

Supporting Information

6 β -N-Heterocyclic Substituted Naltrexamine Derivative BNAP: A Peripherally Selective Mixed MOR/KOR Ligand

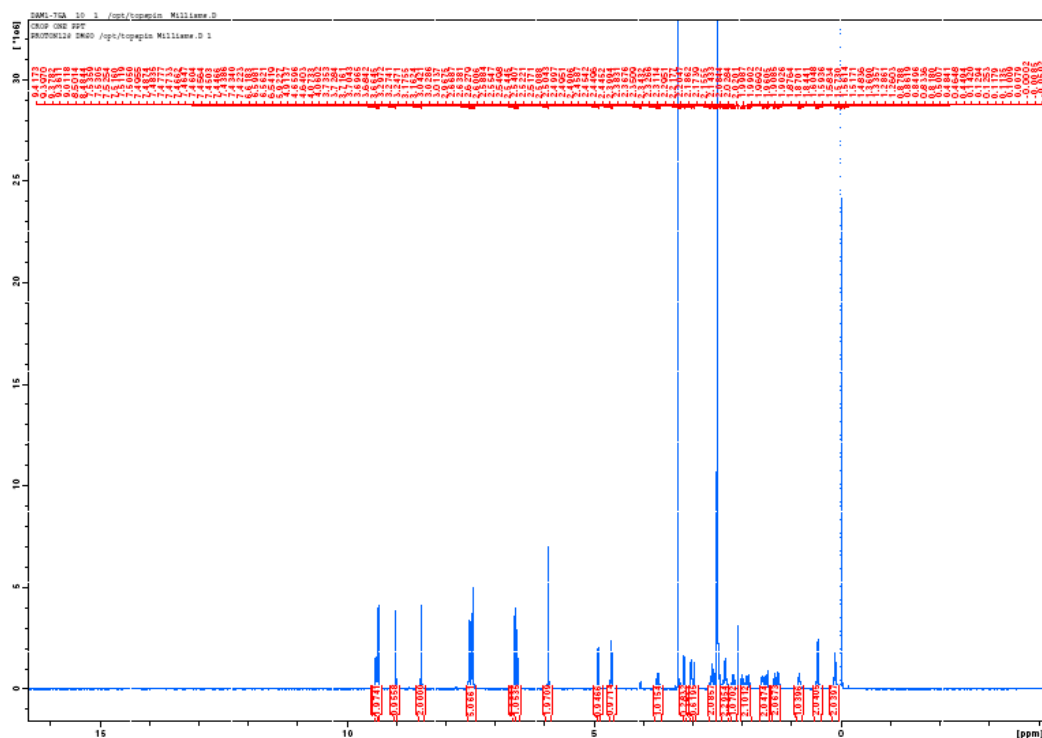
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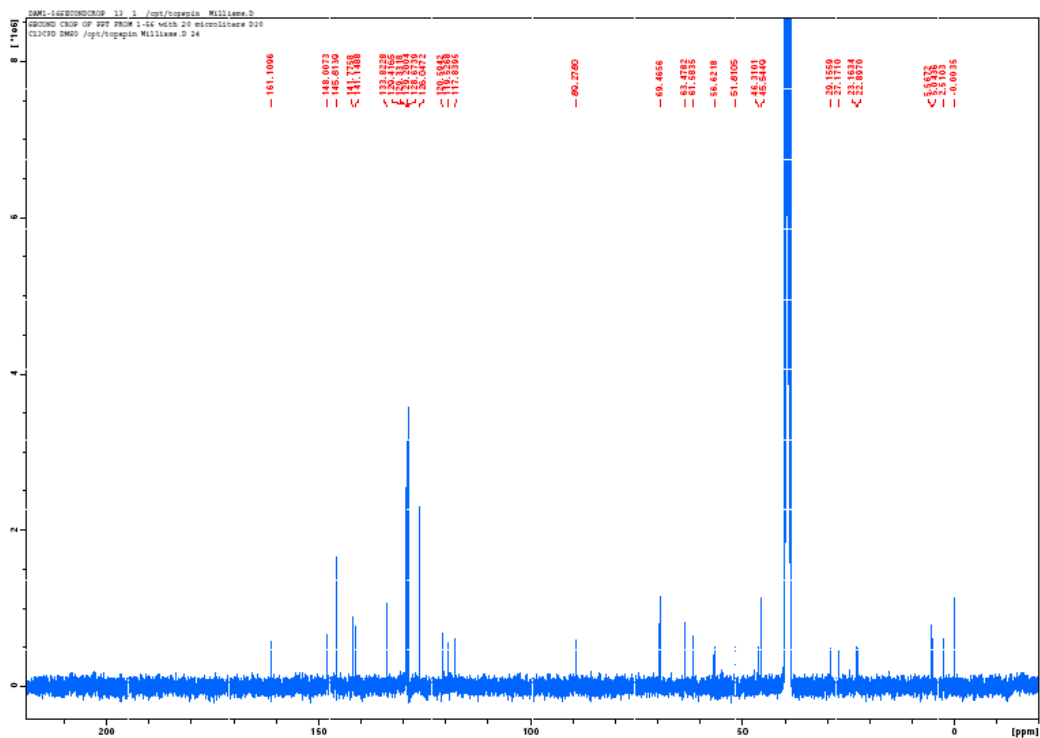
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BNAP characterization (including original spectra):

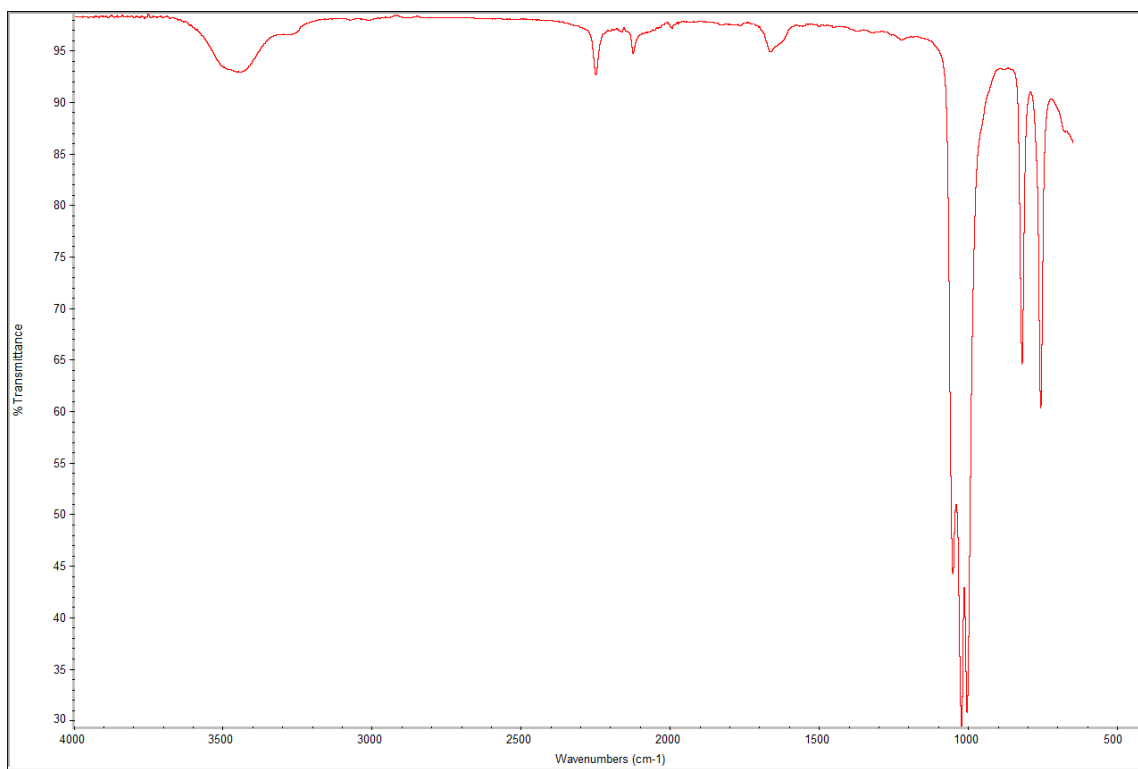
^1H NMR (400 MHz, DMSO- d_6): δ , 9.39-9.42 (1H, d, $J = 8.12$ Hz), 9.38–9.36 (2H, d, $J = 6.84$ Hz), 9.01 (1H, s), 8.50 - 8.48 (2H, d, $J = 6.8$ Hz), 7.48–7.25 (5H, m), 6.61 -6.59 (1H, d, $J = 8.0$ Hz), 6.56 - 6.54 (1H, d, $J = 8.1$ Hz), 5.92 (1H, s), 4.91 (1H, s), 4.65 - 4.64 (1H, d, $J = 7.7$), 3.74 - 3.66 (1H, m), 3.04-2.96 (3H, m) 2.68 - 2.51 (2H, m), 2.39 - 2.30 (2H, m), 2.24 - 2.14 (1H, m), 2.02 - 1.84 (2H, m) 1.63 - 1.26 (4H, m), 0.89 - 0.80 (1H, m), 0.51 - 0.43 (2H, m) 0.14 - 0.11 (2H, m).



^{13}C NMR (100 MHz, DMSO- d_6) δ 161.1, 148.0, 145.8, 141.8, 141.1, 133.8, 129.4, 129.2, 128.7, 126.0, 120.6, 119.5, 117.8, 89.3, 69.5, 63.5, 61.6, 56.6, 51.8, 46.3, 45.5, 29.2, 27.1, 23.2, 22.9, 5.6, 5.0, 2.5.



IR: 3433.29, 2251.06, 2125.05, 1661.09, 1052.38, 1023.83, 1004.68, 821.38, 758.75 .



HPLC:

File c:\star\data\dw\dw-1-75 230nm.run Filetype 325
WTOASCII Parameters: C:\star\WTOASCII.TXT
2 channels
Channel 1 210 nm in AU
Channel 2 230 nm in AU
Base rate 5.0000 Hz Bunch 1 Effective rate 5.00000 Hz. T = 0.003333 min.
4500 points from 0.000 to 15.000 minutes
Sampling every 4 point(s)
Printing points from 0.000 to 15.000 min, point 0 to 4499
Channels 1 to 2
No Results for Channel 1 - 210 nm
Results for Channel 2 - 230 nm
Title: Report Title
Run File: c:\star\data\dw\dw-1-75 230nm.run

Misc Info

Workstation: D92SSP71
Bus Address: 44
Run Time: 0.000 to 15.000 min.

Recalc Info

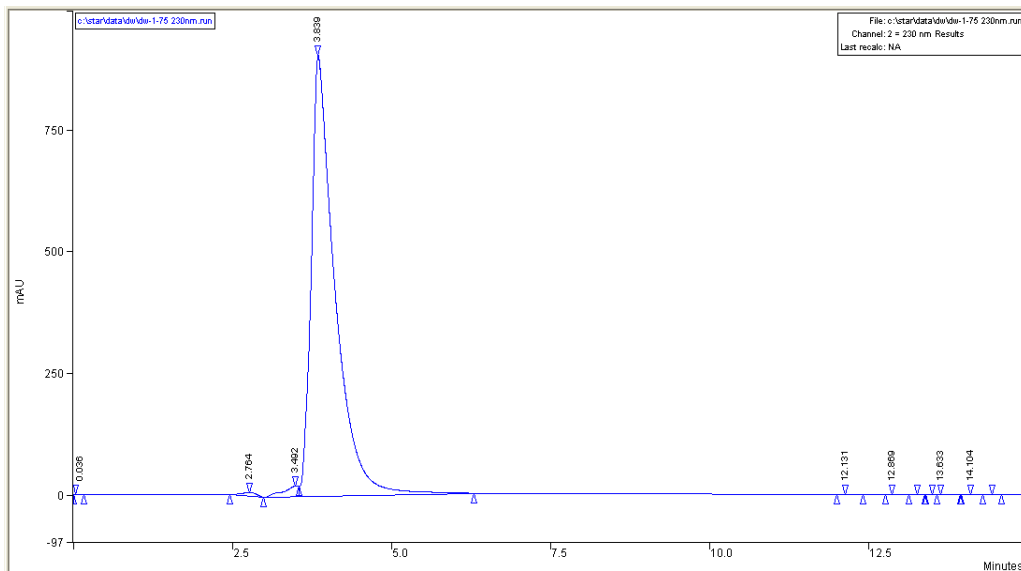
Instrument: Varian Star #1

Notes:

Sample Rate: 5.000 Hz
Measurement Type: 1 - Area
Calculation Type: 1 - %
Normalize Results: No

Peak Info for Channel 2

8 Peaks (tR Timeoffset RRT Sepcode Width Counts Result Name)
0.036 0.000 0.0000 BB 2.96 6065 0.002550
2.764 0.000 0.0000 BP 10.74 1117223 0.468161
3.492 0.000 0.0000 FV 16.16 3707044 1.553399
3.839 0.000 0.0000 VB 21.38 233770624 97.959175
12.131 0.000 0.0000 BB 14.64 12392 0.005193
12.869 0.000 0.0000 BP 7.50 10432 0.004371
13.633 0.000 0.0000 VP 0.00 6938 0.002907
14.104 0.000 0.0000 FV 0.00 10130 0.004245



Mass Spectrum: m/z calc. 538.27 obs. 538.60

snapshot #1-25 RT: 0.01-0.32 AV: 25 NL: 1.36E7
T: + p ESI Full ms [50.00-1000.00]

