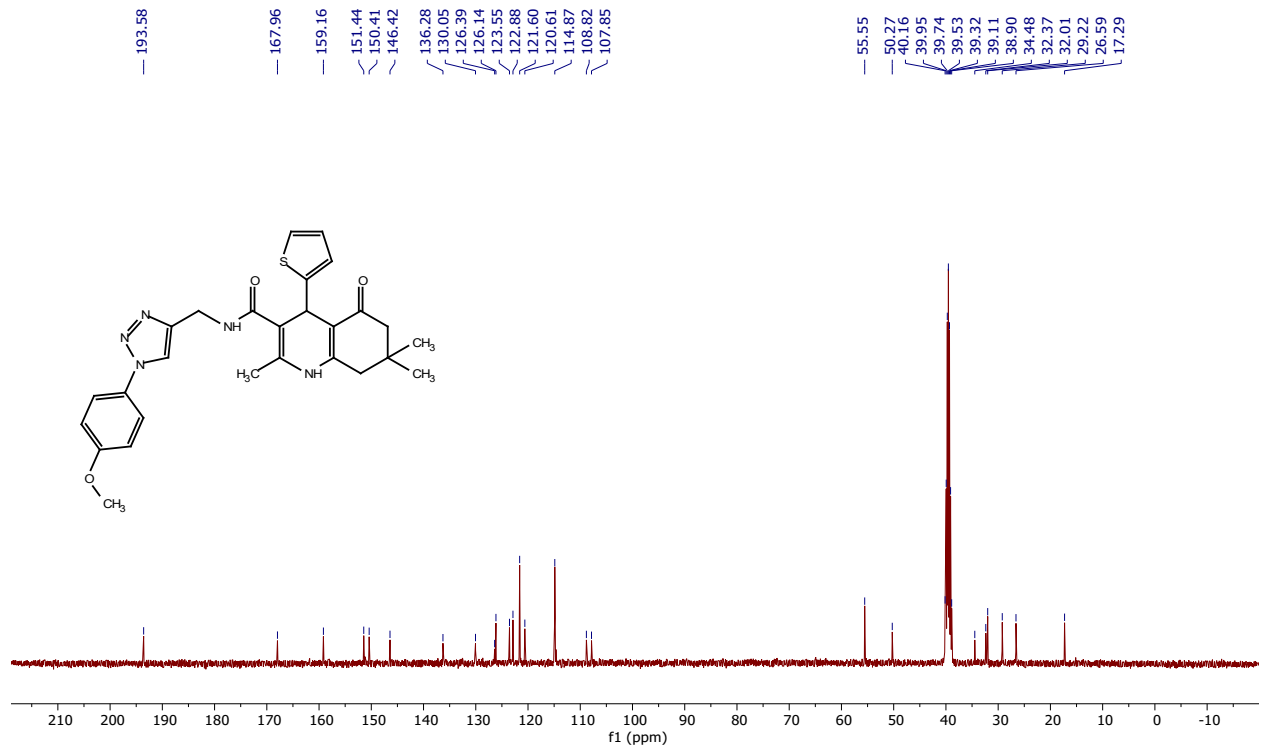
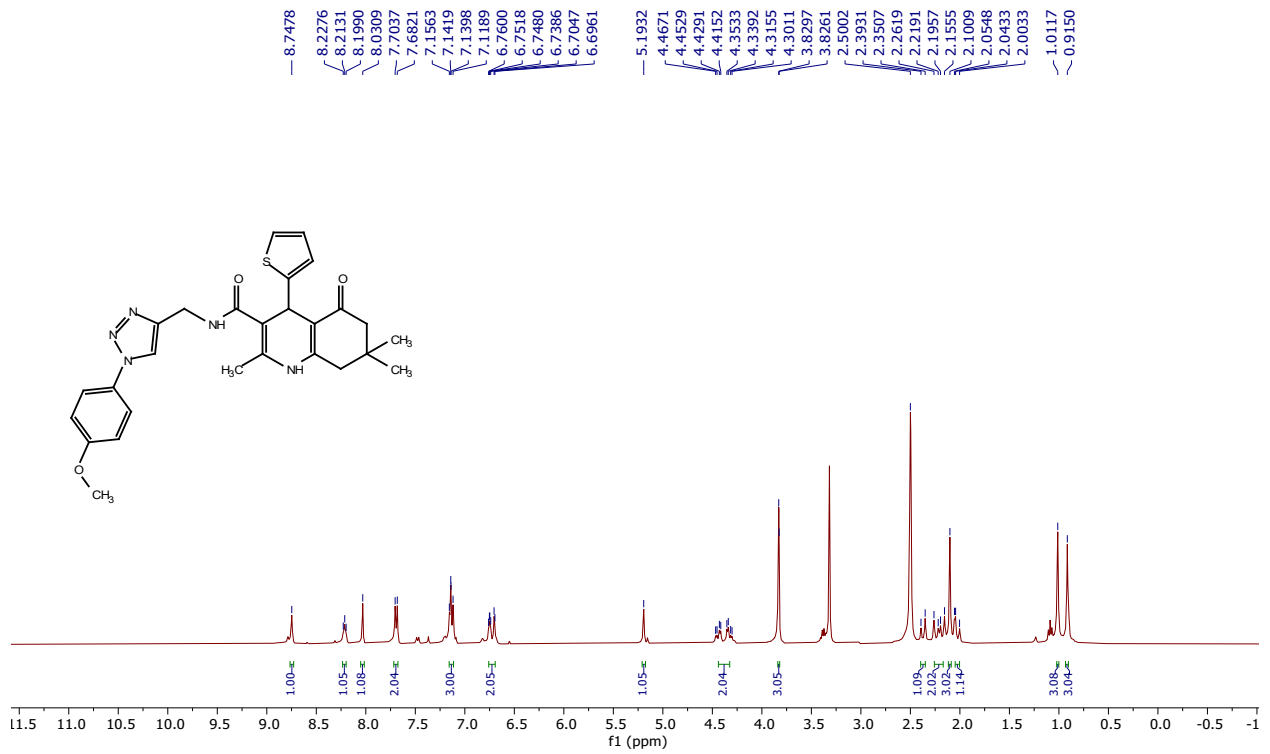
NMR spectrum of compound J25



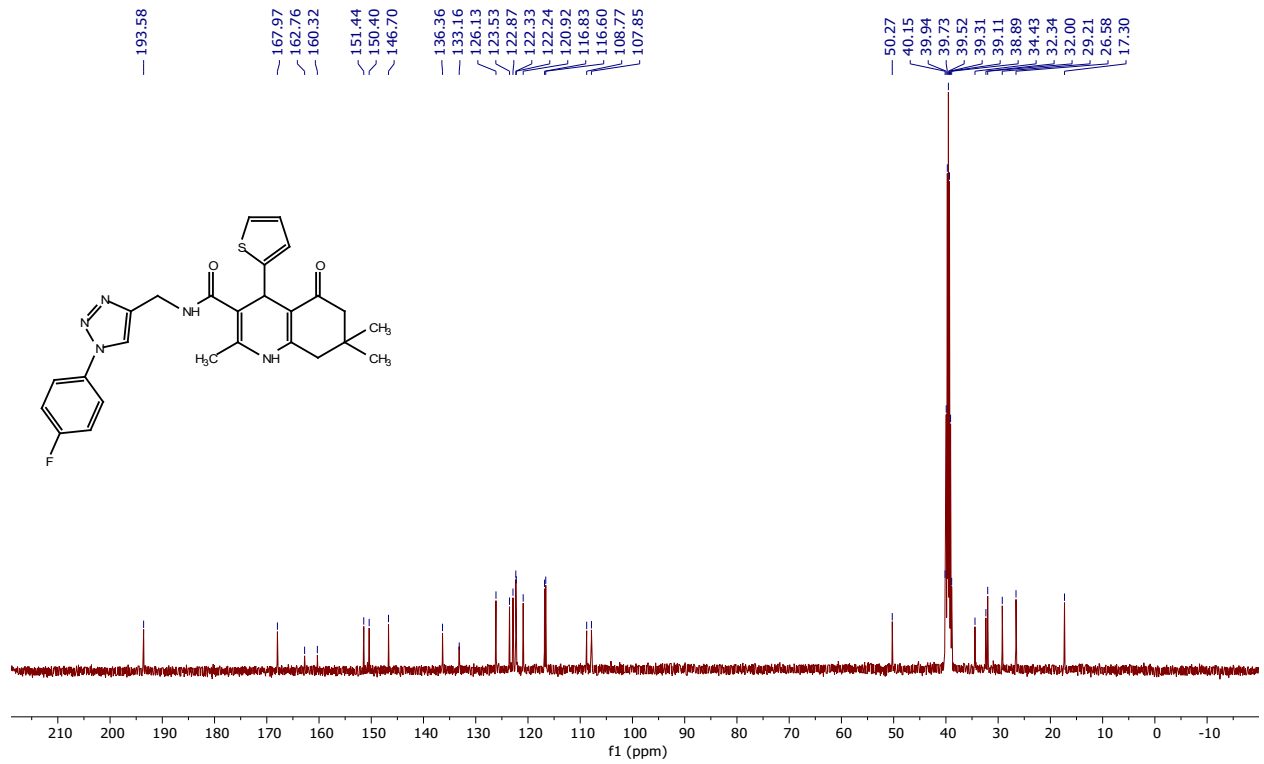
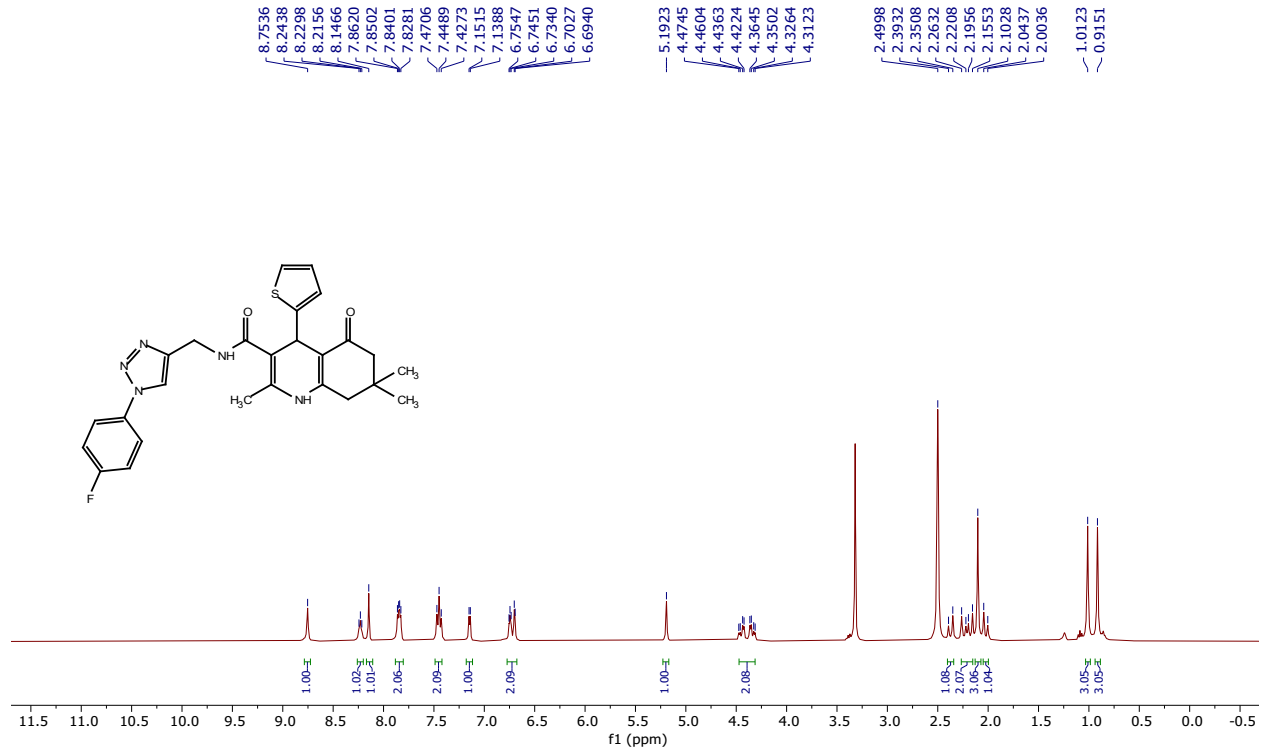
NMR spectrum of compound K1



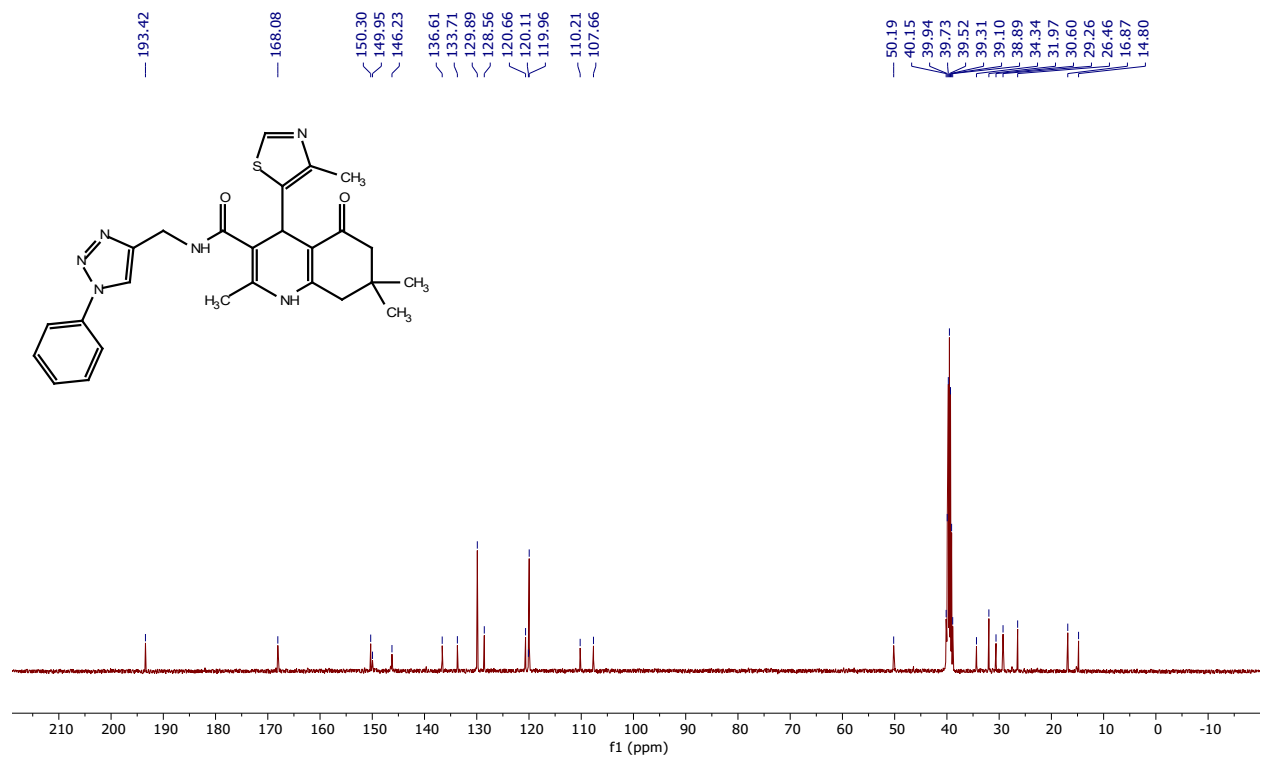
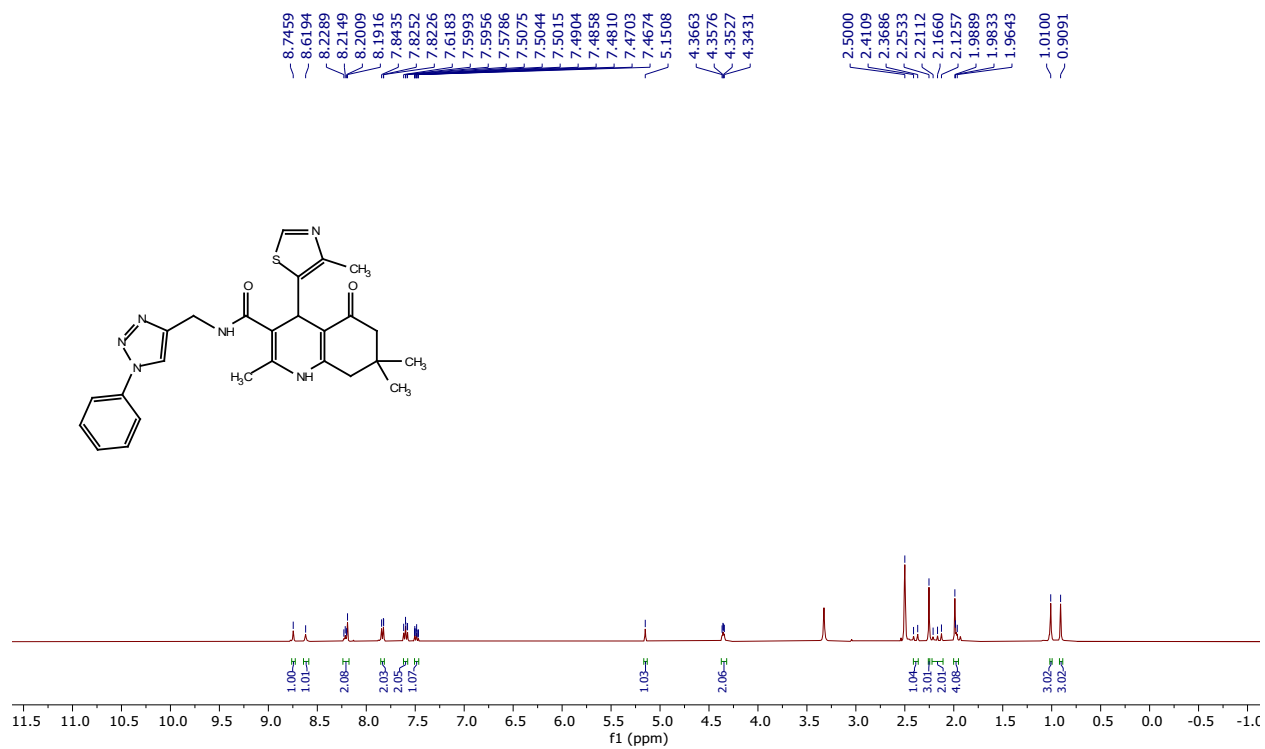
NMR spectrum of compound K2



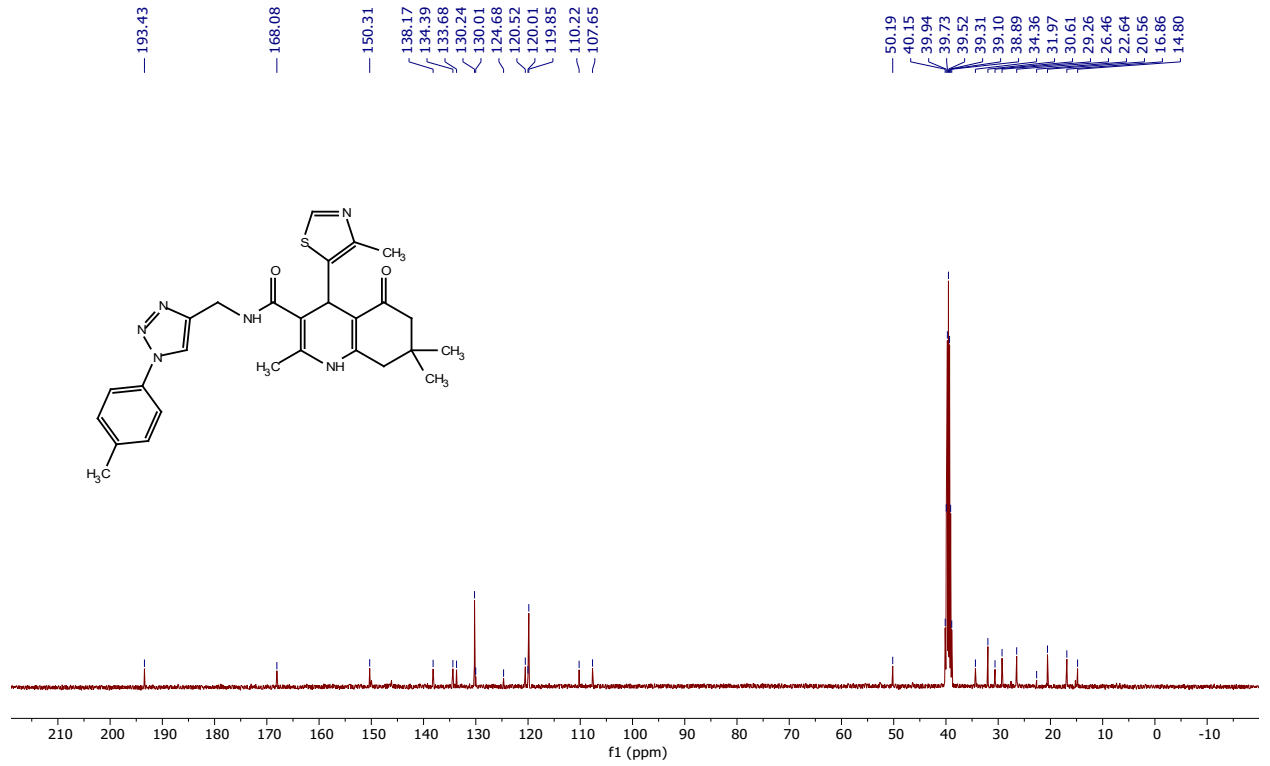
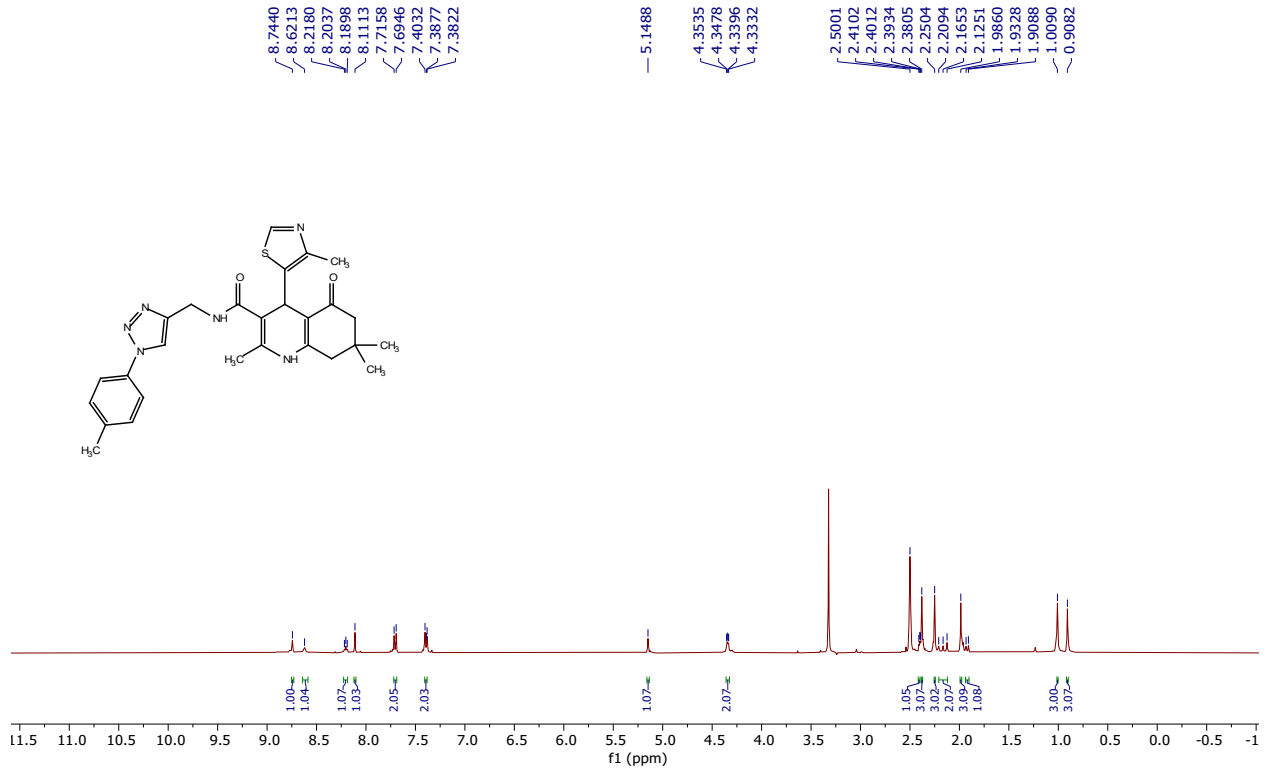
NMR spectrum of compound K3



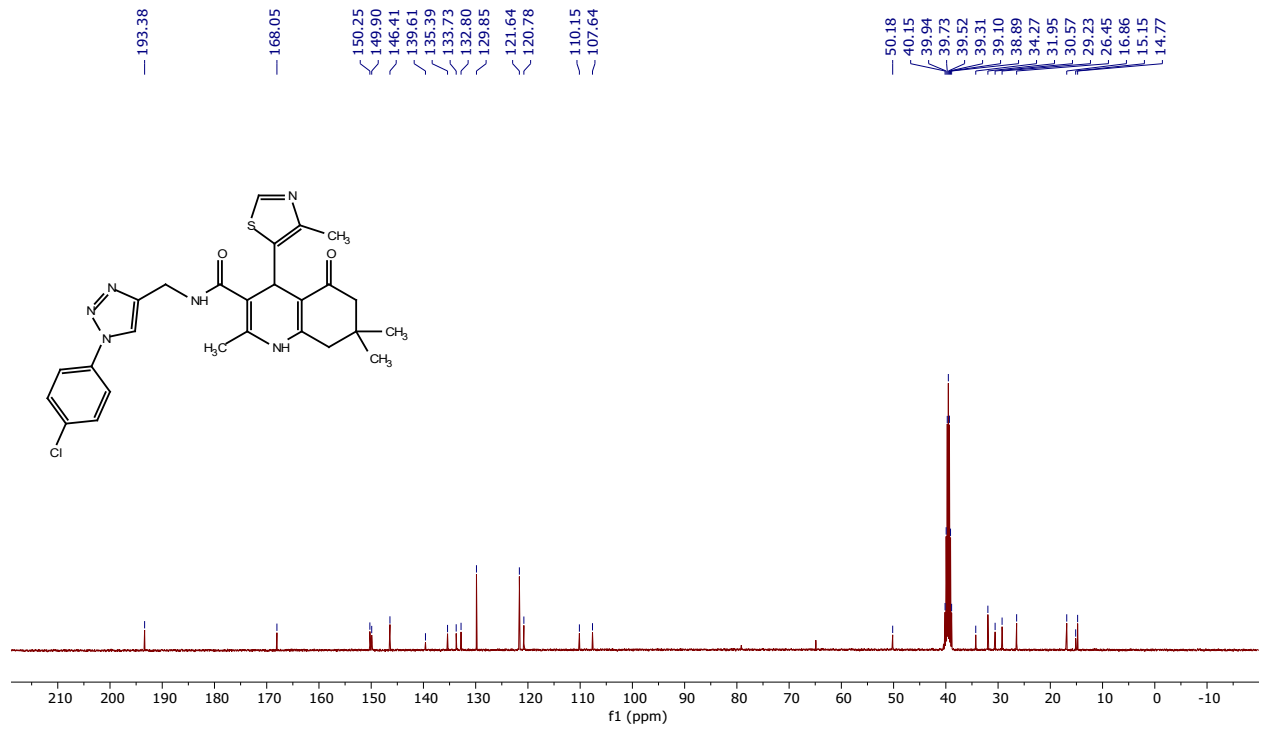
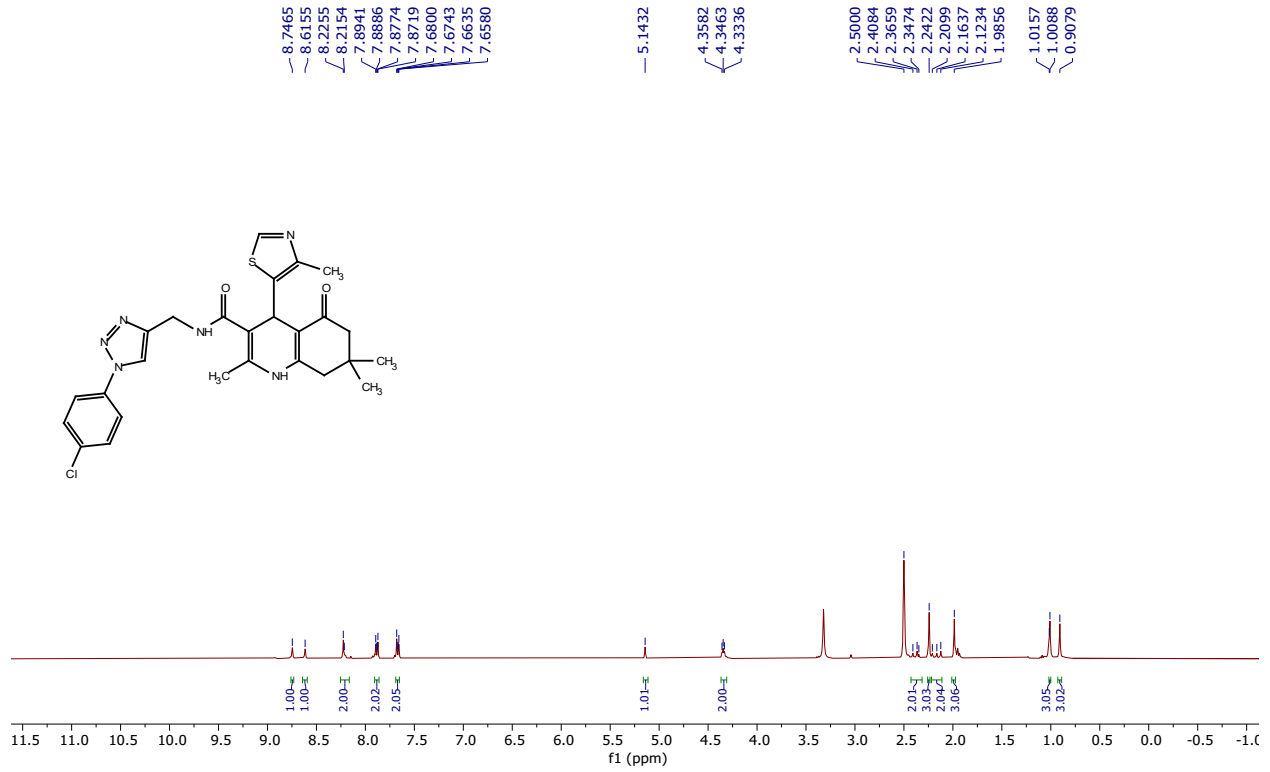
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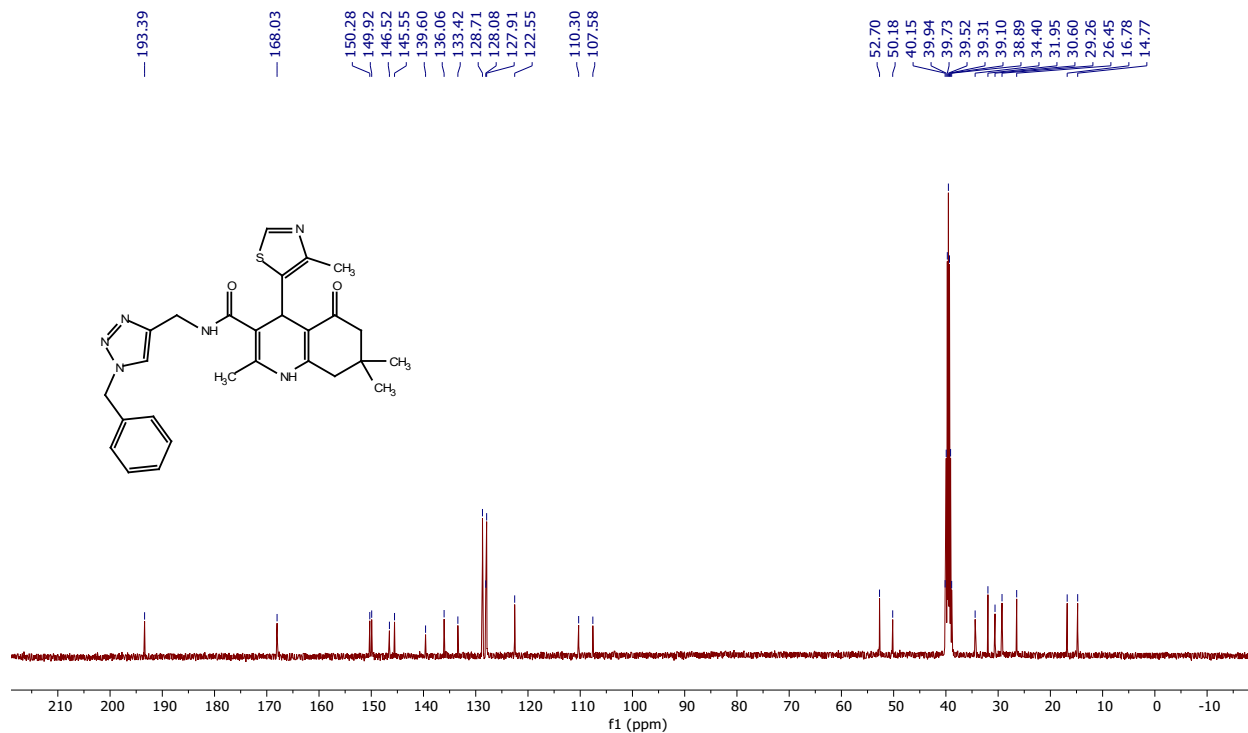
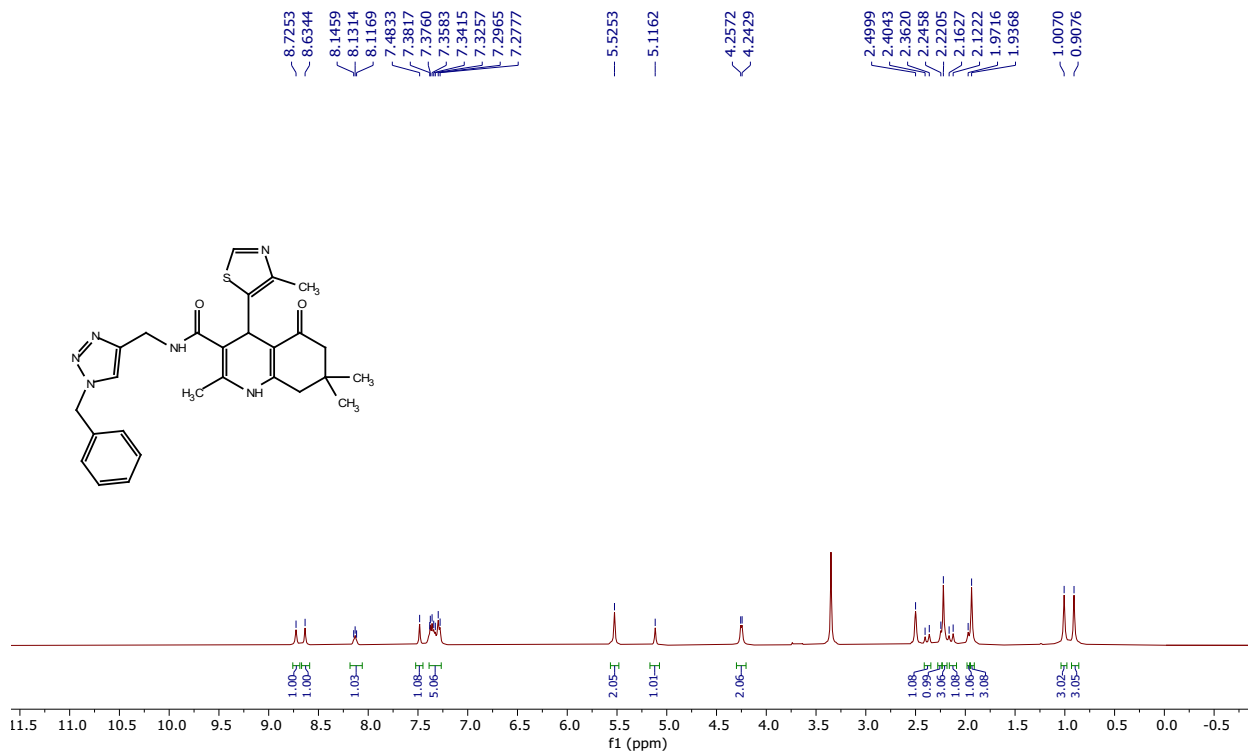
NMR spectrum of compound K5



NMR spectrum of compound K6

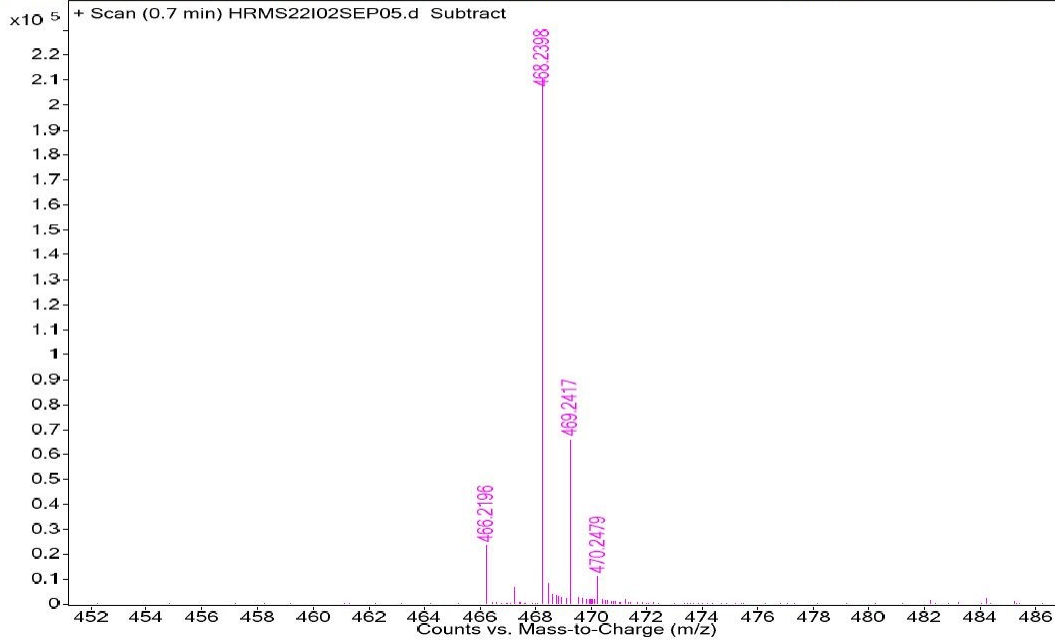


NMR spectrum of compound K7



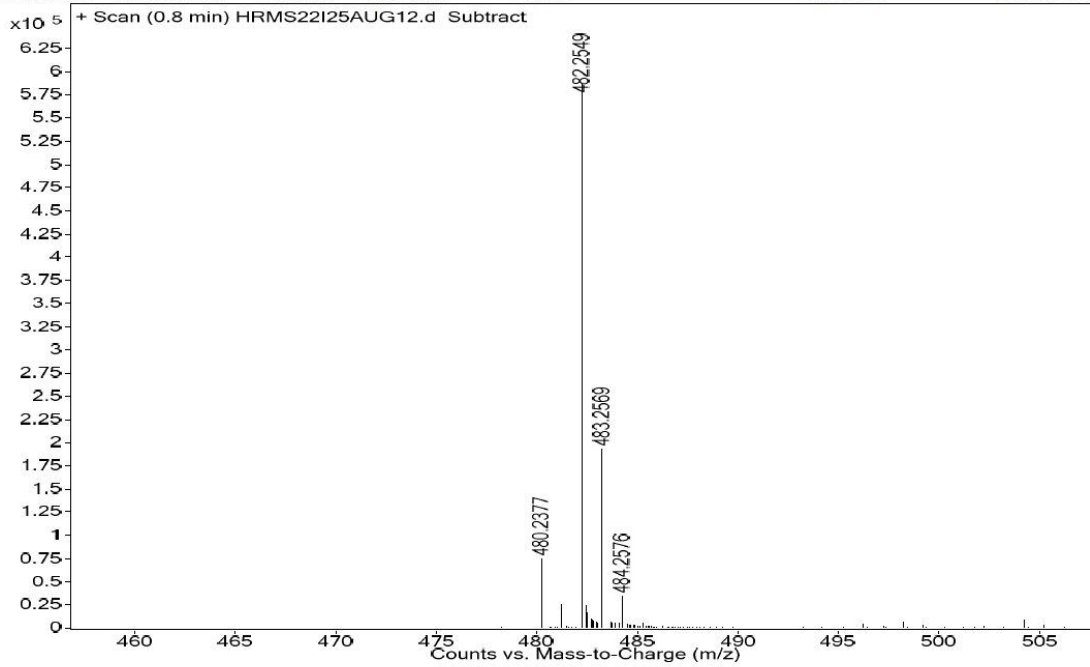
HRMS Spectra of compound J1

| | | | | | | | |
|---------------|------------------|-------------|-------------|-----------------|--------------|------------------------|----------------------|
| Sample Name | KVAJ-DHP-23 | Position | Vial 5 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Some Ions Missed |
| Data Filename | HRMS22102SEP05.d | ACQ Method | ISOCRATIC.m | Comment | | Acquired Time | 9/2/2022 11:28:15 AM |



HRMS Spectra of compound J2

| | | | | | | | |
|---------------|------------------|-------------|-------------|-----------------|--------------|------------------------|-----------------------|
| Sample Name | KVA-DHP-21 | Position | Vial 12 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Some Ions Missed |
| Data Filename | HRMS22125AUG12.d | ACQ Method | ISOCRATIC.m | Comment | | Acquired Time | 8/25/2022 11:54:58 AM |



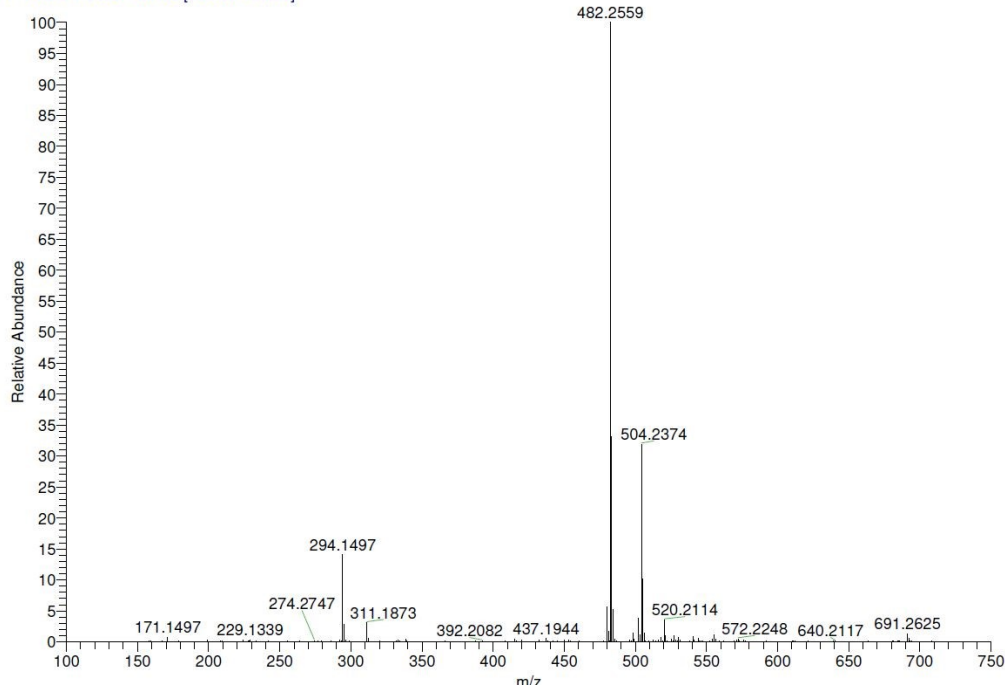
HRMS Spectra of compound J3

D:\INTERNALS 2022\...HRMS22126SEP06

9/26/2022 11:10:40 AM

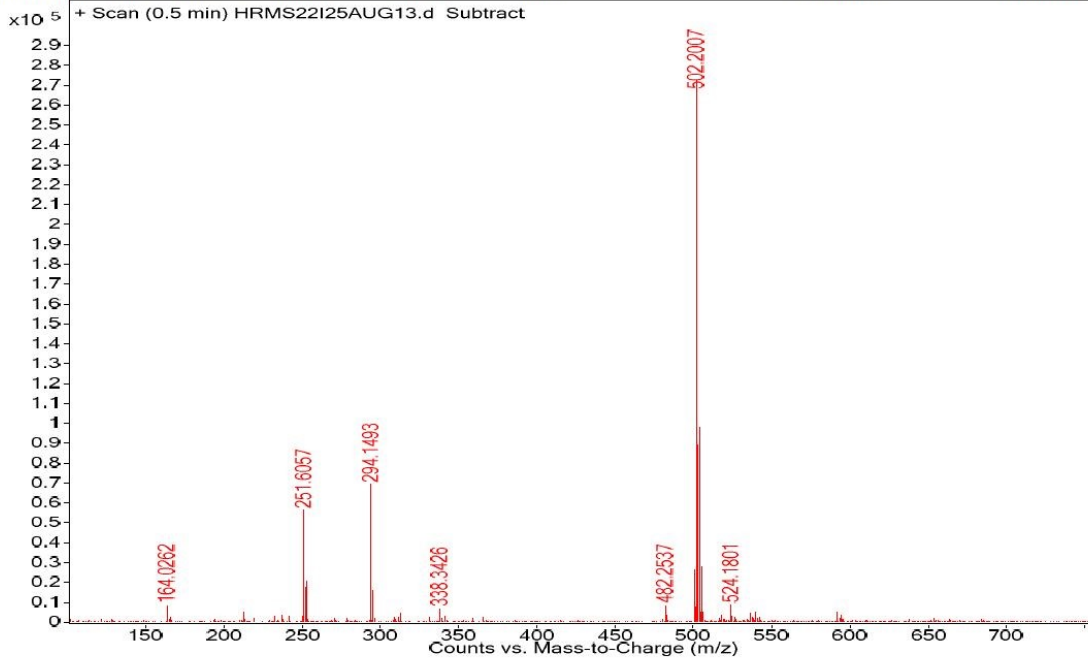
KVAJ-DHP-24

HRMS22126SEP06 #17 RT: 0.14 AV: 1 SB: 6 0.03-0.07 NL: 1.14E6
T: FTMS + c ESI Full ms [100.00-750.00]



HRMS Spectra of compound J4

| Sample Name | KVAJ-DHP-22 | Position | Vial 13 | Instrument Name | Instrument 1 | User Name | |
|---------------|------------------|-------------|-------------|-----------------|--------------|------------------------|-----------------------|
| Inj Vol | 1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Some Ions Missed |
| Data Filename | HRMS22125AUG13.d | ACQ Method | ISOCRATIC.m | Comment | | Acquired Time | 8/25/2022 11:58:01 AM |

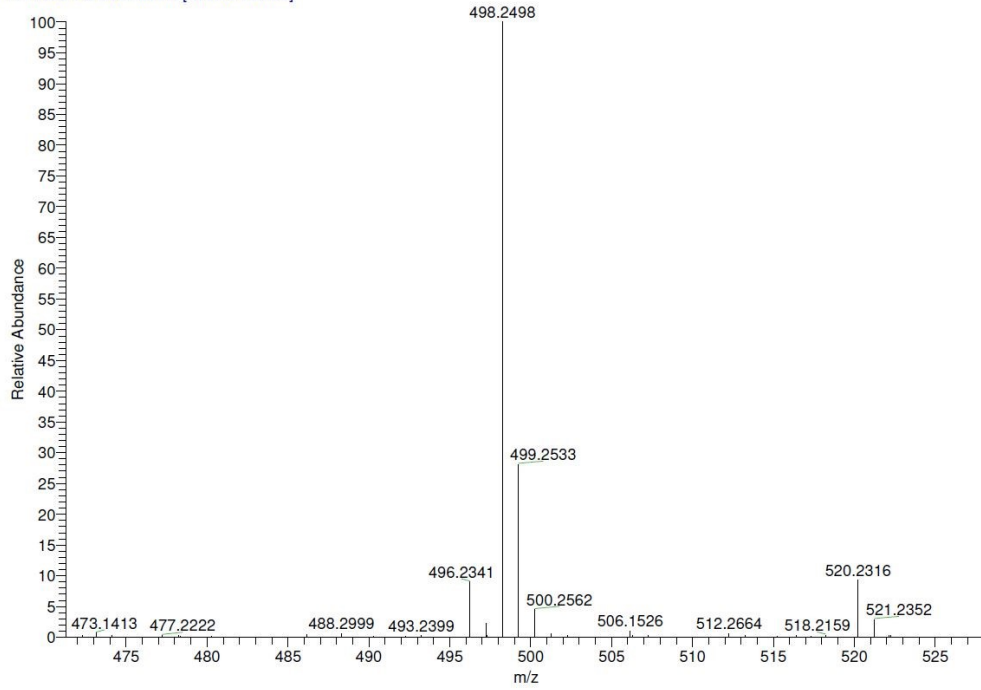


HRMS Spectra of compound J5

D:\internals 2022\NOV22\HRMS22I23NOV08

11/23/2022 11:39:46 AM

HRMS22I23NOV08 #26 RT: 0.21 AV: 1 SB: 1 0.79 NL: 1.28E5
T: FTMS + c ESI Full ms [100.00-750.00]

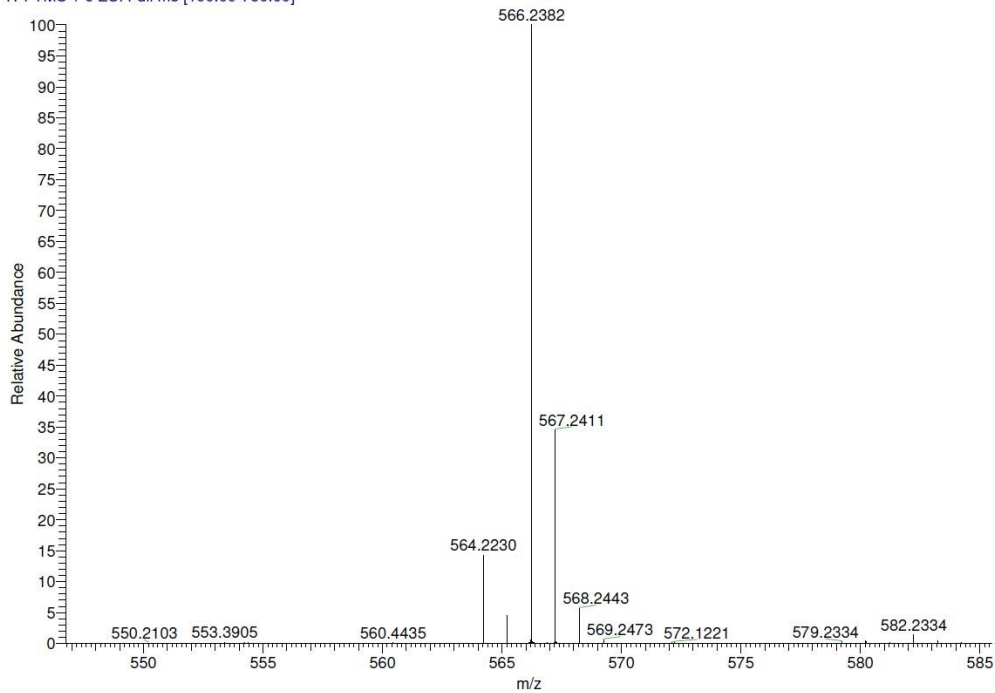


HRMS Spectra of compound J6

D:\internals 2022\...HRMS22I20OCT06

10/20/2022 11:42:03 AM

HRMS22I20OCT06 #25 RT: 0.19 AV: 1 NL: 2.60E6
T: FTMS + c ESI Full ms [100.00-750.00]



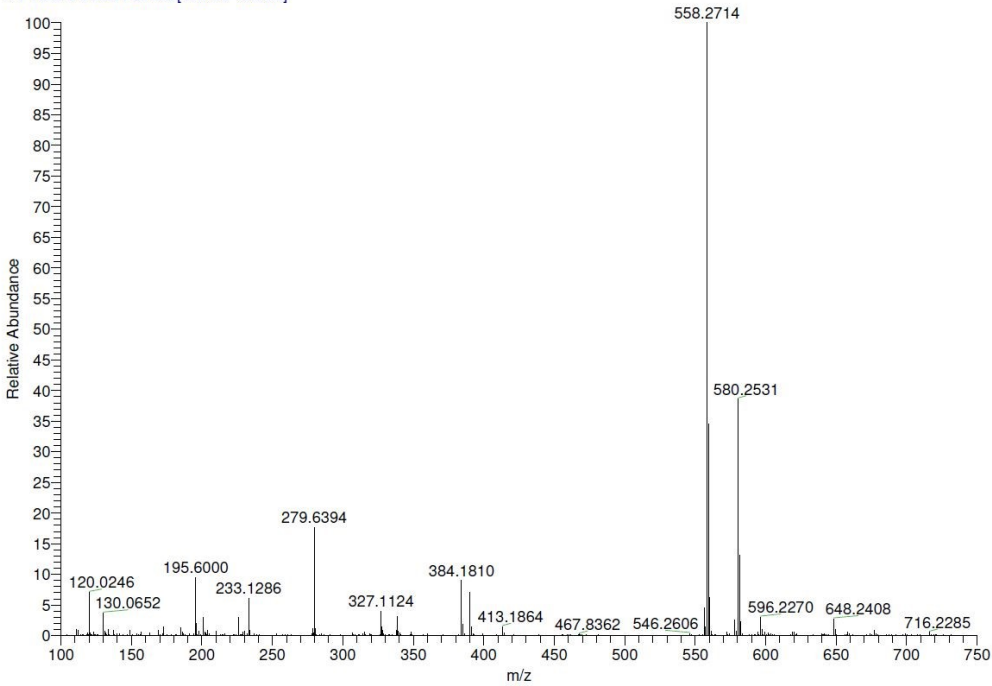
HRMS Spectra of compound J7

D:\INTERNALS 2022\...HRMS22114SEP30

9/14/2022 11:57:18 AM

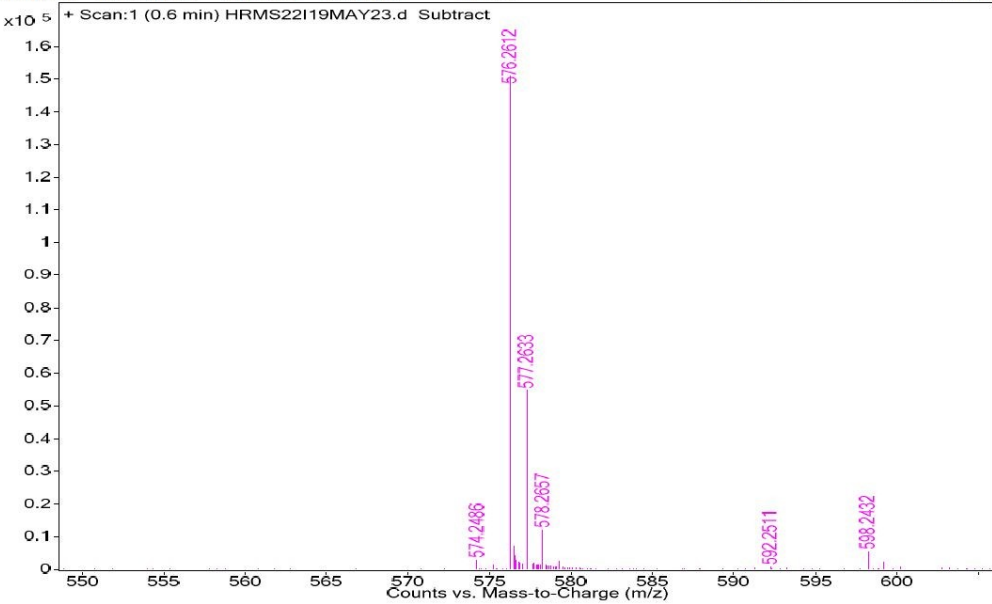
kvaj-bt-12

HRMS22114SEP30 #18 RT: 0.14 AV: 1 SB: 7 0.02-0.07 NL: 1.22E6
T: FTMS + c ESI Full ms [100.00-750.00]



HRMS Spectra of compound J8

| Sample Name | kvaj-dhp6 | Position | Vial 23 | Instrument Name | Instrument 1 | User Name | |
|---------------|------------------|-------------|-------------|-----------------|--------------|------------------------|-----------------------|
| Inj Vol | 1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Some Ions Missed |
| Data Filename | HRMS22119MAY23.d | ACQ Method | ISOCRATIC.m | Comment | | Acquired Time | 5/19/2022 12:56:56 PM |

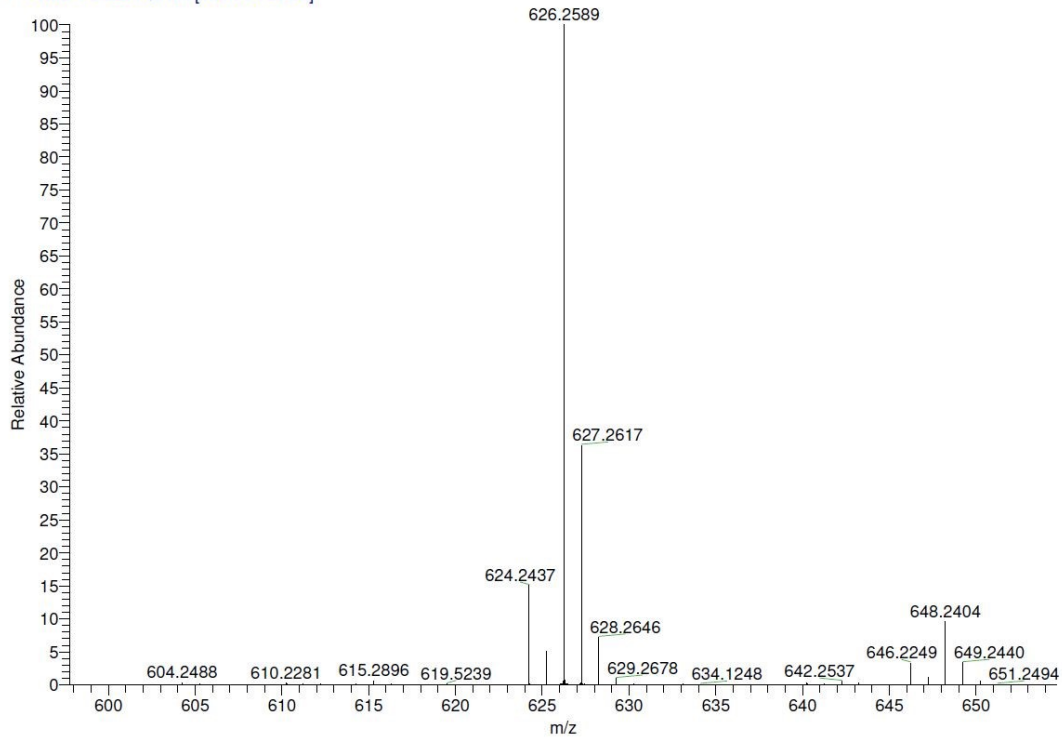


HRMS Spectra of compound J9

D:\internals 2022\NOV22\HRMS22\02NOV19

11/2/2022 11:48:25 AM

HRMS22\02NOV19 #23 RT: 0.19 AV: 1 NL: 1.97E6
T: FTMS + c ESI Full ms [100.00-750.00]

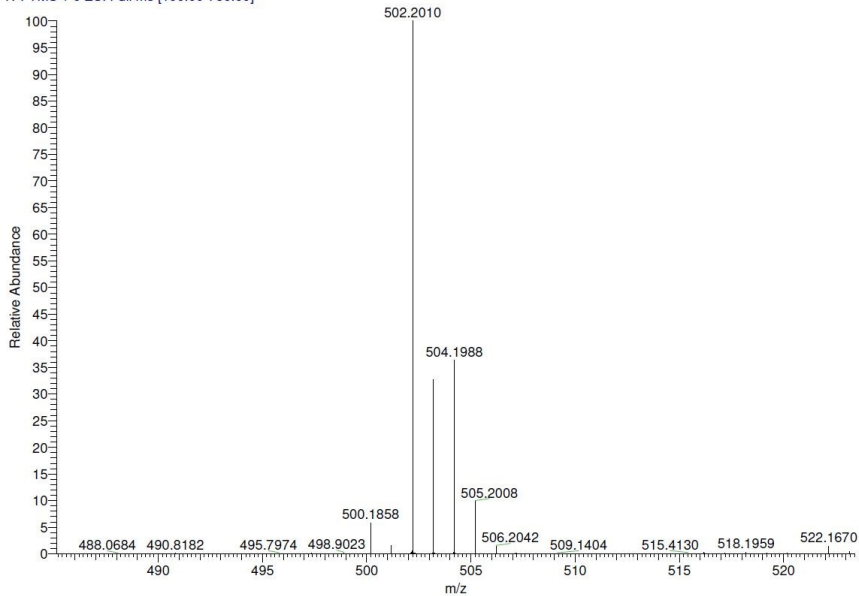


HRMS Spectra of compound J10

D:\internals 2022\...HRMS22\12OCT05

10/12/2022 11:08:44 AM

HRMS22\12OCT05 #16-33 RT: 0.12-0.25 AV: 18 NL: 3.30E6
T: FTMS + c ESI Full ms [100.00-750.00]

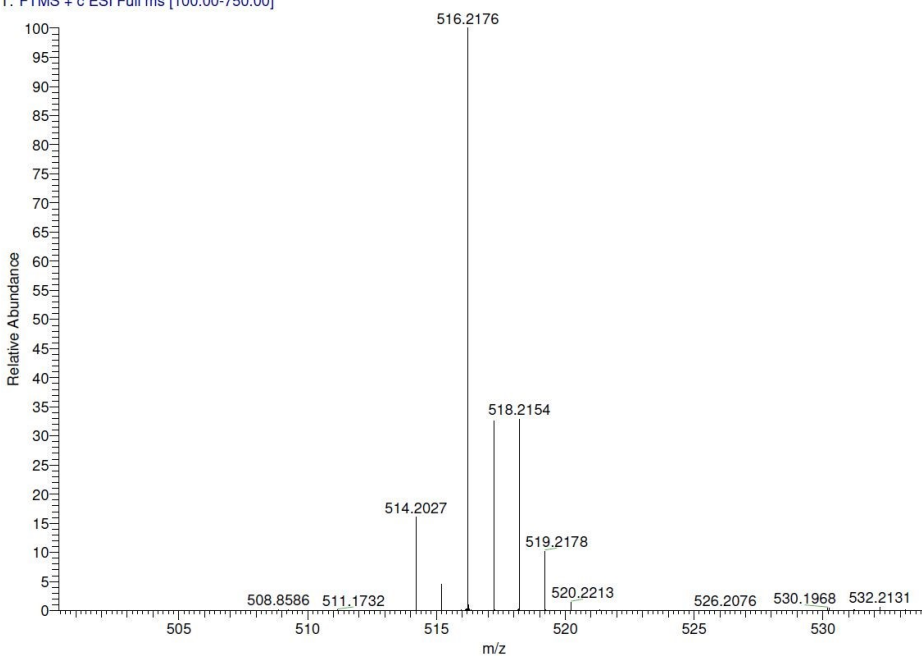


HRMS Spectra of compound J11

D:\internals 2022\...HRMS22120OCT07

10/20/2022 11:44:00 AM

HRMS22120OCT07 #25 RT: 0.19 AV: 1 NL: 1.98E6
T: FTMS + c ESI Full ms [100.00-750.00]

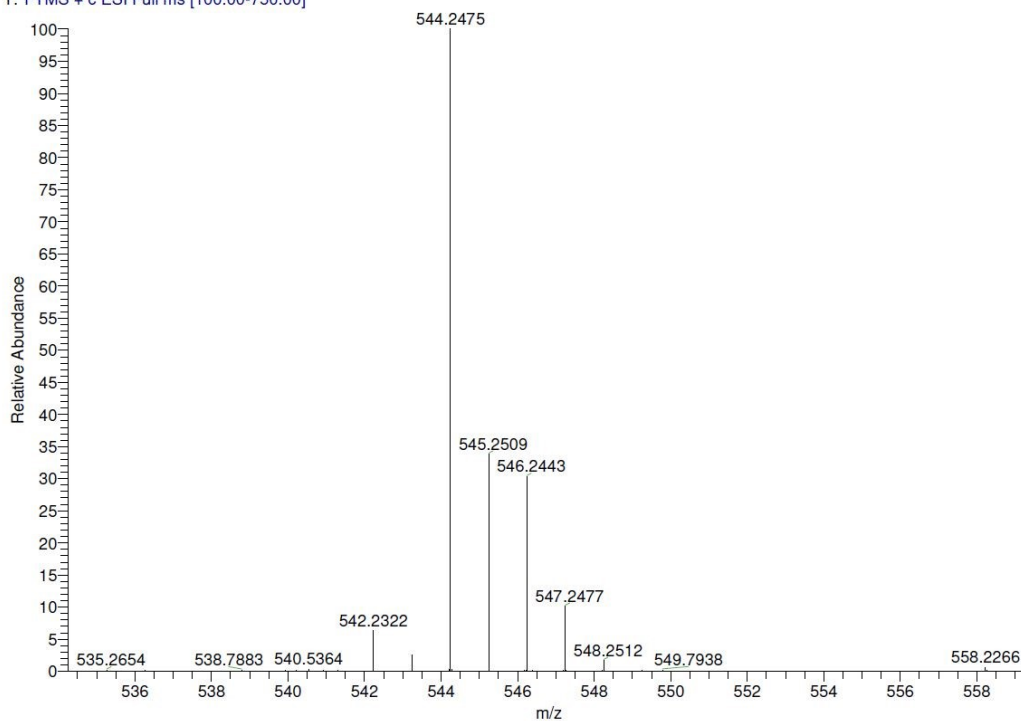


HRMS Spectra of compound J12

D:\INTERNAL 2023\MAR 2023\HRMS23114MAR48

3/14/2023 12:16:21 PM

HRMS23114MAR48 #16 RT: 0.13 AV: 1 SB: 1 0.96 NL: 2.42E5
T: FTMS + c ESI Full ms [100.00-750.00]



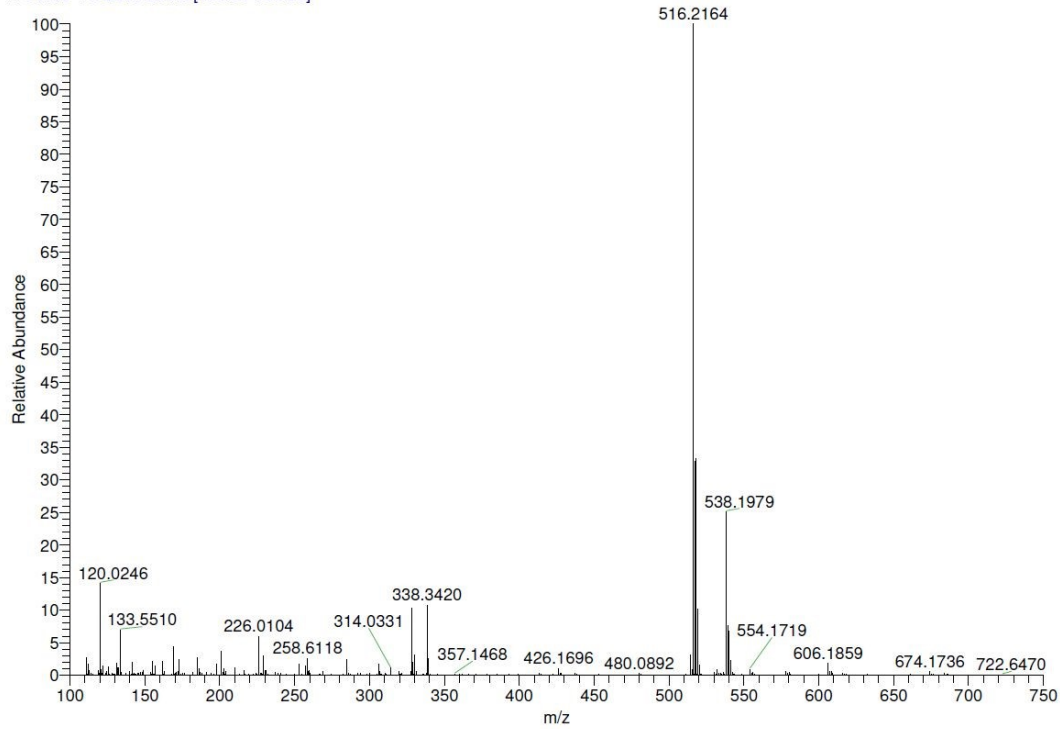
HRMS Spectra of compound J13

D:\INTERNALS 2022\...HRMS22114SEP31

9/14/2022 11:59:15 AM

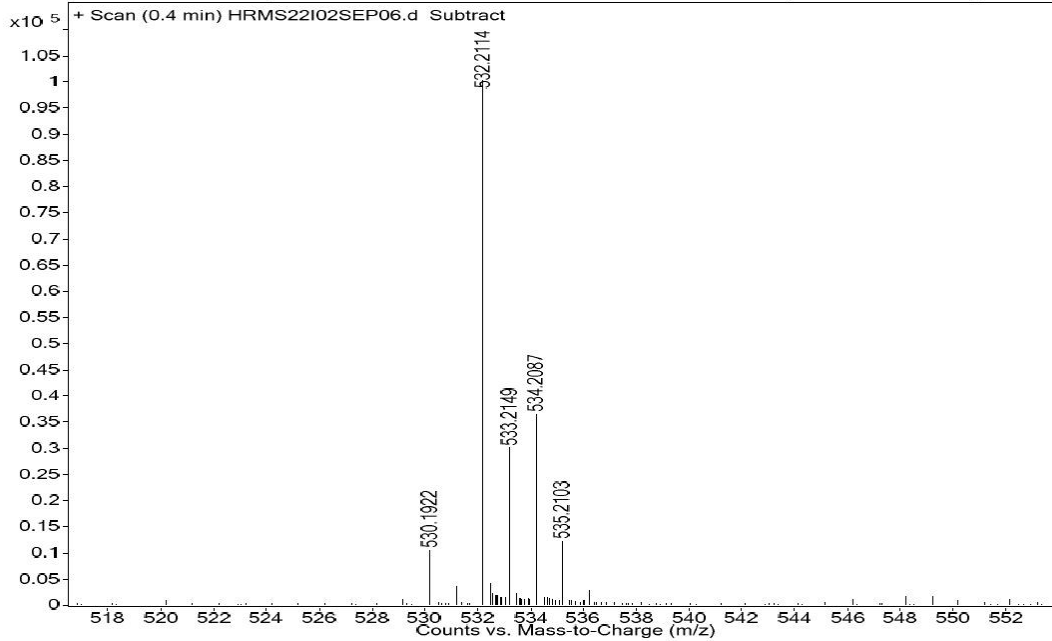
KVAJ-DHP25

HRMS22114SEP31 #31 RT: 0.24 AV: 1 SB: 7 0.03-0.07 NL: 1.56E6
T: FTMS + c ESI Full ms [100.00-750.00]



HRMS Spectra of compound J14

| Sample Name | Position | Vial | Instrument Name | Instrument 1 | User Name |
|------------------|-------------|---------|----------------------|--------------|------------------------|
| kvaj-dhp16 | Vial 6 | 6 | Instrument 1 | Sample | |
| Inj Vol | InjPosition | | SampleType | | IRM Calibration Status |
| 1 | | | | | Some Ions Missed |
| Data Filename | ACQ Method | Comment | Acquired Time | | |
| HRMS22102SEP06.d | ISOCRATIC.m | | 9/2/2022 11:31:24 AM | | |

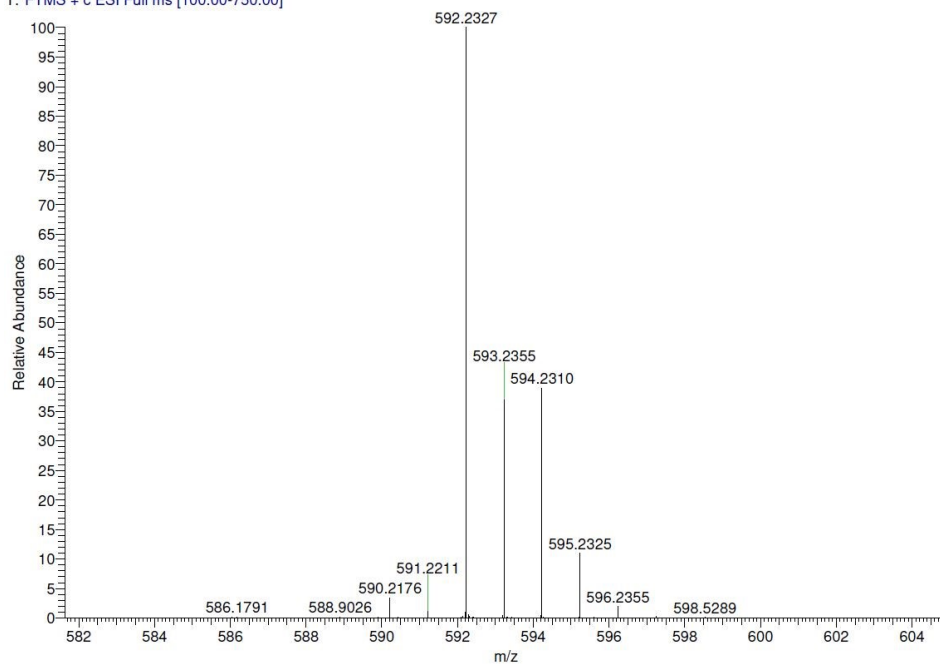


HRMS Spectra of compound J15

D:\INTERNAL 2023\MAR 2023\HRMS23114MAR47

3/14/2023 12:14:24 PM

HRMS23114MAR47 #29 RT: 0.23 AV: 1 SB: 1 0.97 NL: 1.61E6
T: FTMS + c ESI Full ms [100.00-750.00]

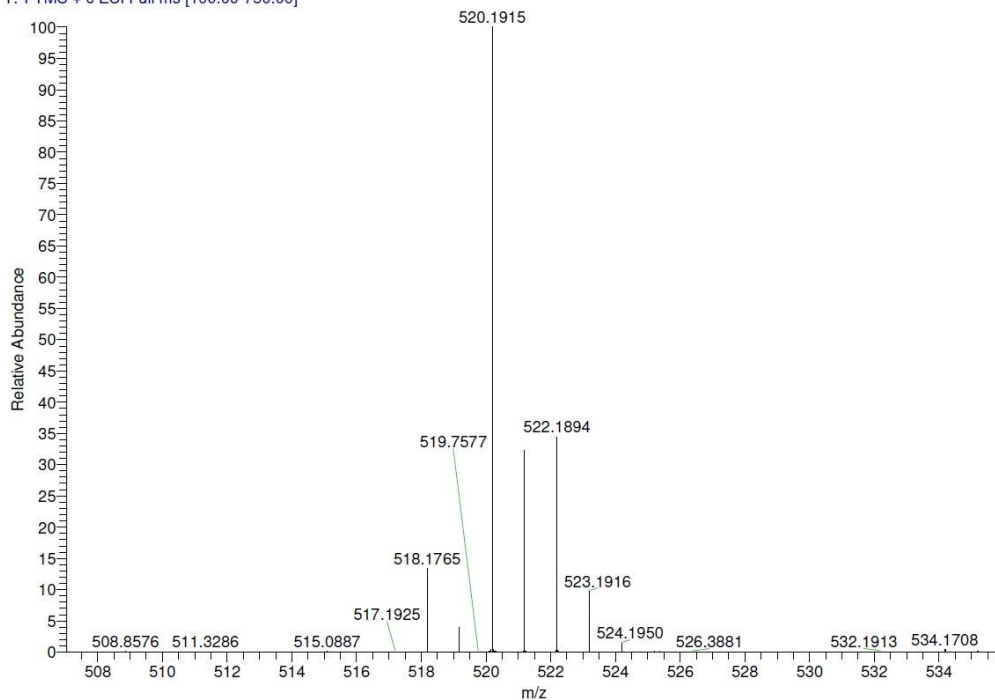


HRMS Spectra of compound J16

D:\internals 2022...\HRMS22112OCT04

10/12/2022 11:06:48 AM

HRMS22112OCT04 #16-33 RT: 0.12-0.25 AV: 18 NL: 1.86E6
T: FTMS + c ESI Full ms [100.00-750.00]



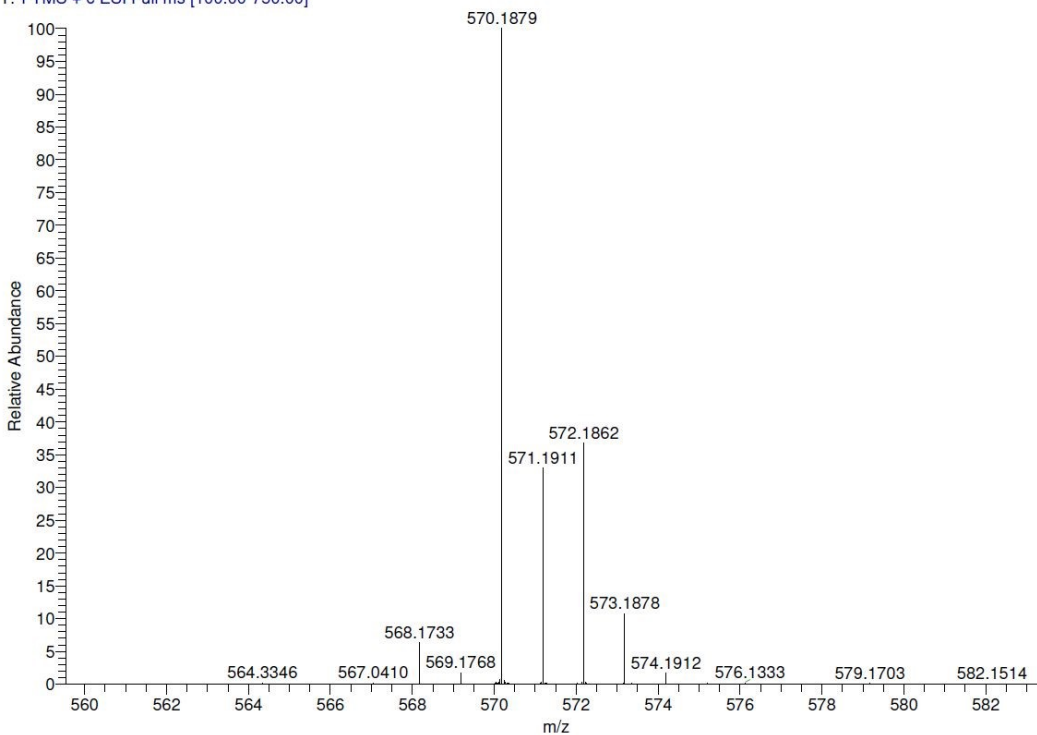
HRMS Spectra of compound J17

D:\INTERNAL 2023\MAR 2023\HRMS23114MAR46

3/14/2023 12:12:28 PM

HRMS23114MAR46 #22 RT: 0.17 AV: 1 SB: 1 0.96 NL: 4.75E6

T: FTMS + c ESI Full ms [100.00-750.00]



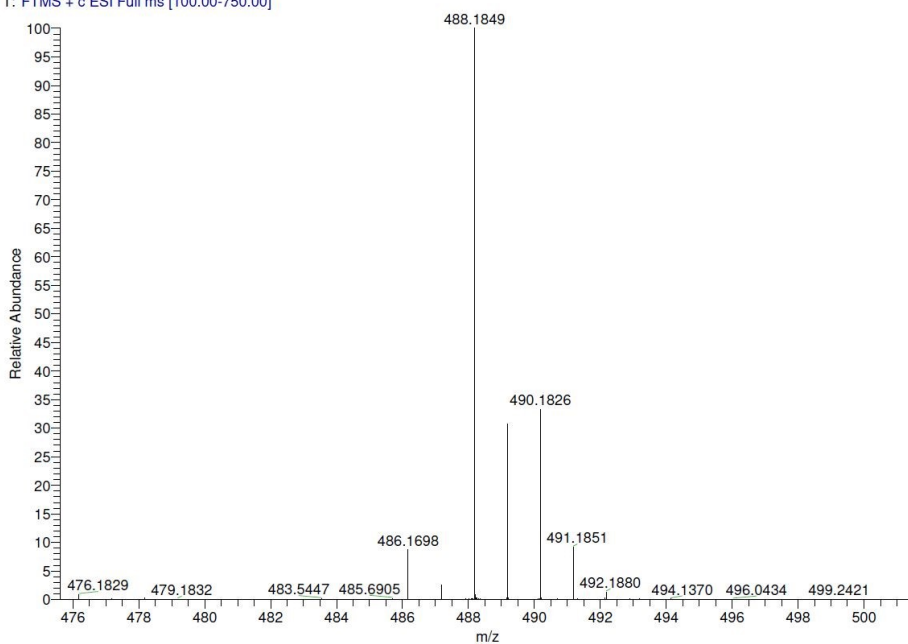
HRMS Spectra of compound J18

D:\INTERNAL 2023\MAR 2023\HRMS23114MAR19

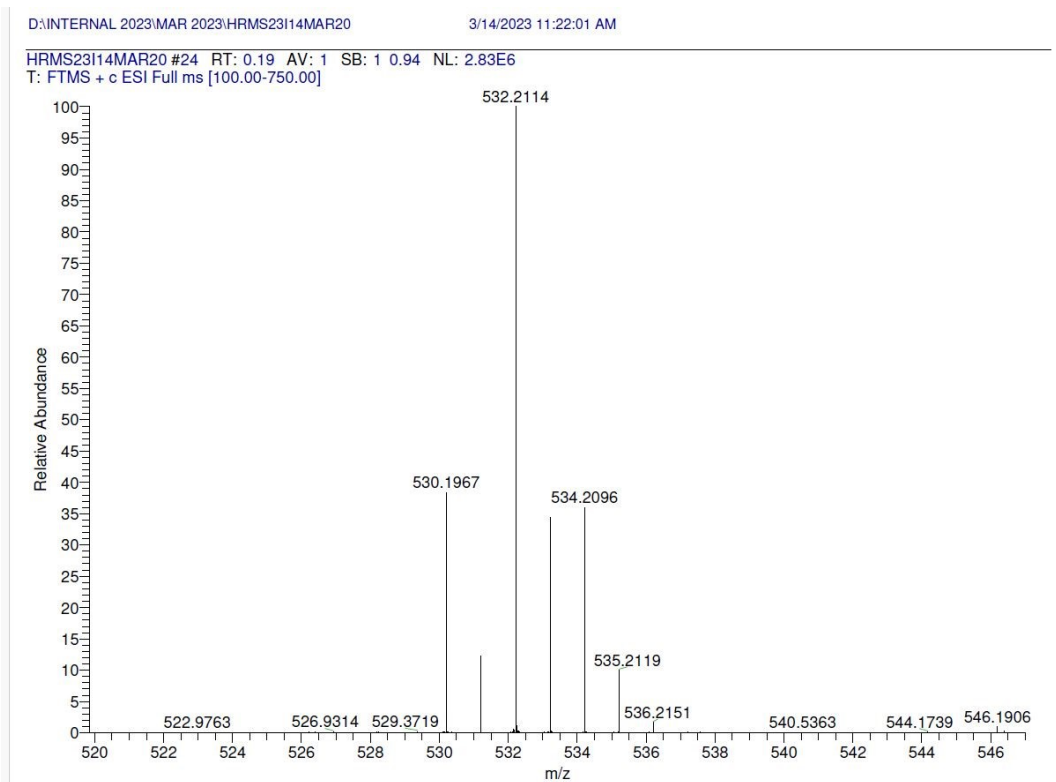
3/14/2023 11:20:04 AM

HRMS23114MAR19 #25 RT: 0.20 AV: 1 SB: 1 0.94 NL: 1.95E6

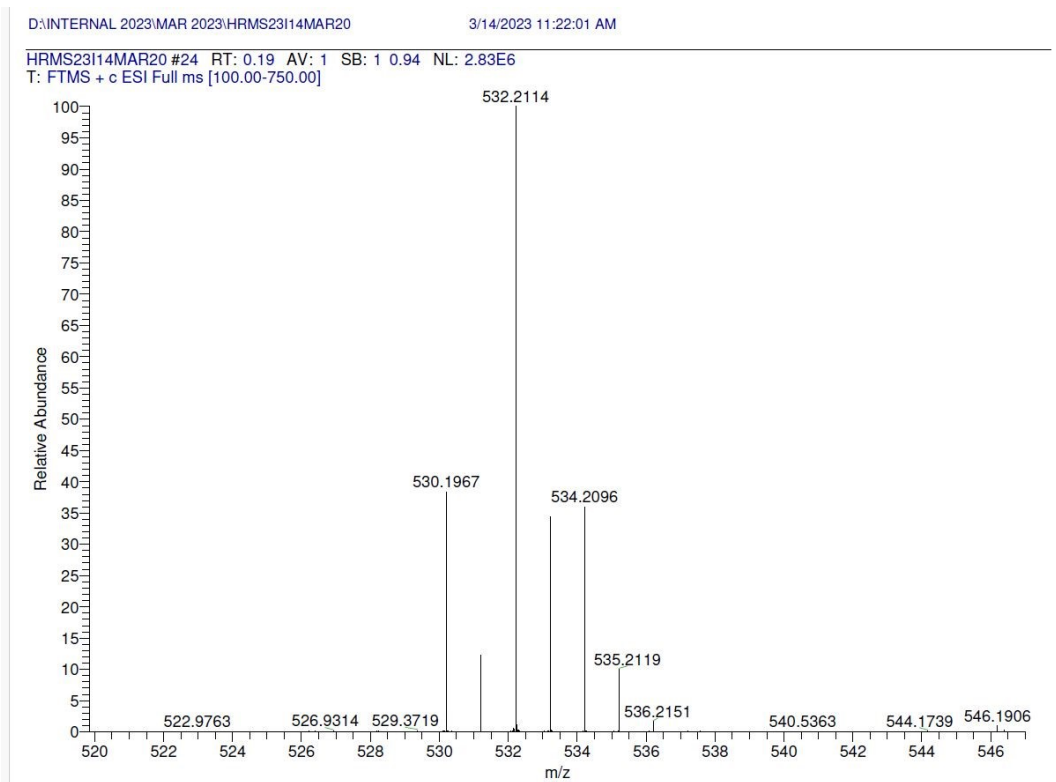
T: FTMS + c ESI Full ms [100.00-750.00]



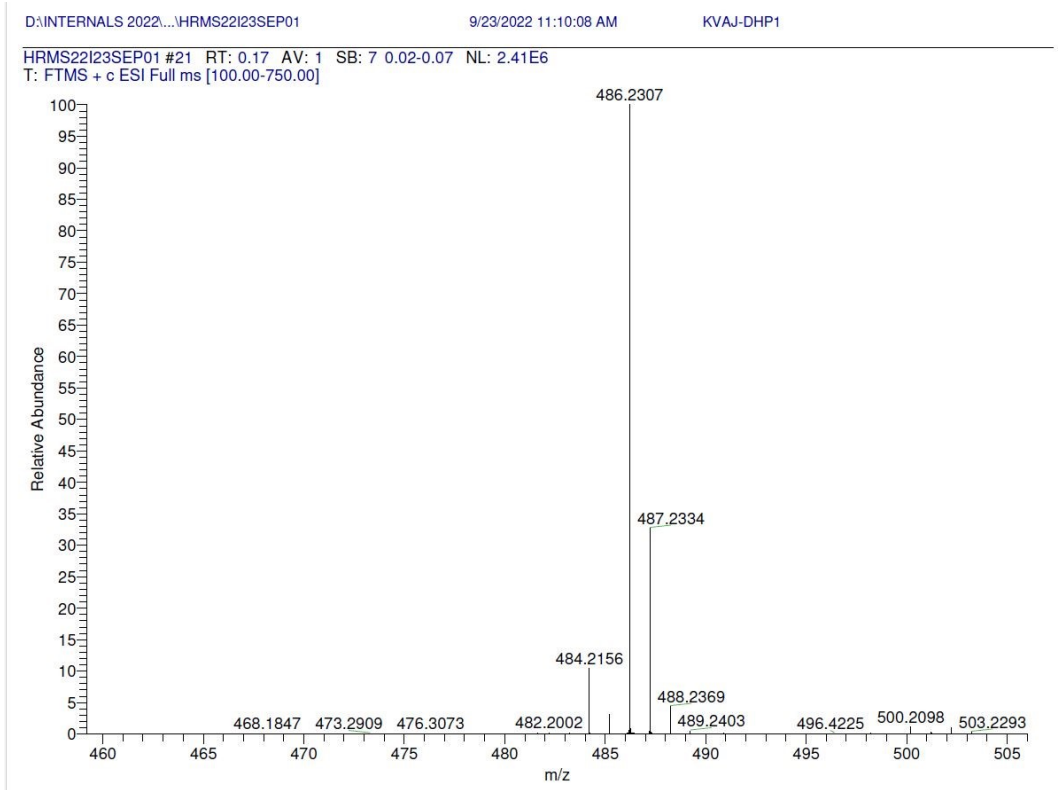
HRMS Spectra of compound J19



HRMS Spectra of compound J20



HRMS Spectra of compound J21

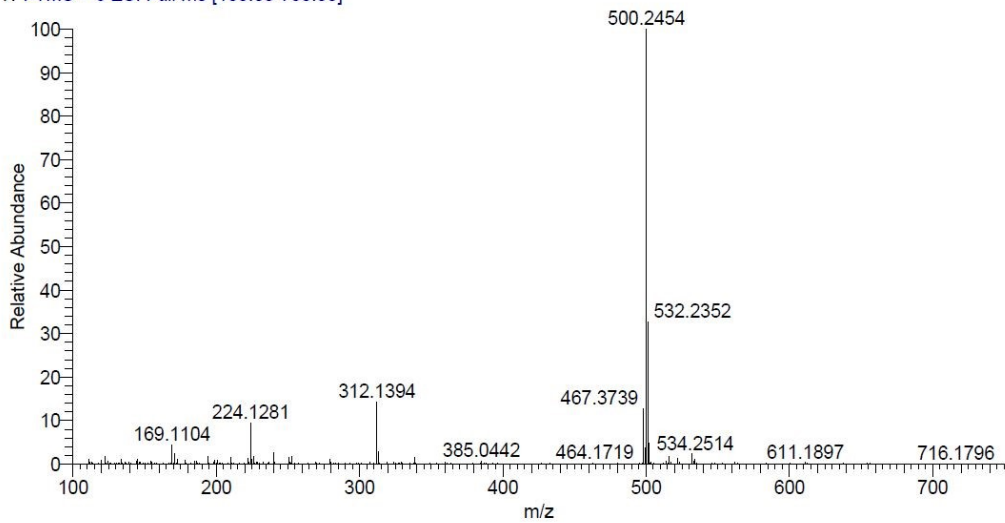


HRMS Spectra of compound J22

SAIF [HRMS Report]

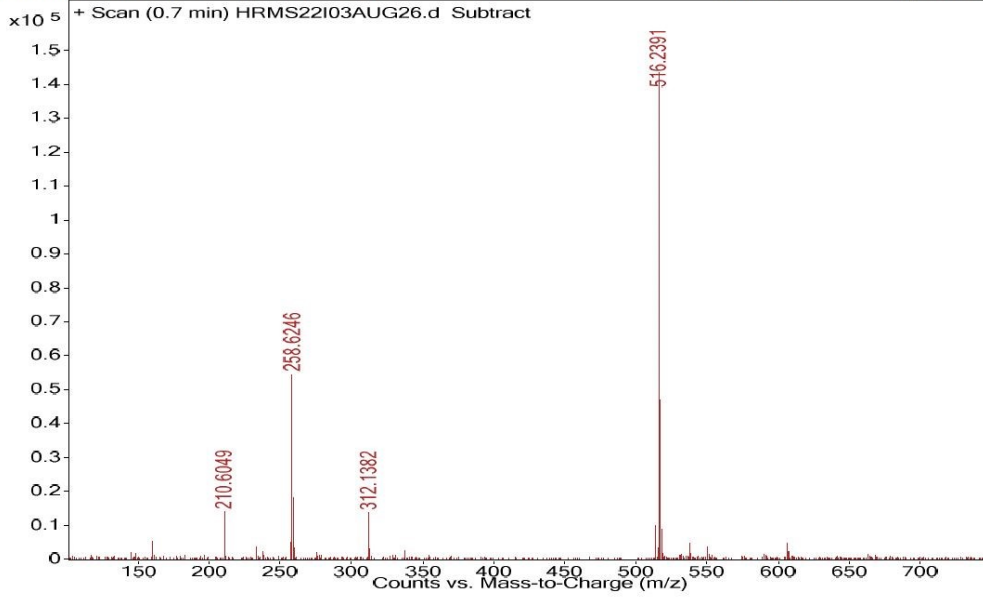
| | | | |
|-------------------|----------------------|-----------------------|---------------------------|
| Data File: | HRMS23I15MAR33 | Original Data Path: | D:\INTERNAL 2023\MAR 2023 |
| Sample ID: | kvaj-dhp-32 | Sample Name: | |
| Acquisition Date: | 03/15/23 11:41:03 AM | Run Time(min): | 0.00 |
| Vial: | CStk1-01:33 | Injection Volume(ul): | 1.00 |

HRMS23I15MAR33 #32-62 RT: 0.25-0.50 AV: 31 SB: 1 0.01 NL: 7.27E5
T: FTMS + c ESI Full ms [100.00-750.00]



HRMS Spectra of compound J23

| | | | | | | | |
|---------------|------------------|-------------|-------------|-----------------|--------------|------------------------|----------------------|
| Sample Name | kvaj-dhp4 | Position | Vial 26 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Some Ions Missed |
| Data Filename | HRMS22I03AUG26.d | ACQ Method | ISOCRATIC.m | Comment | | Acquired Time | 8/3/2022 12:48:41 PM |

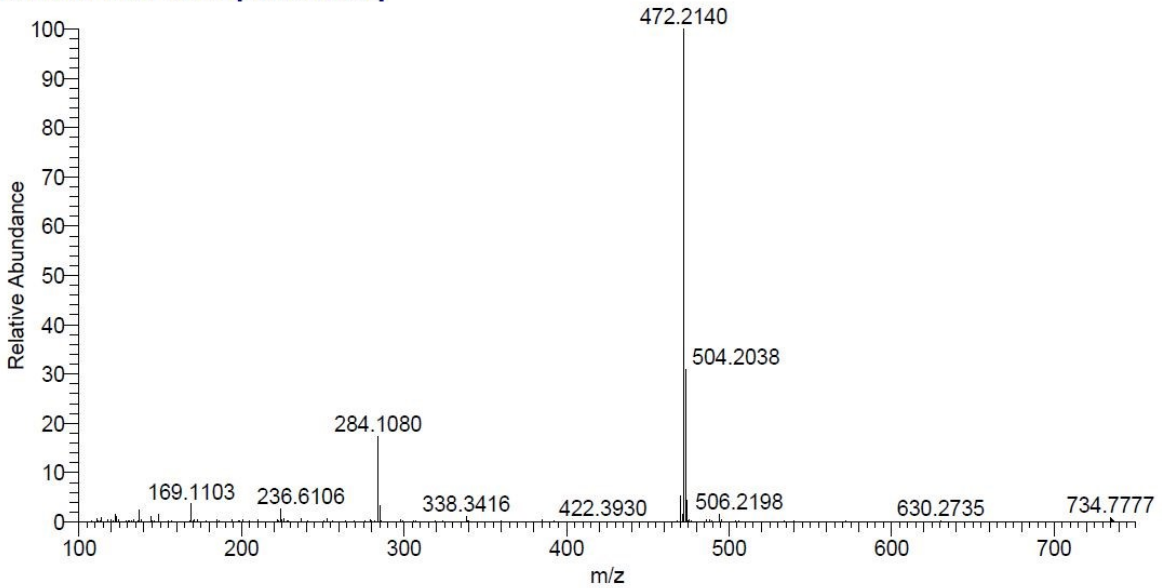


HRMS Spectra of compound J24

SAIF [HRMS Report]

| | | | |
|-------------------|----------------------|-----------------------|---------------------------|
| Data File: | HRMS23I15MAR34 | Original Data Path: | D:\INTERNAL 2023\MAR 2023 |
| Sample ID: | kvaj-dhp-34 | Sample Name: | |
| Acquisition Date: | 03/15/23 11:42:59 AM | Run Time(min): | 0.00 |
| Vial: | CStk1-01:34 | Injection Volume(μl): | 1.00 |

HRMS23I15MAR34 #33-64 RT: 0.25-0.50 AV: 32 SB: 1 0.01 NL: 2.23E6
T: FTMS + c ESI Full ms [100.00-750.00]

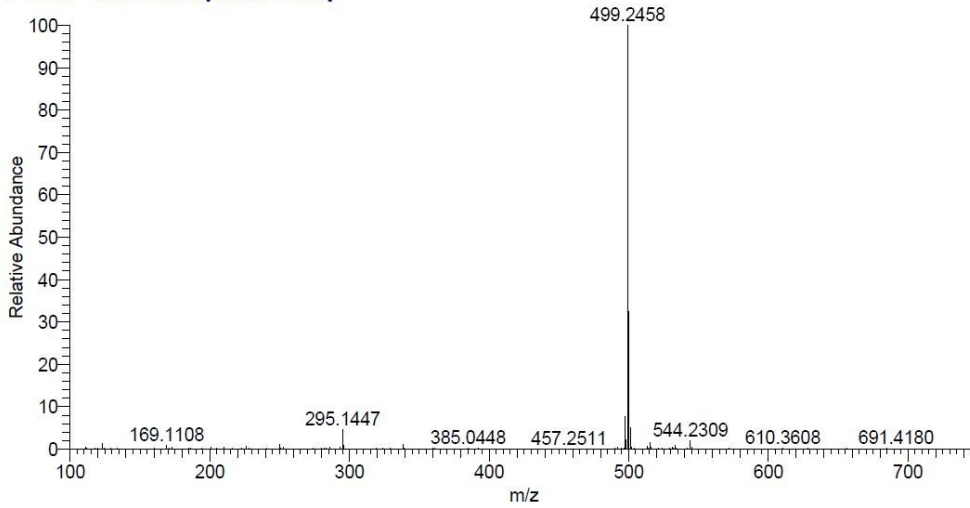


HRMS Spectra of compound J25

SAIF [HRMS Report]

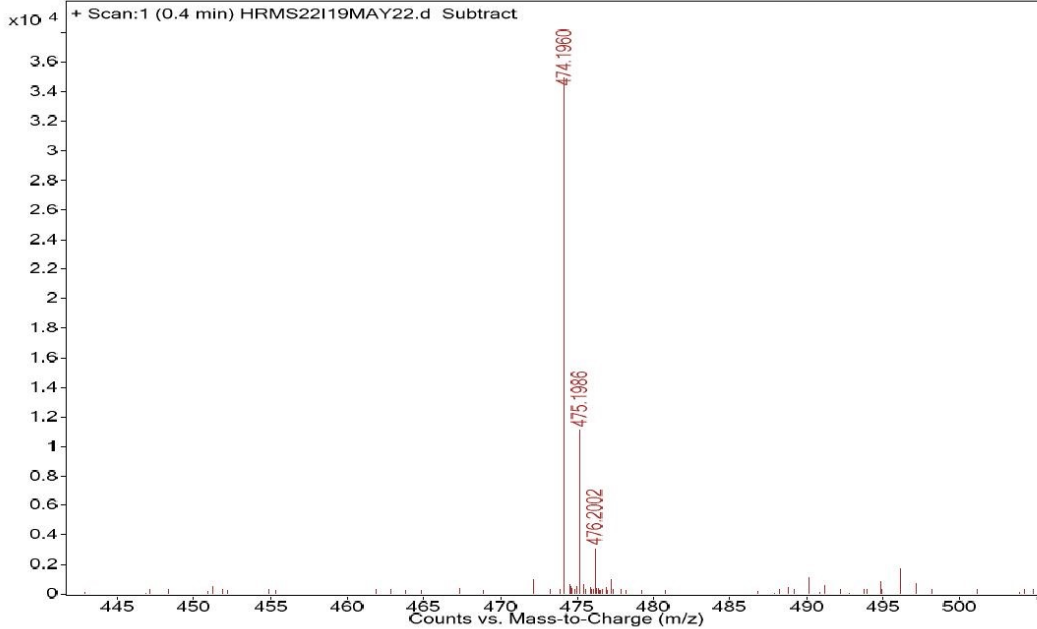
| | | | |
|-------------------|----------------------|-----------------------|---------------------------|
| Data File: | HRMS23I14MAR21 | Original Data Path: | D:\INTERNAL 2023\MAR 2023 |
| Sample ID: | KVAJ-DHP-30 | Sample Name: | |
| Acquisition Date: | 03/14/23 11:23:58 AM | Run Time(min): | 0.00 |
| Vial: | CStk1-01:21 | Injection Volume(μl): | 1.00 |

HRMS23I14MAR21 #33-64 RT: 0.25-0.50 AV: 32 SB: 1 0.01 NL: 1.33E6
T: FTMS + c ESI Full ms [100.00-750.00]



HRMS Spectra of compound K1

| | | | | | | | |
|---------------|------------------|--------------|-------------|-----------------|--------------|------------------------|-----------------------|
| Sample Name | kva-j-dhp5 | Position | Vial 22 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 1 | Inj Position | | Sample Type | Sample | IRM Calibration Status | Some Ions Missed |
| Data Filename | HRMS22I19MAY22.d | ACQ Method | ISOCRATIC.m | Comment | | Acquired Time | 5/19/2022 12:53:51 PM |

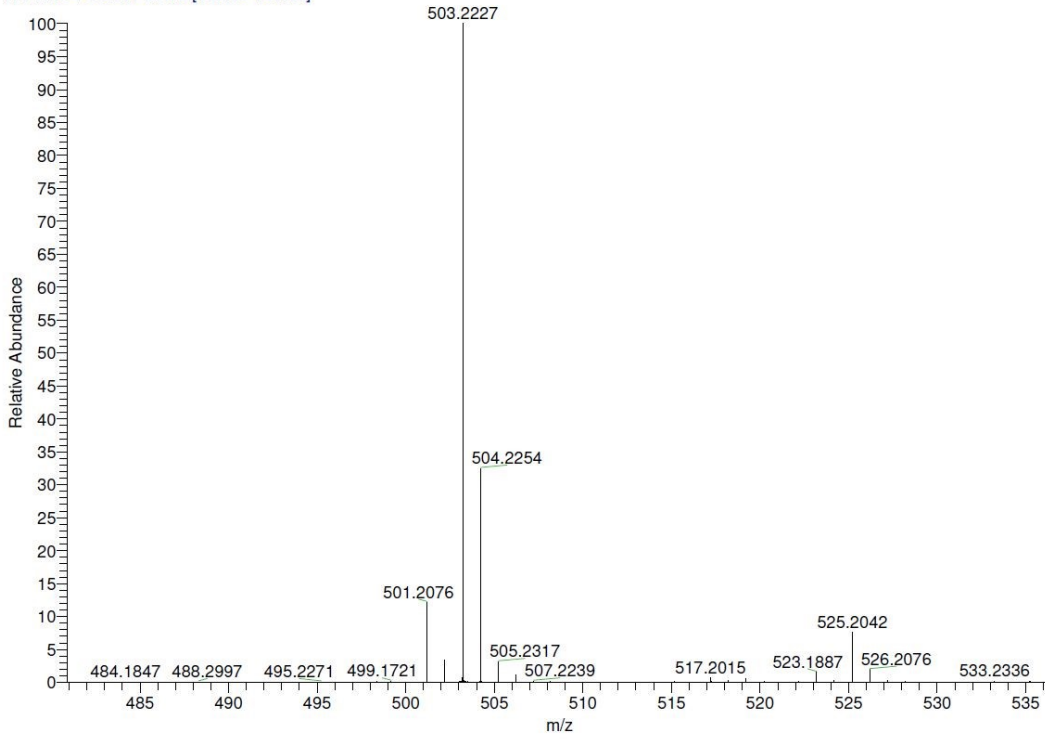


HRMS Spectra of compound K2

D:\internals 2022\NOV22\HRMS22102NOV18

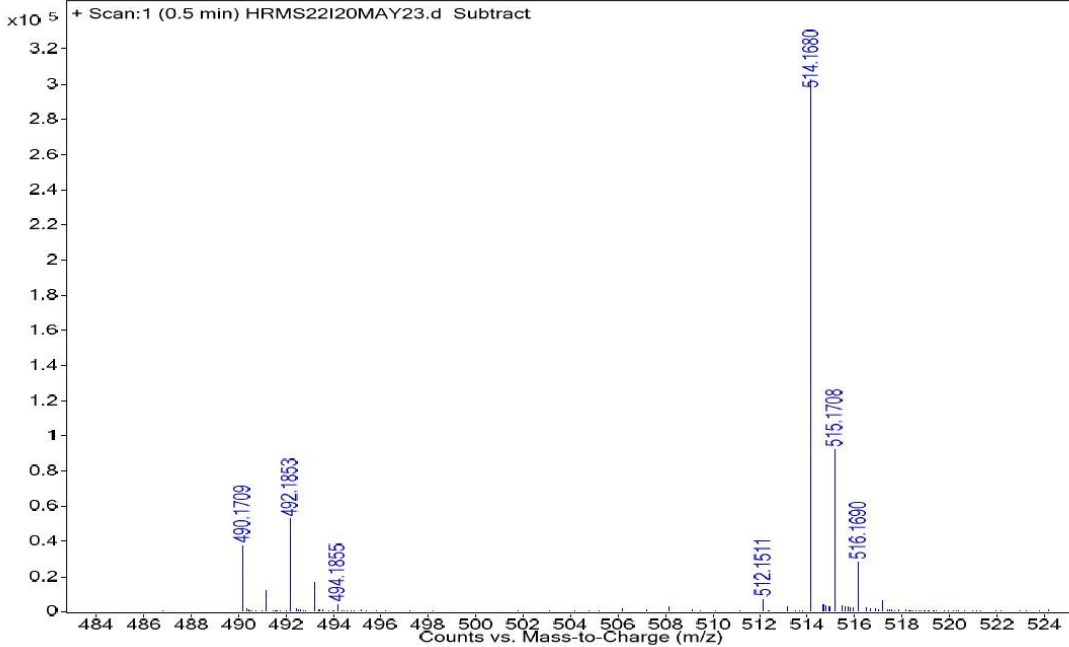
11/2/2022 11:46:29 AM

HRMS22102NOV18 #23 RT: 0.18 AV: 1 NL: 2.06E6
T: FTMS + c ESI Full ms [100.00-750.00]



HRMS Spectra of compound K3

| Sample Name | kvaj-dhp2 | Position | Vial 23 | Instrument Name | Instrument 1 | User Name | |
|---------------|------------------|-------------|-------------|-----------------|--------------|------------------------|----------------------|
| Inj Vol | 1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Some Ions Missed |
| Data Filename | HRMS22120MAY23.d | ACQ Method | ISOCRATIC.m | Comment | | Acquired Time | 5/20/2022 1:12:50 PM |



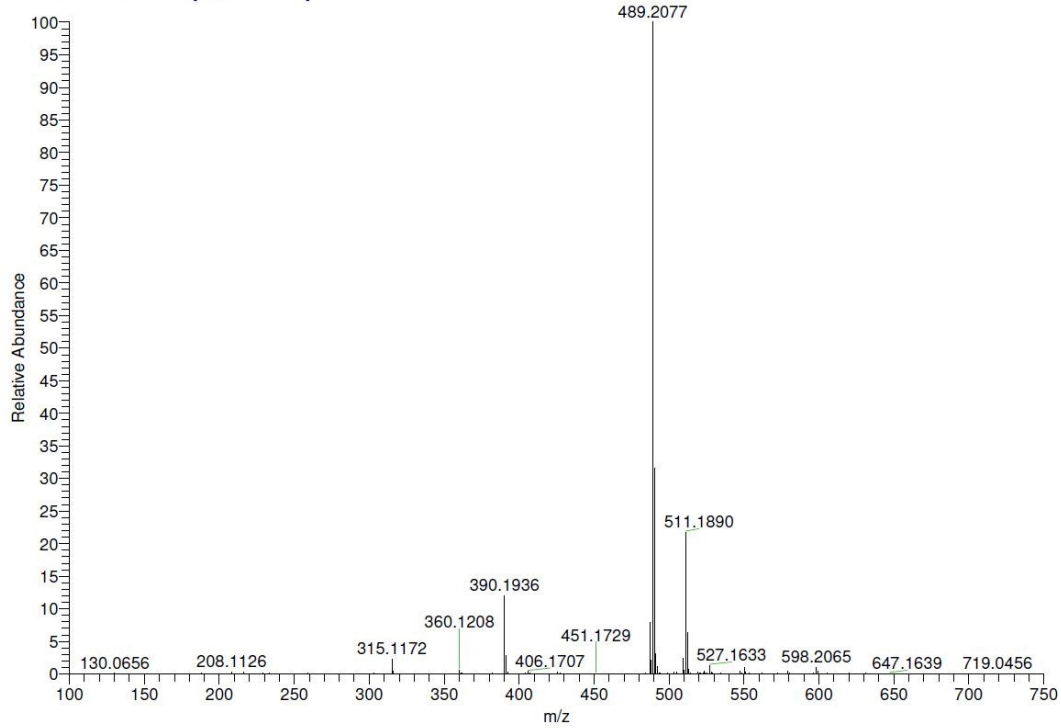
HRMS Spectra of compound K4

D:\INTERNALS 2022\...HRMS22I26SEP07

9/26/2022 11:12:35 AM

KVAJ-DHP-7

HRMS22I26SEP07 #21 RT: 0.17 AV: 1 SB: 6 0.03-0.07 NL: 6.46E6
T: FTMS + c ESI Full ms [100.00-750.00]

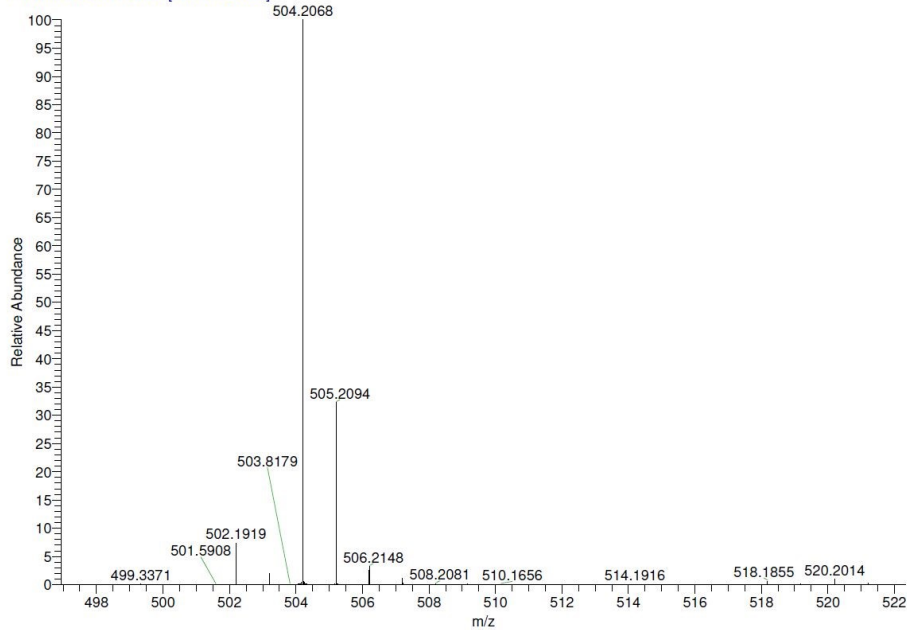


HRMS Spectra of compound K5

D:\internals 2022\NOV22\HRMS22I01NOV21

11/1/2022 11:50:29 AM

HRMS22I01NOV21 #24 RT: 0.19 AV: 1 NL: 4.55E6
T: FTMS + c ESI Full ms [100.00-750.00]

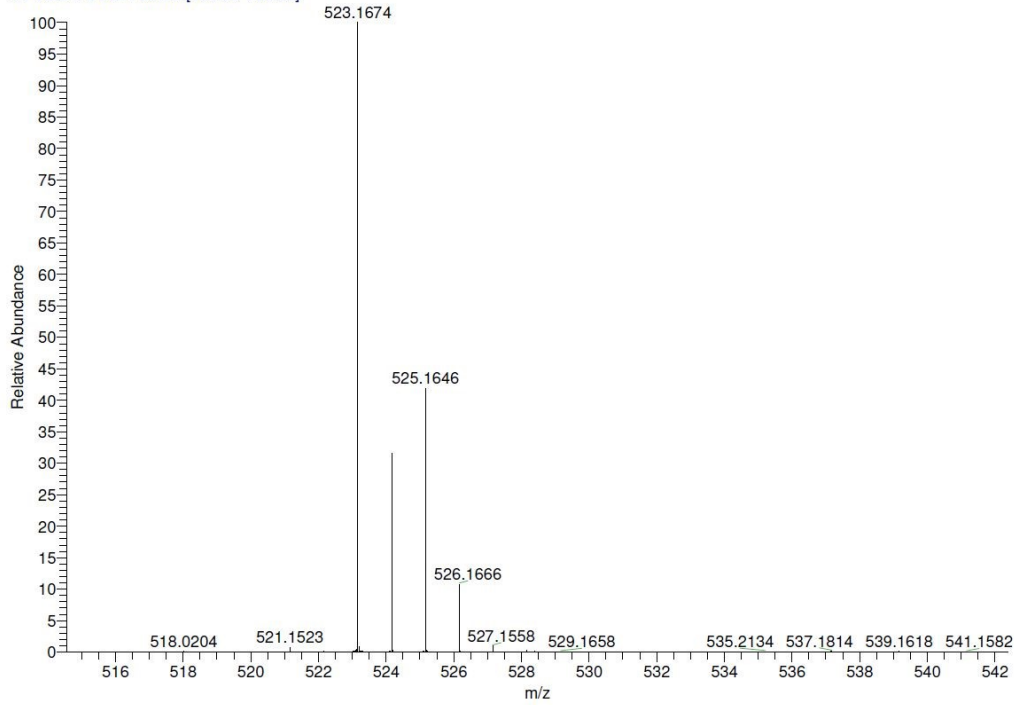


HRMS Spectra of compound K6

D:\internals 2022\NOV22\HRMS22101NOV22

11/1/2022 11:52:26 AM

HRMS22101NOV22 #21 RT: 0.17 AV: 1 NL: 4.23E6
T: FTMS + c ESI Full ms [100.00-750.00]



HRMS Spectra of compound K7

D:\INTERNALS 2022\...HRMS22115SEP20

9/15/2022 11:30:02 AM

kvaj-dhp-26

HRMS22115SEP20 #25 RT: 0.19 AV: 1 SB: 7 0.02-0.07 NL: 4.83E5
T: FTMS + c ESI Full ms [100.00-750.00]

