Supporting Information

Identification and Utilization of a Chemical Probe to Interrogate the Roles of PIKfyve in the Lifecycle of β-Coronaviruses

David H. Drewry[1,2,†], Frances M. Potjewyd[1,†], Armin Bayati[3], Jeffery L. Smith[1], Rebekah J. Dickmander[2,4,5,6], Stefanie Howell[1], Sharon Taft-Benz[4,7], Sophia M. Min[1], Mohammad Anwar Hossain[1], Mark Heise[4,7], Peter S. McPherson[3], Nathaniel J. Moorman[2,4,5], Alison D. Axtman[*,1]

[1] Structural Genomics Consortium, UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599, USA

[2] UNC Lineberger Comprehensive Cancer Center, School of Medicine, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599, USA

[3] Structural Genomics Consortium, Department of Neurology and Neurosurgery, Montreal Neurological Institute, McGill University, Montreal, QC, H3A 2B4, Canada

[4] Rapidly Emerging Antiviral Drug Development Initiative (READDI), Chapel Hill, NC, 27599, USA

[5] Department of Microbiology & Immunology, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599, USA

[6] Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599, USA

[7] Department of Genetics, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599, USA

[†] Authors contributed equally

[*] Corresponding Author E-mail: alison.axtman@unc.edu

Table of Contents

Table S1. Orthogonal assay results for analog **8**

Kinase	DiscoverX PoC value	Assay format (source)	IC$_{50}$ value (nM)
PIP5K1C	0	Enzymatic (Eurofins)	160
PIKFYVE	0	Enzymatic (SignalChem) and NanoBRET (SGC-UNC)	9.3 and 11.4
TYK2(JH2domain-pseudokinase)	10	NanoBRET (RBC)	>10000
MYLK4	14	Enzymatic (RBC)	35
PIP4K2C	15	NanoBRET (SGC-UNC)	76.6
RIPK5	23	Enzymatic (RBC)	3900

Table S2. Enzymatic profiling of analogs **8** and **17** in targeted kinase panel

Compound	PoC at 1 µM[a]																
	HIPK1	MAP4K5	MARK3	MARK4	PAK3	PAK4	PAK5[b]	PAK6	TAOK1	TAOK2	TAOK3	TSSK1	TSSK2	TSSK3	TSSK4	TTBK1	TTBK2
8	73	47	90	73	98	76	79	97	87	77	88	79	68	132	56	97	81
17	88	14	70	97	81	72	89	77	72	79	77	82	77	79	72	92	98

[a] Compounds tested at a single concentration (1 µM) in duplicate

Table S3. Orthogonal assay results for analog **17**

Kinase	DiscoverX PoC value	Assay format (source)	IC$_{50}$ or K$_d$ value (nM)
PIKFYVE	0.1	Enzymatic (SignalChem) and NanoBRET (SGC-UNC)	6.9 and 4.01
MYLK4	1.8	Enzymatic (RBC) and NanoBRET (SGC-UNC)	66 and 265
MEK1	4.5	Enzymatic (Eurofins)	>10000
RIPK5	5.2	Enzymatic (RBC)	>10000
IRAK3	9.2	NT[a]	-
MEK2	9.6	Enzymatic (Eurofins)	>10000
DYRK1A	9.9	Enzymatic (Eurofins)	2040
YSK4	9.9	Enzymatic (RBC)	4020
ULK3	11	Enzymatic (Eurofins)	>10000
MEK4	12	Enzymatic (Eurofins)	>10000
HASPIN	13	Enzymatic (Eurofins)	1400
STK16	14	Enzymatic (Eurofins)	560

CLK2	20	Enzymatic (Eurofins)	290
CDK7	20	Enzymatic (Eurofins)	>10000
IRAK4	21	Enzymatic (Eurofins)	4500
AURKB	23	Enzymatic (Eurofins)	1400
DYRK1B	26	Enzymatic (Eurofins)	380
CLK1	30	Enzymatic (Eurofins)	420
RIOK2	32	NT	-
CLK4	34	Enzymatic (Eurofins)	440
PIP4K2C	53	NanoBRET (SGC-UNC) and binding (DiscoverX)	>10000 and 1900
MAP4K5	96	Enzymatic (Eurofins) and NanoBRET (SGC-UNC)	89 and >10000

[a] NT: not tested, no assay available.
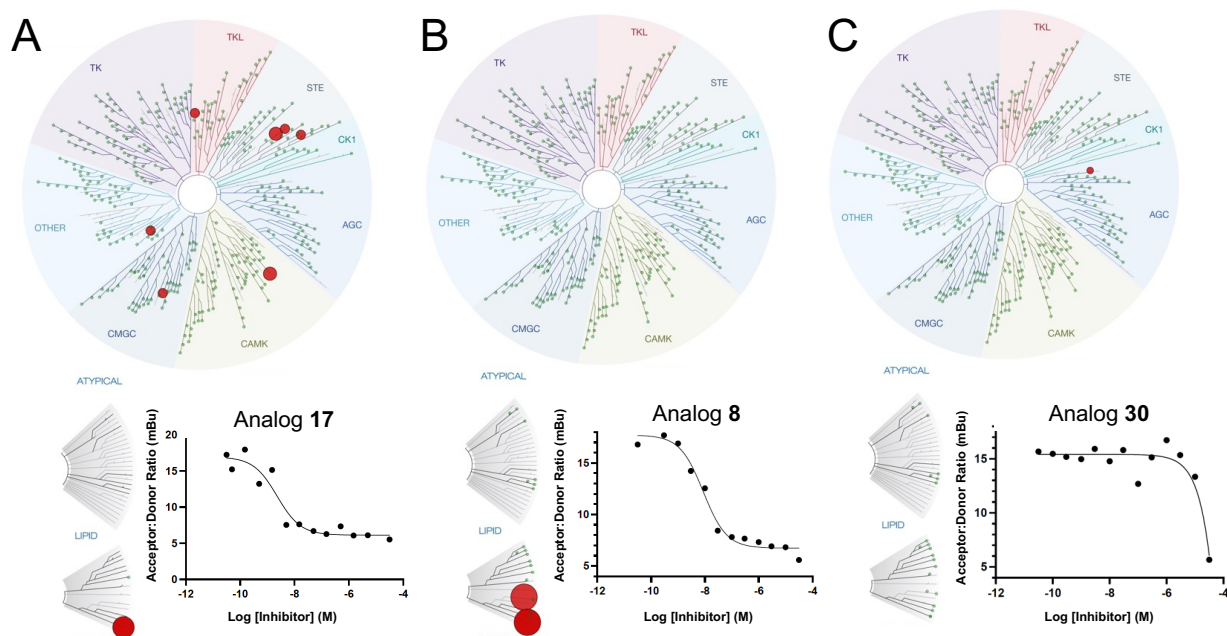
Figure S1. Visualization of DiscoverX *scanMAX* results and PIKfyve NanoBRET curves for chemical probe candidates (A) **17** (S_{10}(1 µM)) and (B) **8** (S_{10}(1 µM)) and (C) negative control compound **30** (S_{35}(1 µM)).

MAP4K5-NL

$IC_{50} >10000$
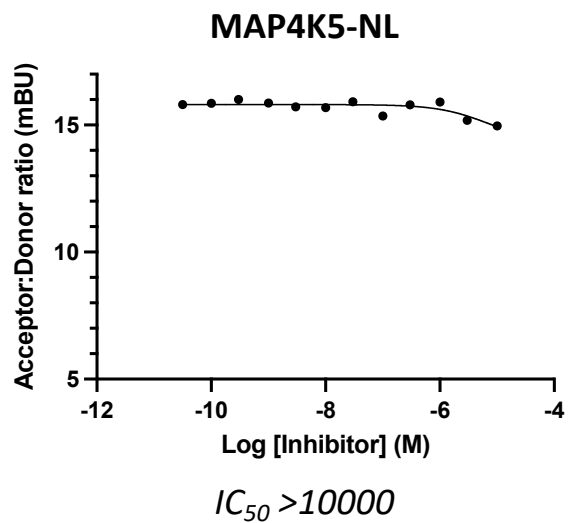
MYLK4-NL

$IC_{50} = 265\ nM$
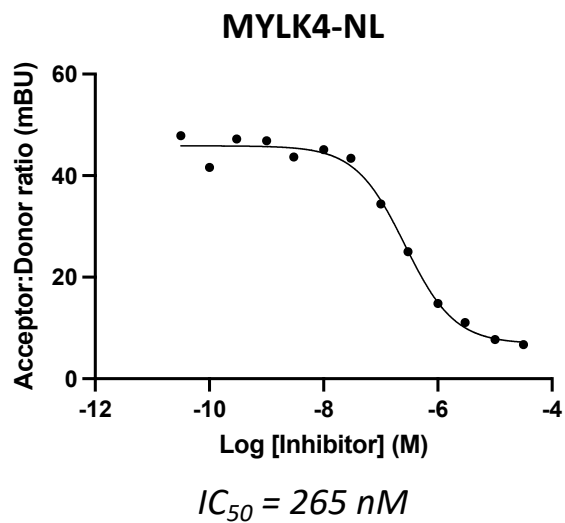
Figure S2. NanoBRET curves and corresponding IC_{50} values for chemical probe candidate **17** versus most potent off-target kinases.
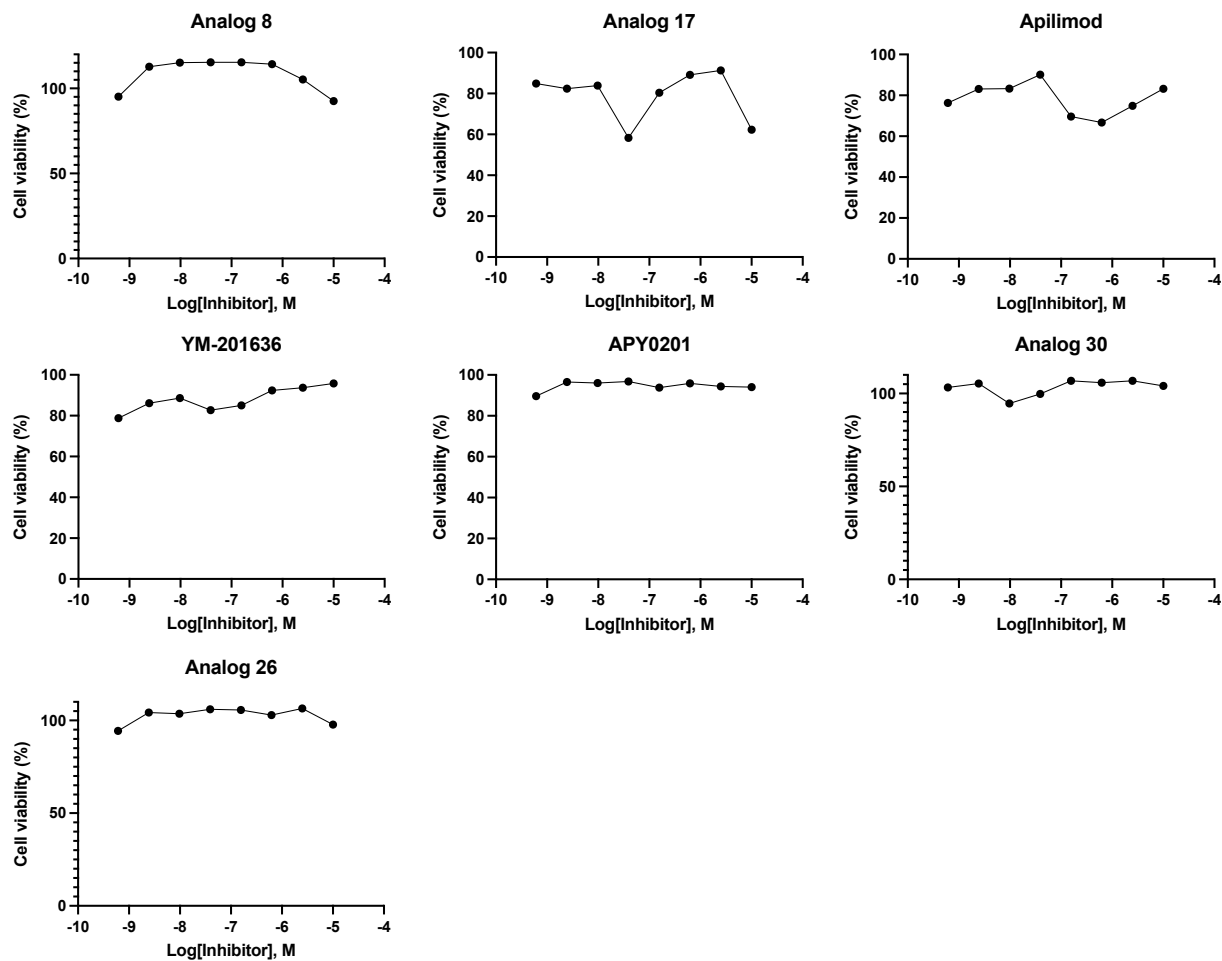
Figure S3. Cell viability data determined by LDH assay in DBT cells after 10 h of continuous treatment. Plot of average values from n = 3 for compounds that exhibit IC_{50} <100 nM in MHV-nLuc assay and negative control **30**.
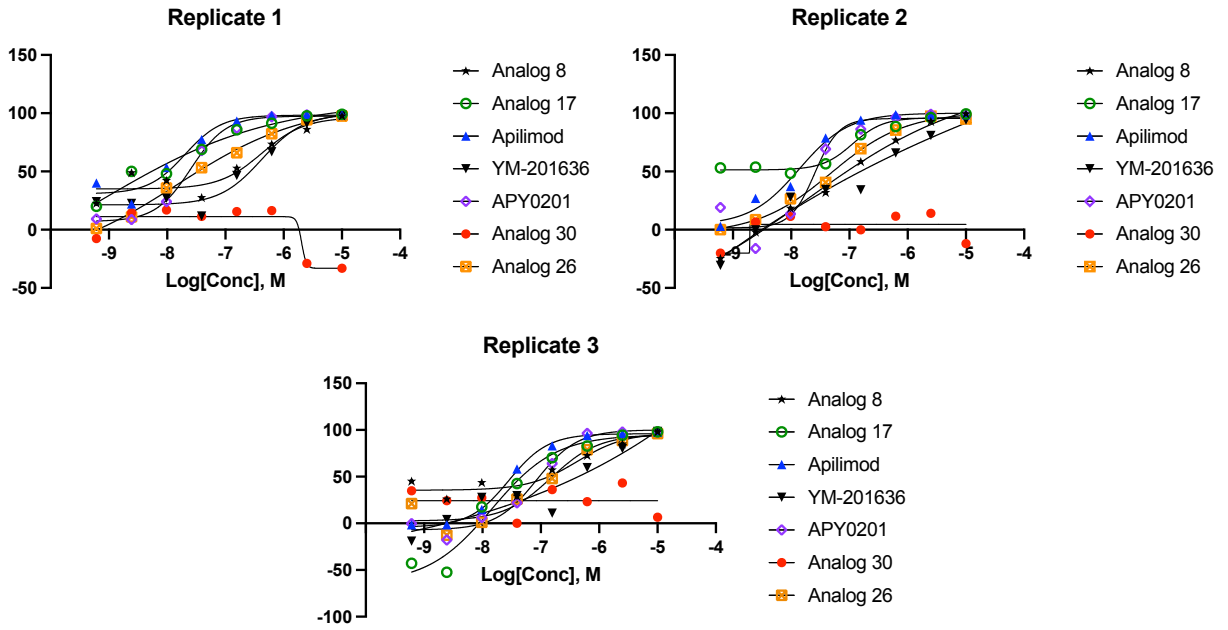
Figure S4. Individual replicates corresponding to effect of PIKfyve inhibitors on replication of MHV-nLuc in DBT cells in Figure 4A.

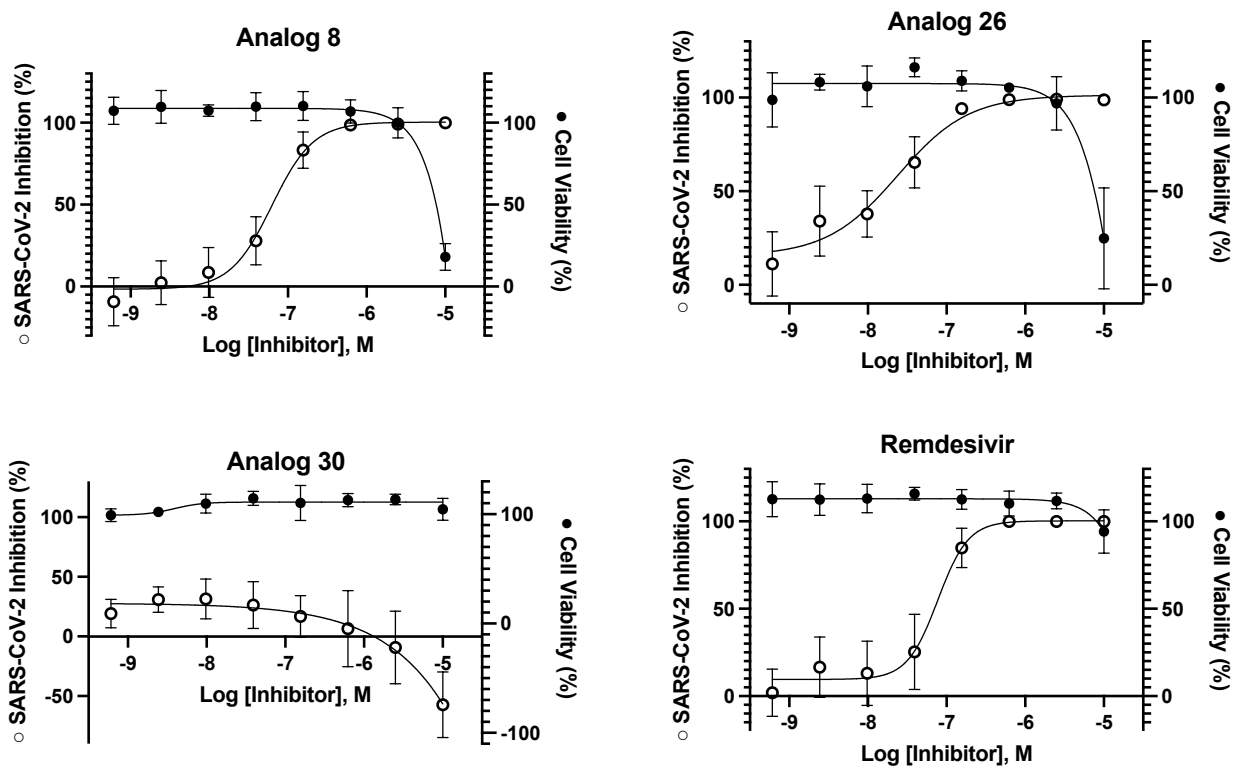**Figure S5.** Effect of indolyl pyrimidinamines and remdesivir (positive control) on viral replication (open circles) in A549–ACE2 cells infected with SARS-CoV-2-nLuc (n = 4). Cell viability determined by LDH assay (closed circles) in A549–ACE2 cells (n = 2). These individual graphs correspond with the compounds included in Figure 4C. Error bars represent SEM.
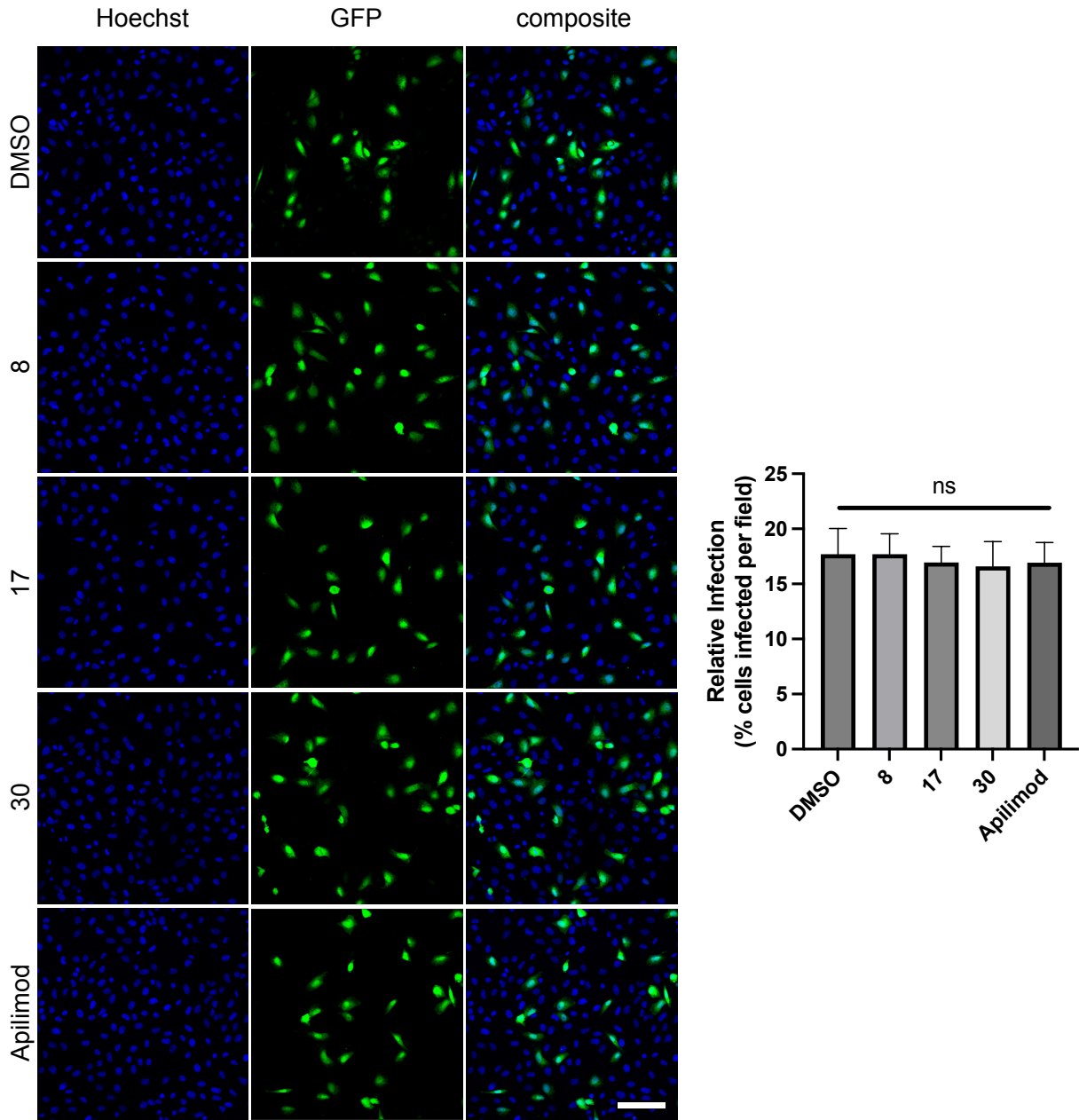
Figure S6. Uptake of bald GFP lentivirus is not inhibited by PIKfyve inhibitors. Calu-3 cells were incubated with 1 μM of each compound (or DMSO) for 1 h followed by the addition of the bald GFP lentivirus for 12 h. Cells were fixed and stained with Hoechst to label nuclei. Cells were also imaged for GFP, following transduction from the pseudovirus. Scale bar (shown in white in the bottom right corner of images) = 100 μm. Bar graph shows the quantification of bald GFP lentivirus infection from experiments: n = 9 from three independent experiments, mean ± SD; one-way *ANOVA* followed Tukey's test; ns = not significant when p >0.05.

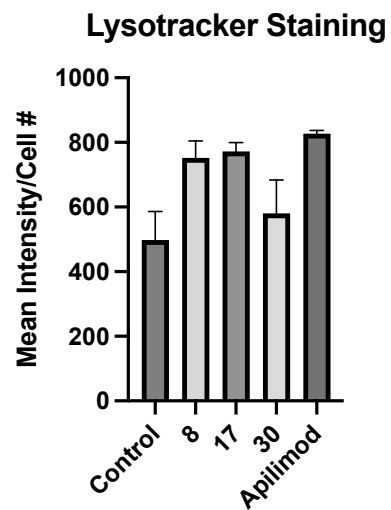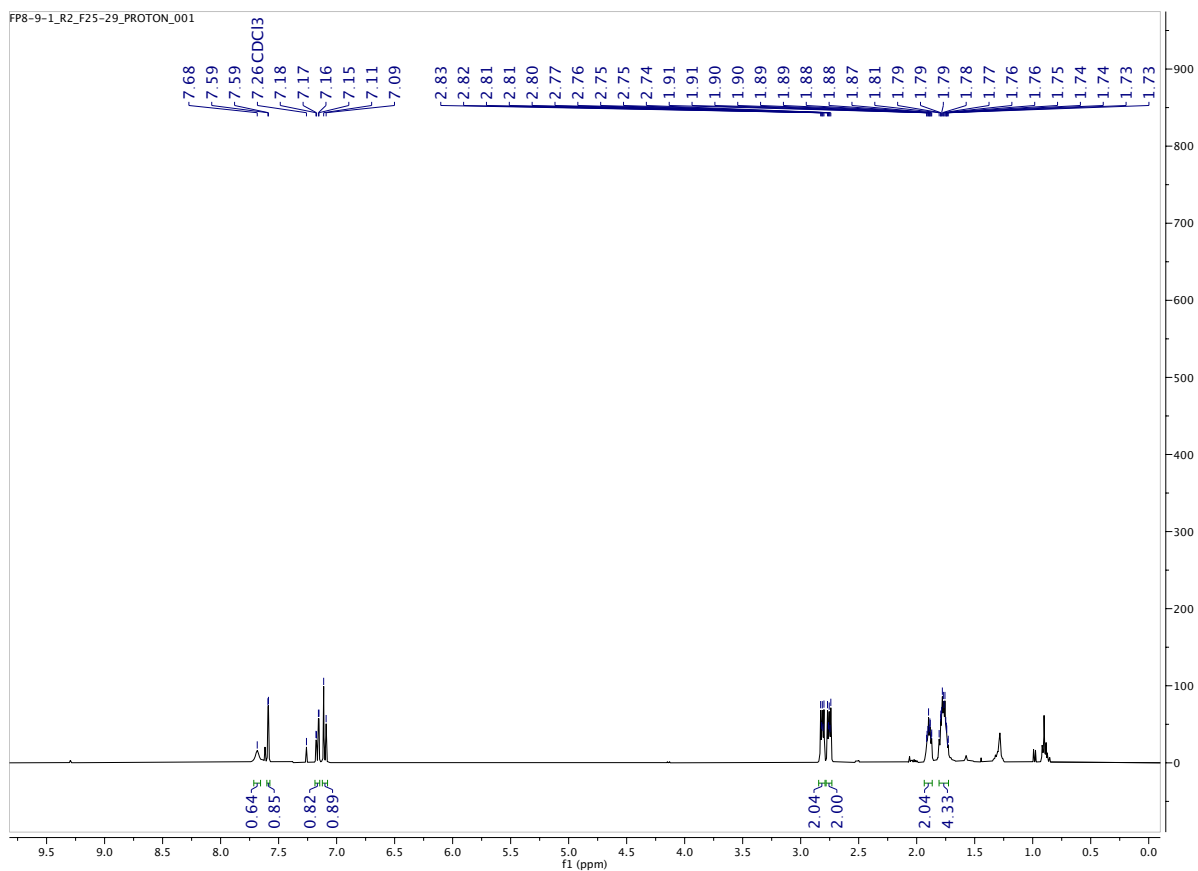**Lysotracker Staining**

Figure S7. Quantification of fluorescence from Lysotracker staining in Figure 7.

Compound Characterization – Experimental Spectra

2-bromo-5,6,7,8,9,10-hexahydrocyclohepta[b]indol (34).
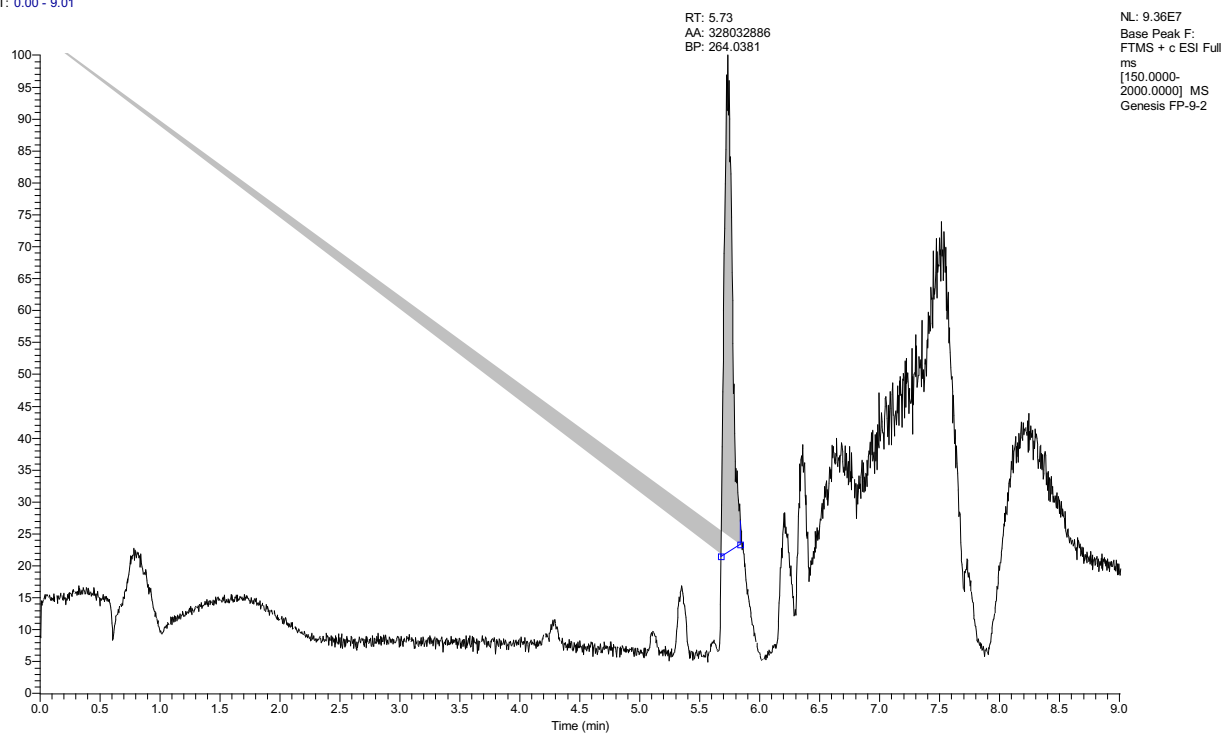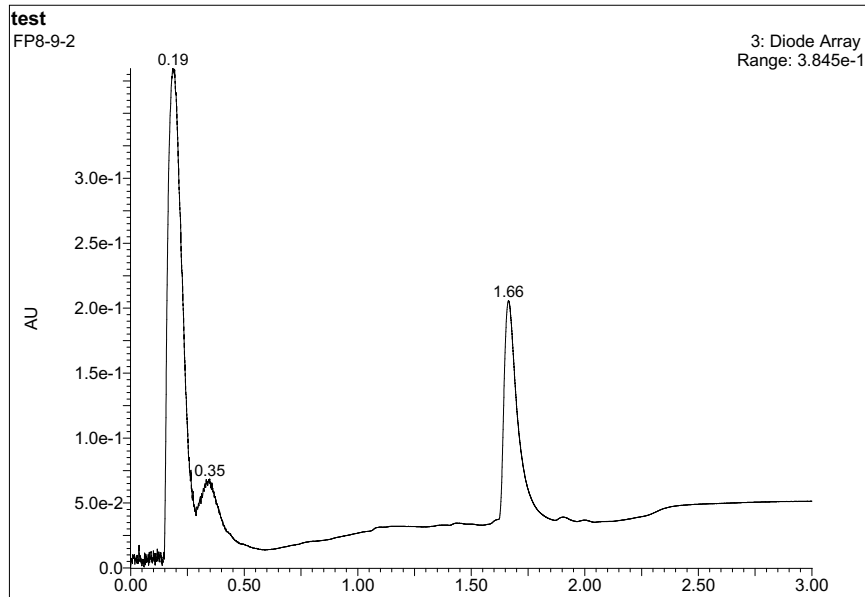**¹H NMR**

^{13}C NMR
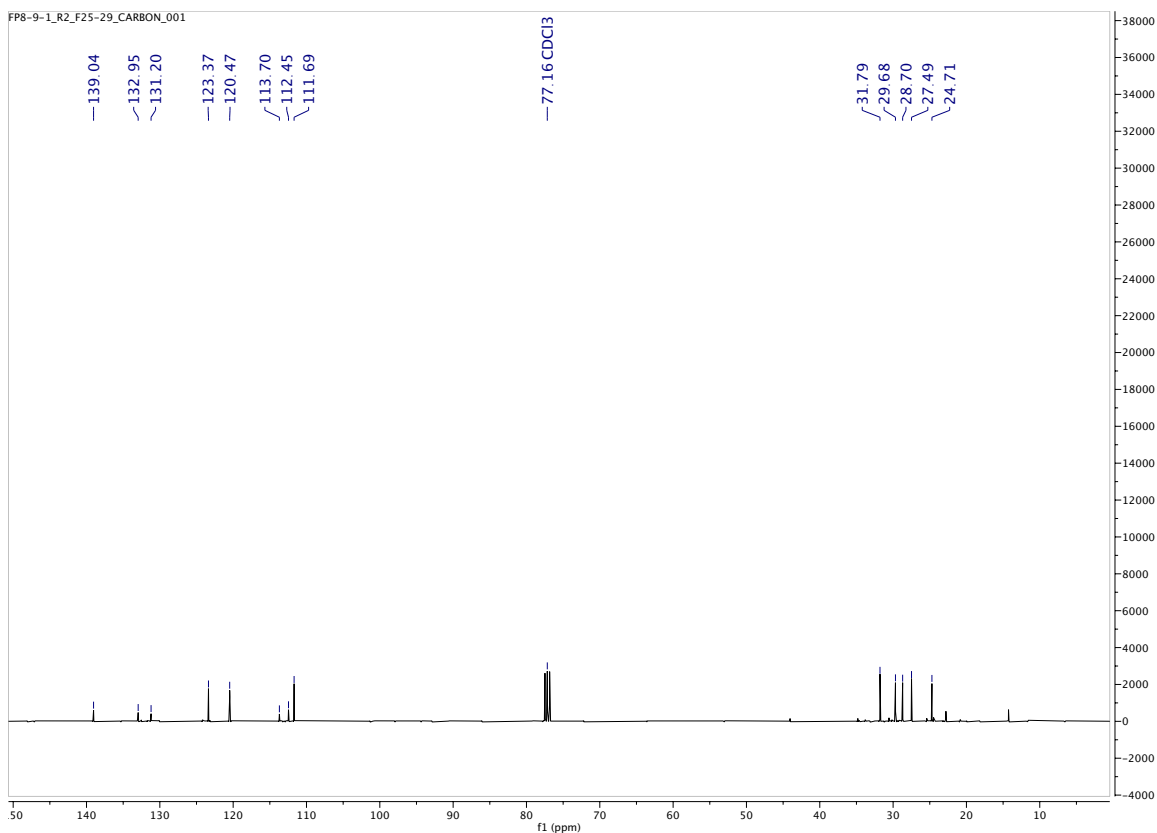
FP8-9-1_R2_F25-29_CARBON_001

139.04
132.95
131.20
123.37
120.47
113.70
112.45
111.69
77.16 CDCl3
31.79
29.68
28.70
27.49
24.71

f1 (ppm)

LC Chromatogram HRMS

RT: 0.00 - 9.01

RT: 5.73
AA: 328032886
BP: 264.0381

NL: 9.36E7
Base Peak F:
FTMS + c ESI Full
ms
[150.0000-
2000.0000] MS
Genesis FP-9-2

Time (min)
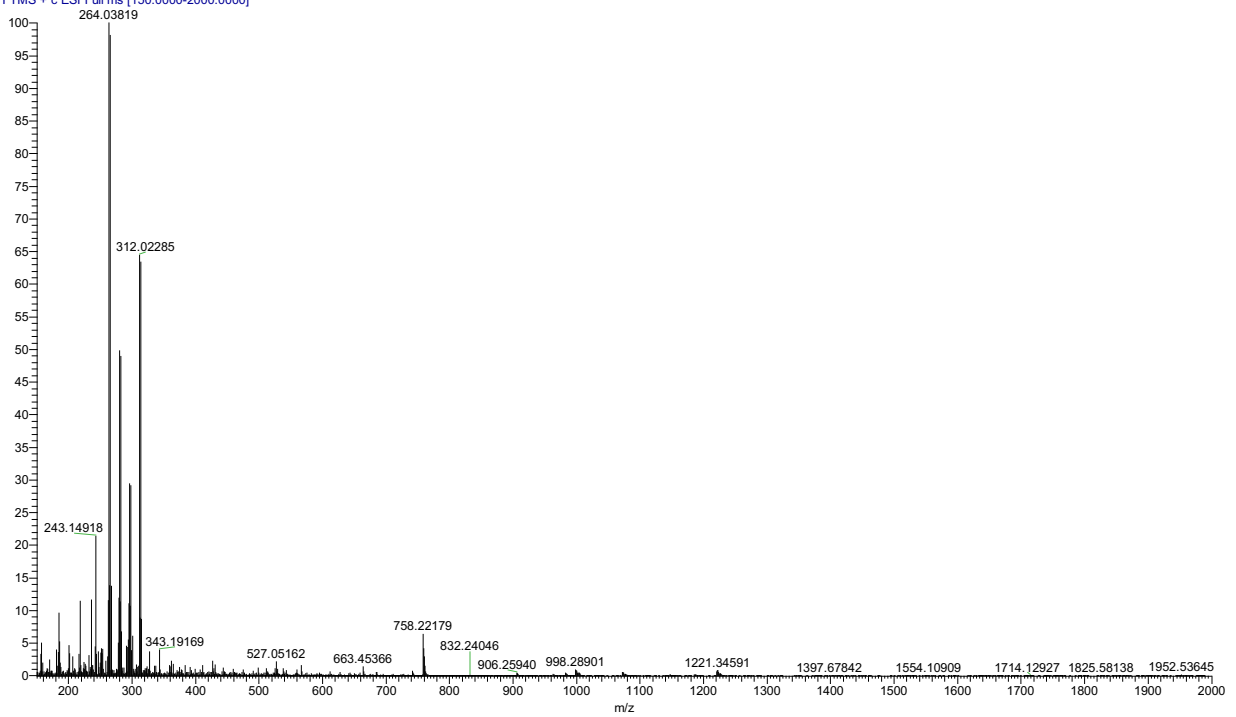
LC Chromatogram LCMS
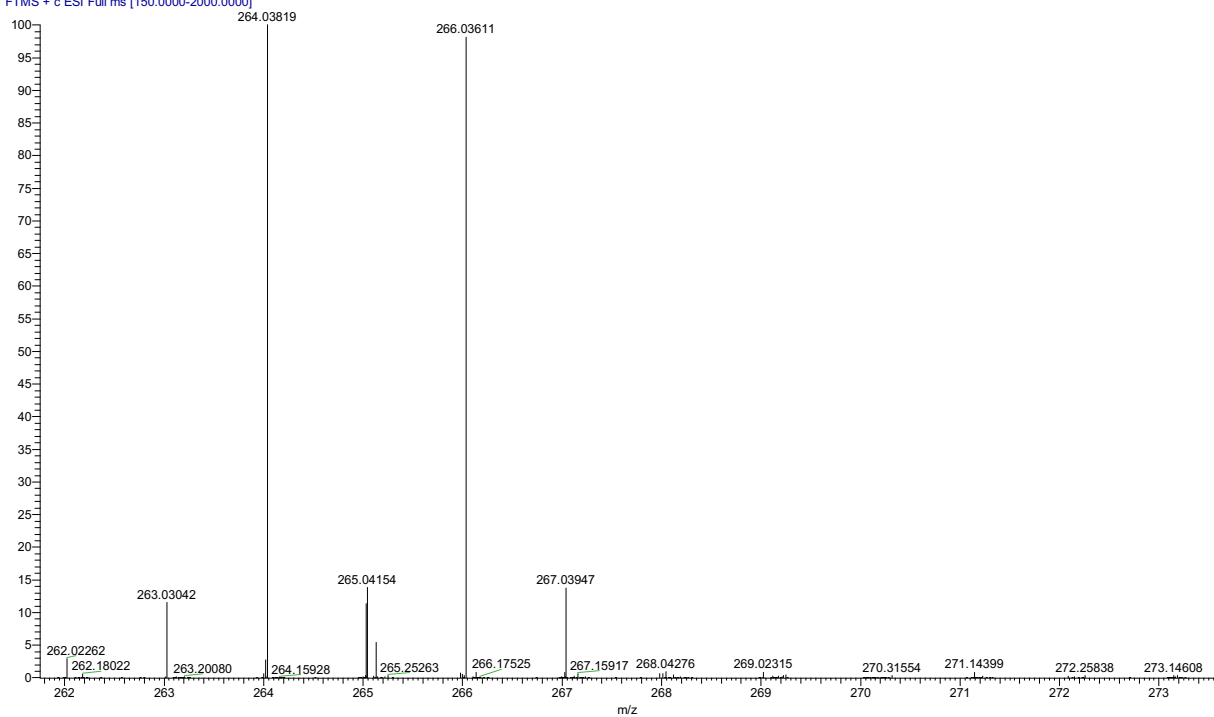
HRMS

*6-bromo-1,2,3,9-tetrahydro-4H-carbazol-4-one (**36**).*
¹H NMR
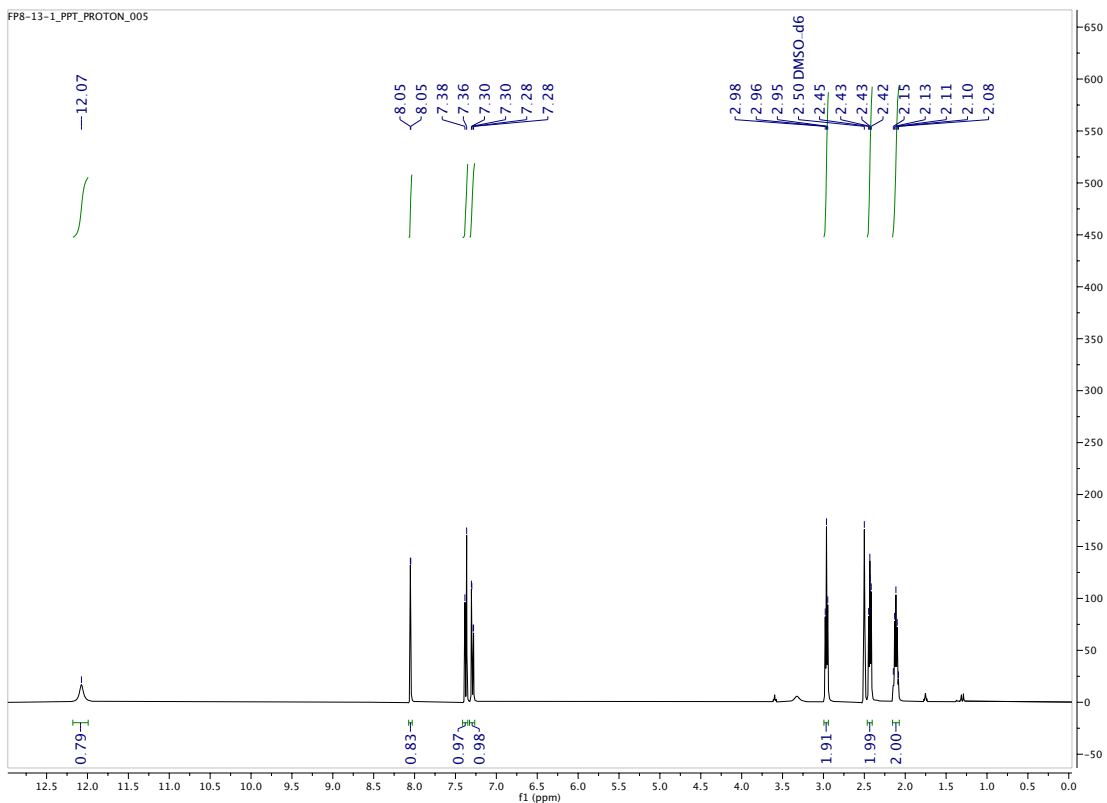
^{13}C NMR
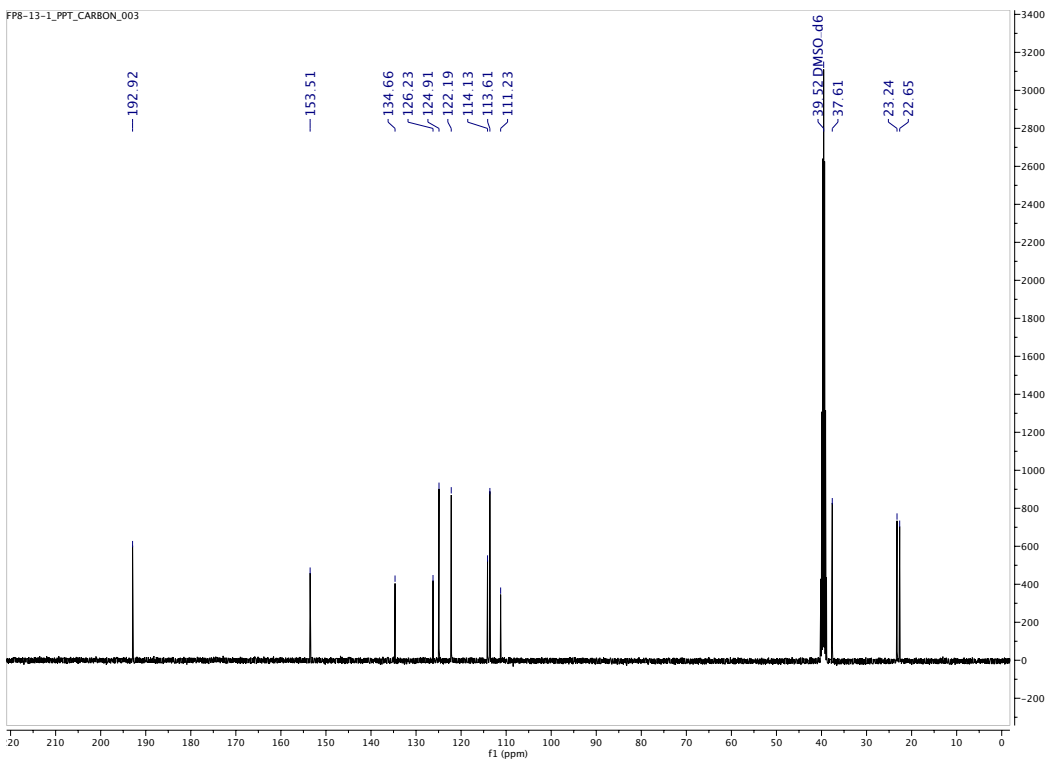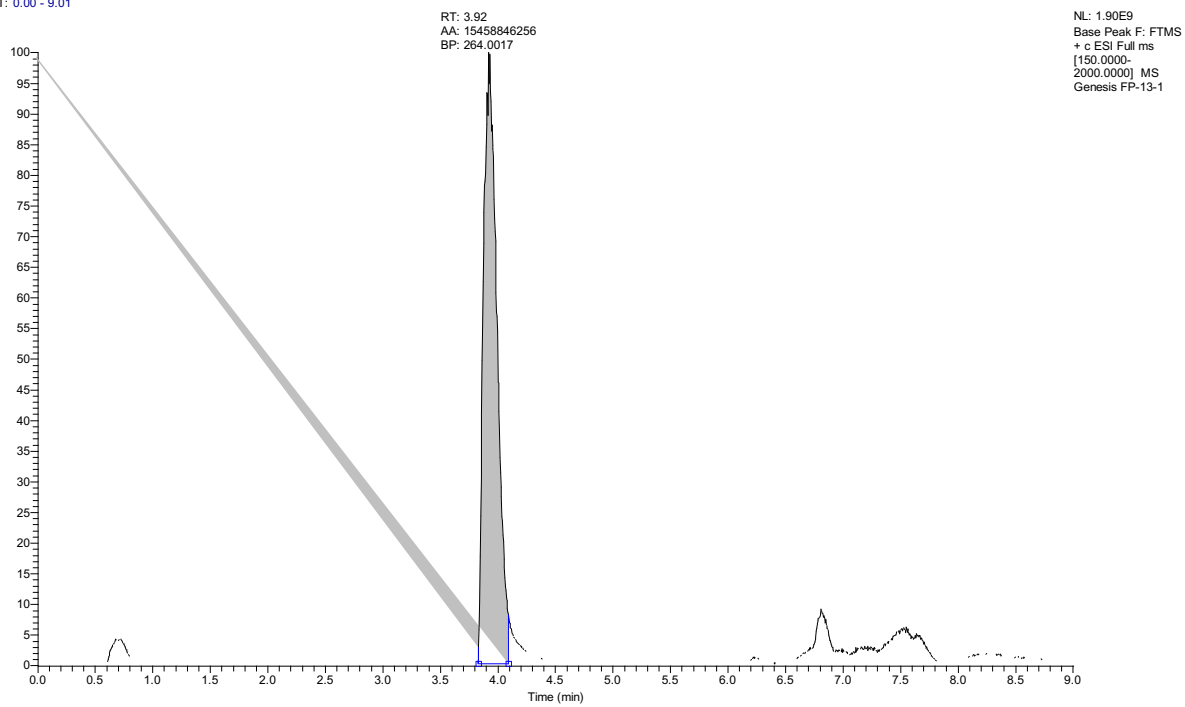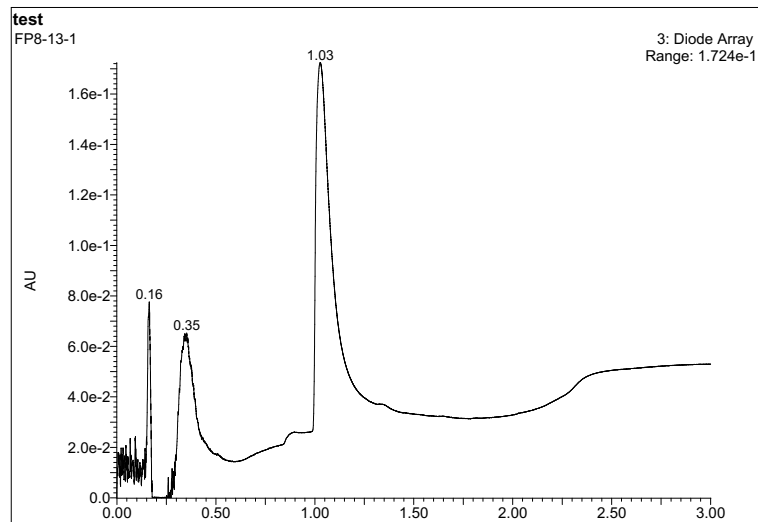
FP8-13-1_PPT_CARBON_003

192.92
153.51
134.66
126.23
124.91
122.19
114.13
113.61
111.23
39.52 DMSO-d6
37.61
23.24
22.65

f1 (ppm)

LC Chromatogram HRMS

RT: 0.00 - 9.01

RT: 3.92
AA: 15458846256
BP: 264.0017

NL: 1.90E9
Base Peak F: FTMS
+ c ESI Full ms
[150.0000-
2000.0000] MS
Genesis FP-13-1

Time (min)

LC Chromatogram LCMS

test
FP8-13-1

3: Diode Array
Range: 1.724e-1
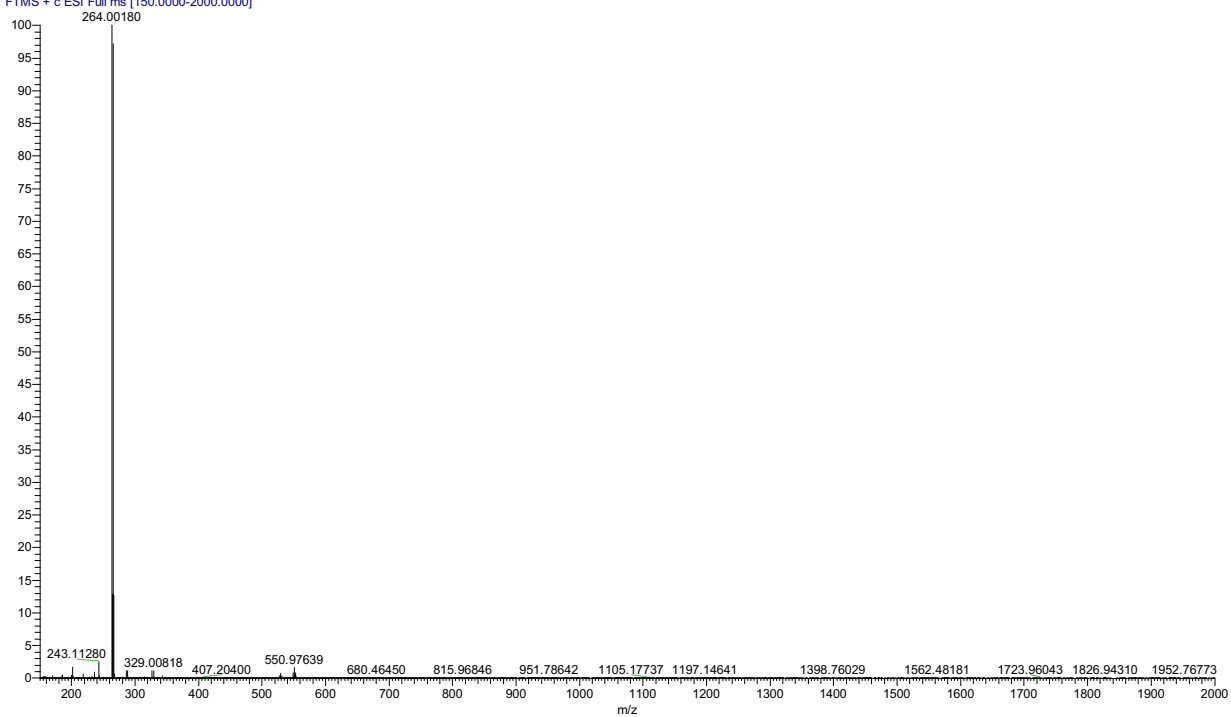
HRMS

*2-bromo-6,7,8,9-tetrahydrocyclohepta[b]indol-10(5H)-one (**37**).*

¹H NMR

¹³C NMR

LC Chromatogram HRMS

RT: 4.21
AA: 11940895429
BP: 278.0174

RT: 6.60
AA: 9371195611
BP: 684.2034
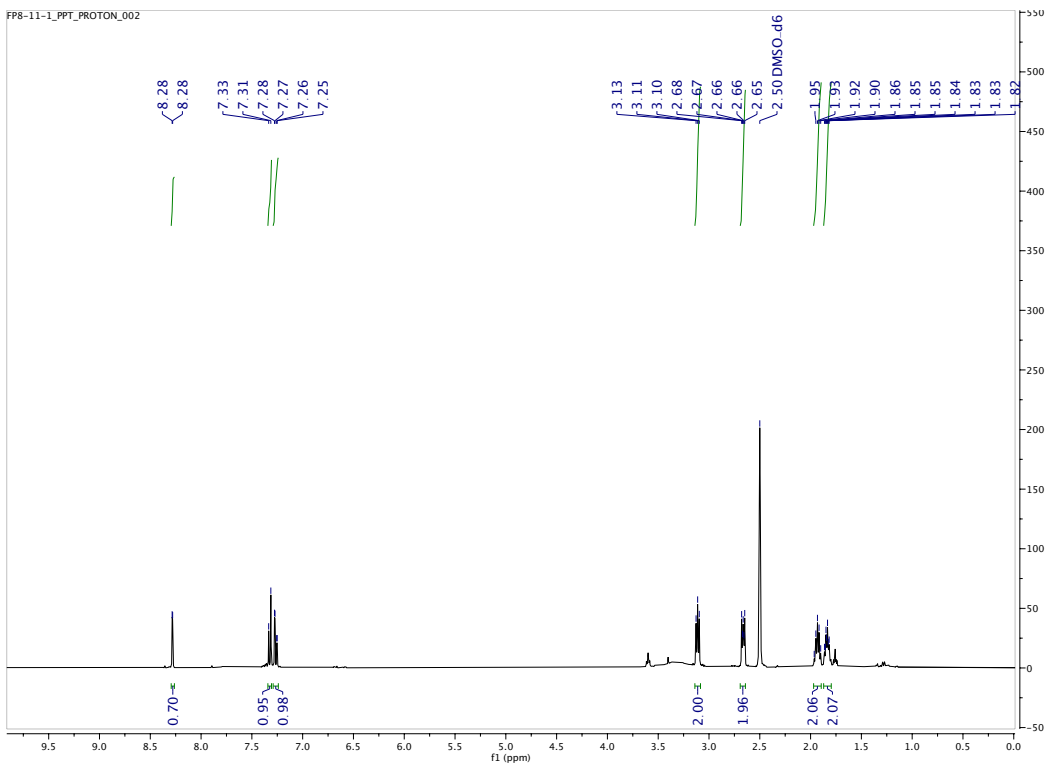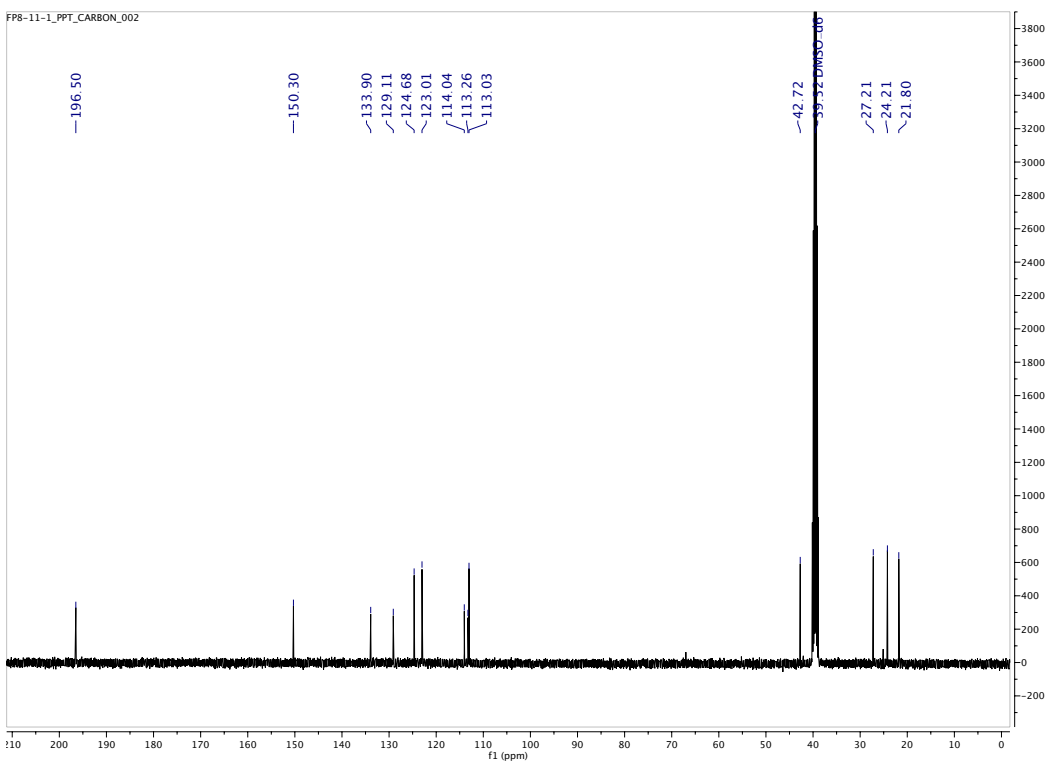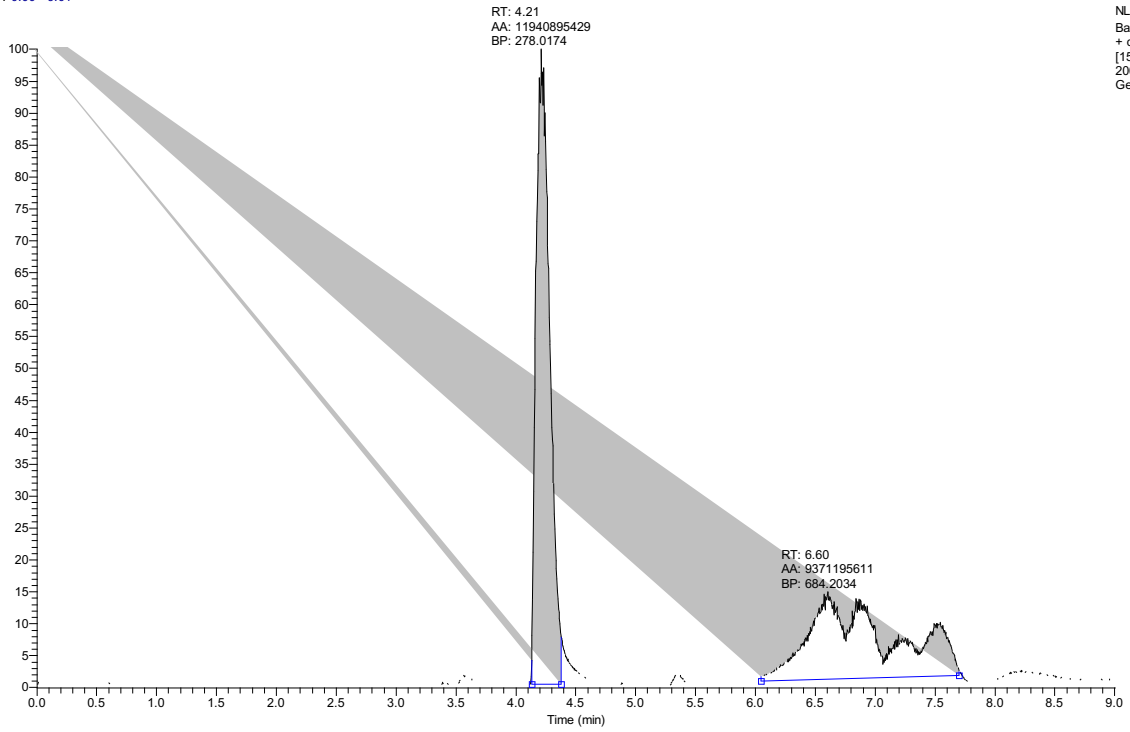
NL: 1.52E9
Base Peak F: FTMS
+ c ESI Full ms
[150.0000-
2000.0000] MS
Genesis FP-11-2

Time (min)

LC Chromatogram LCMS

test

FP8-11-2

3: Diode Array
Range: 8.069e-2

0.16

0.35

1.15

0.00

AU

S17
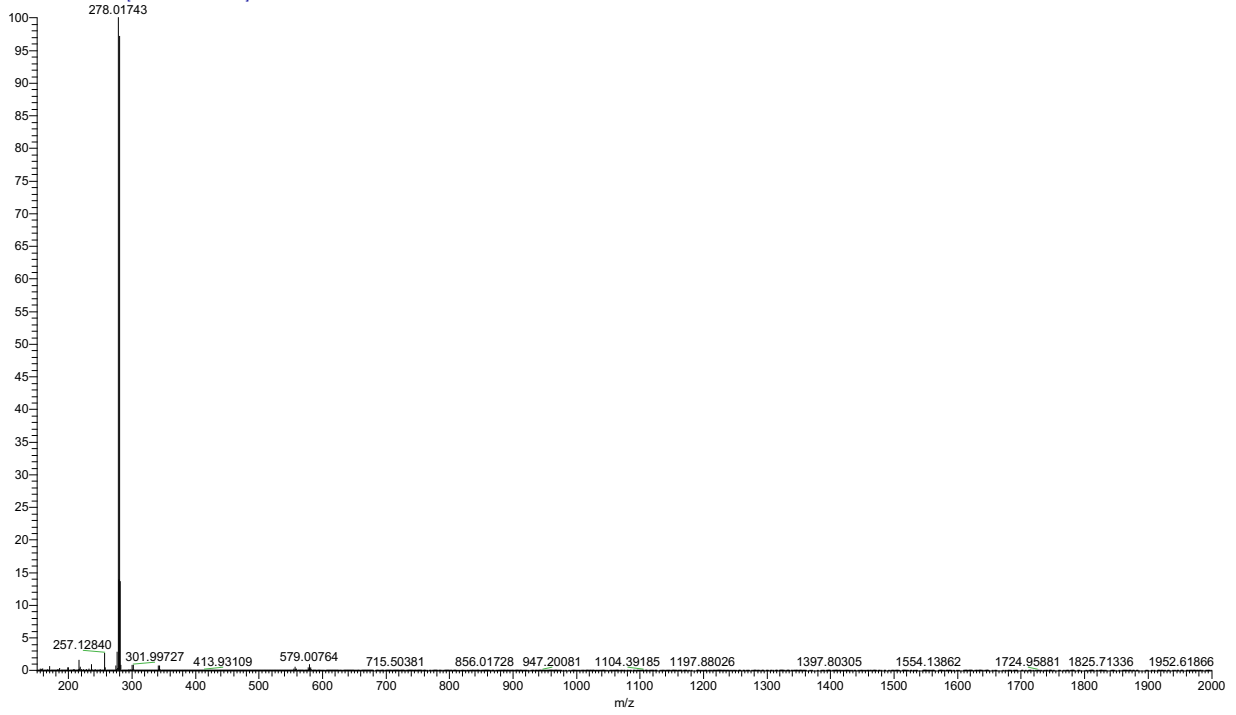
HRMS

2-bromo-5,6,7,8,9,10-hexahydro-11H-cycloocta[b]indol-11-one (38).
^{1}H NMR
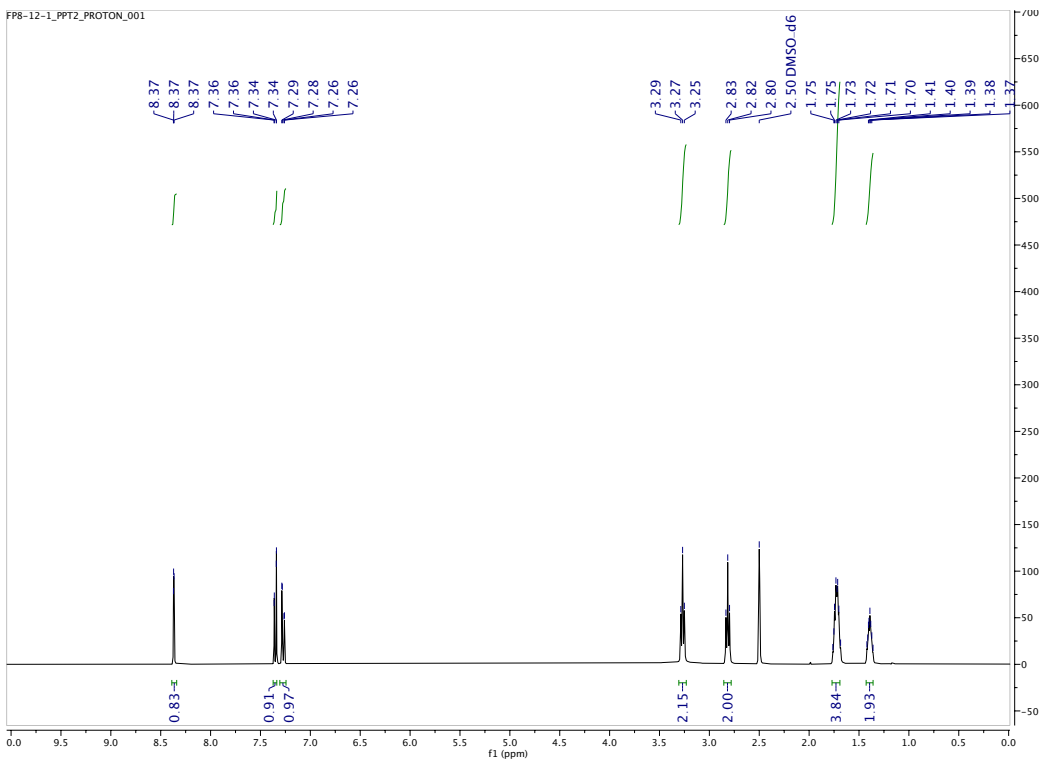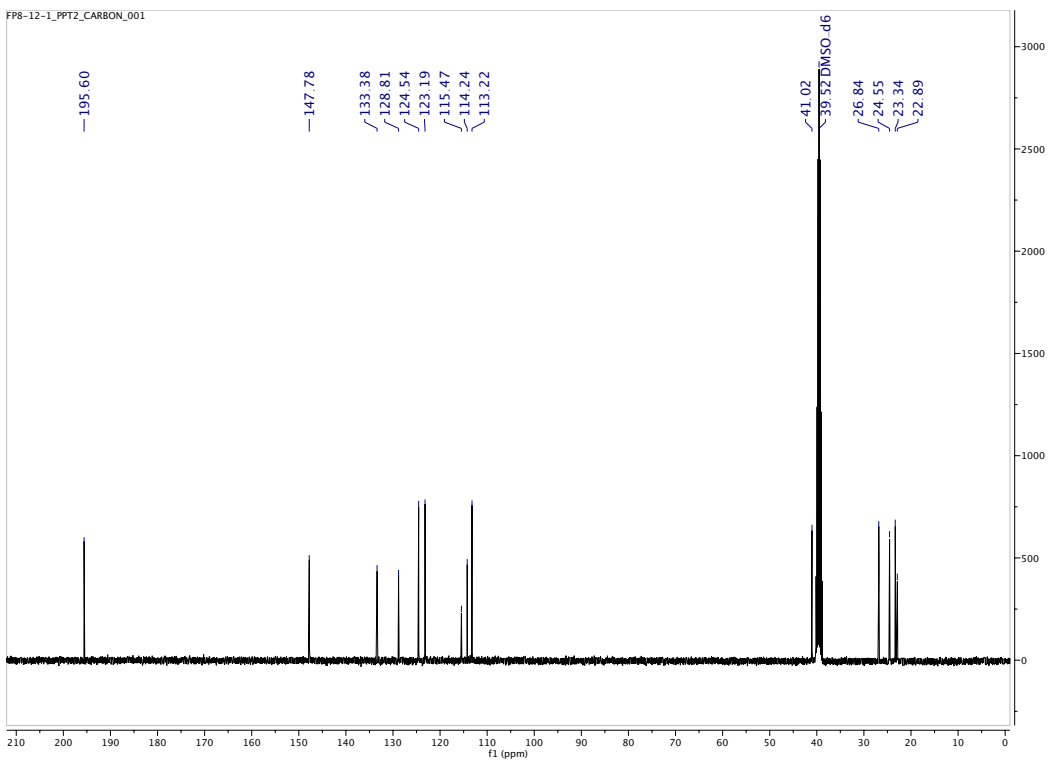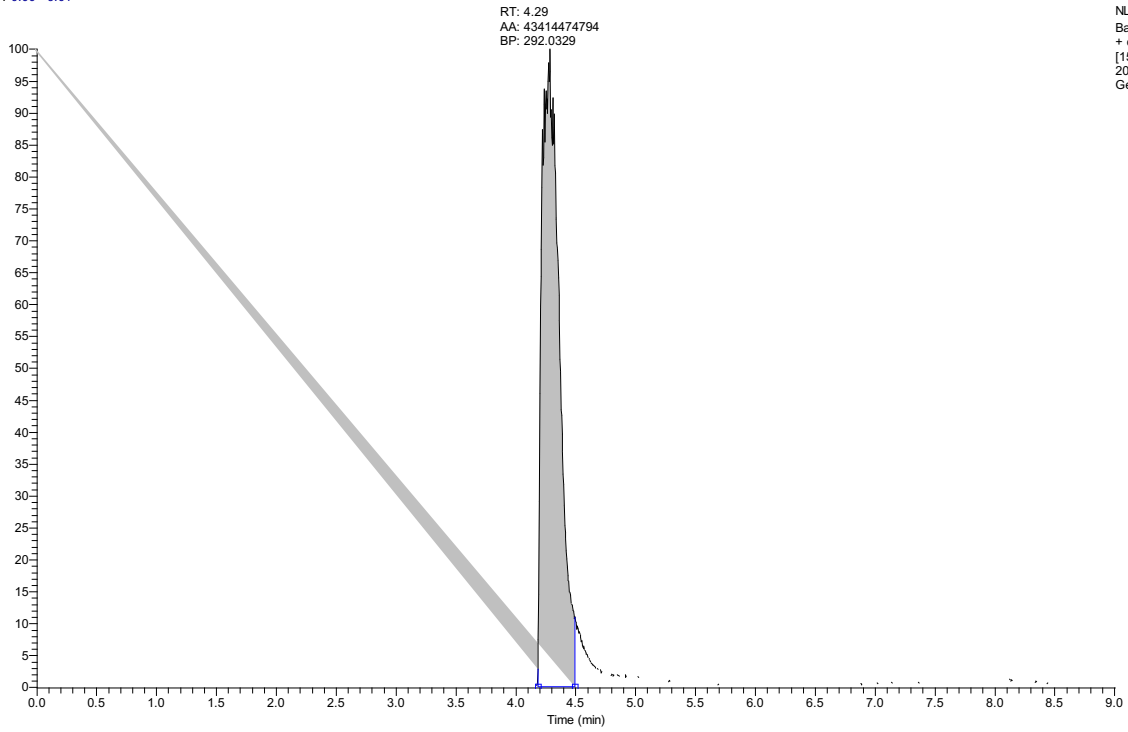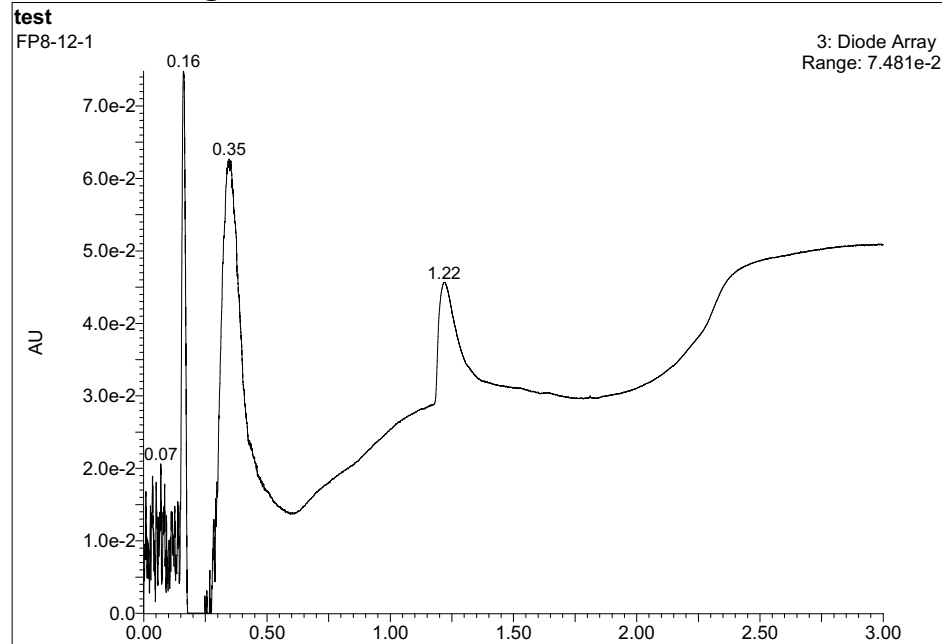
FP8-12-1_PPT2_PROTON_001

8.37
8.37
8.37
7.36
7.34
7.34
7.29
7.28
7.26
7.26

3.29
3.27
3.25
2.83
2.82
2.80
2.50 DMSO.d6
1.75
1.75
1.73
1.72
1.71
1.70
1.41
1.40
1.39
1.38
1.37

0.83
0.91
0.97
2.15
2.00
3.84
1.93

^{13}C NMR

FP8-12-1_PPT2_CARBON_001

195.60

147.78

133.38
128.81
124.54
123.19
115.47
114.24
113.22

41.02
39.52 DMSO.d6
26.84
24.55
23.34
22.89

LC Chromatogram HRMS

RT: 0.00 - 9.01

RT: 4.29
AA: 43414474794
BP: 292.0329

NL: 4.27E9
Base Peak F: FTMS
+ c ESI Full ms
[150.0000-
2000.0000] MS
Genesis FP-12-1

Time (min)

LC Chromatogram LCMS

test
FP8-12-1

3: Diode Array
Range: 7.481e-2

0.16

0.35

1.22

0.07

AU
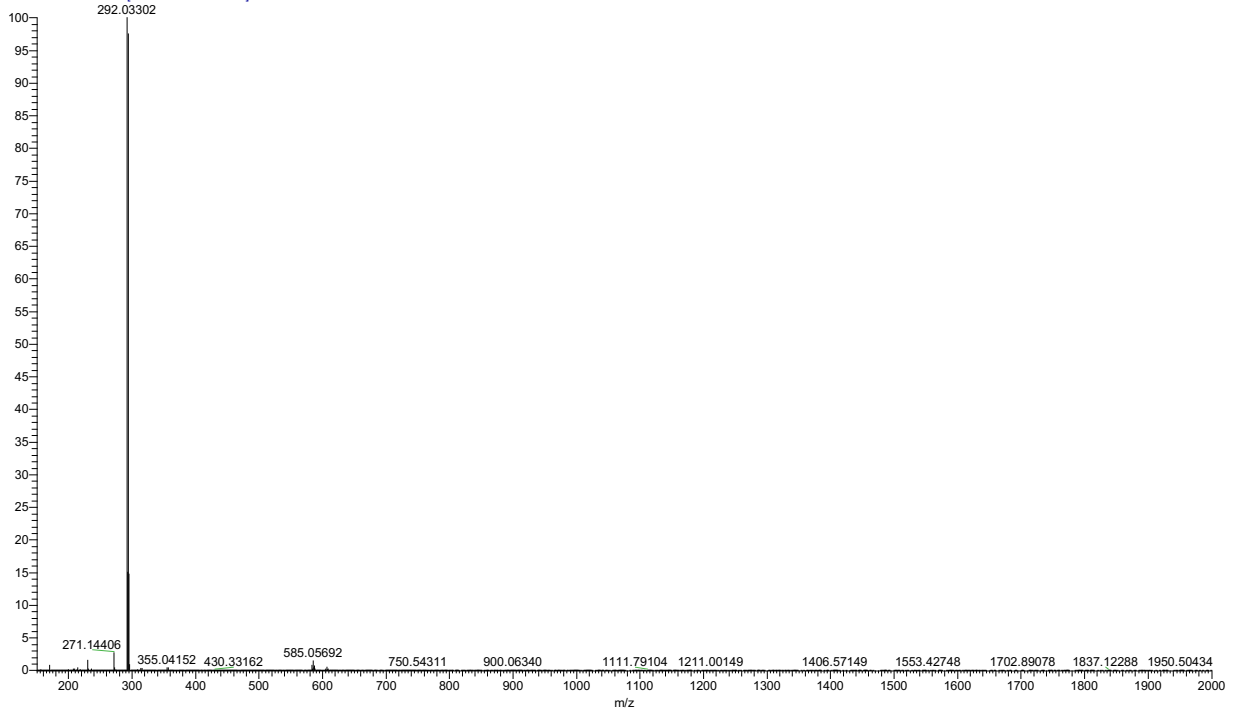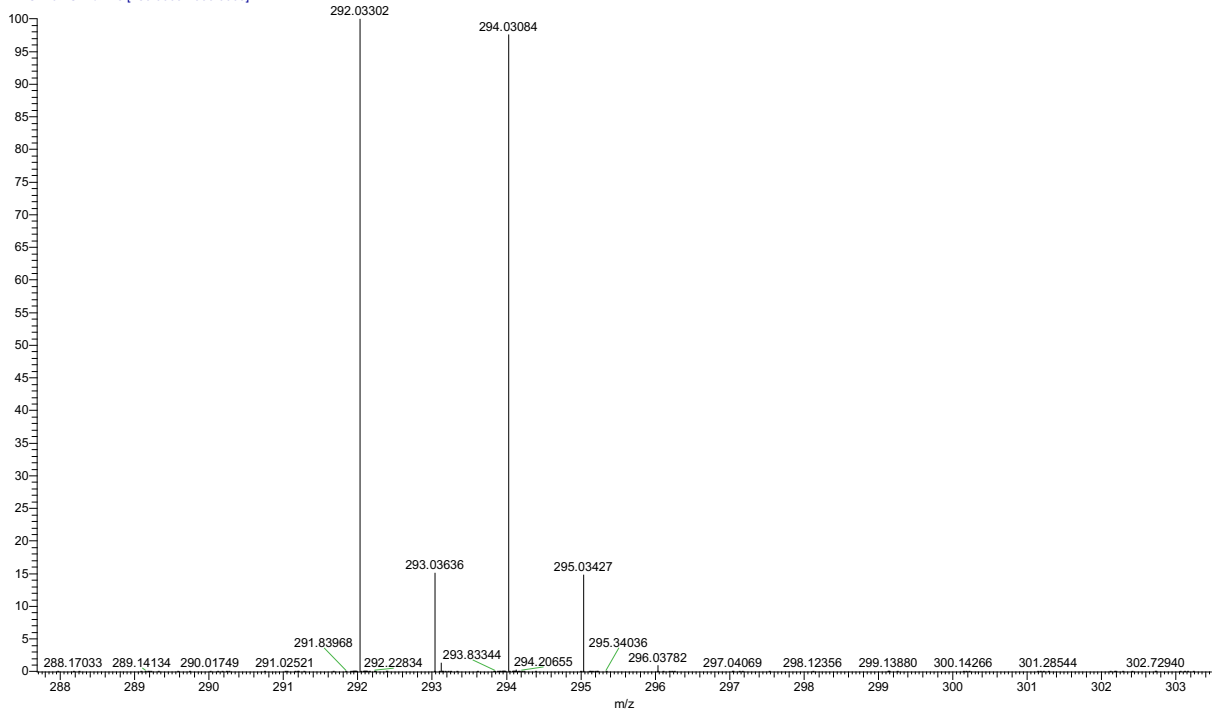
HRMS

*10-bromo-6,7-dihydro-5H-pyrimido[5,4-c]carbazol-2-amine (**42**).*
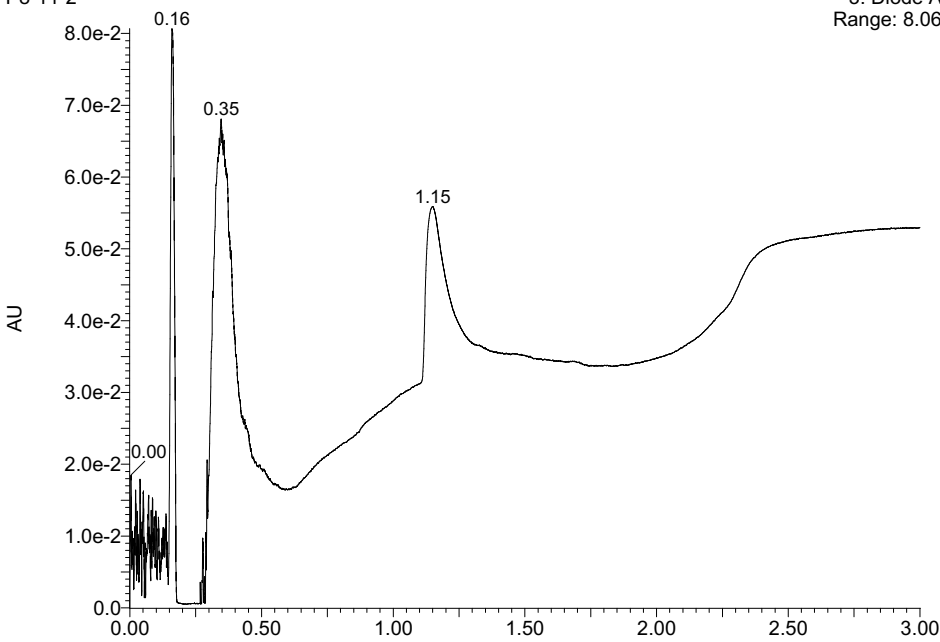
¹H NMR

¹³C NMR

LC Chromatogram HRMS

RT: 3.19
AA: 10041088601
BP: 315.0237

NL: 1.12E9
Base Peak F: FTMS
+ c ESI Full ms
[150.0000-
2000.0000] MS
Genesis FP-19-2
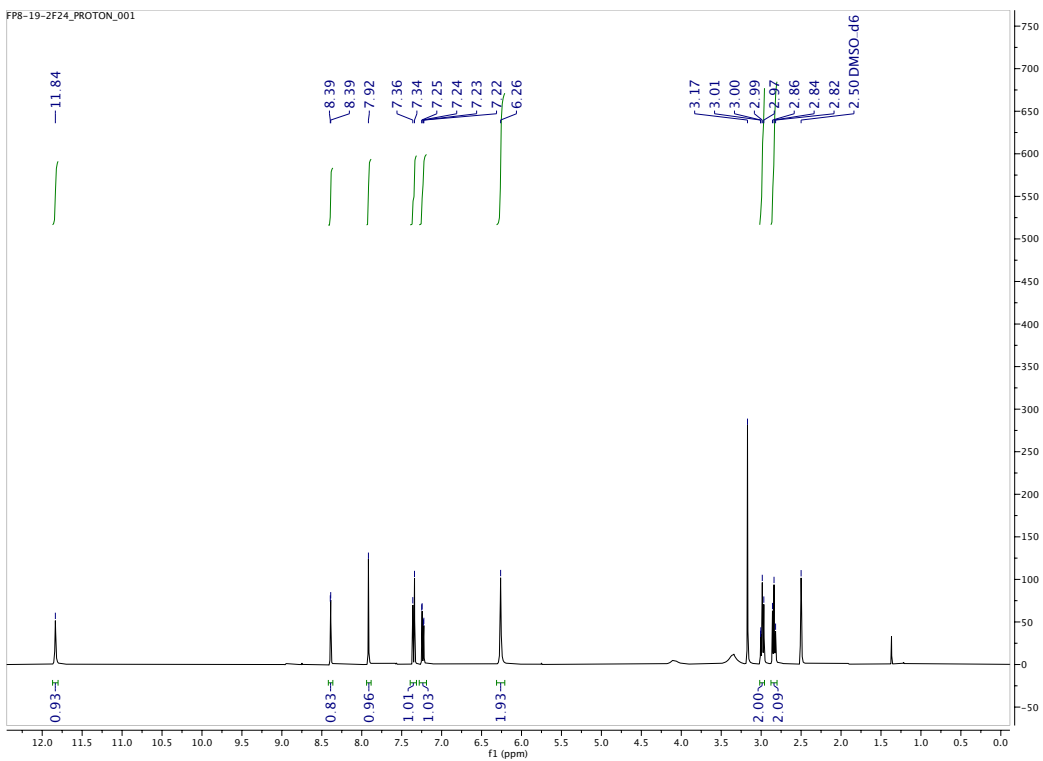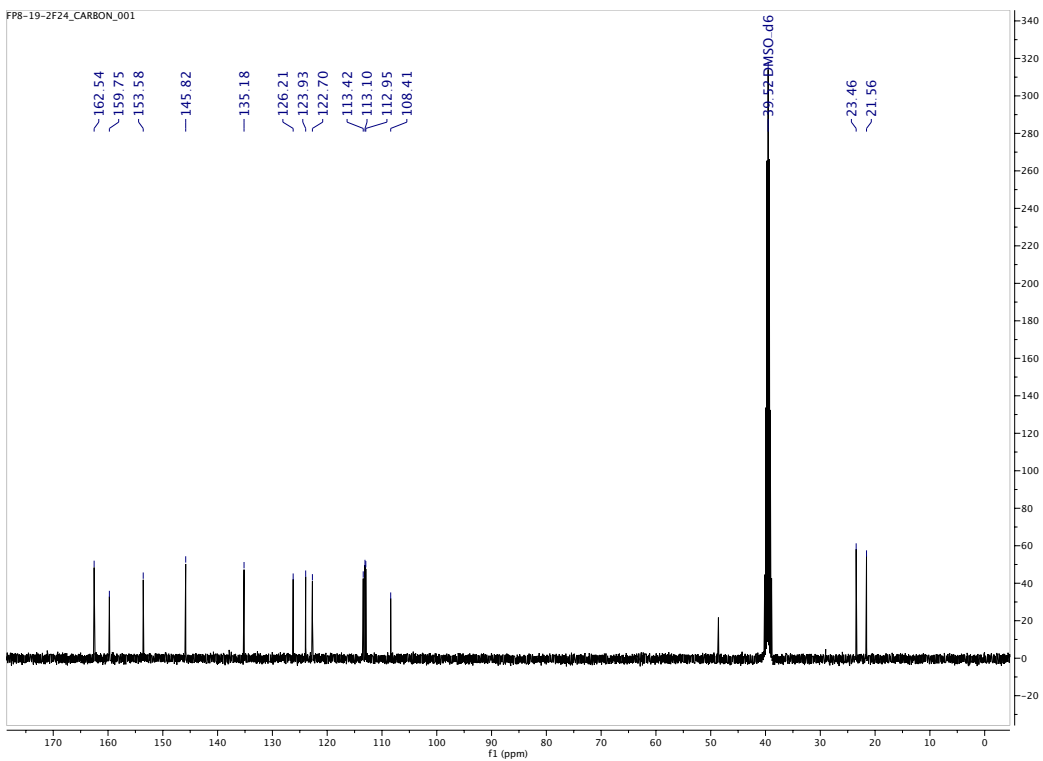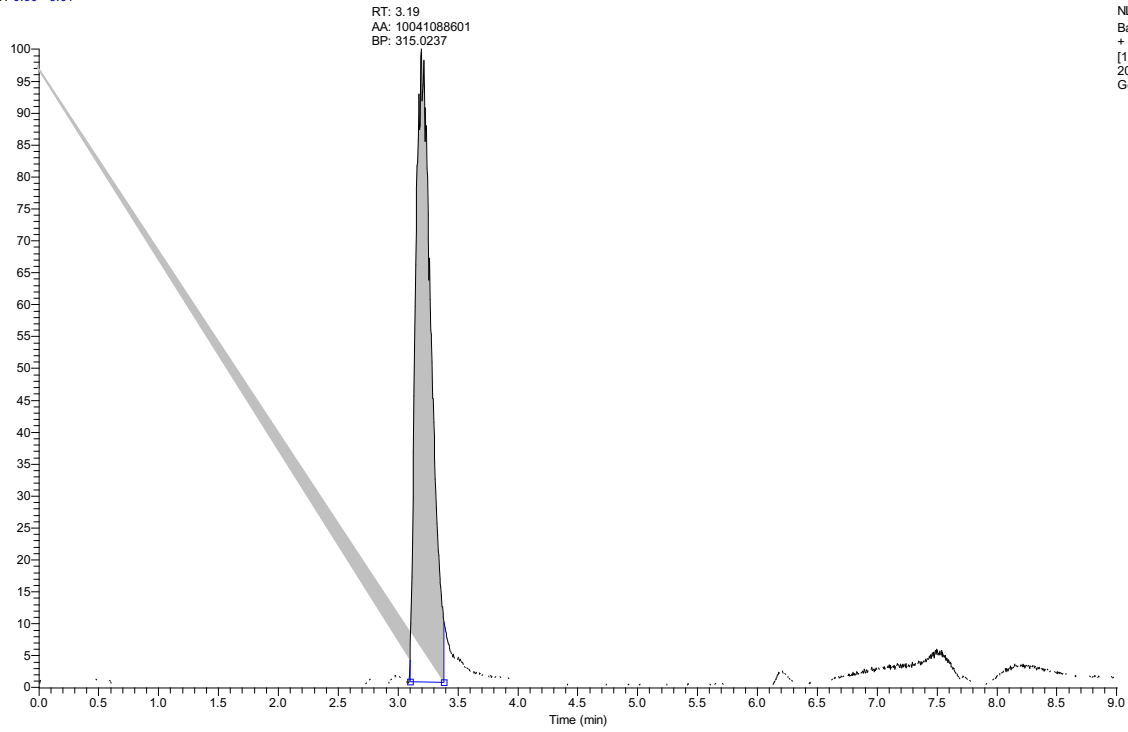
HRMS

FP-19-2 #723-783   RT: 3.12-3.38   AV: 61   NL: 6.33E8
T: FTMS + c ESI Full ms [150.0000-2000.0000]

315.02387

236.12812   345.03443   555.11404   635.02239   730.96435   880.55676   981.79657   1064.59802   1199.39148   1398.50540   1553.73222   1637.64056   1826.56751   1952.48433
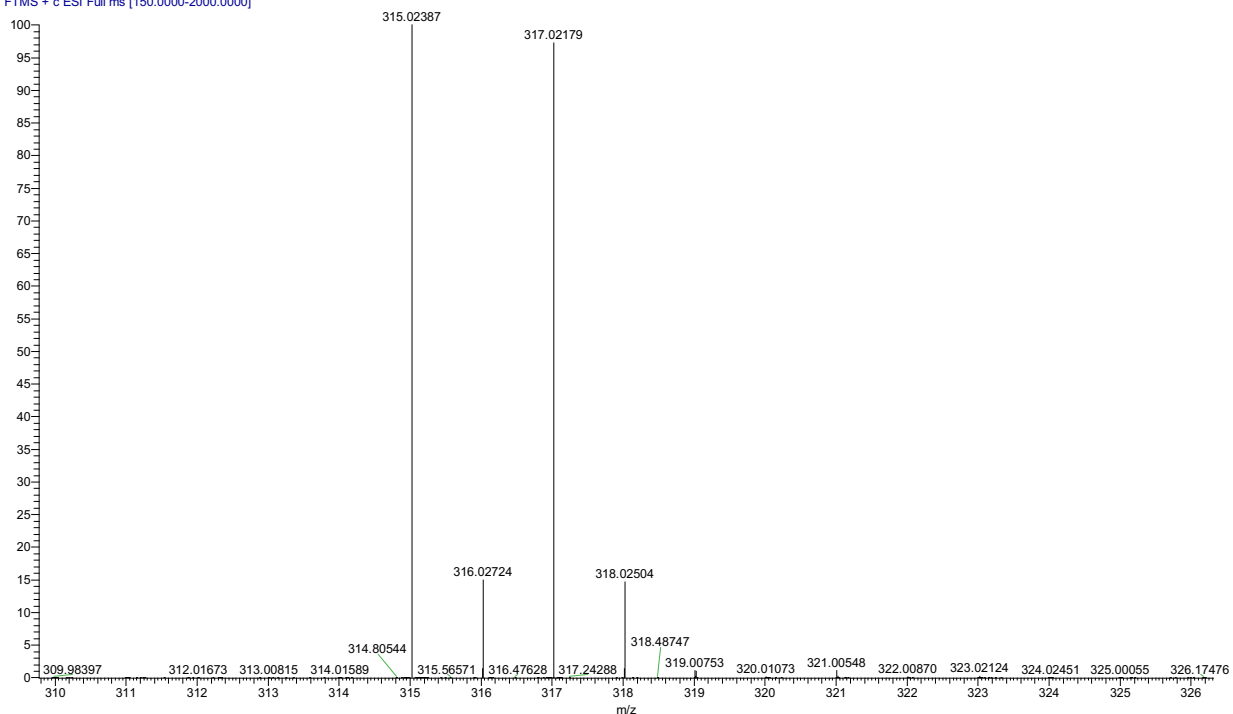
11-bromo-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-2-amine (43).
¹H NMR

¹³C NMR

FP8-22-1_F28_CARBON_001

164.10, 163.01, 156.66, 146.06, 136.50, 130.73, 126.47, 125.86, 122.82, 114.66, 112.74, 111.55, 31.23, 30.72, 25.49

LC Chromatogram HRMS

RT: 0.00 - 9.01

RT: 3.07
AA: 12977780841
BP: 329.0396

NL: 1.24E9
Base Peak F: FTMS
+ c ESI Full ms
[150.0000-
2000.0000] MS
Genesis FP-22-1

LC Chromatogram LCMS

test
FP8-22-1

3: Diode Array
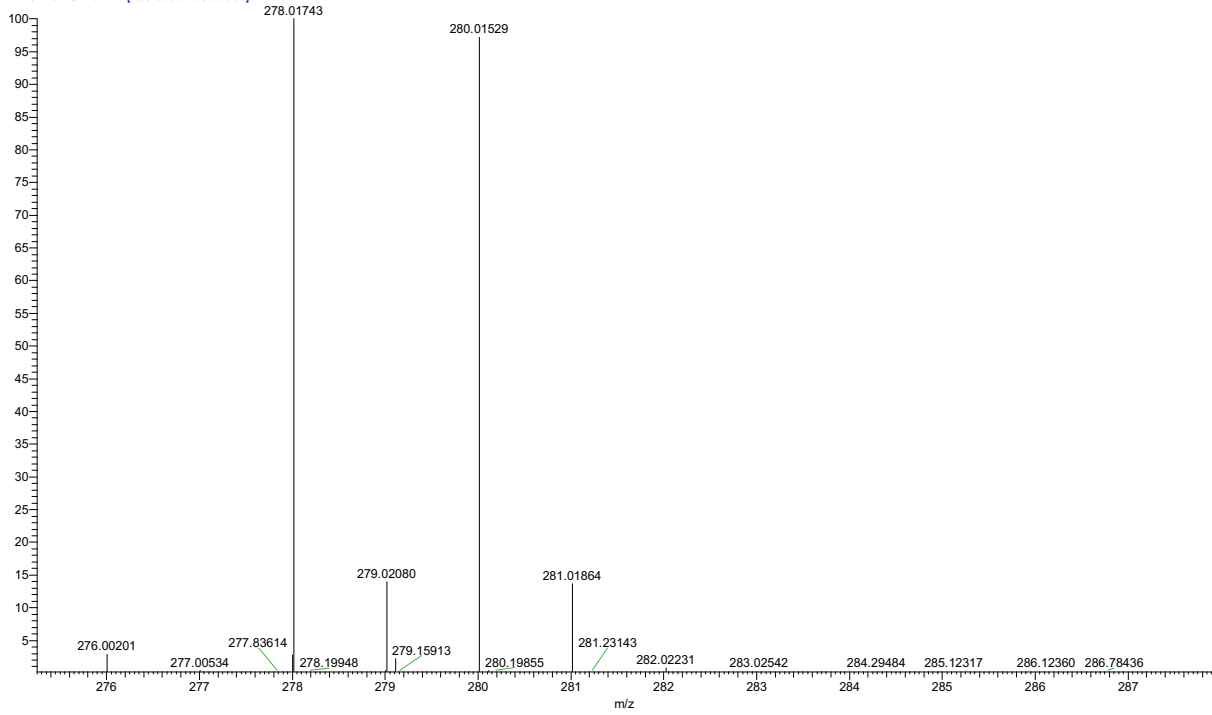Range: 1.285e-1

AU

0.74

0.34

0.16

1.08

1.2e-1
1.1e-1
1.0e-1
9.0e-2
8.0e-2
7.0e-2
6.0e-2
5.0e-2
4.0e-2
3.0e-2
2.0e-2
1.0e-2
0.0

0.00   0.50   1.00   1.50   2.00   2.50   3.00
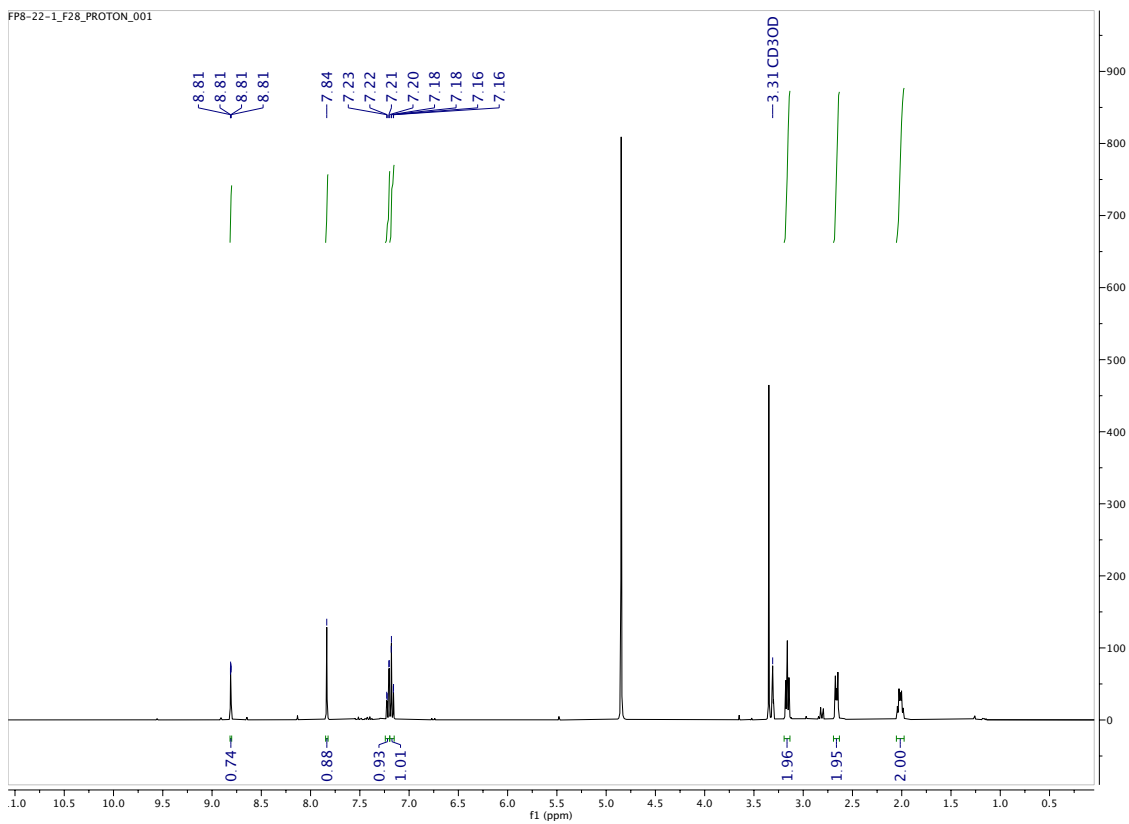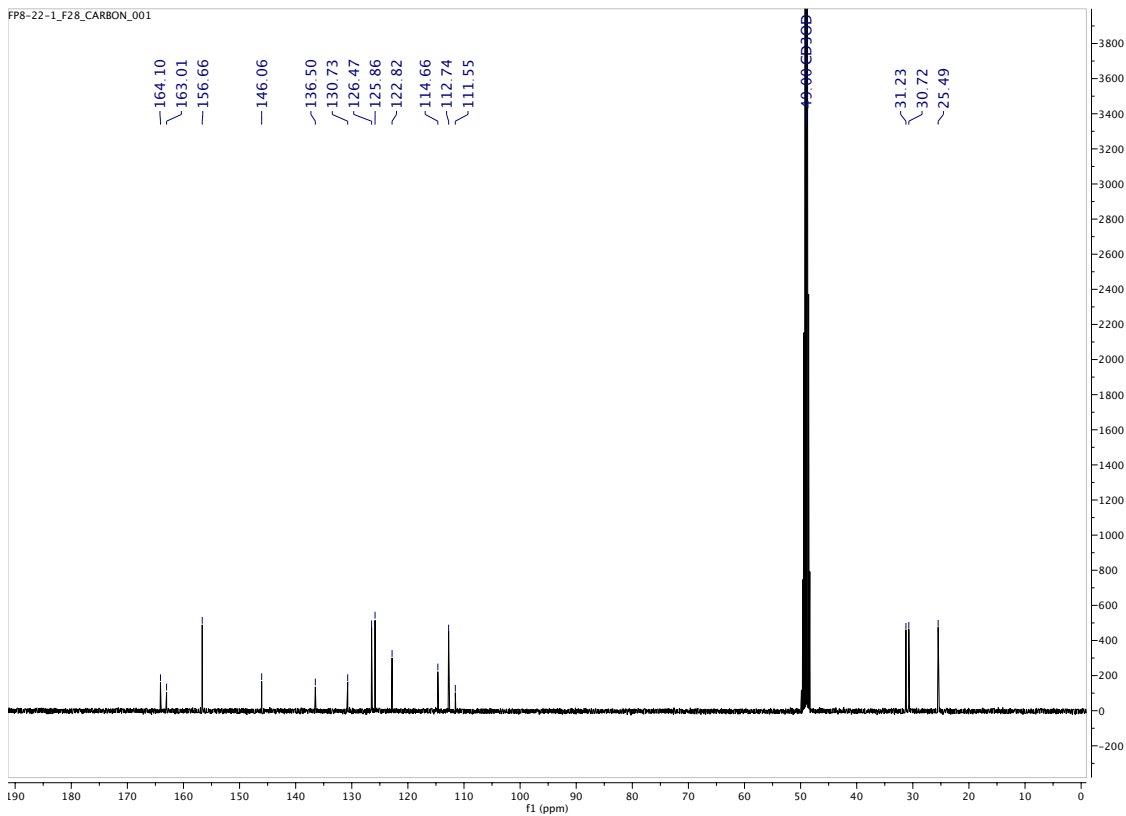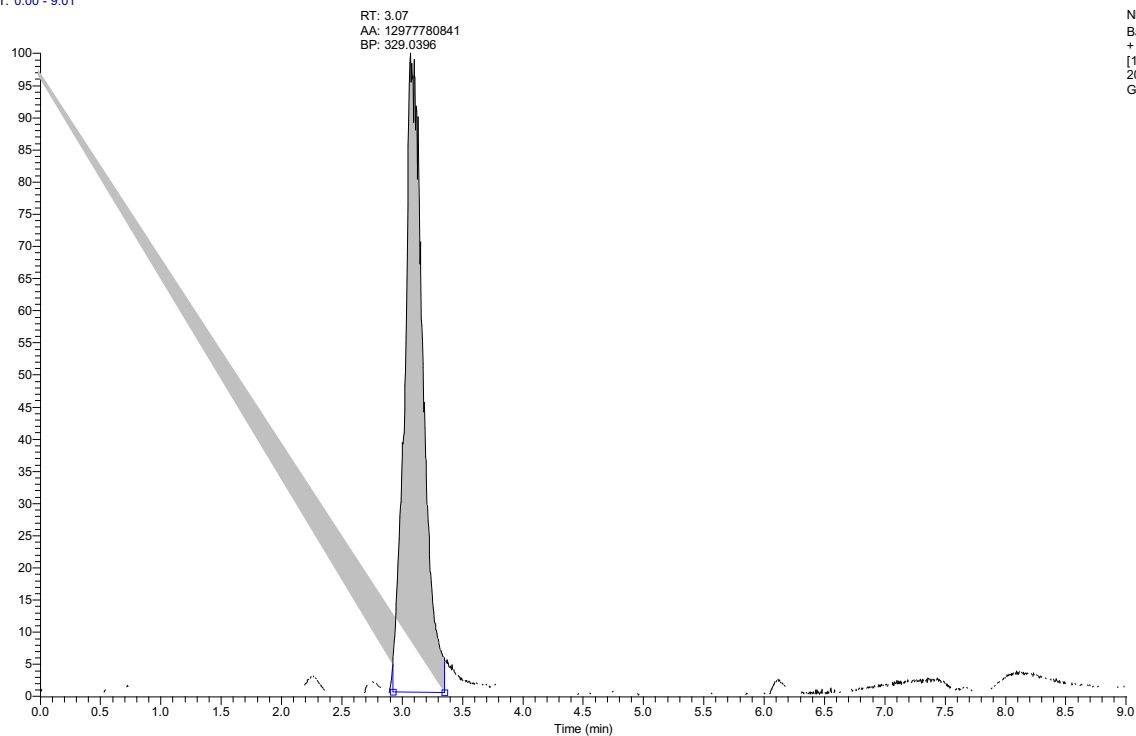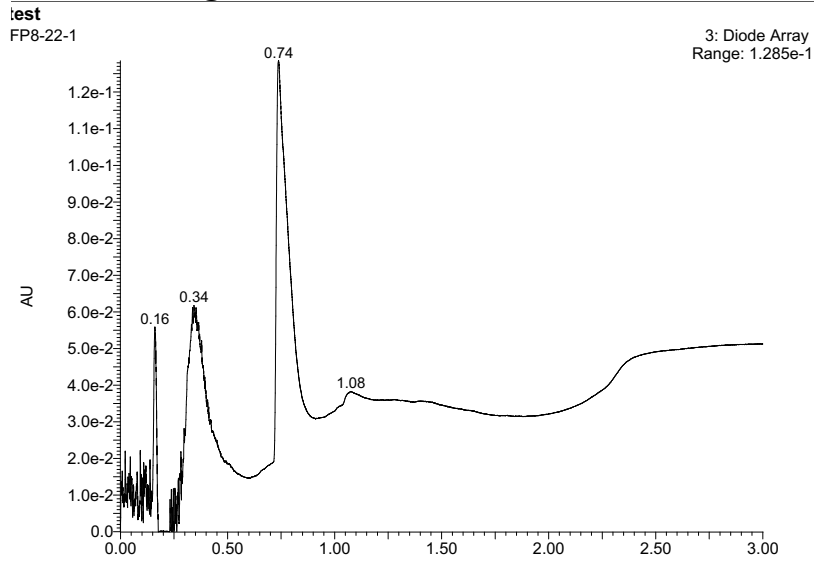
HRMS

FP-22-1 #683-758 RT: 2.95-3.28 AV: 76 NL: 6.39E8
T: FTMS + c ESI Full ms [150.0000-2000.0000]

329.03951

100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0

199.98791   298.12367   366.03487   446.11860   527.14736   659.06994   777.16901   857.66888   1055.41309   1212.30325   1398.68433   1553.16269   1745.66855 1837.67570 1950.36915

200   300   400   500   600   700   800   900   1000   1100   1200   1300   1400   1500   1600   1700   1800   1900   2000
m/z
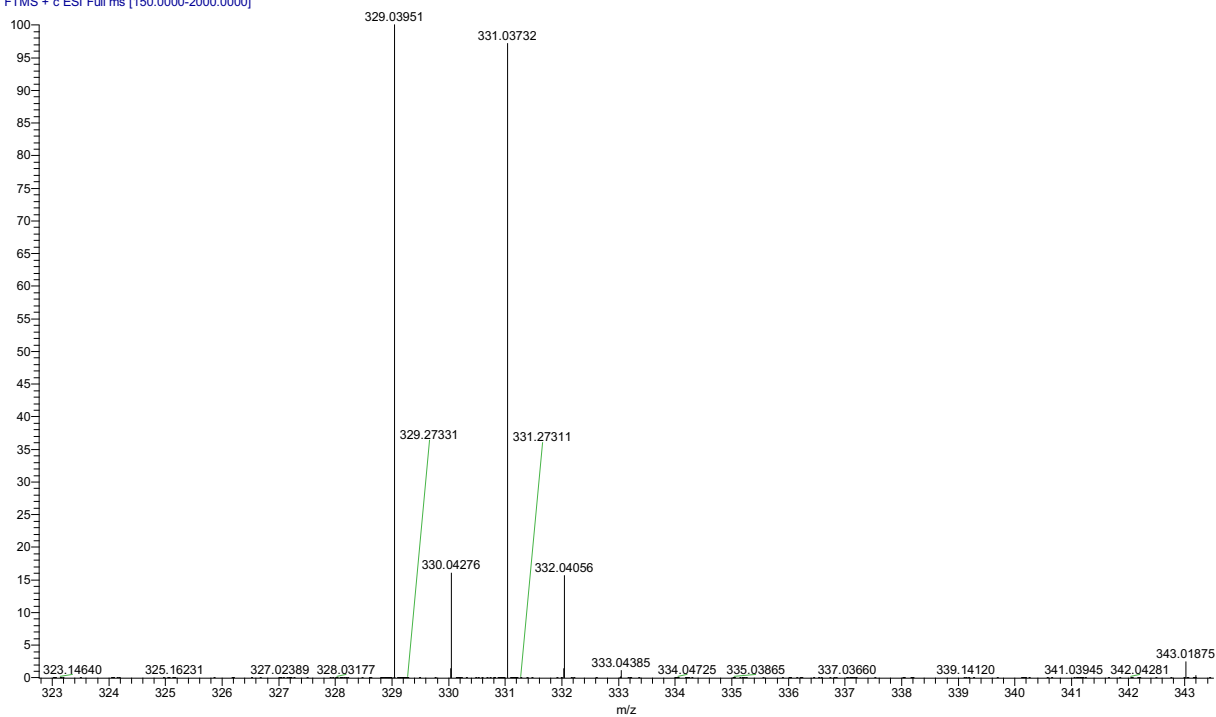
*12-bromo-6,7,8,9-tetrahydro-5H-pyrimido[4',5':3,4]cycloocta[1,2-b]indol-2-amine (**44**).*
¹H NMR
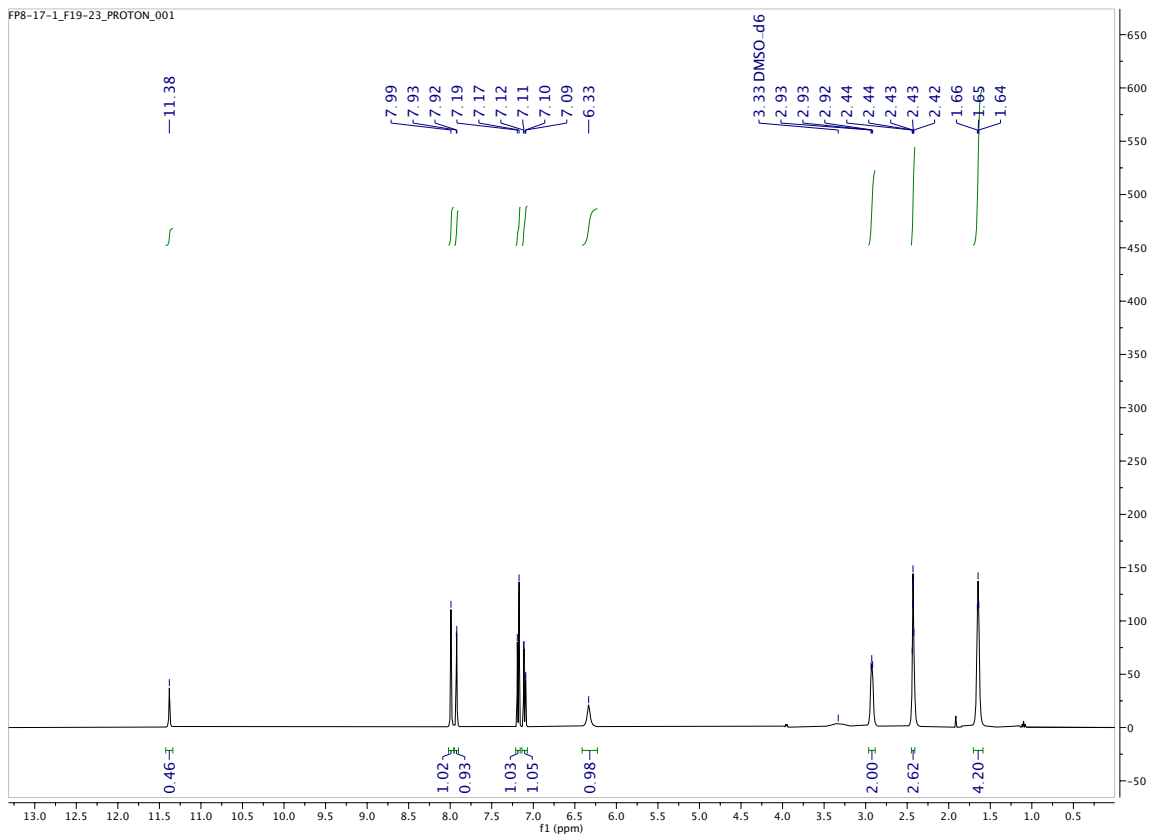
^{13}C NMR
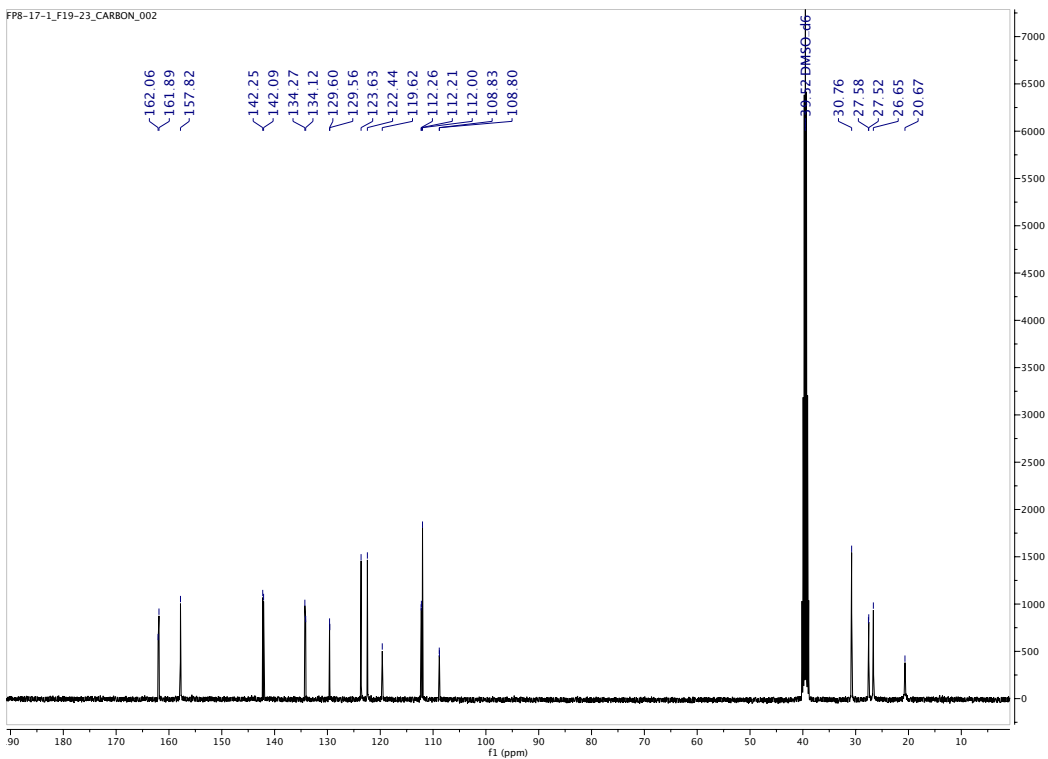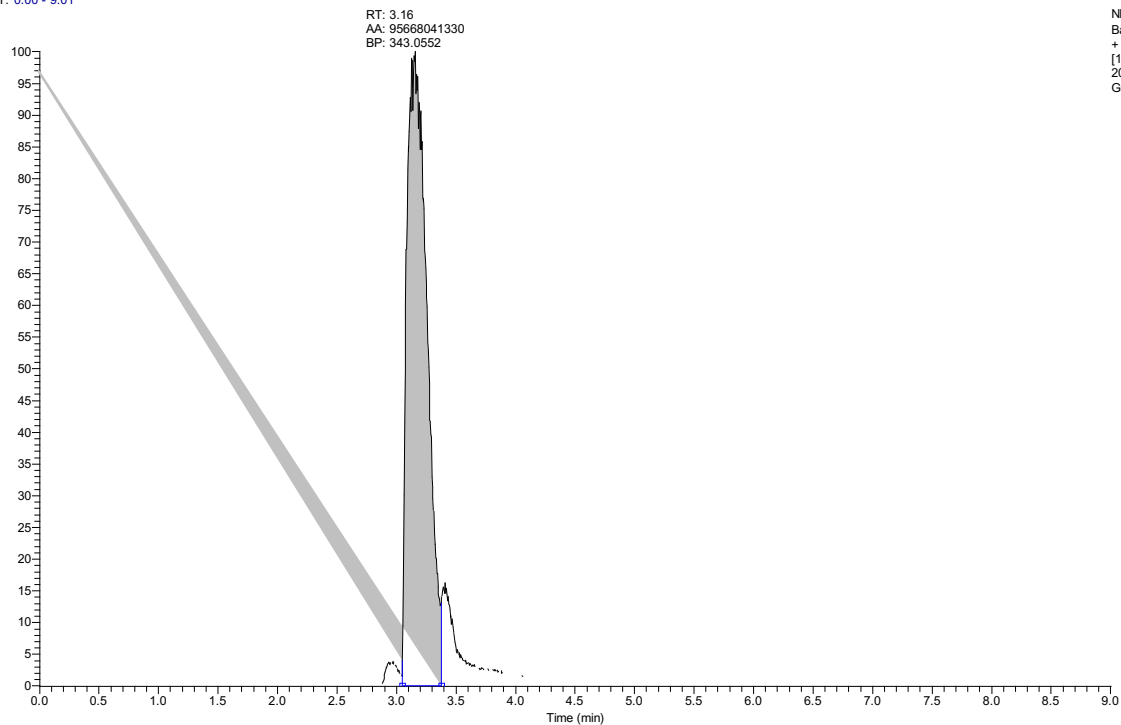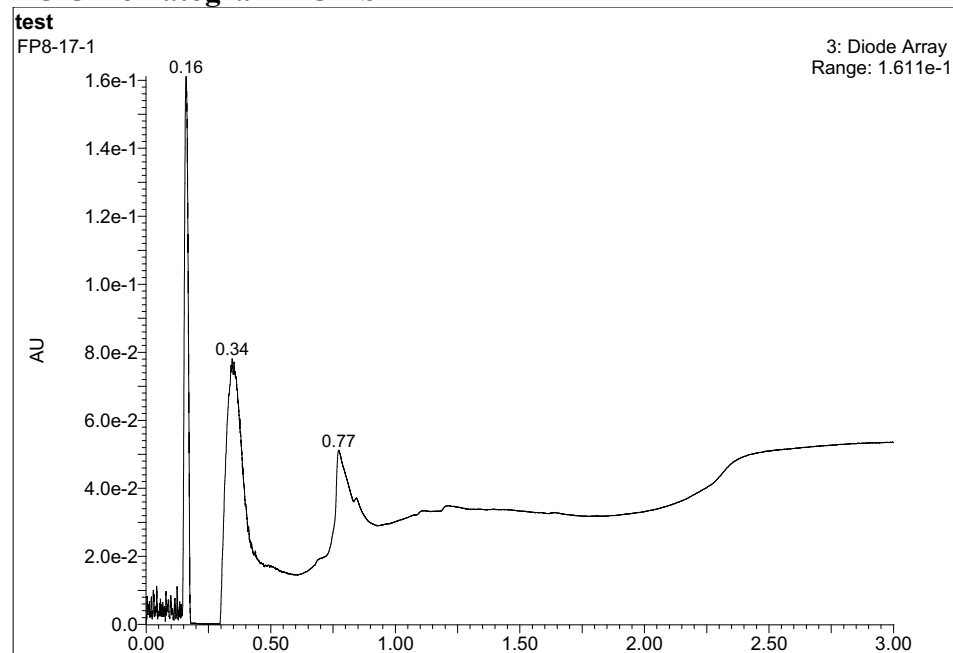
FP8-17-1_F19-23_CARBON_002

Peaks: 162.06, 161.89, 157.82, 142.25, 142.09, 134.27, 134.12, 129.60, 129.56, 123.63, 122.44, 119.62, 112.26, 112.21, 112.00, 108.83, 108.80, 39.52 DMSO-d6, 30.76, 27.58, 27.52, 26.65, 20.67

LC Chromatogram HRMS

RT: 0.00 - 9.01

RT: 3.16
AA: 95668041330
BP: 343.0552

NL: 8.14E9
Base Peak F: FTMS
+ c ESI Full ms
[150.0000-
2000.0000] MS
Genesis FP-17-1

LC Chromatogram LCMS

3: Diode Array
Range: 1.611e-1

HRMS
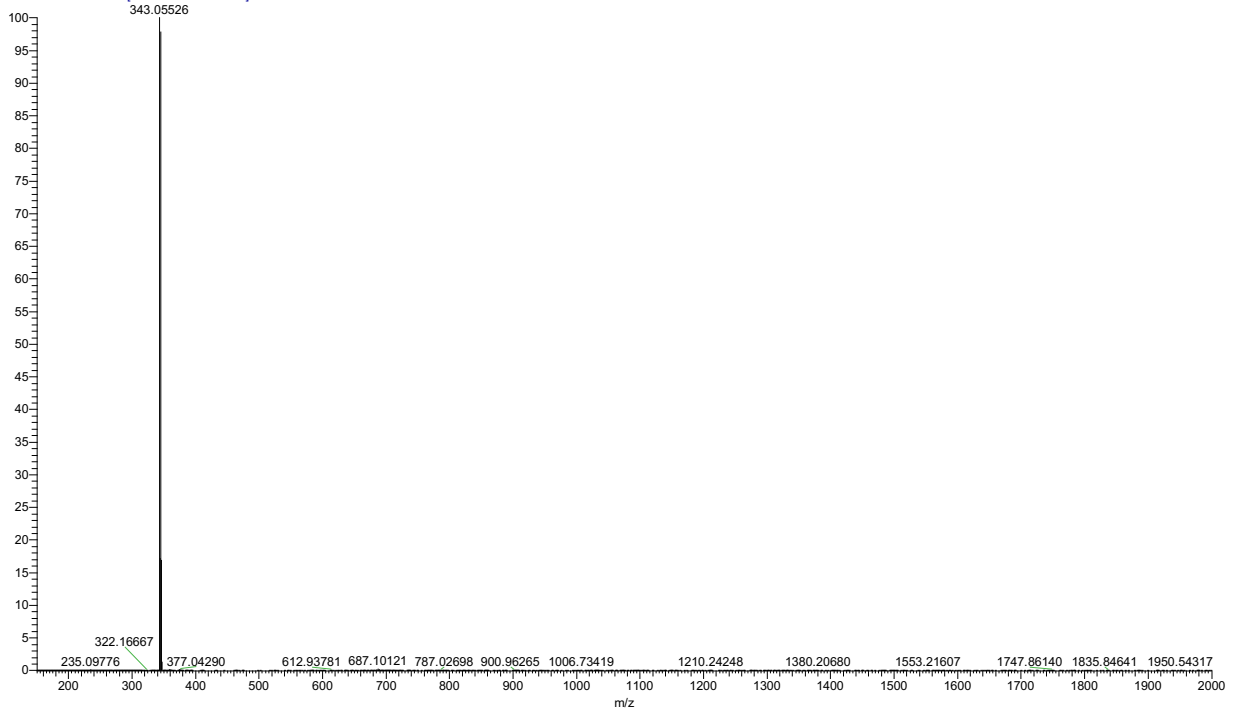
S30
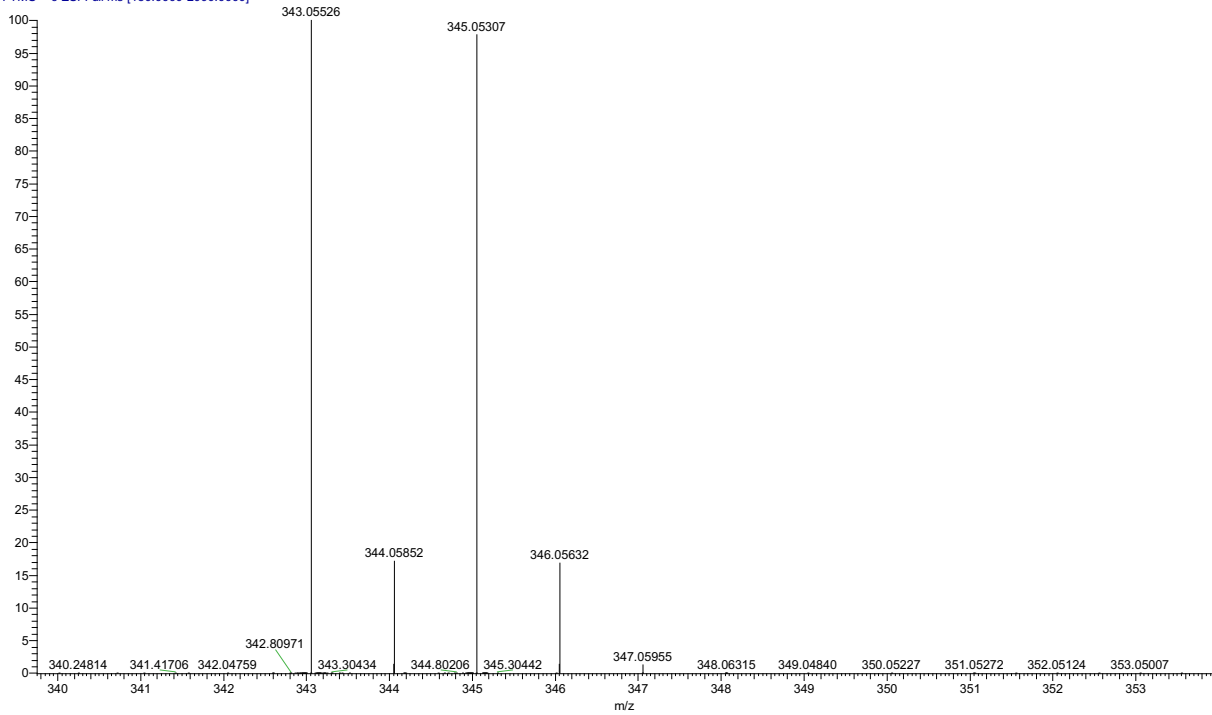
*4-(2-amino-6,7-dihydro-5H-pyrimido[5,4-c]carbazol-10-yl)-2-methylbut-3-yn-2-ol (**1**).*

^{1}H NMR

^{13}C NMR

LC Chromatogram

O602765$1
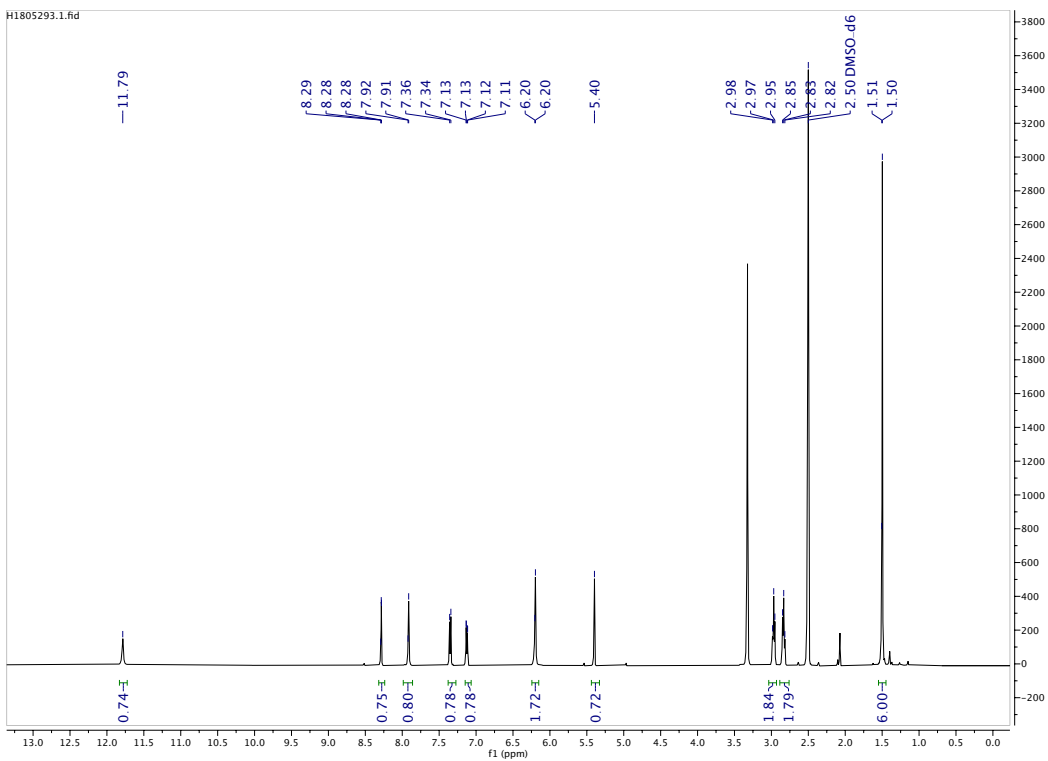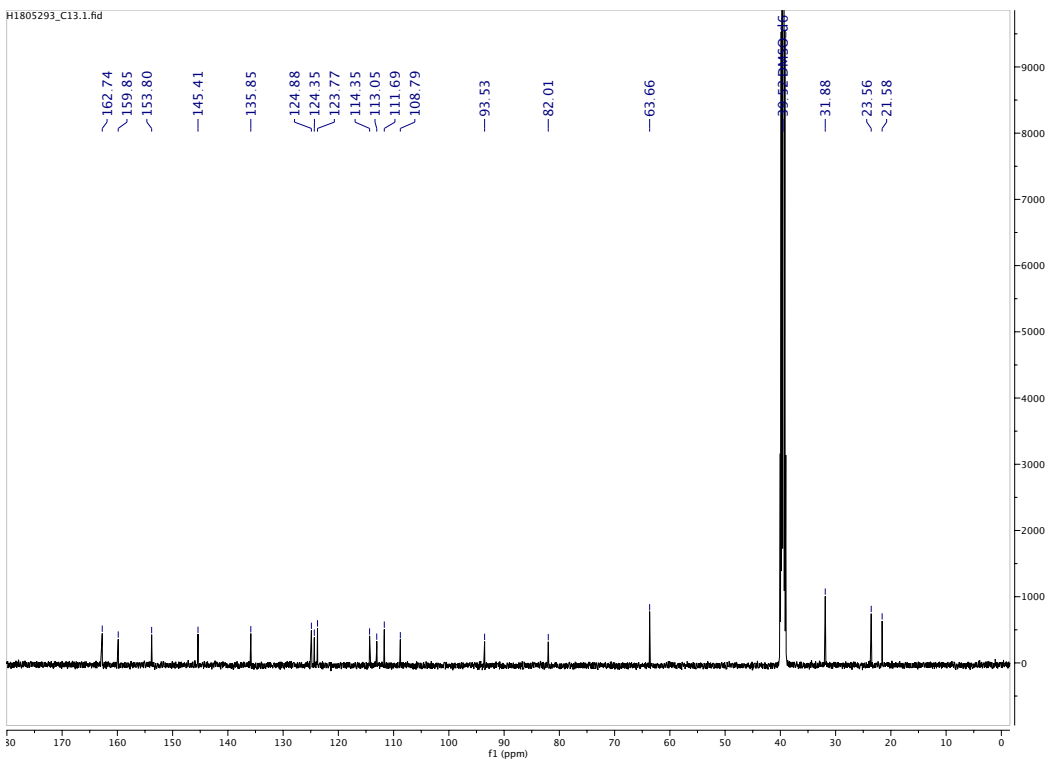
MaxPeak: 95.03%
Ret_Time: 0.916 min
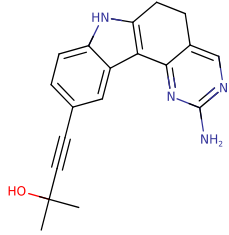
Mol Wt   318.37
Exact Mass   318.17

```
#  Time    Area%
-----------------
1  0.916   95.03
2  0.973   4.97
```

DAD1 A, Sig=215,16 Ref=off (D:\DATA\08.2019\02-\L179092R\002-D5F-F1-O602765$1.D)

0.916
0.973

DAD1 B, Sig=254,16 Ref=off (D:\DATA\08.2019\02-\L179092R\002-D5F-F1-O602765$1.D)

MSD1 TIC, MS File (D:\DATA\08.2019\02-\L179092R\002-D5F-F1-O602765$1.D) ES-API, Scan, Frag: 100, "PO

0.926
0.982

MSD2 TIC, MS File (D:\DATA\08.2019\02-\L179092R\002-D5F-F1-O602765$1.D) ES-API, Scan, Frag: 100, "NE

0.925
0.984

ADC1 A, ELSD (D:\DATA\08.2019\02-\L179092R\002-D5F-F1-O602765$1.D)

*MSD1 SPC, time=0.929 of D:\DATA\08.2019\02-\L179092R\002-D5F-F1-O602765$1.D ES-API, Scan, Frag: 100, "POS"

RT 0.926
319.2
320.2

*MSD1 SPC, time=0.979 of D:\DATA\08.2019\02-\L179092R\002-D5F-F1-O602765$1.D ES-API, Scan, Frag: 100, "POS"

RT 0.982
403.2
404.2
487.2

*MSD2 SPC, time=0.925 of D:\DATA\08.2019\02-\L179092R\002-D5F-F1-O602765$1.D ES-API, Scan, Frag: 100, "NEG"

RT 0.925
317.0
318.2

*MSD2 SPC, time=0.983 of D:\DATA\08.2019\02-\L179092R\002-D5F-F1-O602765$1.D ES-API, Scan, Frag: 100, "NEG"

RT 0.984
401.2
402.0
485.2
487.2

Inj.Date 8/2/2019   CH   <invalid> -8-   Acq. Method C:\Chem32\->   ->

HRMS

Target Compound Screening Report

Data File	H1805293.d	**Sample Name**	H1805293
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 6:14:09 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C19H18N4O	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 6:14:09 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C19 H18 N4 O; 2.165	82.72	0.85	C19 H18 N4 O	2.165	318.1481	318.1483

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
319.1555	2.165	318.1483	C19 H18 N4 O	318.1481	0.85	Find By Formula	

Compound Chromatograms
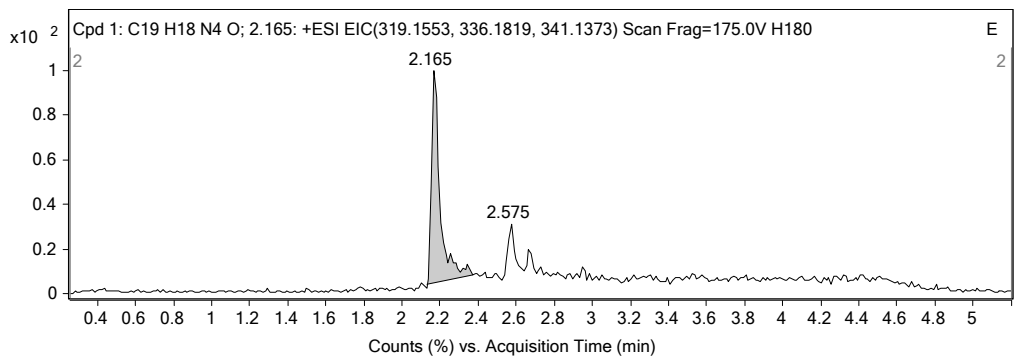
MS Zoomed Spectrum

4-(2-amino-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-11-yl)-2-methylbut-3-yn-2-ol (AMG28).

¹H NMR
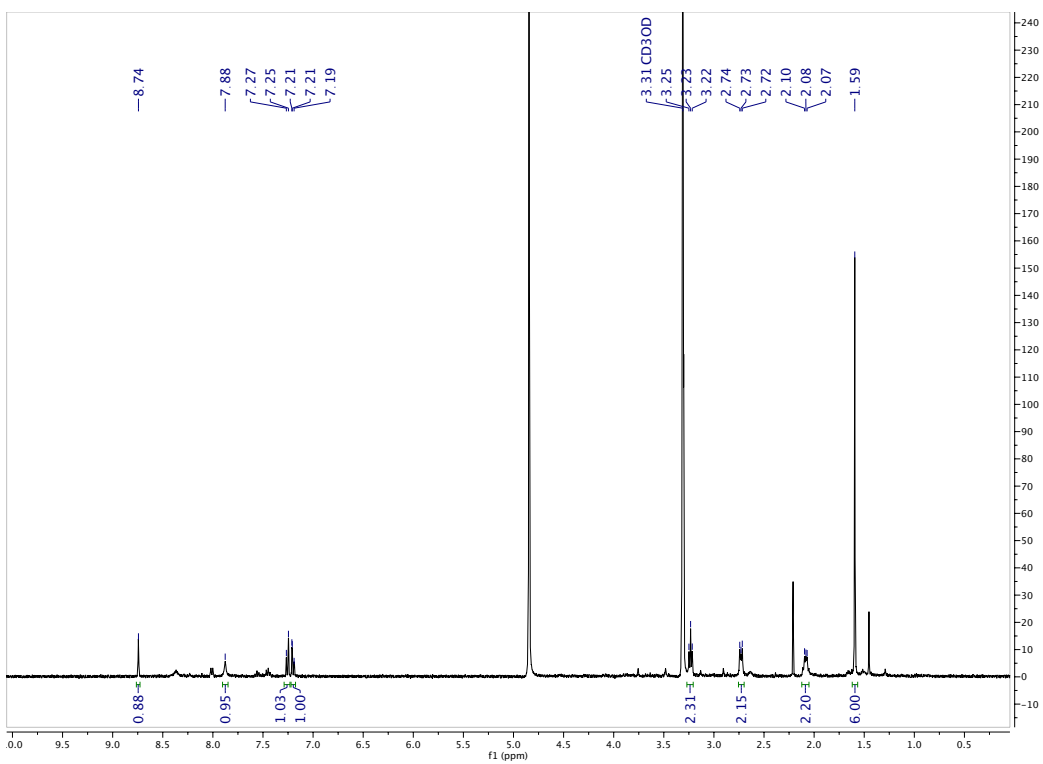
LC Chromatogram

MaxPeak: 96.35%
Ret_Time: 0.961 min
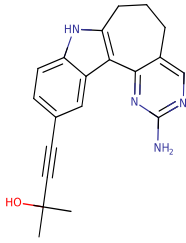
Mol Wt   **332.4**
Exact Mass   **332.19**

```
#   Time    Area%
-----------------
1   0.940   3.65
2   0.961   96.35
```

O546425$2

DAD1 A, Sig=215,16 Ref=off (D:\DATA\0729\L177756R\002-D6F-A1-O546425$2.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATA\0729\L177756R\002-D6F-A1-O546425$2.D)

MSD1 TIC, MS File (D:\DATA\0729\L177756R\002-D6F-A1-O546425$2.D) ES-API, Scan, Frag: 100, "POS"

MSD2 TIC, MS File (D:\DATA\0729\L177756R\002-D6F-A1-O546425$2.D) ES-API, Scan, Frag: 100, "NEG"

ELS1 A, ELS1A, ELSD Signal (D:\DATA\0729\L177756R\002-D6F-A1-O546425$2.D)

*MSD1 SPC, time=0.971 of D:\DATA\0729\L177756R\002-D6F-A1-O546425$2.D ES-API, Scan, Frag: 100, "POS"

RT 0.973

*MSD2 SPC, time=0.975 of D:\DATA\0729\L177756R\002-D6F-A1-O546425$2.D ES-API, Scan, Frag: 100, "NEG"

RT 0.973

Inj.Date 7/29/2019   LT   \<invalid\> 13   Acq. Method C:\Chem32\->   ->

*4-(2-amino-6,7,8,9-tetrahydro-5H-pyrimido[4',5':3,4]cycloocta[1,2-b]indol-12-yl)-2-methylbut-3-yn-2-ol (**2**).*

^{1}H NMR
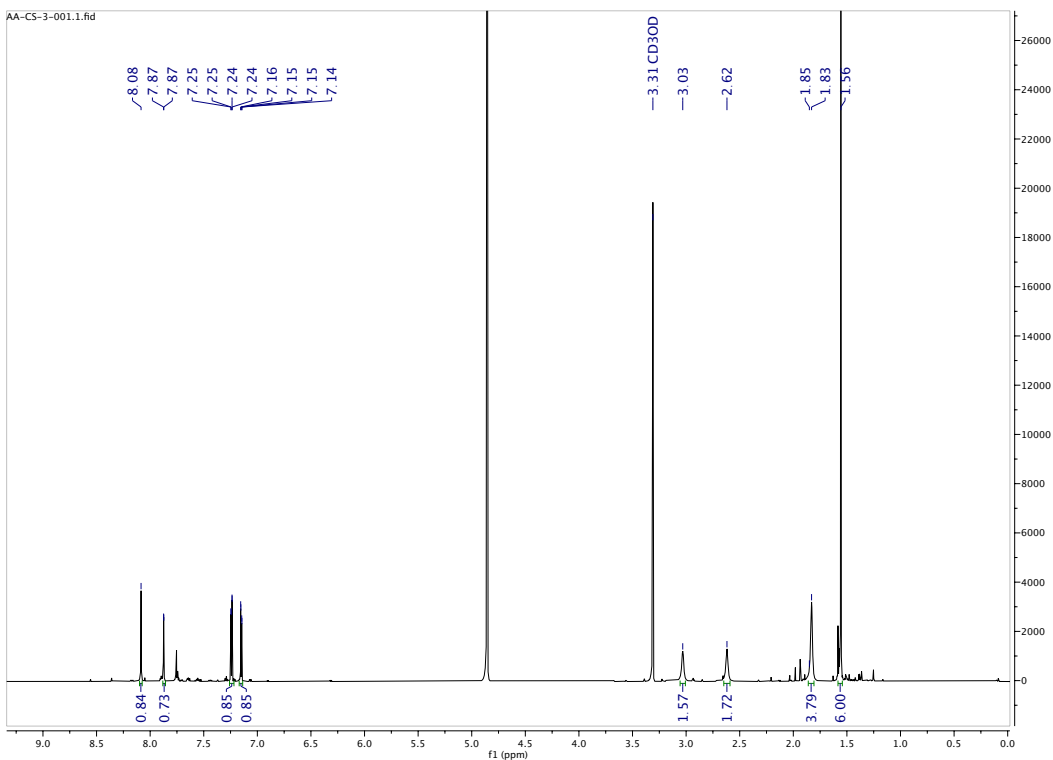
^{13}C NMR
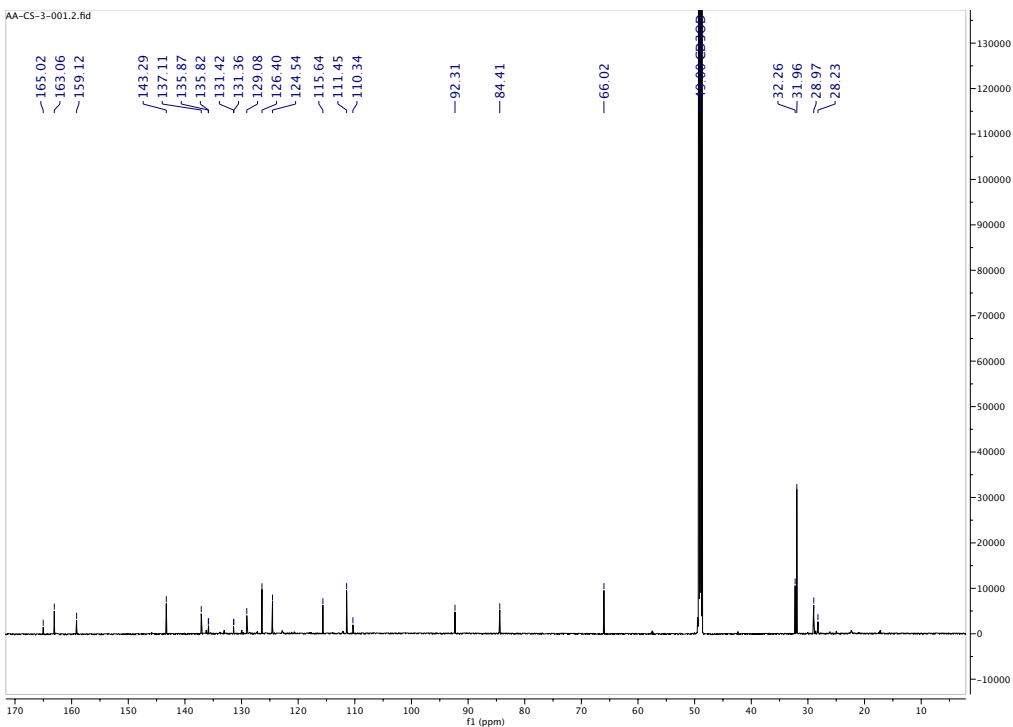
LC Chromatogram

MaxPeak: 95.56%
Ret_Time: 0.990 min
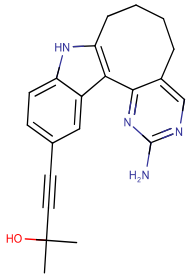
Mol Wt 346.43
Exact Mass 346.21

```
#  Time    Area%
-----------------
1  0.990   95.56
2  1.055   2.18
3  1.141   2.26
```

O518950$2

DAD1 A, Sig=215,16 Ref=off (D:\DATA\0718\L175406R\007-D6B-A6-O518950$2.D)

0.990
1.055 1.141

DAD1 B, Sig=254,16 Ref=off (D:\DATA\0718\L175406R\007-D6B-A6-O518950$2.D)

MSD1 TIC, MS File (D:\DATA\0718\L175406R\007-D6B-A6-O518950$2.D) ES-API, Scan, Frag: 100, "POS"

1.001
1.059 1.154

MSD2 TIC, MS File (D:\DATA\0718\L175406R\007-D6B-A6-O518950$2.D) ES-API, Scan, Frag: 100, "NEG"

1.002
1.066

ELS1 A, ELS1A, ELSD Signal (D:\DATA\0718\L175406R\007-D6B-A6-O518950$2.D)

*MSD1 SPC, time=1.004 of D:\DATA\0718\L175406R\007-D6B-A6-O518950$2.D ES-API, Scan, Frag: 100, "POS"

RT 1.001
347.2
348.2

*MSD1 SPC, time=1.062 of D:\DATA\0718\L175406R\007-D6B-A6-O518950$2.D ES-API, Scan, Frag: 100, "POS"

RT 1.059
101.0 130.0 179.0 293.2 343.0 373.0 418.2 462.0 347.2 515.4 517.2 599

*MSD1 SPC, time=1.154 of D:\DATA\0718\L175406R\007-D6B-A6-O518950$2.D ES-API, Scan, Frag: 100, "POS"

RT 1.154
263.2 525.2 527.2

*MSD2 SPC, time=1.000 of D:\DATA\0718\L175406R\007-D6B-A6-O518950$2.D ES-API, Scan, Frag: 100, "NEG"

RT 1.002
345.2 346.2 383.0

Inj.Date 7/18/2019   LT   <invalid> 13   Acq. Method C:\Chem32\->   ->

HRMS

Target Compound Screening Report

Data File	H1785737.d	**Sample Name**	H1785737
Sample Type	Sample	**Position**	P1-D4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 8:03:12 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C21H22N4O	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 8:03:12 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 2: C21 H22 N4 O; 2.294	98.87	0.5	C21 H22 N4 O	2.294	346.1794	346.1795
Cpd 1: C21 H22 N4 O; 2.409	78.19	-0.43	C21 H22 N4 O	2.409	346.1794	346.1792

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
347.1868	2.294	346.1795	C21 H22 N4 O	346.1794	0.5	Find By Formula	

Compound Chromatograms
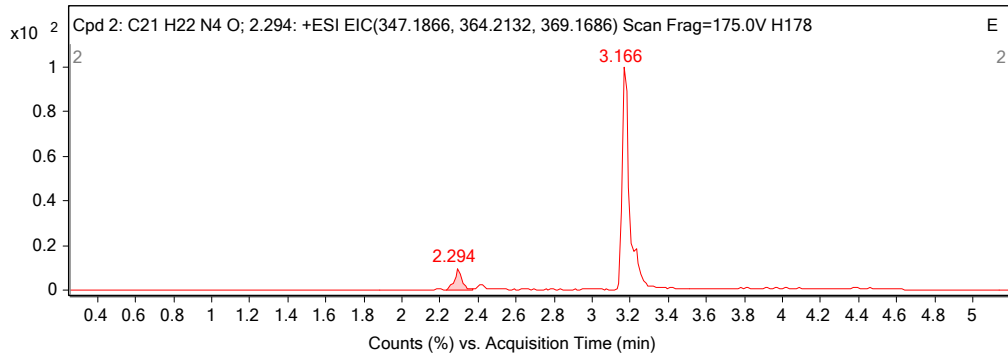
MS Zoomed Spectrum

*4-(3-(2-aminopyrimidin-4-yl)-1H-indol-5-yl)-2-methylbut-3-yn-2-ol (**3**).*

¹H NMR
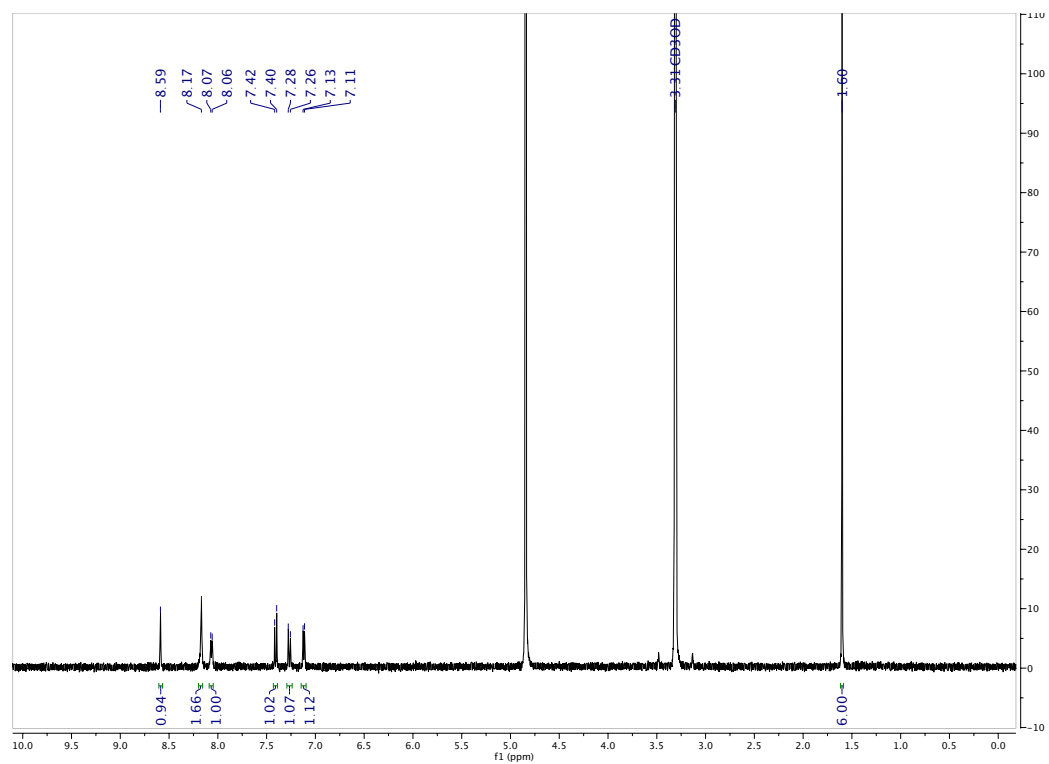
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 0.771 min
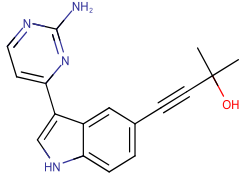
Mol Wt 292.33
Exact Mass 292.15

```
# Time  Area%
-----------------
1 0.771 100.00
```

P961853$3

DAD1 A, Sig=215,16 Ref=off (D:\DATE\FEB\1502\VST\L226516R\003-D1B-A2-P961853$3.D)

mAU
400
200
0.771

DAD1 B, Sig=254,16 Ref=off (D:\DATE\FEB\1502\VST\L226516R\003-D1B-A2-P961853$3.D)

mAU
200
100
0
-100

MSD1 TIC, MS File (D:\DATE\FEB\1502\VST\L226516R\003-D1B-A2-P961853$3.D) ES-API, Fast Scan, Frag:

2000000
1500000
1000000
500000
0
0.780

MSD2 TIC, MS File (D:\DATE\FEB\1502\VST\L226516R\003-D1B-A2-P961853$3.D) ES-API, Fast Scan, Frag:

80000
60000
40000
20000
0
0.782

ELS1 A, ELS1A, ELSD Signal (D:\DATE\FEB\1502\VST\L226516R\003-D1B-A2-P961853$3.D)

LSU
84.5
84
83.5

*MSD1 SPC, time=0.776 of D:\DATE\FEB\1502\VST\L226516R\003-D1B-A2-P961853$3.D ES-API, Fast Scan, Frag: 100, "POS"

RT 0.780

50
0
157.0
293.0
294.0

*MSD2 SPC, time=0.782 of D:\DATE\FEB\1502\VST\L226516R\003-D1B-A2-P961853$3.D ES-API, Fast Scan, Frag: 100, "NEG"

RT 0.782

30
20
10
0
291.0
292.0
328.0
458.8

S40

HRMS

Target Compound Screening Report

Data File	H2233612a.d	**Sample Name**	H2233612
Sample Type	Sample	**Position**	P1-E2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 9:01:20 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C17H16N4O	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 9:01:20 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C17 H16 N4 O; 2.110	96.35	-0.02	C17 H16 N4 O	2.11	292.1324	292.1324

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
293.1397	2.11	292.1324	C17 H16 N4 O	292.1324	-0.02	Find By Formula	

Compound Chromatograms
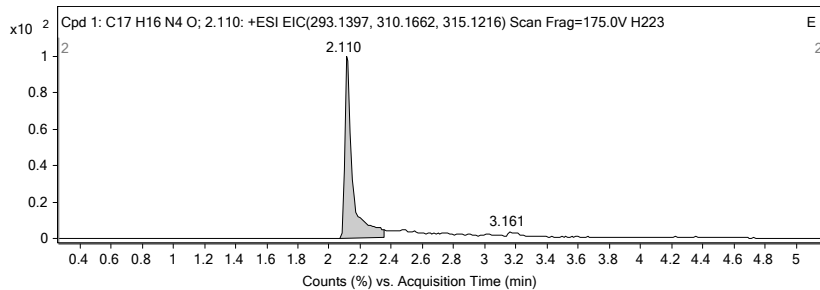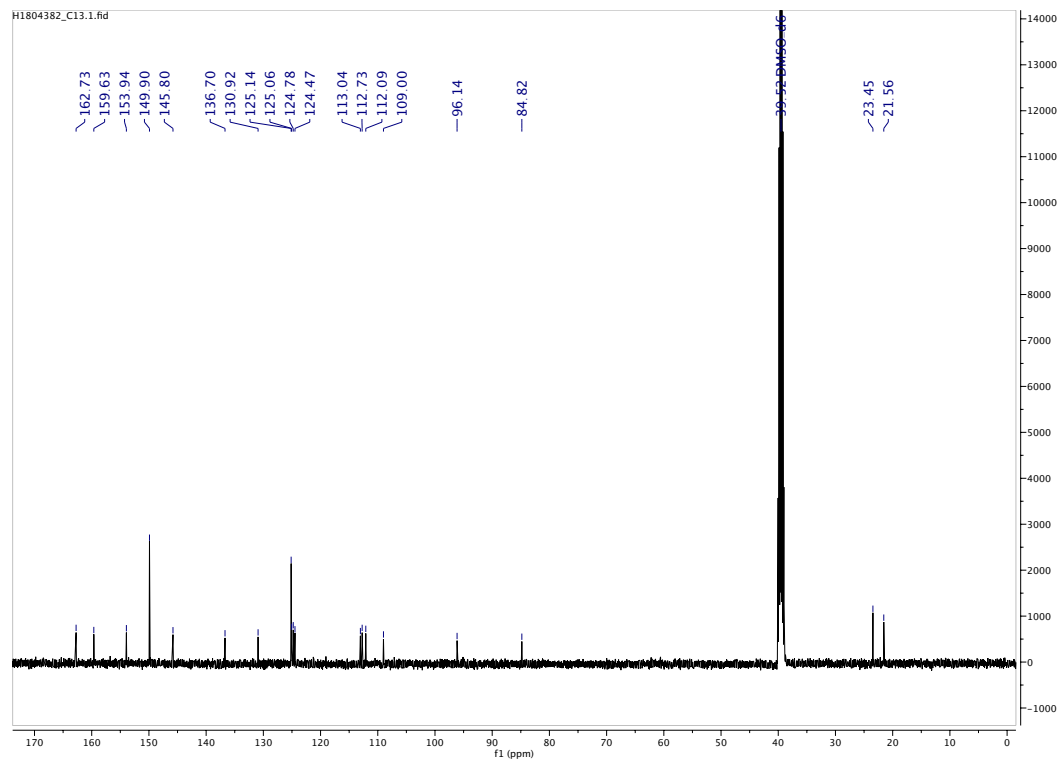

MS Zoomed Spectrum

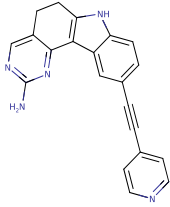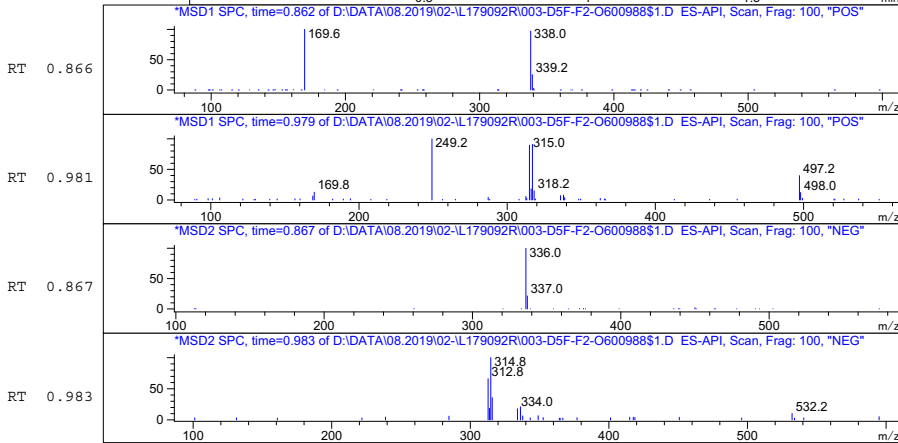*10-(pyridin-4-ylethynyl)-6,7-dihydro-5H-pyrimido[5,4-c]carbazol-2-amine (4).*
1H NMR
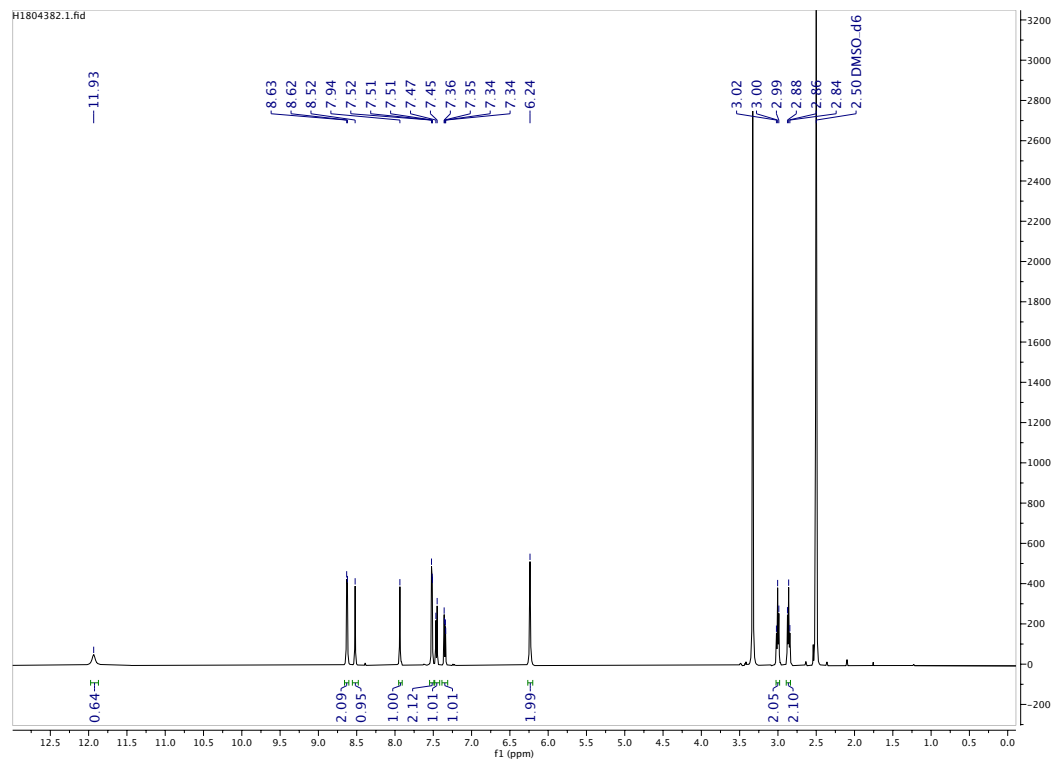
13C NMR

LC Chromatogram

MaxPeak: 96.28%
Ret_Time: 0.858 min

Mol Wt   337.38
Exact Mass   337.15

```
#   Time    Area%
-----------------
1   0.858   96.28
2   0.975    3.72
```

O600988$1

DAD1 A, Sig=215,16 Ref=off (D:\DATA\08.2019\02-\L179092R\003-D5F-F2-O600988$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATA\08.2019\02-\L179092R\003-D5F-F2-O600988$1.D)

MSD1 TIC, MS File (D:\DATA\08.2019\02-\L179092R\003-D5F-F2-O600988$1.D) ES-API, Scan, Frag: 100, "PO

MSD2 TIC, MS File (D:\DATA\08.2019\02-\L179092R\003-D5F-F2-O600988$1.D) ES-API, Scan, Frag: 100, "NE

ADC1 A, ELSD (D:\DATA\08.2019\02-\L179092R\003-D5F-F2-O600988$1.D)

*MSD1 SPC, time=0.862 of D:\DATA\08.2019\02-\L179092R\003-D5F-F2-O600988$1.D ES-API, Scan, Frag: 100, "POS"
RT 0.866

*MSD1 SPC, time=0.979 of D:\DATA\08.2019\02-\L179092R\003-D5F-F2-O600988$1.D ES-API, Scan, Frag: 100, "POS"
RT 0.981

*MSD2 SPC, time=0.867 of D:\DATA\08.2019\02-\L179092R\003-D5F-F2-O600988$1.D ES-API, Scan, Frag: 100, "NEG"
RT 0.867

*MSD2 SPC, time=0.983 of D:\DATA\08.2019\02-\L179092R\003-D5F-F2-O600988$1.D ES-API, Scan, Frag: 100, "NEG"
RT 0.983

Inj.Date 8/2/2019   CH   <invalid> -8-   Acq. Method C:\Chem32\->   ->

HRMS

Target Compound Screening Report

Data File	H1804382.d	**Sample Name**	H1804382
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 6:38:24 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C21H15N5	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 6:38:24 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H15 N5; 2.012	81.24	-0.22	C21 H15 N5	2.012	337.1327	337.1327

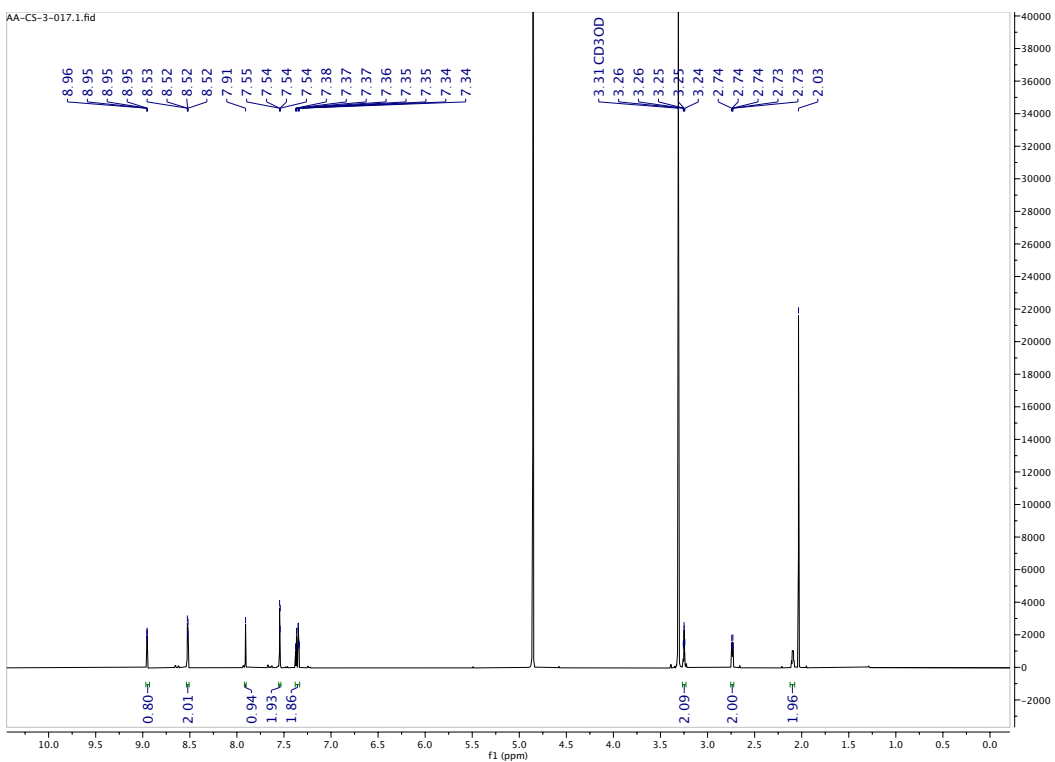| Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
338.1393	2.012	337.1327	C21 H15 N5	337.1327	-0.22	Find By Formula	

Compound Chromatograms
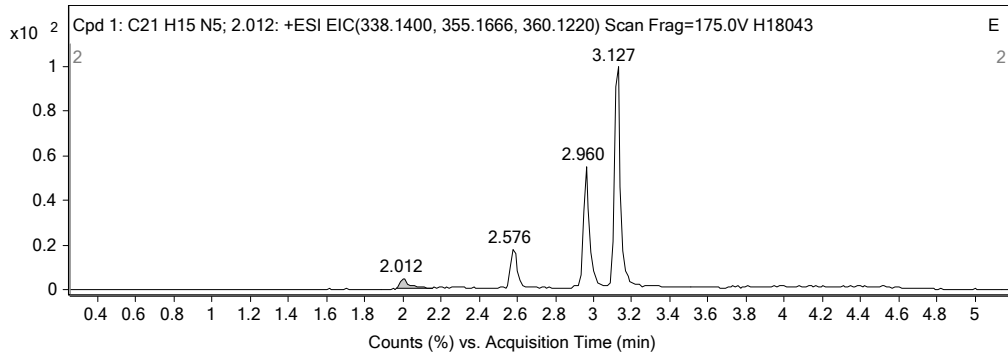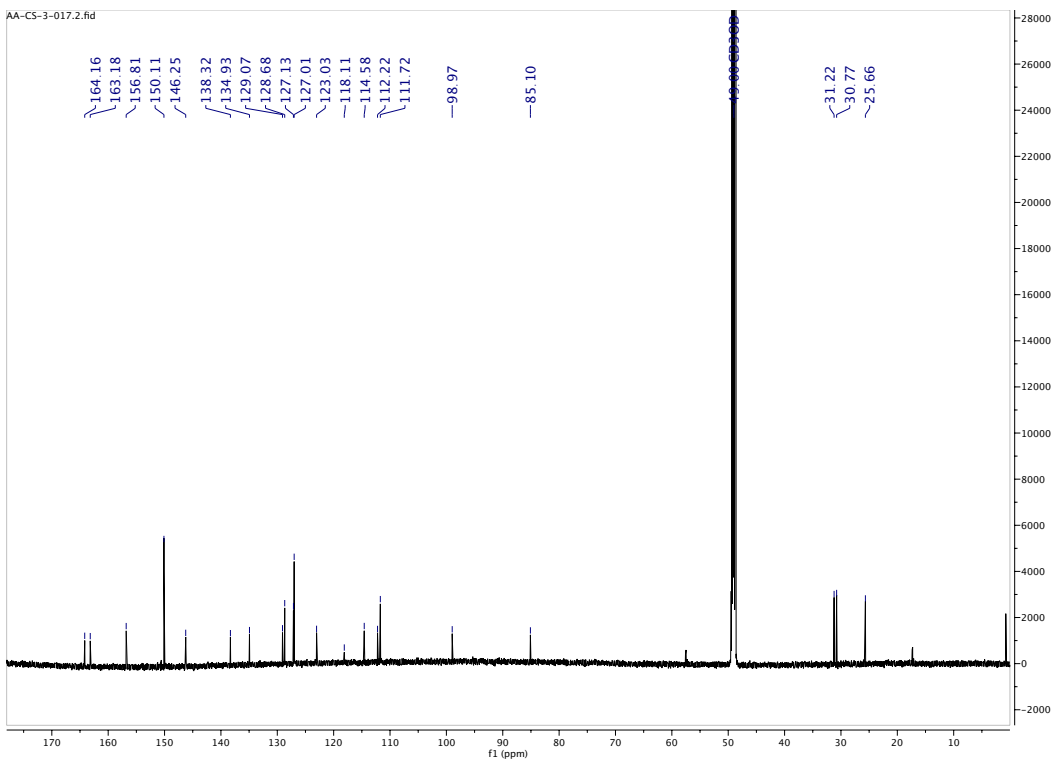

MS Zoomed Spectrum

11-(pyridin-4-ylethynyl)-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-2-amine (5).
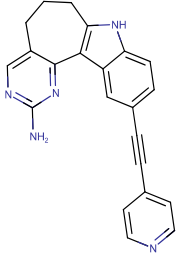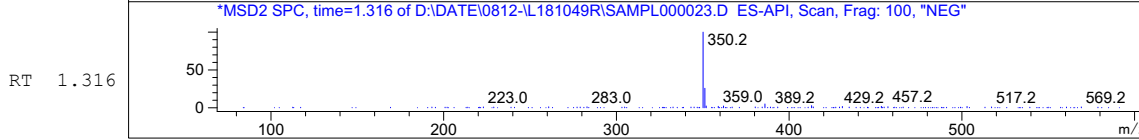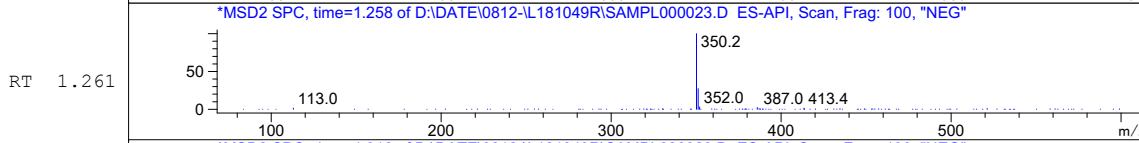
¹H NMR

¹³C NMR

LC Chromatogram

MaxPeak: 96.99%
Ret_Time: 1.253 min

Mol Wt **351.4**
Exact Mass **351.17**

#	Time	Area%
1	1.253	96.99
2	1.336	3.01
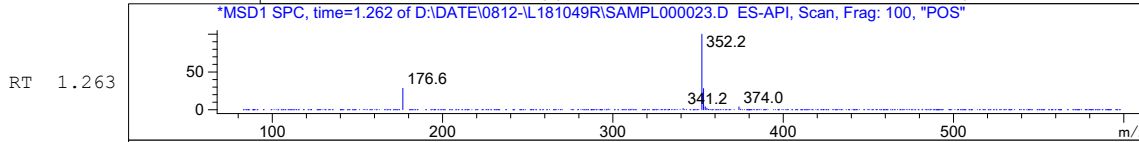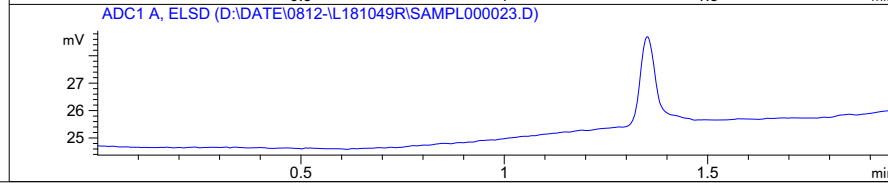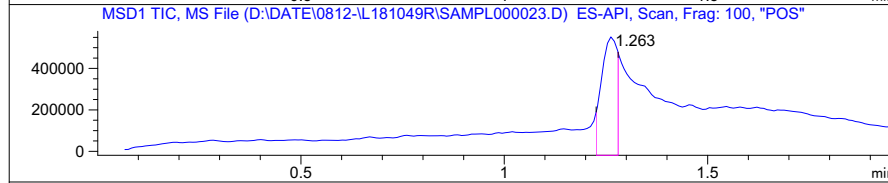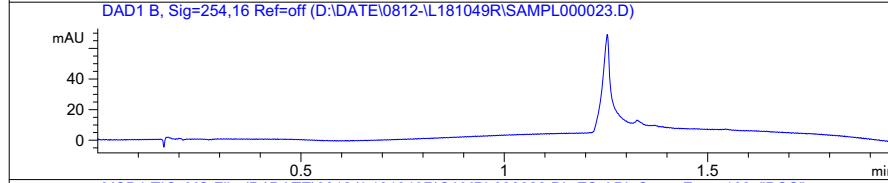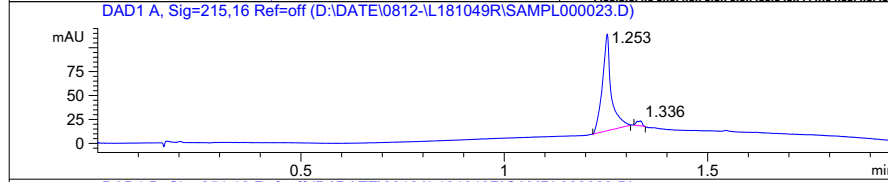
DAD1 A, Sig=215,16 Ref=off (D:\DATE\0812-\L181049R\SAMPL000023.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATE\0812-\L181049R\SAMPL000023.D)
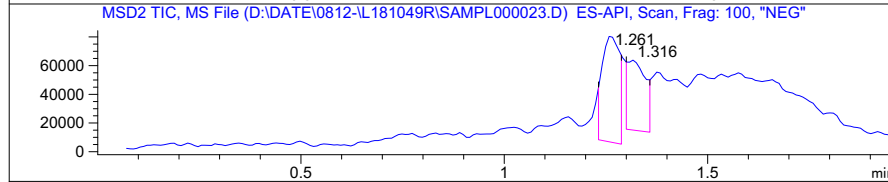
MSD1 TIC, MS File (D:\DATE\0812-\L181049R\SAMPL000023.D) ES-API, Scan, Frag: 100, "POS"

MSD2 TIC, MS File (D:\DATE\0812-\L181049R\SAMPL000023.D) ES-API, Scan, Frag: 100, "NEG"

ADC1 A, ELSD (D:\DATE\0812-\L181049R\SAMPL000023.D)

*MSD1 SPC, time=1.262 of D:\DATE\0812-\L181049R\SAMPL000023.D ES-API, Scan, Frag: 100, "POS"
RT 1.263

*MSD2 SPC, time=1.258 of D:\DATE\0812-\L181049R\SAMPL000023.D ES-API, Scan, Frag: 100, "NEG"
RT 1.261

*MSD2 SPC, time=1.316 of D:\DATE\0812-\L181049R\SAMPL000023.D ES-API, Scan, Frag: 100, "NEG"
RT 1.316

HRMS
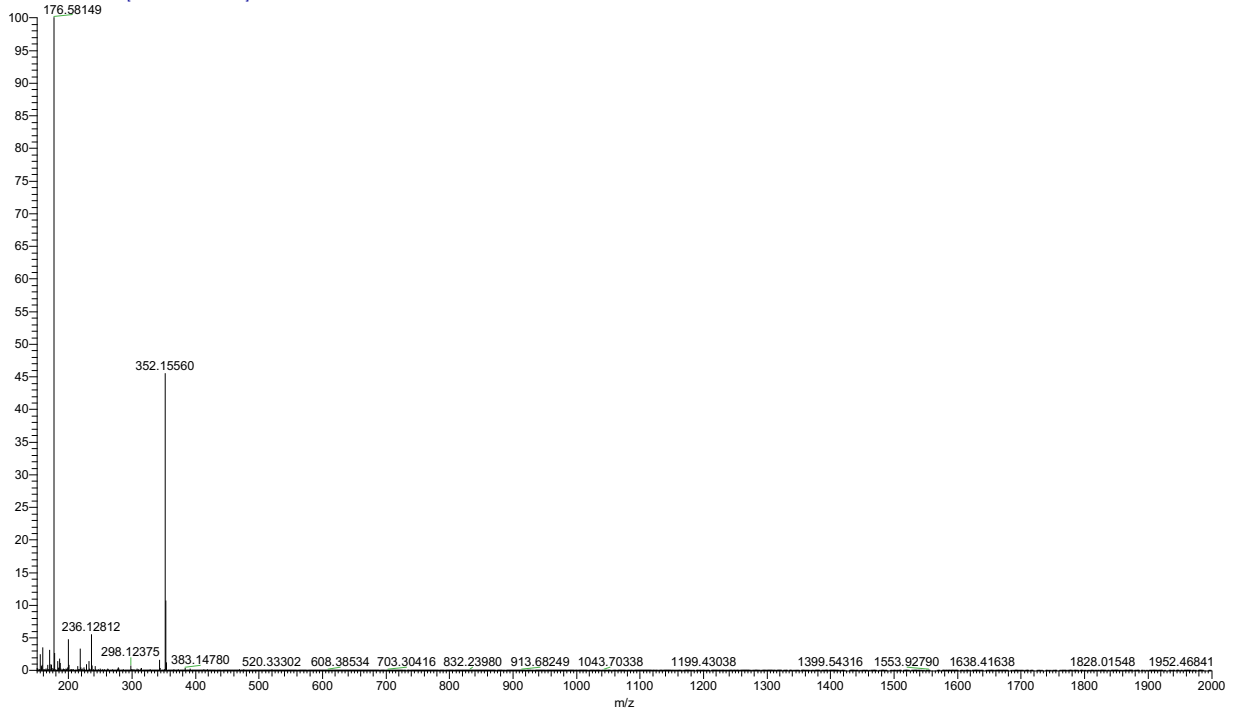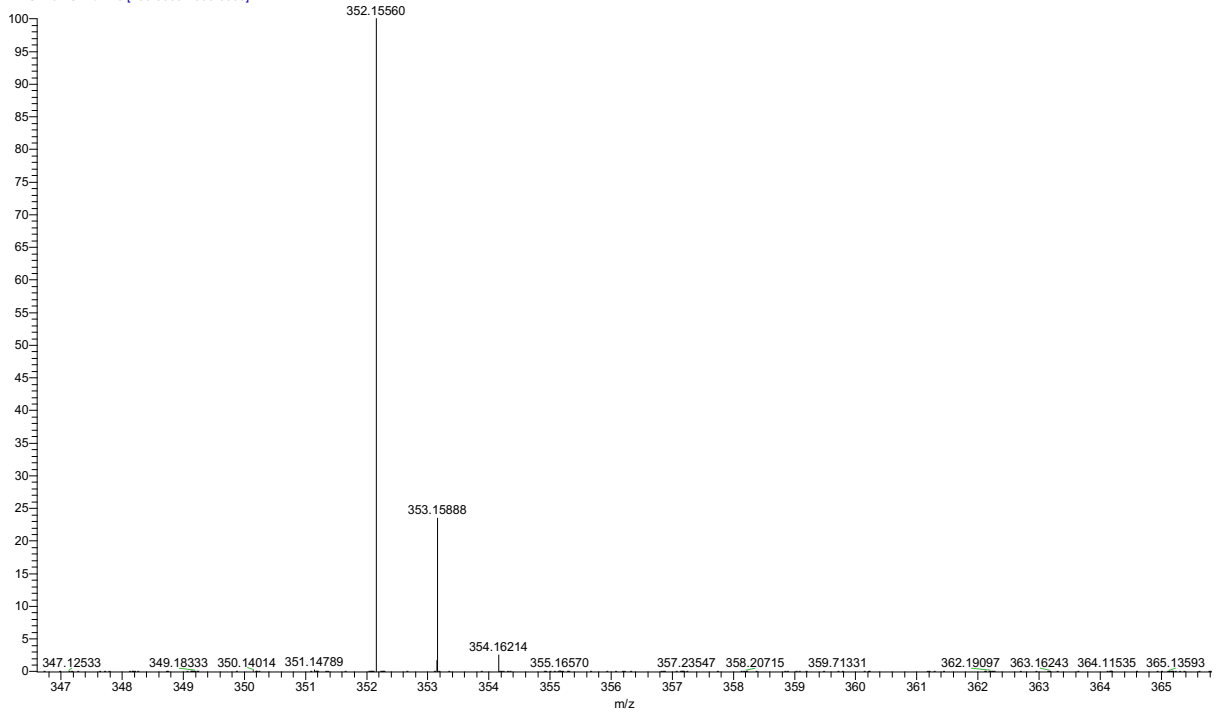
12-(pyridin-4-ylethynyl)-6,7,8,9-tetrahydro-5H-pyrimido[4',5':3,4]cycloocta[1,2-b]indol-2-amine (6).

¹H NMR
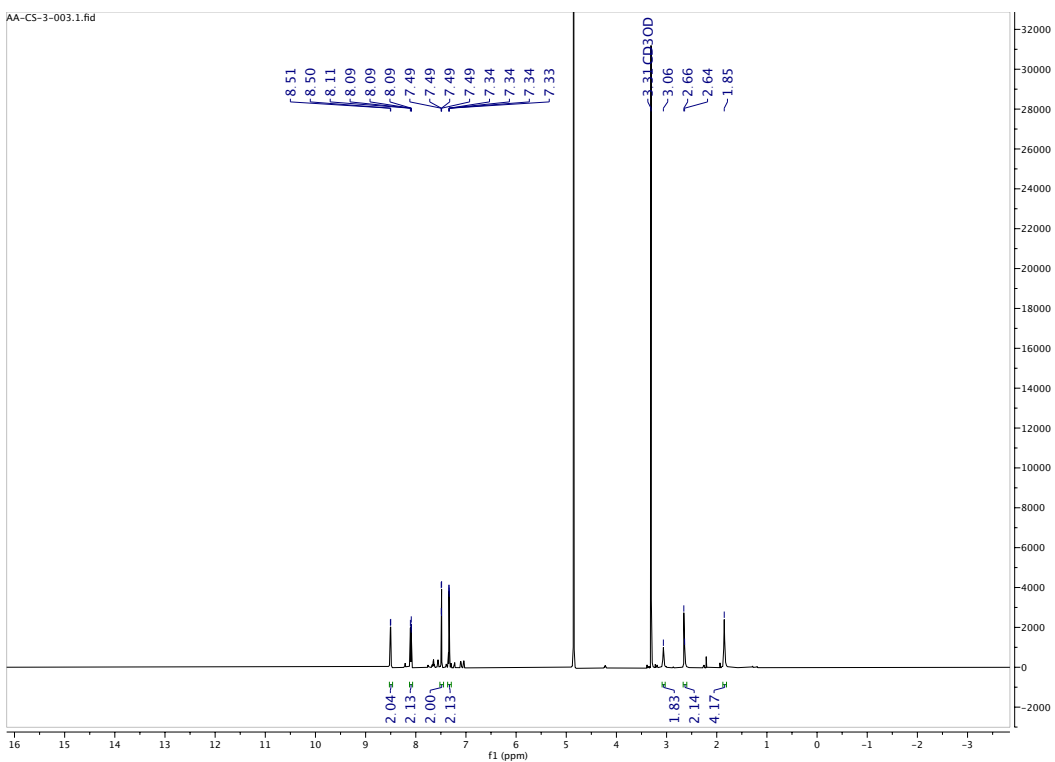
¹³C NMR
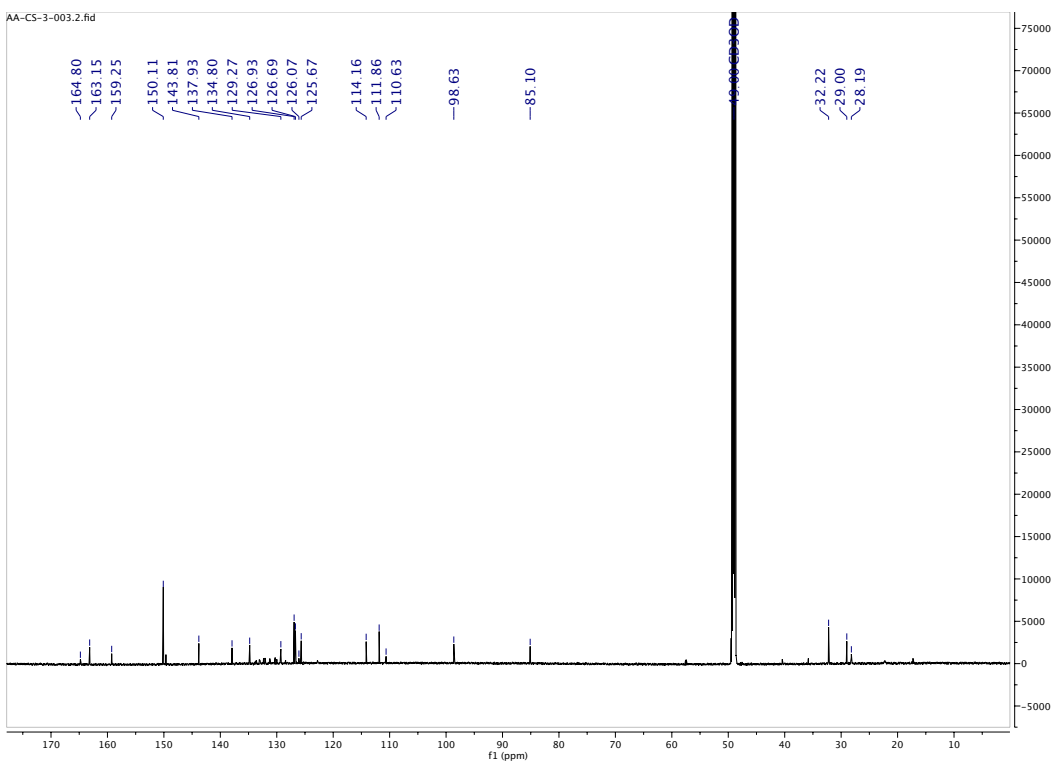
LC Chromatogram

MaxPeak: 97.95%
Ret_Time: 0.929 min
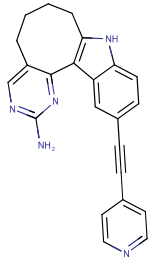
Mol Wt **365.43**
Exact Mass **365.19**

```
#  Time   Area%
-----------------
1  0.929  97.95
2  1.041   2.05
```

O519555$2

DAD1 A, Sig=215,16 Ref=off (D:\DATA\0718\L175406R\004-D6B-A3-O519555$2.D)
mAU
400
200
0.929
1.041

DAD1 B, Sig=254,16 Ref=off (D:\DATA\0718\L175406R\004-D6B-A3-O519555$2.D)
mAU
300
200
100
0

MSD1 TIC, MS File (D:\DATA\0718\L175406R\004-D6B-A3-O519555$2.D) ES-API, Scan, Frag: 100, "POS"
800000
600000
400000
200000
0.941
1.050

MSD2 TIC, MS File (D:\DATA\0718\L175406R\004-D6B-A3-O519555$2.D) ES-API, Scan, Frag: 100, "NEG"
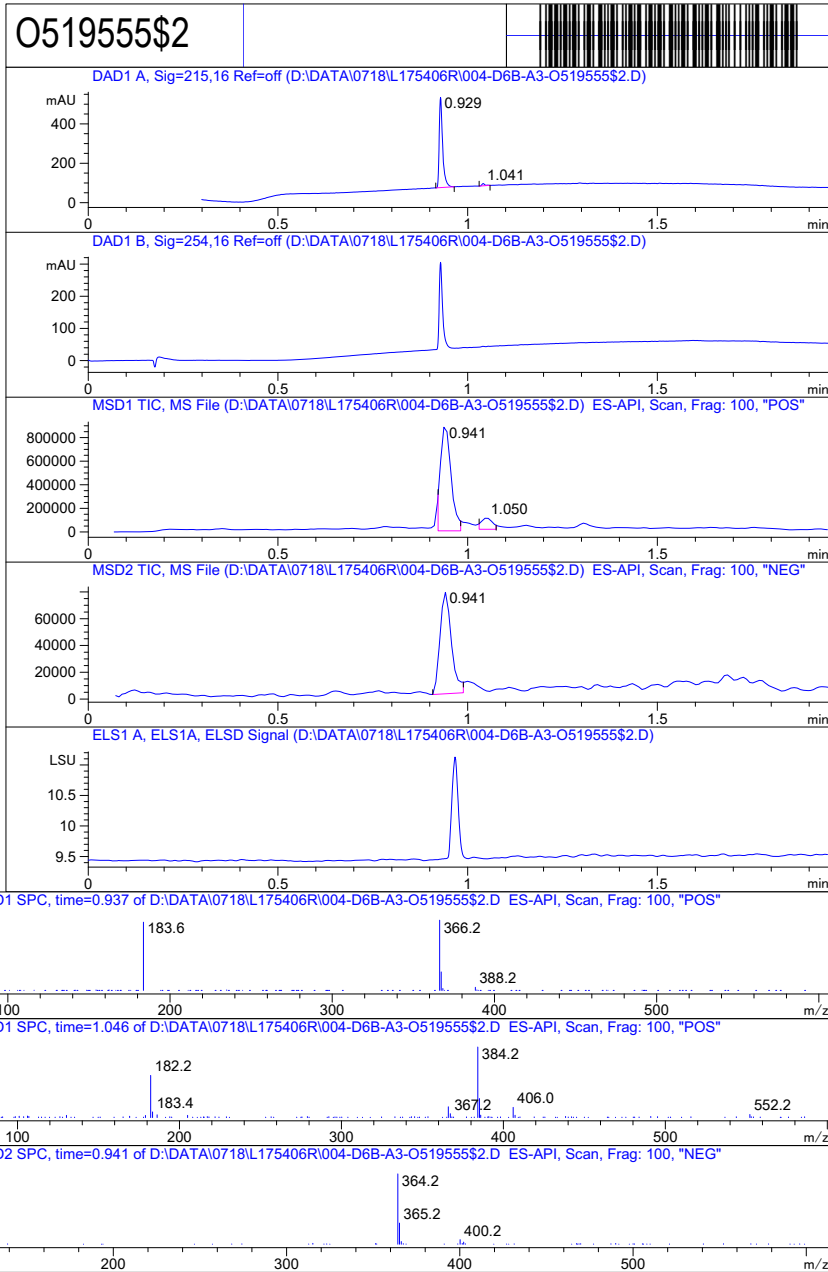60000
40000
20000
0.941

ELS1 A, ELS1A, ELSD Signal (D:\DATA\0718\L175406R\004-D6B-A3-O519555$2.D)
LSU
10.5
10
9.5

*MSD1 SPC, time=0.937 of D:\DATA\0718\L175406R\004-D6B-A3-O519555$2.D ES-API, Scan, Frag: 100, "POS"
RT 0.941
50
183.6   366.2   388.2

*MSD1 SPC, time=1.046 of D:\DATA\0718\L175406R\004-D6B-A3-O519555$2.D ES-API, Scan, Frag: 100, "POS"
RT 1.050
50
182.2 183.4 384.2 367.2 406.0 552.2

*MSD2 SPC, time=0.941 of D:\DATA\0718\L175406R\004-D6B-A3-O519555$2.D ES-API, Scan, Frag: 100, "NEG"
RT 0.941
50
364.2 365.2 400.2

Inj.Date 7/18/2019   LT   <invalid> 13   Acq. Method C:\Chem32\->   ->

S49

HRMS

Target Compound Screening Report

Data File	H1785733a.d	**Sample Name**	H1785733
Sample Type	Sample	**Position**	P1-F2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/10/2021 11:50:40 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C23H19N5	**Stream Name**	LC 1
Acquisition Time (Local)	5/10/2021 11:50:40 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H19 N5; 2.077	97.71	-0.54	C23 H19 N5	2.077	365.164	365.1638

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
366.1711	2.077	365.1638	C23 H19 N5	365.164	-0.54	Find By Formula	

Compound Chromatograms

Cpd 1: C23 H19 N5; 2.077: +ESI EIC(366.1713, 383.1979, 388.1533) Scan Frag=175.0V H17857
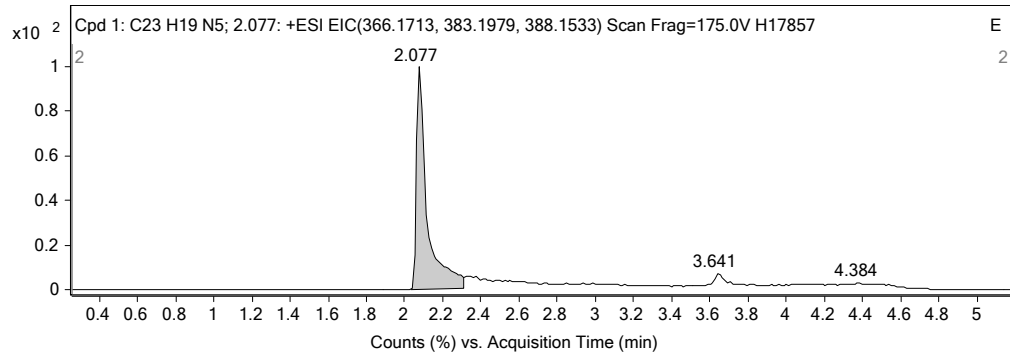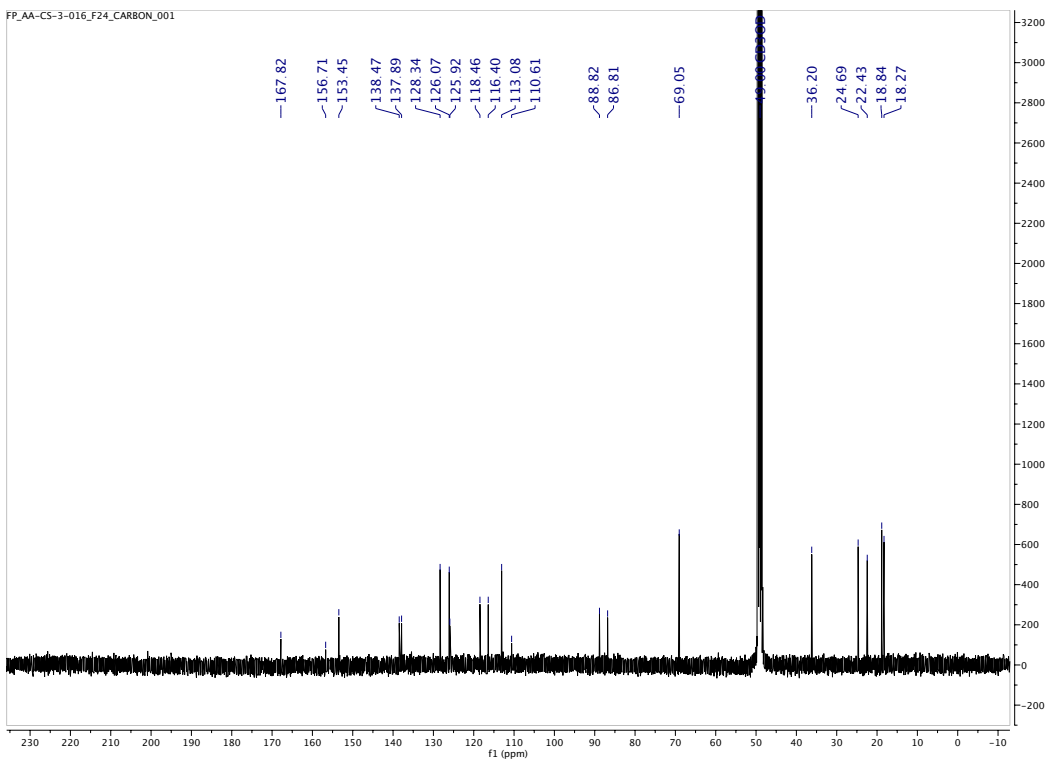
MS Zoomed Spectrum

*1-(2-amino-6,7-dihydro-5H-pyrimido[5,4-c]carbazol-10-yl)-4-methylpent-1-yn-3-ol (**10**).*
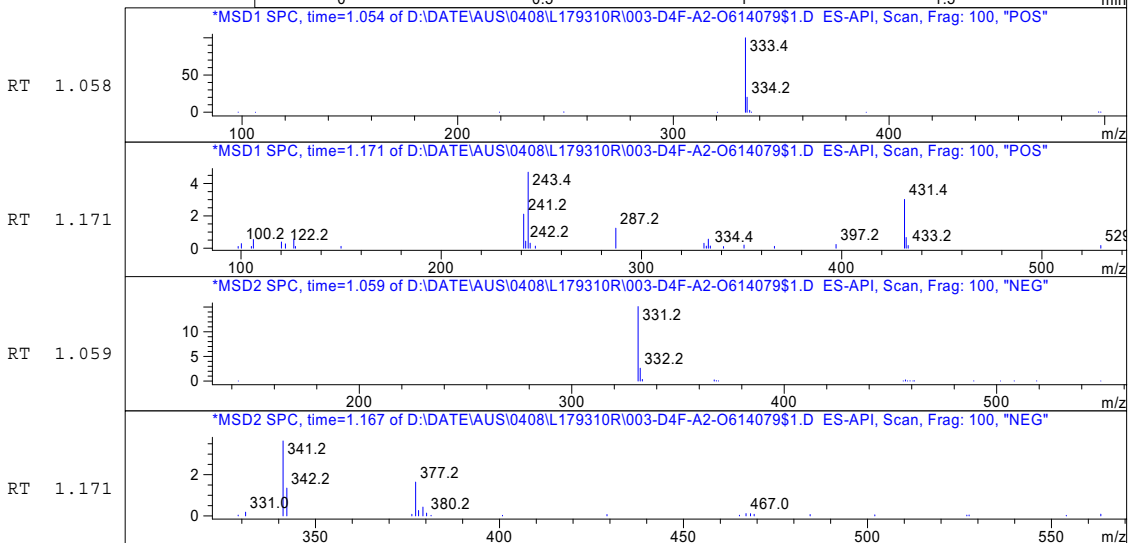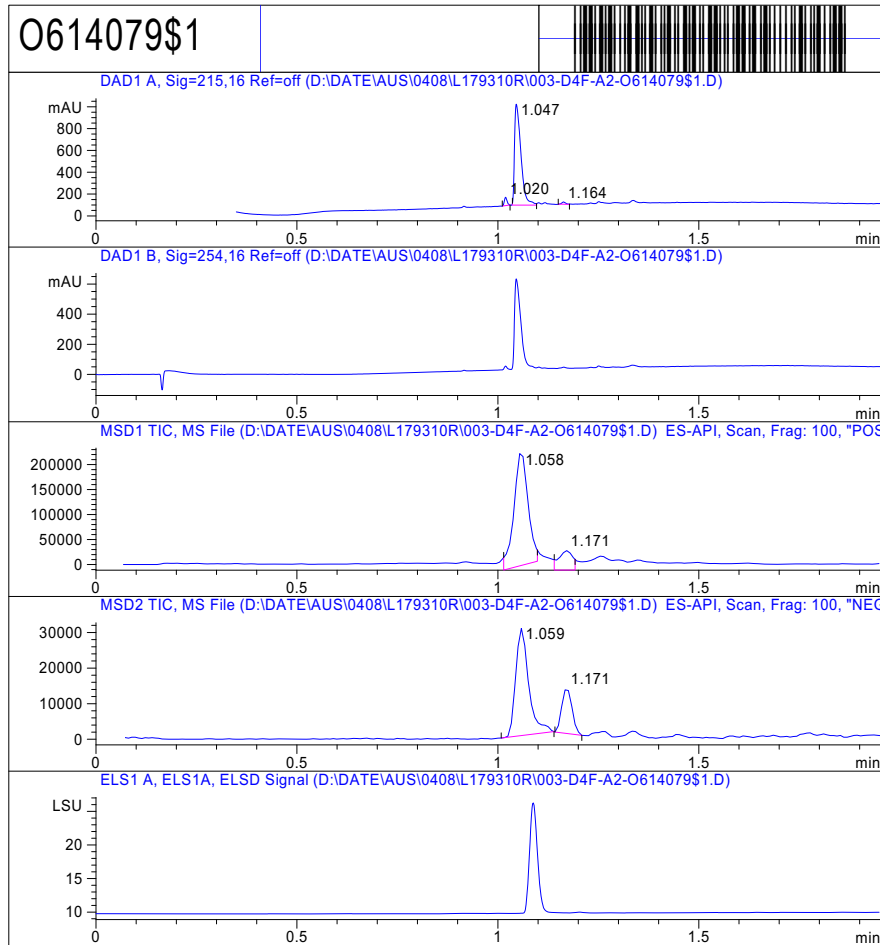
¹H NMR
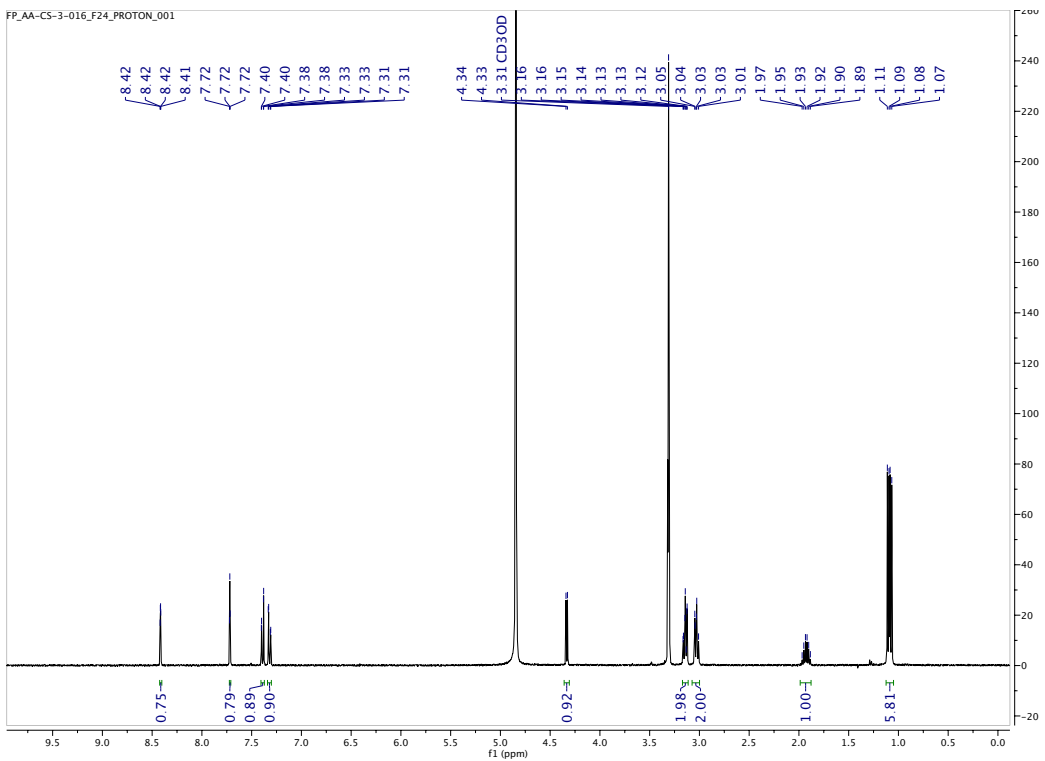
¹³C NMR

LC Chromatogram

MaxPeak: 95.34%
Ret_Time: 1.047 min
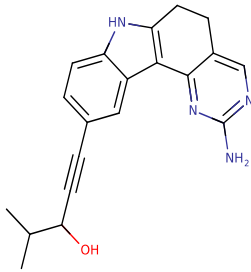
Mol Wt 332.4
Exact Mass 332.19

#	Time	Area%
1	1.020	3.34
2	1.047	95.34
3	1.164	1.33

O614079$1

DAD1 A, Sig=215,16 Ref=off (D:\DATE\AUS\0408\L179310R\003-D4F-A2-O614079$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATE\AUS\0408\L179310R\003-D4F-A2-O614079$1.D)

MSD1 TIC, MS File (D:\DATE\AUS\0408\L179310R\003-D4F-A2-O614079$1.D) ES-API, Scan, Frag: 100, "POS"

MSD2 TIC, MS File (D:\DATE\AUS\0408\L179310R\003-D4F-A2-O614079$1.D) ES-API, Scan, Frag: 100, "NEG"

ELS1 A, ELS1A, ELSD Signal (D:\DATE\AUS\0408\L179310R\003-D4F-A2-O614079$1.D)

RT 1.058 *MSD1 SPC, time=1.054 of D:\DATE\AUS\0408\L179310R\003-D4F-A2-O614079$1.D ES-API, Scan, Frag: 100, "POS"

RT 1.171 *MSD1 SPC, time=1.171 of D:\DATE\AUS\0408\L179310R\003-D4F-A2-O614079$1.D ES-API, Scan, Frag: 100, "POS"

RT 1.059 *MSD2 SPC, time=1.059 of D:\DATE\AUS\0408\L179310R\003-D4F-A2-O614079$1.D ES-API, Scan, Frag: 100, "NEG"

RT 1.171 *MSD2 SPC, time=1.167 of D:\DATE\AUS\0408\L179310R\003-D4F-A2-O614079$1.D ES-API, Scan, Frag: 100, "NEG"

Inj.Date 8/4/2019   Y   <invalid> -14-   Acq. Method C:\Chem32\-> ->

HRMS

Target Compound Screening Report

Data File	H1806657.d	**Sample Name**	H1806657
Sample Type	Sample	**Position**	P1-D5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 8:09:18 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C20H20N4O	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 8:09:18 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 2: C20 H20 N4 O; 2.259	80.03	-0.57	C20 H20 N4 O	2.259	332.1637	332.1635
Cpd 1: C20 H20 N4 O; 2.323	71.87	0.52	C20 H20 N4 O	2.323	332.1637	332.1639

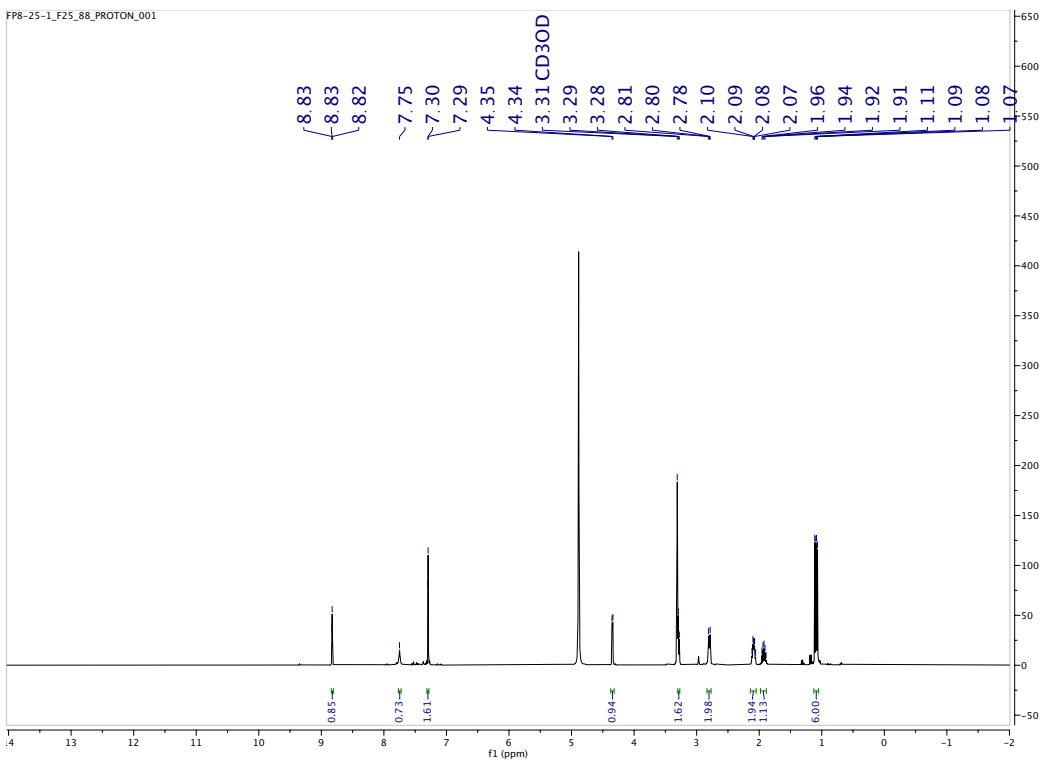| Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
333.1703	2.259	332.1635	C20 H20 N4 O	332.1637	-0.57	Find By Formula	

Compound Chromatograms
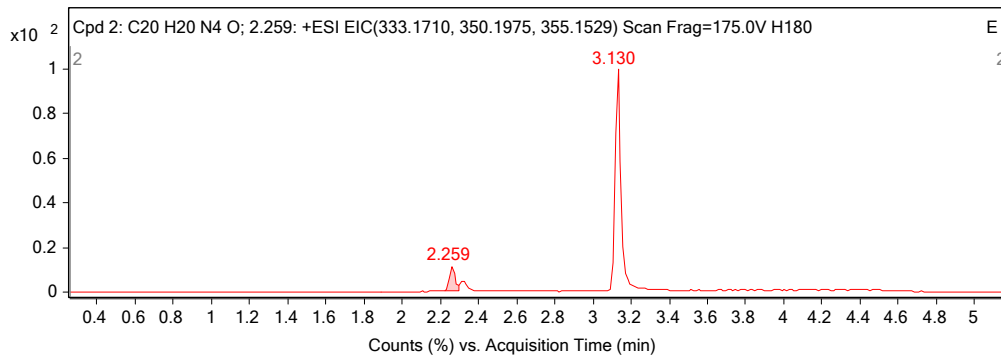
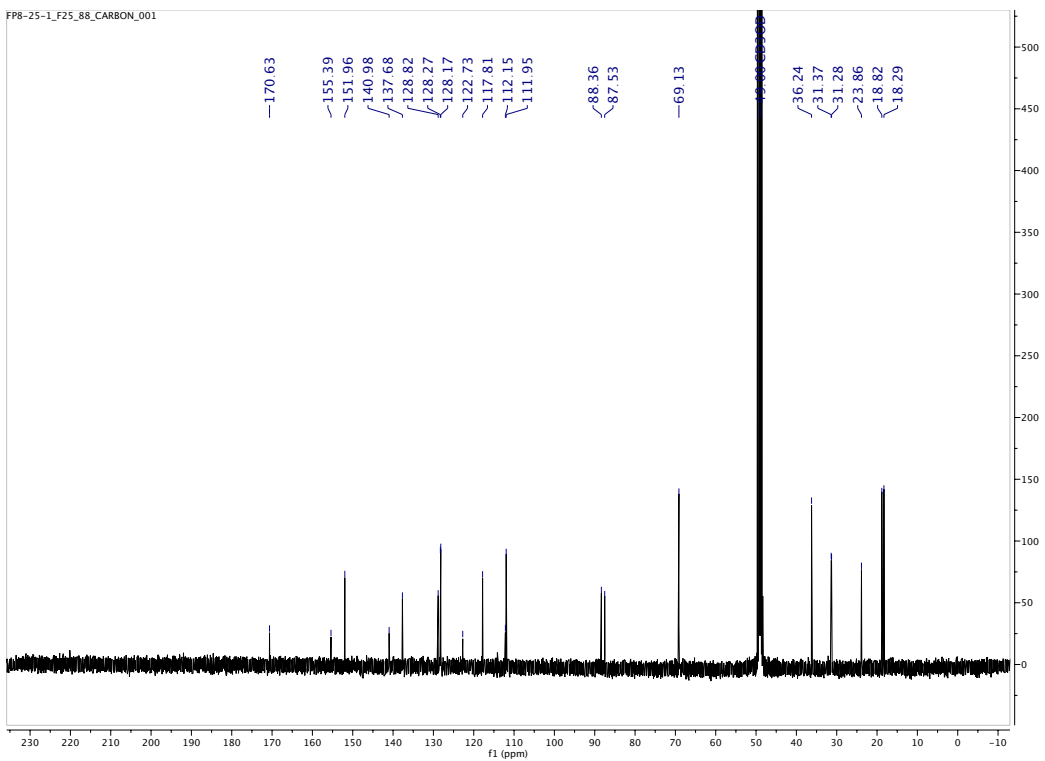

MS Zoomed Spectrum

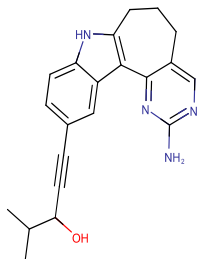*1-(2-amino-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-11-yl)-4-methylpent-1-yn-3-ol (11).*
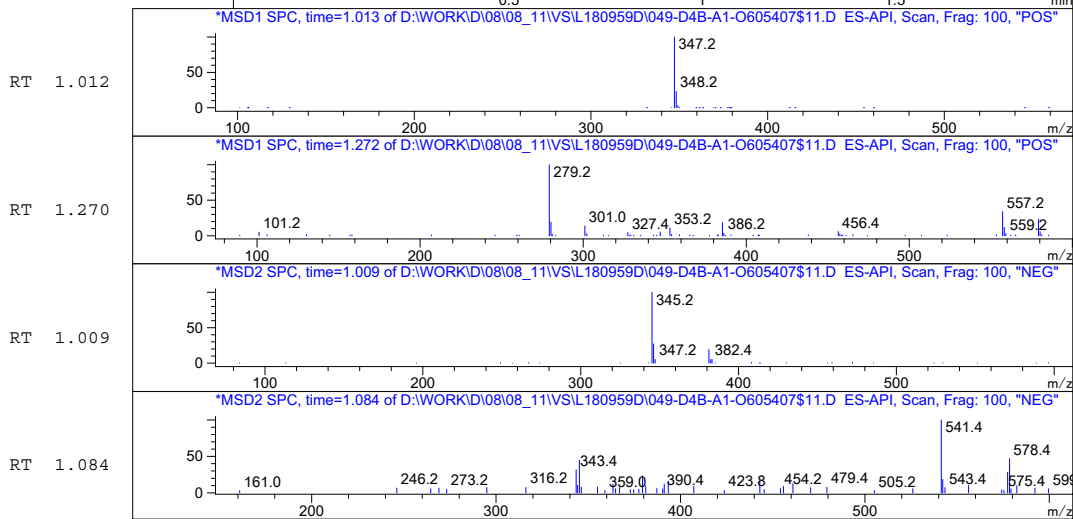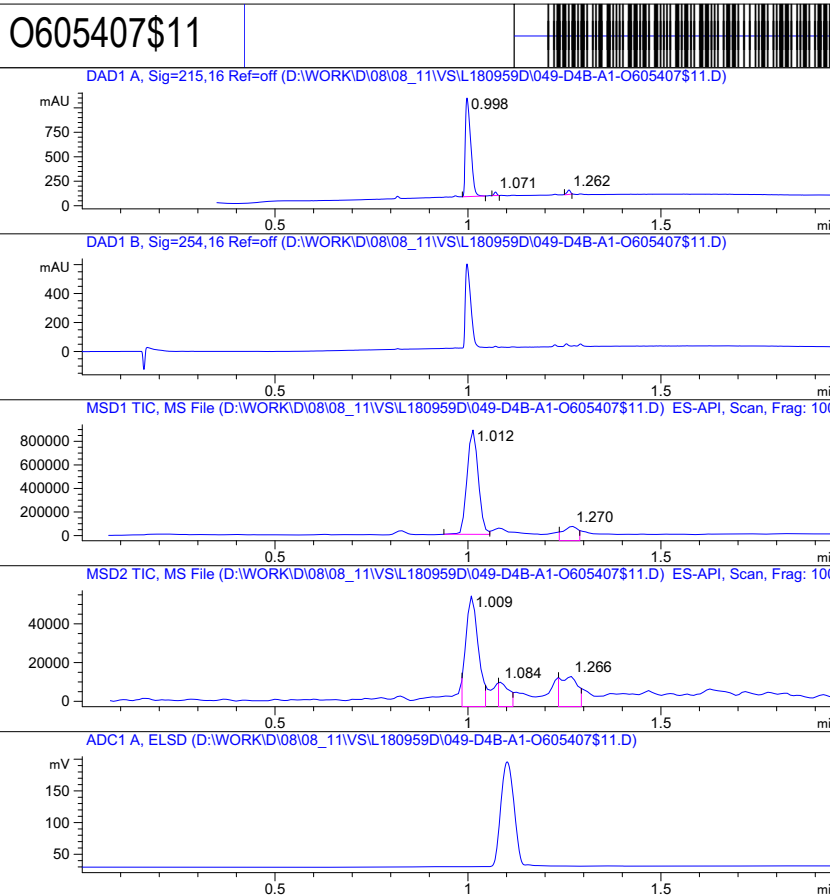
¹H NMR

¹³C NMR

LC Chromatogram

MaxPeak: 95.56%
Ret_Time: 0.998 min

Mol Wt 346.43
Exact Mass 346.21

```
#  Time   Area%
----------------
1  0.998  95.56
2  1.071   1.72
3  1.262   2.72
```


O605407$11

DAD1 A, Sig=215,16 Ref=off (D:\WORK\D\08\08_11\VS\L180959D\049-D4B-A1-O605407$11.D)
DAD1 B, Sig=254,16 Ref=off (D:\WORK\D\08\08_11\VS\L180959D\049-D4B-A1-O605407$11.D)
MSD1 TIC, MS File (D:\WORK\D\08\08_11\VS\L180959D\049-D4B-A1-O605407$11.D) ES-API, Scan, Frag: 100,
MSD2 TIC, MS File (D:\WORK\D\08\08_11\VS\L180959D\049-D4B-A1-O605407$11.D) ES-API, Scan, Frag: 100,
ADC1 A, ELSD (D:\WORK\D\08\08_11\VS\L180959D\049-D4B-A1-O605407$11.D)

RT 1.012 — *MSD1 SPC, time=1.013 of D:\WORK\D\08\08_11\VS\L180959D\049-D4B-A1-O605407$11.D ES-API, Scan, Frag: 100, "POS"

RT 1.270 — *MSD1 SPC, time=1.272 of D:\WORK\D\08\08_11\VS\L180959D\049-D4B-A1-O605407$11.D ES-API, Scan, Frag: 100, "POS"

RT 1.009 — *MSD2 SPC, time=1.009 of D:\WORK\D\08\08_11\VS\L180959D\049-D4B-A1-O605407$11.D ES-API, Scan, Frag: 100, "NEG"

RT 1.084 — *MSD2 SPC, time=1.084 of D:\WORK\D\08\08_11\VS\L180959D\049-D4B-A1-O605407$11.D ES-API, Scan, Frag: 100, "NEG"

Inj.Date 8/11/2019   K   <invalid> -9-   Acq. Method C:\Chem32\-> ->
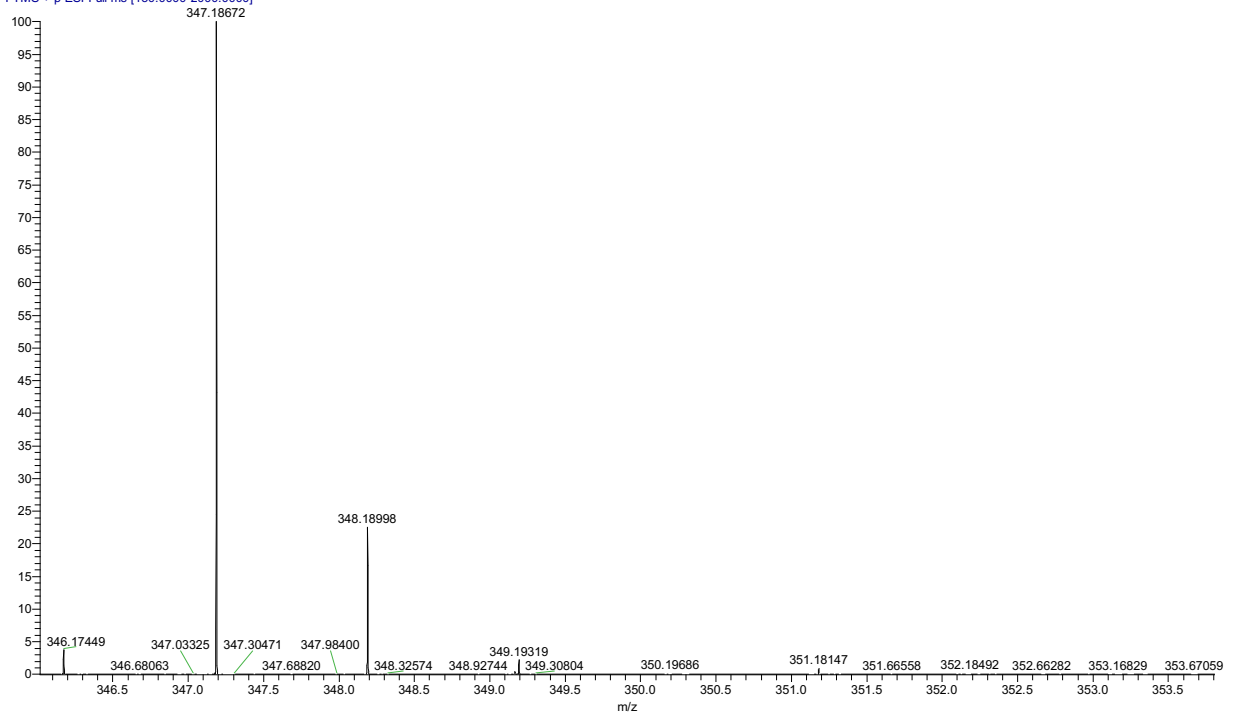
HRMS

FP-25-1 #5-100 RT: 0.02-0.43 AV: 96 NL: 9.88E8
T: FTMS + p ESI Full ms [150.0000-2000.0000]

347.18672

317.24118

217.08370   284.33131   368.42528   511.20519   693.36676   764.57468   1009.63358   1185.04485   1412.28332   1557.94101   1720.04596   1844.22560   1946.57482
536.61351

m/z

FP-25-1 #5-100 RT: 0.02-0.43 AV: 96 NL: 9.88E8
T: FTMS + p ESI Full ms [150.0000-2000.0000]

347.18672

348.18998

346.17449   347.03325   347.30471   347.98400   348.32574   348.92744   349.19319   350.19686   351.18147   351.66558   352.18492   352.66282   353.16829   353.67059
346.68063   347.68820   349.30804

m/z
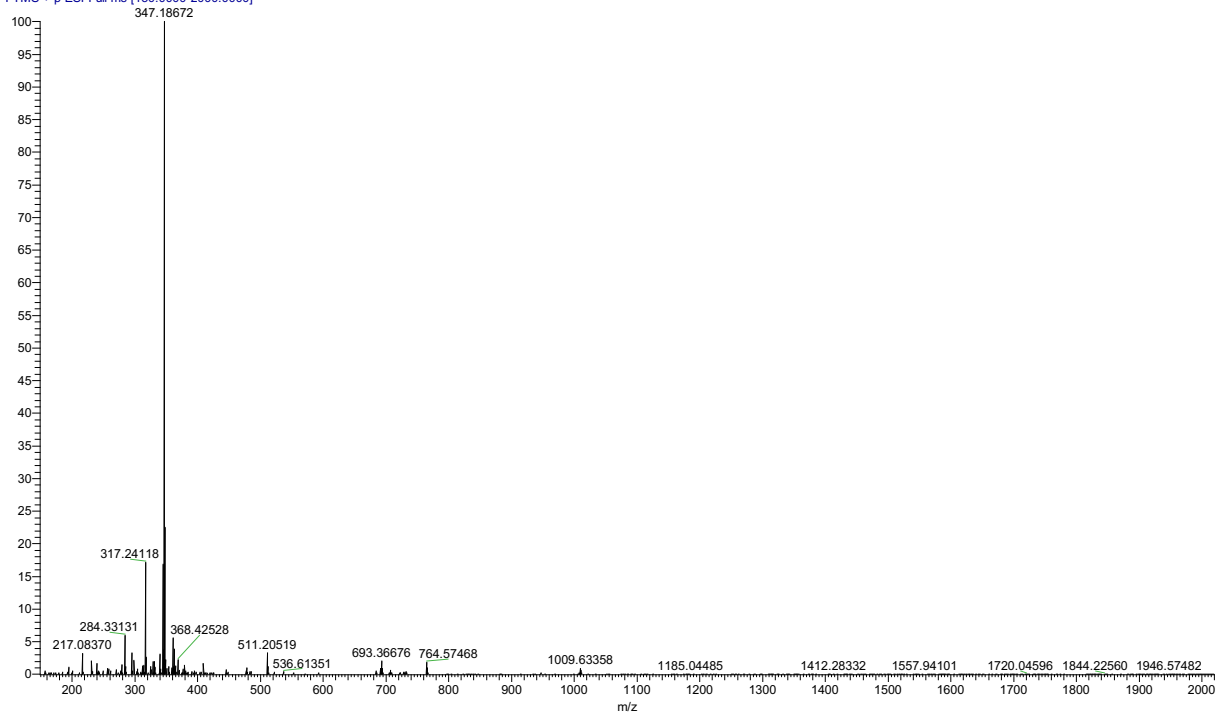
*10-((1-methyl-1H-imidazol-5-yl)ethynyl)-6,7-dihydro-5H-pyrimido[5,4-c]carbazol-2-amine (**14**).*
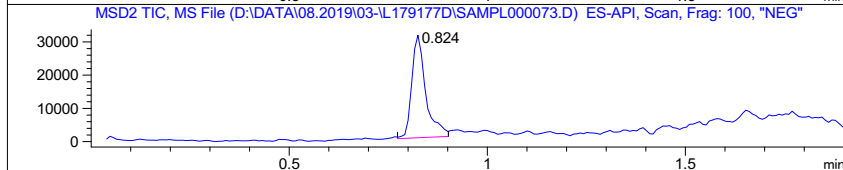**¹H NMR**
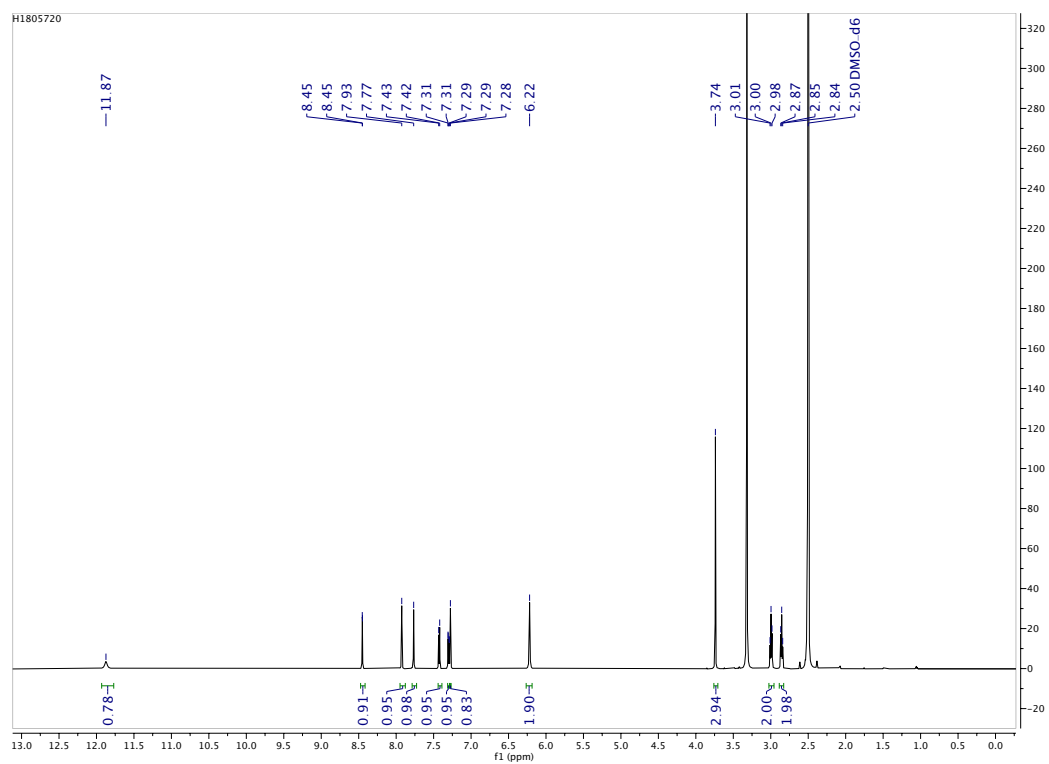
¹³C NMR
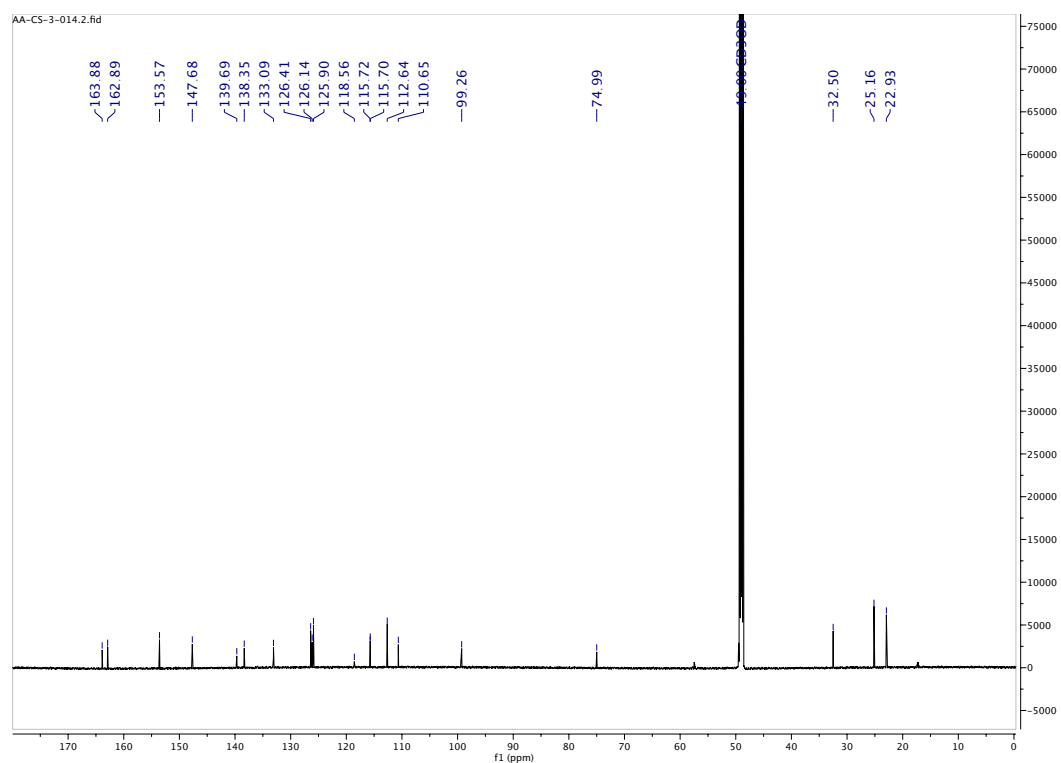
LC Chromatogram

MaxPeak: 98.86%
Ret_Time: 0.810 min
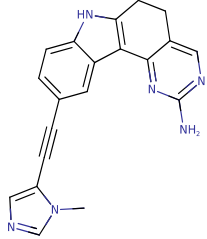
Mol Wt   **340.38**
Exact Mass   **340.16**

```
#  Time   Area%
-----------------
1  0.810  98.86
2  1.021   1.14
```

O604497$1

DAD1 A, Sig=215,16 Ref=off (D:\DATA\08.2019\03-\L179177D\SAMPL000073.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATA\08.2019\03-\L179177D\SAMPL000073.D)

MSD1 TIC, MS File (D:\DATA\08.2019\03-\L179177D\SAMPL000073.D) ES-API, Scan, Frag: 100, "POS"

MSD2 TIC, MS File (D:\DATA\08.2019\03-\L179177D\SAMPL000073.D) ES-API, Scan, Frag: 100, "NEG"

ADC1 A, ELSD (D:\DATA\08.2019\03-\L179177D\SAMPL000073.D)

*MSD1 SPC, time=0.821 of D:\DATA\08.2019\03-\L179177D\SAMPL000073.D ES-API, Scan, Frag: 100, "POS"
RT 0.825

*MSD1 SPC, time=1.038 of D:\DATA\08.2019\03-\L179177D\SAMPL000073.D ES-API, Scan, Frag: 100, "POS"
RT 1.038

*MSD2 SPC, time=0.825 of D:\DATA\08.2019\03-\L179177D\SAMPL000073.D ES-API, Scan, Frag: 100, "NEG"
RT 0.824

HRMS

Target Compound Screening Report

Data File	H1805720.d	**Sample Name**	H1805720
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 7:14:44 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C20H16N6	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 7:14:44 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C20 H16 N6; 2.944	54.57	2.51	C20 H16 N6	2.944	340.1436	340.1445

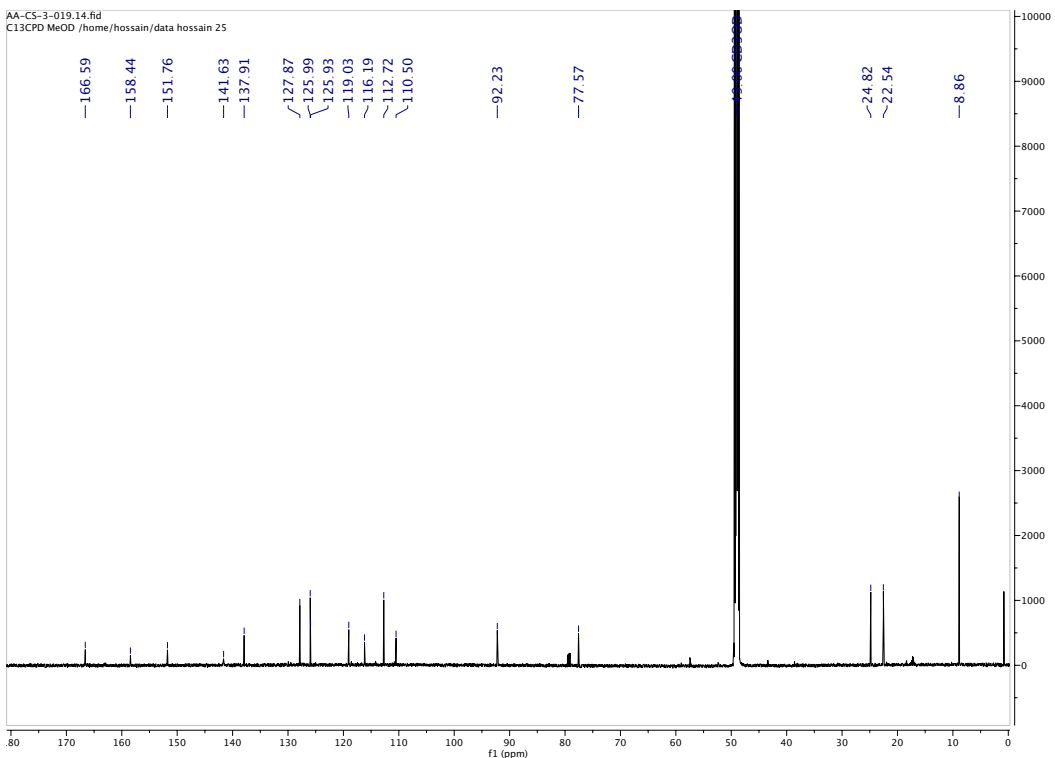| Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
363.1347	2.944	340.1445	C20 H16 N6	340.1436	2.51	Find By Formula	

Compound Chromatograms
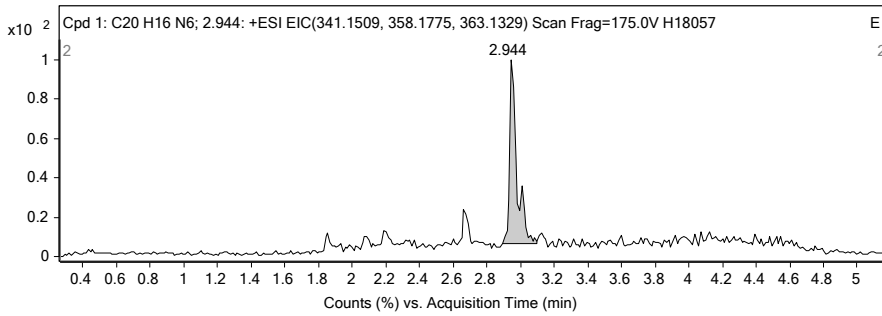
MS Zoomed Spectrum

*10-(cyclopropylethynyl)-6,7-dihydro-5H-pyrimido[5,4-c]carbazol-2-amine (**15**).*
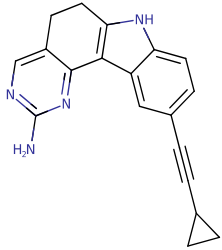**¹H NMR**
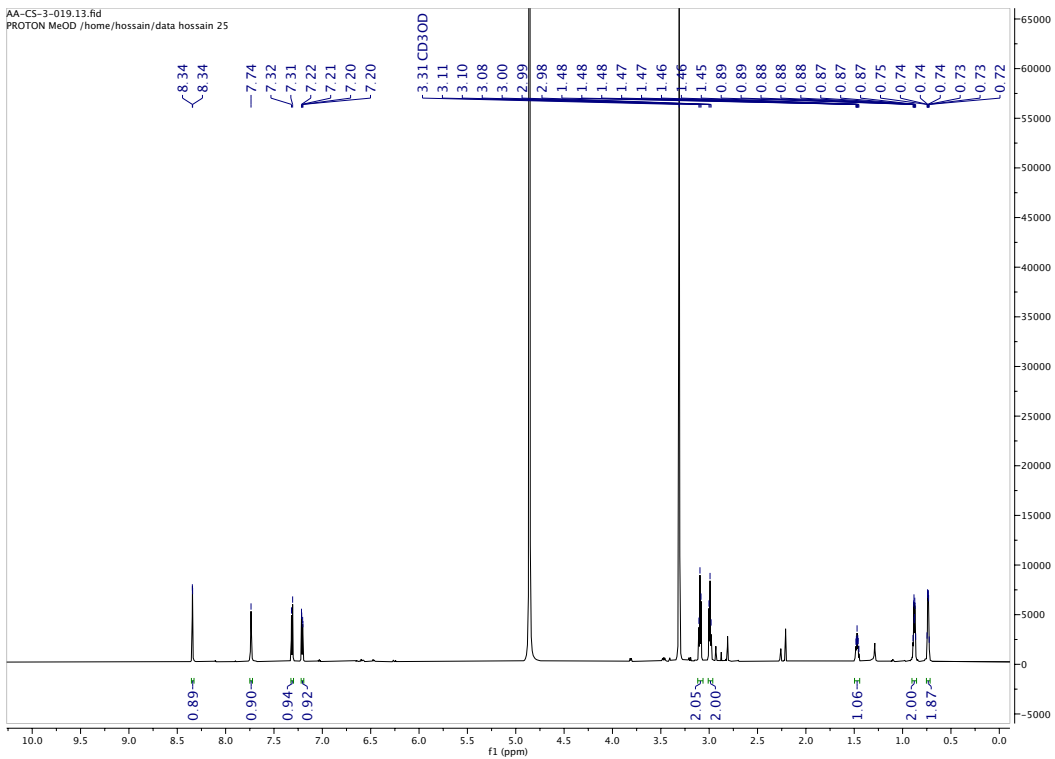
¹³C NMR
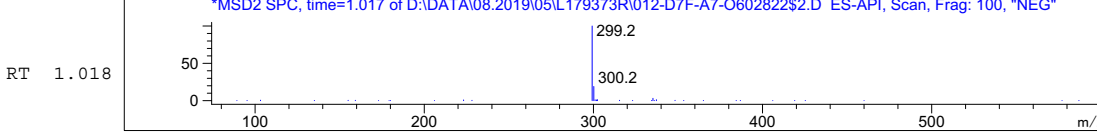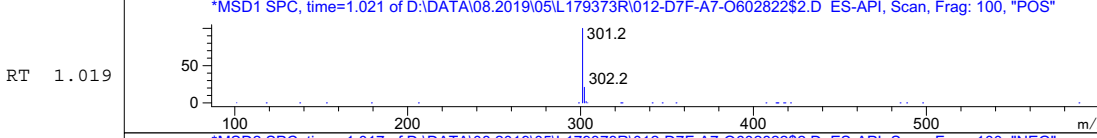
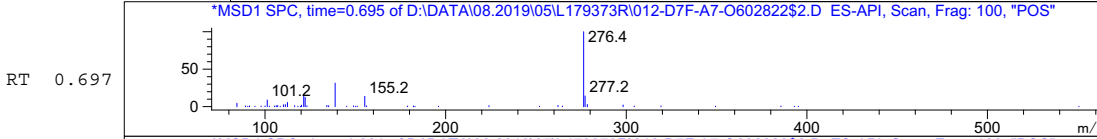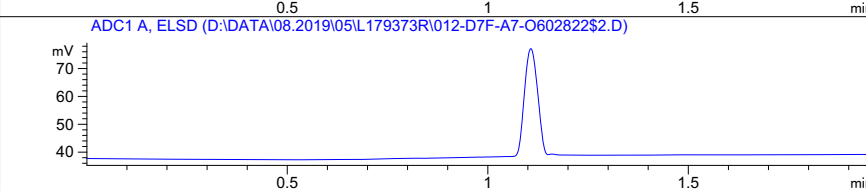## LC Chromatogram

MaxPeak: 96.33%
Ret_Time: 1.007 min

Mol Wt 300.36
Exact Mass 300.16

```
#  Time   Area%
----------------
1  0.691  3.67
2  1.007  96.33
```

O602822$2

DAD1 A, Sig=215,16 Ref=off (D:\DATA\08.2019\05\L179373R\012-D7F-A7-O602822$2.D)

mAU

1.007

0.691

DAD1 B, Sig=254,16 Ref=off (D:\DATA\08.2019\05\L179373R\012-D7F-A7-O602822$2.D)

mAU

MSD1 TIC, MS File (D:\DATA\08.2019\05\L179373R\012-D7F-A7-O602822$2.D) ES-API, Scan, Frag: 100, "PO

1.019

0.697

MSD2 TIC, MS File (D:\DATA\08.2019\05\L179373R\012-D7F-A7-O602822$2.D) ES-API, Scan, Frag: 100, "NE

1.018

ADC1 A, ELSD (D:\DATA\08.2019\05\L179373R\012-D7F-A7-O602822$2.D)

mV

*MSD1 SPC, time=0.695 of D:\DATA\08.2019\05\L179373R\012-D7F-A7-O602822$2.D ES-API, Scan, Frag: 100, "POS"

RT 0.697

276.4
277.2
101.2 155.2

*MSD1 SPC, time=1.021 of D:\DATA\08.2019\05\L179373R\012-D7F-A7-O602822$2.D ES-API, Scan, Frag: 100, "POS"

RT 1.019

301.2
302.2

*MSD2 SPC, time=1.017 of D:\DATA\08.2019\05\L179373R\012-D7F-A7-O602822$2.D ES-API, Scan, Frag: 100, "NEG"

RT 1.018

299.2
300.2

HRMS

10-(3-(dimethylamino)prop-1-yn-1-yl)-6,7-dihydro-5H-pyrimido[5,4-c]carbazol-2-amine (16).
¹H NMR

¹³C NMR

AA-CS-3-027.1.fid

164.25
161.84
149.41
149.23
138.55
127.20
126.42
126.02
115.97
115.69
112.78
110.58
90.73
78.97
43.51
25.00
22.76

f1 (ppm)
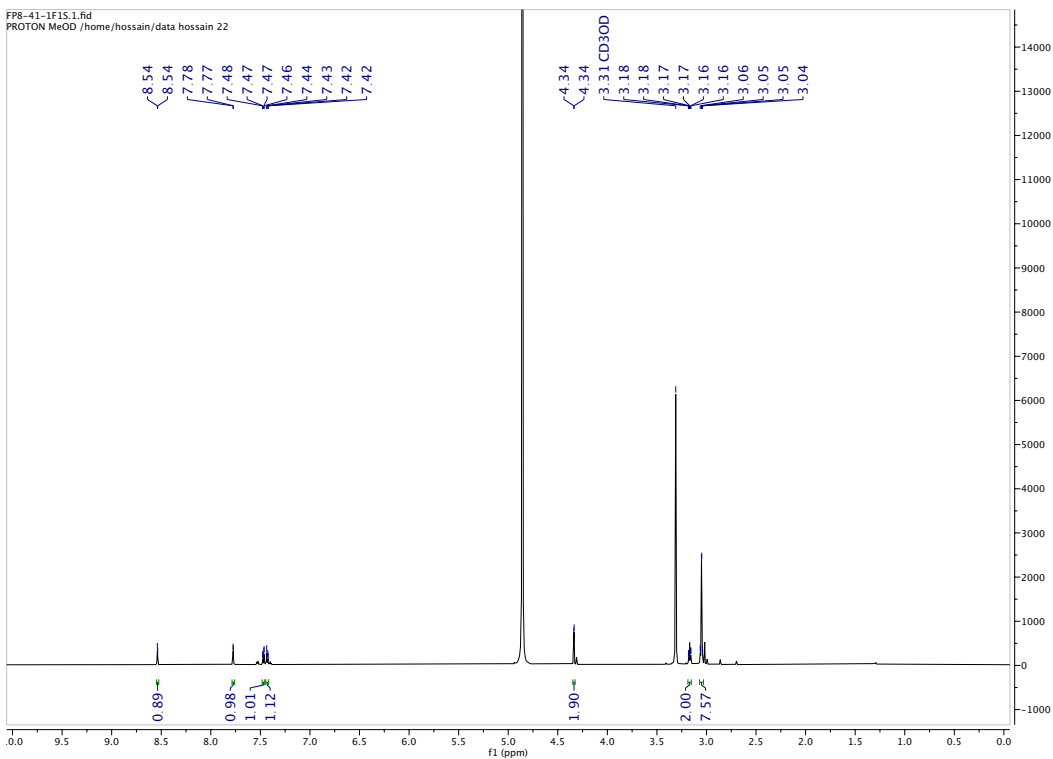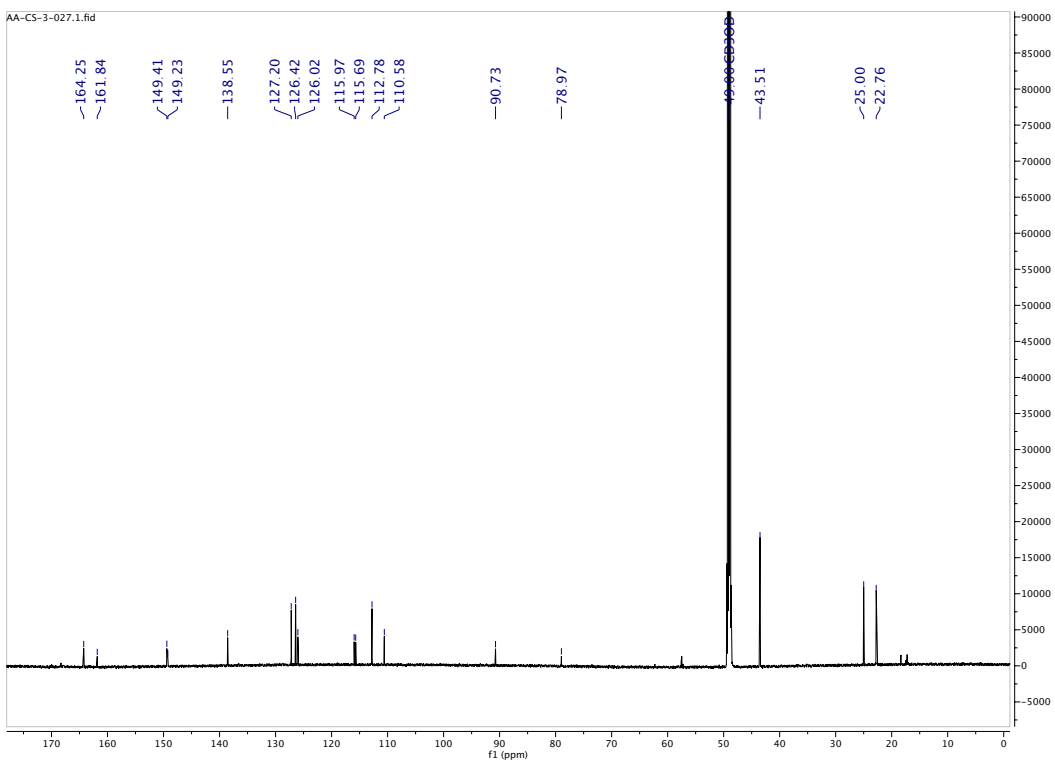
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 0.689 min
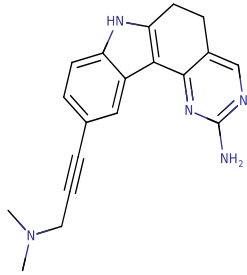
Mol Wt   **317.39**
Exact Mass   **317.19**

```
#   Time    Area%
-----------------
1   0.689  100.00
```
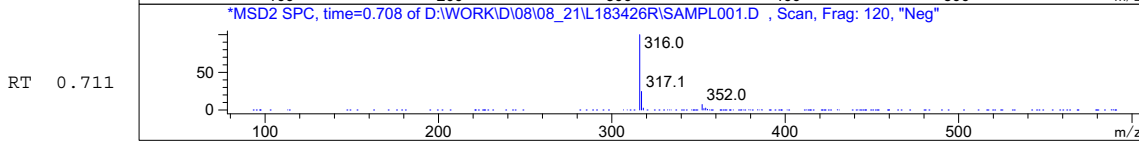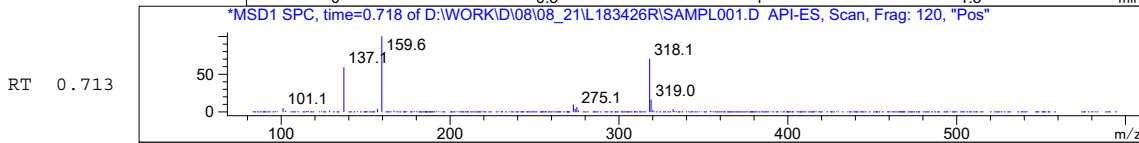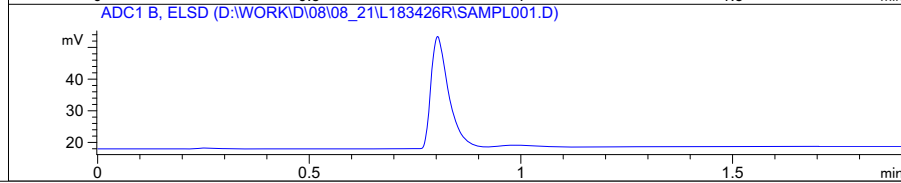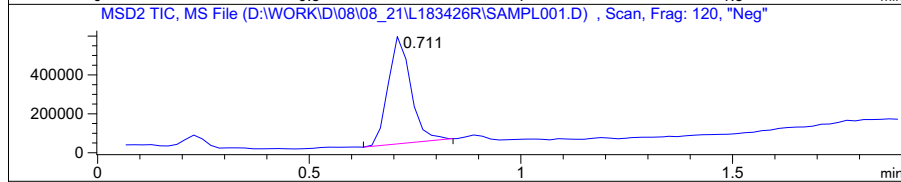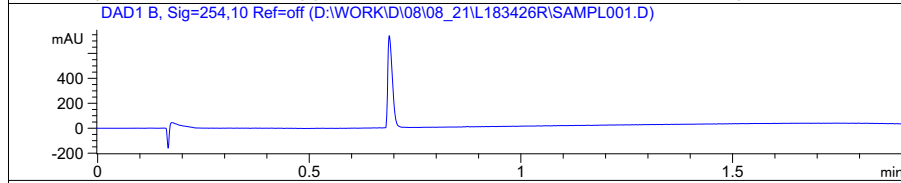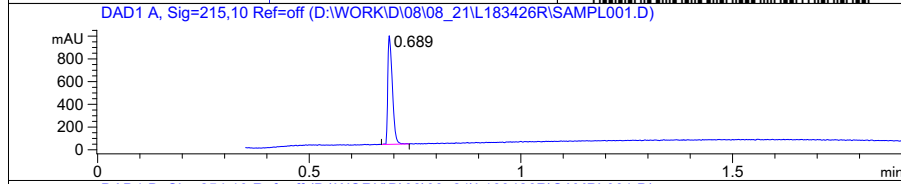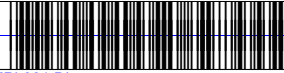
O696137$1

DAD1 A, Sig=215,10 Ref=off (D:\WORK\D\08\08_21\L183426R\SAMPL001.D)

0.689

DAD1 B, Sig=254,10 Ref=off (D:\WORK\D\08\08_21\L183426R\SAMPL001.D)

MSD1 TIC, MS File (D:\WORK\D\08\08_21\L183426R\SAMPL001.D) API-ES, Scan, Frag: 120, "Pos"

0.713

MSD2 TIC, MS File (D:\WORK\D\08\08_21\L183426R\SAMPL001.D) , Scan, Frag: 120, "Neg"

0.711

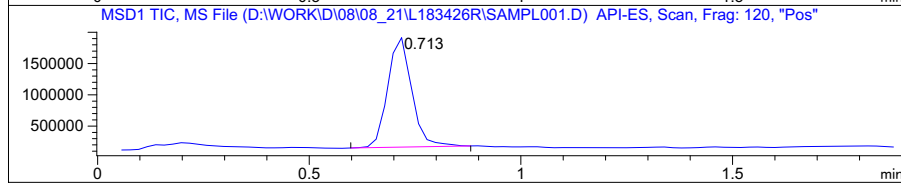ADC1 B, ELSD (D:\WORK\D\08\08_21\L183426R\SAMPL001.D)

*MSD1 SPC, time=0.718 of D:\WORK\D\08\08_21\L183426R\SAMPL001.D API-ES, Scan, Frag: 120, "Pos"

RT 0.713

101.1 137.1 159.6 275.1 318.1 319.0

*MSD2 SPC, time=0.708 of D:\WORK\D\08\08_21\L183426R\SAMPL001.D , Scan, Frag: 120, "Neg"

RT 0.711

316.0 317.1 352.0

HRMS
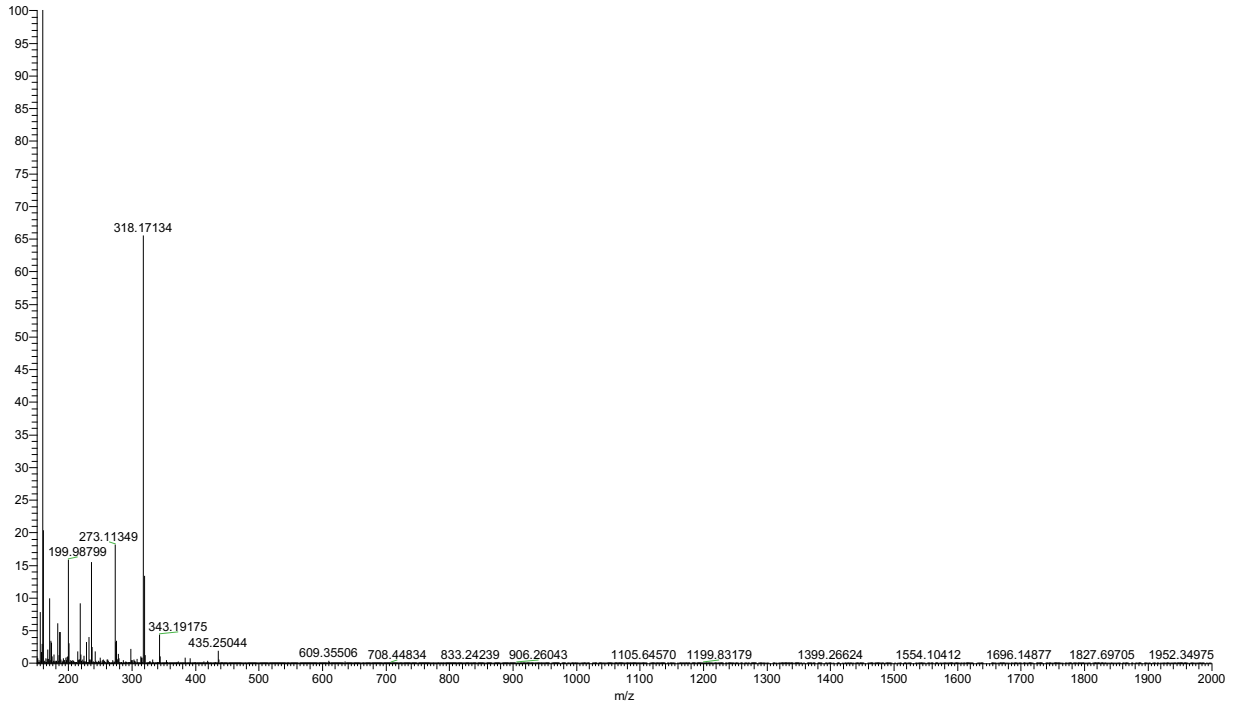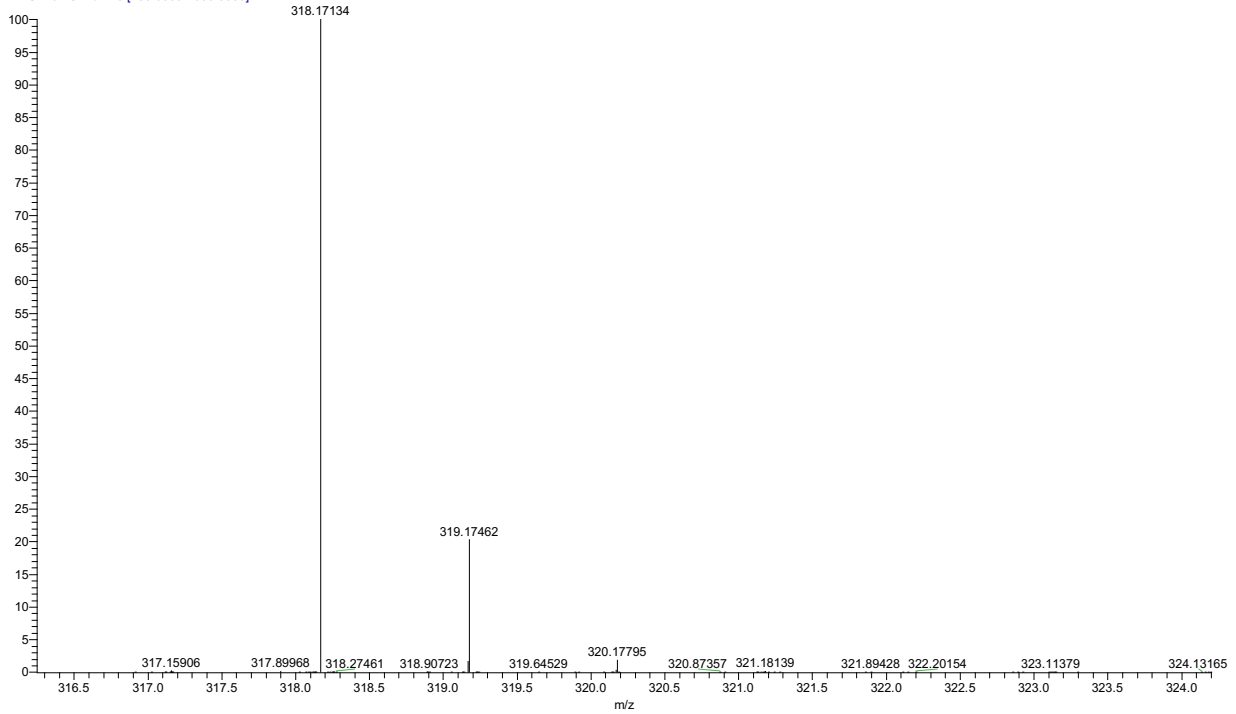
11-(3-(dimethylamino)prop-1-yn-1-yl)-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-2-amine (17).

^{1}H NMR
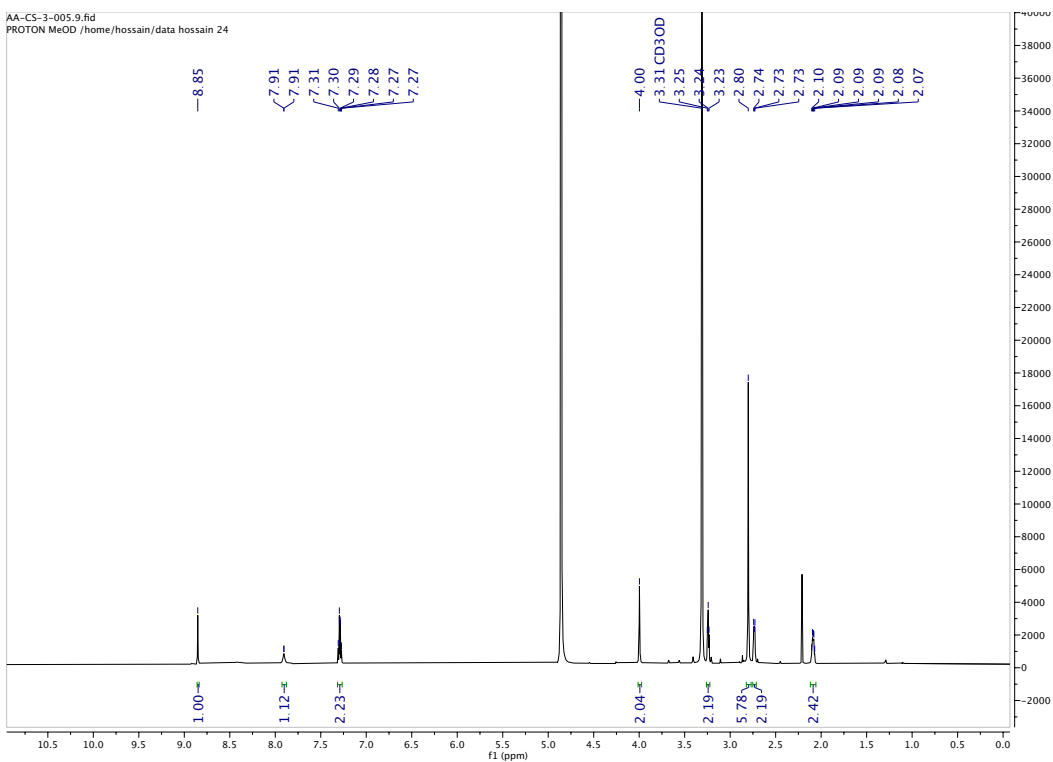
^{13}C NMR
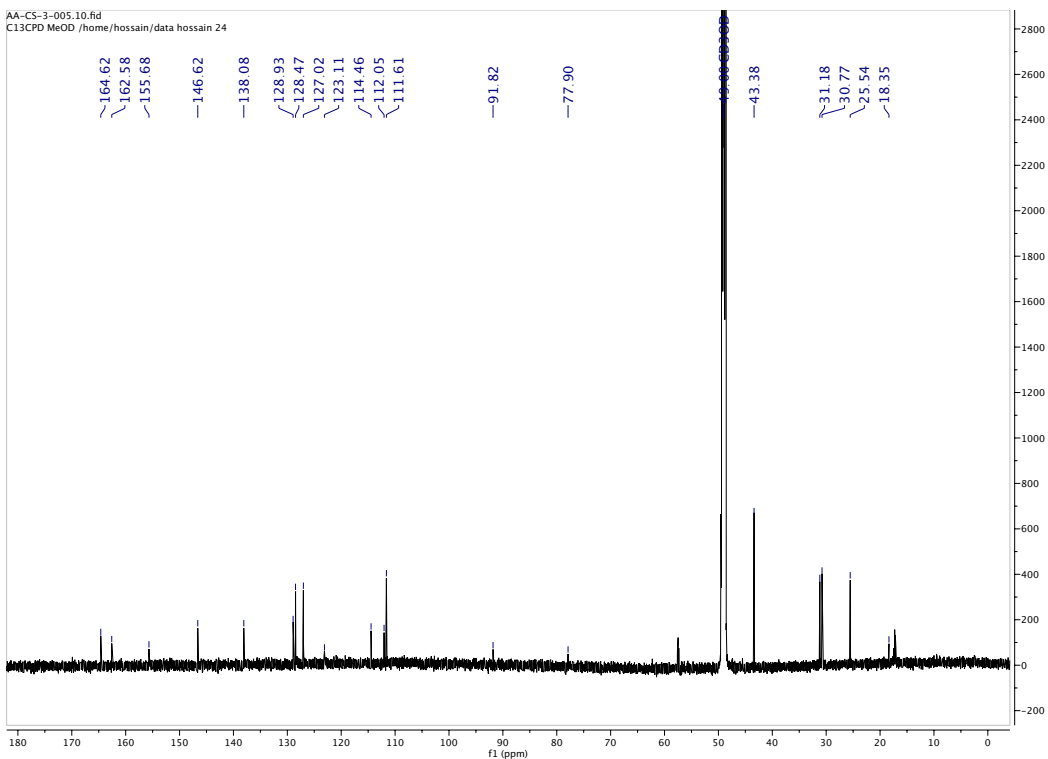
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 0.723 min
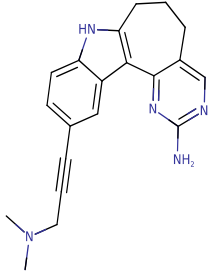
Mol Wt   **331.41**
Exact Mass   **331.21**

```
#   Time    Area%
-----------------
1   0.723   100.00
```

O694483$1
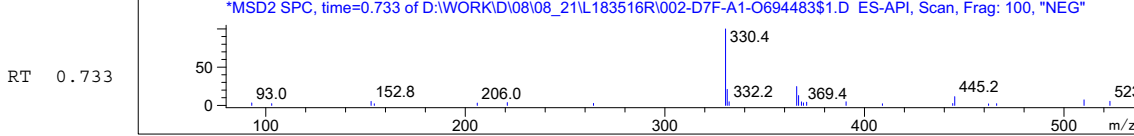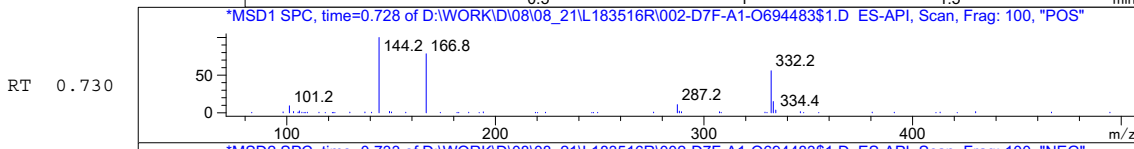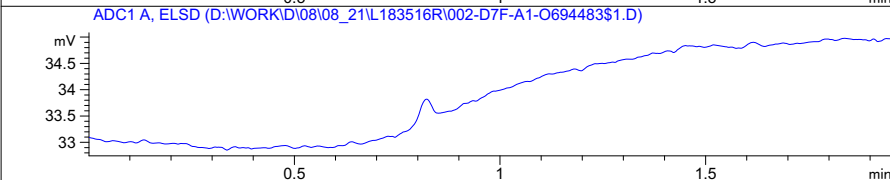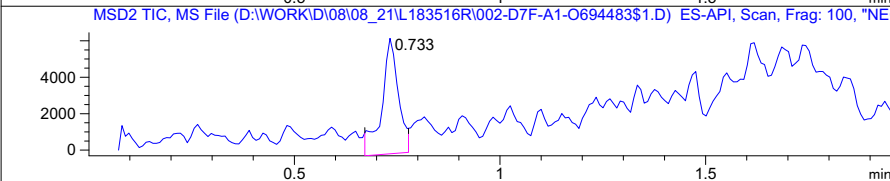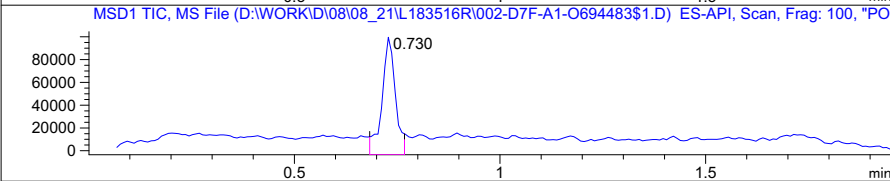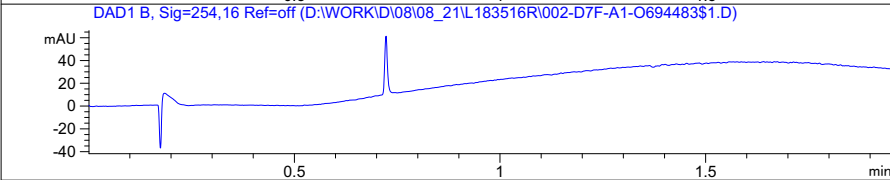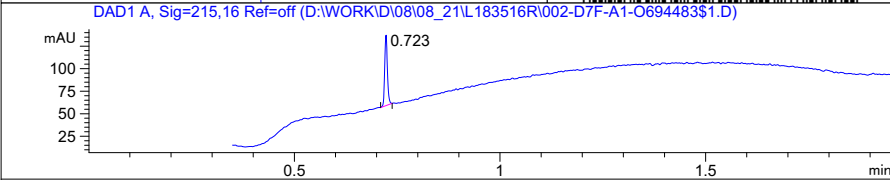
DAD1 A, Sig=215,16 Ref=off (D:\WORK\D\08\08_21\L183516R\002-D7F-A1-O694483$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\WORK\D\08\08_21\L183516R\002-D7F-A1-O694483$1.D)

MSD1 TIC, MS File (D:\WORK\D\08\08_21\L183516R\002-D7F-A1-O694483$1.D) ES-API, Scan, Frag: 100, "PO

MSD2 TIC, MS File (D:\WORK\D\08\08_21\L183516R\002-D7F-A1-O694483$1.D) ES-API, Scan, Frag: 100, "NE

ADC1 A, ELSD (D:\WORK\D\08\08_21\L183516R\002-D7F-A1-O694483$1.D)

*MSD1 SPC, time=0.728 of D:\WORK\D\08\08_21\L183516R\002-D7F-A1-O694483$1.D ES-API, Scan, Frag: 100, "POS"

RT 0.730

*MSD2 SPC, time=0.733 of D:\WORK\D\08\08_21\L183516R\002-D7F-A1-O694483$1.D ES-API, Scan, Frag: 100, "NEG"

RT 0.733

HRMS
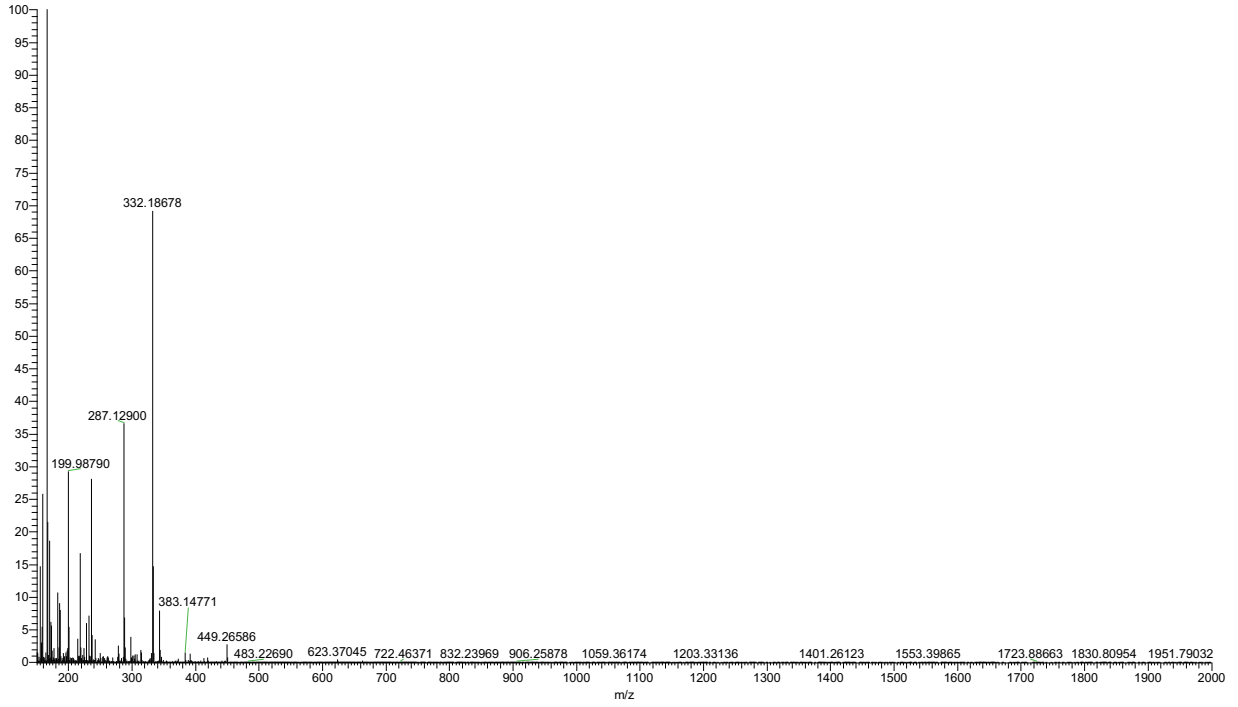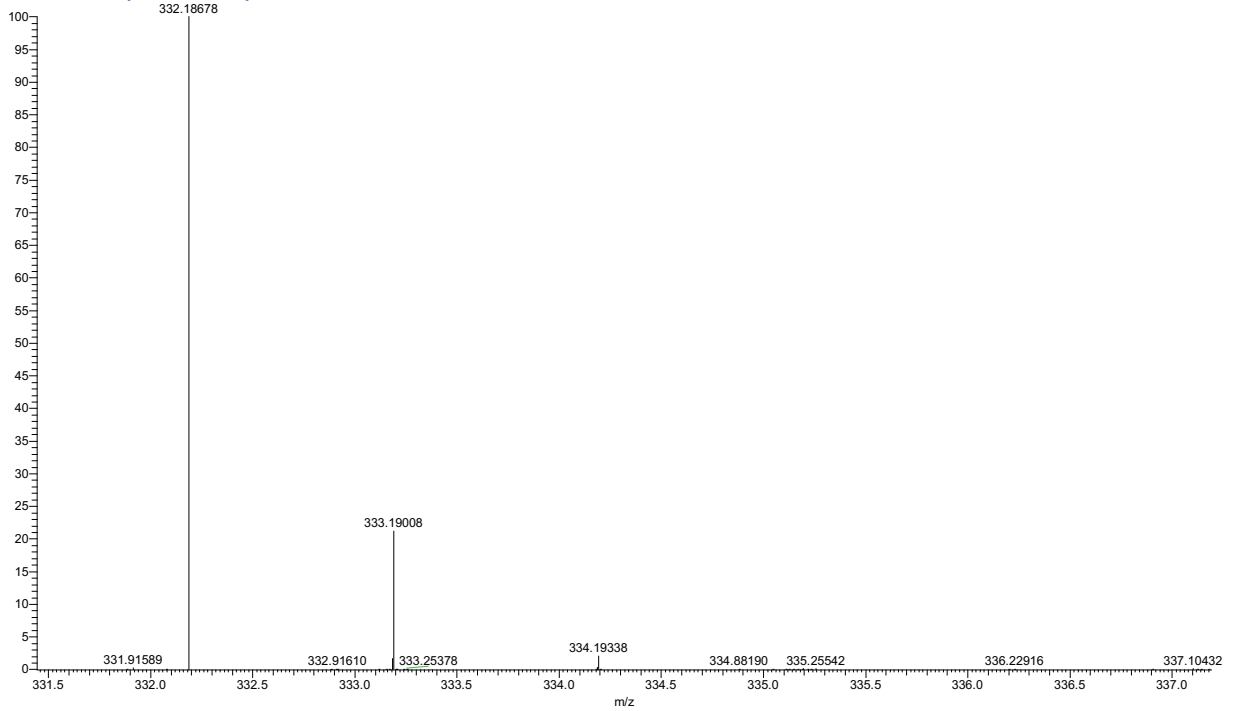
12-(1-methyl-1H-imidazol-5-yl)ethynyl)-6,7,8,9-tetrahydro-5H-pyrimido[4',5':3,4] cycloocta[1,2-b]indol-2-amine (27).

¹H NMR
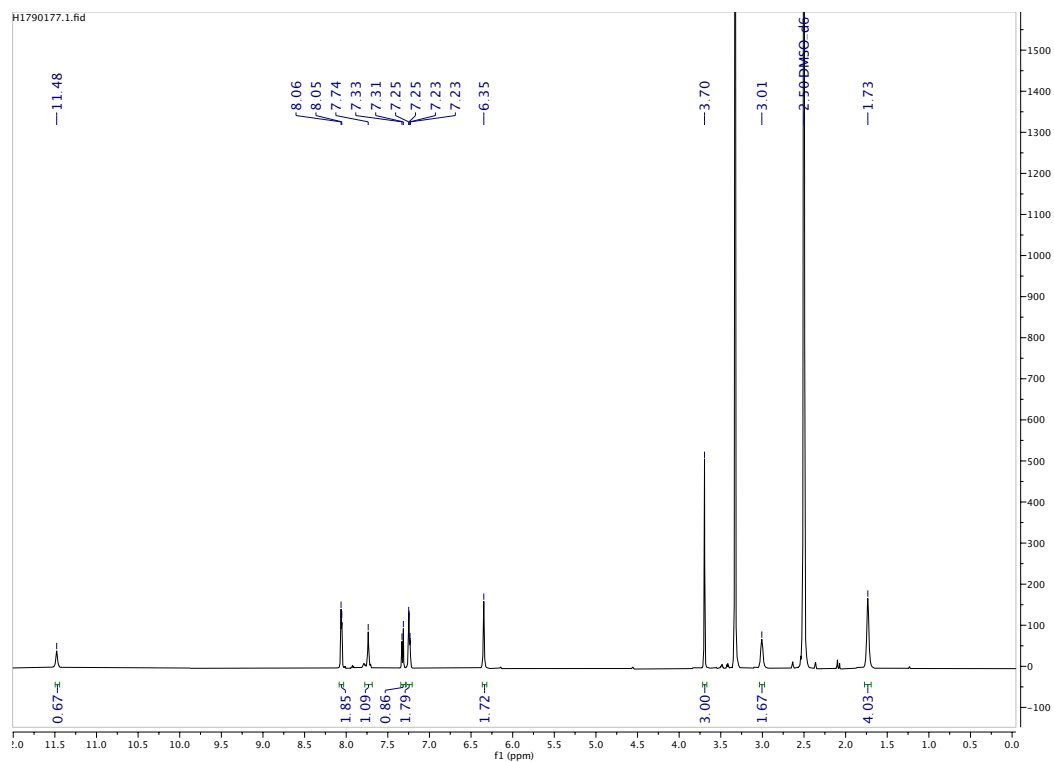
¹³C NMR

LC Chromatogram
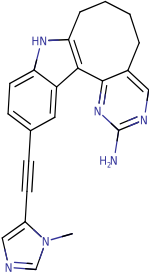
Mol Wt   **368.43**
Exact Mass   **368.2**

```
#  Time   Area%
-----------------
1  0.855  100.00
```

O541246$2

DAD1 A, Sig=215,16 Ref=off (D:\WORK\D\07\07_23\L176509R\005-D6B-A4-O541246$2.D)

DAD1 B, Sig=254,16 Ref=off (D:\WORK\D\07\07_23\L176509R\005-D6B-A4-O541246$2.D)

MSD1 TIC, MS File (D:\WORK\D\07\07_23\L176509R\005-D6B-A4-O541246$2.D) ES-API, Scan, Frag: 100, "PO

MSD2 TIC, MS File (D:\WORK\D\07\07_23\L176509R\005-D6B-A4-O541246$2.D) ES-API, Scan, Frag: 100, "NE

ELS1 A, ELS1A, ELSD Signal (D:\WORK\D\07\07_23\L176509R\005-D6B-A4-O541246$2.D)

*MSD1 SPC, time=0.862 of D:\WORK\D\07\07_23\L176509R\005-D6B-A4-O541246$2.D ES-API, Scan, Frag: 100, "POS"

RT 0.865

*MSD2 SPC, time=0.866 of D:\WORK\D\07\07_23\L176509R\005-D6B-A4-O541246$2.D ES-API, Scan, Frag: 100, "NEG"

RT 0.866

HRMS

Target Compound Screening Report

Data File	H1790176a.d	**Sample Name**	H1790176
Sample Type	Sample	**Position**	P1-E1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 8:55:19 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C22H20N6	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 8:55:19 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H20 N6; 1.969	97.19	0.04	C22 H20 N6	1.969	368.1749	368.175

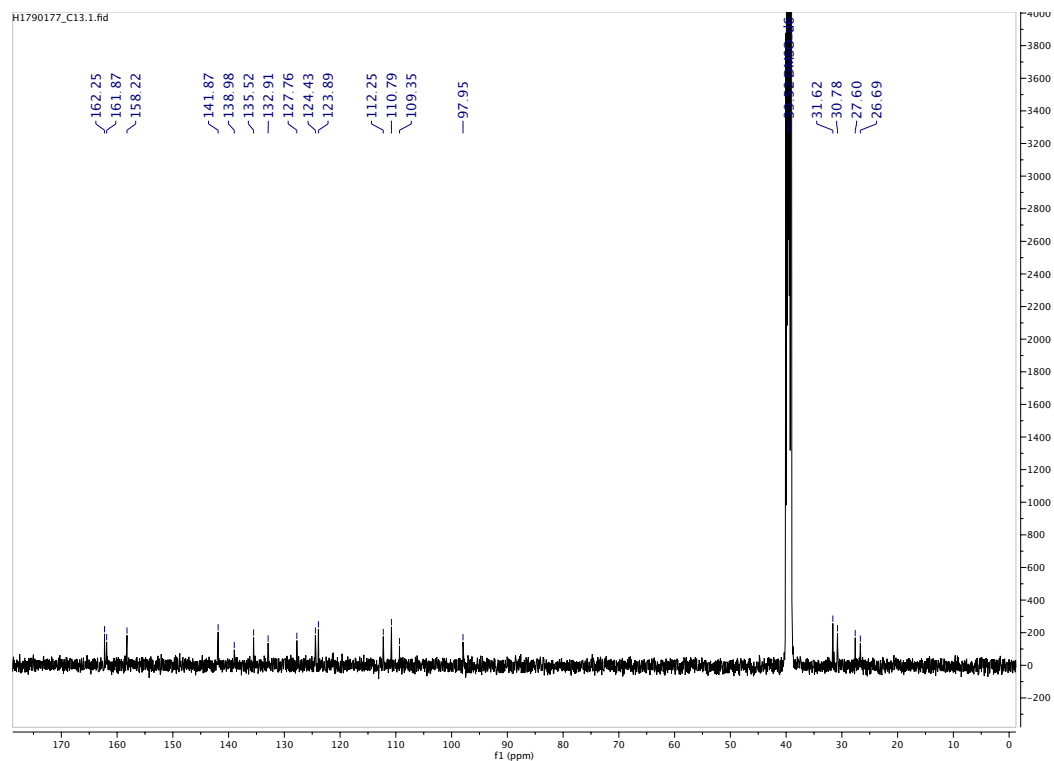| Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
369.1822	1.969	368.175	C22 H20 N6	368.1749	0.04	Find By Formula	

Compound Chromatograms
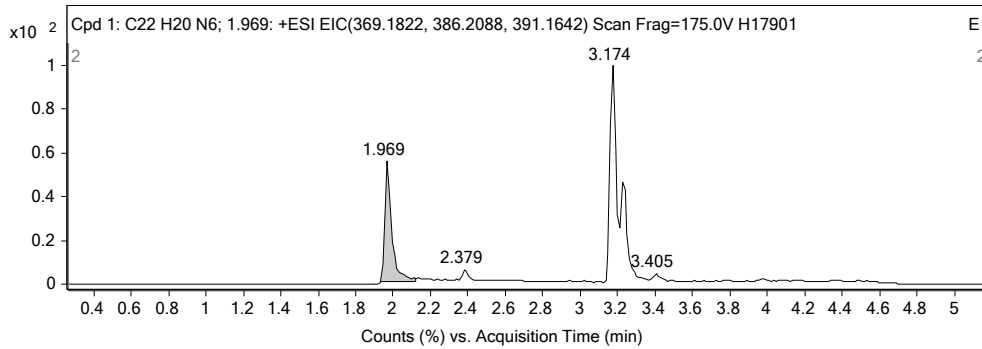
MS Zoomed Spectrum

12-(cyclopropylethynyl)-6,7,8,9-tetrahydro-5H-pyrimido[4',5':3,4]cycloocta[1,2-b]indol-2-amine (28).
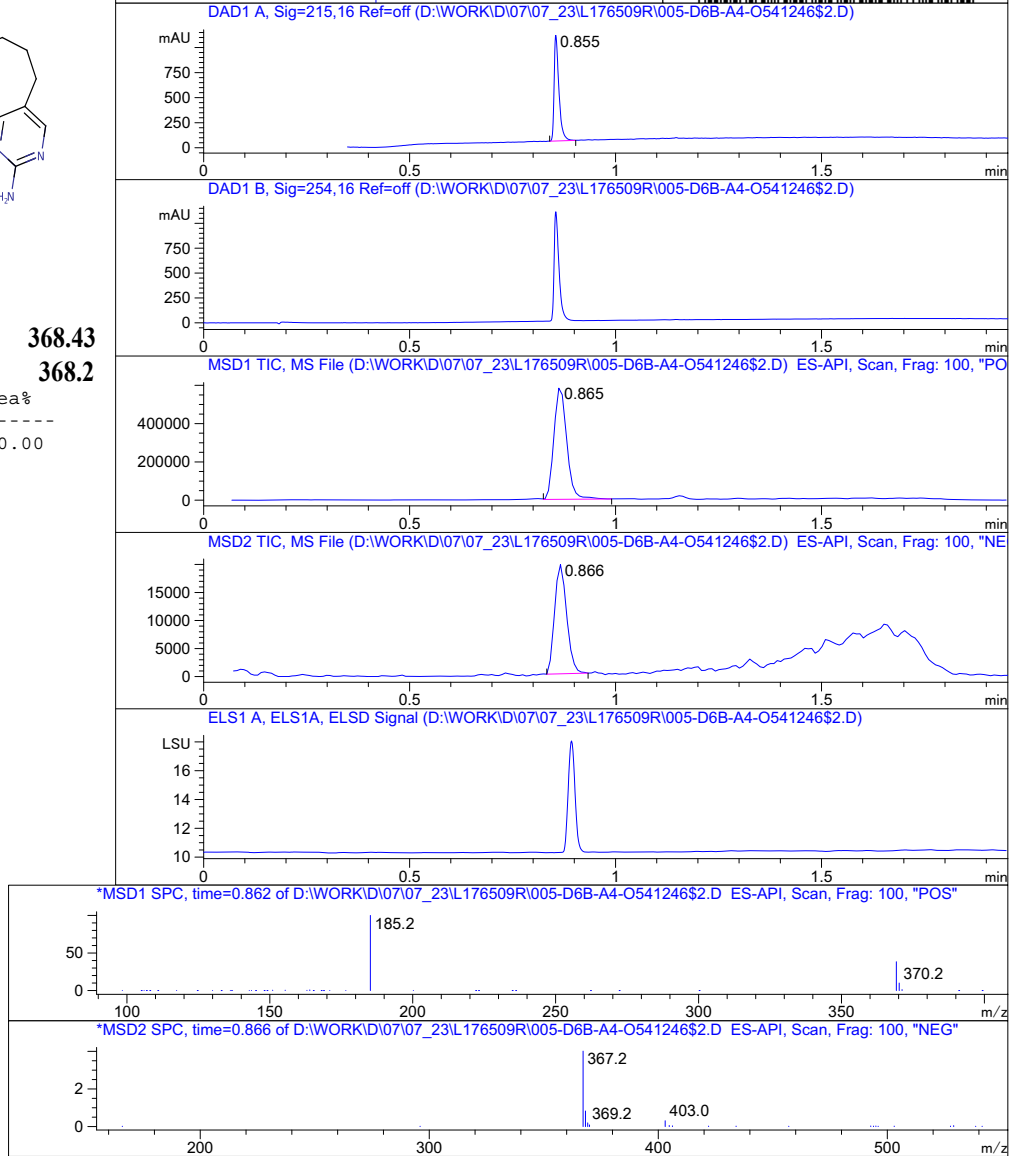
¹H NMR
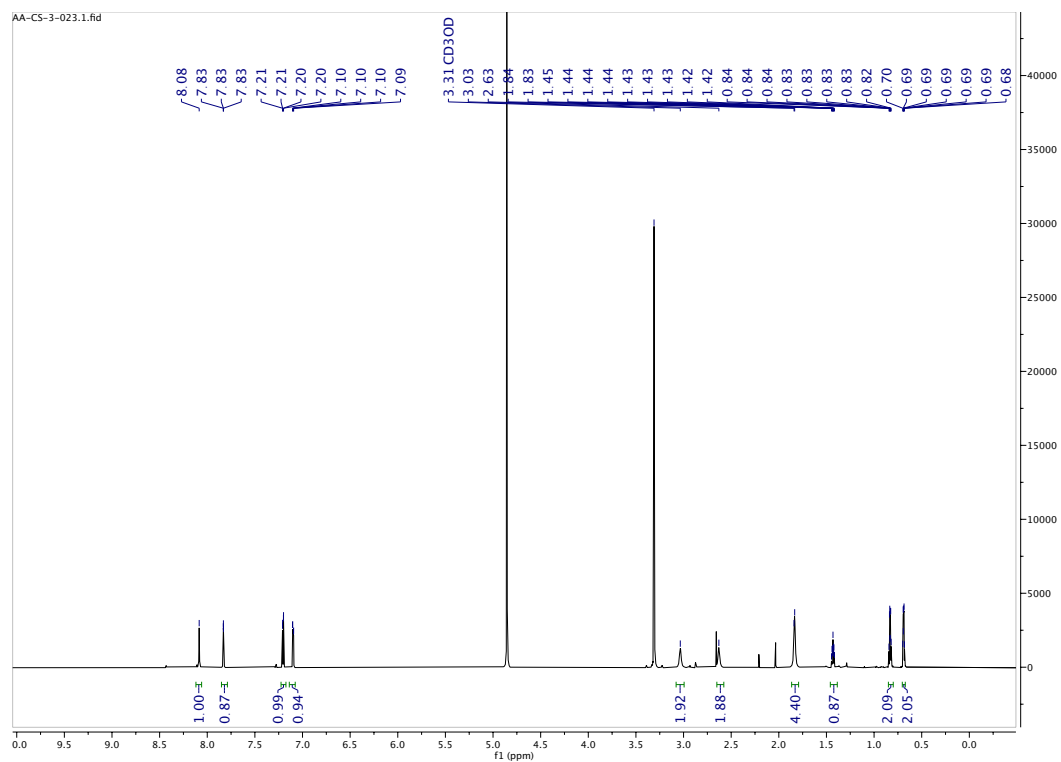
¹³C NMR
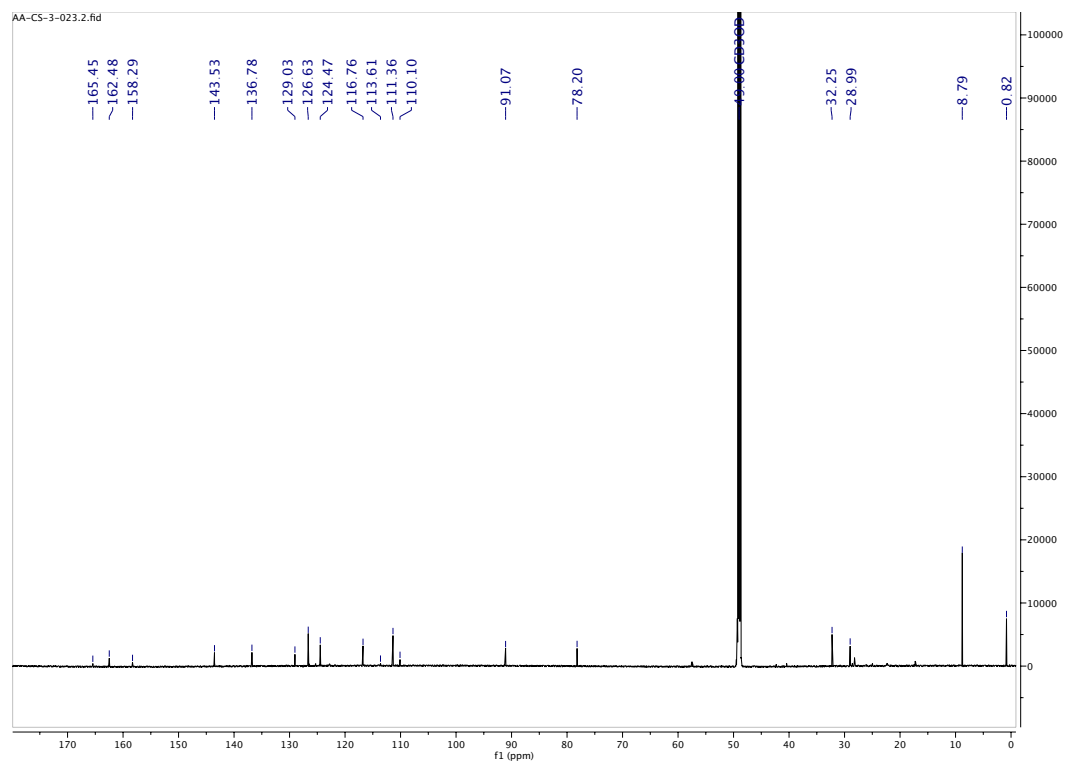
LC Chromatogram
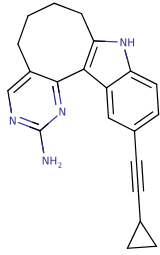
Mol Wt   **328.41**
Exact Mass   **328.2**

```
#  Time    Area%
-----------------
1  1.100   97.53
2  1.318   2.47
```

O617249$1
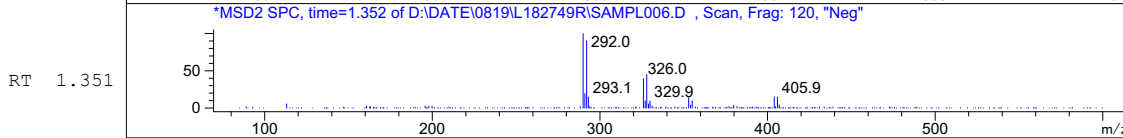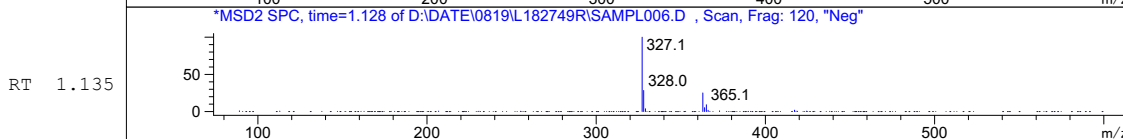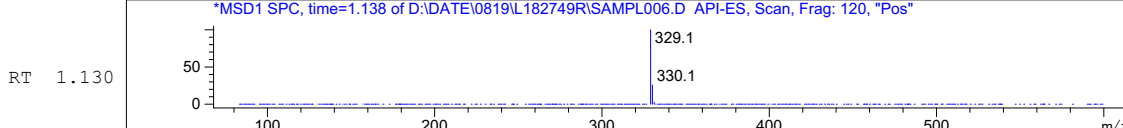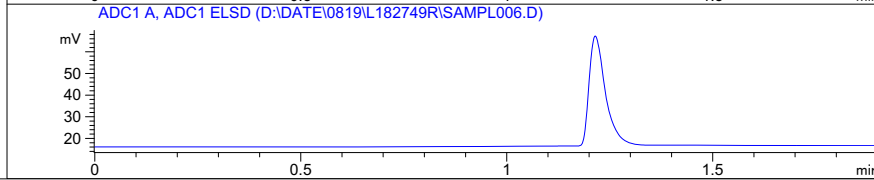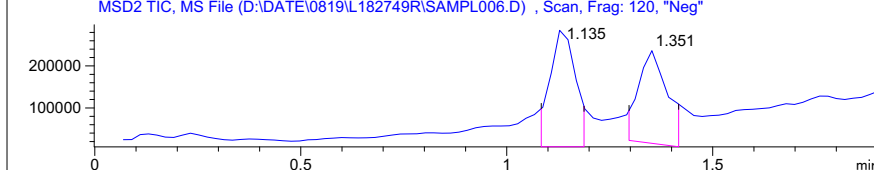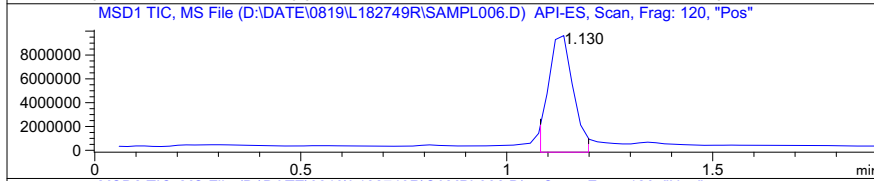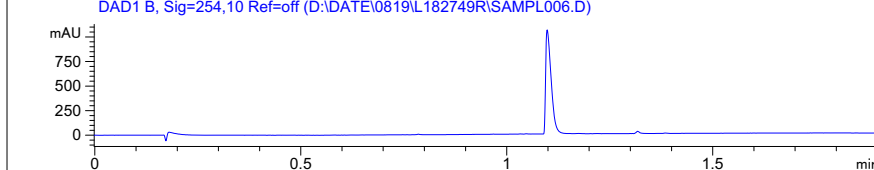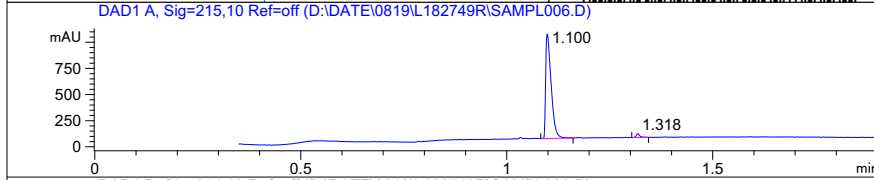
DAD1 A, Sig=215,10 Ref=off (D:\DATE\0819\L182749R\SAMPL006.D)

1.100
1.318

DAD1 B, Sig=254,10 Ref=off (D:\DATE\0819\L182749R\SAMPL006.D)

MSD1 TIC, MS File (D:\DATE\0819\L182749R\SAMPL006.D) API-ES, Scan, Frag: 120, "Pos"

1.130

MSD2 TIC, MS File (D:\DATE\0819\L182749R\SAMPL006.D) , Scan, Frag: 120, "Neg"

1.135
1.351

ADC1 A, ADC1 ELSD (D:\DATE\0819\L182749R\SAMPL006.D)

*MSD1 SPC, time=1.138 of D:\DATE\0819\L182749R\SAMPL006.D API-ES, Scan, Frag: 120, "Pos"

RT 1.130

329.1
330.1

*MSD2 SPC, time=1.128 of D:\DATE\0819\L182749R\SAMPL006.D , Scan, Frag: 120, "Neg"

RT 1.135

327.1
328.0
365.1

*MSD2 SPC, time=1.352 of D:\DATE\0819\L182749R\SAMPL006.D , Scan, Frag: 120, "Neg"

RT 1.351

292.0
293.1
326.0
329.9
405.9

HRMS
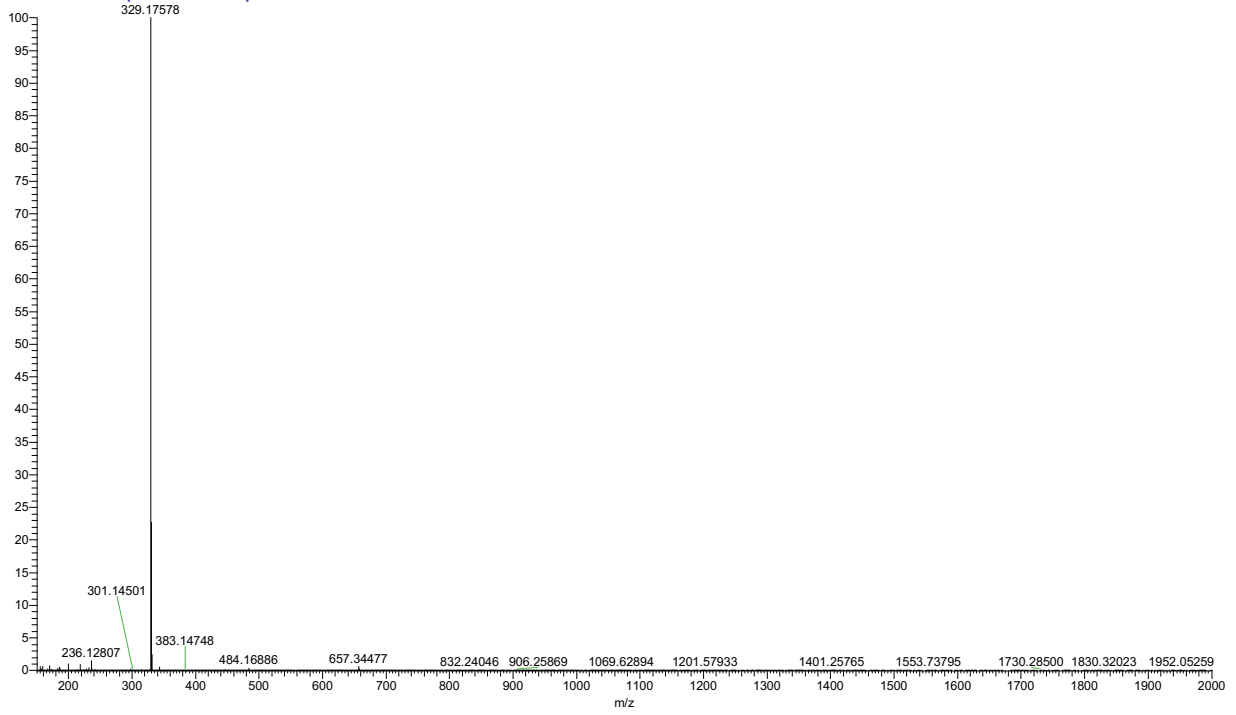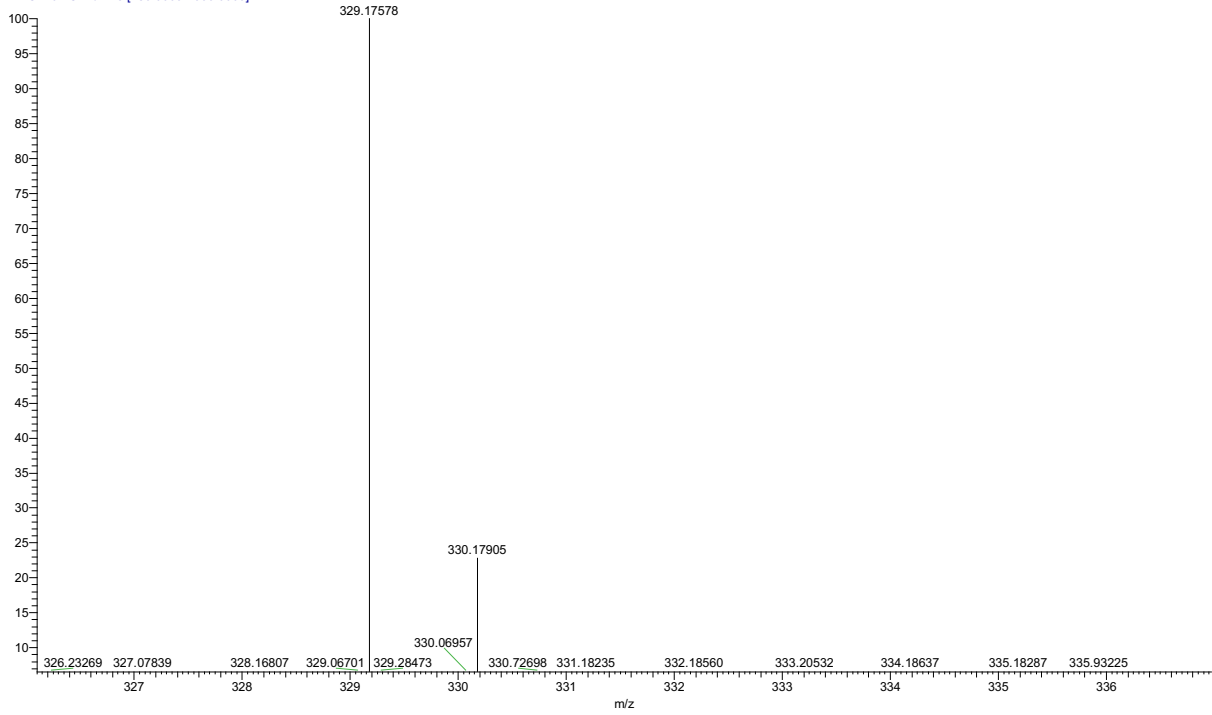
12-(3-(dimethylamino)prop-1-yn-1-yl)-6,7,8,9-tetrahydro-5H-pyrimido[4',5':3,4] cycloocta[1,2-b]indol-2-amine (29).

¹H NMR
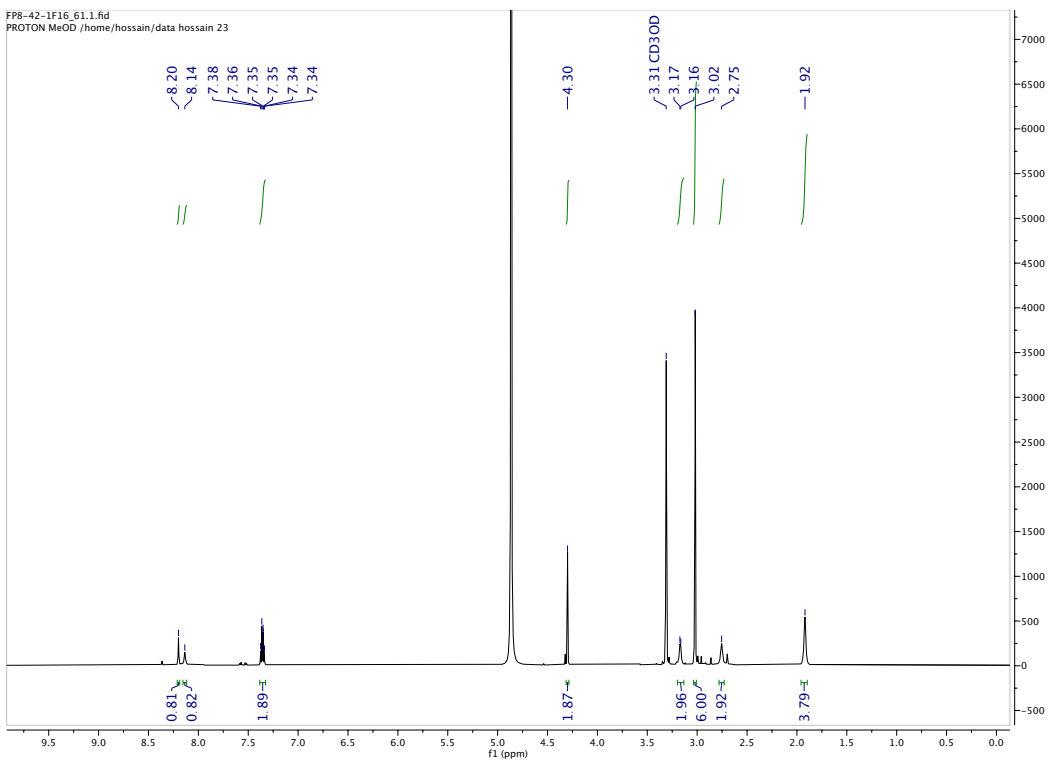
¹³C NMR
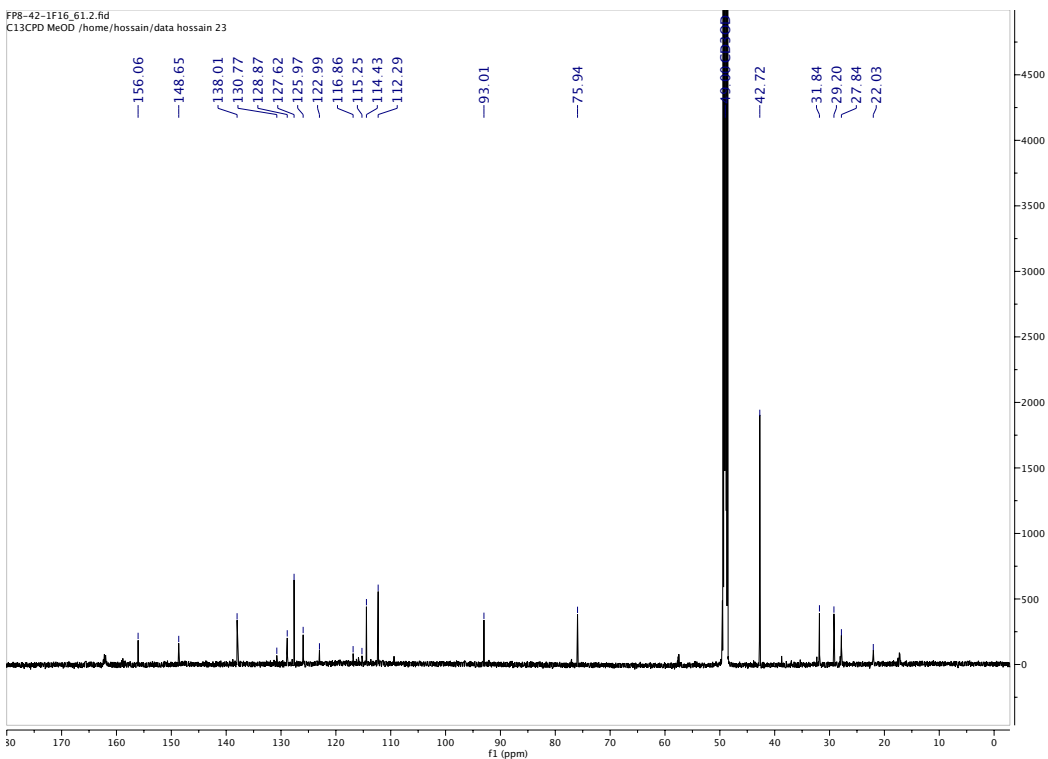
LC Chromatogram
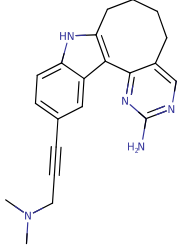
Mol Wt   345.44
Exact Mass   345.23

```
#  Time    Area%
----------------
1  0.646   2.02
2  0.793   95.61
3  1.104   2.36
```


O696164$1
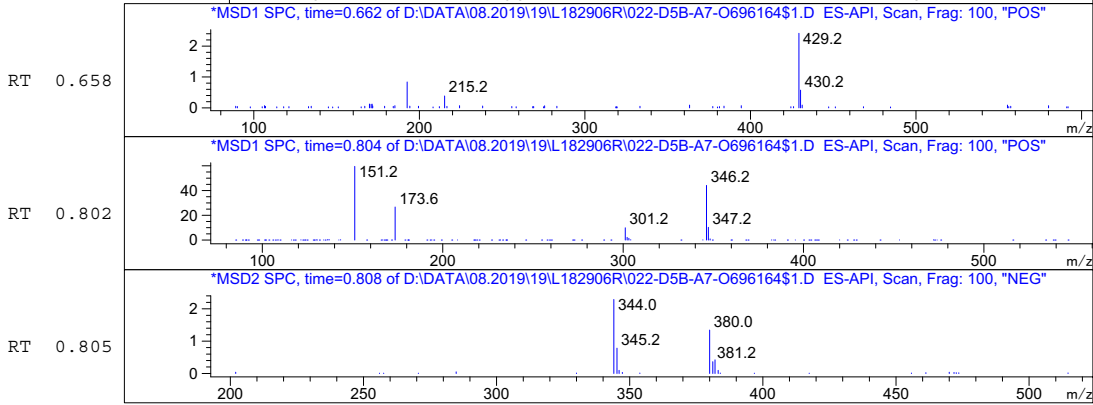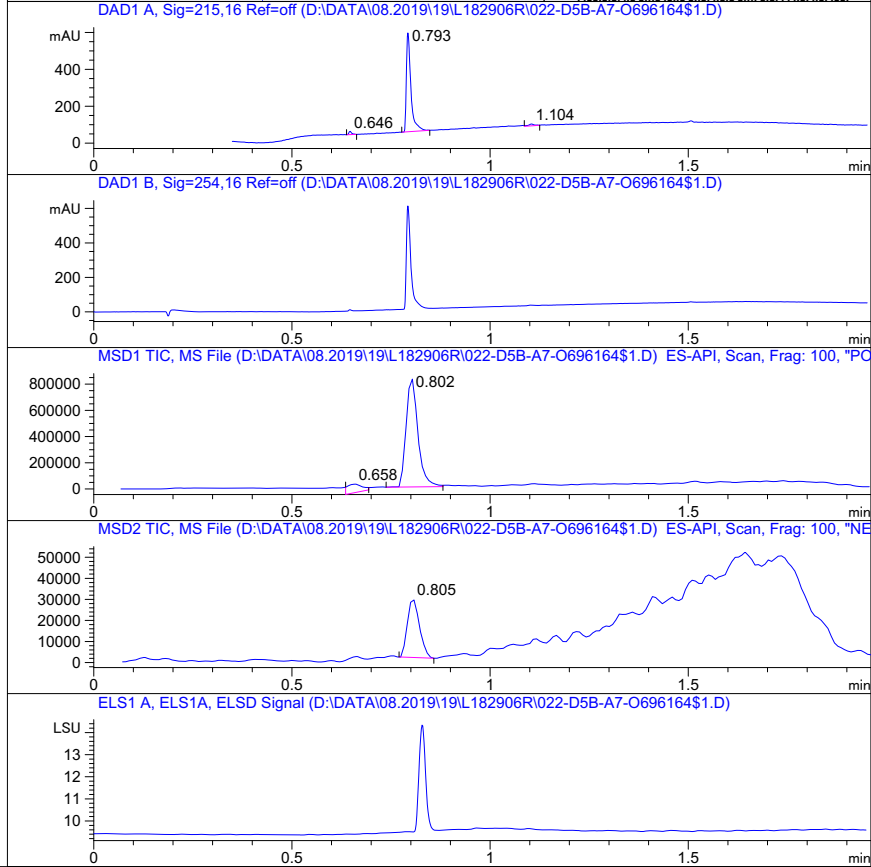
DAD1 A, Sig=215,16 Ref=off (D:\DATA\08.2019\19\L182906R\022-D5B-A7-O696164$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATA\08.2019\19\L182906R\022-D5B-A7-O696164$1.D)

MSD1 TIC, MS File (D:\DATA\08.2019\19\L182906R\022-D5B-A7-O696164$1.D) ES-API, Scan, Frag: 100, "PO

MSD2 TIC, MS File (D:\DATA\08.2019\19\L182906R\022-D5B-A7-O696164$1.D) ES-API, Scan, Frag: 100, "NE

ELS1 A, ELS1A, ELSD Signal (D:\DATA\08.2019\19\L182906R\022-D5B-A7-O696164$1.D)

*MSD1 SPC, time=0.662 of D:\DATA\08.2019\19\L182906R\022-D5B-A7-O696164$1.D ES-API, Scan, Frag: 100, "POS"

RT 0.658

*MSD1 SPC, time=0.804 of D:\DATA\08.2019\19\L182906R\022-D5B-A7-O696164$1.D ES-API, Scan, Frag: 100, "POS"

RT 0.802

*MSD2 SPC, time=0.808 of D:\DATA\08.2019\19\L182906R\022-D5B-A7-O696164$1.D ES-API, Scan, Frag: 100, "NEG"

RT 0.805

HRMS
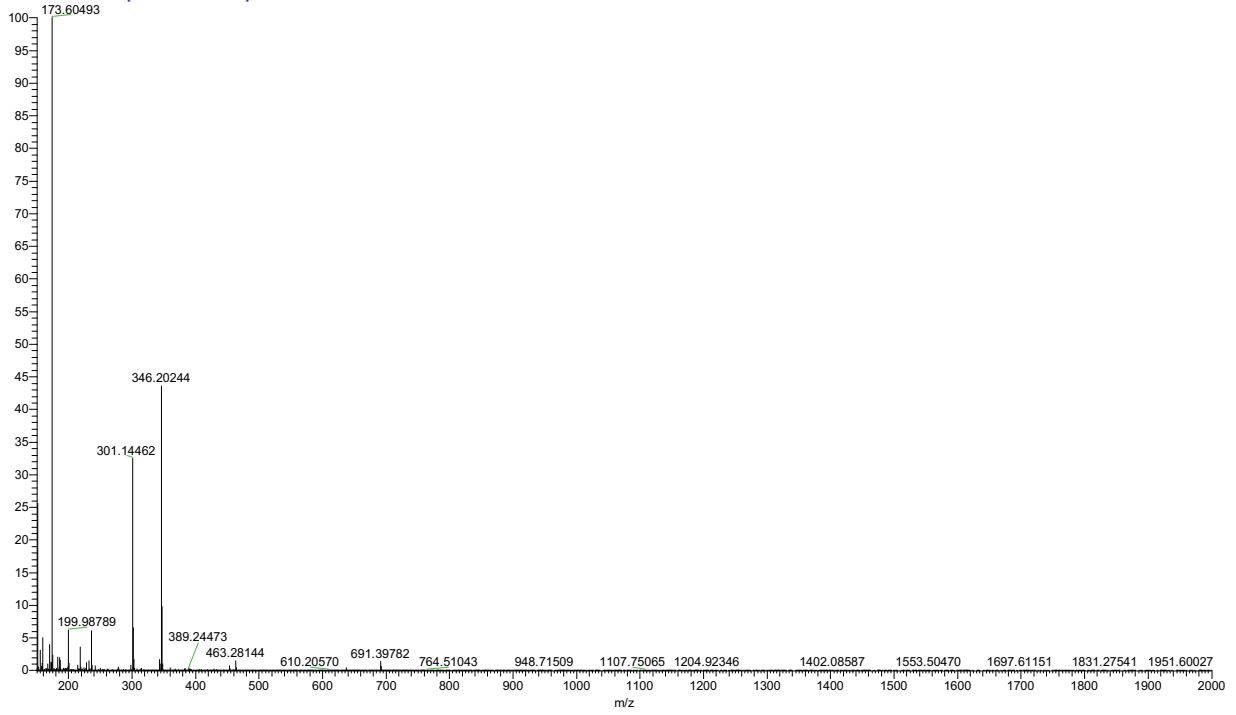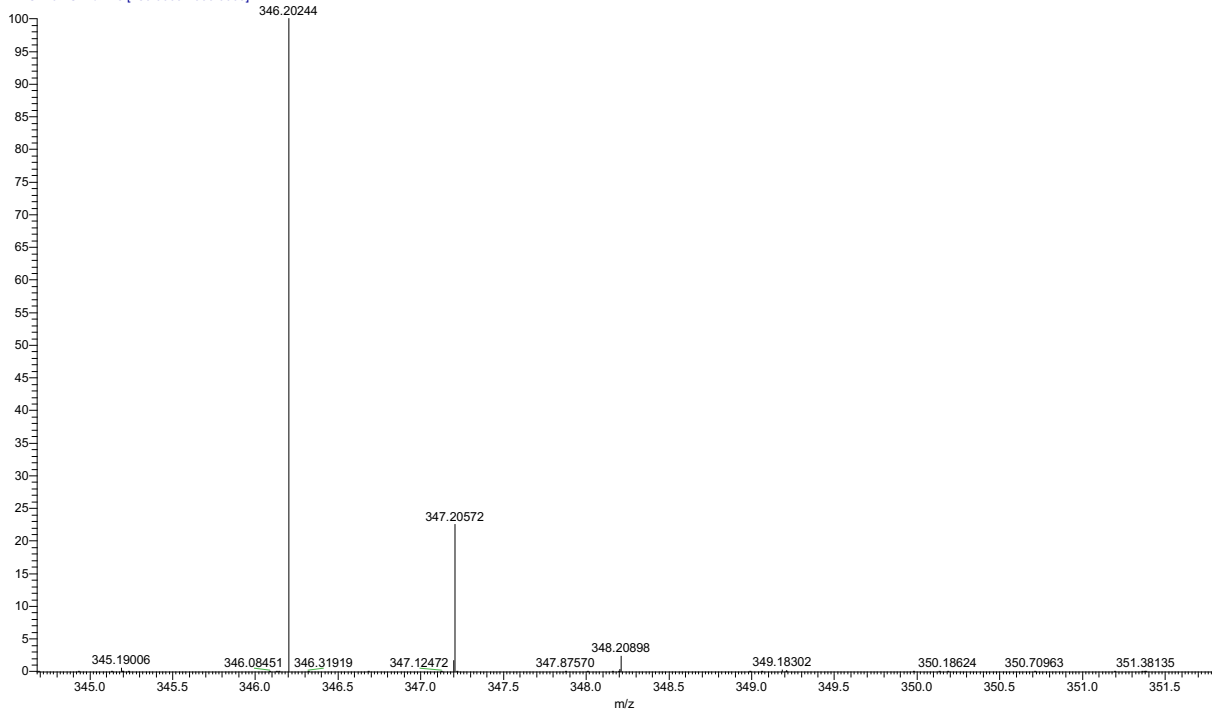
*N-(4-2-amino-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-11-yl)-2-methylbut-3-yn-2-yl)acetamide (**18**).*

¹H NMR
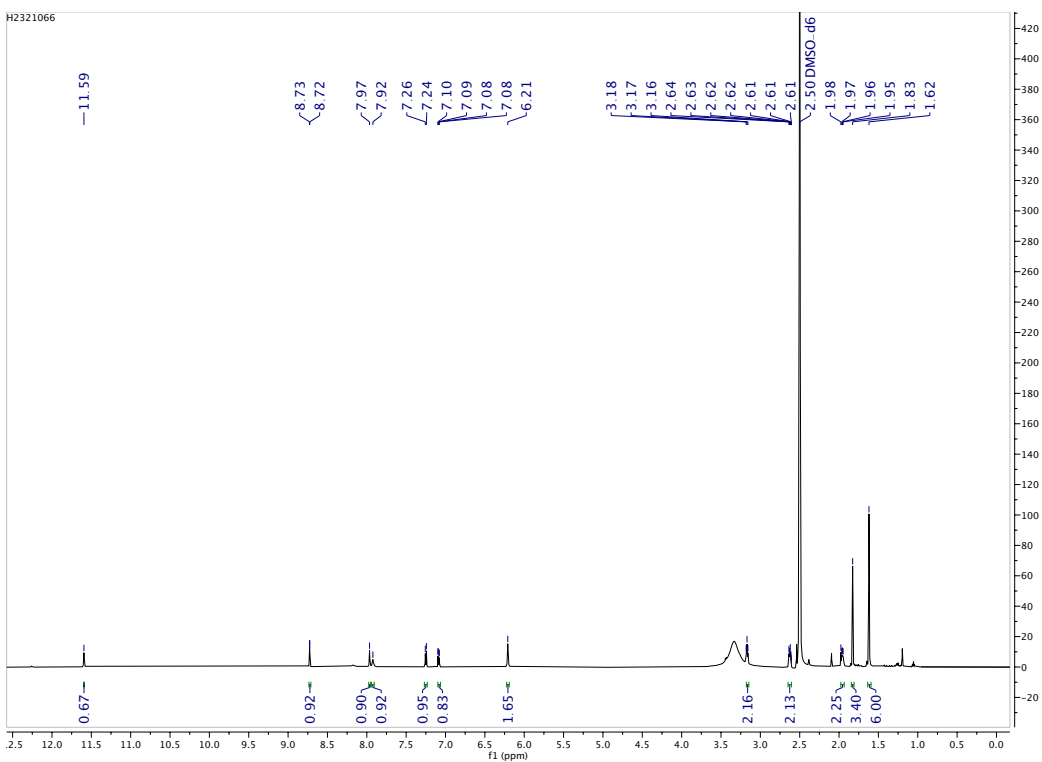
¹³C NMR
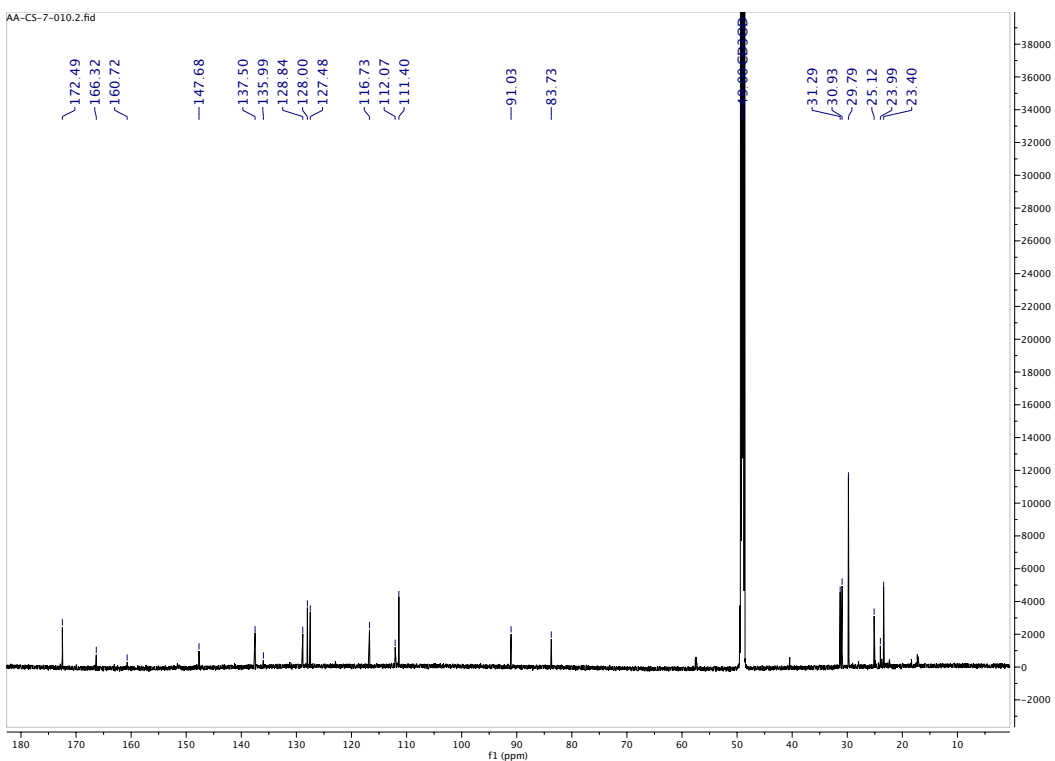
LC Chromatogram

MaxPeak: 97.62%
Ret_Time: 0.796 min
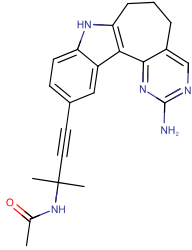
Mol Wt 373.45
Exact Mass 373.22

```
# Time    Area%
-----------------
1 0.784   2.38
2 0.796   97.62
```

Q301618$2

DAD1 A, Sig=215,16 Ref=off (D:\DATA\04\09\L239331R\010-D6F-A9-Q301618$2.D)

mAU
300
200
100
0.796
0.784

DAD1 B, Sig=254,16 Ref=off (D:\DATA\04\09\L239331R\010-D6F-A9-Q301618$2.D)

mAU
100
50
0
-50

MSD1 TIC, MS File (D:\DATA\04\09\L239331R\010-D6F-A9-Q301618$2.D) ES-API, Fast Scan, Frag: 100, "POS"

1000000
800000
600000
400000
200000
0
0.805

MSD2 TIC, MS File (D:\DATA\04\09\L239331R\010-D6F-A9-Q301618$2.D) ES-API, Fast Scan, Frag: 100, "NEG"

60000
40000
20000
0
0.809

ELS1 A, ELS1A, ELSD Signal (D:\DATA\04\09\L239331R\010-D6F-A9-Q301618$2.D)

LSU
10.2
10
9.8

*MSD1 SPC, time=0.803 of D:\DATA\04\09\L239331R\010-D6F-A9-Q301618$2.D ES-API, Fast Scan, Frag: 100, "POS"

RT 0.805
50
0
374.2
375.2

*MSD2 SPC, time=0.808 of D:\DATA\04\09\L239331R\010-D6F-A9-Q301618$2.D ES-API, Fast Scan, Frag: 100, "NEG"

RT 0.809
50
0
372.2
373.2
410.2

Inj.Date 4/8/2020   LB   Acq. Method C:\Users\ ->   ->

HRMS

Target Compound Screening Report

Data File	H2321066.d	**Sample Name**	H2321066
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 7:32:58 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C22H23N5O	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 7:32:58 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H23 N5 O; 2.217	77.35	-2.66	C22 H23 N5 O	2.217	373.1903	373.1893

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
374.1975	2.217	373.1893	C22 H23 N5 O	373.1903	-2.66	Find By Formula	

Compound Chromatograms
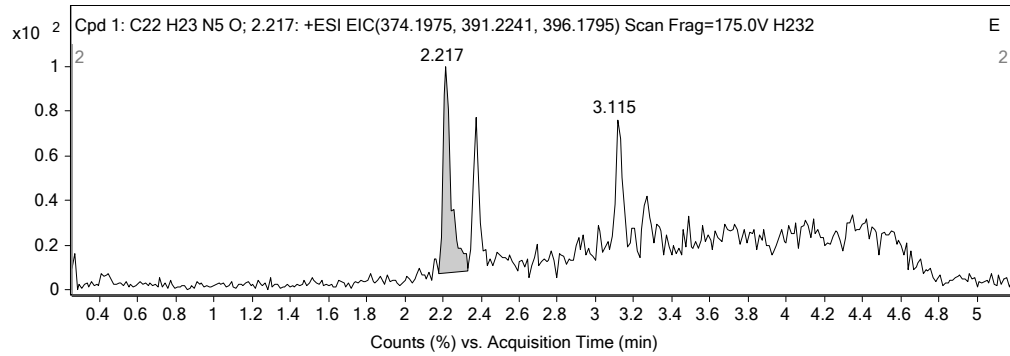
MS Zoomed Spectrum

*N-(4-(2-amino-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-11-yl)-2-methylbut-3-yn-2-yl)methanesulfonamide (**19**).*

¹H NMR
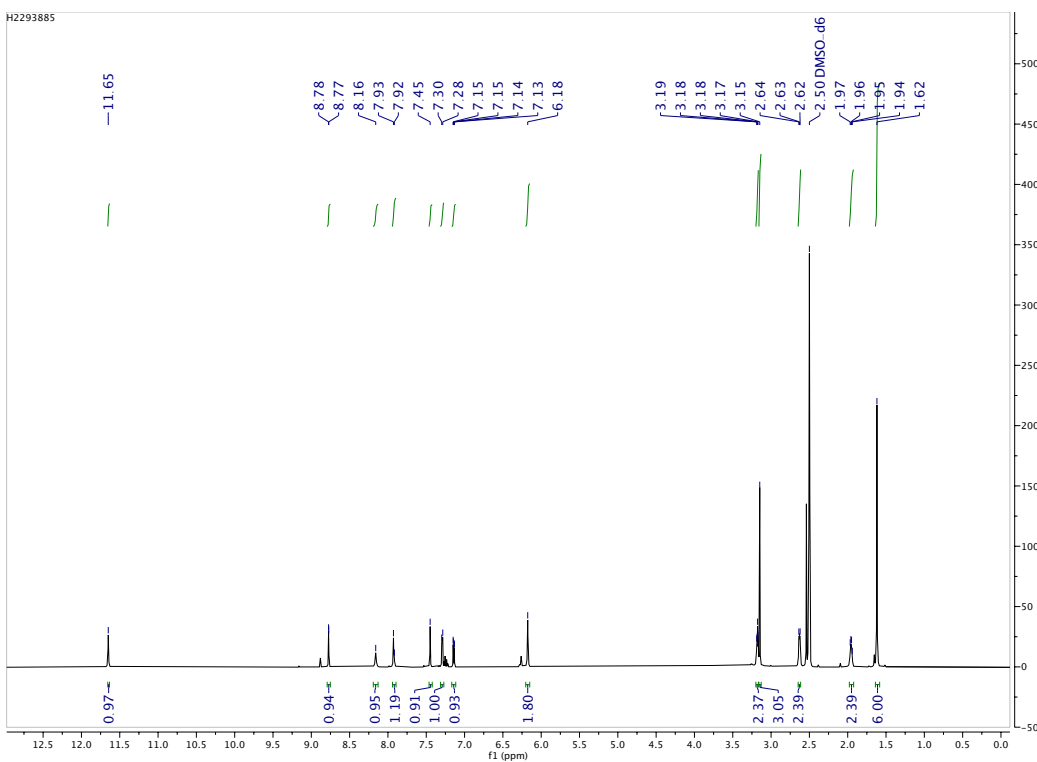
¹³C NMR
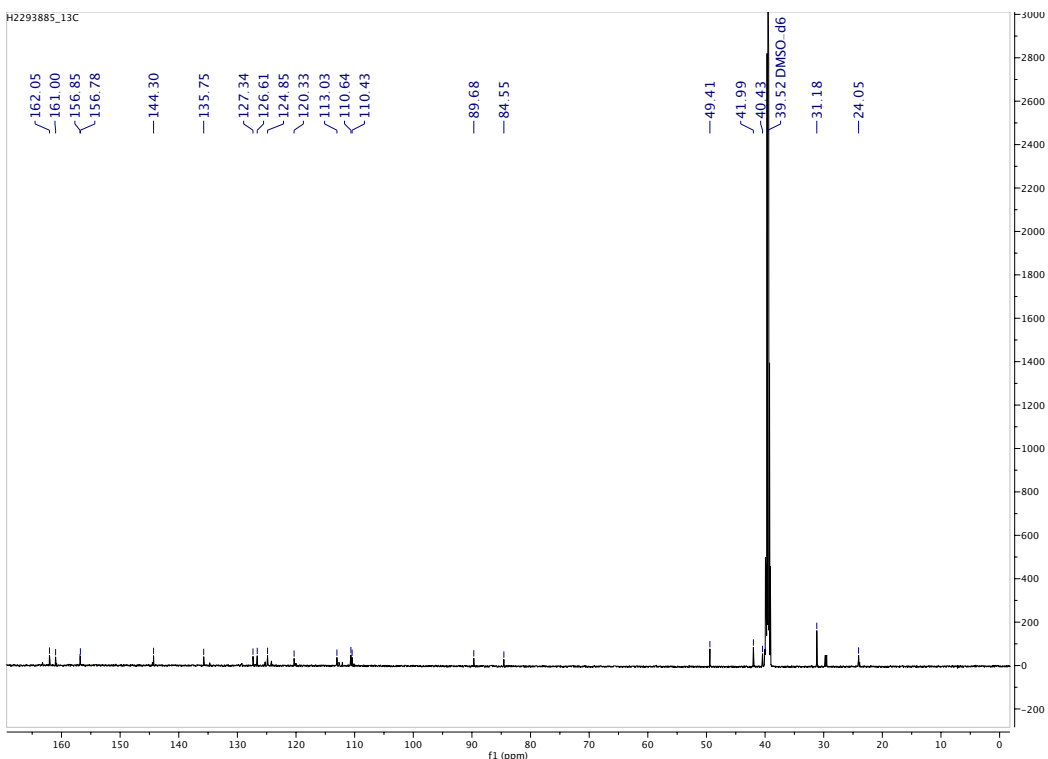
LC Chromatogram

MaxPeak: 95.31%
Ret_Time: 0.749 min
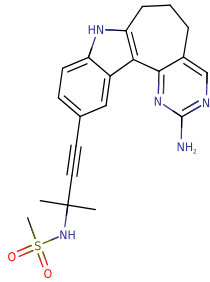
Mol Wt   **409.5**
Exact Mass   **409.18**

```
#  Time    Area%
----------------
1  0.731   4.69
2  0.749   95.31
```

Q184368$2

DAD1 A, Sig=215,16 Ref=off (D:\DATA\03\0323\L234990R\006-D5B-A5-Q184368$2.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATA\03\0323\L234990R\006-D5B-A5-Q184368$2.D)

MSD1 TIC, MS File (D:\DATA\03\0323\L234990R\006-D5B-A5-Q184368$2.D) ES-API, Fast Scan, Frag: 100, "P

MSD2 TIC, MS File (D:\DATA\03\0323\L234990R\006-D5B-A5-Q184368$2.D) ES-API, Fast Scan, Frag: 100, "N

ELS1 A, ELS1A, ELSD Signal (D:\DATA\03\0323\L234990R\006-D5B-A5-Q184368$2.D)

*MSD1 SPC, time=0.756 of D:\DATA\03\0323\L234990R\006-D5B-A5-Q184368$2.D ES-API, Fast Scan, Frag: 100, "POS"

RT 0.758

*MSD2 SPC, time=0.762 of D:\DATA\03\0323\L234990R\006-D5B-A5-Q184368$2.D ES-API, Fast Scan, Frag: 100, "NEG"

RT 0.761

Inj.Date 3/23/2020   LT   Acq. Method C:\Users\ ->   ->

HRMS

Target Compound Screening Report

Data File	H2293885.d	**Sample Name**	H2293885
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 6:32:18 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C21H23N5O2S	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 6:32:18 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H23 N5 O2 S; 2.262	85.33	0.65	C21 H23 N5 O2 S	2.262	409.1572	409.1575

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
410.1645	2.262	409.1575	C21 H23 N5 O2 S	409.1572	0.65	Find By Formula	

Compound Chromatograms
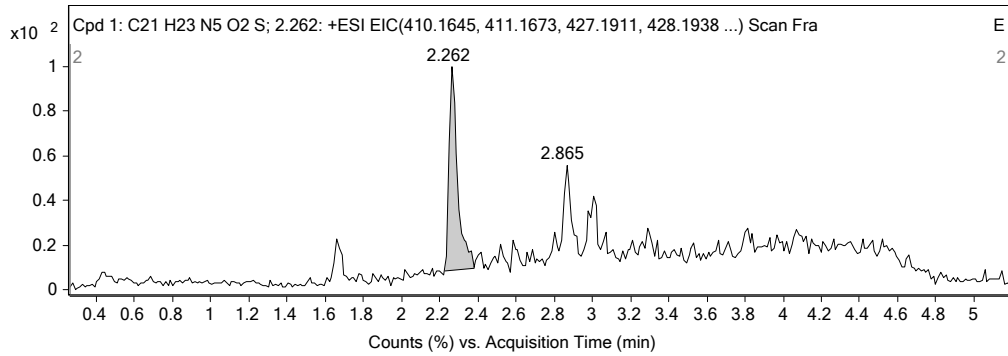
MS Zoomed Spectrum

11-(3-methoxy-3-methylbut-1-yn-1-yl)-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-2-amine (20).

1H NMR
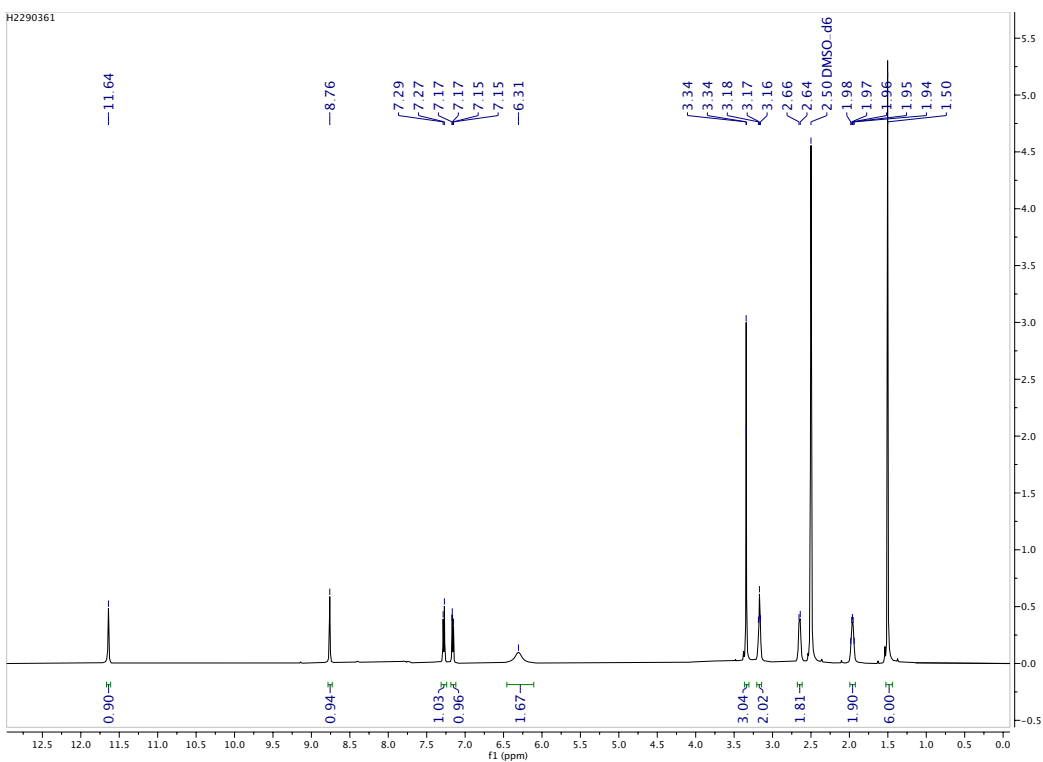
13C NMR
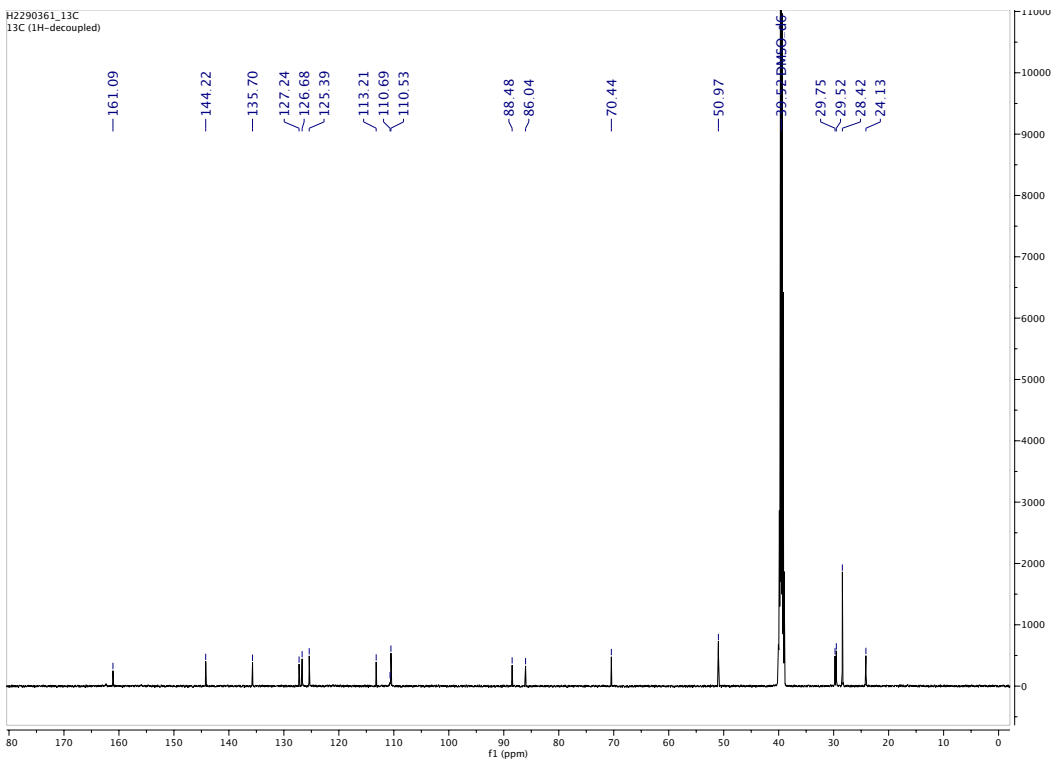
LC Chromatogram

MaxPeak: 98.70%
Ret_Time: 2.208 min
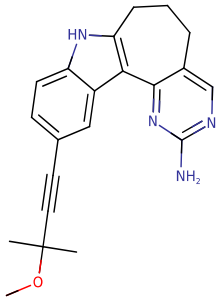
Mol Wt   **346.43**
Exact Mass **346.21**

```
#  Time    Area%
-----------------
1  2.170   1.30
2  2.208   98.70
```

Q184058$1

DAD1 A, Sig=215,16 Ref=off (D:\DATE\0317\L233659R\014-D6B-B1-Q184058$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATE\0317\L233659R\014-D6B-B1-Q184058$1.D)

MSD1 TIC, MS File (D:\DATE\0317\L233659R\014-D6B-B1-Q184058$1.D) ES-API, Scan, Frag: 100, "POS"

MSD2 TIC, MS File (D:\DATE\0317\L233659R\014-D6B-B1-Q184058$1.D) ES-API, Scan, Frag: 100, "NEG"

ELS1 A, ELS1A, ELSD Signal (D:\DATE\0317\L233659R\014-D6B-B1-Q184058$1.D)

*MSD1 SPC, time=2.220 of D:\DATE\0317\L233659R\014-D6B-B1-Q184058$1.D ES-API, Scan, Frag: 100, "POS"

RT 2.223

*MSD2 SPC, time=2.224 of D:\DATE\0317\L233659R\014-D6B-B1-Q184058$1.D ES-API, Scan, Frag: 100, "NEG"

RT 2.221

HRMS

Target Compound Screening Report

Data File	H2290361.d	**Sample Name**	H2290361
Sample Type	Sample	**Position**	P1-B3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 6:56:35 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C21H22N4O	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 6:56:35 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H22 N4 O; 2.409	98.44	-0.79	C21 H22 N4 O	2.409	346.1794	346.1791

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
347.1863	2.409	346.1791	C21 H22 N4 O	346.1794	-0.79	Find By Formula	

Compound Chromatograms
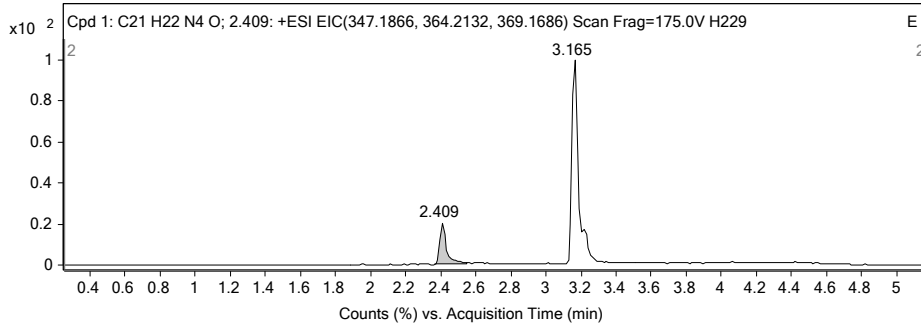
MS Zoomed Spectrum

4-(2-amino-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-11-yl)but-3-yn-2-ol (21).

¹H NMR
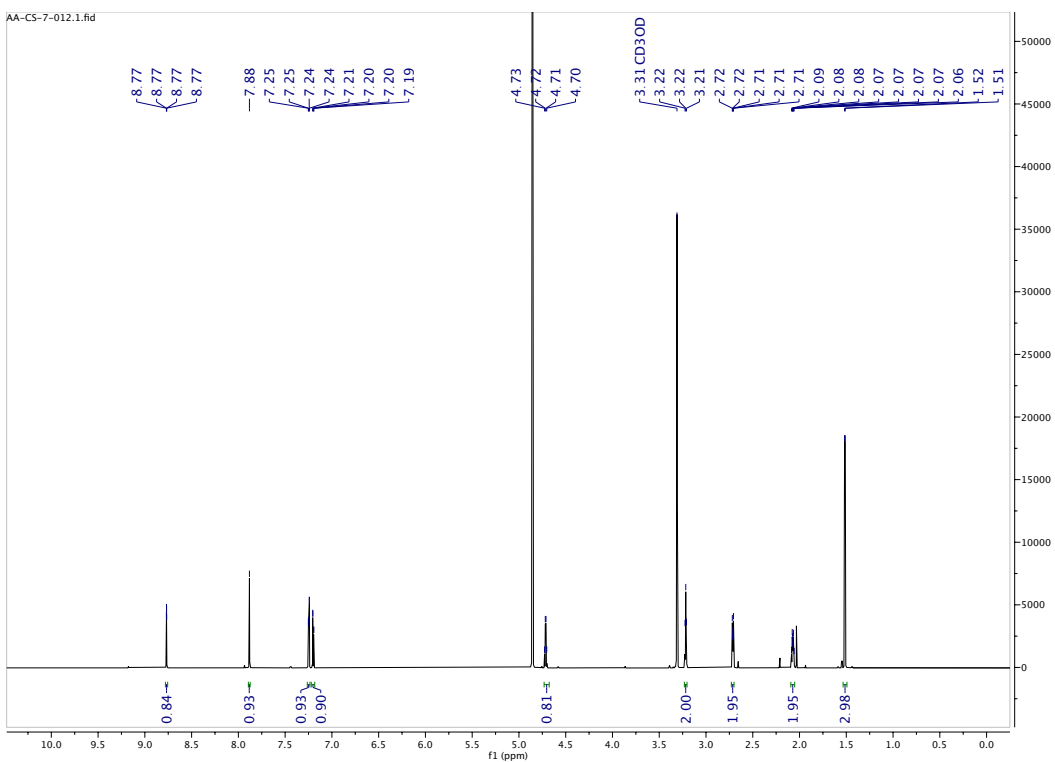
¹³C NMR
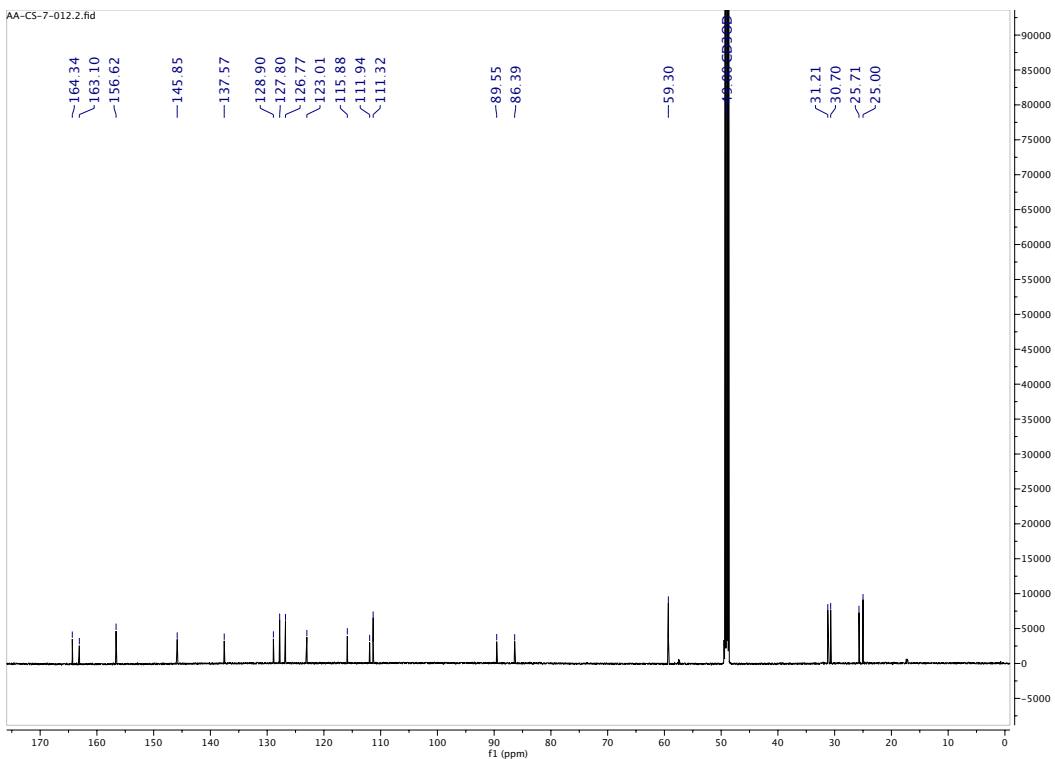
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 0.748 min
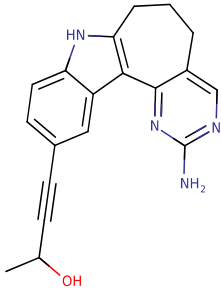
Mol Wt **318.37**
Exact Mass **318.17**

```
#  Time    Area%
-----------------
1  0.748   100.00
```

Q301253$1

DAD1 A, Sig=215,16 Ref=off (D:\DATE\0414\L240396R\006-D5F-A3-Q301253$1.D)

0.748

DAD1 B, Sig=254,16 Ref=off (D:\DATE\0414\L240396R\006-D5F-A3-Q301253$1.D)

MSD1 TIC, MS File (D:\DATE\0414\L240396R\006-D5F-A3-Q301253$1.D) ES-API, Fast Scan, Frag: 100, "PO

0.758

MSD2 TIC, MS File (D:\DATE\0414\L240396R\006-D5F-A3-Q301253$1.D) ES-API, Fast Scan, Frag: 100, "NE

0.762

ELS1 A, ELS1A, ELSD Signal (D:\DATE\0414\L240396R\006-D5F-A3-Q301253$1.D)

*MSD1 SPC, time=0.754 of D:\DATE\0414\L240396R\006-D5F-A3-Q301253$1.D ES-API, Fast Scan, Frag: 100, "POS"

RT 0.758

157.0   319.2   320.2

*MSD2 SPC, time=0.760 of D:\DATE\0414\L240396R\006-D5F-A3-Q301253$1.D ES-API, Fast Scan, Frag: 100, "NEG"

RT 0.762

317.2   318.2   369.0

Inj.Date 4/14/2020   E   Acq. Method C:\Users\ ->   ->

HRMS
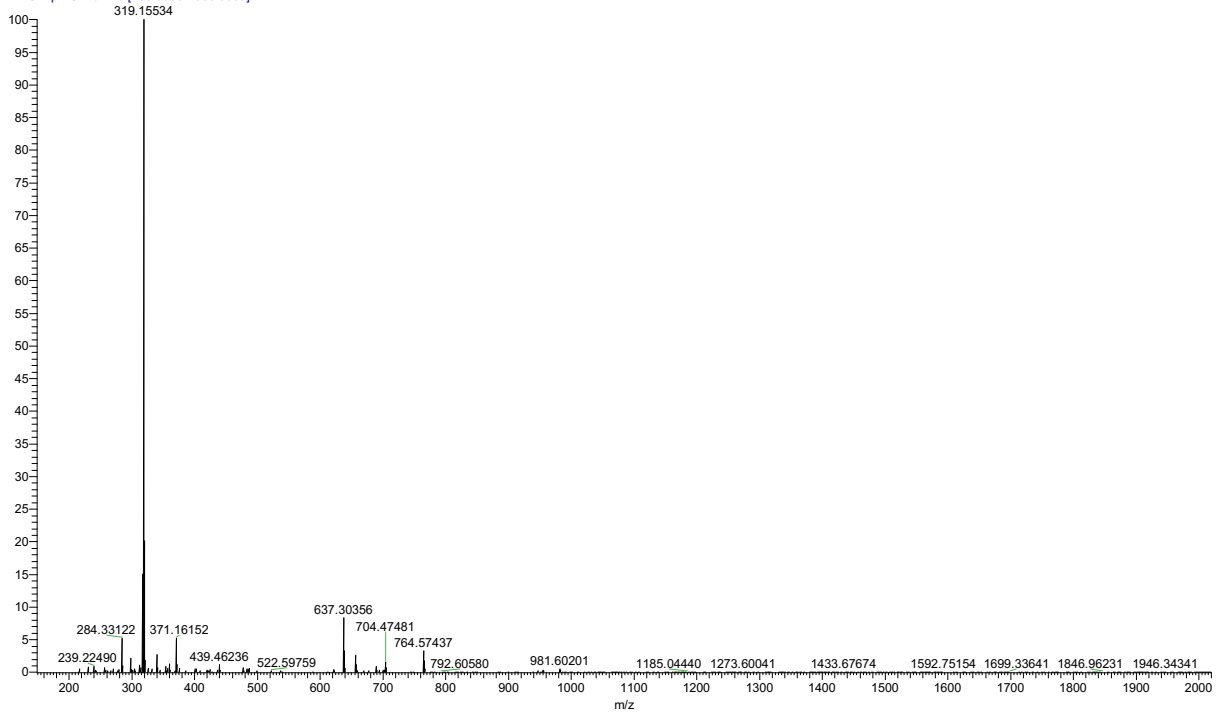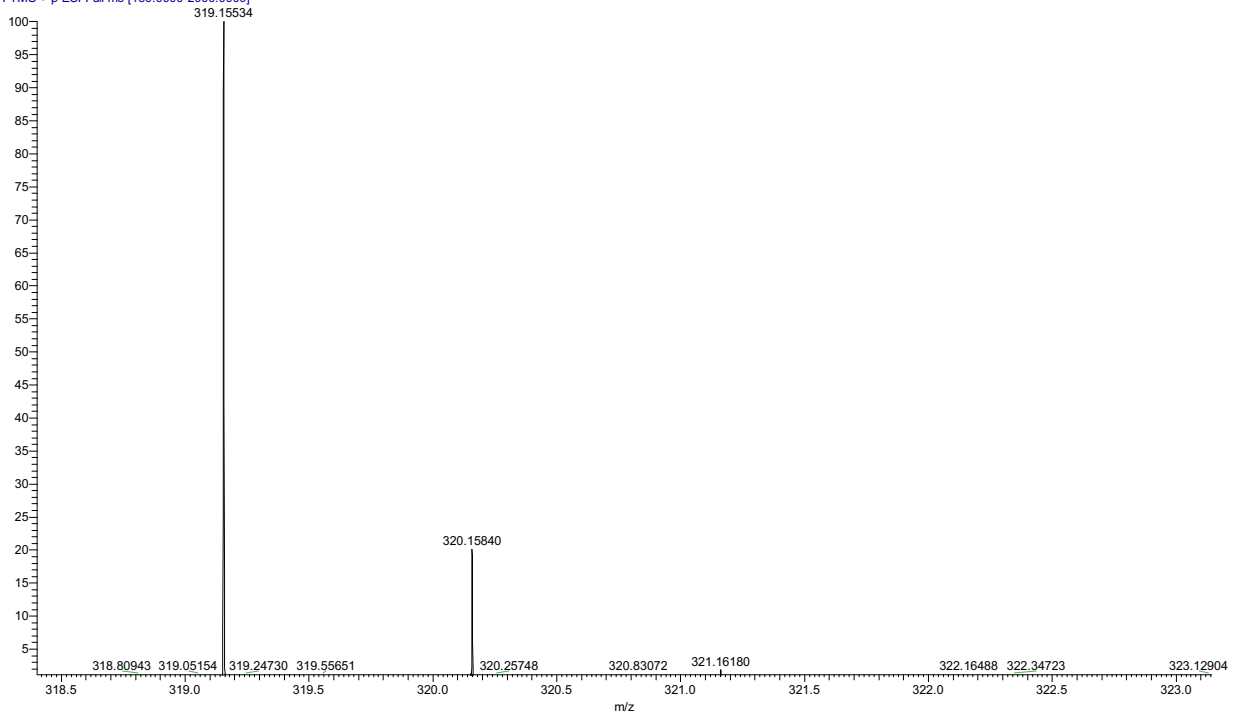
4-(2-amino-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-11-yl)but-3-yn-1-ol (22).

¹H NMR
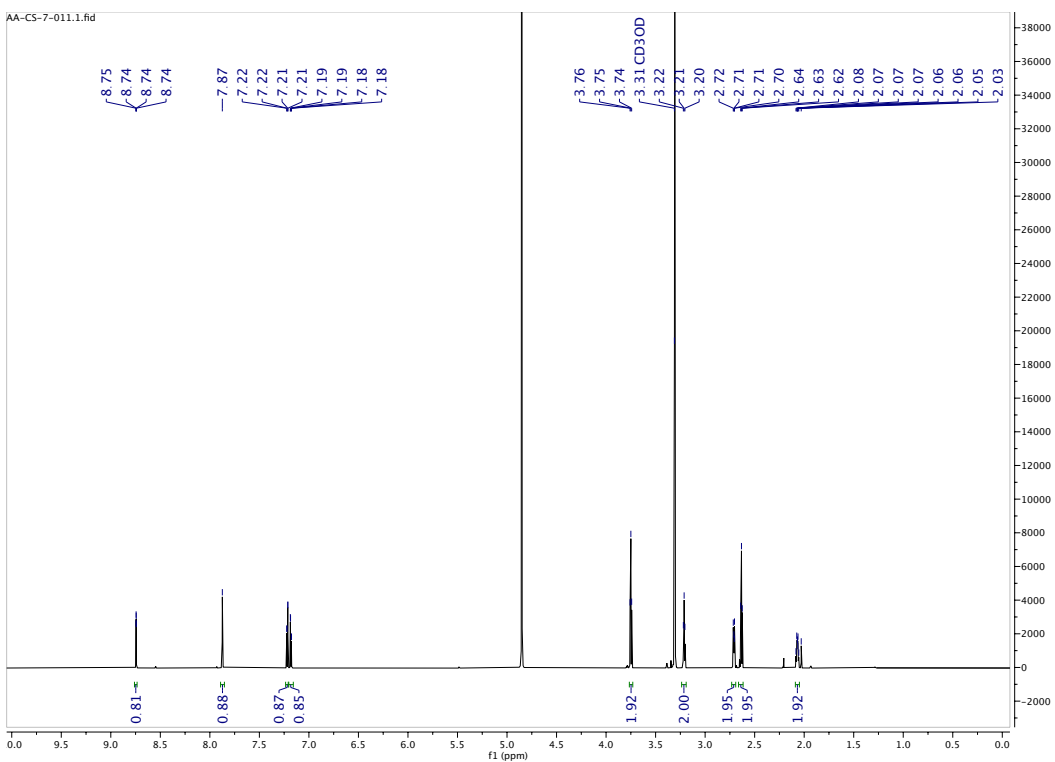
¹³C NMR
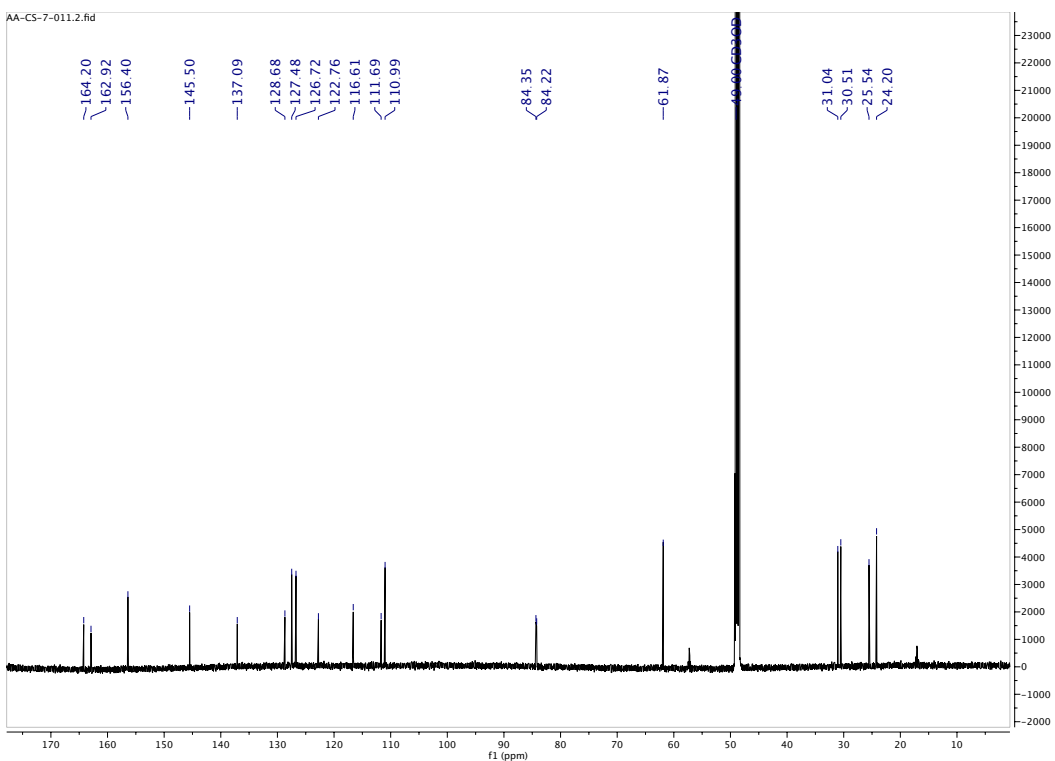
LC Chromatogram
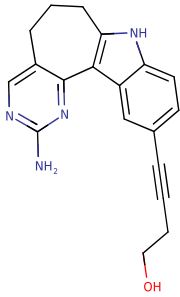
Mol Wt   **318.37**
Exact Mass   **318.17**

```
#   Time    Area%
-----------------
1   0.731   100.00
```


Q301616$1

DAD1 A, Sig=215,16 Ref=off (D:\DATE\0414\L240396R\007-D5F-A4-Q301616$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATE\0414\L240396R\007-D5F-A4-Q301616$1.D)

MSD1 TIC, MS File (D:\DATE\0414\L240396R\007-D5F-A4-Q301616$1.D) ES-API, Fast Scan, Frag: 100, "PO

MSD2 TIC, MS File (D:\DATE\0414\L240396R\007-D5F-A4-Q301616$1.D) ES-API, Fast Scan, Frag: 100, "NE

ELS1 A, ELS1A, ELSD Signal (D:\DATE\0414\L240396R\007-D5F-A4-Q301616$1.D)

*MSD1 SPC, time=0.743 of D:\DATE\0414\L240396R\007-D5F-A4-Q301616$1.D ES-API, Fast Scan, Frag: 100, "POS"

RT 0.744

*MSD2 SPC, time=0.749 of D:\DATE\0414\L240396R\007-D5F-A4-Q301616$1.D ES-API, Fast Scan, Frag: 100, "NEG"

RT 0.743
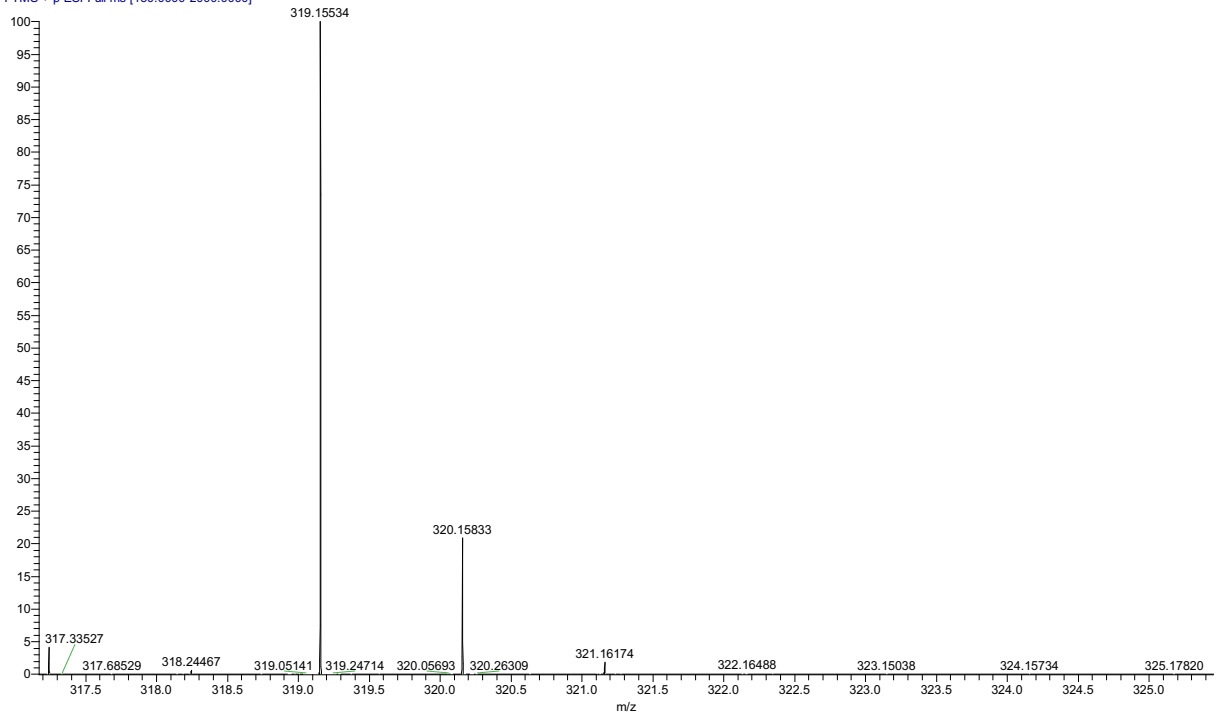
HRMS

4-(2-amino-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-11-yl)-2,2-dimethylbut-3-yn-1-ol (23).

¹H NMR
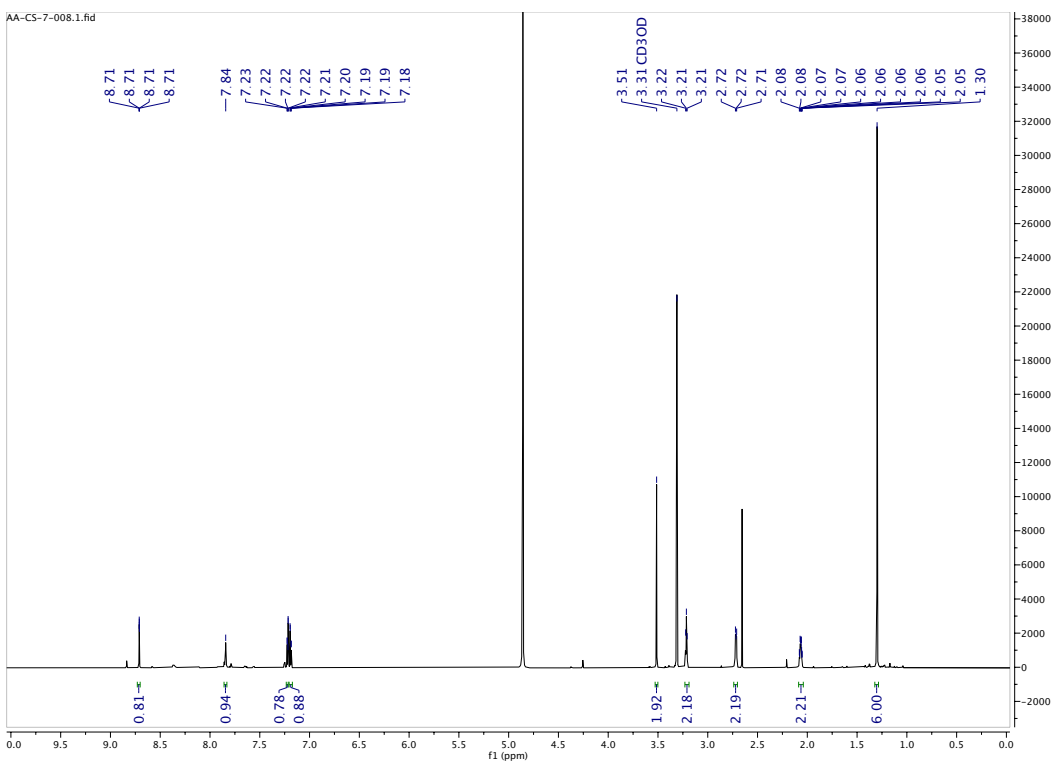
¹³C NMR

LC Chromatogram
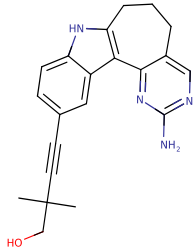
Mol Wt 346.43
Exact Mass 346.21

```
#  Time   Area%
------------------
1  0.964  98.28
2  1.251   1.72
```

Q158596$2

DAD1 A, Sig=215,16 Ref=off (D:\DATA\0312\L232517R\003-D2F-A2-Q158596$2.D)

mAU
800
600
400
200
0
0.964
1.251

DAD1 B, Sig=254,16 Ref=off (D:\DATA\0312\L232517R\003-D2F-A2-Q158596$2.D)

mAU
400
200
0

MSD1 TIC, MS File (D:\DATA\0312\L232517R\003-D2F-A2-Q158596$2.D) ES-API, Scan, Frag: 100, "POS"

1000000
500000
0.979
1.258

MSD2 TIC, MS File (D:\DATA\0312\L232517R\003-D2F-A2-Q158596$2.D) ES-API, Scan, Frag: 100, "NEG"

50000
40000
30000
20000
10000
0.978

ELS1 A, ELS1A, ELSD Signal (D:\DATA\0312\L232517R\003-D2F-A2-Q158596$2.D)

LSU
20
15
10

*MSD1 SPC, time=0.979 of D:\DATA\0312\L232517R\003-D2F-A2-Q158596$2.D ES-API, Scan, Frag: 100, "POS"

RT 0.979
50
0
347.2
348.2
375.2

*MSD1 SPC, time=1.255 of D:\DATA\0312\L232517R\003-D2F-A2-Q158596$2.D ES-API, Scan, Frag: 100, "POS"

RT 1.258
50
0
279.0
280.0
347.2
558.2

*MSD2 SPC, time=0.975 of D:\DATA\0312\L232517R\003-D2F-A2-Q158596$2.D ES-API, Scan, Frag: 100, "NEG"

RT 0.978
50
0
345.2
347.2
373.0
381.0

HRMS

S95

5-(2-amino-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-11-yl)-2-methylpent-4-yn-2-ol (24).

¹H NMR
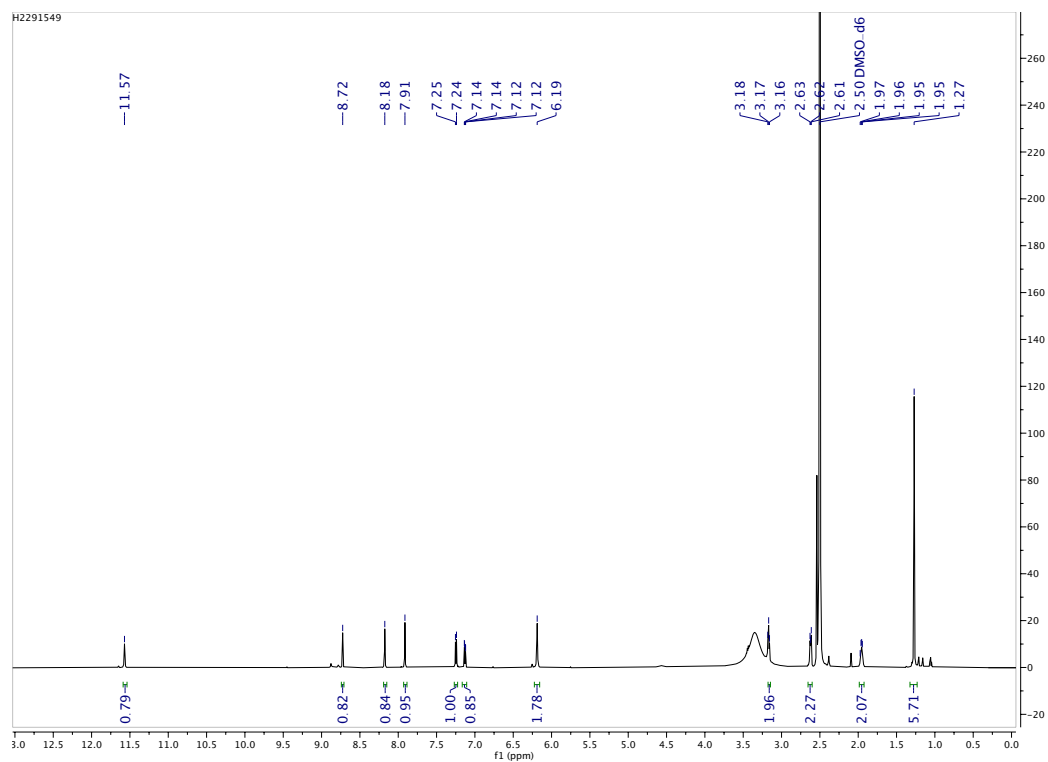
¹³C NMR
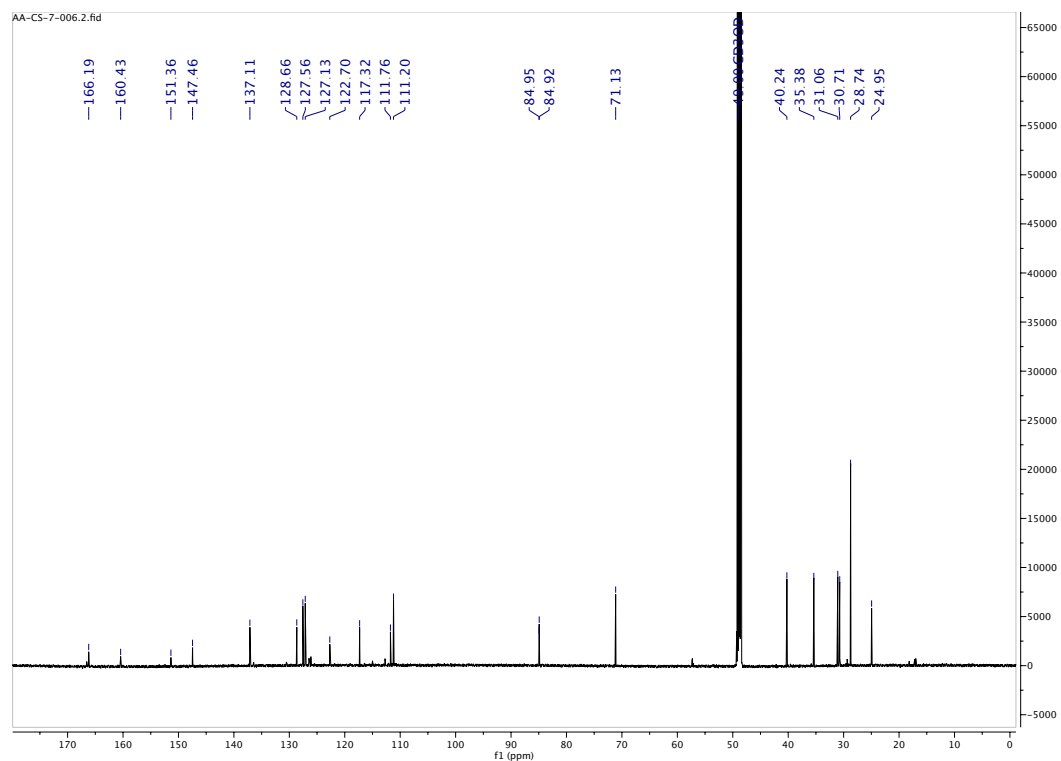
LC Chromatogram

MaxPeak: 95.86%
Ret_Time: 0.749 min
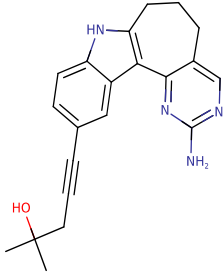
Mol Wt   **346.43**
Exact Mass   **346.21**

```
#   Time    Area%
-----------------
1   0.712   1.50
2   0.749   95.86
3   0.801   2.64
```

Q184300$1

DAD1 A, Sig=215,16 Ref=off (D:\DATA\03\0323\L234990R\007-D5B-A6-Q184300$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATA\03\0323\L234990R\007-D5B-A6-Q184300$1.D)

MSD1 TIC, MS File (D:\DATA\03\0323\L234990R\007-D5B-A6-Q184300$1.D) ES-API, Fast Scan, Frag: 100, "F

MSD2 TIC, MS File (D:\DATA\03\0323\L234990R\007-D5B-A6-Q184300$1.D) ES-API, Fast Scan, Frag: 100, "N

ELS1 A, ELS1A, ELSD Signal (D:\DATA\03\0323\L234990R\007-D5B-A6-Q184300$1.D)

*MSD1 SPC, time=0.756 of D:\DATA\03\0323\L234990R\007-D5B-A6-Q184300$1.D ES-API, Fast Scan, Frag: 100, "POS"
RT 0.760

*MSD1 SPC, time=0.814 of D:\DATA\03\0323\L234990R\007-D5B-A6-Q184300$1.D ES-API, Fast Scan, Frag: 100, "POS"
RT 0.814

*MSD2 SPC, time=0.715 of D:\DATA\03\0323\L234990R\007-D5B-A6-Q184300$1.D ES-API, Fast Scan, Frag: 100, "NEG"
RT 0.717

*MSD2 SPC, time=0.762 of D:\DATA\03\0323\L234990R\007-D5B-A6-Q184300$1.D ES-API, Fast Scan, Frag: 100, "NEG"
RT 0.761

Inj.Date 3/23/2020   LT   Acq. Method C:\Users\ ->   ->

HRMS

Target Compound Screening Report

Data File	H2291549.d	**Sample Name**	H2291549
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 7:51:06 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C21H22N4O	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 7:51:06 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 2: C21 H22 N4 O; 2.291	97.59	-0.91	C21 H22 N4 O	2.291	346.1794	346.179
Cpd 1: C21 H22 N4 O; 2.419	61.78	2	C21 H22 N4 O	2.419	346.1794	346.1801

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
347.1865	2.291	346.179	C21 H22 N4 O	346.1794	-0.91	Find By Formula	

Compound Chromatograms
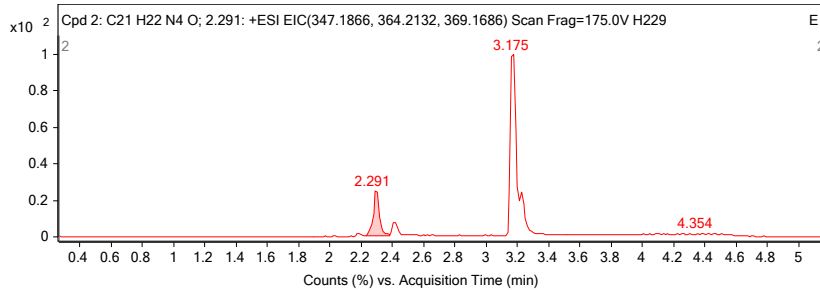
MS Zoomed Spectrum

1-(2-amino-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-11-yl)-3-methylpent-1-yn-3-ol (25).

¹H NMR
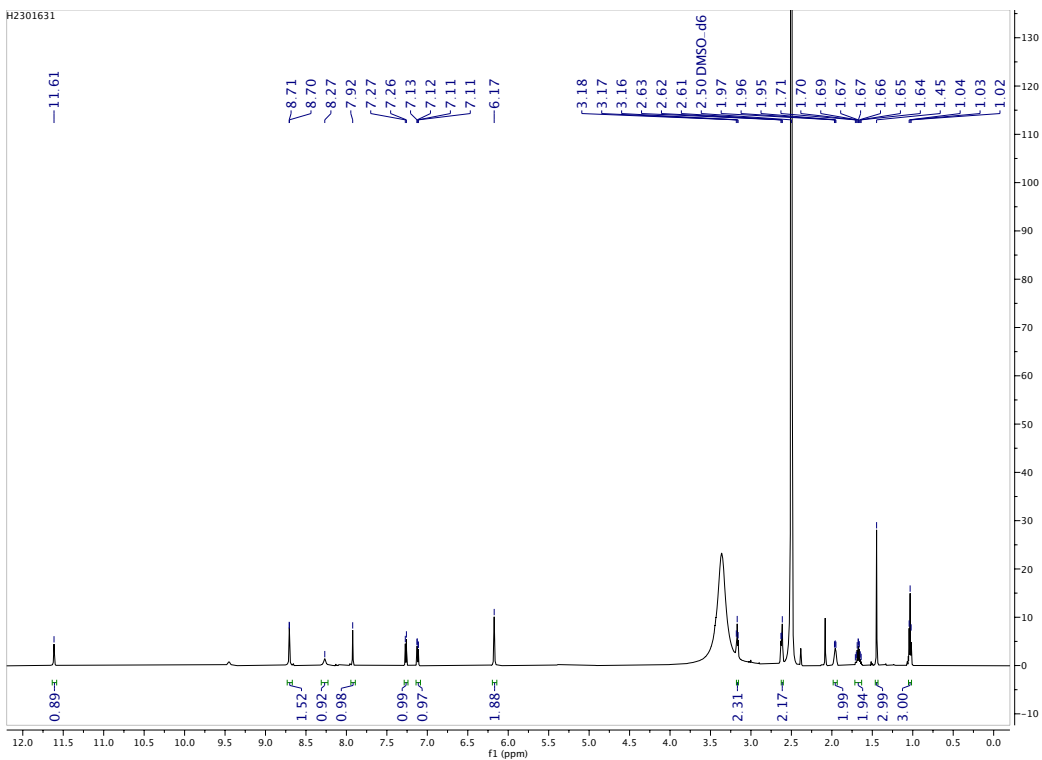
¹³C NMR
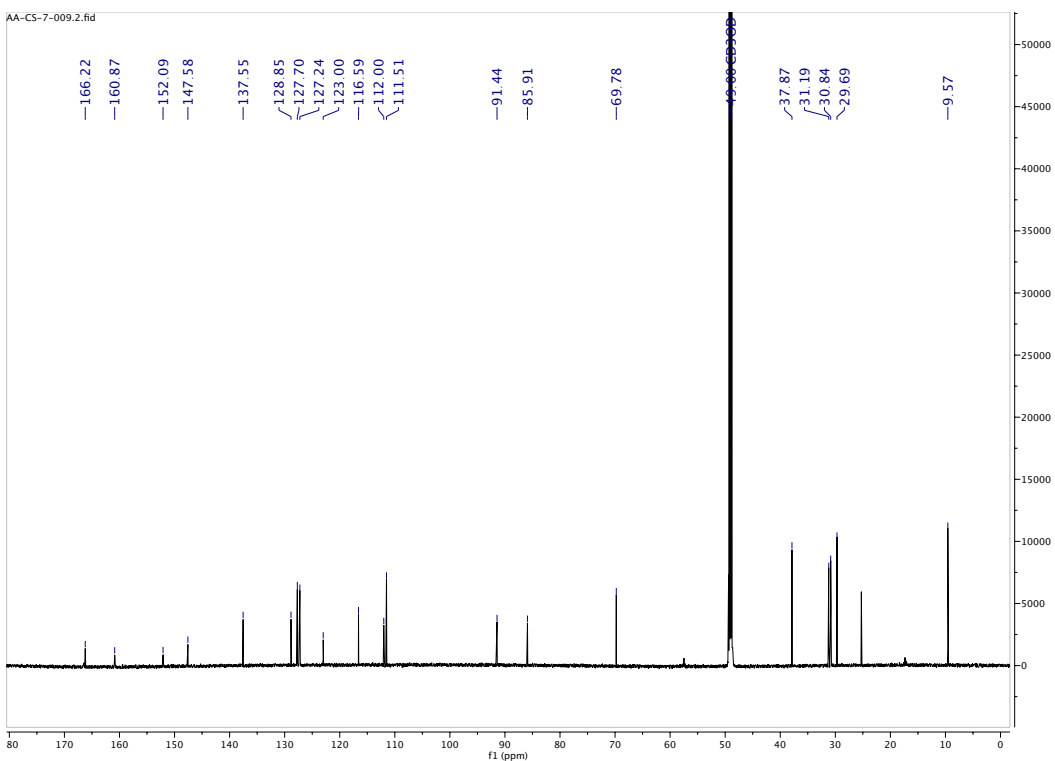
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 2.135 min
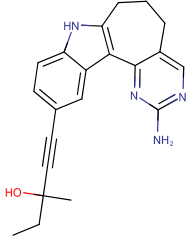
Mol Wt   **346.43**
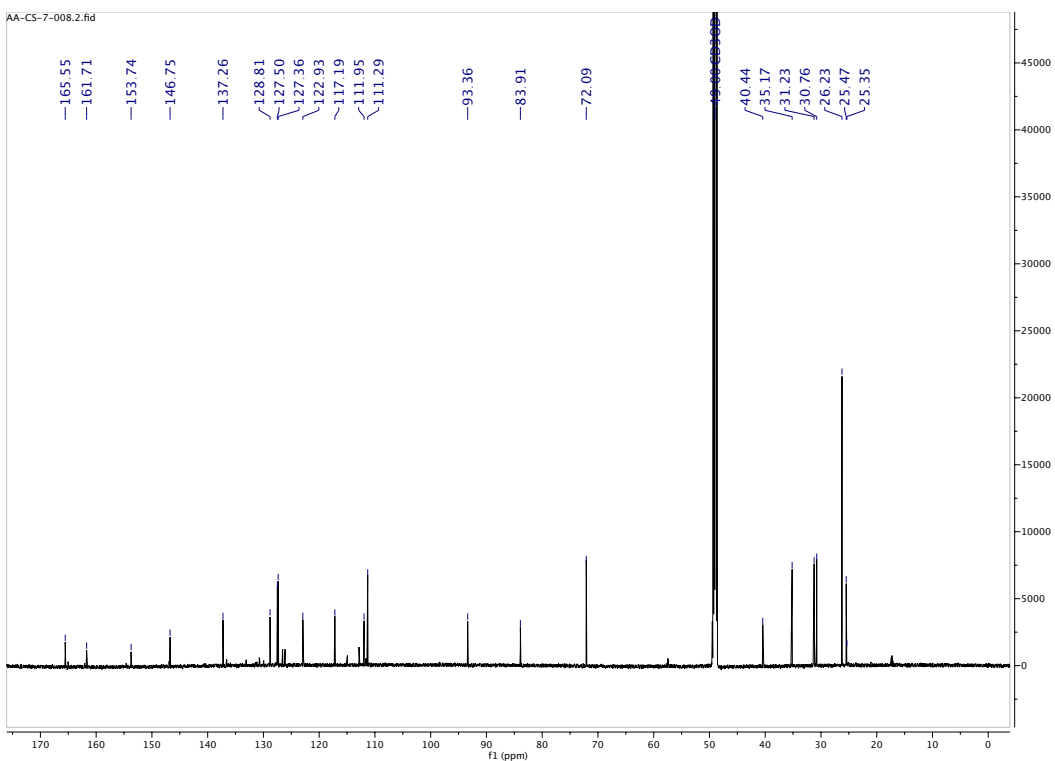**Exact Mass**   **346.21**

```
#  Time    Area%
-----------------
1  2.135  100.00
```

Q227419$1

DAD1 A, Sig=215,16 Ref=off (D:\DATA\0325\L235658R\011-D5B-A9-Q227419$1.D)

mAU

2.135

DAD1 B, Sig=254,16 Ref=off (D:\DATA\0325\L235658R\011-D5B-A9-Q227419$1.D)

mAU

MSD1 TIC, MS File (D:\DATA\0325\L235658R\011-D5B-A9-Q227419$1.D) ES-API, Scan, Frag: 100, "POS"

2.151

MSD2 TIC, MS File (D:\DATA\0325\L235658R\011-D5B-A9-Q227419$1.D) ES-API, Scan, Frag: 100, "NEG"

2.153

ADC1 B, ELSD (D:\DATA\0325\L235658R\011-D5B-A9-Q227419$1.D)

mAu

*MSD1 SPC, time=2.152 of D:\DATA\0325\L235658R\011-D5B-A9-Q227419$1.D ES-API, Scan, Frag: 100, "POS"

RT 2.151

347.2
348.2

*MSD2 SPC, time=2.156 of D:\DATA\0325\L235658R\011-D5B-A9-Q227419$1.D ES-API, Scan, Frag: 100, "NEG"

RT 2.153

345.2
346.2

HRMS

Target Compound Screening Report

Data File	5-2.d	**Sample Name**	EQNO
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/18/2021 11:13:32 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	QualDAMethod.m
Comment			
Sample Group		**Info.**	
MFC	C21H22N4O	**Stream Name**	LC 1
Acquisition Time (Local)	5/18/2021 11:13:32 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H22 N4 O; 2.329	95.9	-1.66	C21 H22 N4 O	2.329	346.1794	346.1788

Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
347.186	2.329	346.1788	C21 H22 N4 O	346.1794	-1.66	Find By Formula	

Compound Chromatograms

Cpd 1: C21 H22 N4 O; 2.329: +ESI EIC(347.1866, 364.2132, 369.1686) Scan Frag=175.0V 5-2.d
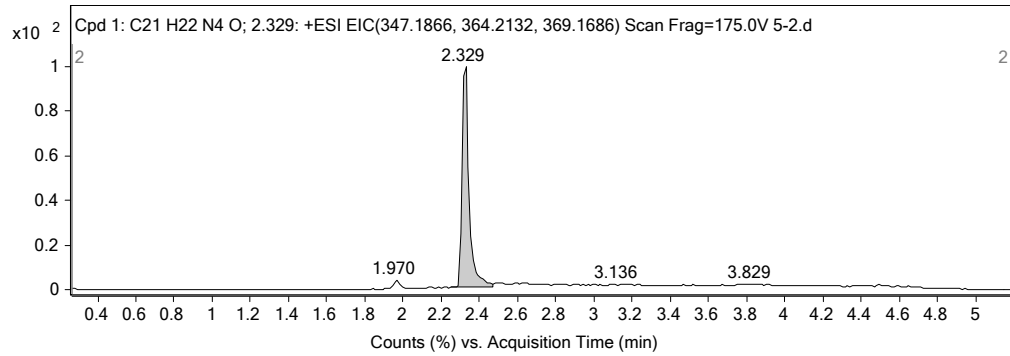
MS Zoomed Spectrum

1-(2-amino-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-11-yl)-3-ethylpent-1-yn-3-ol (26).

1H NMR
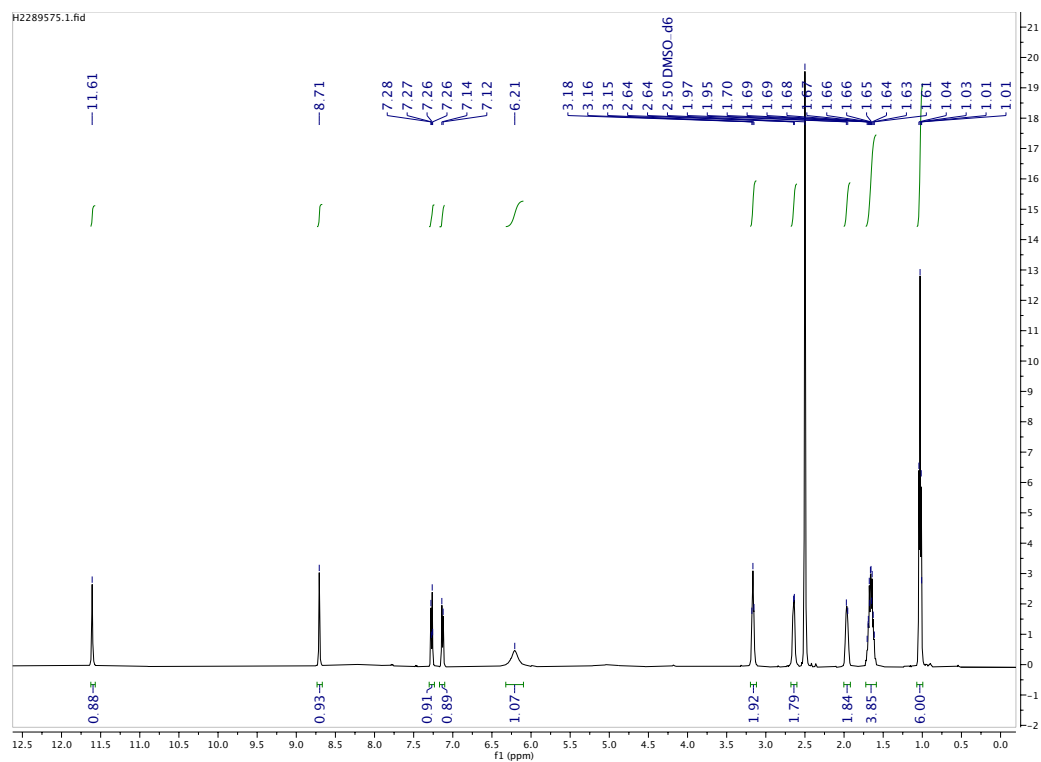
13C NMR
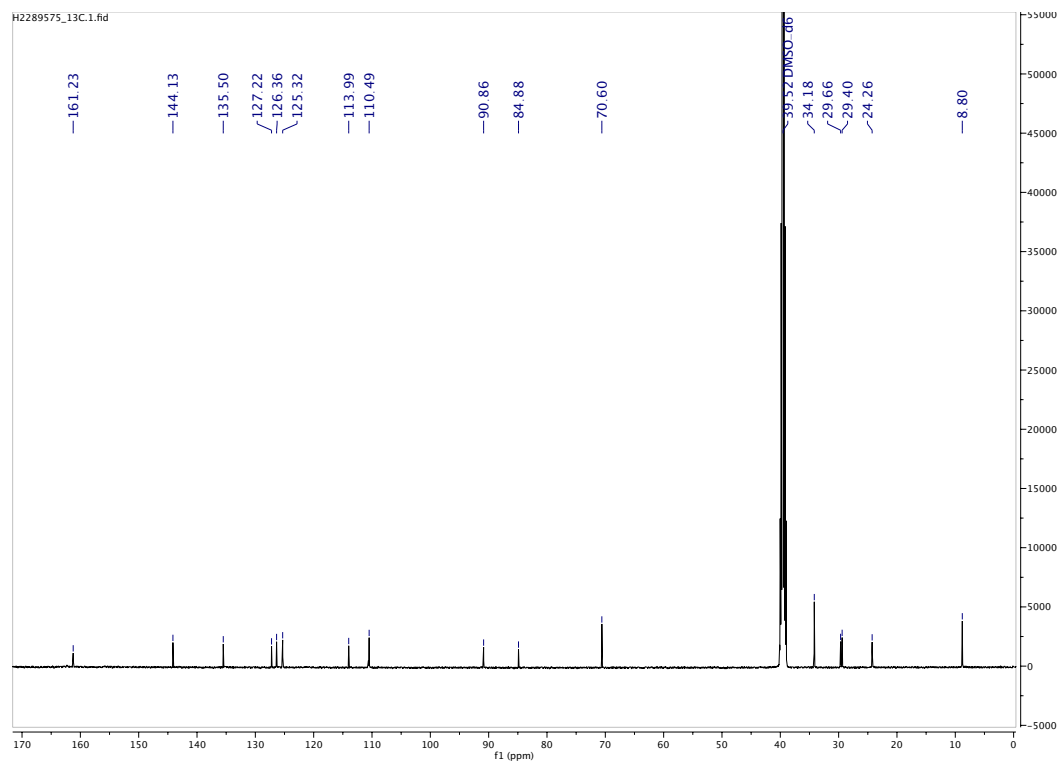
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 2.443 min
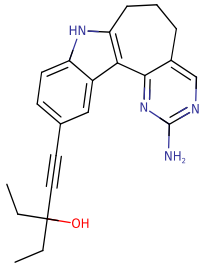
Mol Wt 360.45
Exact Mass 360.23

```
#  Time    Area%
----------------
1  2.443   100.00
```

Q184057$1

DAD1 A, Sig=215,16 Ref=off (D:\DATA\03\0317\L233584R\013-D6F-A6-Q184057$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATA\03\0317\L233584R\013-D6F-A6-Q184057$1.D)

MSD1 TIC, MS File (D:\DATA\03\0317\L233584R\013-D6F-A6-Q184057$1.D) ES-API, Scan, Frag: 100, "POS"

MSD2 TIC, MS File (D:\DATA\03\0317\L233584R\013-D6F-A6-Q184057$1.D) ES-API, Scan, Frag: 100, "NEG"

ADC1 A, ELSD (D:\DATA\03\0317\L233584R\013-D6F-A6-Q184057$1.D)

RT 2.460

*MSD1 SPC, time=2.461 of D:\DATA\03\0317\L233584R\013-D6F-A6-Q184057$1.D ES-API, Scan, Frag: 100, "POS"

RT 2.464

*MSD2 SPC, time=2.465 of D:\DATA\03\0317\L233584R\013-D6F-A6-Q184057$1.D ES-API, Scan, Frag: 100, "NEG"

HRMS

Target Compound Screening Report

Data File	H2289575.d	**Sample Name**	H2289575
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 5:49:49 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C22H24N4O	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 5:49:49 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H24 N4 O; 2.419	67.71	-0.18	C22 H24 N4 O	2.419	360.195	360.1949

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
361.2026	2.419	360.1949	C22 H24 N4 O	360.195	-0.18	Find By Formula	

Compound Chromatograms
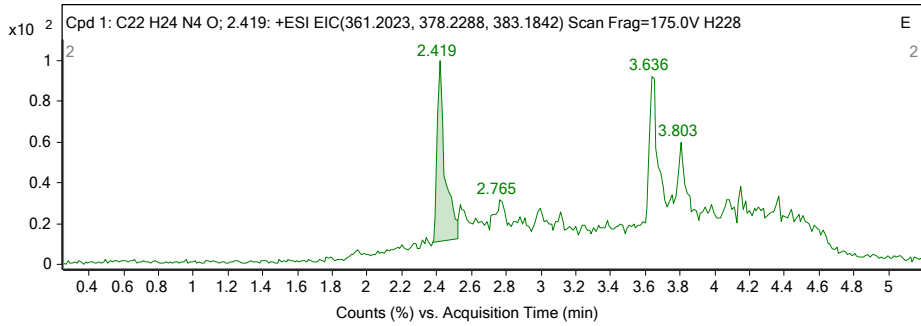
MS Zoomed Spectrum

*10-(4-fluorophenyl)-6,7-dihydro-5H-pyrimido[5,4-c]carbazol-2-amine (**7**).*

¹H NMR

H1799969.1.fid

¹³C NMR

H1799969_C13.1.fid
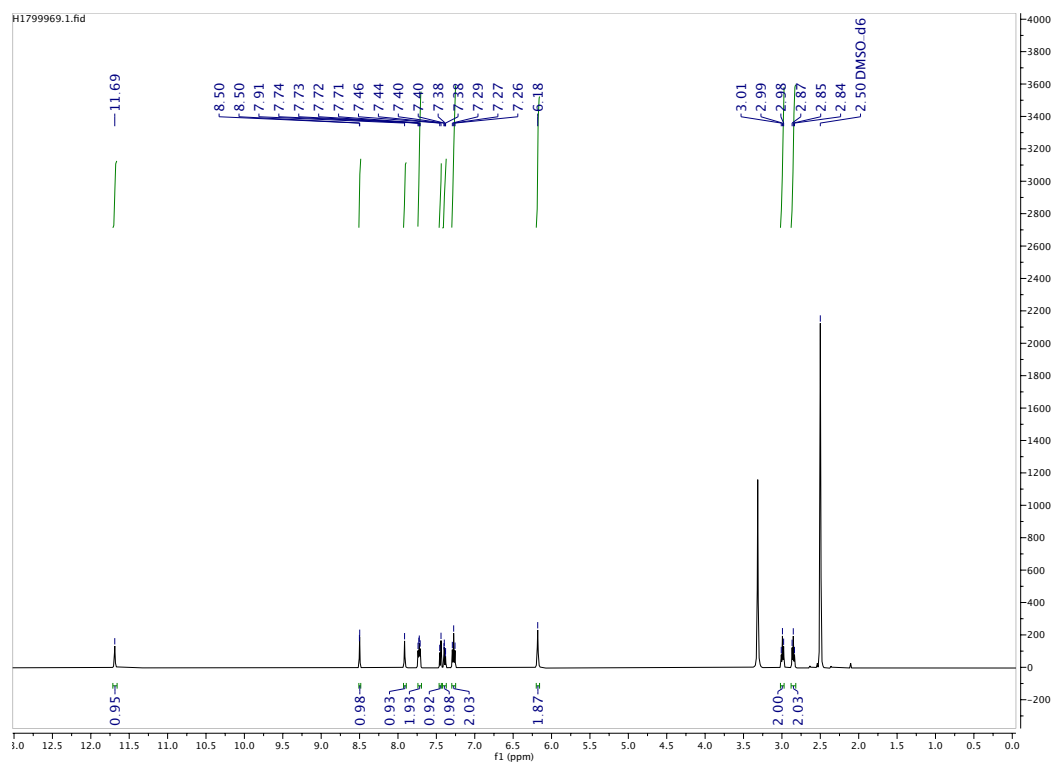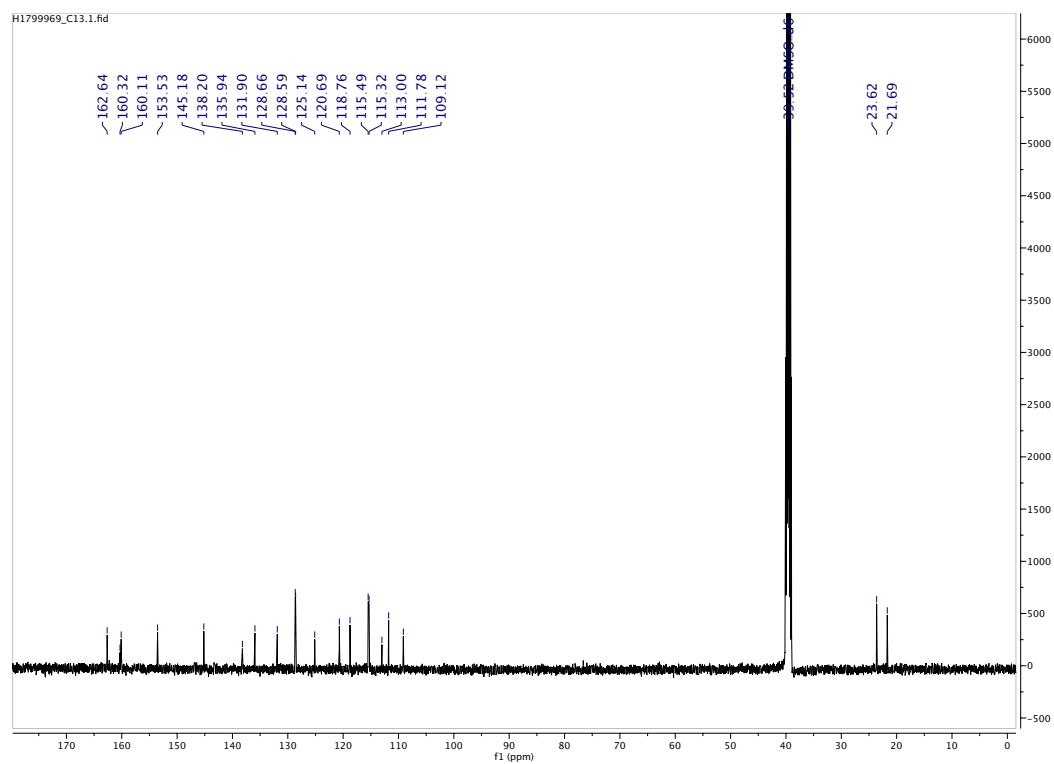
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 1.093 min
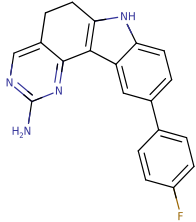
Mol Wt   **330.36**
Exact Mass   **330.15**

```
#  Time    Area%
-----------------
1  1.093  100.00
```


O578492$1

DAD1 A, Sig=215,16 Ref=off (D:\D\07_29B\1177654D\035-2-O578492$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\D\07_29B\1177654D\035-2-O578492$1.D)

MSD1 TIC, MS File (D:\D\07_29B\1177654D\035-2-O578492$1.D) ES-API, Scan, Frag: 100, "POS"

MSD2 TIC, MS File (D:\D\07_29B\1177654D\035-2-O578492$1.D) ES-API, Scan, Frag: 100, "NEG"

ADC1 A, ELSD (D:\D\07_29B\1177654D\035-2-O578492$1.D)

*MSD1 SPC, time=1.105 of D:\D\07_29B\1177654D\035-2-O578492$1.D ES-API, Scan, Frag: 100, "POS"

RT 1.107

*MSD2 SPC, time=1.109 of D:\D\07_29B\1177654D\035-2-O578492$1.D ES-API, Scan, Frag: 100, "NEG"

RT 1.108

Inj.Date 7/29/2019   N   Vial 2   -7-   Acq. Method C:\Chem32\->   ->

HRMS

Target Compound Screening Report

Data File	H1799969.d	**Sample Name**	H1799969
Sample Type	Sample	**Position**	P1-B4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 7:02:37 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C20H15FN4	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 7:02:37 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C20 H15 F N4; 2.482	94.69	-0.37	C20 H15 F N4	2.482	330.1281	330.128

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
331.1352	2.482	330.128	C20 H15 F N4	330.1281	-0.37	Find By Formula	

Compound Chromatograms
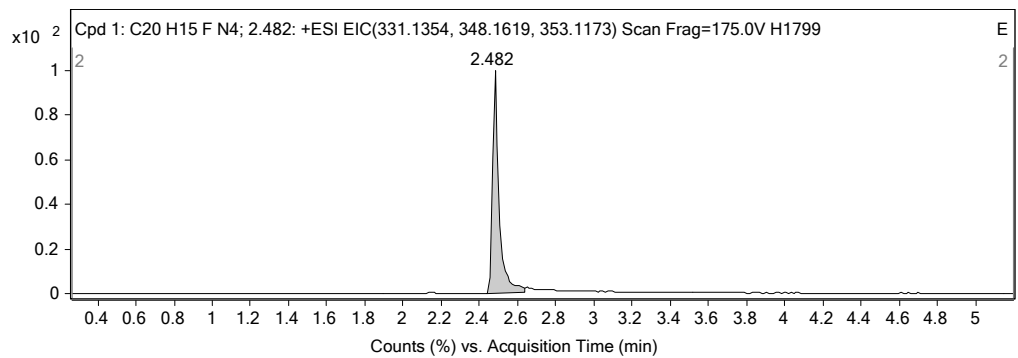
MS Zoomed Spectrum

*11-(4-fluorophenyl)-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-2-amine (**8**).*

¹H NMR
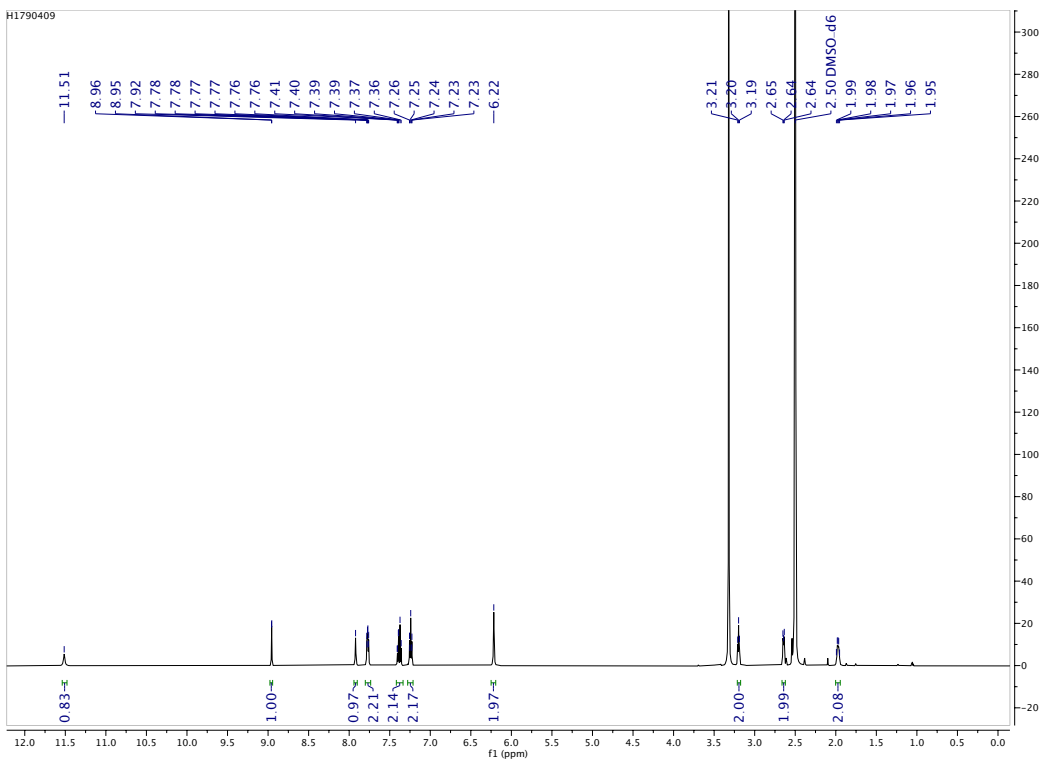
¹³C NMR
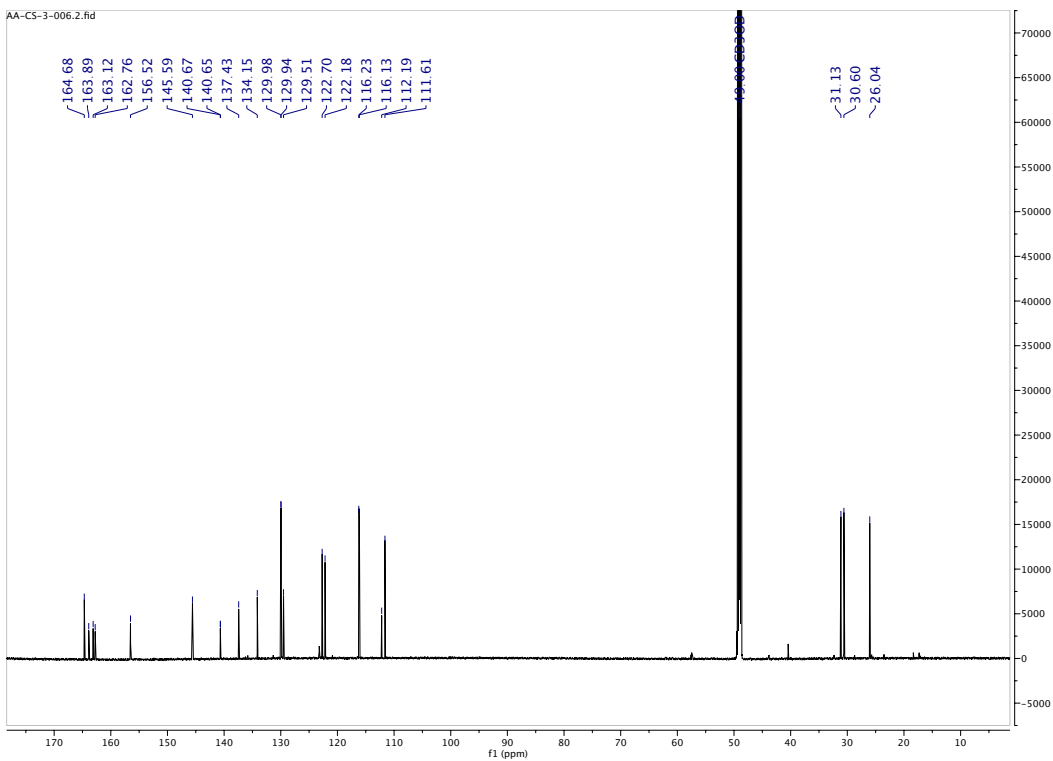
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 1.043 min
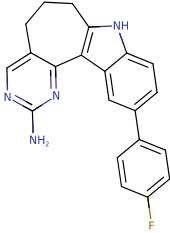
Mol Wt   **344.38**
Exact Mass **344.17**

```
#  Time   Area%
-----------------
1  1.043  100.00
```

O541244$1

DAD1 A, Sig=215,16 Ref=off (D:\DATA\07\23\L176391R\006-D2F-A5-O541244$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATA\07\23\L176391R\006-D2F-A5-O541244$1.D)

MSD1 TIC, MS File (D:\DATA\07\23\L176391R\006-D2F-A5-O541244$1.D) ES-API, Scan, Frag: 100, "POS"

MSD2 TIC, MS File (D:\DATA\07\23\L176391R\006-D2F-A5-O541244$1.D) ES-API, Scan, Frag: 100, "NEG"

ADC1 A, ADC1A, ELSD (D:\DATA\07\23\L176391R\006-D2F-A5-O541244$1.D)

*MSD1 SPC, time=1.055 of D:\DATA\07\23\L176391R\006-D2F-A5-O541244$1.D ES-API, Scan, Frag: 100, "POS"

RT 1.056

*MSD2 SPC, time=1.059 of D:\DATA\07\23\L176391R\006-D2F-A5-O541244$1.D ES-API, Scan, Frag: 100, "NEG"

RT 1.057

Inj.Date 7/23/2019   LB   <invalid> -11-   Acq. Method C:\Chem32\->   ->

HRMS

Target Compound Screening Report

Data File	H1790409.d	**Sample Name**	H1790409
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 7:08:41 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C21H17FN4	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 7:08:41 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H17 F N4; 2.509	95.81	0.28	C21 H17 F N4	2.509	344.1437	344.1438

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
345.1511	2.509	344.1438	C21 H17 F N4	344.1437	0.28	Find By Formula	

Compound Chromatograms

Cpd 1: C21 H17 F N4; 2.509: +ESI EIC(345.1510, 362.1776, 367.1329) Scan Frag=175.0V H1790
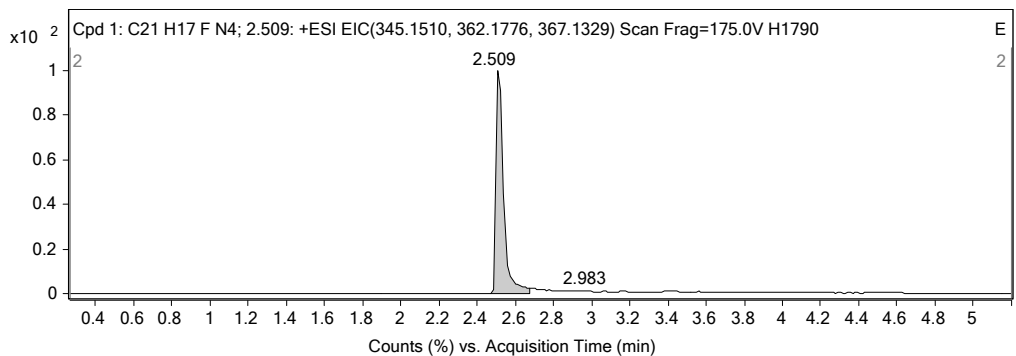
MS Zoomed Spectrum

12-(4-fluorophenyl)-6,7,8,9-tetrahydro-5H-pyrimido[4',5':3,4]cycloocta[1,2-b]indol-2-amine (9).

^{1}H NMR
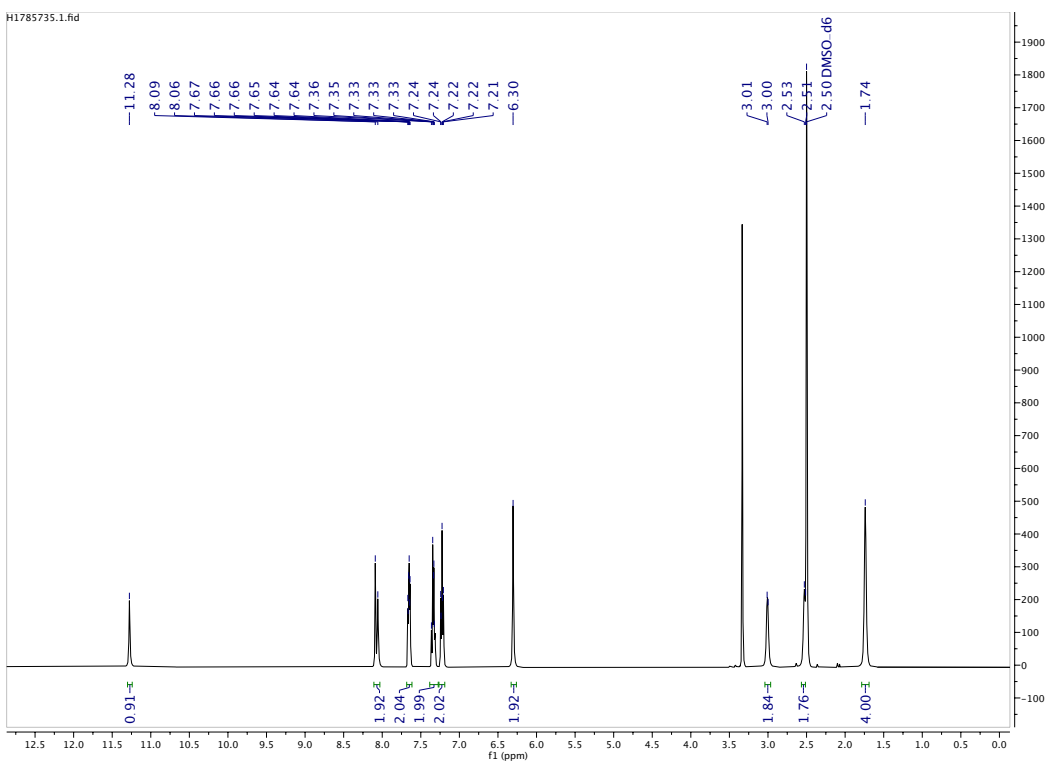
^{13}C NMR
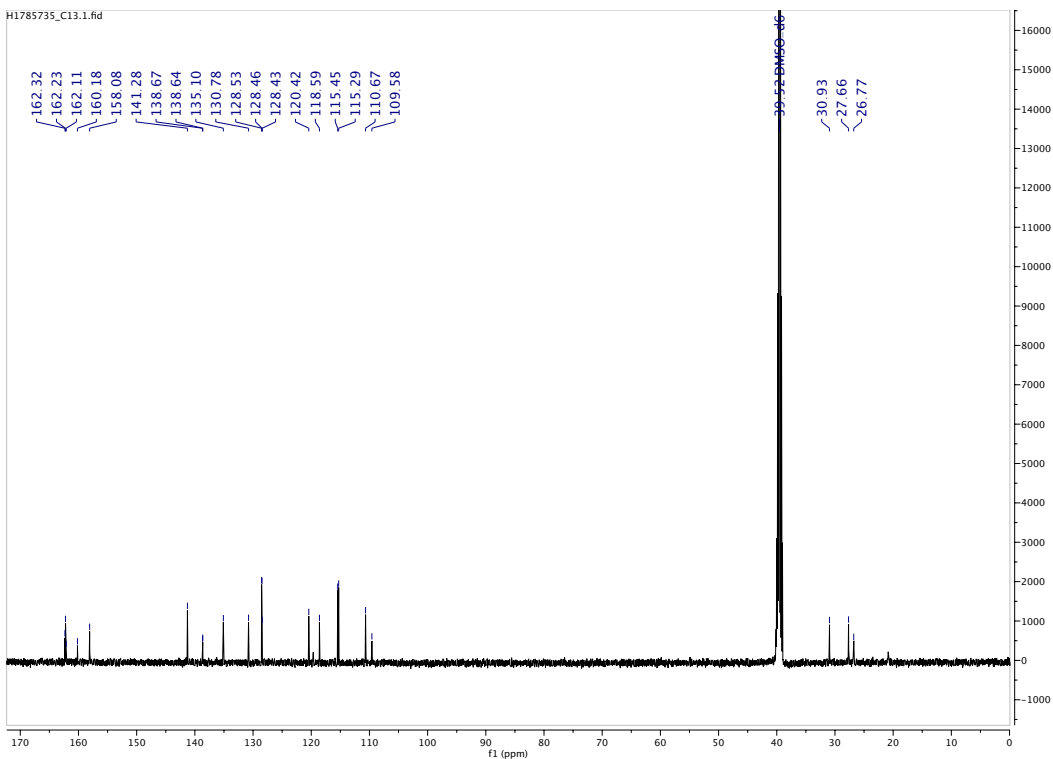
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 1.169 min
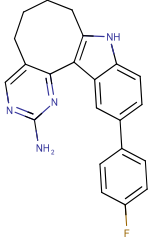
Mol Wt **358.41**
Exact Mass **358.19**

```
#  Time    Area%
-----------------
1  1.169  100.00
```


O521269$1

DAD1 A, Sig=215,16 Ref=off (D:\DATA\0718\L175406R\005-D6B-A4-O521269$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\DATA\0718\L175406R\005-D6B-A4-O521269$1.D)

MSD1 TIC, MS File (D:\DATA\0718\L175406R\005-D6B-A4-O521269$1.D) ES-API, Scan, Frag: 100, "POS"

MSD2 TIC, MS File (D:\DATA\0718\L175406R\005-D6B-A4-O521269$1.D) ES-API, Scan, Frag: 100, "NEG"

ELS1 A, ELS1A, ELSD Signal (D:\DATA\0718\L175406R\005-D6B-A4-O521269$1.D)

*MSD1 SPC, time=1.179 of D:\DATA\0718\L175406R\005-D6B-A4-O521269$1.D ES-API, Scan, Frag: 100, "POS"
RT 1.182

*MSD2 SPC, time=1.183 of D:\DATA\0718\L175406R\005-D6B-A4-O521269$1.D ES-API, Scan, Frag: 100, "NEG"
RT 1.183

Inj.Date 7/18/2019   LT   <invalid> 13   Acq. Method C:\Chem32\->   ->

HRMS

Target Compound Screening Report

Data File	H1785735.d	**Sample Name**	H1785735
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 6:26:15 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C22H19FN4	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 6:26:15 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H19 F N4; 2.572	96.64	-0.12	C22 H19 F N4	2.572	358.1594	358.1593

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
359.1668	2.572	358.1593	C22 H19 F N4	358.1594	-0.12	Find By Formula	

Compound Chromatograms
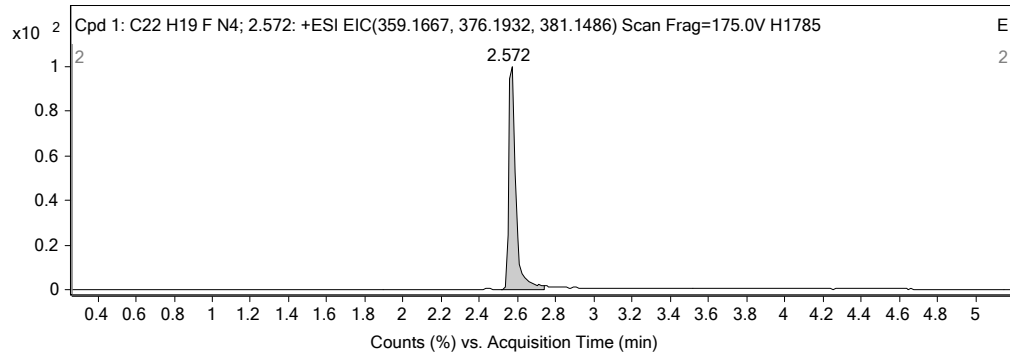
MS Zoomed Spectrum

*10-(1-methyl-1H-pyrazol-4-yl)-6,7-dihydro-5H-pyrimido[5,4-c]carbazol-2-amine (**12**).*

^{1}H NMR

H1799968.1.fid

11.56

8.45
8.07
7.90
7.89
7.35
7.33
7.31
7.31
6.21

3.88
2.99
2.97
2.96
2.86
2.84
2.82
2.50 DMSO.d6

0.93

0.96
0.95
2.00
1.99

1.90

3.04

2.00
2.00

f1 (ppm)

^{13}C NMR

H1799968_C13.1.fid

162.64
160.09
153.49

144.56

135.79
135.15
127.01
125.12
125.00
123.28
119.33
116.96
112.88
111.62
108.81

39.52 DMSO.d6
38.58

23.59
21.66

f1 (ppm)
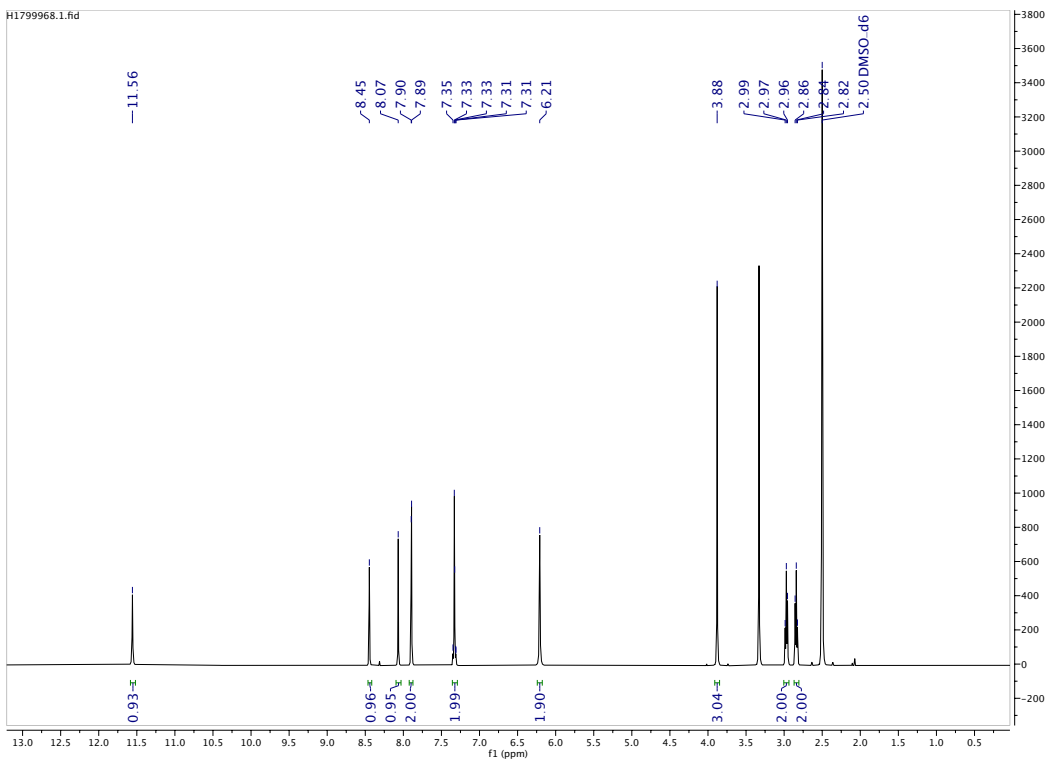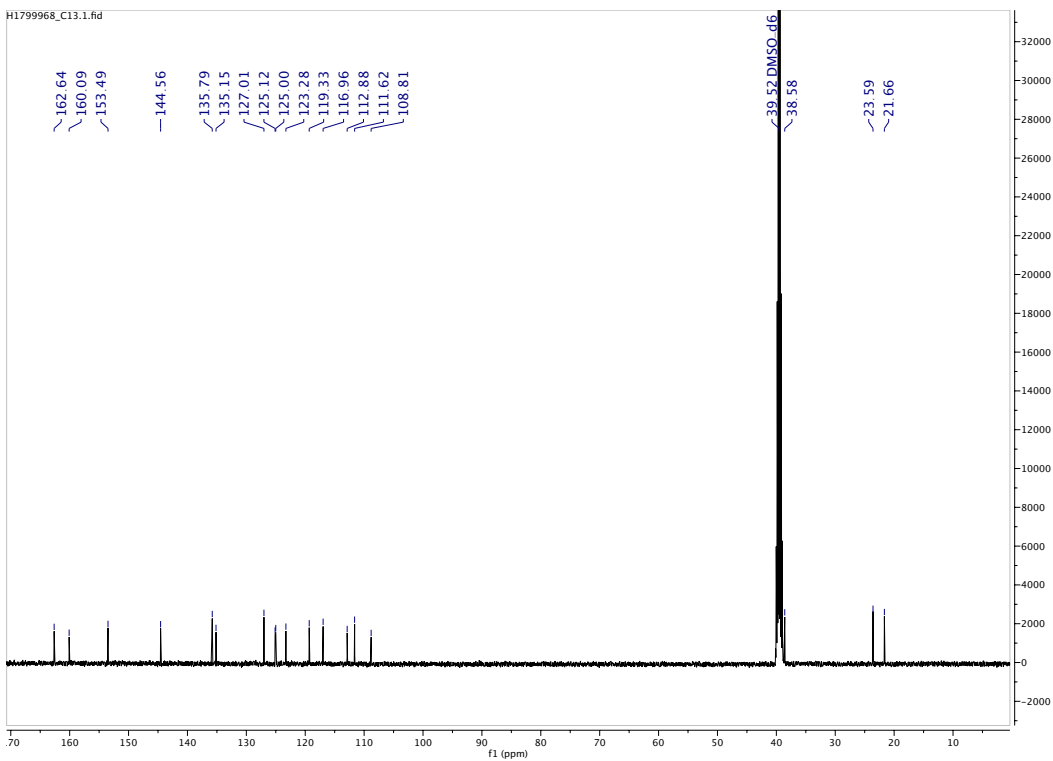
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 0.885 min
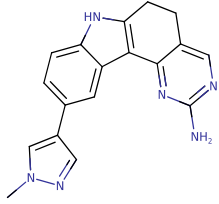
Mol Wt   316.36
Exact Mass   316.16

```
#  Time   Area%
-----------------
1  0.885  100.00
```

O578496$1

DAD1 A, Sig=215,16 Ref=off (D:\D\07_29B\1177654D\034-1-O578496$1.D)

DAD1 B, Sig=254,16 Ref=off (D:\D\07_29B\1177654D\034-1-O578496$1.D)

MSD1 TIC, MS File (D:\D\07_29B\1177654D\034-1-O578496$1.D) ES-API, Scan, Frag: 100, "POS"

MSD2 TIC, MS File (D:\D\07_29B\1177654D\034-1-O578496$1.D) ES-API, Scan, Frag: 100, "NEG"

ADC1 A, ELSD (D:\D\07_29B\1177654D\034-1-O578496$1.D)

*MSD1 SPC, time=0.904 of D:\D\07_29B\1177654D\034-1-O578496$1.D ES-API, Scan, Frag: 100, "POS"

RT 0.900

*MSD2 SPC, time=0.900 of D:\D\07_29B\1177654D\034-1-O578496$1.D ES-API, Scan, Frag: 100, "NEG"

RT 0.900

Inj.Date 7/29/2019   N   Vial 1   -7-   Acq. Method C:\Chem32\->   ->

HRMS

Target Compound Screening Report

Data File	H1799968.d	**Sample Name**	H1799968
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 5:55:50 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C18H16N6	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 5:55:50 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C18 H16 N6; 2.092	77.64	4.59	C18 H16 N6	2.092	316.1436	316.1451

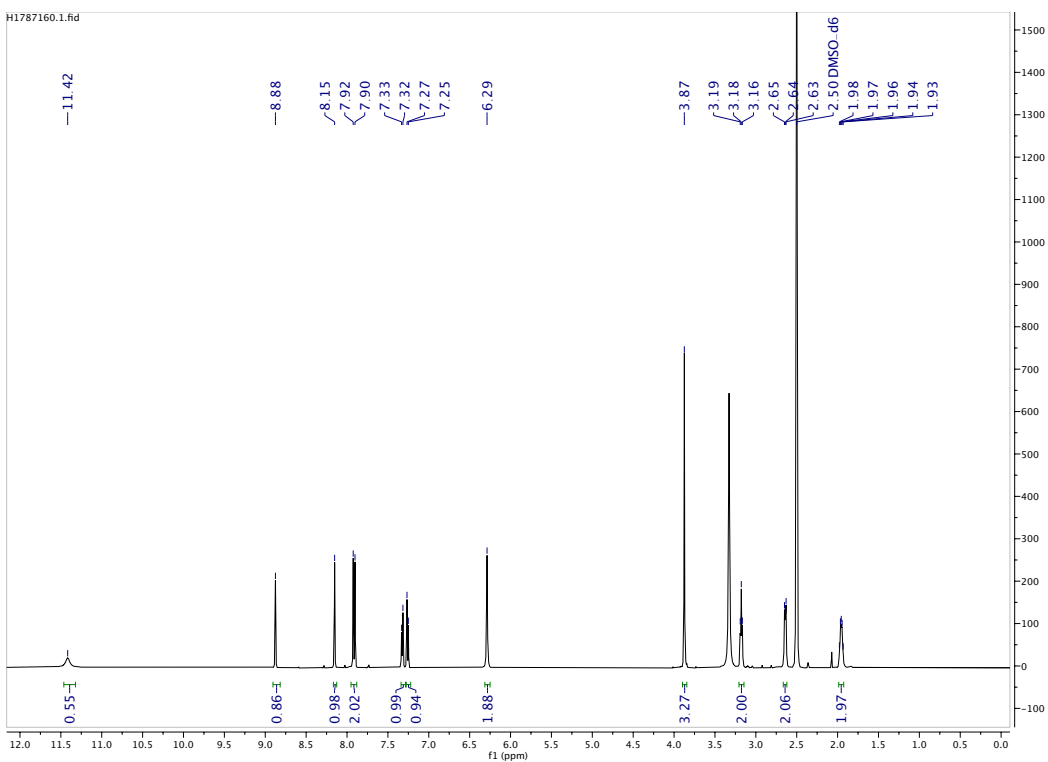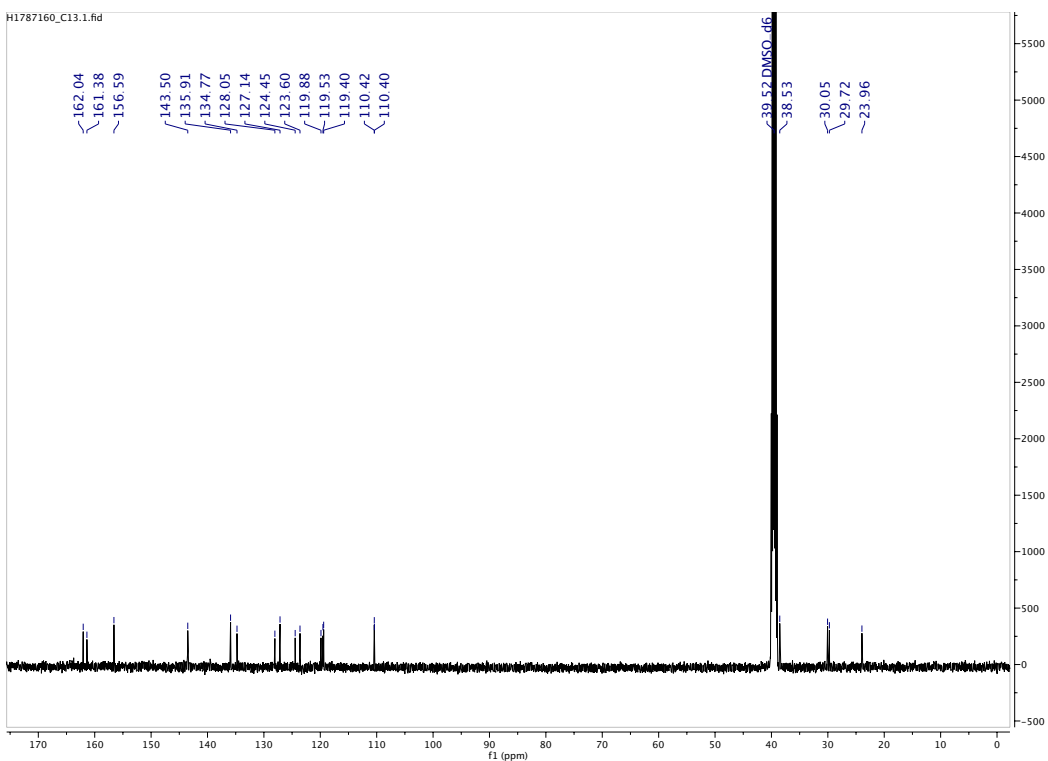| Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
317.1522	2.092	316.1451	C18 H16 N6	316.1436	4.59	Find By Formula	

Compound Chromatograms
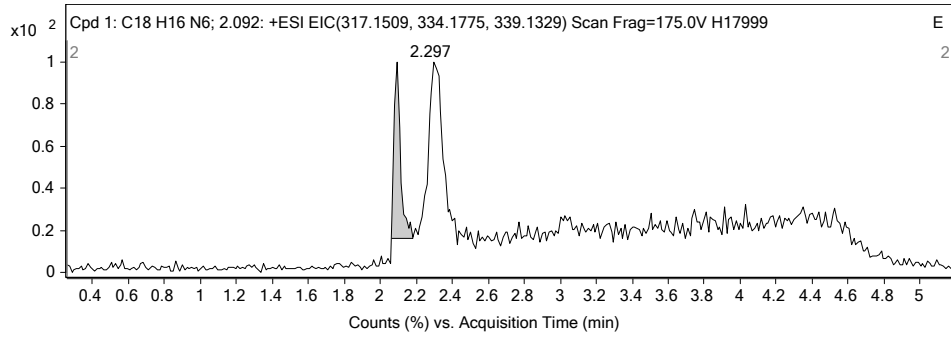
MS Zoomed Spectrum

11-(1-methyl-1H-pyrazol-4-yl)-5,6,7,8-tetrahydropyrimido[4',5':3,4]cyclohepta[1,2-b]indol-2-amine (13).
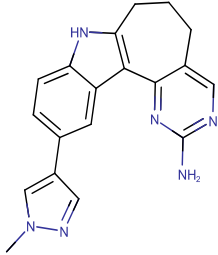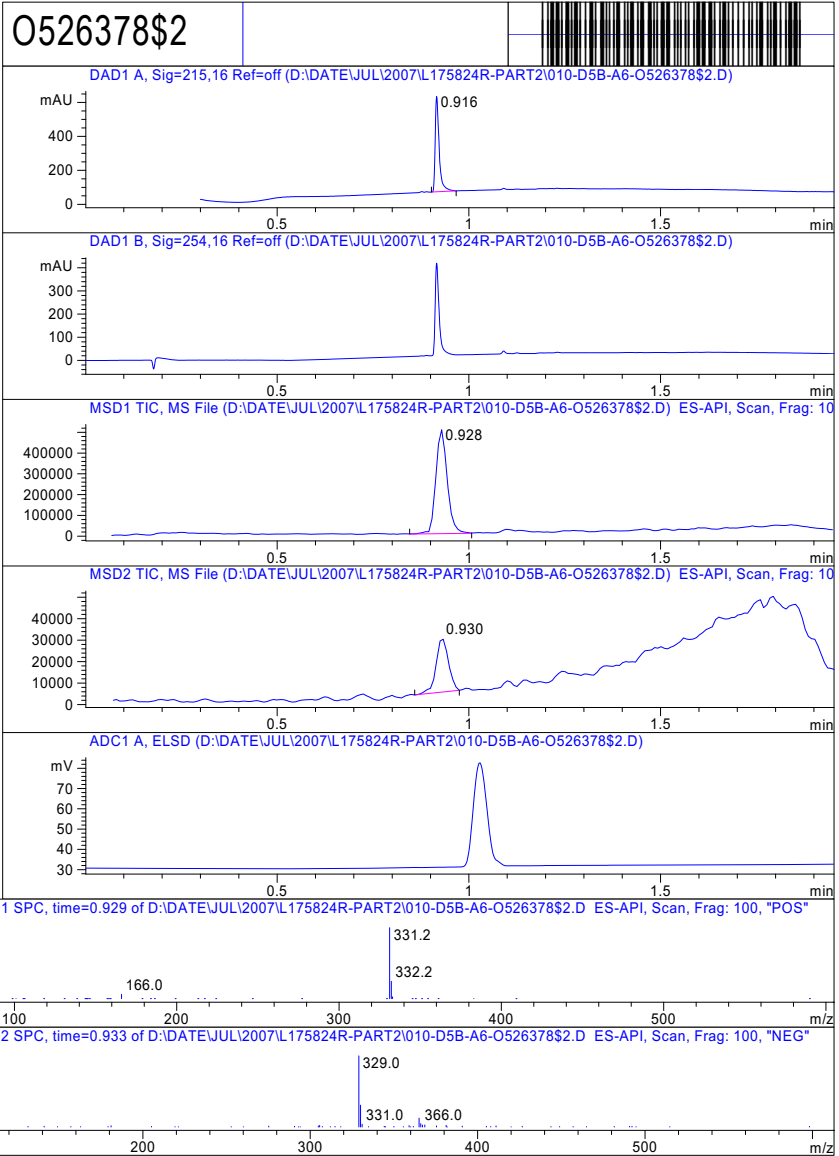
¹H NMR

¹³C NMR

LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 0.916 min

Mol Wt   **330.39**
Exact Mass   **330.18**

```
#   Time     Area%
-----------------
1   0.916    100.00
```

O526378$2

DAD1 A, Sig=215,16 Ref=off (D:\DATE\JUL\2007\L175824R-PART2\010-D5B-A6-O526378$2.D)

0.916

DAD1 B, Sig=254,16 Ref=off (D:\DATE\JUL\2007\L175824R-PART2\010-D5B-A6-O526378$2.D)

MSD1 TIC, MS File (D:\DATE\JUL\2007\L175824R-PART2\010-D5B-A6-O526378$2.D) ES-API, Scan, Frag: 10

0.928

MSD2 TIC, MS File (D:\DATE\JUL\2007\L175824R-PART2\010-D5B-A6-O526378$2.D) ES-API, Scan, Frag: 10

0.930

ADC1 A, ELSD (D:\DATE\JUL\2007\L175824R-PART2\010-D5B-A6-O526378$2.D)

*MSD1 SPC, time=0.929 of D:\DATE\JUL\2007\L175824R-PART2\010-D5B-A6-O526378$2.D ES-API, Scan, Frag: 100, "POS"

RT 0.928

331.2
332.2
166.0

*MSD2 SPC, time=0.933 of D:\DATE\JUL\2007\L175824R-PART2\010-D5B-A6-O526378$2.D ES-API, Scan, Frag: 100, "NEG"

RT 0.930

329.0
331.0 366.0

Inj.Date 7/19/2019   Y   <invalid> -7-   Acq. Method C:\Chem32\->   ->

HRMS

Target Compound Screening Report

Data File	H1787160.d	**Sample Name**	H1787160
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	5/7/2021 6:50:30 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	Fast_Gradient_HRMS_pos_Lock_08272019.m
Comment			
Sample Group		**Info.**	
MFC	C19H18N6	**Stream Name**	LC 1
Acquisition Time (Local)	5/7/2021 6:50:30 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C19 H18 N6; 2.154	77.33	-2.38	C19 H18 N6	2.154	330.1593	330.1585

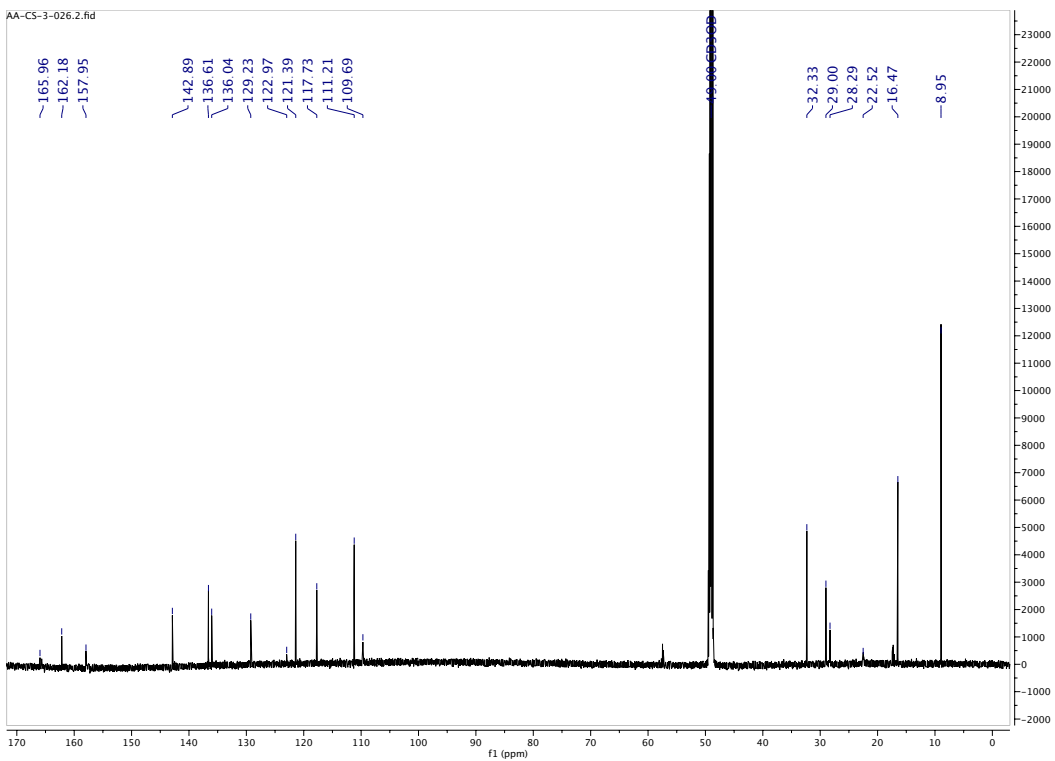| Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
331.1661	2.154	330.1585	C19 H18 N6	330.1593	-2.38	Find By Formula	

Compound Chromatograms
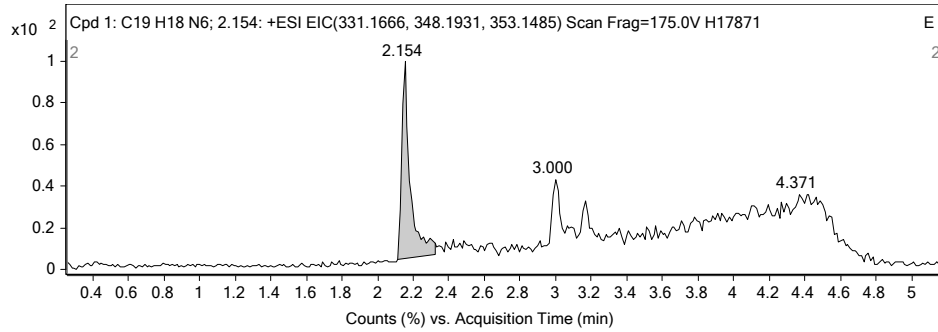
MS Zoomed Spectrum

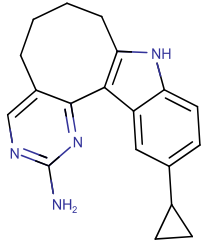*12-cyclopropyl-6,7,8,9-tetrahydro-5H-pyrimido[4',5':3,4]cycloocta[1,2-b]indol-2-amine (**30**).*

¹H NMR
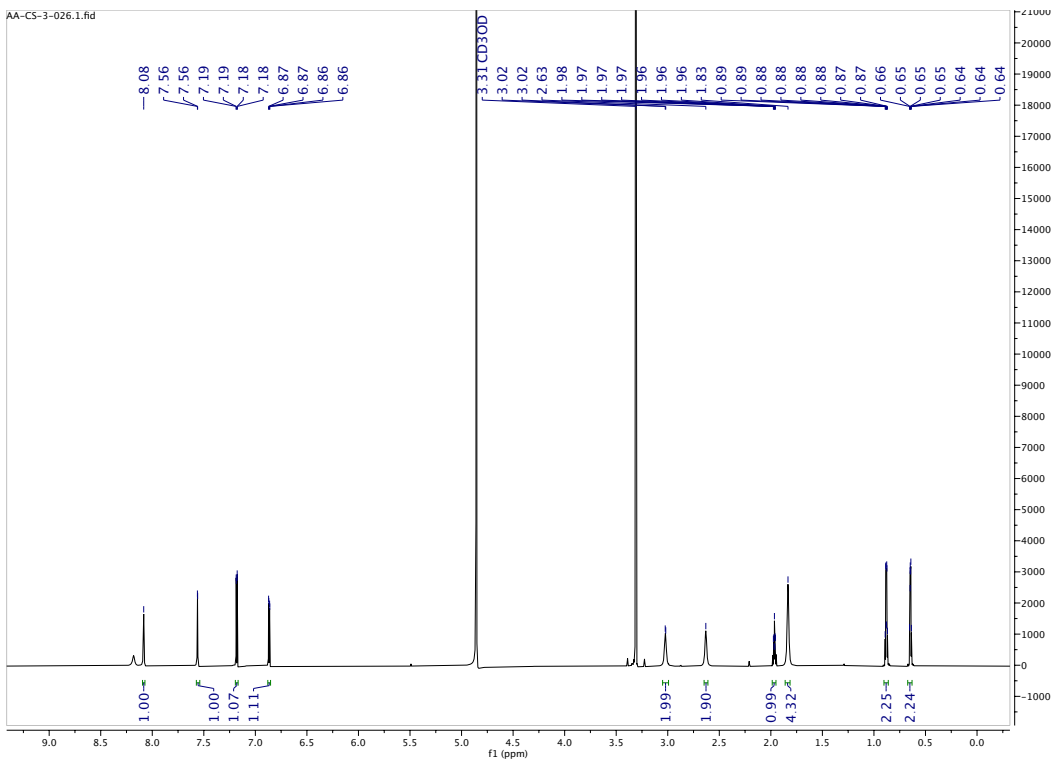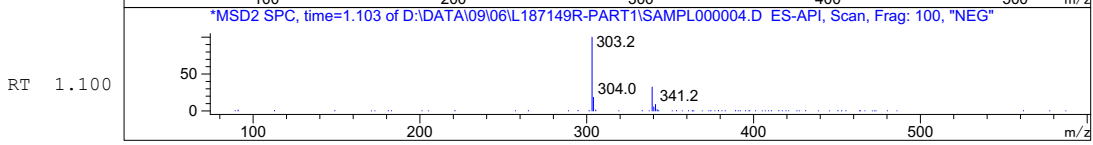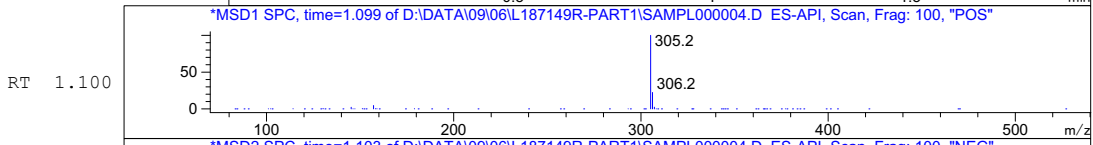

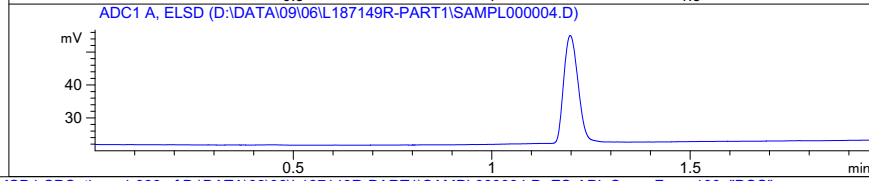**¹³C NMR**
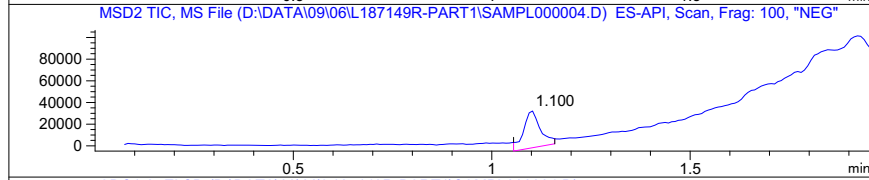
LC Chromatogram

MaxPeak: 100.00%
Ret_Time: 1.083 min

Mol Wt **304.39**
Exact Mass **304.2**

#	Time	Area%
1	1.083	100.00

O713582$1

DAD1 A, Sig=215,16 Ref=off (D:\DATA\09\06\L187149R-PART1\SAMPL000004.D)

mAU
600
400
200
0
1.083
0.5   1   1.5   min

DAD1 B, Sig=254,16 Ref=off (D:\DATA\09\06\L187149R-PART1\SAMPL000004.D)

mAU
50
0
-50
0.5   1   1.5   min

MSD1 TIC, MS File (D:\DATA\09\06\L187149R-PART1\SAMPL000004.D) ES-API, Scan, Frag: 100, "POS"

1000000
750000
500000
250000
0
1.100
0.5   1   1.5   min

MSD2 TIC, MS File (D:\DATA\09\06\L187149R-PART1\SAMPL000004.D) ES-API, Scan, Frag: 100, "NEG"

80000
60000
40000
20000
0
1.100
0.5   1   1.5   min

ADC1 A, ELSD (D:\DATA\09\06\L187149R-PART1\SAMPL000004.D)

mV
40
30
0.5   1   1.5   min

*MSD1 SPC, time=1.099 of D:\DATA\09\06\L187149R-PART1\SAMPL000004.D ES-API, Scan, Frag: 100, "POS"

RT 1.100
50
0
305.2
306.2
100   200   300   400   500   m/z

*MSD2 SPC, time=1.103 of D:\DATA\09\06\L187149R-PART1\SAMPL000004.D ES-API, Scan, Frag: 100, "NEG"

RT 1.100
50
0
303.2
304.0
341.2
100   200   300   400   500   m/z

Inj.Date 9/6/2019   LB   P2-B-03 -3-   Acq. Method C:\CHEM32\->   ->

HRMS