Supporting information

1,4,9-Triazaspiro[5.5]undecan-2-one derivatives as potent and selective METTL3 inhibitors

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Figure S1: Thermal shift first derivative curves for UZH2 and SAH with METTL3/METTL14 2

Figure S2: Thermal shift first derivative curves for UZH2 and SAH with METTL16 2

Figure S3: Thermal shift first derivative curves for UZH2 and SAH with METTL1 3

Figure S4: Cell viability curves of MOLM13 and PC-3 cells upon UZH2 incubation for 3 days. ... 4

Figure S5: Western blotting of METTL3 in MOLM-13 cells after UZH2 treatment for 16 h 4

X-ray data collection and refinement statistics 5

NMR traces of final compounds 7

HPLC traces of final compounds 28

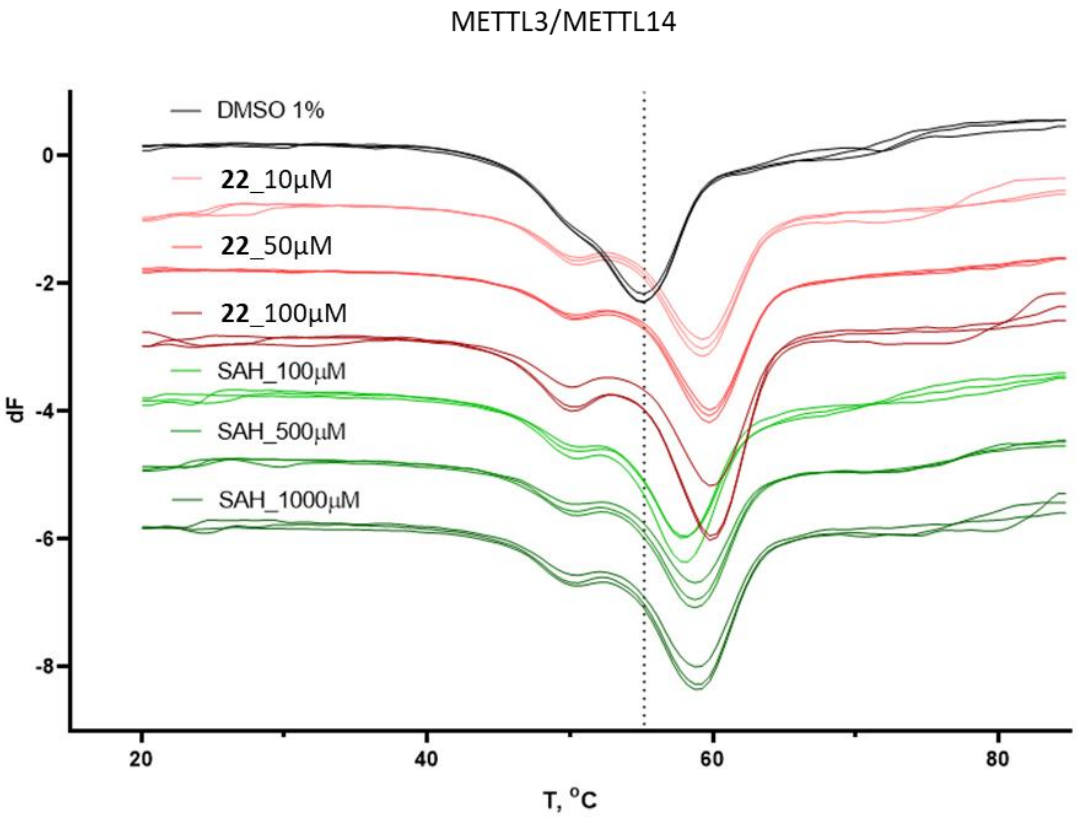


Figure S1: Thermal shift assay results. Shown are the first derivative of the melting curves of METTL3/METTL14 for inhibitor **UZH2** or **SAH**.

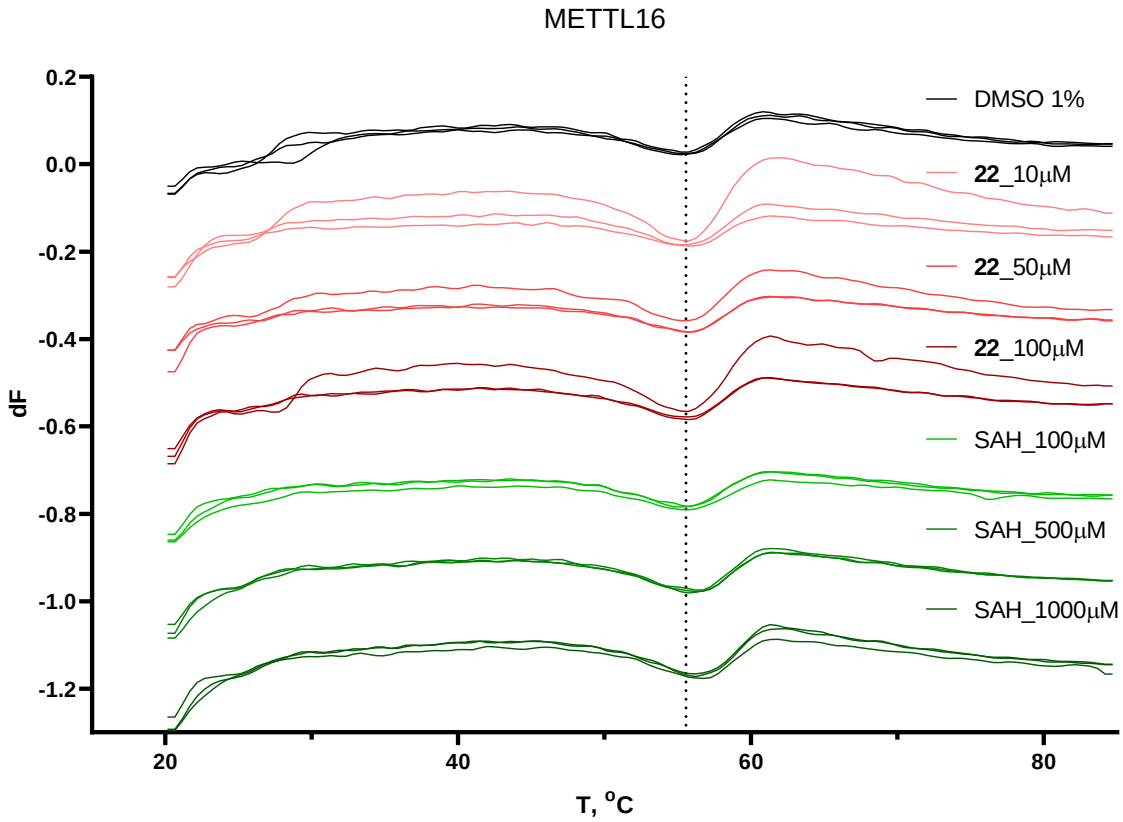


Figure S2: Thermal shift assay results. Shown are the first derivative of the melting curves of METTL16 for inhibitor **UZH2** or **SAH**. **UZH2** does not shift the melting temperature of METTL16.

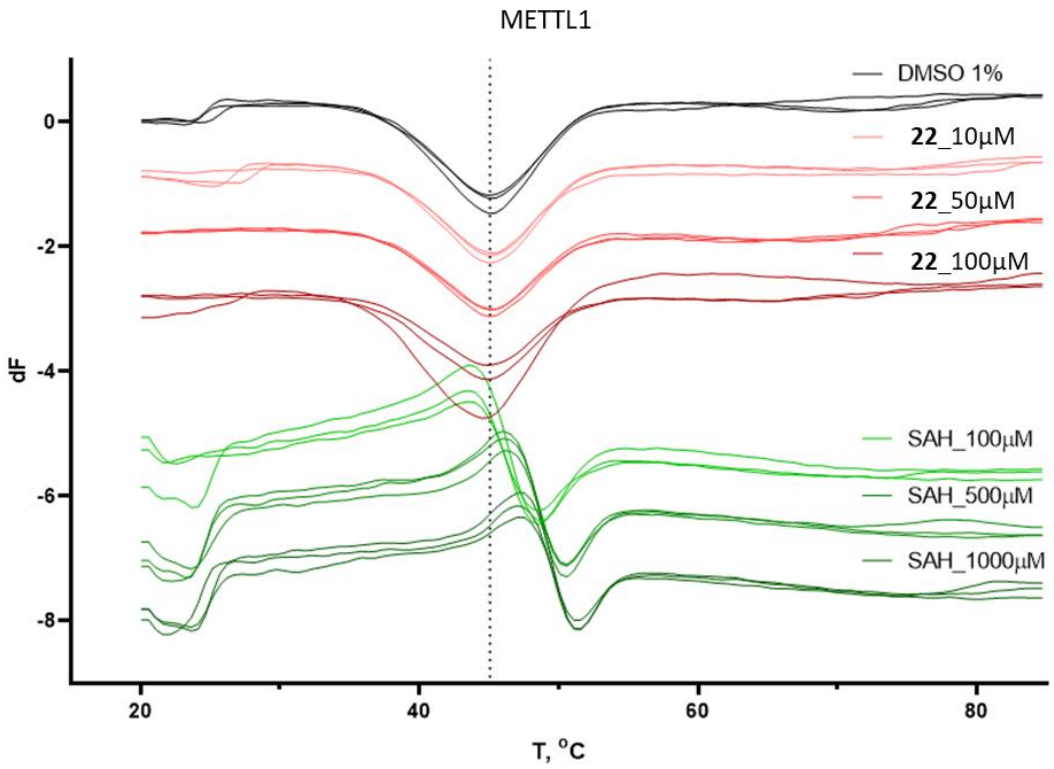


Figure S3: Thermal shift assay results. Shown are the first derivative of the melting curves of METTL1 for inhibitor **UZH2** or **SAH**. **UZH2** does not shift the melting temperature of METTL1.

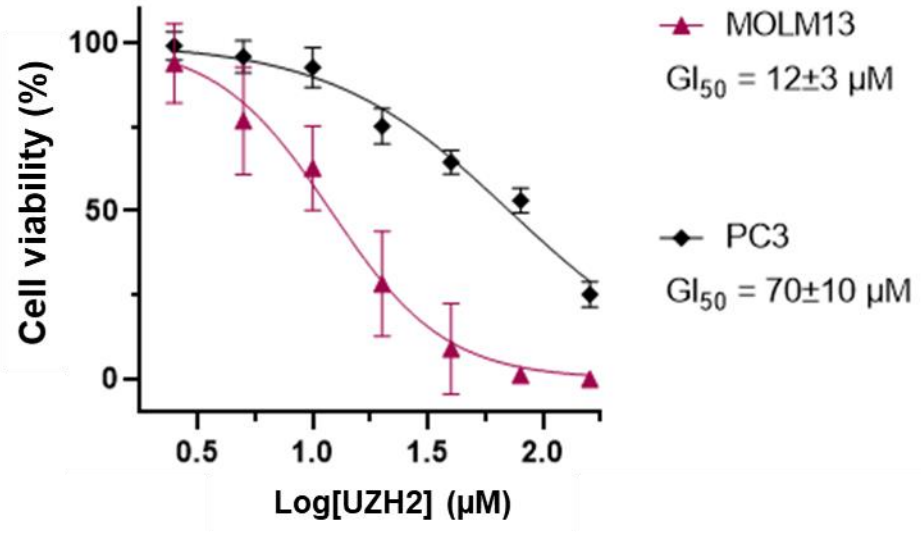


Figure S4: Cell viability curves of MOLM13 and PC-3 cells upon **UZH2** incubation for 3 days.

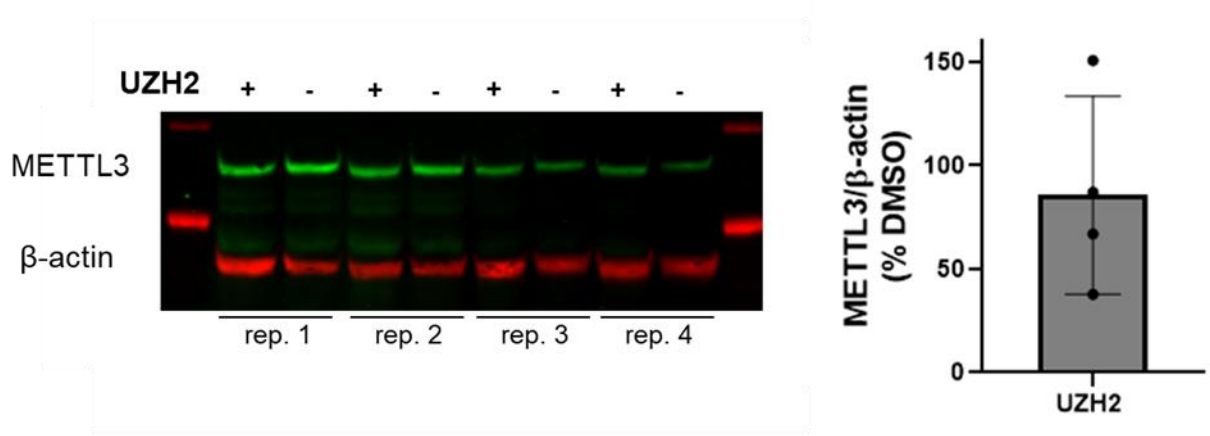


Figure S5: Western blotting of METTL3 in MOLM-13 cells after **UZH2** treatment (10 µM) for 16 h. METTL3/β-actin (90 ± 40)% of DMSO control.

X-ray data collection and refinement statistics

Table S1: PDB codes, X-ray data collection and refinement statistics for structures of ternary complexes of METTL3, METTL14 and selected compounds developed in this study.

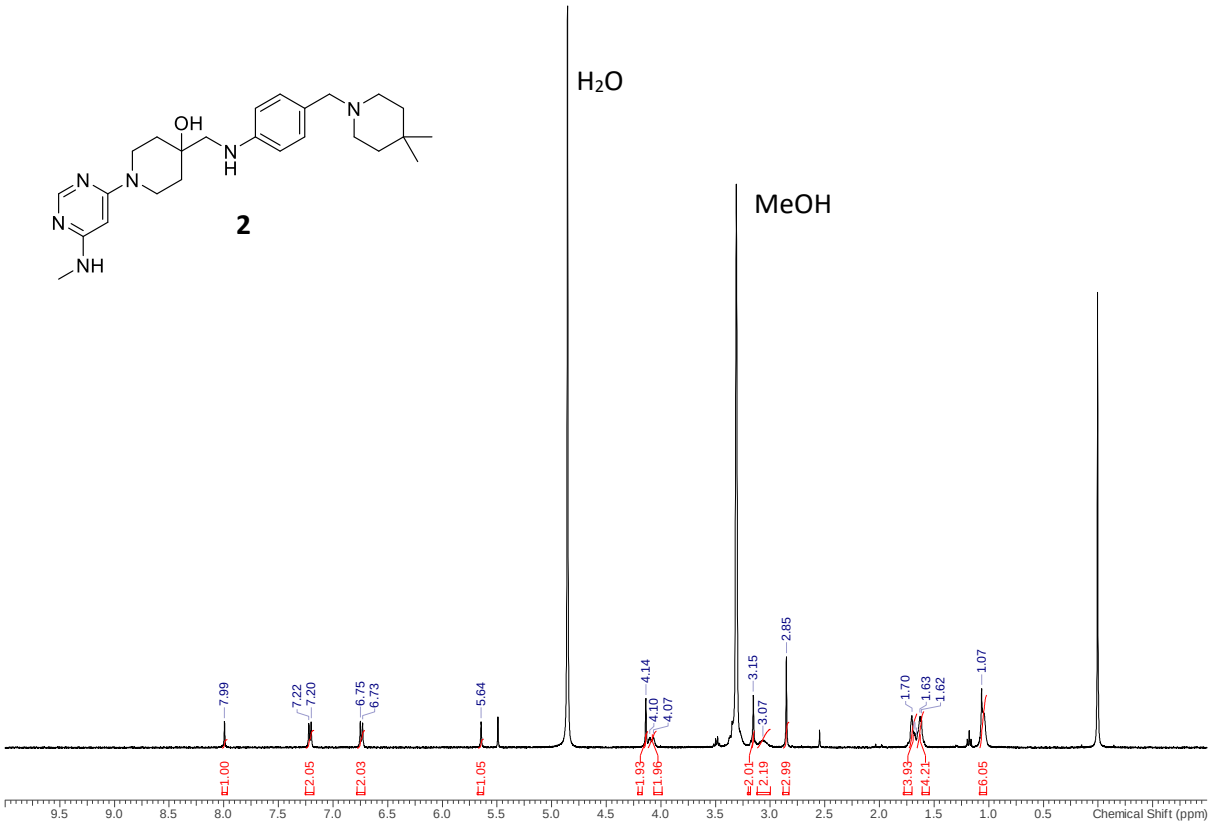
PDB ID:	7NHI	7O08	7O09
Compound	**1**	**5**	**7**
Data Collection			
Space group	$P3_221$	$P3_221$	$P3_221$
Cell dimension a, b, c (Å)	63.89, 63.89, 225.77	63.8, 63.81, 225.99	63.89, 63.89, 225.7
Cell dimension α, β, γ (°)	90, 90, 120	90, 90, 120	90, 90, 120
Resolution (Å)	44.58 (1.85)	49.64 (2)	45.2 (1.8)
Unique reflections*	46100 (7322)	31729 (5871)	50869 (8076)
Completeness*	98.2 (98.9)	100 (99.8)	99.9 (99.7)
Redundancy*	6.14 (5.26)	13.06 (13.65)	9.77 (9.53)
R_{merge}*	8.3 (141.4)	12.6 (128.6)	8.4 (158.3)
CC (1/2)	99.9 (45.8)	99.9 (70.5)	100 (55.1)
I/σI	15.17 (1.11)	17.69 (2.1)	19.93 (1.43)
Refinement			
R_{work}/R_{free}	19.81/22.18	18.9/22.6	19.28/22.51
RMSD bond (Å)	0.008	0.008	0.008
RMSD angle (°)	0.989	0.898	1.027
B-factor (Å^2)**	34.92/42.86/41.82	34.67/41.14/41.35	33.66/42.2/41.79
Ramanchandran Favored	97.64	97.23	97.16
Ramanchandran allowed	2.12	2.08	2.6
Ramanchandran Disallowed	0.24	0.69	0.24
PDB ID:	7O0L	7O29	7O2E
Compound	**8**	**20**	**21**
Data Collection			
Space group	$P3_221$	$P3_221$	$P3_221$
Cell dimension a, b, c (Å)	64.13, 64.13, 225.85	64.15, 64.15, 225.65	63.8, 63.8, 224.91
Cell dimension α, β, γ (°)	90, 90, 120	90, 90, 120	90, 90, 120
Resolution (Å)	45.18 (1.9)	45.13 (2.75)	44.92 (2.5)
Unique reflections*	43655 (6908)	14906 (2374)	19442 (3082)
Completeness*	99.7 (99.2)	99.9 (100)	99.9 (99.8)
Redundancy*	9.84 (10.04)	9.53 (9.28)	8.14 (8.55)
R_{merge}*	9.7 (195.1)	11.4 (107.5)	10.7 (160.8)
CC (1/2)	100 (18.4)	99.9 (71.4)	99.9 (49.6)
I/σI	19.28 (1.29)	19.12 (2.12)	17.13 (1.41)
Refinement			
R_{work}/R_{free}	19.6/22.63	20.23/25.54	20.57/27.3
RMSD bond (Å)	0.009	0.009	0.009
RMSD angle (°)	1.012	1.073	1.067
B-factor (Å^2)**	38.22/44.34/42.67	56.99/59.35/49.38	62.3/63.56/57.07
Ramanchandran Favored	96.52	93.78	95.31
Ramanchandran allowed	3.02	5.3	4.46
Ramanchandran Disallowed	0.46	0.92	0.23

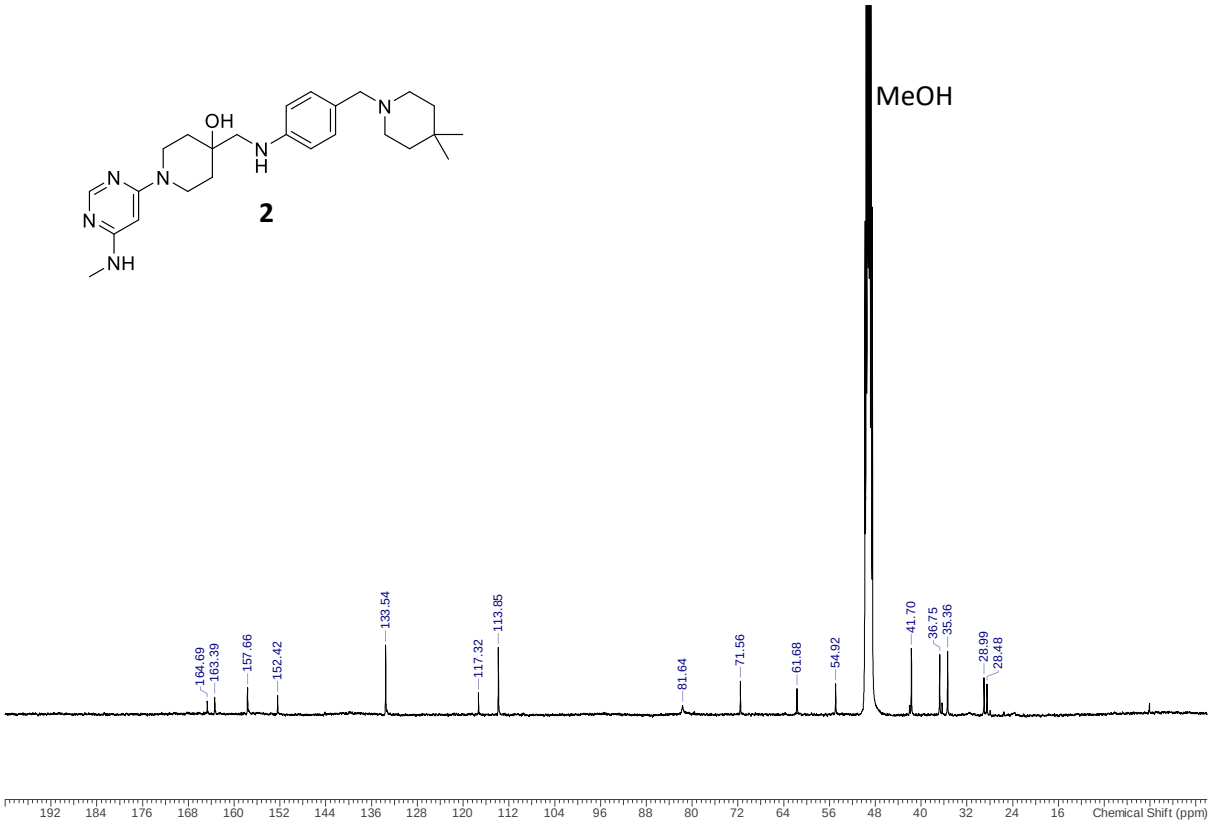
*Statistics for the highest resolution shell shown in parentheses. ** P/L/W indicate protein, ligand/ion and water molecules, respectively.

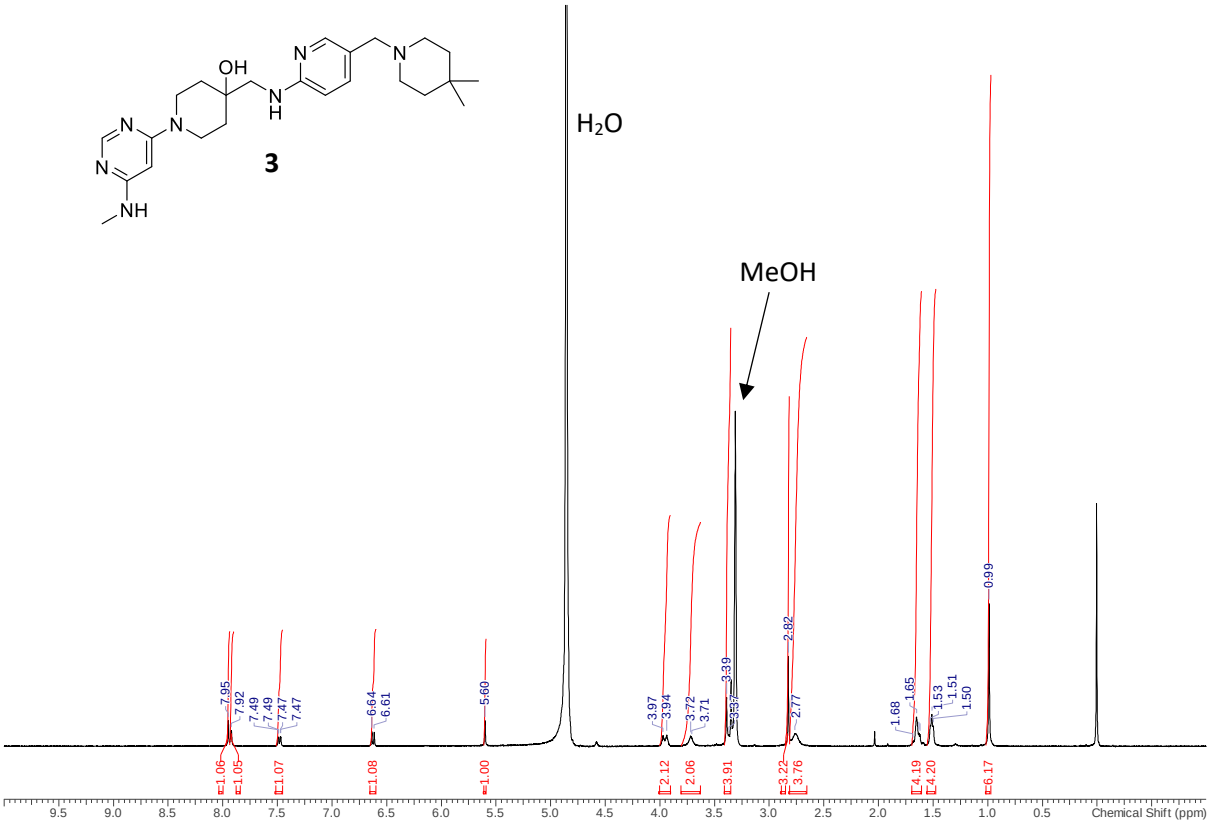
PDB ID:	7O2F
Compound	**22** (**UZH2**)
Data Collection	
Space group	$P3_221$
Cell dimension a, b, c (Å)	63.87, 63.87, 224.51
Cell dimension α, β, γ (°)	90, 90, 120
Resolution (Å)	44.74 (2.1)
Unique reflections*	32606 (5099)
Completeness*	99.3 (98.1)
Redundancy*	6.56 (4.96)
R_{merge}*	9.5 (87.8)
CC (1/2)	99.8 (61.4)
I/σI	12.77 (1.48)
Refinement	
R_{work}/R_{free}	19.71/24.21
RMSD bond (Å)	0.008
RMSD angle (°)	0.963
B-factor (Å^2)**	40.17/41.12/42.7
Ramanchandran Favored	96.32
Ramanchandran allowed	3.22
Ramanchandran Disallowed	0.46

*Statistics for the highest resolution shell shown in parentheses. ** P/L/W indicate protein, ligand/ion and water molecules, respectively.

NMR traces of final compounds



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H
N
N
N
NH
3
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7.47
6.64
6.61
5.60
3.97
3.94
3.72
3.71
3.39
2.82
2.77
1.68
1.65
1.53
1.51
1.50
0.99
1.06
1.05
1.07
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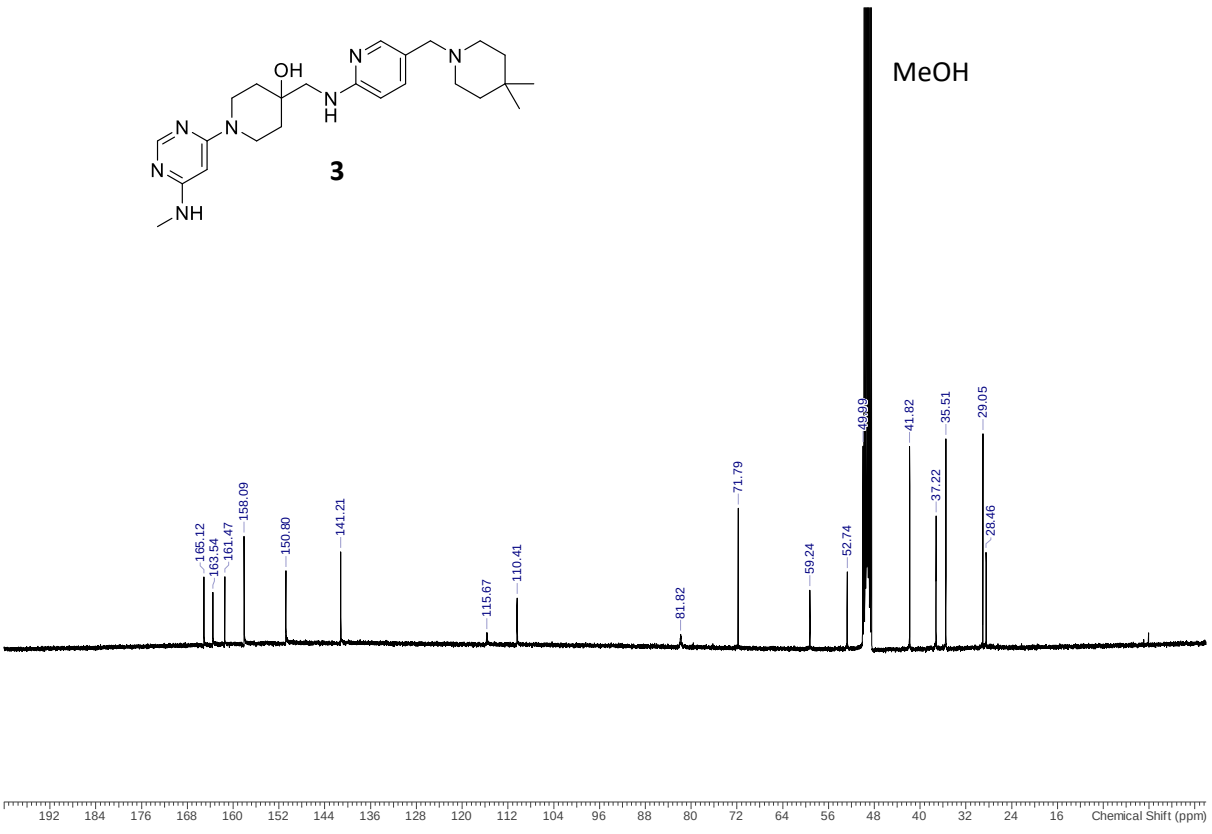
6.17
Chemical Shift (ppm)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H
N
N
N
NH
3
MeOH
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163.54
161.47
158.09
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141.21
115.67
110.41
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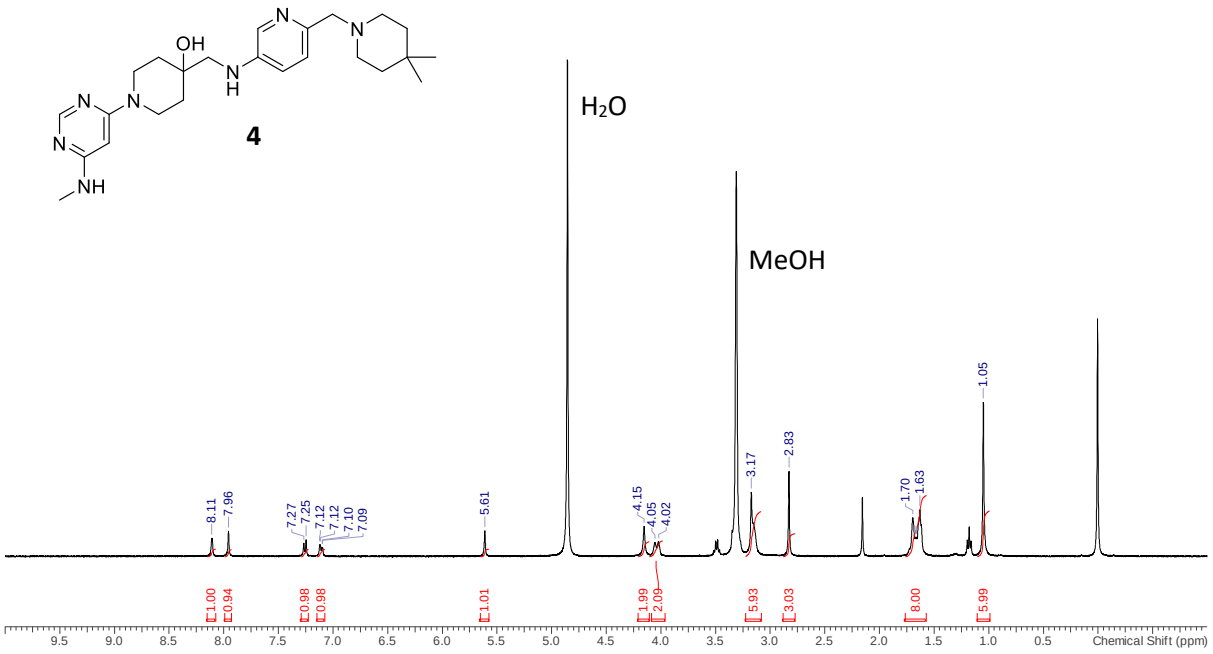
28.46
Chemical Shift (ppm)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NH
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MeOH
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7.25
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7.10
7.09
5.61
4.15
4.05
4.02
3.17
2.83
1.70
1.63
1.05
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1.99
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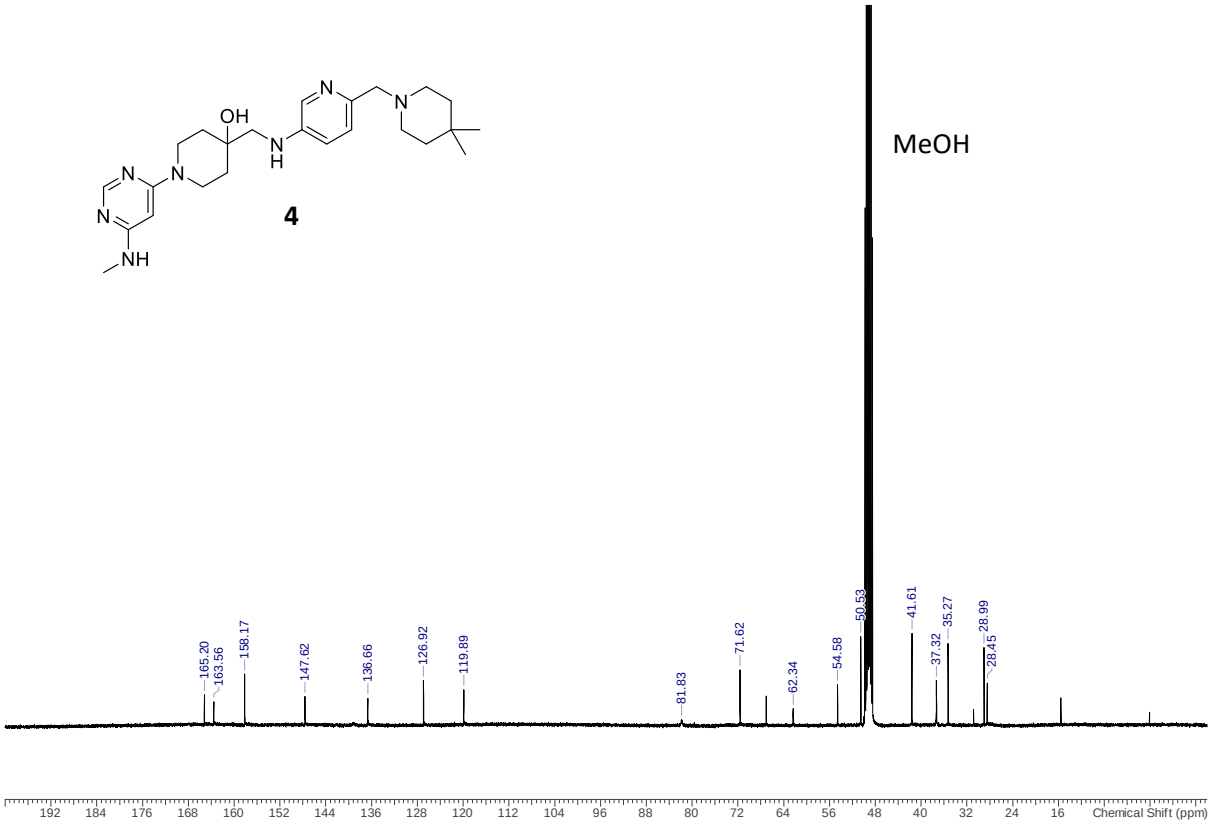
3.03
8.00
5.99
Chemical Shift (ppm)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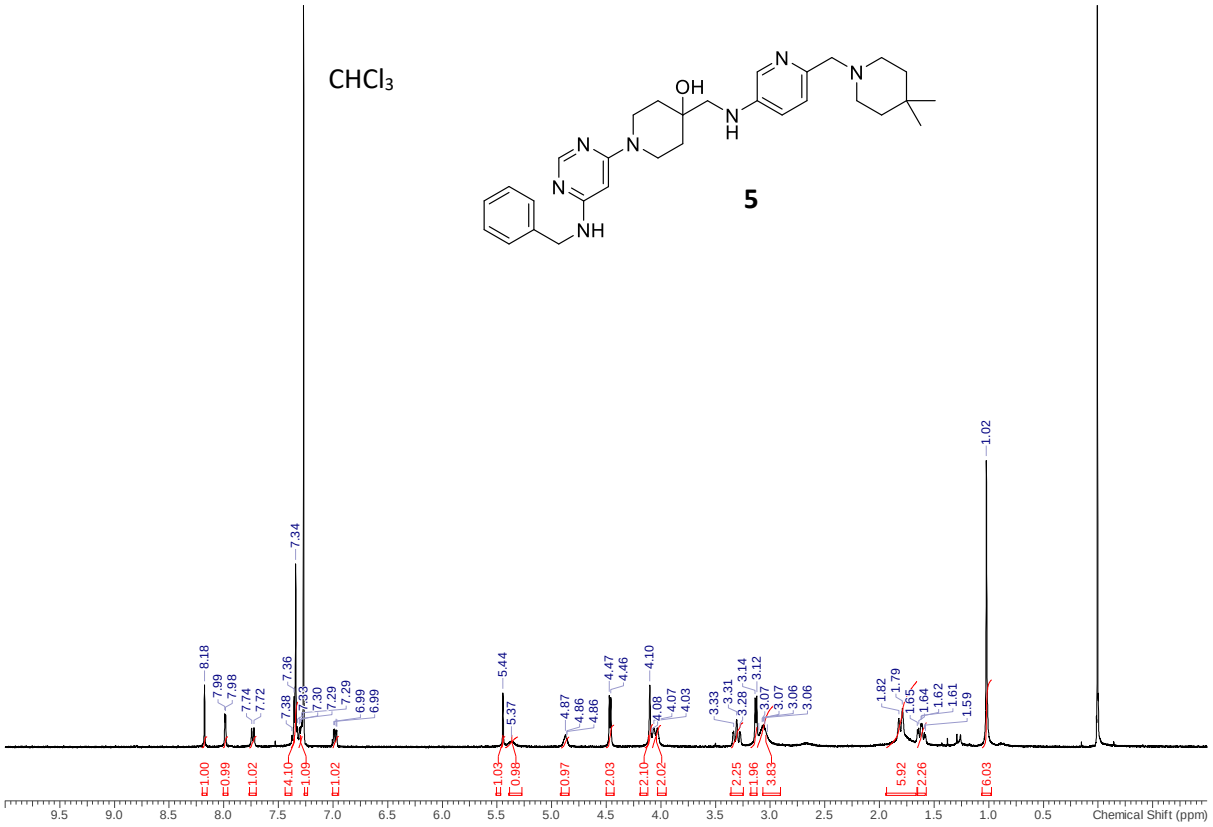
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H
N
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N
N
N
NH
5
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7.98
7.74
7.72
7.38
7.36
7.34
7.30
7.29
7.29
6.99
6.99
5.44
5.37
4.87
4.86
4.86
4.47
4.46
4.10
4.08
4.07
4.03
3.33
3.31
3.28
3.14
3.12
3.07
3.07
3.06
3.06
1.82
1.79
1.65
1.64
1.62
1.61
1.59
1.02
1.00
0.99
1.02
4.10
1.09
1.02
1.03
0.98
0.97
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2.10
2.02
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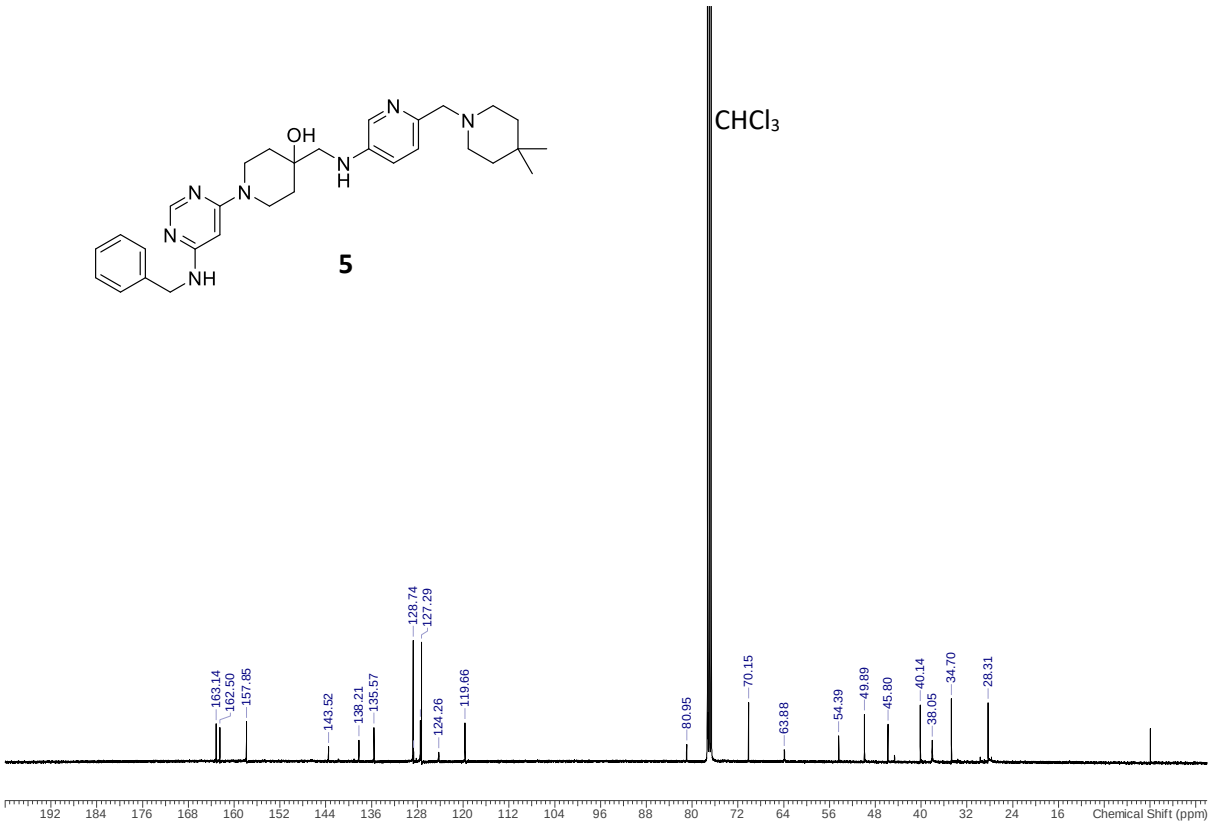
5.92
2.26
6.03
Chemical Shift (ppm)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H
N
N
N
N
N
NH
5
CHCl3
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162.50
157.85
143.52
138.21
135.57
128.74
127.29
124.26
119.66
80.95
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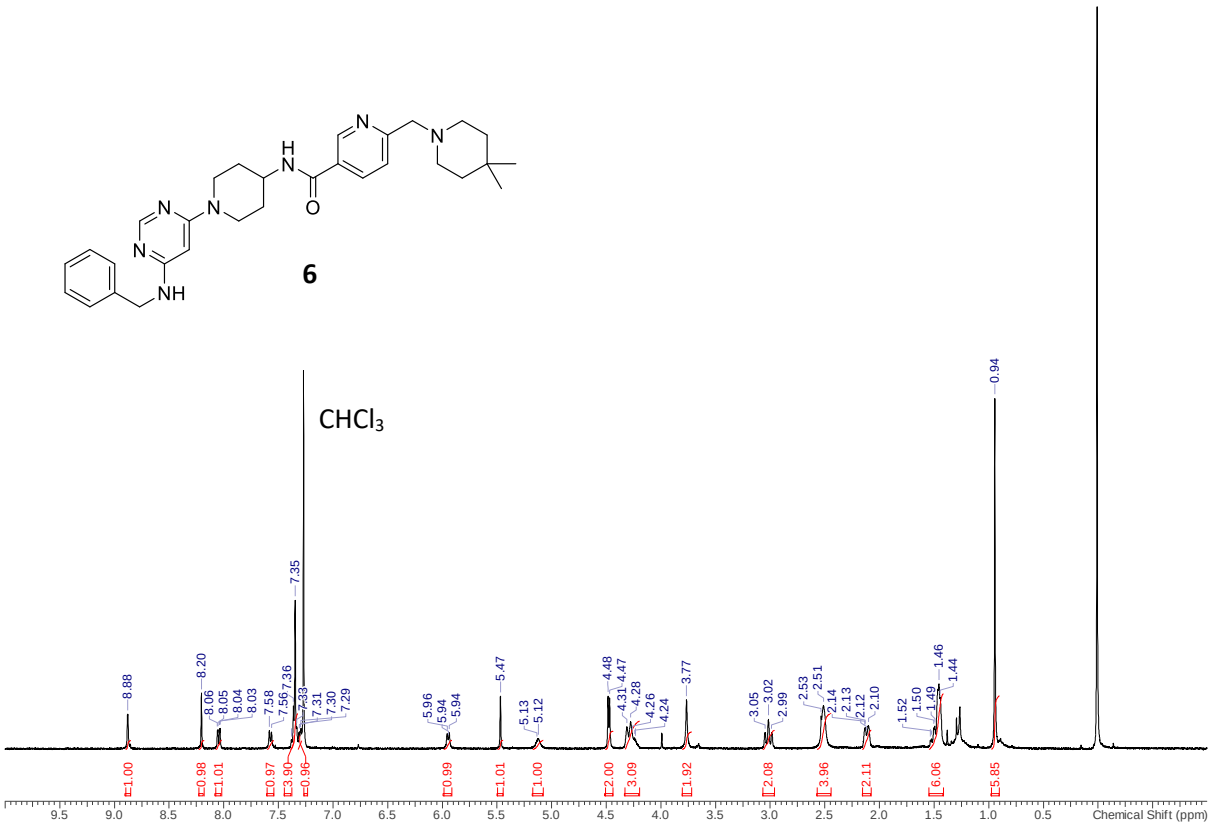
49.89
45.80
40.14
38.05
34.70
28.31
Chemical Shift (ppm)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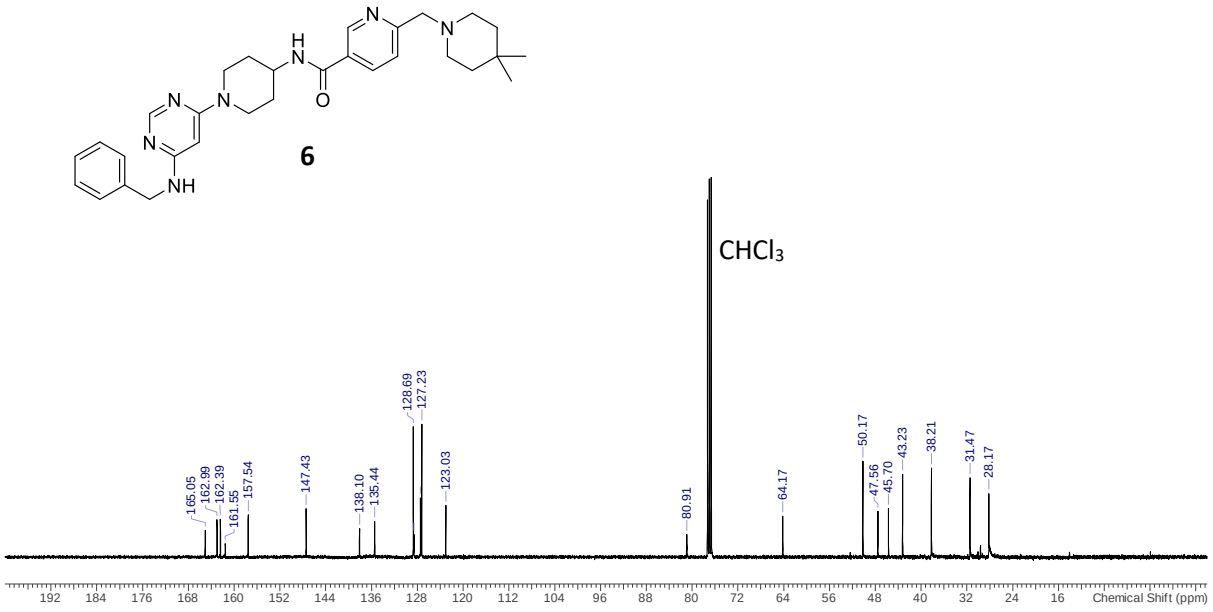
Chemical Shift (ppm)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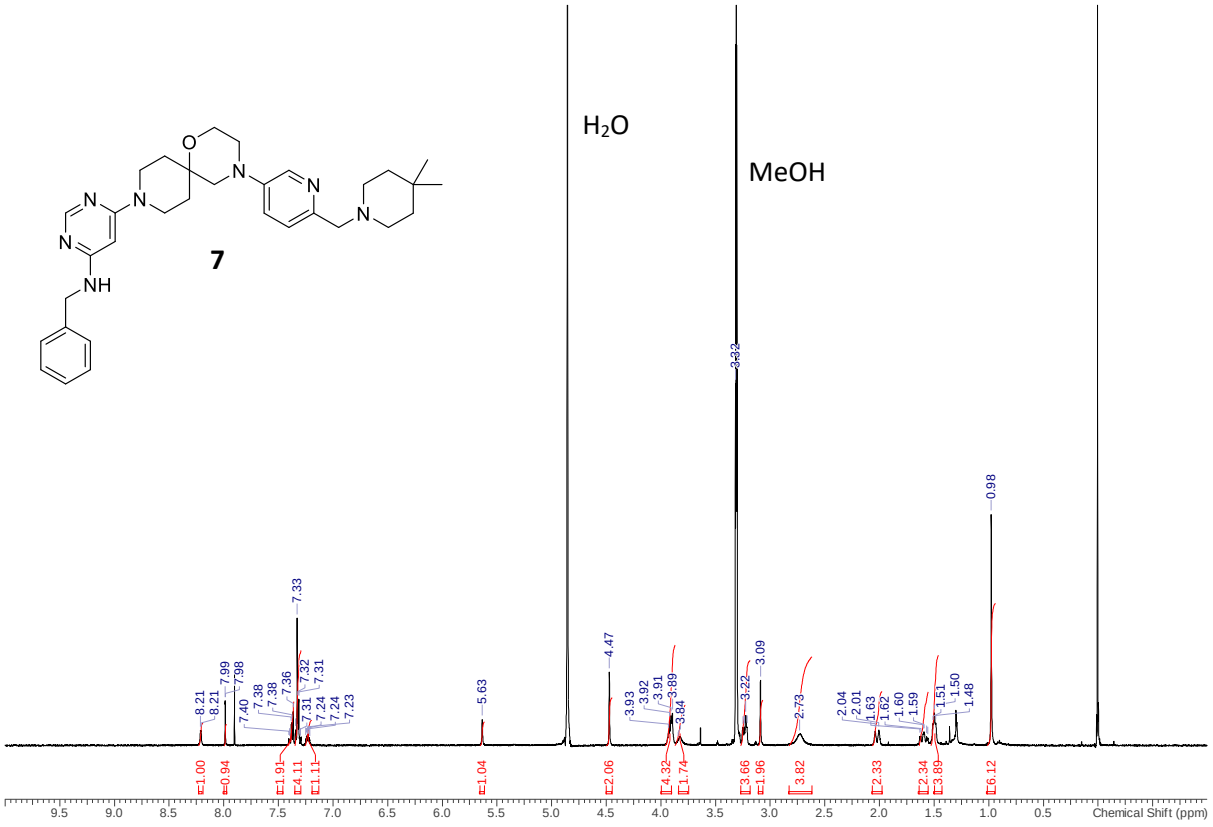
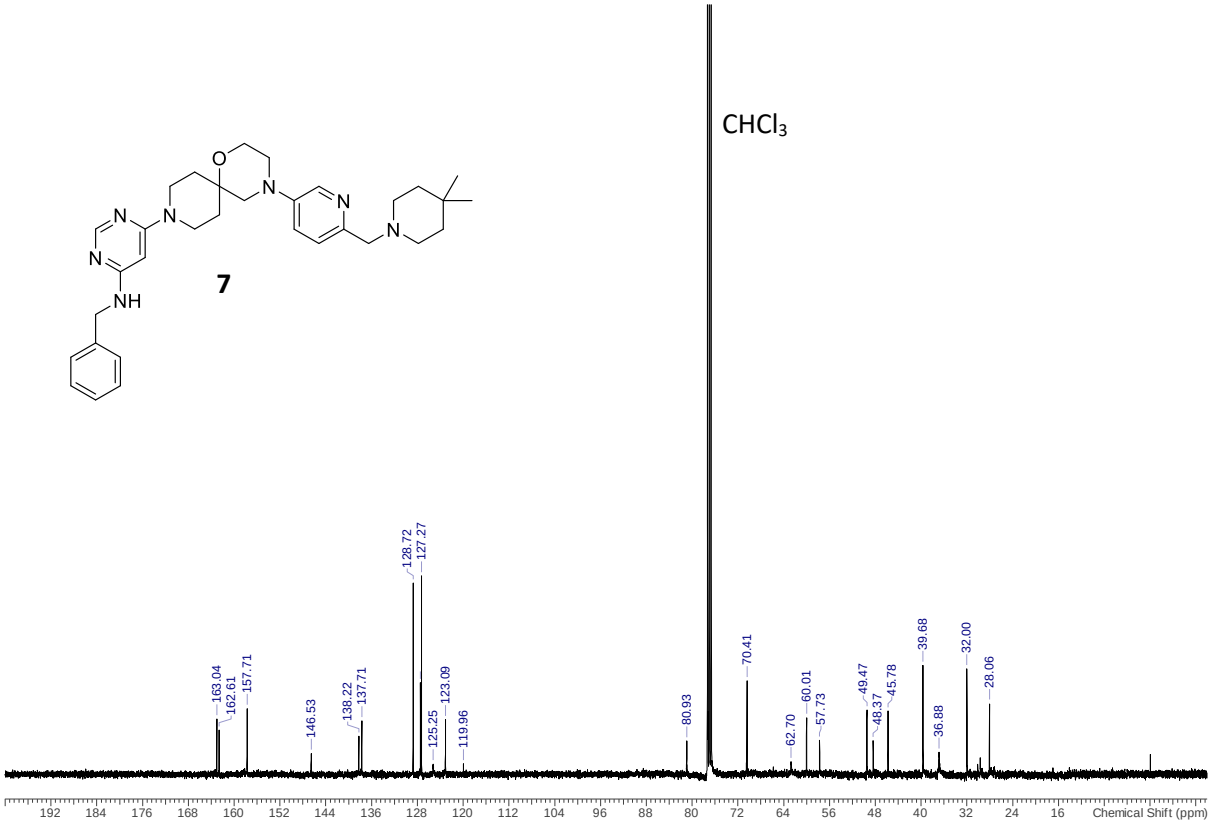

7
H2O
MeOH
Chemical Shift (ppm)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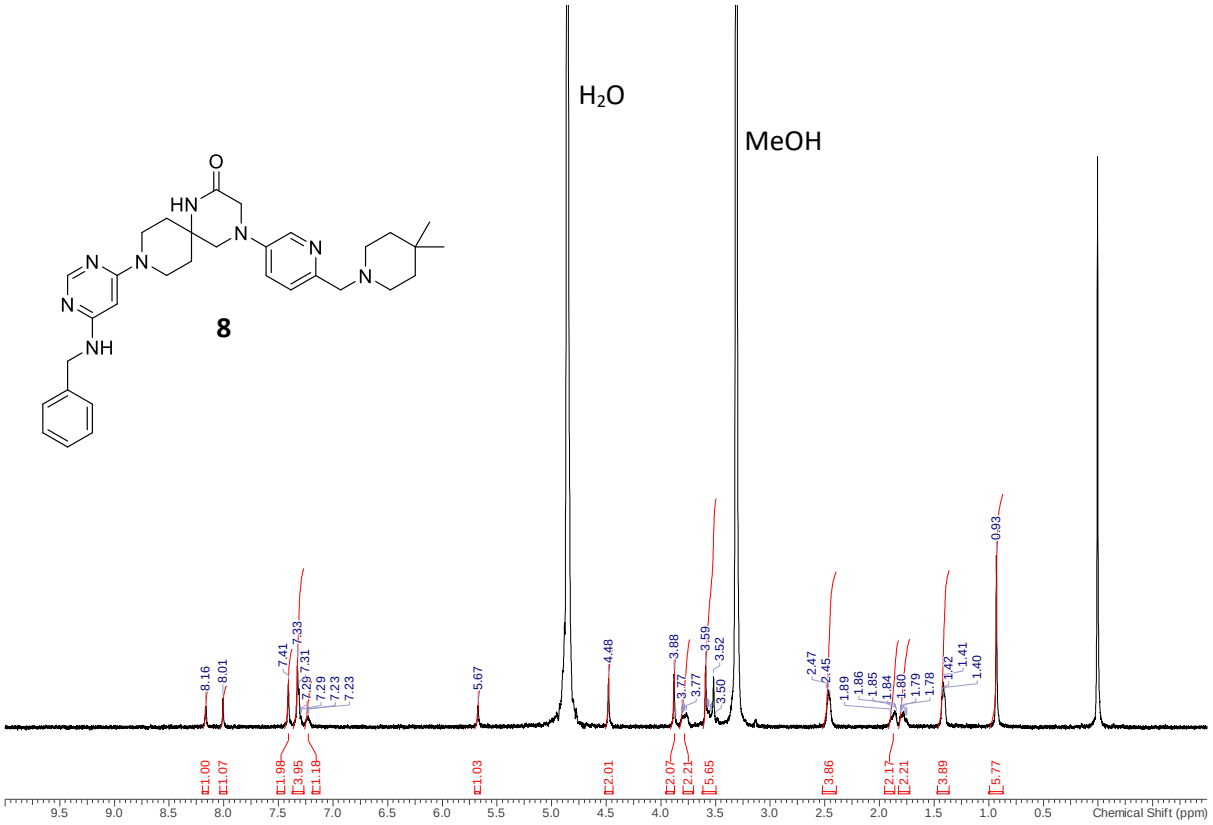
CHCl3
Chemical Shift (ppm)


H2O
MeOH
8
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8.01
7.41
7.33
7.31
7.29
7.23
7.23
5.67
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3.77
3.77
3.59
3.52
3.50
2.47
2.45
1.89
1.86
1.85
1.84
1.80
1.79
1.78
1.42
1.41
1.40
0.93
1.00
1.07
1.98
3.95
1.18
1.03
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2.07
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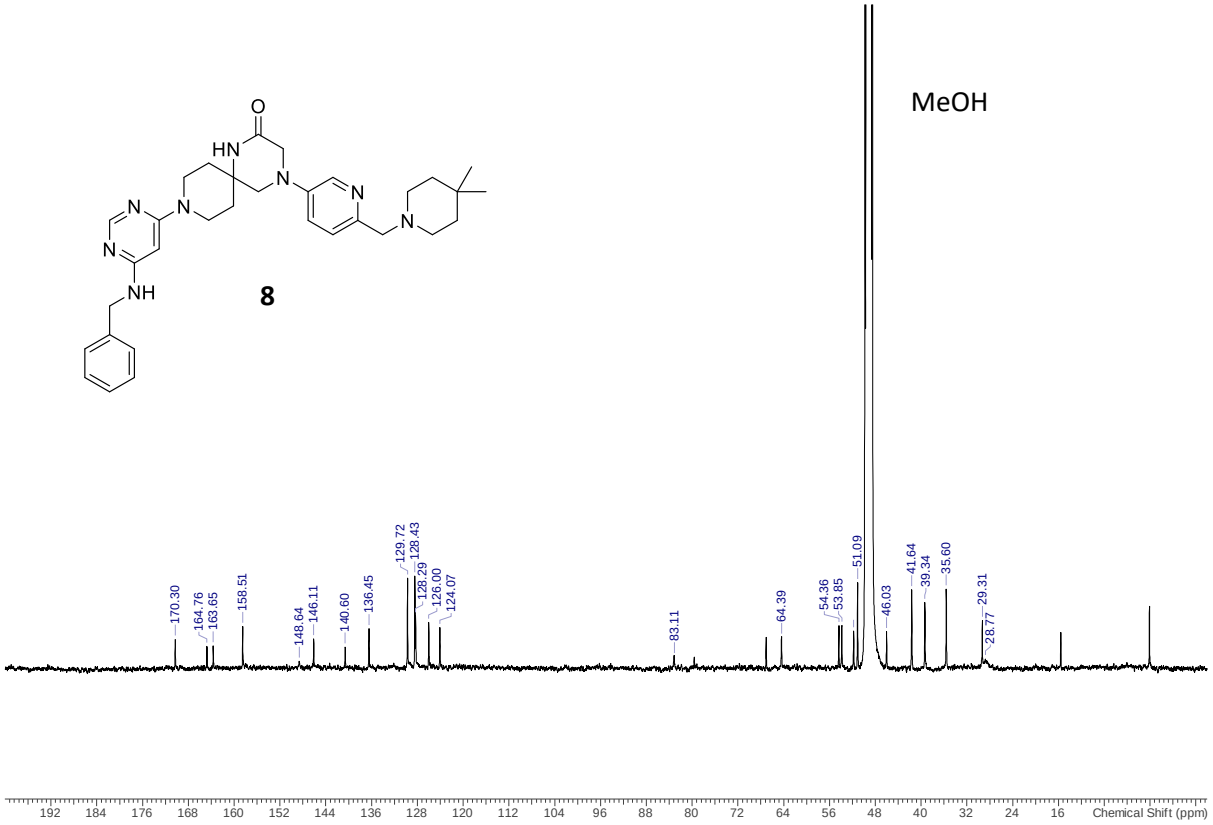
5.77
Chemical Shift (ppm)


MeOH
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158.51
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129.72
128.43
128.29
126.00
124.07
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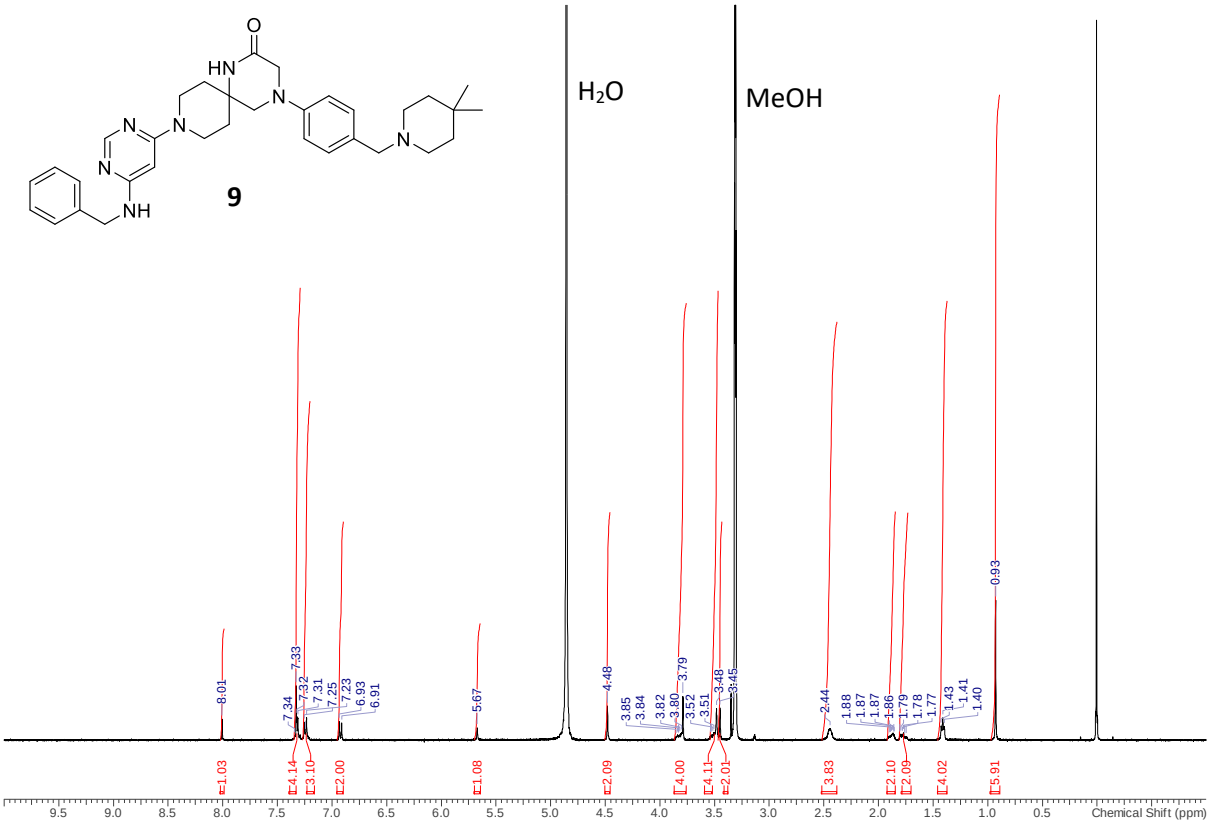
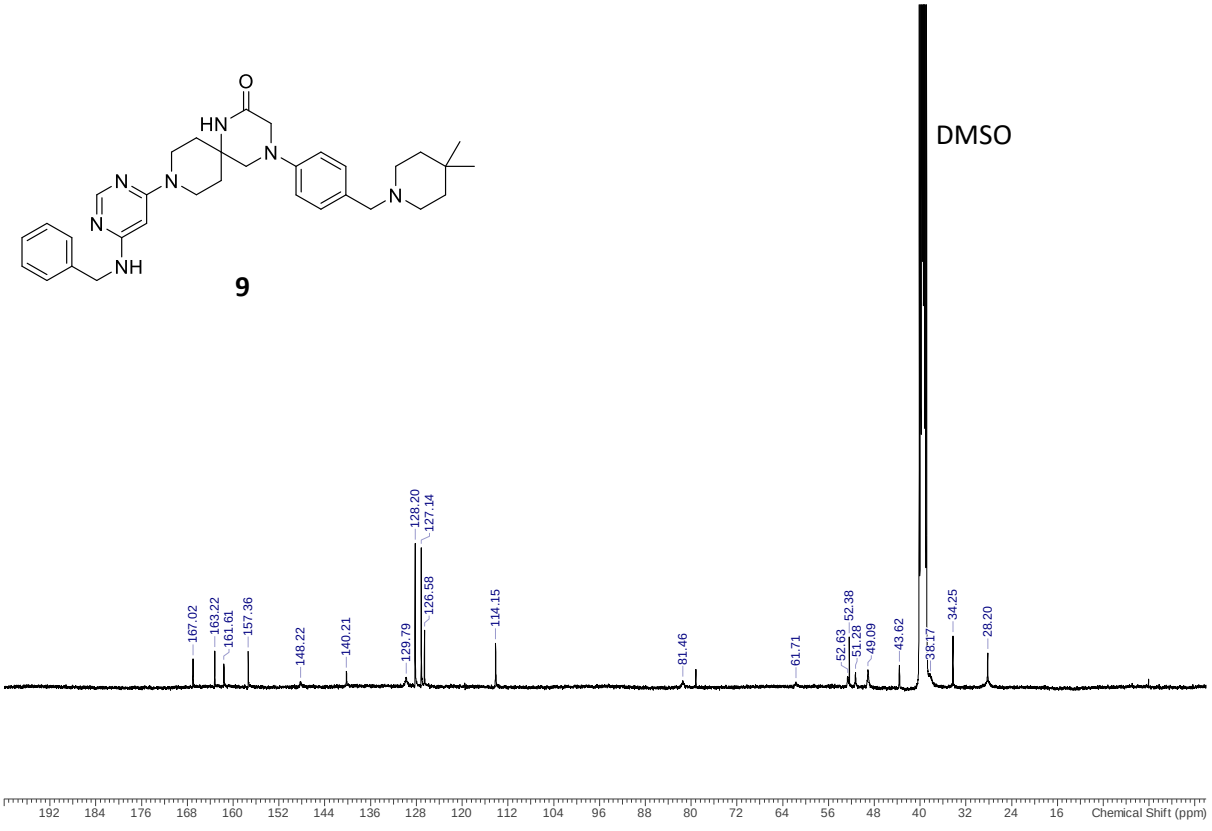
28.77
Chemical Shift (ppm)


H2O
MeOH
9
Chemical Shift (ppm)


DMSO
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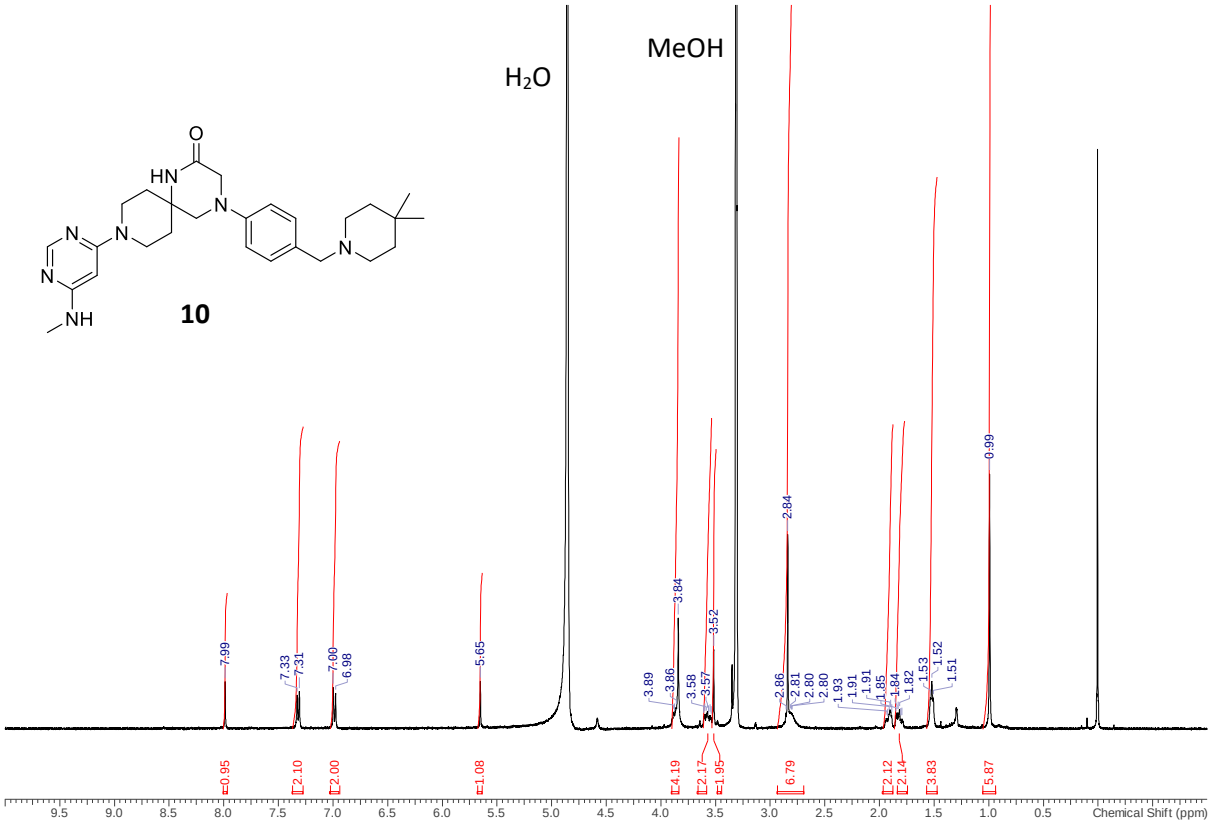
Chemical Shift (ppm)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MeOH
O
HN
N
N
N
N
NH
10
7.99
7.33
7.31
7.00
6.98
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3.86
3.84
3.58
3.57
3.52
2.86
2.84
2.81
2.80
2.80
1.93
1.91
1.91
1.85
1.84
1.82
1.53
1.52
1.51
0.99
0.95
2.10
2.00
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4.19
2.17
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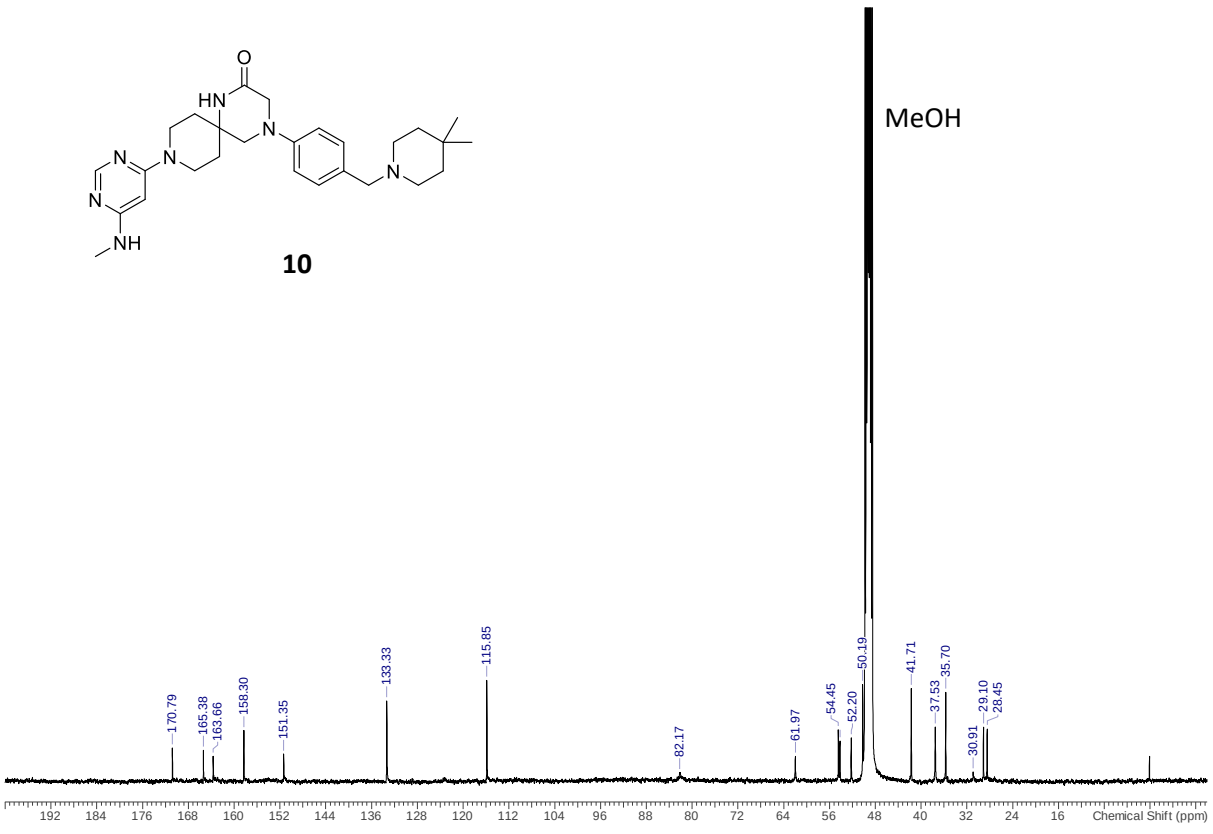
6.79
2.12
2.14
3.83
5.87
Chemical Shift (ppm)


O
HN
N
N
N
N
NH
10
MeOH
170.79
165.38
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158.30
151.35
133.33
115.85
82.17
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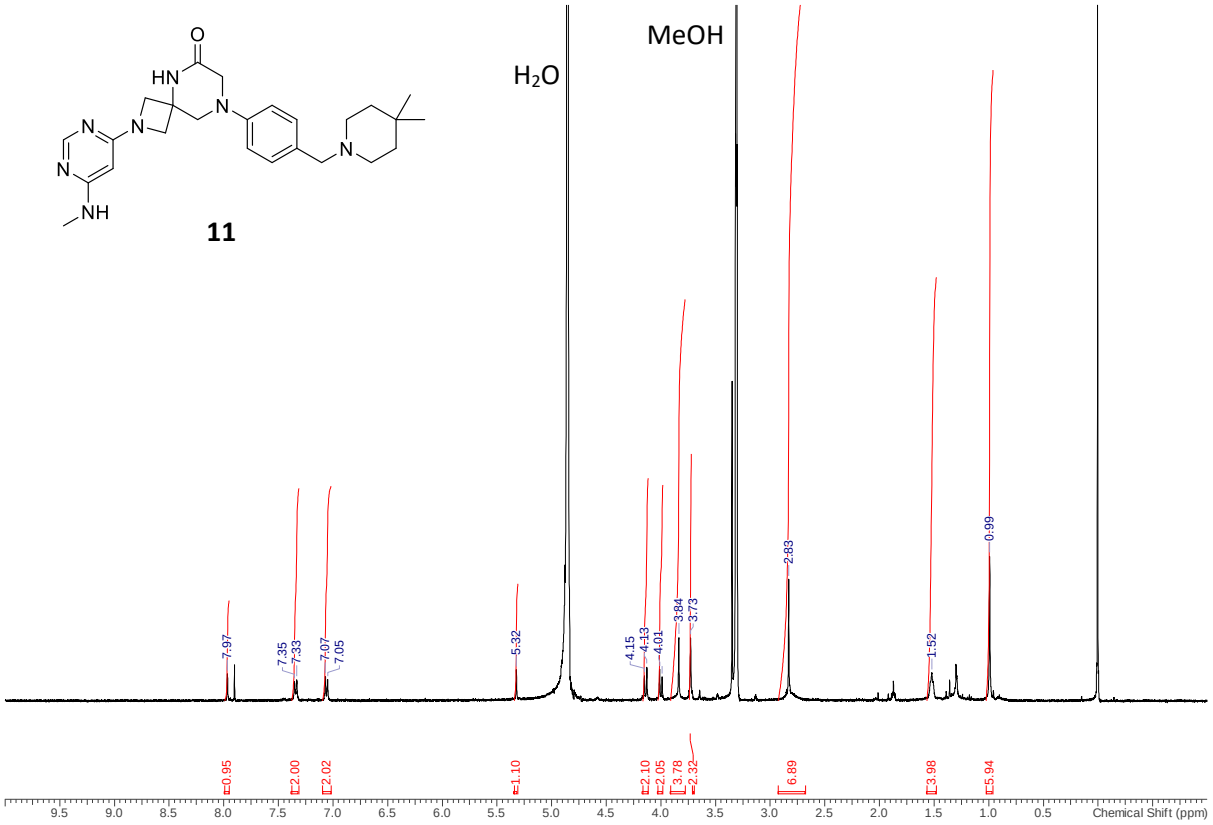
50.19
41.71
37.53
35.70
30.91
29.10
28.45
Chemical Shift (ppm)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HN
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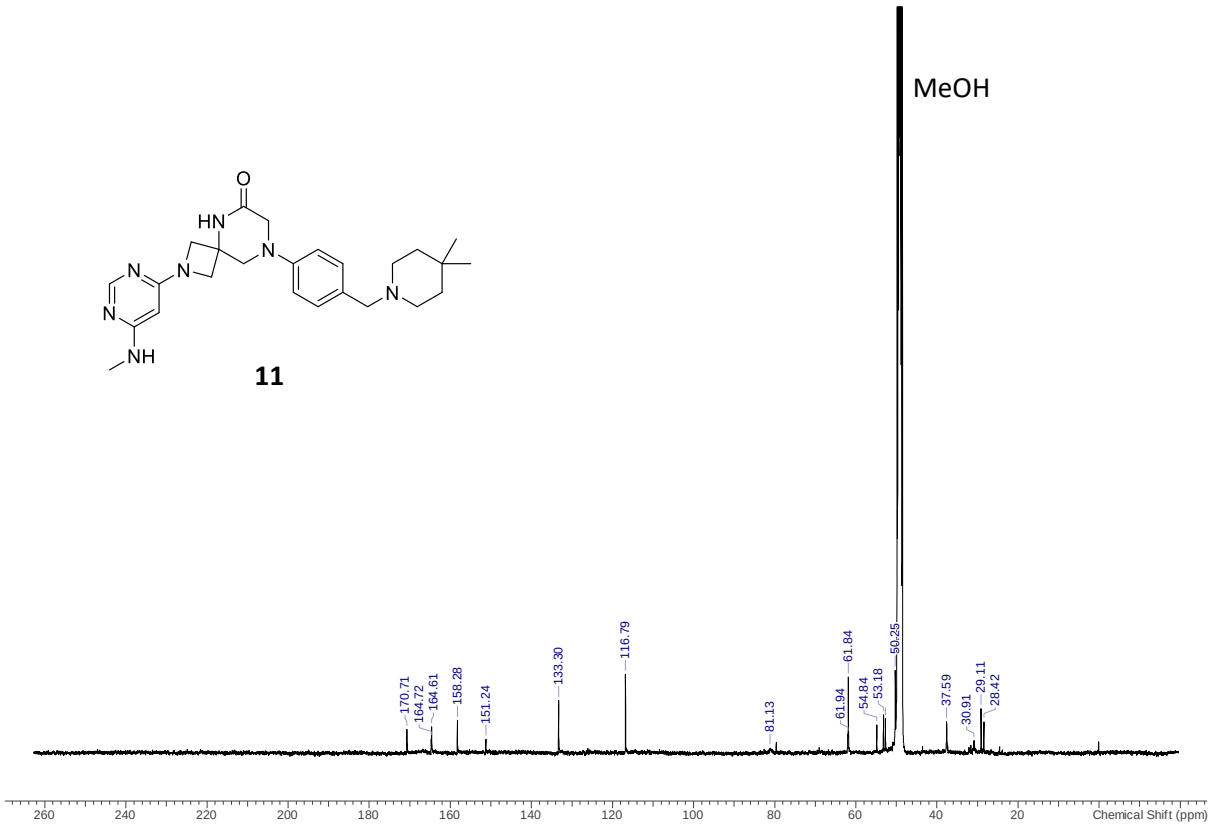
N
N
N
NH
11
H2O
MeOH
7.97
7.35
7.33
7.07
7.05
5.32
4.15
4.13
4.01
3.84
3.73
2.83
1.52
0.99
1.00
2.00
2.02
1.10
2.10
2.05
3.78
2.32
6.89
3.98
5.94
Chemical Shift (ppm)


O
HN
N
N
N
N
NH
11
MeOH
170.71
164.72
164.61
158.28
151.24
133.30
116.79
81.13
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54.84
53.18
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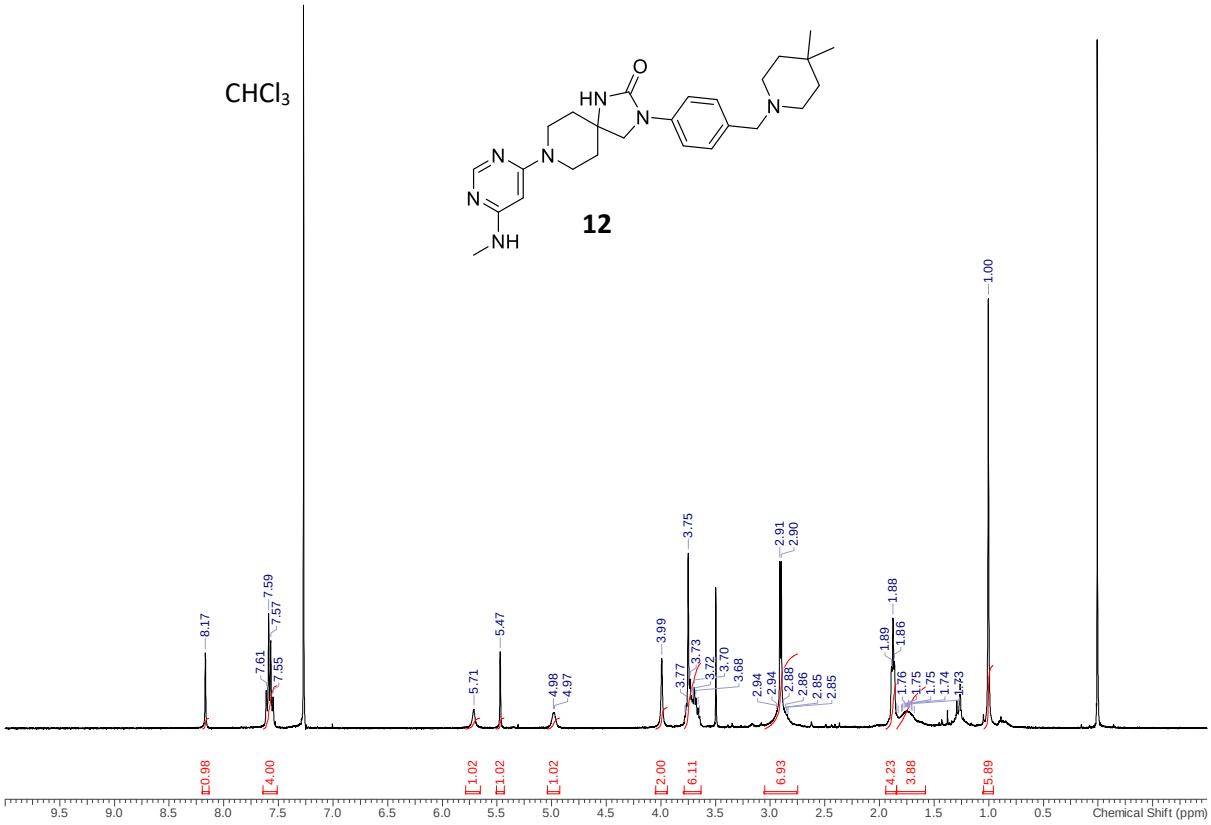
37.59
30.91
29.11
28.42
Chemical Shift (ppm)


CHCl3
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8.17
7.61
7.59
7.57
7.55
5.71
5.47
4.98
4.97
3.99
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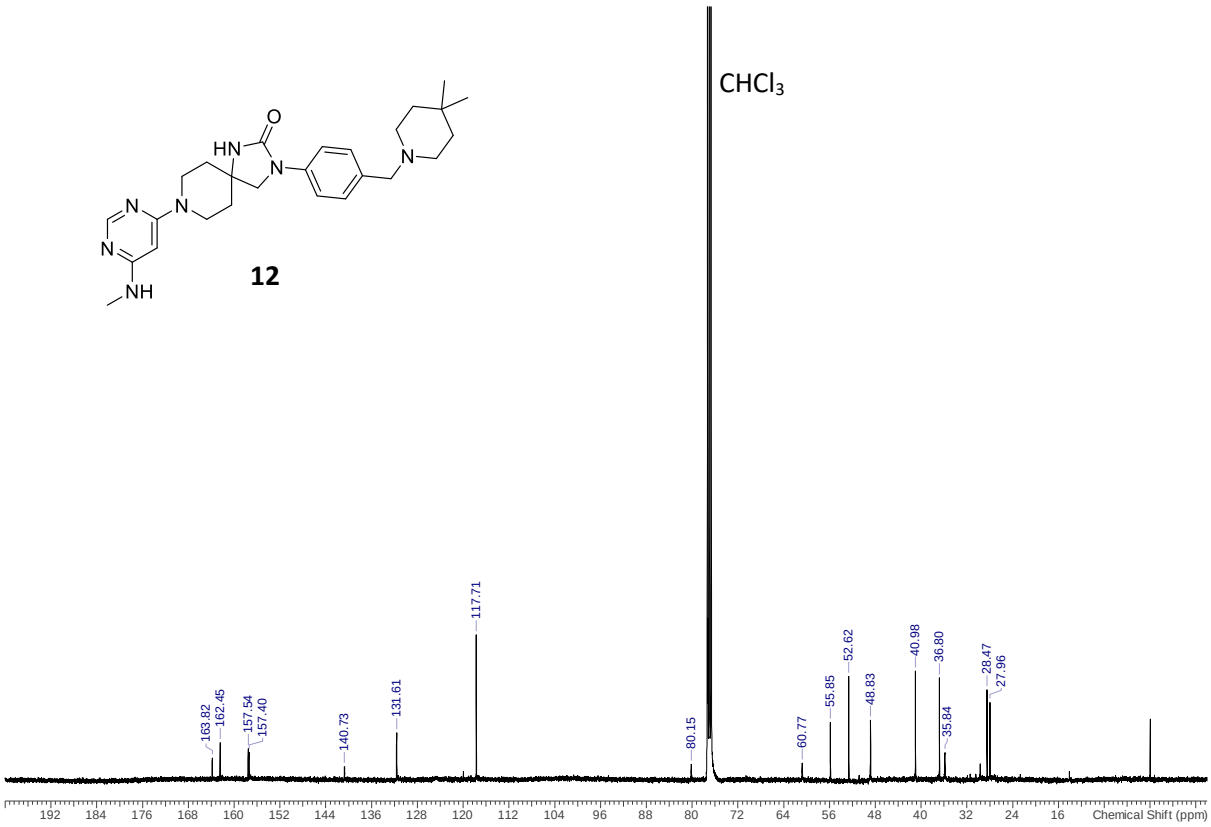
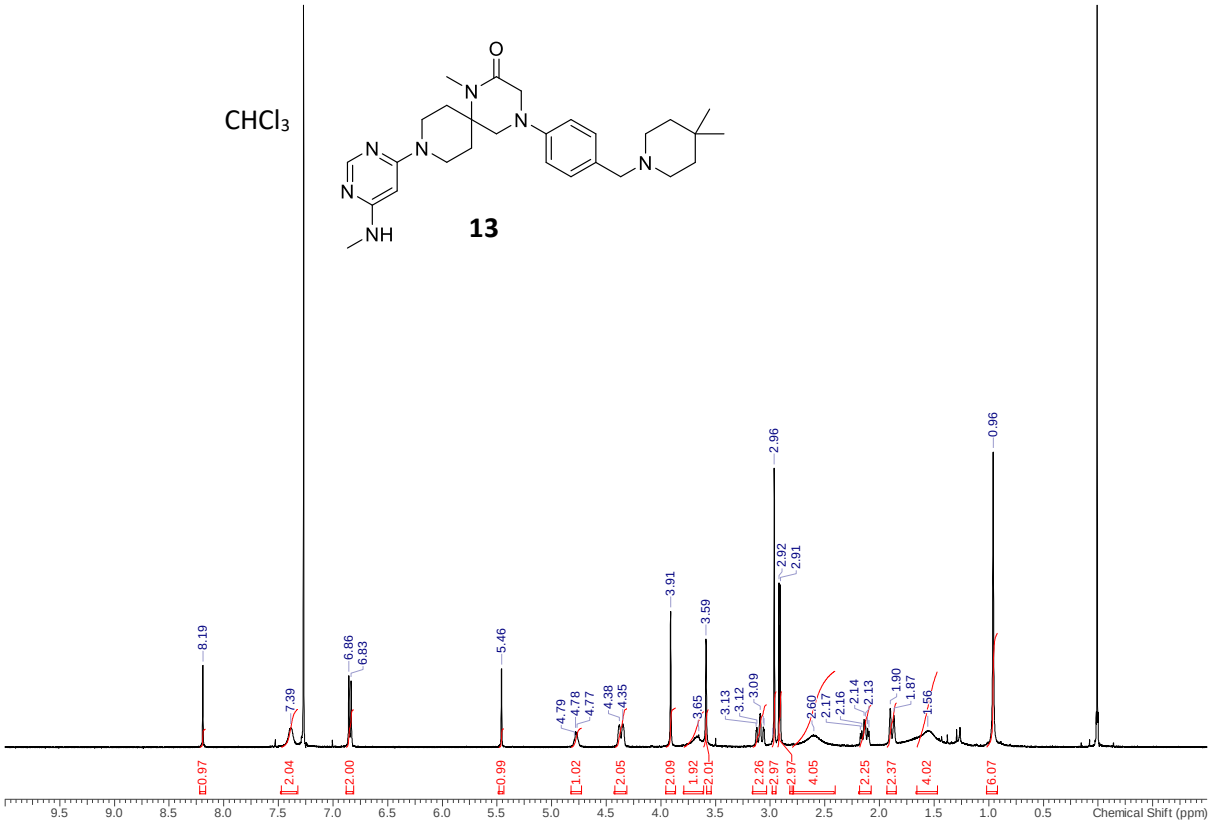
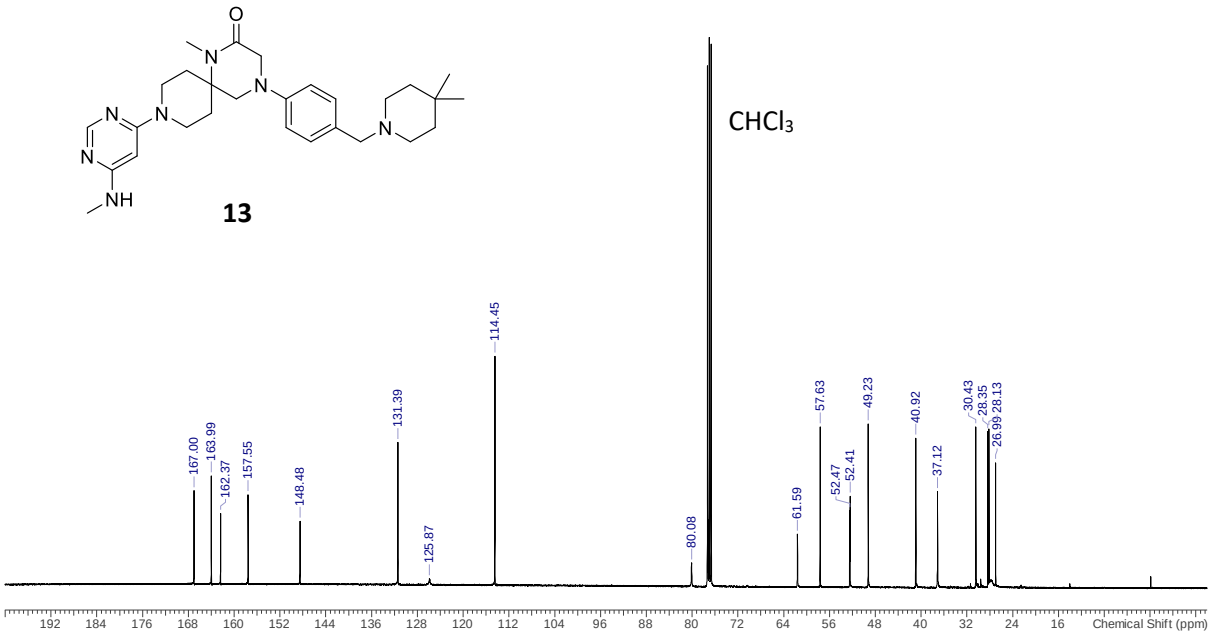
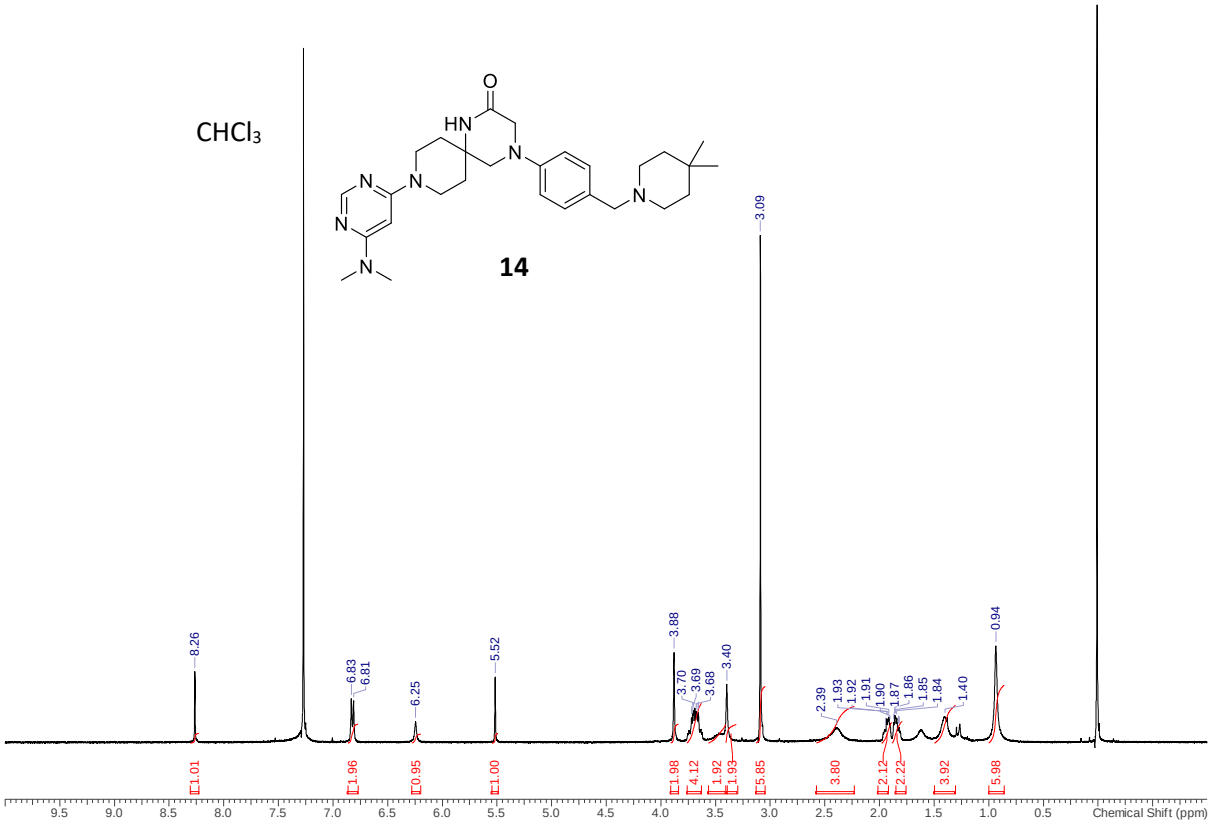
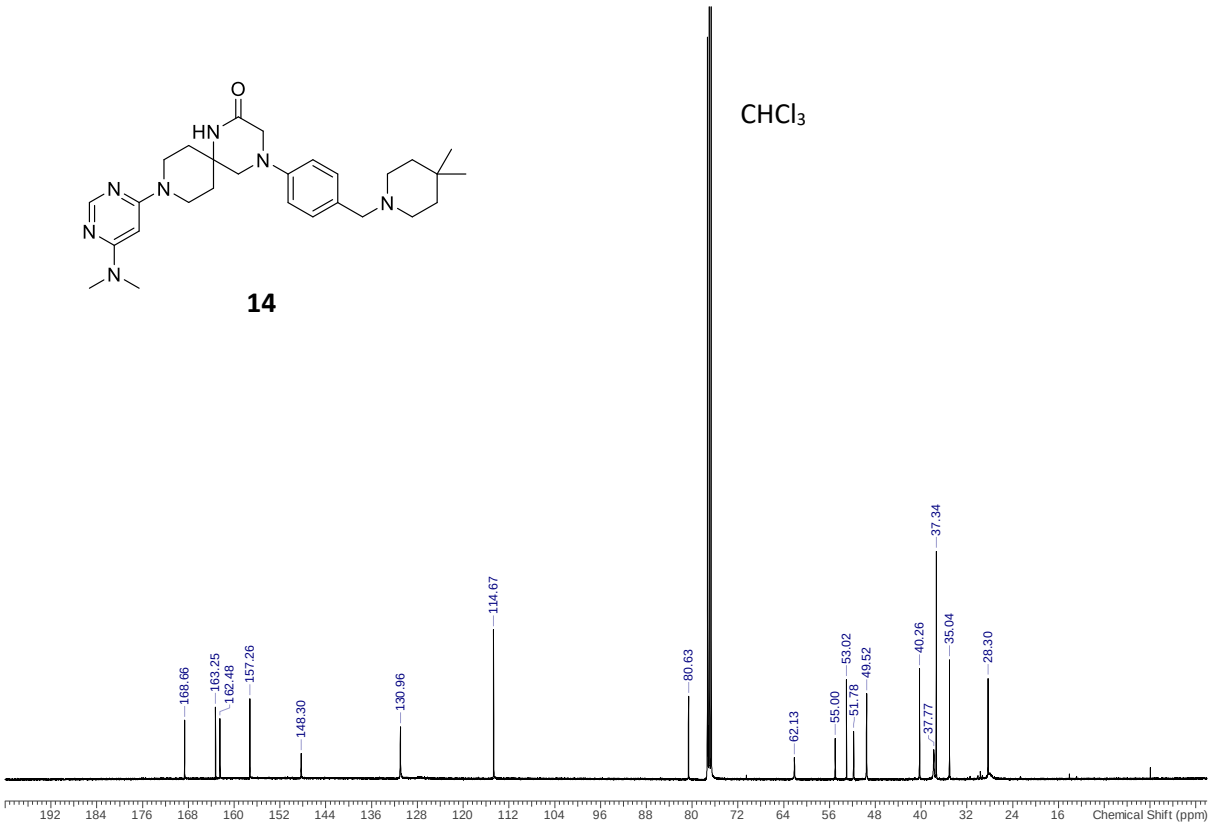
3.75
3.73
3.72
3.70
3.68
2.94
2.91
2.90
2.88
2.86
2.85
2.85
1.89
1.88
1.86
1.76
1.75
1.75
1.74
1.73
1.00
0.98
4.00
1.02
1.02
1.02
2.00
6.11
6.93
4.23
3.88
5.89
Chemical Shift (ppm)

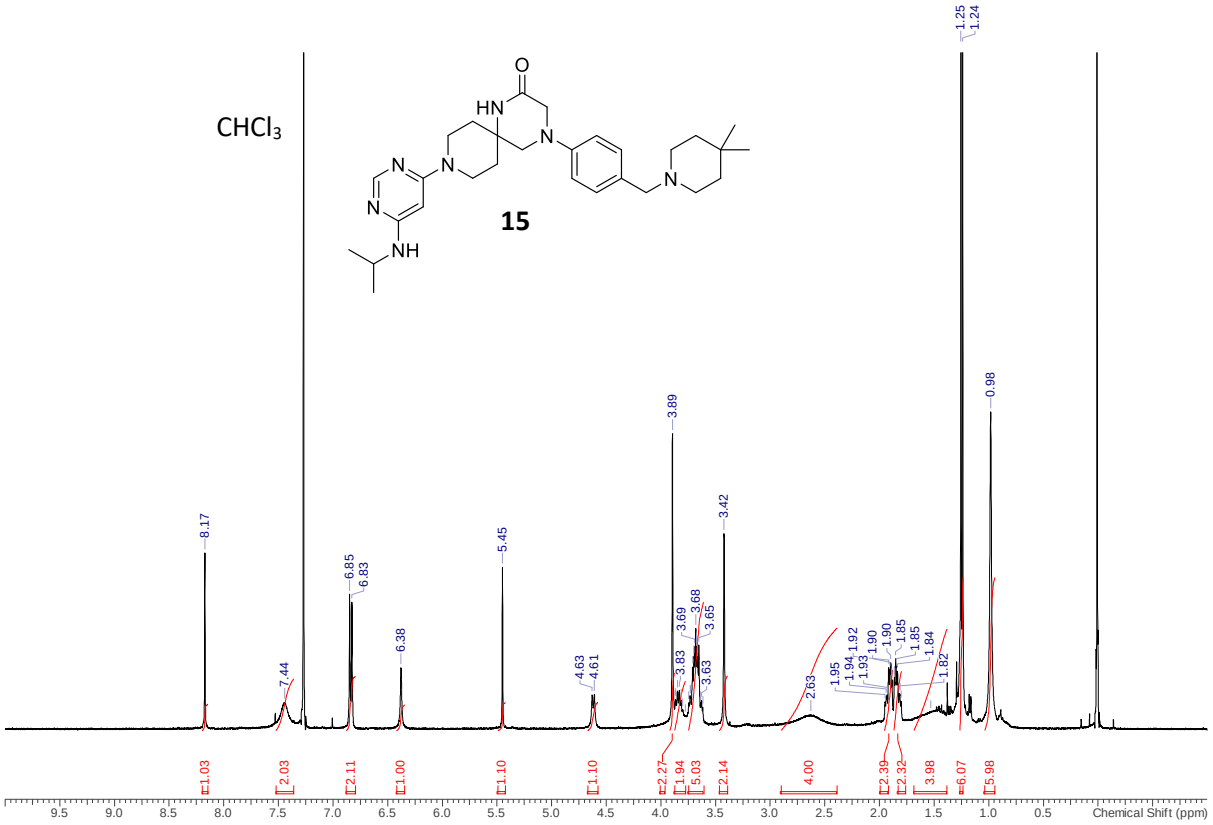

12
CHCl3
163.82
162.45
157.54
157.40
140.73
131.61
117.71
80.15
60.77
55.85
52.62
48.83
40.98
36.80
35.84
28.47
27.96
Chemical Shift (ppm)

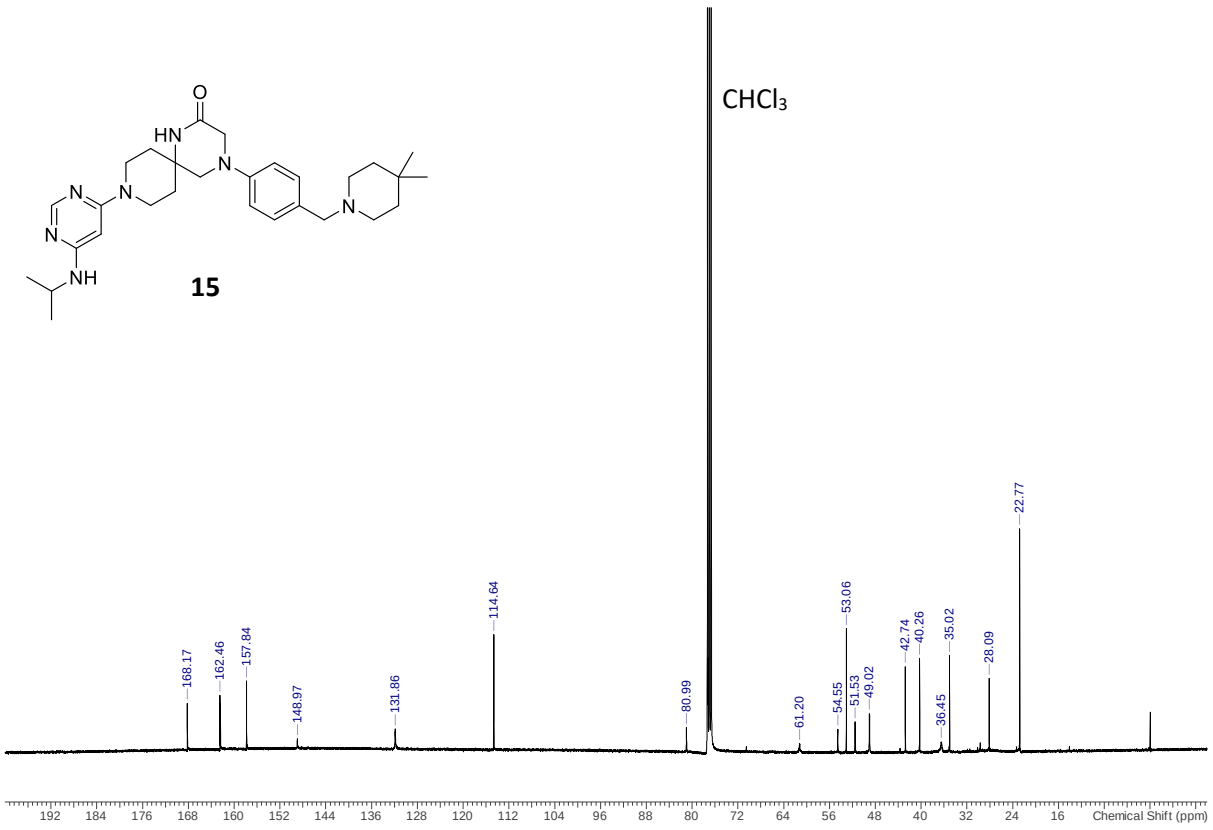

CHCl3
13
8.19
7.39
6.86
6.83
5.46
4.79
4.78
4.77
4.38
4.35
3.91
3.65
3.59
3.13
3.12
3.09
2.96
2.92
2.91
2.60
2.17
2.16
2.14
2.13
1.90
1.87
1.56
0.96
Chemical Shift (ppm)

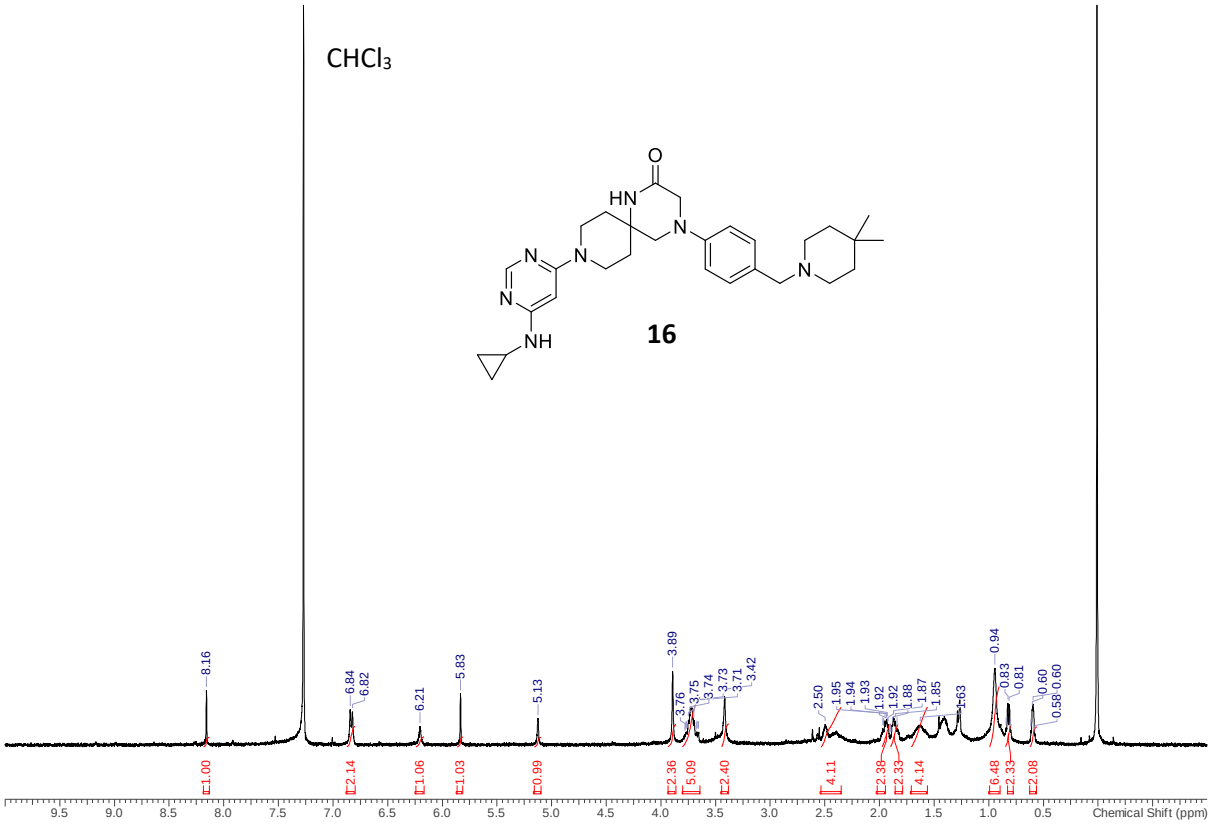

13
CHCl3
167.00
163.99
162.37
157.55
148.48
131.39
125.87
114.45
80.08
61.59
57.63
52.47
52.41
49.23
40.92
37.12
30.43
28.35
26.99
28.13
Chemical Shift (ppm)

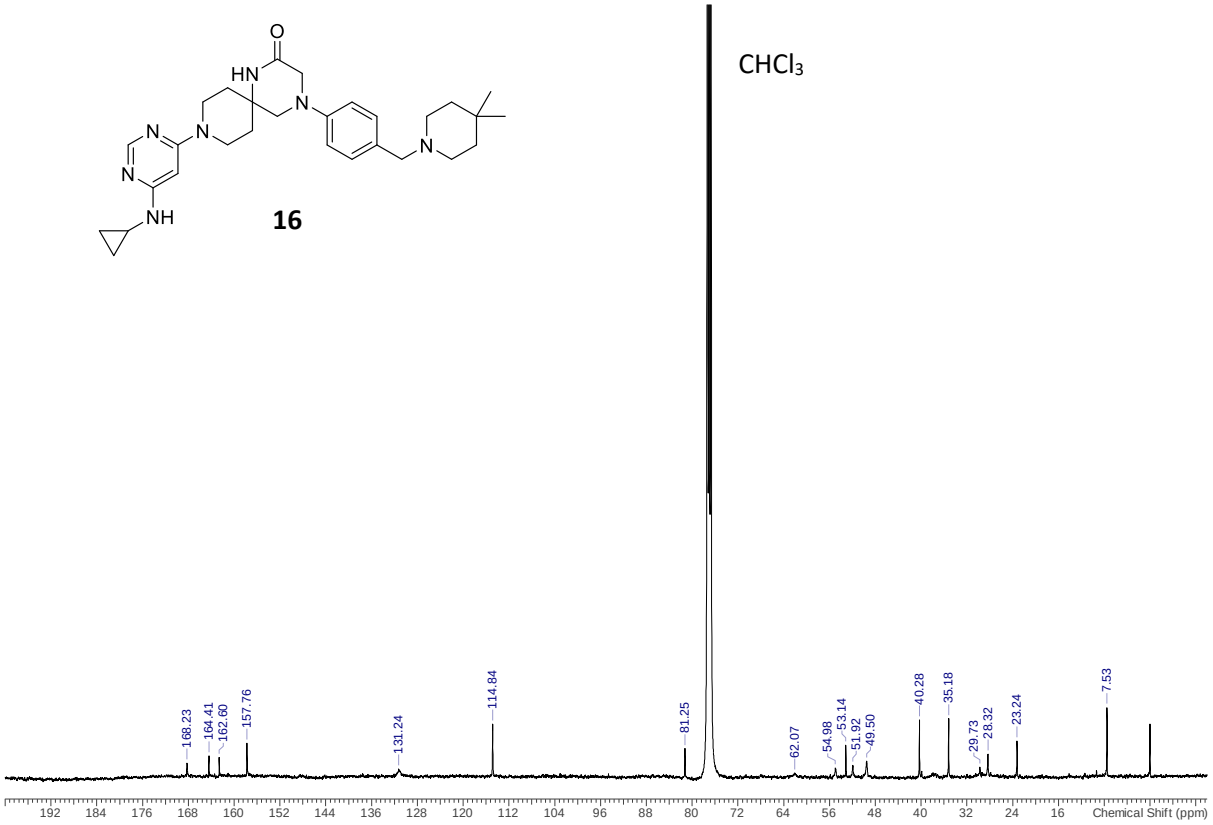

CHCl3
O
HN
N
N
N
N
N
N
14
8.26
6.83
6.81
6.25
5.52
3.88
3.70
3.69
3.68
3.40
3.09
2.39
1.93
1.92
1.91
1.90
1.87
1.86
1.85
1.84
1.40
0.94
1.01
1.96
0.95
1.00
1.98
4.12
1.92
1.93
5.85
3.80
2.12
2.22
3.92
5.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
Chemical Shift (ppm)

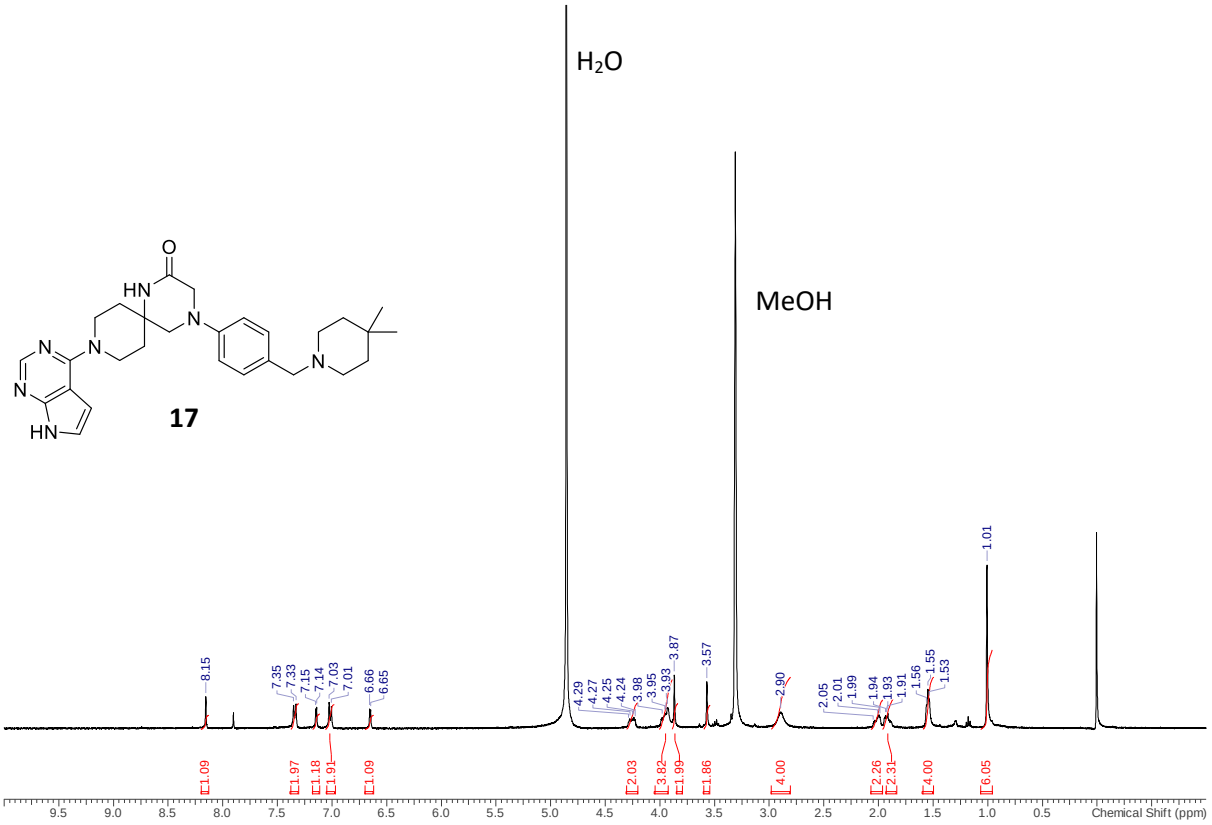

O
HN
N
N
N
N
N
N
14
CHCl3
168.66
163.25
162.48
157.26
148.30
130.96
114.67
80.63
62.13
55.00
53.02
51.78
49.52
40.26
37.77
37.34
35.04
28.30
192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16
Chemical Shift (ppm)

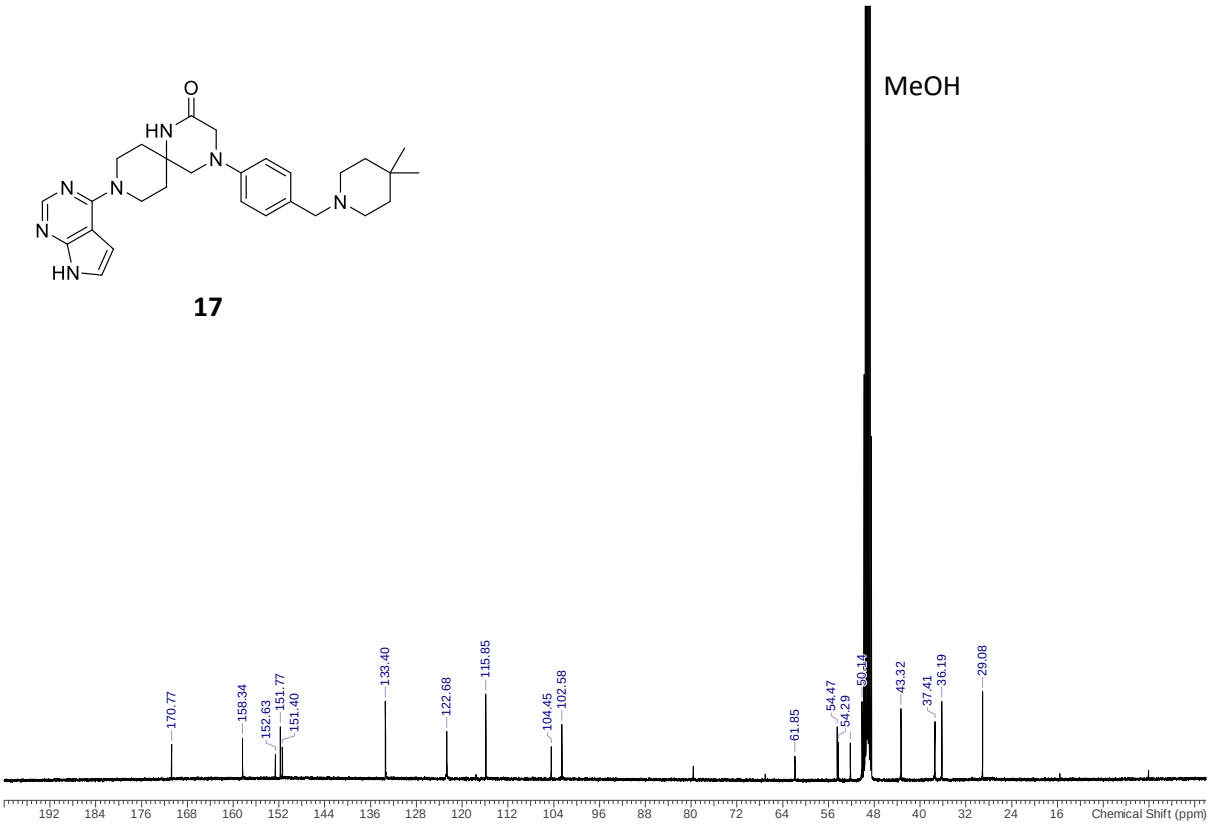

CHCl3
15
8.17
7.44
6.85
6.83
6.38
5.45
4.63
4.61
3.89
3.69
3.68
3.65
3.83
3.63
3.42
2.63
1.95
1.94
1.93
1.92
1.90
1.90
1.85
1.85
1.84
1.82
1.25
1.24
0.98
1.03
2.03
2.11
1.00
1.10
1.10
2.27
1.94
5.03
2.14
4.00
2.39
2.32
3.98
6.07
5.98
Chemical Shift (ppm)

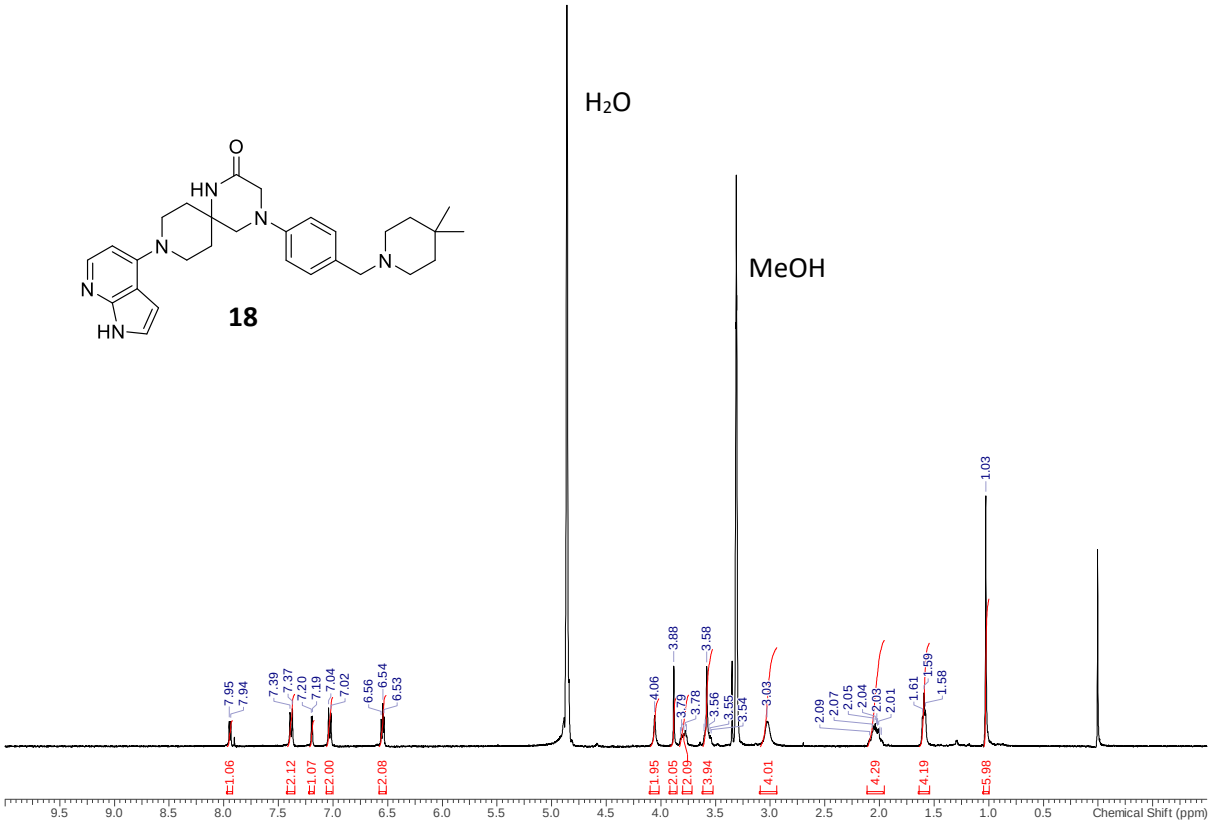

15
CHCl3
168.17
162.46
157.84
148.97
131.86
114.64
80.99
61.20
54.55
53.06
51.53
49.02
42.74
40.26
36.45
35.02
28.09
22.77
Chemical Shift (ppm)

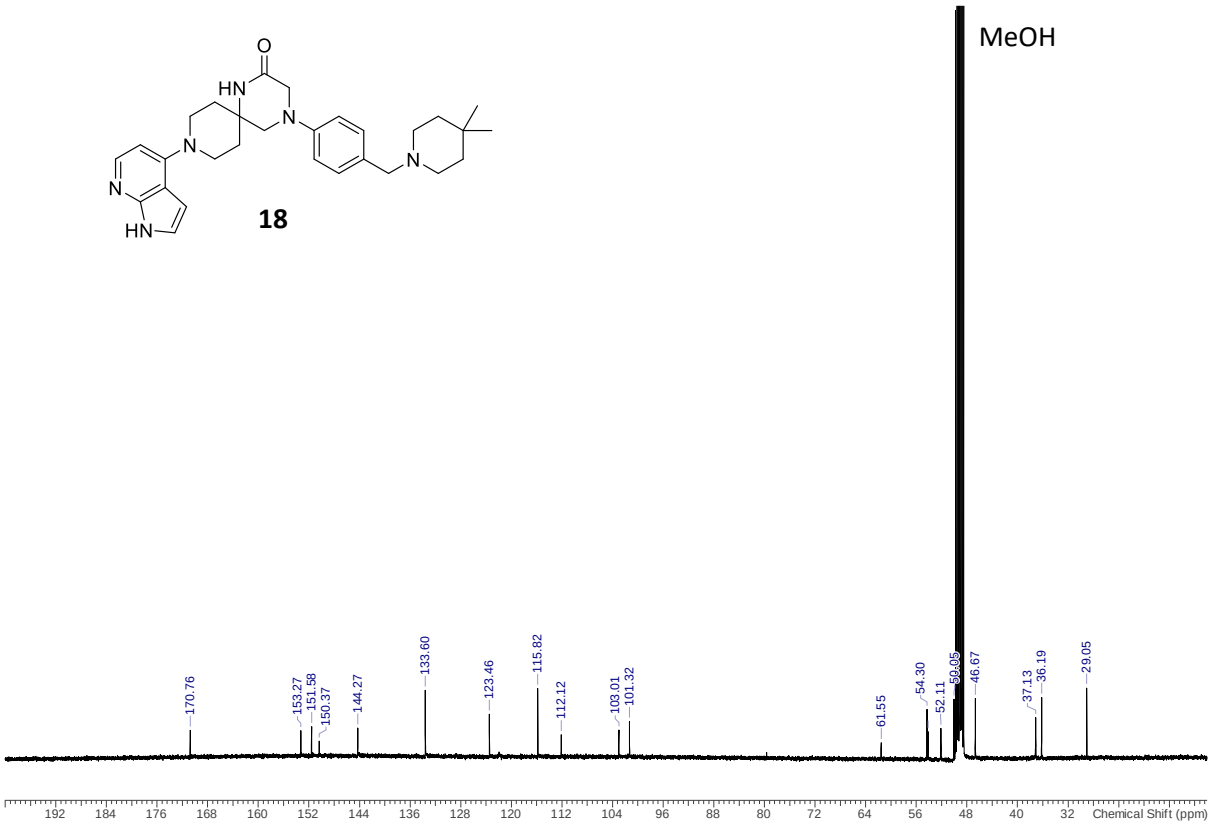

CHCl3
16
8.16
6.84
6.82
6.21
5.83
5.13
3.89
3.76
3.75
3.74
3.73
3.71
3.42
2.50
1.95
1.94
1.93
1.92
1.92
1.88
1.87
1.85
1.63
0.94
0.83
0.81
0.60
0.58 0.60
1.00
2.14
1.06
1.03
0.99
2.36
5.09
2.40
4.11
2.38
2.33
4.14
6.48
2.33
2.08
Chemical Shift (ppm)

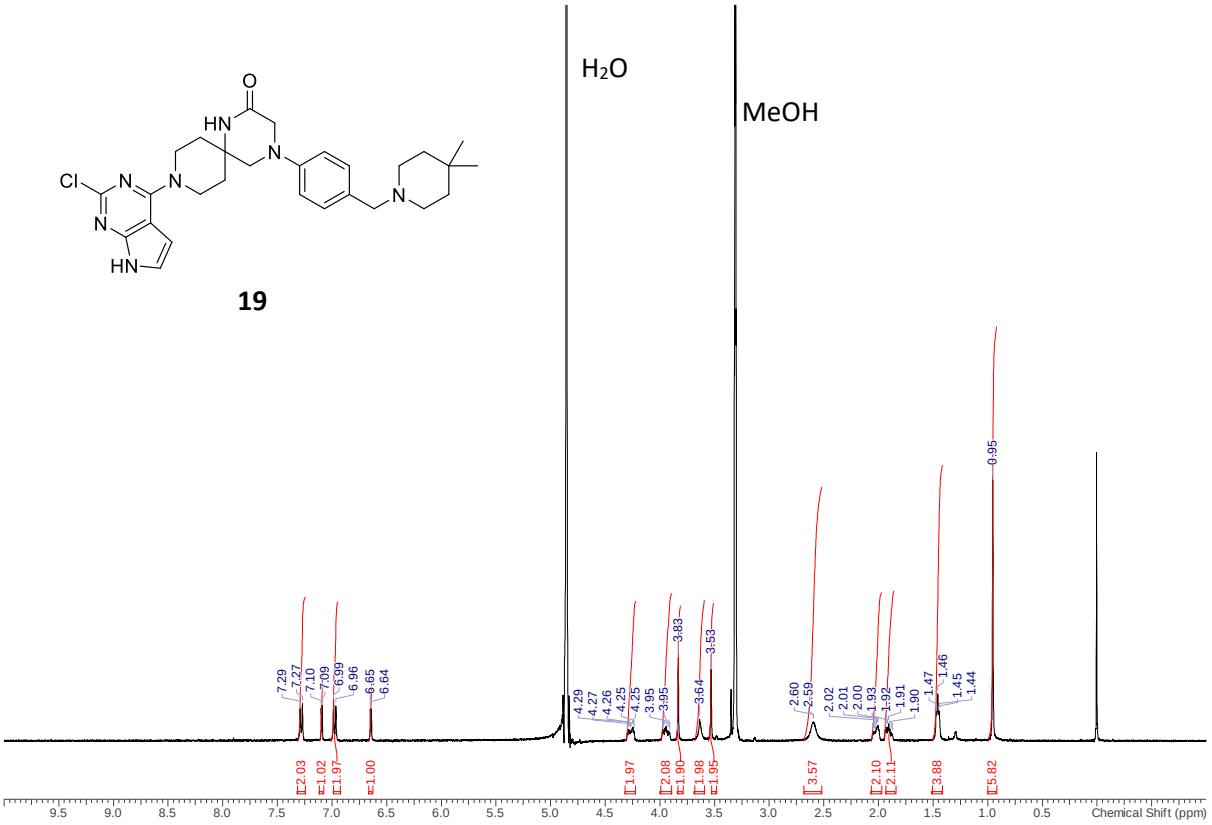

16
CHCl3
168.23
164.41
162.60
157.76
131.24
114.84
81.25
62.07
54.98
53.14
51.92
49.50
40.28
35.18
29.73
28.32
23.24
7.53
Chemical Shift (ppm)

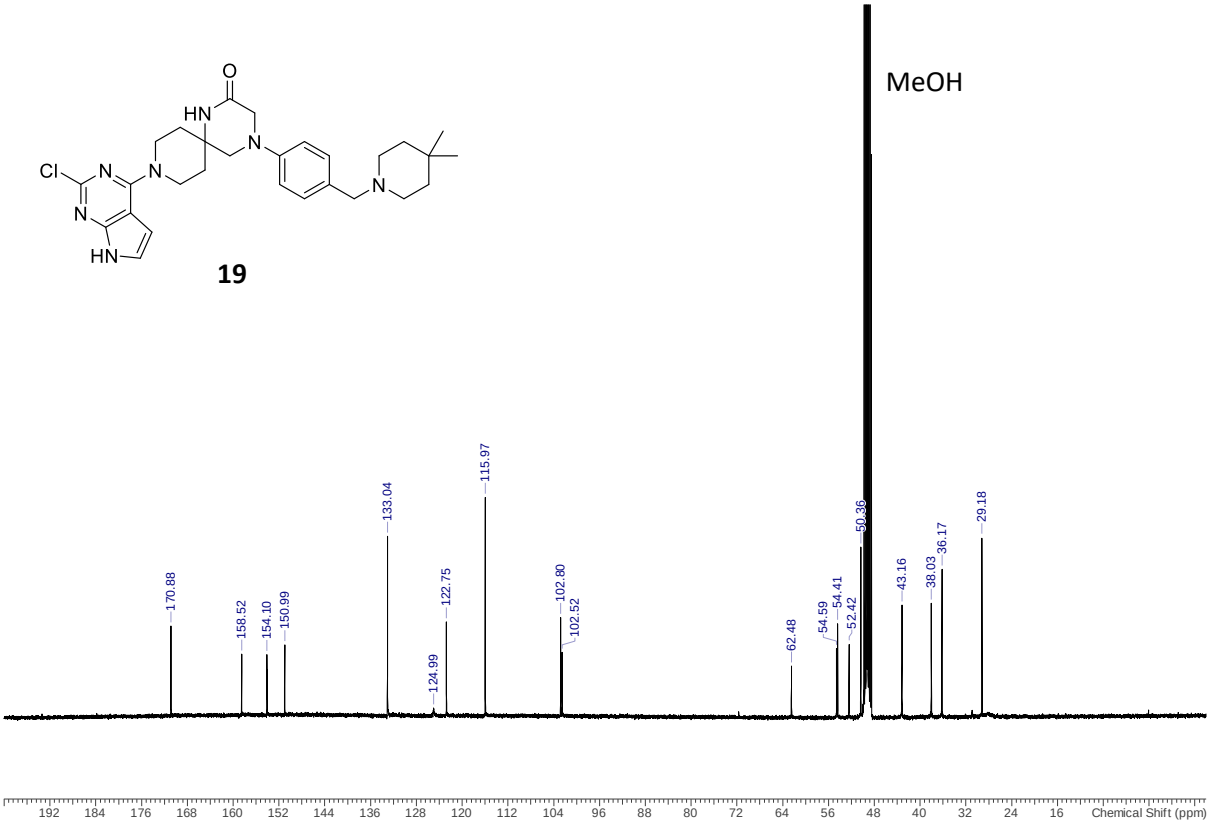

H2O
MeOH
17
8.15
7.35
7.33
7.15
7.14
7.03
7.01
6.66
6.65
4.29
4.27
4.25
4.24
3.98
3.95
3.93
3.87
3.57
2.90
2.05
2.01
1.99
1.94
1.93
1.91
1.56
1.55
1.53
1.01
1.09
1.97
1.18
1.91
1.09
2.03
3.82
1.99
1.86
4.00
2.26
2.31
4.00
6.05
Chemical Shift (ppm)

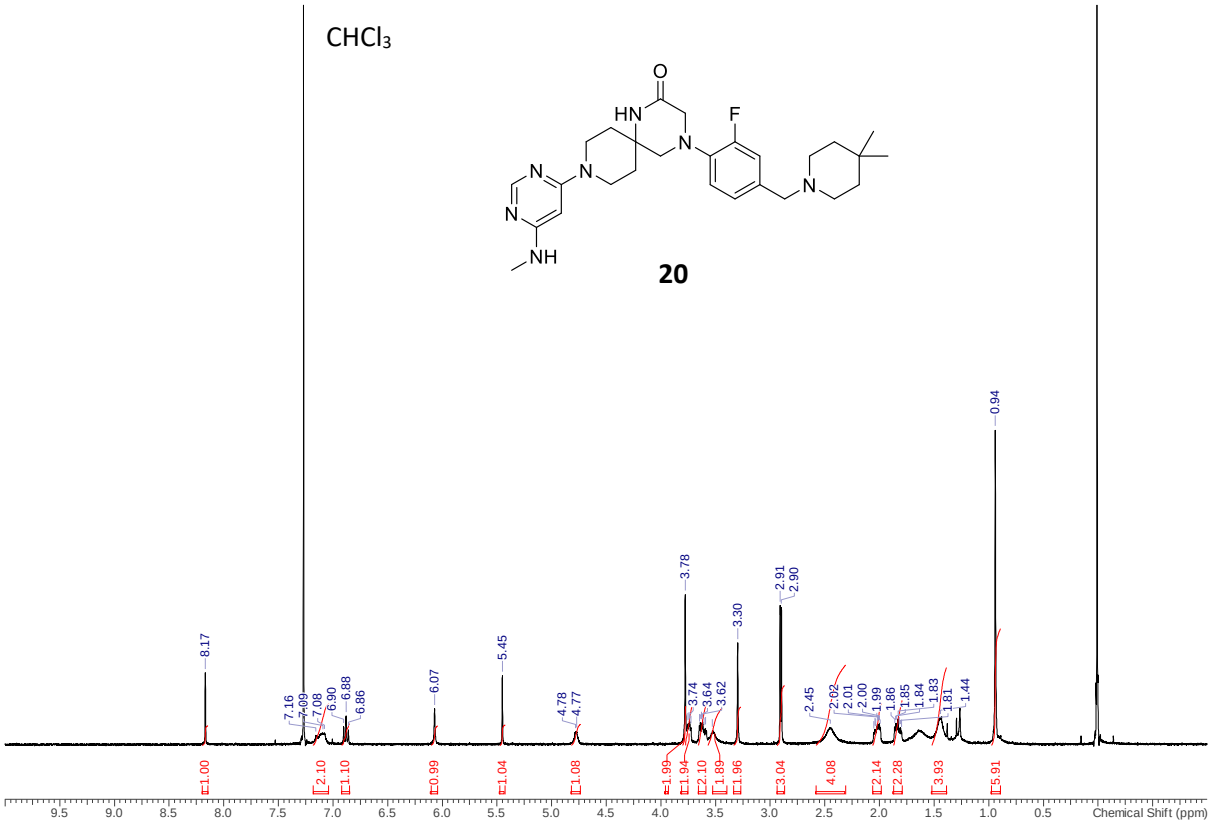

MeOH
17
170.77
158.34
152.63
151.77
151.40
133.40
122.68
115.85
104.45
102.58
61.85
54.47
54.29
50.14
43.32
37.41
36.19
29.08
Chemical Shift (ppm)

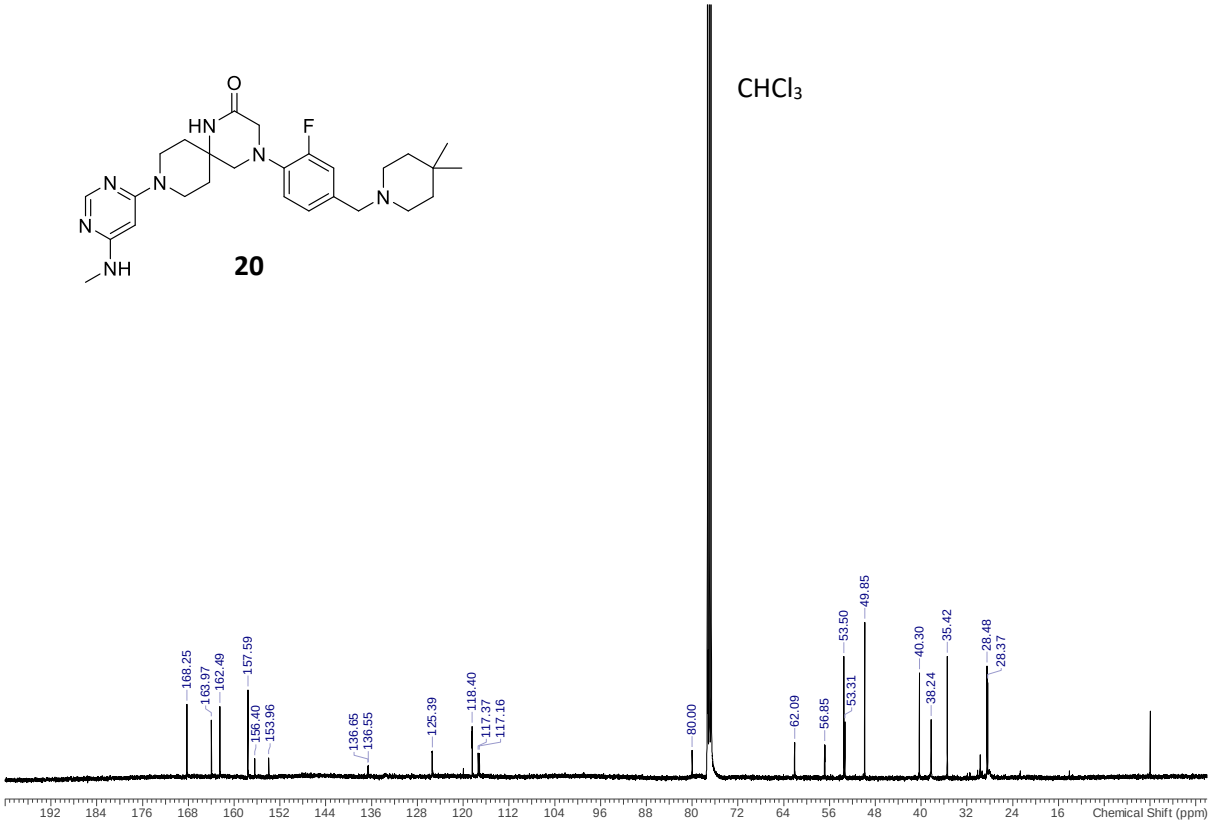

H2O
MeOH
18
7.95
7.94
7.39
7.37
7.20
7.19
7.04
7.02
6.56
6.54
6.53
4.06
3.88
3.79
3.78
3.58
3.56
3.55
3.54
3.03
2.09
2.07
2.05
2.04
2.03
2.01
1.61
1.59
1.58
1.03
Chemical Shift (ppm)

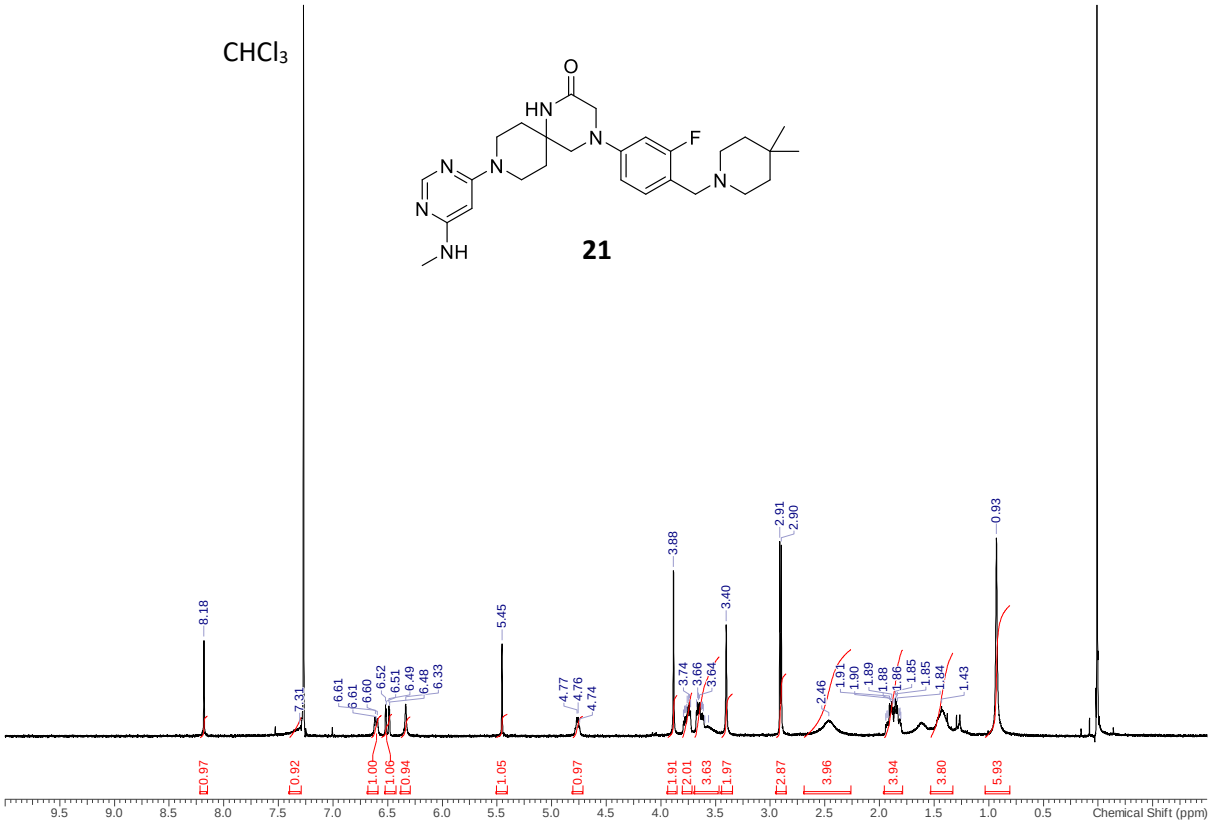

MeOH
18
170.76
153.27
151.58
150.37
144.27
133.60
123.46
115.82
112.12
103.01
101.32
61.55
54.30
52.11
49.05
46.67
37.13
36.19
29.05
Chemical Shift (ppm)

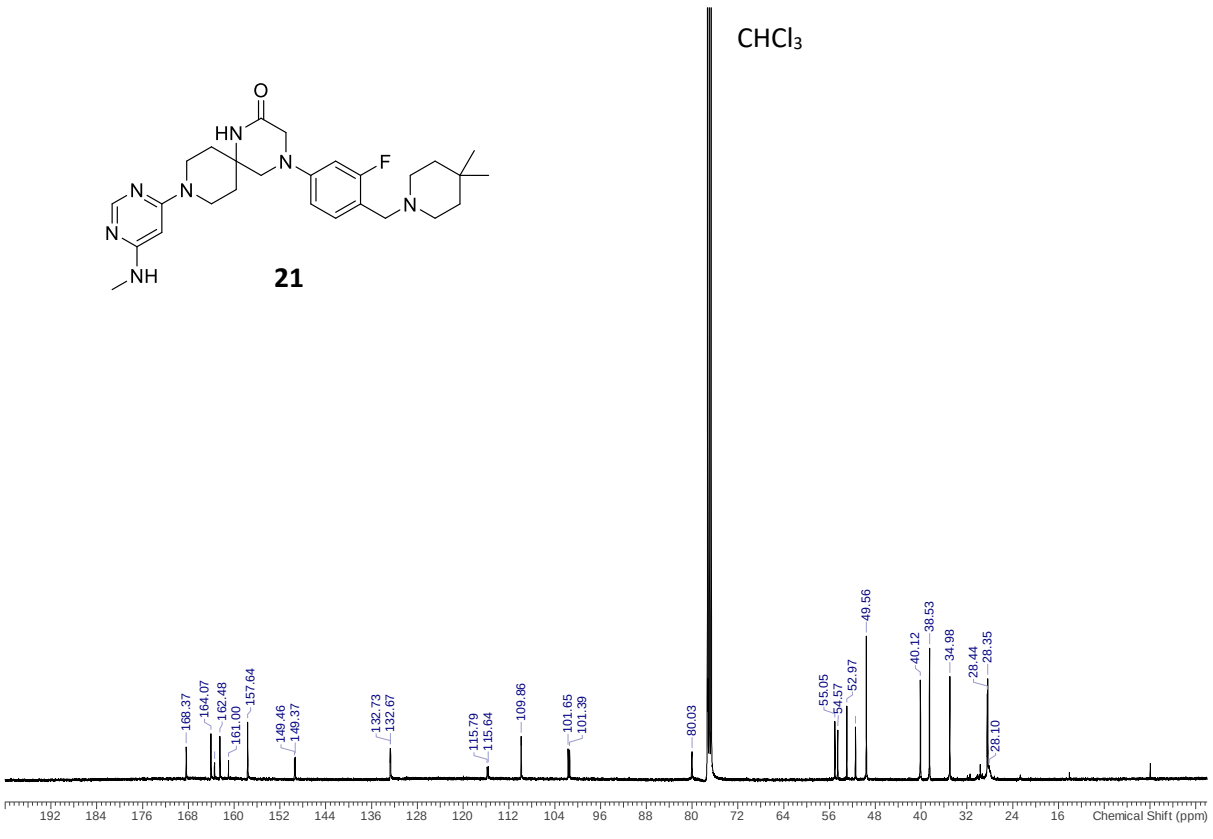

H2O
MeOH
19
Chemical Shift (ppm)


MeOH
19
Chemical Shift (ppm)

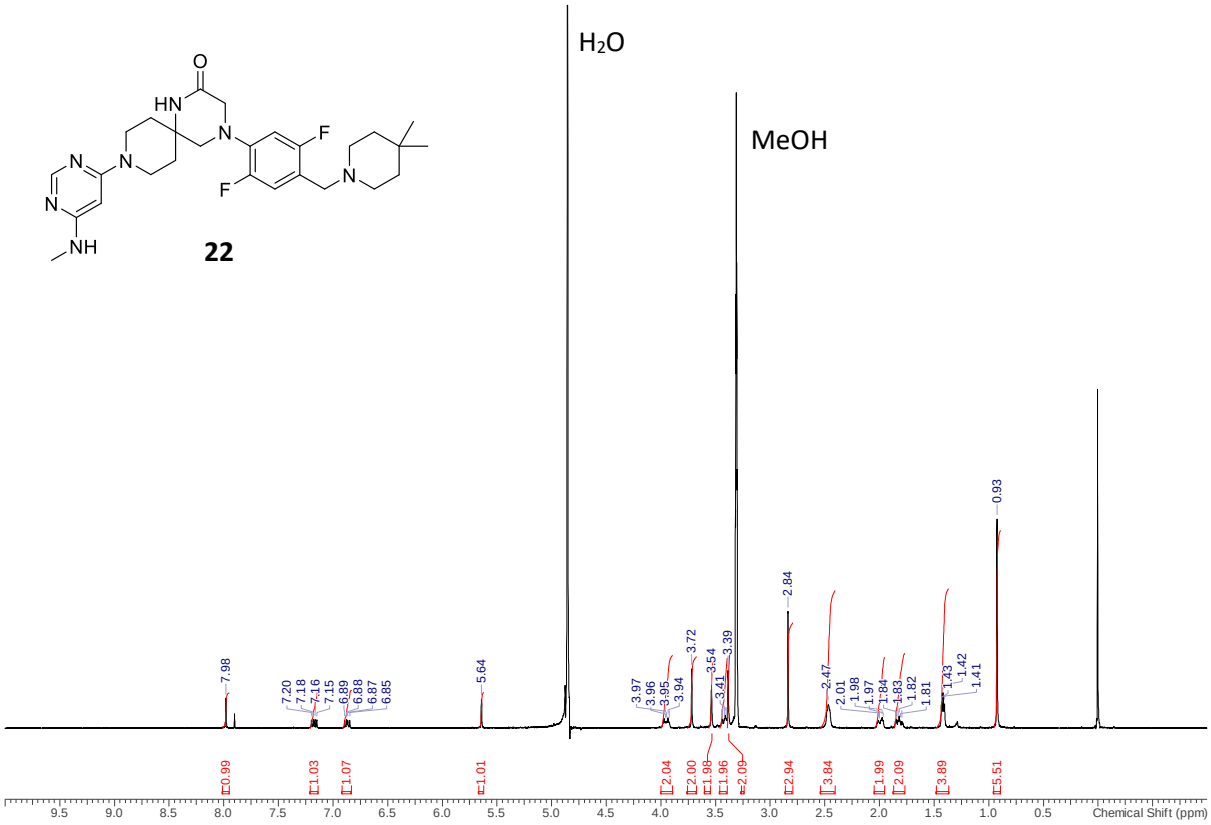

CHCl3
O
HN
F
N
N
N
N
N
NH
20
8.17
7.16
7.09
7.08
6.90
6.88
6.86
6.07
5.45
4.78
4.77
3.78
3.74
3.64
3.62
3.30
2.91
2.90
2.45
2.02
2.01
2.00
1.99
1.86
1.85
1.84
1.83
1.81
1.44
0.94
1.00
2.10
1.10
0.99
1.04
1.08
1.99
1.94
2.10
1.89
1.96
3.04
4.08
2.14
2.28
3.93
5.91
Chemical Shift (ppm)


O
HN
F
N
N
N
N
N
NH
20
CHCl3
168.25
163.97
162.49
157.59
156.40
153.96
136.65
136.55
125.39
118.40
117.37
117.16
80.00
62.09
56.85
53.50
53.31
49.85
40.30
38.24
35.42
28.48
28.37
Chemical Shift (ppm)

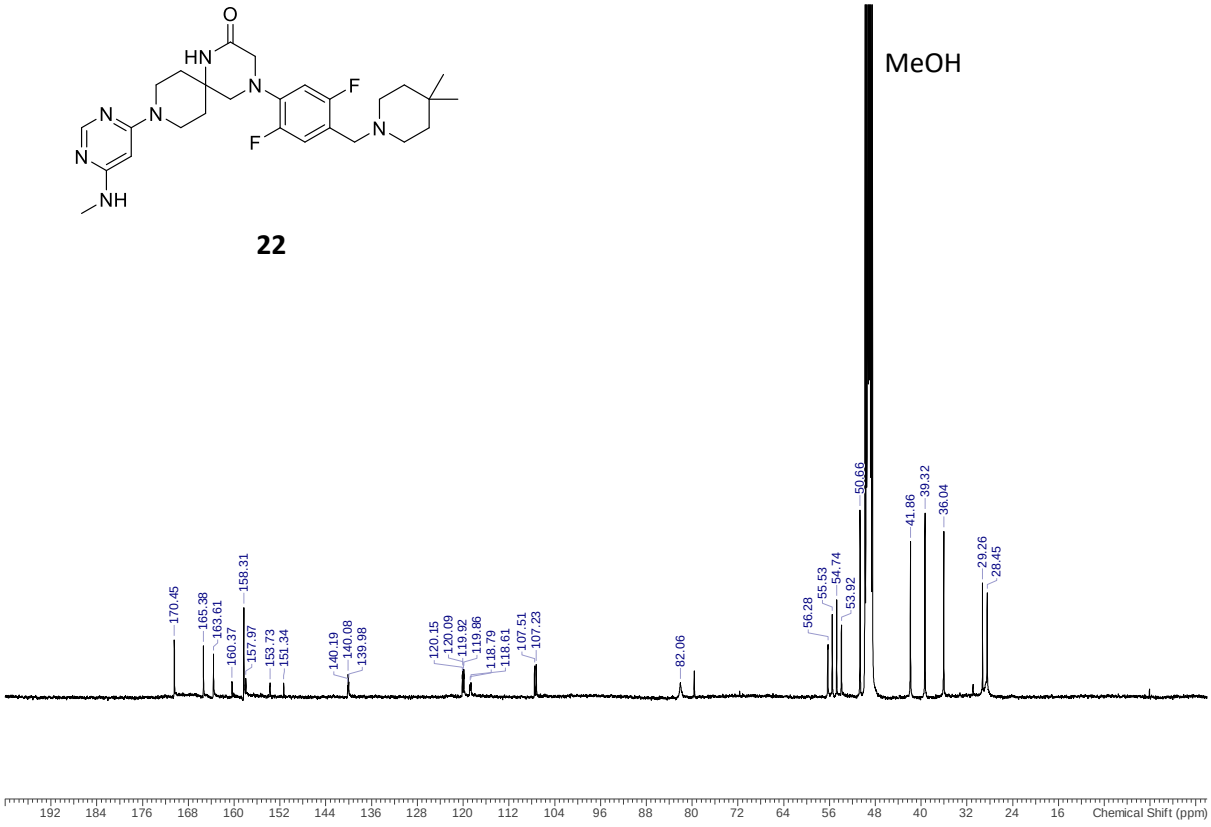

CHCl3
O
HN
N
N
F
N
N
N
NH
21
8.18
7.31
6.61
6.61
6.60
6.52
6.51
6.49
6.48
6.33
5.45
4.77
4.76
4.74
3.88
3.74
3.66
3.64
3.40
2.91
2.90
2.46
1.91
1.90
1.89
1.88
1.86
1.85
1.85
1.84
1.43
0.93
0.97
0.92
1.00
1.06
0.94
1.05
0.97
1.91
2.01
3.63
1.97
2.87
3.96
3.94
3.80
5.93
Chemical Shift (ppm)


CHCl3
O
HN
N
N
F
N
N
N
NH
21
168.37
164.07
162.48
161.00
157.64
149.46
149.37
132.73
132.67
115.79
115.64
109.86
101.65
101.39
80.03
55.05
54.57
52.97
49.56
40.12
38.53
34.98
28.44
28.35
28.10
Chemical Shift (ppm)

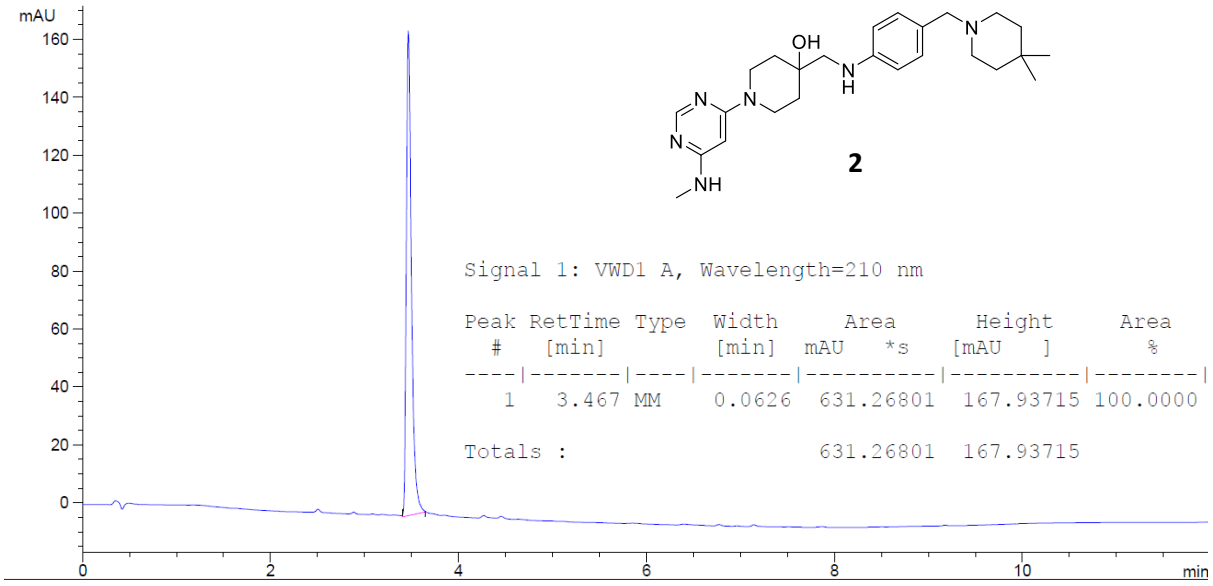
22

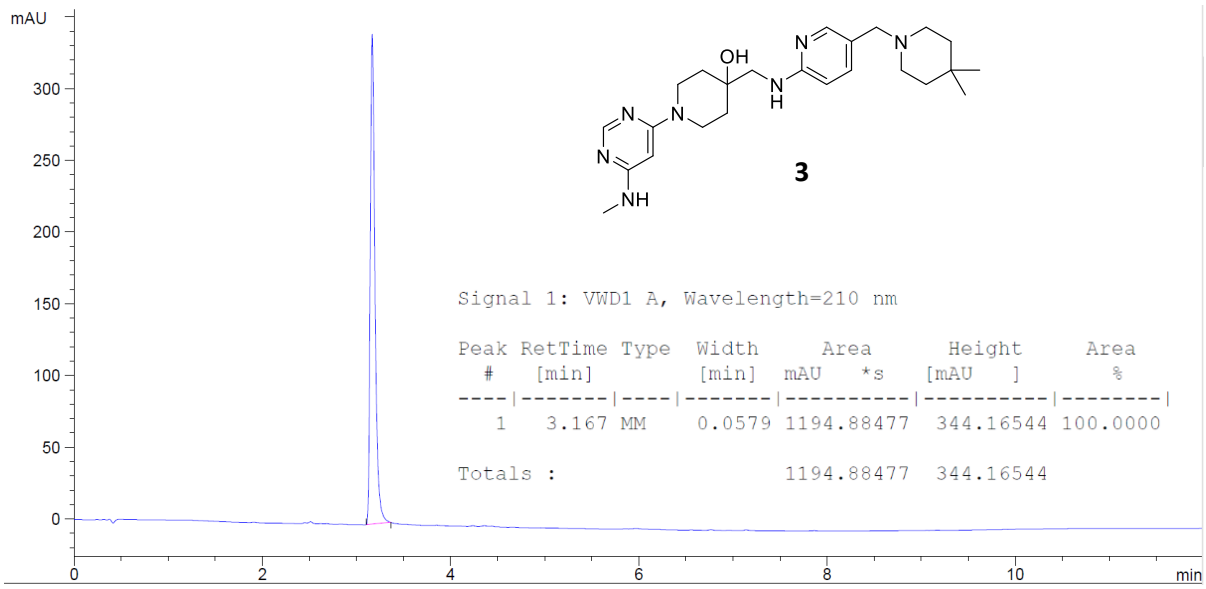

H2O
MeOH
7.98
7.20
7.18
7.16
7.15
6.89
6.88
6.87
6.85
5.64
3.97
3.96
3.95
3.94
3.72
3.54
3.41
3.39
2.84
2.47
2.01
1.98
1.97
1.84
1.83
1.82
1.81
1.43
1.42
1.41
0.93
Chemical Shift (ppm)

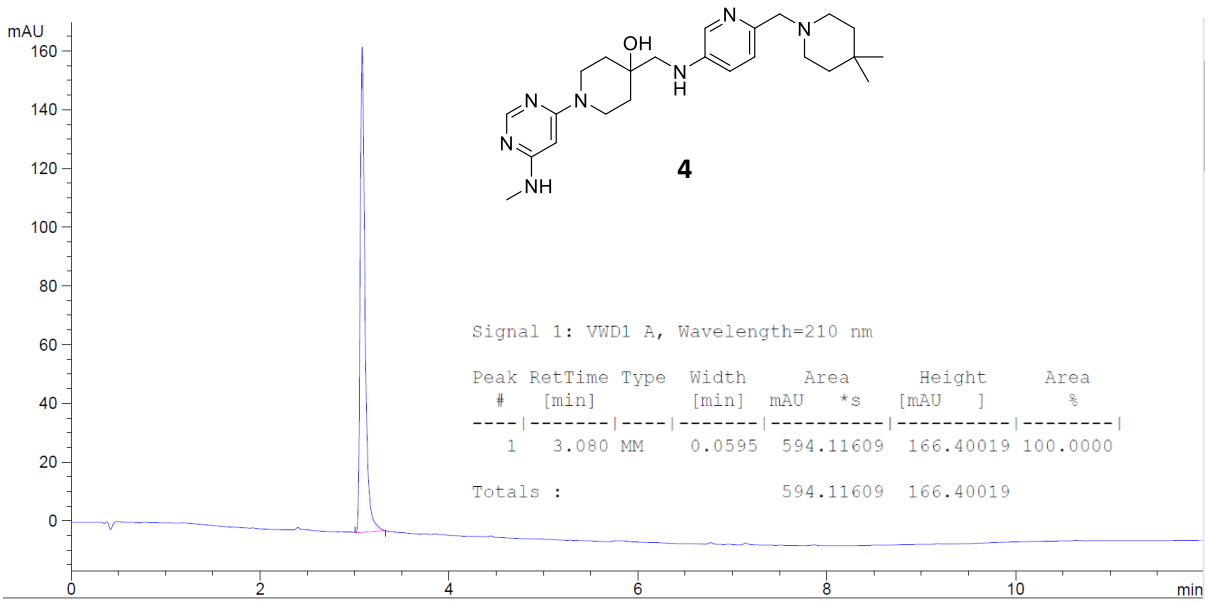
22


MeOH
170.45
165.38
163.61
160.37
158.31
157.97
153.73
151.34
140.19
140.08
139.98
120.15
120.09
119.92
119.86
118.79
118.61
107.51
107.23
82.06
56.28
55.53
54.74
53.92
50.66
41.86
39.32
36.04
29.26
28.45
Chemical Shift (ppm)

HPLC traces of final compounds

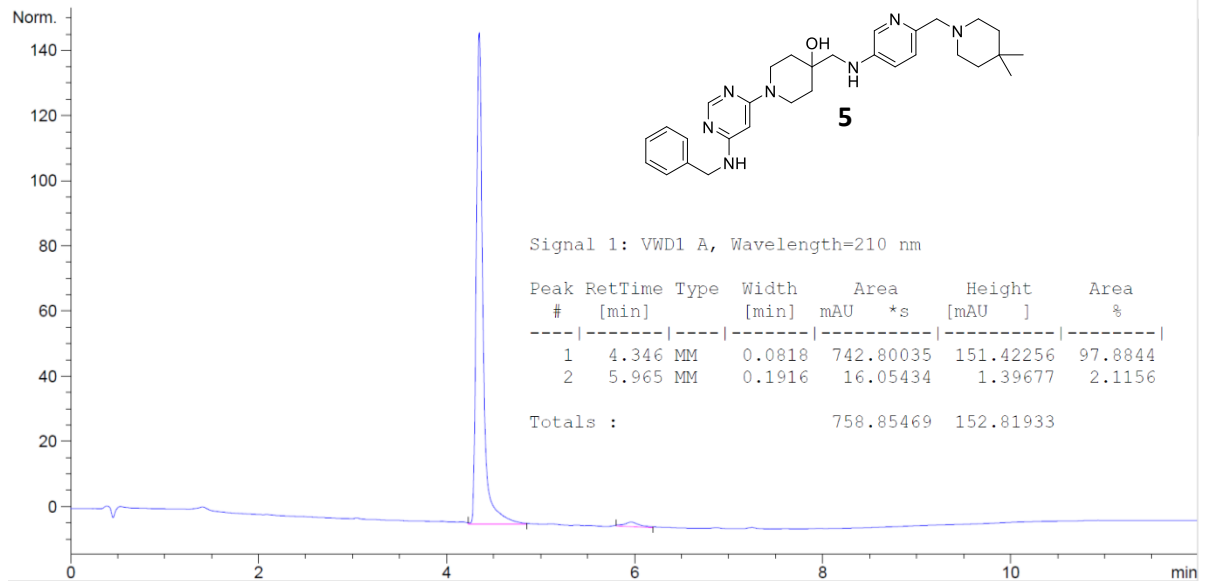






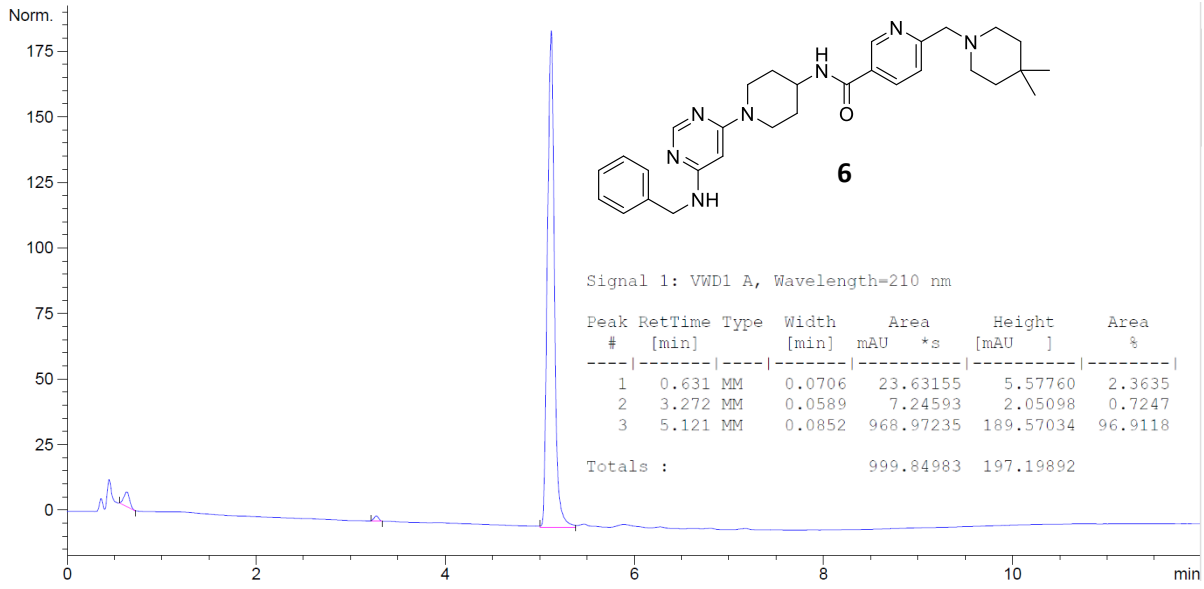
Signal 1: VWD1 A, Wavelength=210 nm

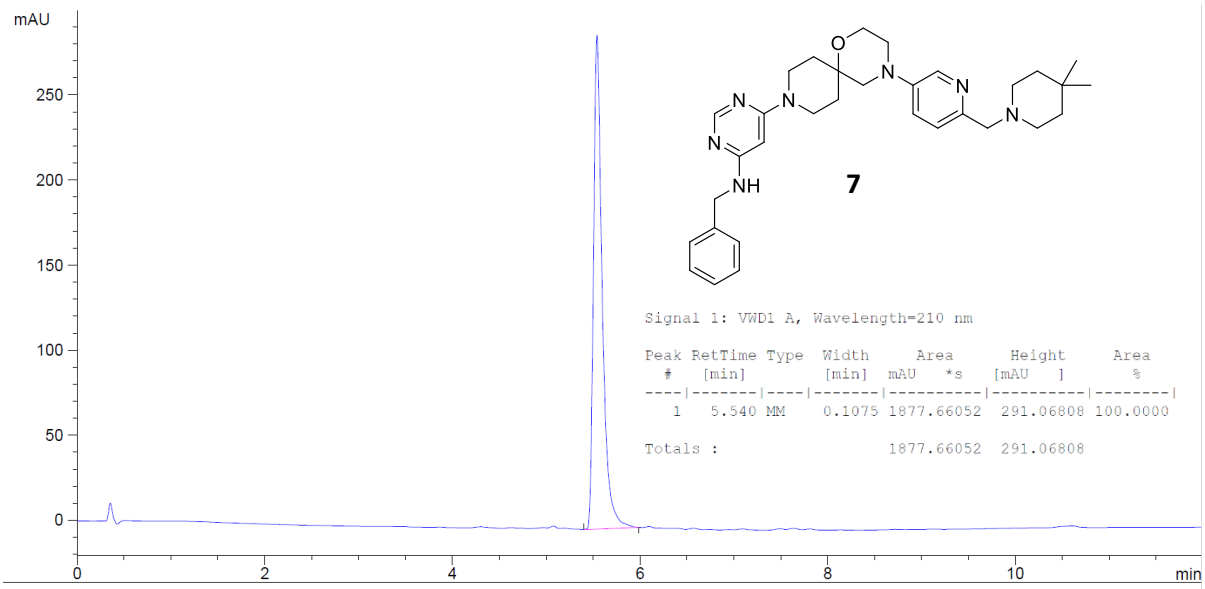
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	3.080	MM	0.0595	594.11609	166.40019	100.0000
Totals :				594.11609	166.40019	

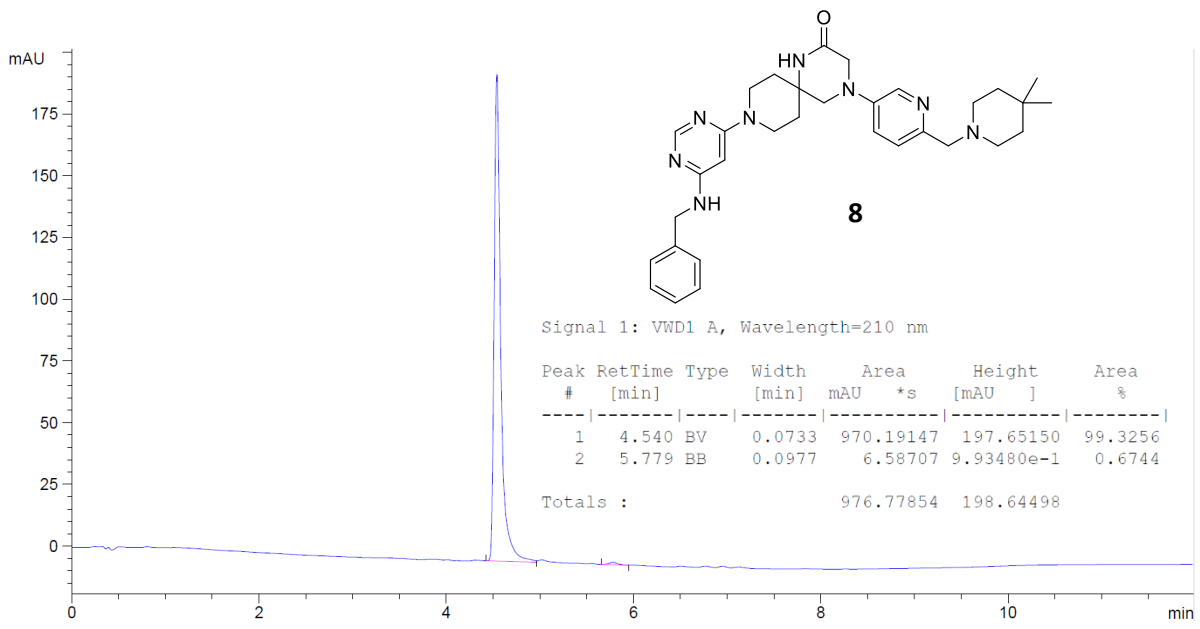


Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.346	MM	0.0818	742.80035	151.42256	97.8844
2	5.965	MM	0.1916	16.05434	1.39677	2.1156
Totals :				758.85469	152.81933	


Norm.
175
150
125
100
75
50
25
0
0
2
4
6
8
10
min
6
Signal 1: VWD1 A, Wavelength=210 nm
Peak RetTime Type Width Area Height Area
[min] [min] mAU *s [mAU] %
1 0.631 MM 0.0706 23.63155 5.57760 2.3635
2 3.272 MM 0.0589 7.24593 2.05098 0.7247
3 5.121 MM 0.0852 968.97235 189.57034 96.9118
Totals : 999.84983 197.19892

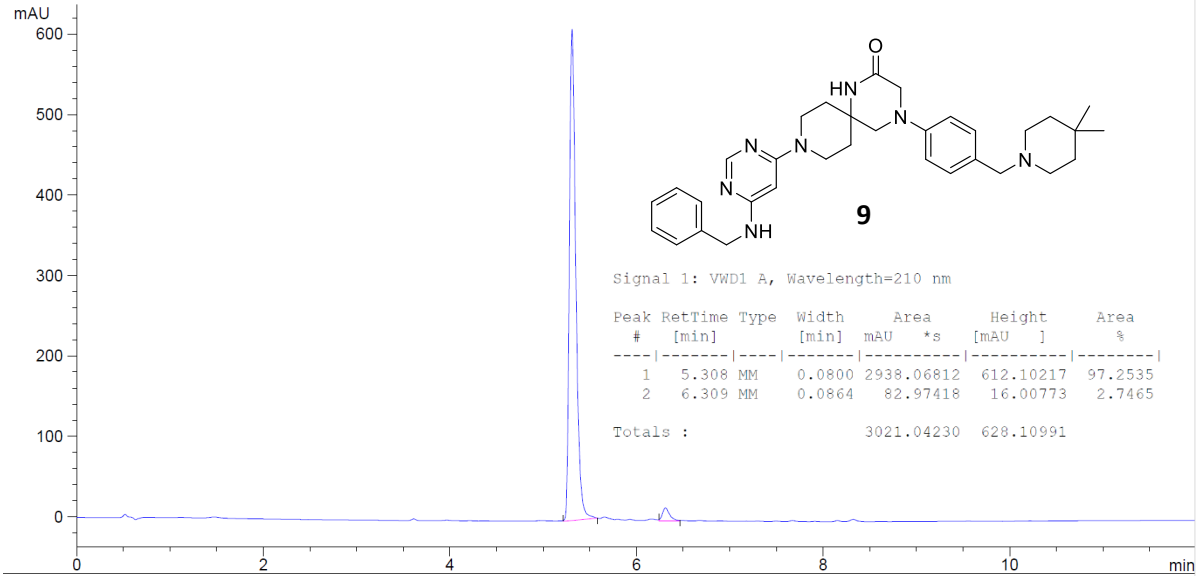

mAU
250
200
150
100
50
0
0
2
4
6
8
10
min
7
Signal 1: VWD1 A, Wavelength=210 nm
Peak RetTime Type Width Area Height Area
[min] [min] mAU *s [mAU] %
1 5.540 MM 0.1075 1877.66052 291.06808 100.0000
Totals : 1877.66052 291.06808



8

Signal 1: VWD1 A, Wavelength=210 nm

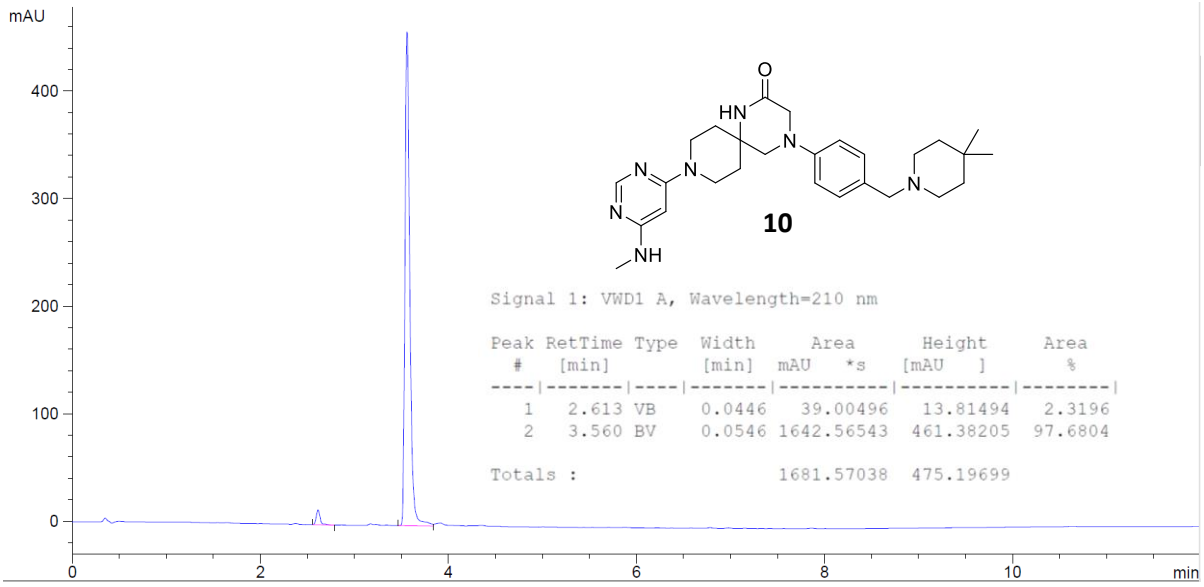
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.540	BV	0.0733	970.19147	197.65150	99.3256
2	5.779	BB	0.0977	6.58707	9.93480e-1	0.6744
Totals :				976.77854	198.64498	



9

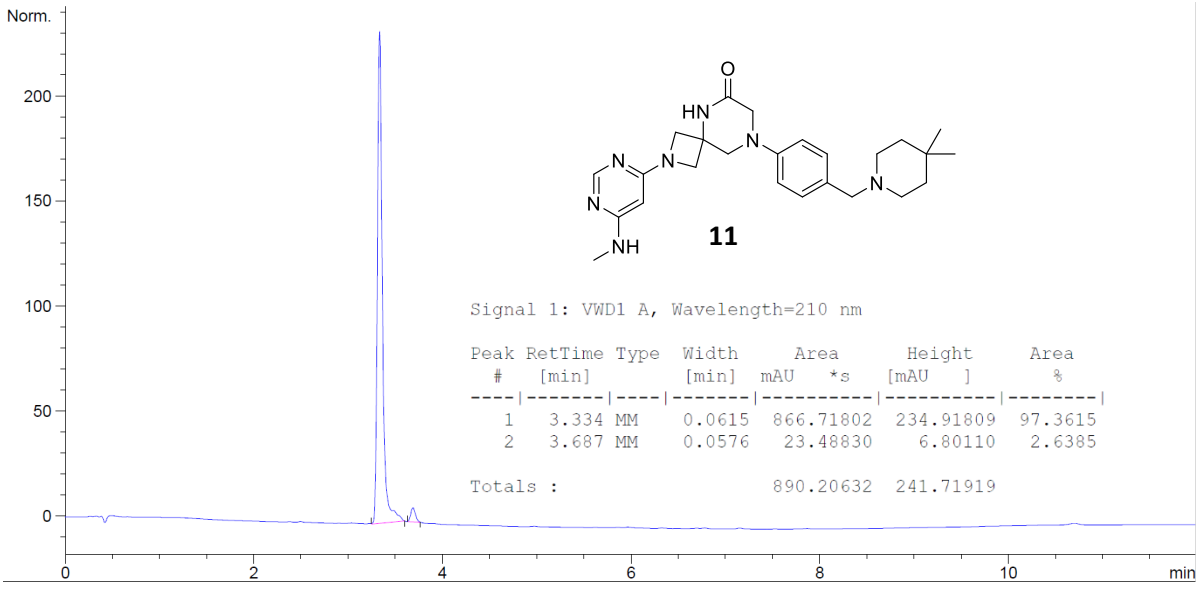
Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.308	MM	0.0800	2938.06812	612.10217	97.2535
2	6.309	MM	0.0864	82.97418	16.00773	2.7465
Totals :				3021.04230	628.10991	



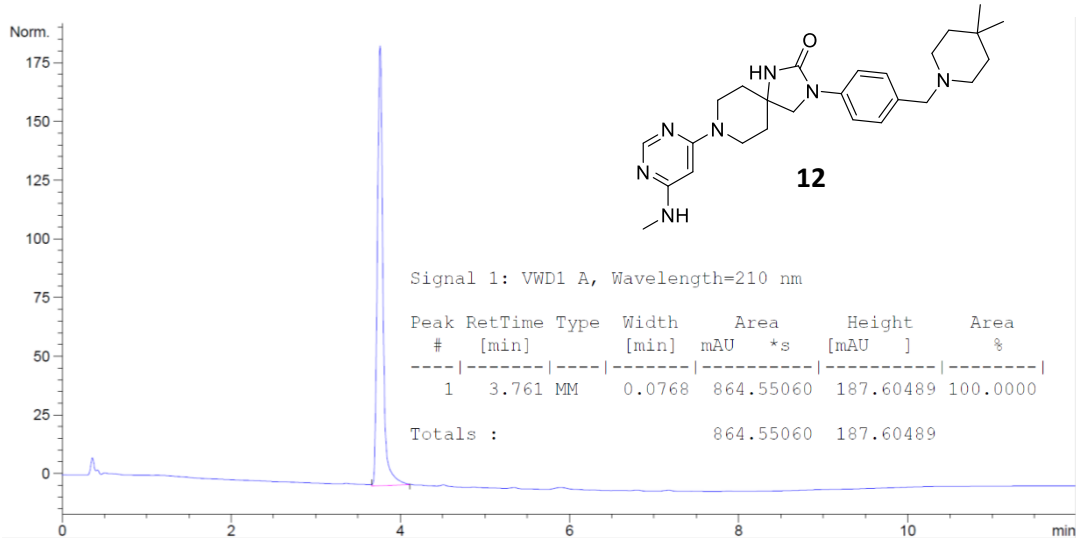
Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.613	VB	0.0446	39.00496	13.81494	2.3196
2	3.560	BV	0.0546	1642.56543	461.38205	97.6804
Totals :				1681.57038	475.19699	



Signal 1: VWD1 A, Wavelength=210 nm

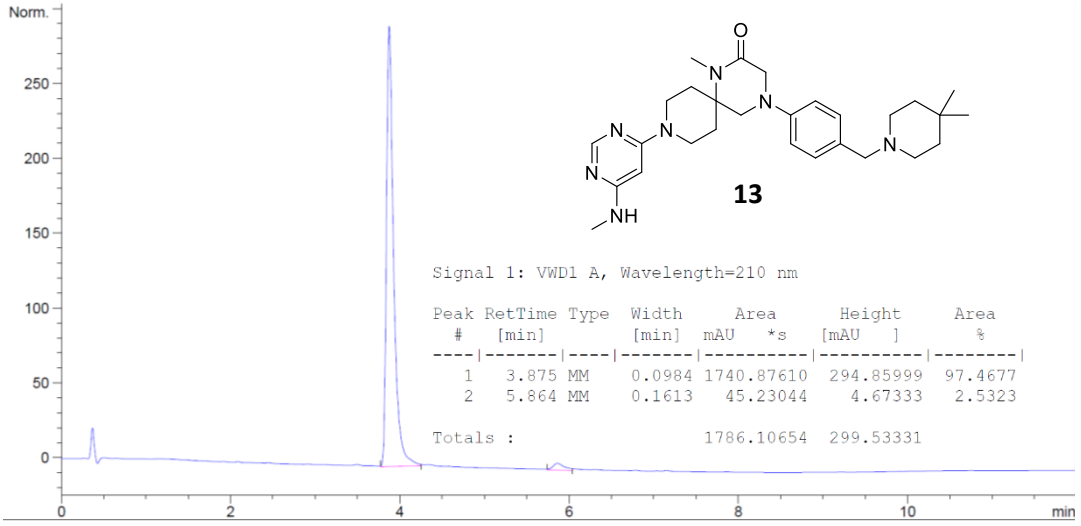
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	3.334	MM	0.0615	866.71802	234.91809	97.3615
2	3.687	MM	0.0576	23.48830	6.80110	2.6385
Totals :				890.20632	241.71919	



12

Signal 1: VWD1 A, Wavelength=210 nm

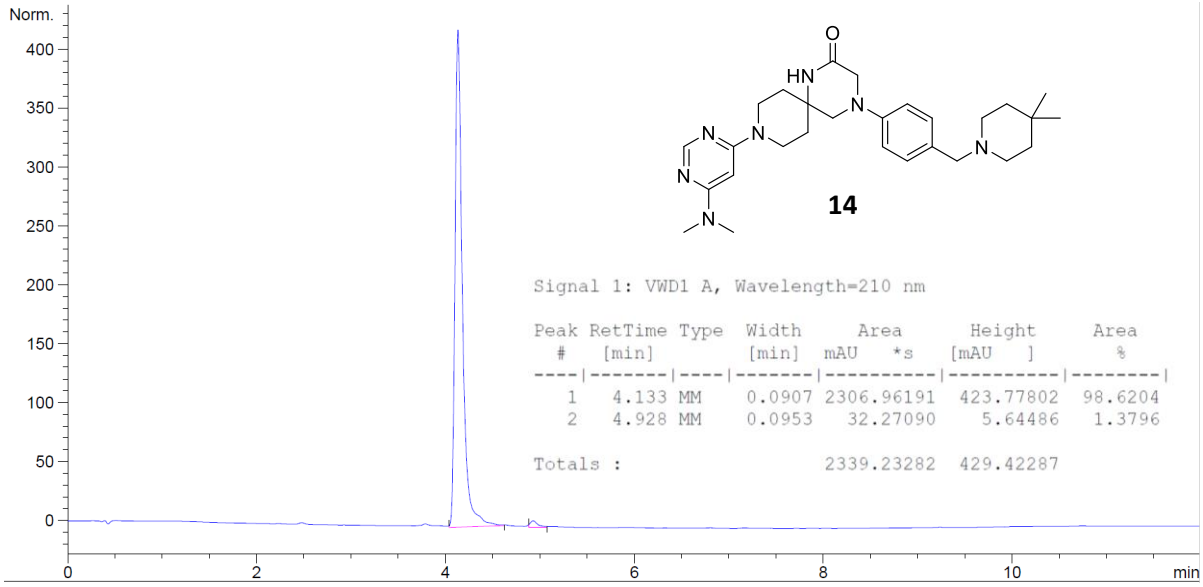
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	3.761	MM	0.0768	864.55060	187.60489	100.0000
Totals :				864.55060	187.60489	



13

Signal 1: VWD1 A, Wavelength=210 nm

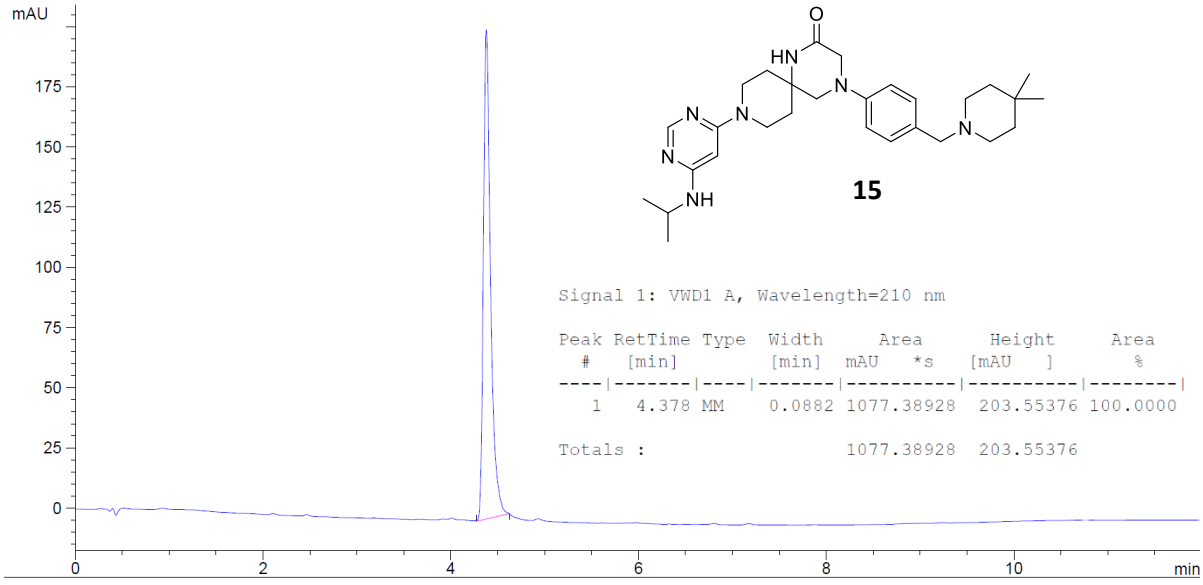
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	3.875	MM	0.0984	1740.87610	294.85999	97.4677
2	5.864	MM	0.1613	45.23044	4.67333	2.5323
Totals :				1786.10654	299.53331	



14

Signal 1: VWD1 A, Wavelength=210 nm

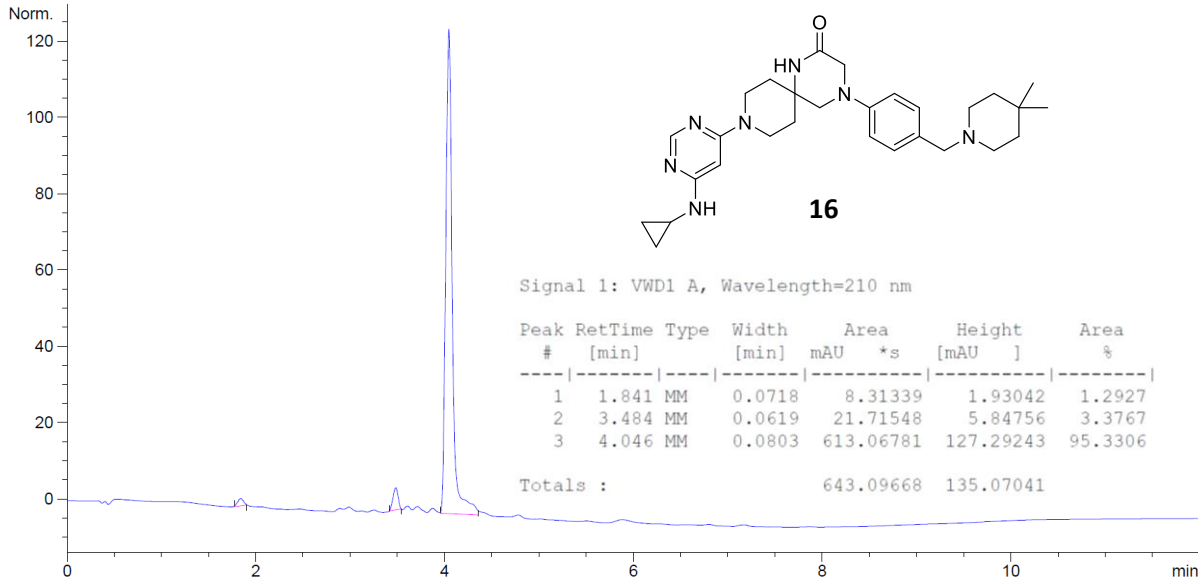
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.133	MM	0.0907	2306.96191	423.77802	98.6204
2	4.928	MM	0.0953	32.27090	5.64486	1.3796
Totals :				2339.23282	429.42287	



15

Signal 1: VWD1 A, Wavelength=210 nm

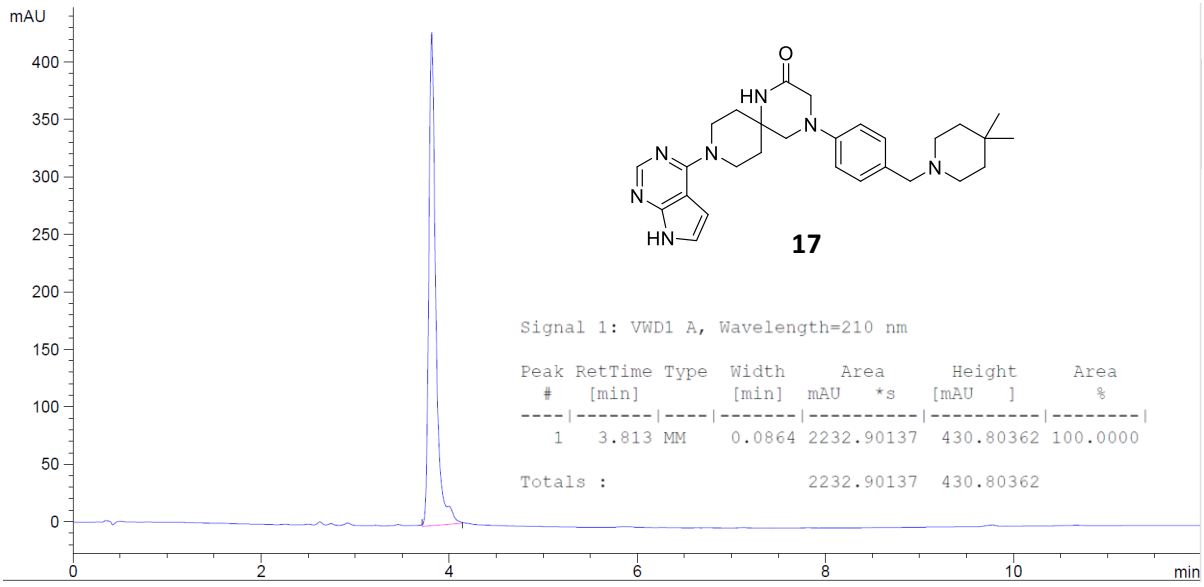
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.378	MM	0.0882	1077.38928	203.55376	100.0000
Totals :				1077.38928	203.55376	



16

Signal 1: VWD1 A, Wavelength=210 nm

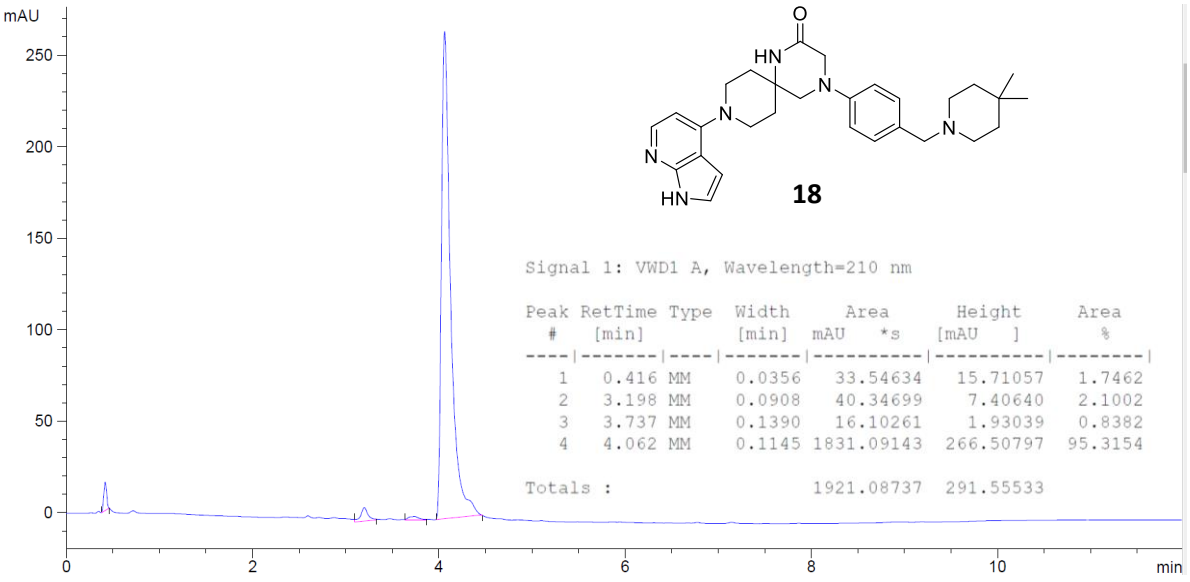
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	1.841	MM	0.0718	8.31339	1.93042	1.2927
2	3.484	MM	0.0619	21.71548	5.84756	3.3767
3	4.046	MM	0.0803	613.06781	127.29243	95.3306
Totals :				643.09668	135.07041	



17

Signal 1: VWD1 A, Wavelength=210 nm

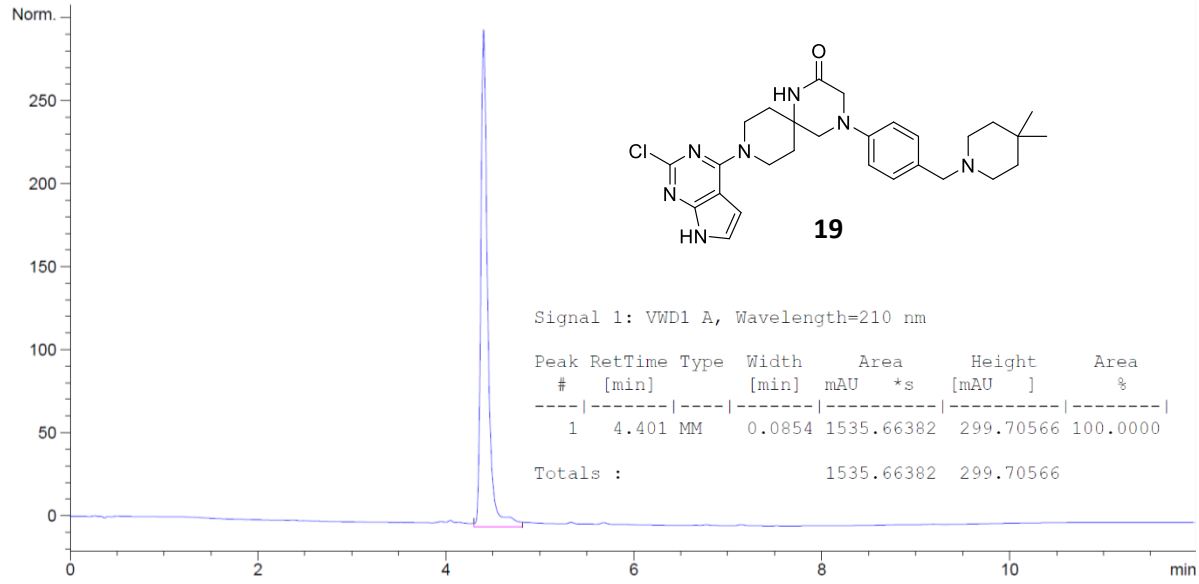
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	3.813	MM	0.0864	2232.90137	430.80362	100.0000
Totals :				2232.90137	430.80362	



18

Signal 1: VWD1 A, Wavelength=210 nm

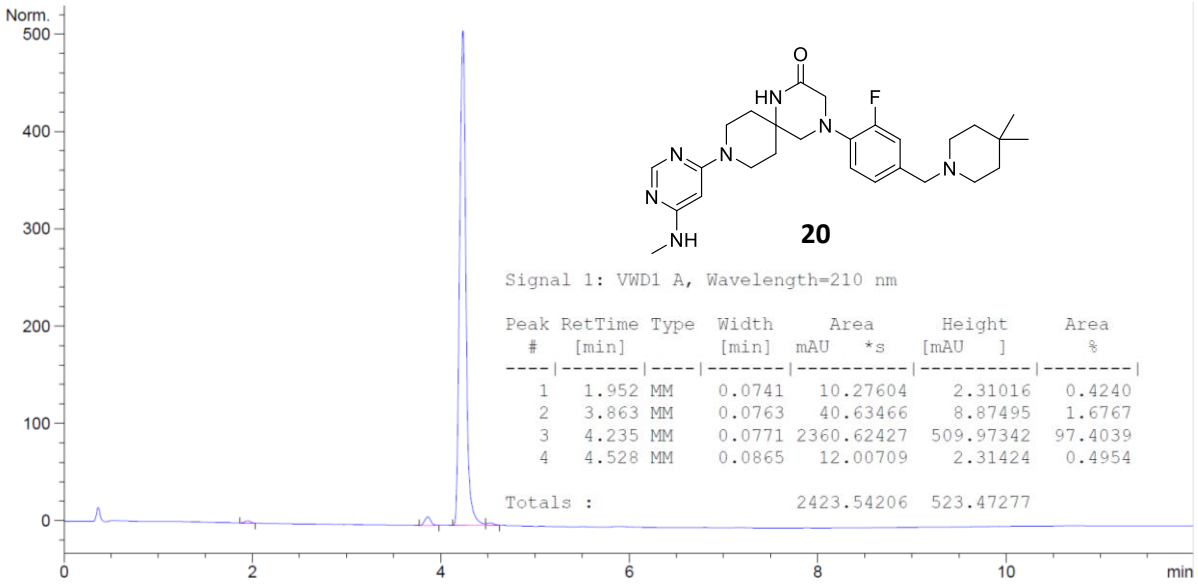
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	0.416	MM	0.0356	33.54634	15.71057	1.7462
2	3.198	MM	0.0908	40.34699	7.40640	2.1002
3	3.737	MM	0.1390	16.10261	1.93039	0.8382
4	4.062	MM	0.1145	1831.09143	266.50797	95.3154
Totals :				1921.08737	291.55533	



19

Signal 1: VWD1 A, Wavelength=210 nm

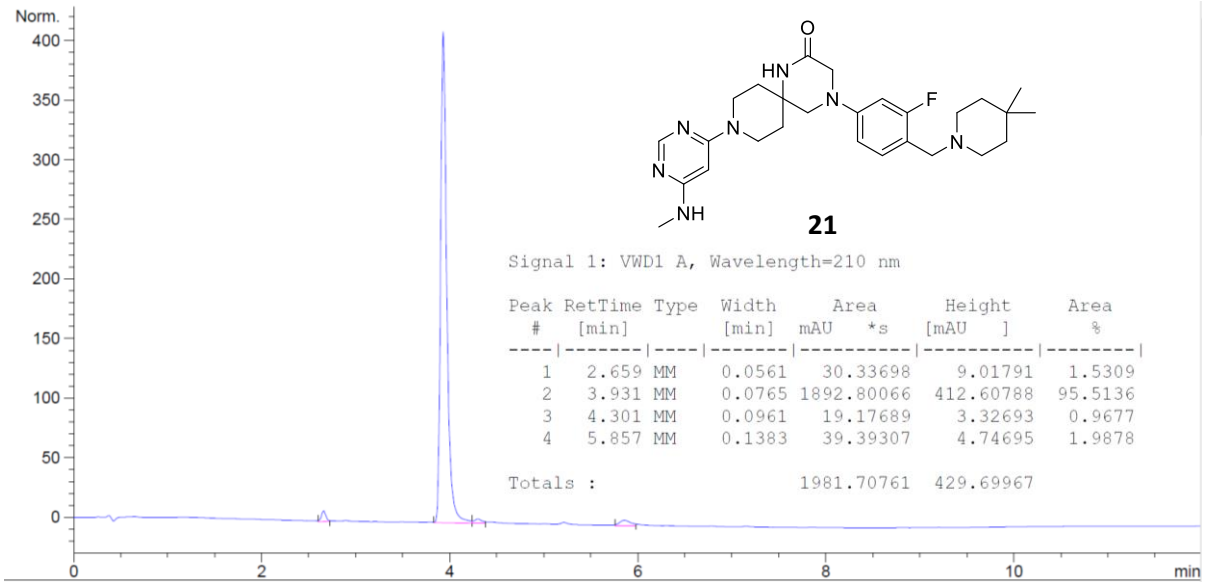
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.401	MM	0.0854	1535.66382	299.70566	100.0000
Totals :				1535.66382	299.70566	



20

Signal 1: VWD1 A, Wavelength=210 nm

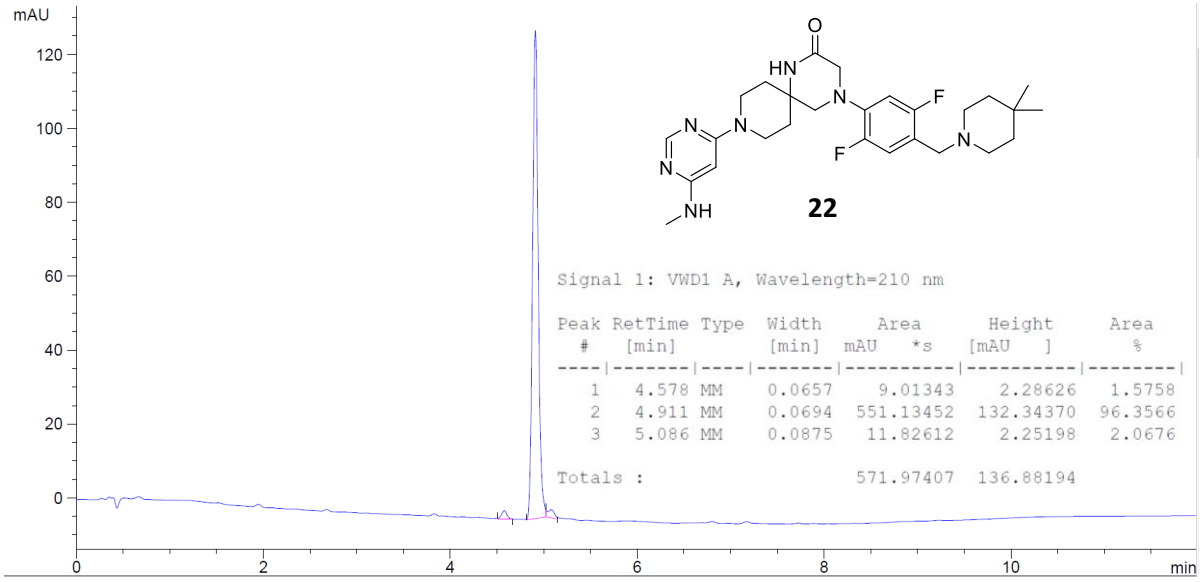
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	1.952	MM	0.0741	10.27604	2.31016	0.4240
2	3.863	MM	0.0763	40.63466	8.87495	1.6767
3	4.235	MM	0.0771	2360.62427	509.97342	97.4039
4	4.528	MM	0.0865	12.00709	2.31424	0.4954
Totals :				2423.54206	523.47277	



21

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.659	MM	0.0561	30.33698	9.01791	1.5309
2	3.931	MM	0.0765	1892.80066	412.60788	95.5136
3	4.301	MM	0.0961	19.17689	3.32693	0.9677
4	5.857	MM	0.1383	39.39307	4.74695	1.9878
Totals :				1981.70761	429.69967	



22

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.578	MM	0.0657	9.01343	2.28626	1.5758
2	4.911	MM	0.0694	551.13452	132.34370	96.3566
3	5.086	MM	0.0875	11.82612	2.25198	2.0676
Totals :				571.97407	136.88194	