

SUPPORTING INFORMATION

Identification of Spirodioxolane nsP2 Helicase Inhibitors with Antialphaviral Activity

Hans J. Oh,^{ab} John D. Sears,^{bc} Bose Muthu Ramalingam,^{ab} Rahman Shah Zaib Saleem,^{bd} Zachary W. Davis-Gilbert,^{ab} Mohammed Anwar Hossain,^{ab} Stella R. Moorman,^{bc} Durbadal Ohja,^{bc} Sabian A. Martinez,^{be} Jane E. Burdick,^{be} Rafael M. Couñago,^{abf} Nathaniel J. Moorman,^{bc} Mark T. Heise,^{bce} Matthew H. Todd,^{bd} and Timothy M. Willson^{*ab}

^a Structural Genomics Consortium, UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA

^b READDI AViDD Center, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA

^c Department of Microbiology and Immunology, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA

^d Structural Genomics Consortium, Department of Pharmaceutical and Biological Chemistry, School of Pharmacy, University College London, London WC1N 1AX, UK

^e Department of Genetics, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA

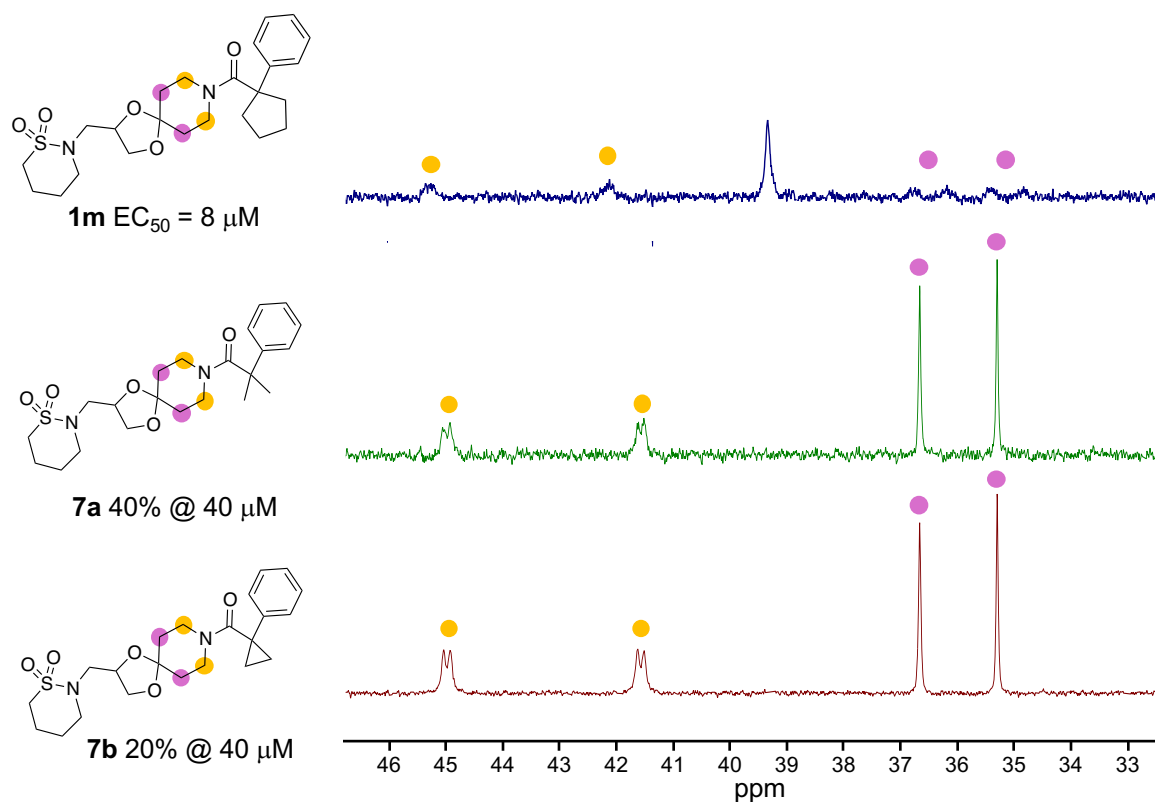
^f Center of Medicinal Chemistry, Center for Molecular Biology and Genetic Engineering, University of Campinas, 13083-886-Campinas, SP, Brazil

* E-mail: tim.willson@unc.edu

Table of Contents

		<u>Page</u>
Figure S1	¹³ C NMR of Acetamide Spirodioxolanes	S2
Figures S2–S161	NMR spectra of final compounds	S3–S82
Figures S162–S251	HPLC analyses	S83–S115

Fig. S1 ^{13}C NMR of Spirodioxolanes



^{13}C NMR spectra recorded at 126 MHz in CD_3OD at 25 °C. The region from 33–46 ppm is displayed, which contains the signals for the carbons on the piperidine ring (orange and magenta dots). For active analog **1m** (CHIKV-nLuc $\text{EC}_{50} = 8 \mu\text{M}$), signals from the four piperidine carbons are broad. The signal at 39.3 ppm is from two carbons of the cyclopentane ring. With weakly active analogs **7a** and **7b** (CHIKV-nLuc <50% at $40 \mu\text{M}$), sharp signals are seen from the carbons adjacent to the nitrogen of the piperidine (magenta dots) while the other piperidine carbons (orange dots) appear as doublets.

Figure S2: ^1H NMR (500 MHz, CD_3OD) for intermediate II

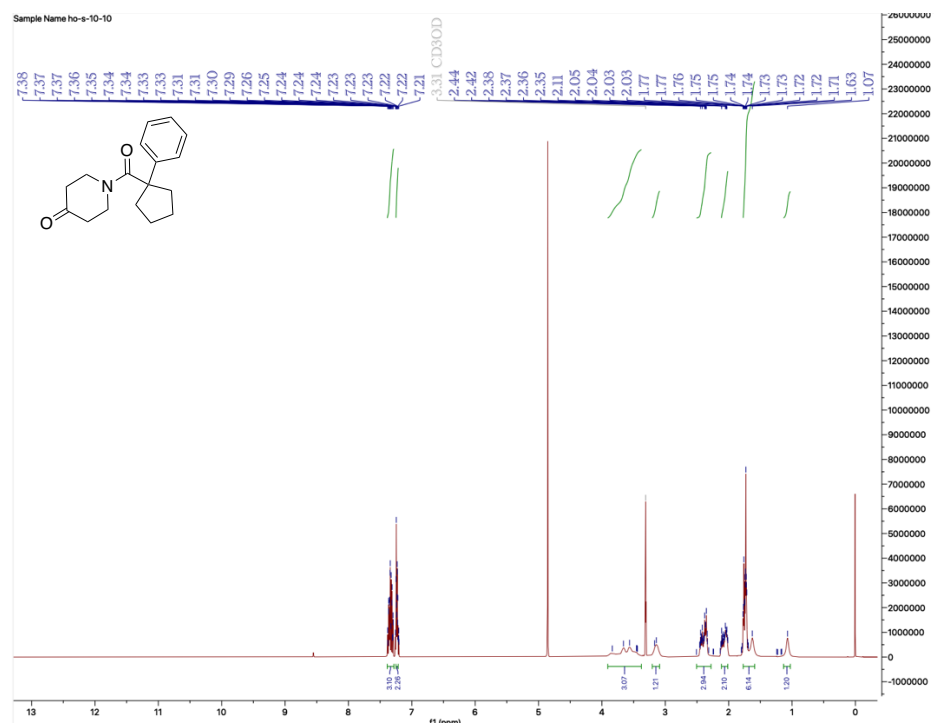
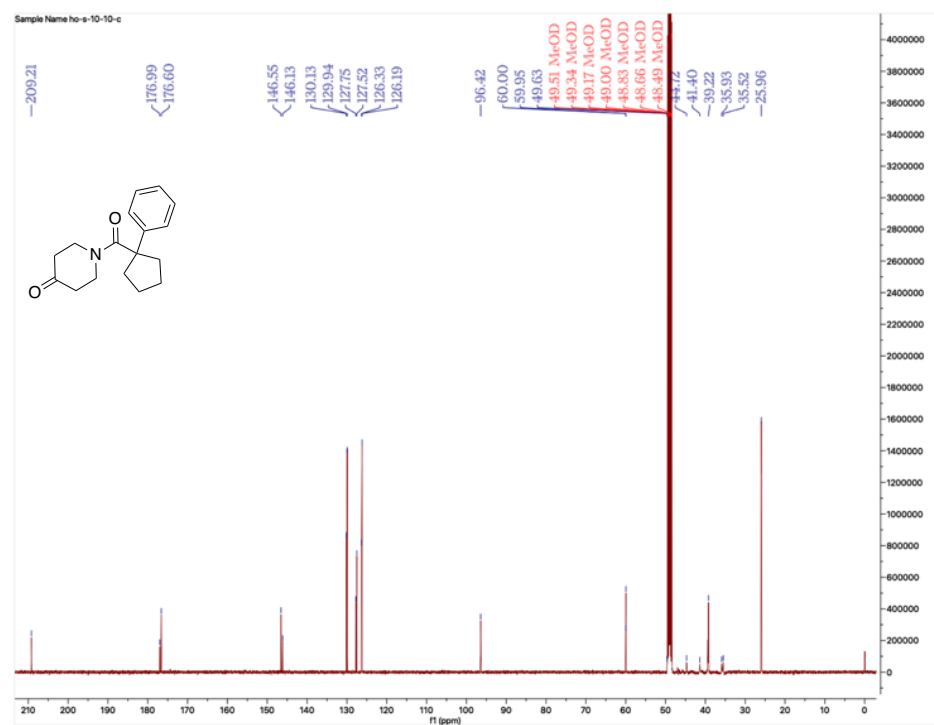


Figure S3: ^{13}C NMR (126 MHz, CD_3OD) for intermediate II



Chemical structure of compound 10a is shown above the spectrum. The spectrum displays peaks corresponding to the structure, with integration values indicated below the baseline and a list of chemical shifts (ppm) provided on the right side of the plot.

Sample Name ho-s-25-c

Chemical structure of 10a is shown. The spectrum displays peaks corresponding to the structure, with chemical shifts labeled in ppm:

- 176.57
- 146.52
- 146.45
- 129.94
- 127.55
- 127.52
- 126.20
- 126.18
- 108.97
- 76.36
- 67.62
- 59.91
- 49.85
- 49.63
- 49.51 MeOD
- 49.45
- 49.34 MeOD
- 49.28
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 48.33 MeOD
- 47.88
- 46.79
- 46.16
- 45.27
- 42.06
- 40.13
- 39.35
- 36.77
- 35.31
- 25.97
- 25.94
- 25.93

Figure S6: ^1H NMR (500 MHz, CD_3OD) for **1b**

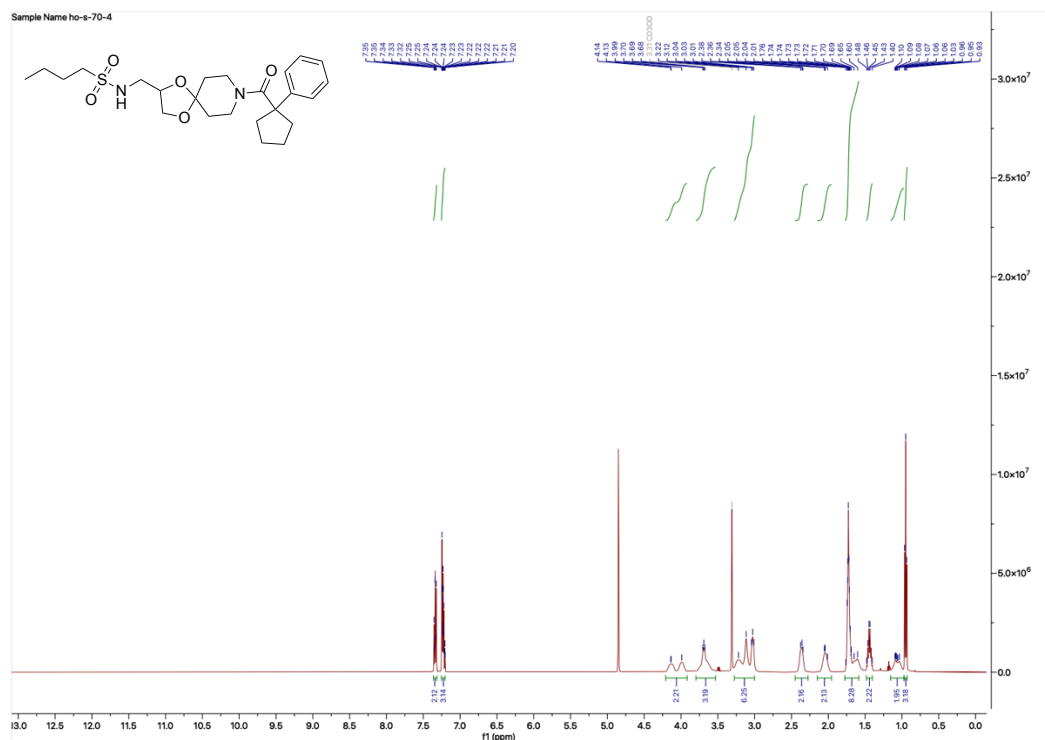


Figure S7: ^{13}C NMR (126 MHz, CD_3OD) for **1b**

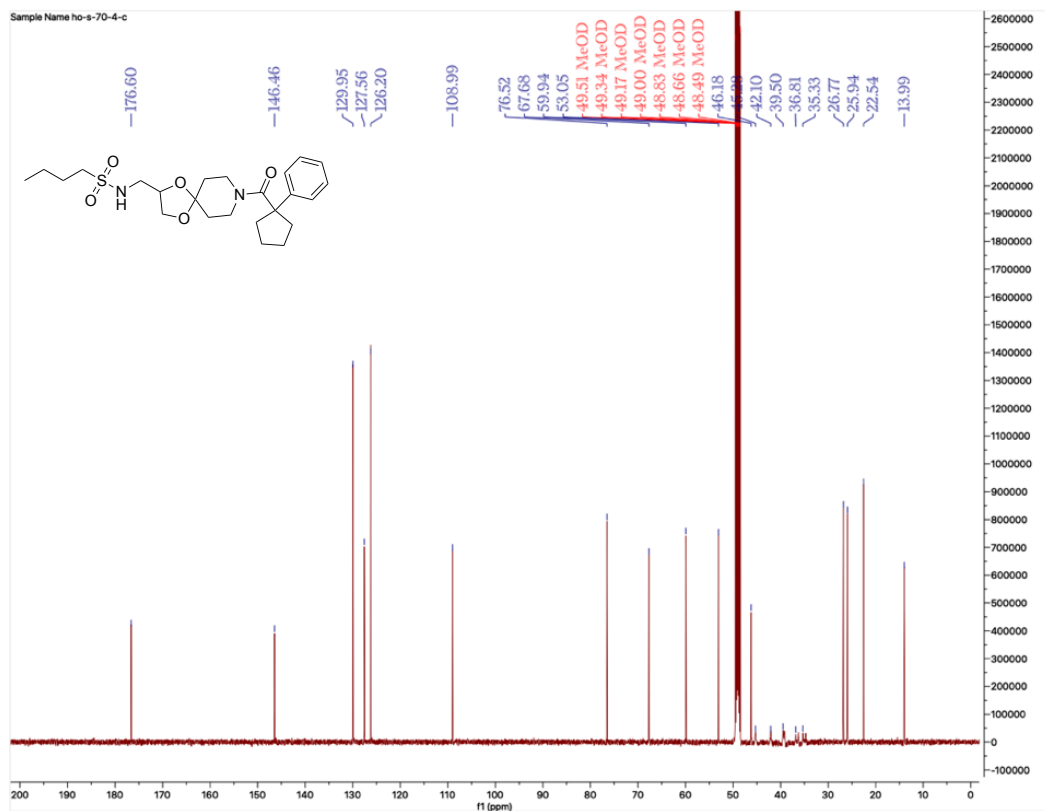


Figure S8: ^1H NMR (500 MHz, CD_3OD) for **1c**

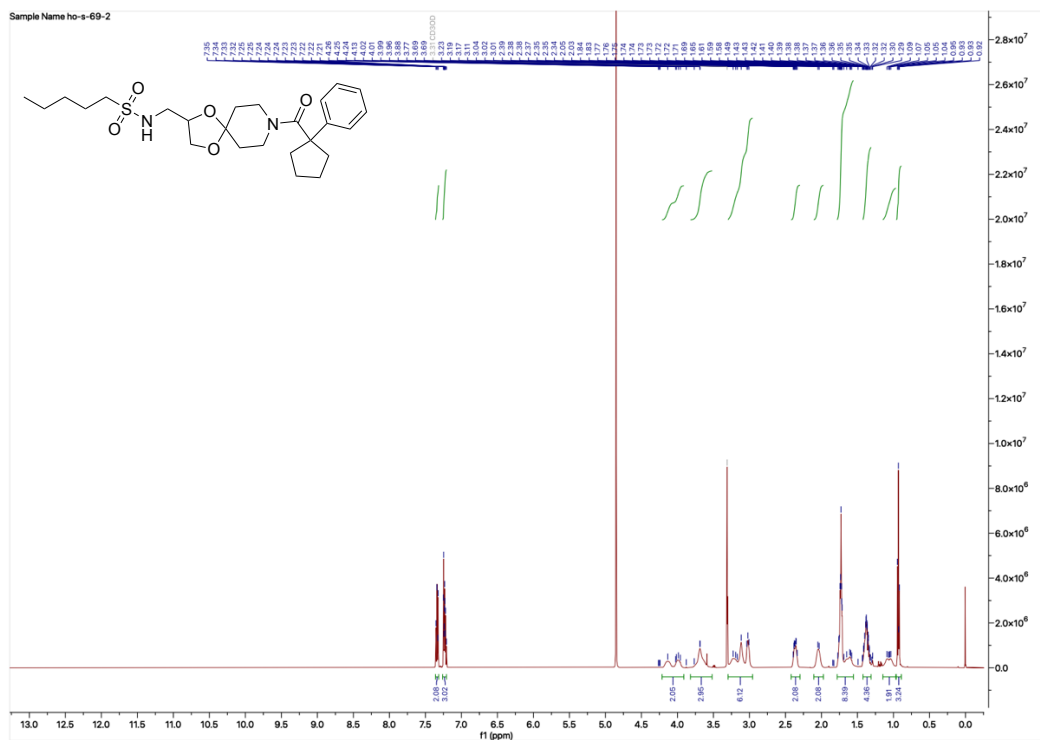


Figure S9: ^{13}C NMR (126 MHz, CD_3OD) for **1c**

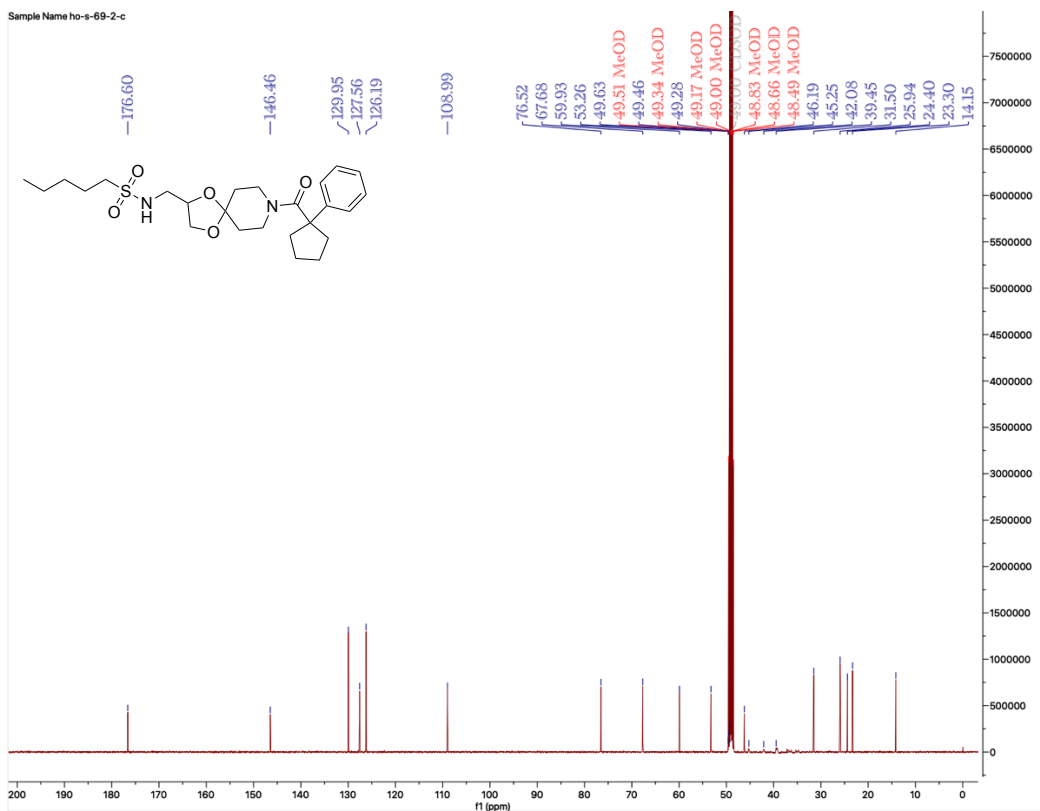


Figure S10: ^1H NMR (500 MHz, CD_3OD) for **1d**

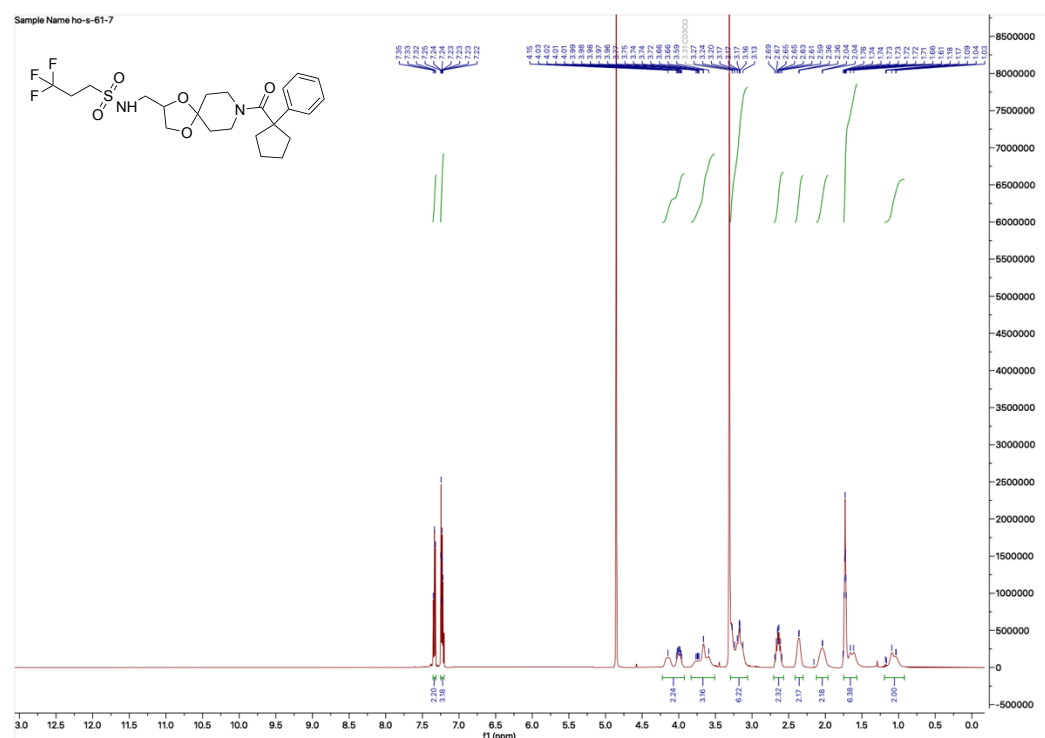


Figure S11: ^{13}C NMR (126 MHz, CD_3OD) for **1d**

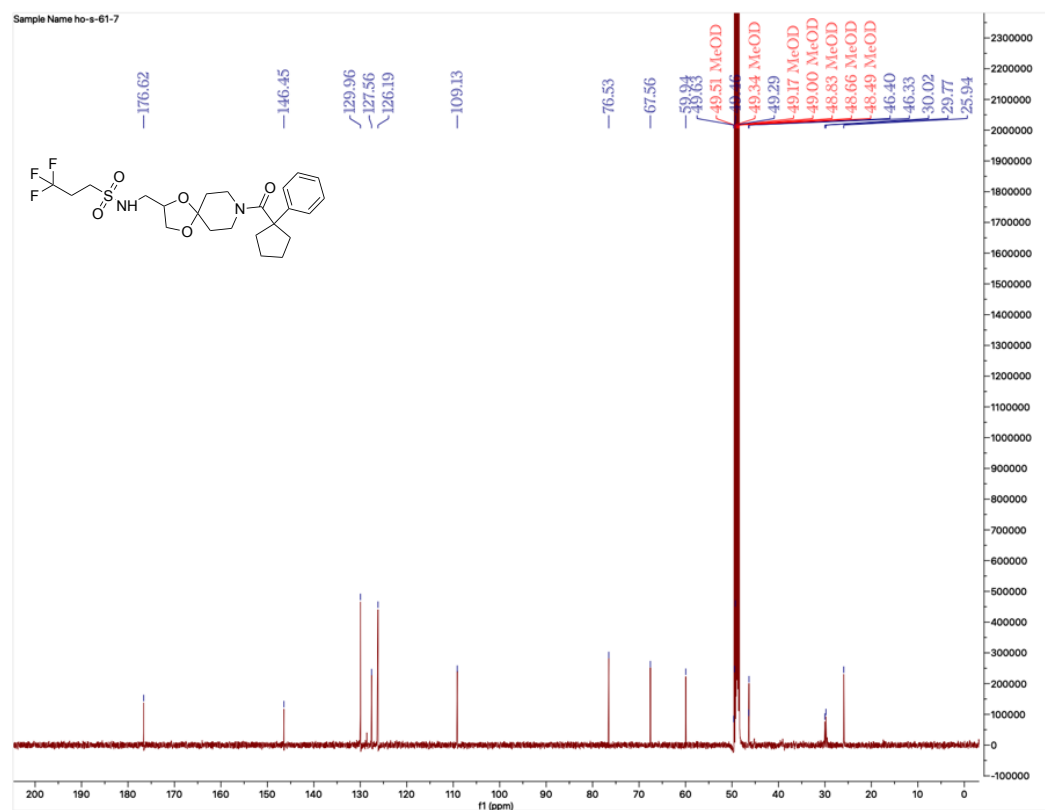


Figure S12: ^1H NMR (500 MHz, CD_3OD) for **1e**

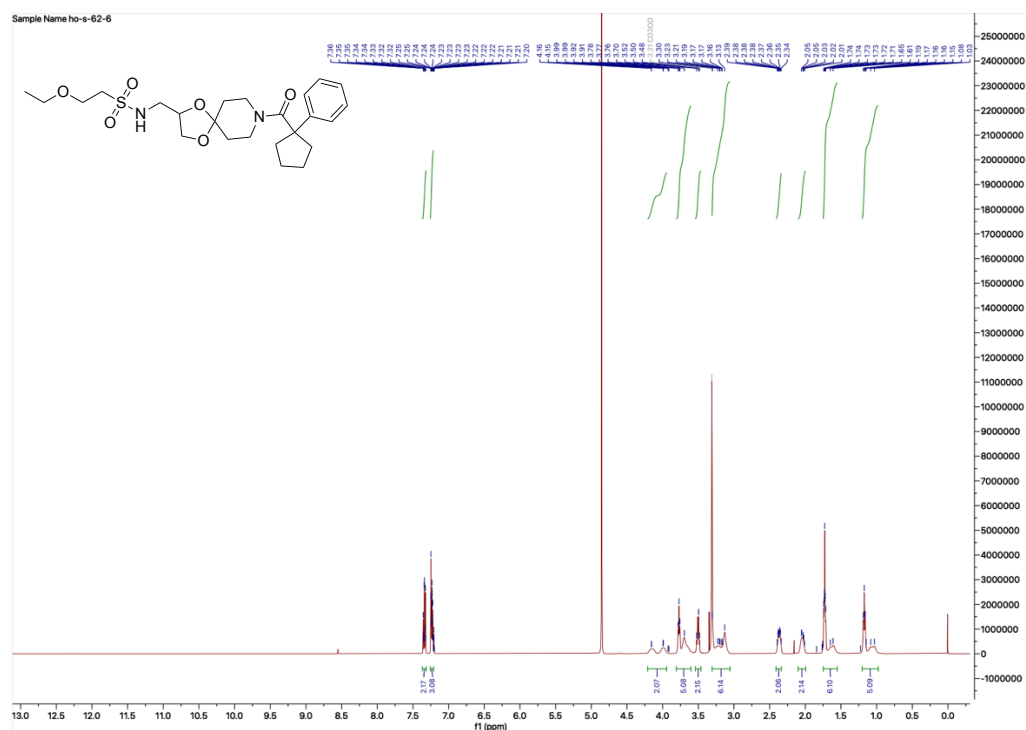
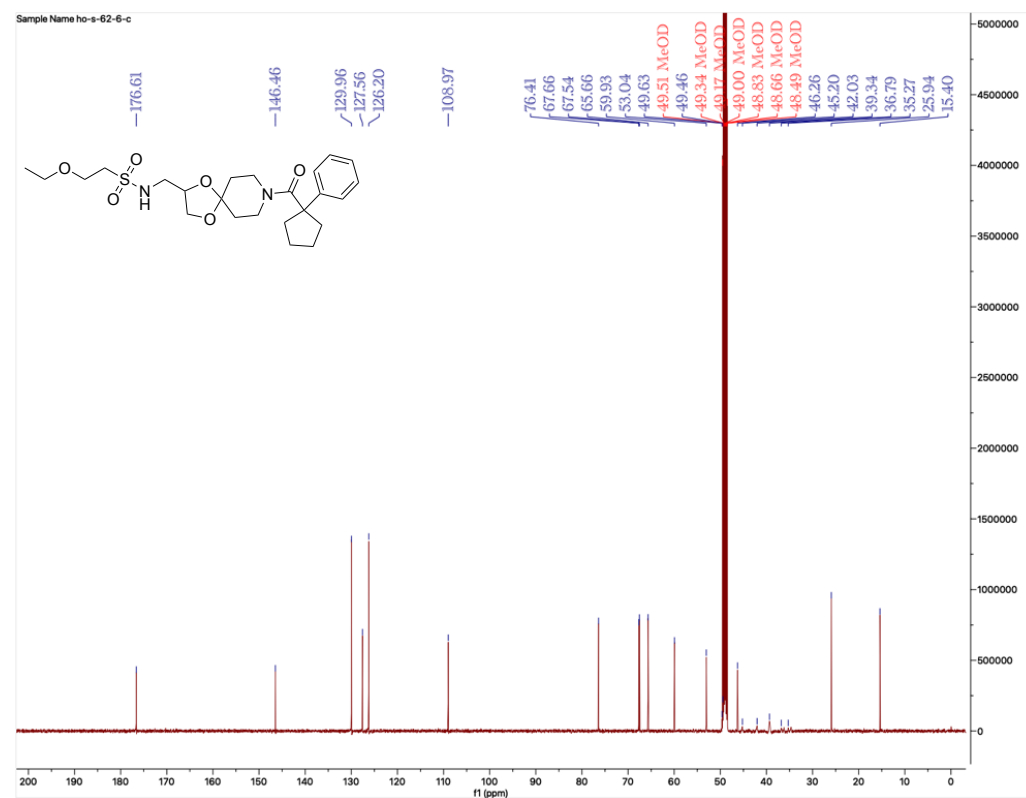


Figure S13: ^{13}C NMR (126 MHz, CD_3OD) for **1e**



[illegible]

Sample Name ho-a-83-1-c

Chemical structure of compound 10:

O=C1C(=O)N1CC2(CCC2)C(=O)N(CCC(F)(F)F)C3=CC=CC=C3

¹H NMR (CDCl₃) peaks (ppm):

- ~7.35 (m, 2H, aromatic)
- ~7.25 (m, 2H, aromatic)
- ~7.15 (m, 2H, aromatic)
- ~4.00 (s, 3H, OCH₃)
- ~3.90 (s, 3H, OCH₃)
- ~3.80 (s, 3H, OCH₃)
- ~3.70 (s, 3H, OCH₃)
- ~3.60 (s, 3H, OCH₃)
- ~3.50 (s, 3H, OCH₃)
- ~3.40 (s, 3H, OCH₃)
- ~3.30 (s, 3H, OCH₃)
- ~3.20 (s, 3H, OCH₃)
- ~3.10 (s, 3H, OCH₃)
- ~3.00 (s, 3H, OCH₃)
- ~2.90 (s, 3H, OCH₃)
- ~2.80 (s, 3H, OCH₃)
- ~2.70 (s, 3H, OCH₃)
- ~2.60 (s, 3H, OCH₃)
- ~2.50 (s, 3H, OCH₃)
- ~2.40 (s, 3H, OCH₃)
- ~2.30 (s, 3H, OCH₃)
- ~2.20 (s, 3H, OCH₃)
- ~2.10 (s, 3H, OCH₃)
- ~2.00 (s, 3H, OCH₃)
- ~1.90 (s, 3H, OCH₃)
- ~1.80 (s, 3H, OCH₃)
- ~1.70 (s, 3H, OCH₃)
- ~1.60 (s, 3H, OCH₃)
- ~1.50 (s, 3H, OCH₃)
- ~1.40 (s, 3H, OCH₃)
- ~1.30 (s, 3H, OCH₃)
- ~1.20 (s, 3H, OCH₃)
- ~1.10 (s, 3H, OCH₃)
- ~1.00 (s, 3H, OCH₃)
- ~0.90 (s, 3H, OCH₃)
- ~0.80 (s, 3H, OCH₃)
- ~0.70 (s, 3H, OCH₃)
- ~0.60 (s, 3H, OCH₃)
- ~0.50 (s, 3H, OCH₃)
- ~0.40 (s, 3H, OCH₃)
- ~0.30 (s, 3H, OCH₃)
- ~0.20 (s, 3H, OCH₃)
- ~0.10 (s, 3H, OCH₃)
- ~0.00 (s, 3H, OCH₃)

¹³C NMR (CDCl₃) peaks (ppm):

- ~160.00 (C=O)
- ~150.00 (C=O)
- ~140.00 (C=O)
- ~130.00 (aromatic)
- ~125.00 (aromatic)
- ~120.00 (aromatic)
- ~115.00 (aromatic)
- ~110.00 (aromatic)
- ~105.00 (aromatic)
- ~100.00 (aromatic)
- ~95.00 (aromatic)
- ~90.00 (aromatic)
- ~85.00 (aromatic)
- ~80.00 (aromatic)
- ~75.00 (aromatic)
- ~70.00 (aromatic)
- ~65.00 (aromatic)
- ~60.00 (aromatic)
- ~55.00 (aromatic)
- ~50.00 (aromatic)
- ~45.00 (aromatic)
- ~40.00 (aromatic)
- ~35.00 (aromatic)
- ~30.00 (aromatic)
- ~25.00 (aromatic)
- ~20.00 (aromatic)
- ~15.00 (aromatic)
- ~10.00 (aromatic)
- ~5.00 (aromatic)
- ~0.00 (aromatic)

[illegible]

Sample Name ho-s-57

Chemical structure of compound 10: ClCCCN(=O)C1CC2(C1)CCN(C2)C(=O)C3CCCC3

Peak assignments (ppm):

- 176.62
- 146.47
- 129.97
- 127.57
- 126.21
- 109.05
- 76.50
- 67.65
- 59.94
- 50.70
- 49.63
- 49.51 MeOD
- 49.46
- 49.34 MeOD
- 49.28
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 43.85
- 28.24
- 25.99

Figure S18: ^1H NMR (500 MHz, CD_3OD) for **1h**

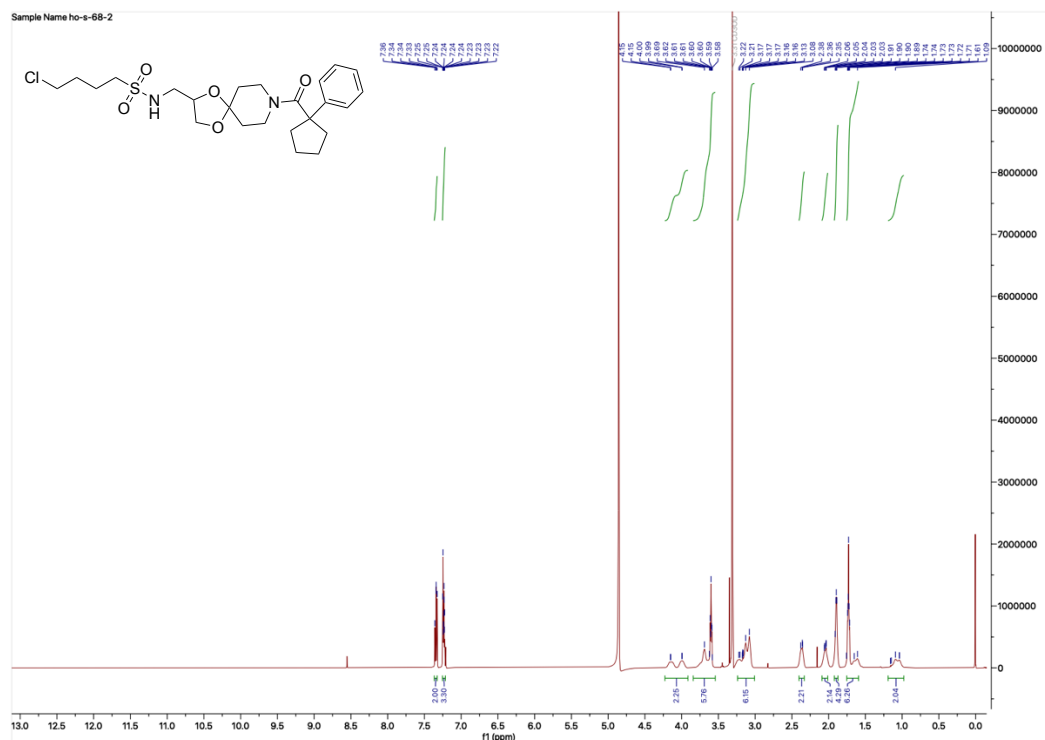


Figure S19: ^{13}C NMR (126 MHz, CD_3OD) for **1h**

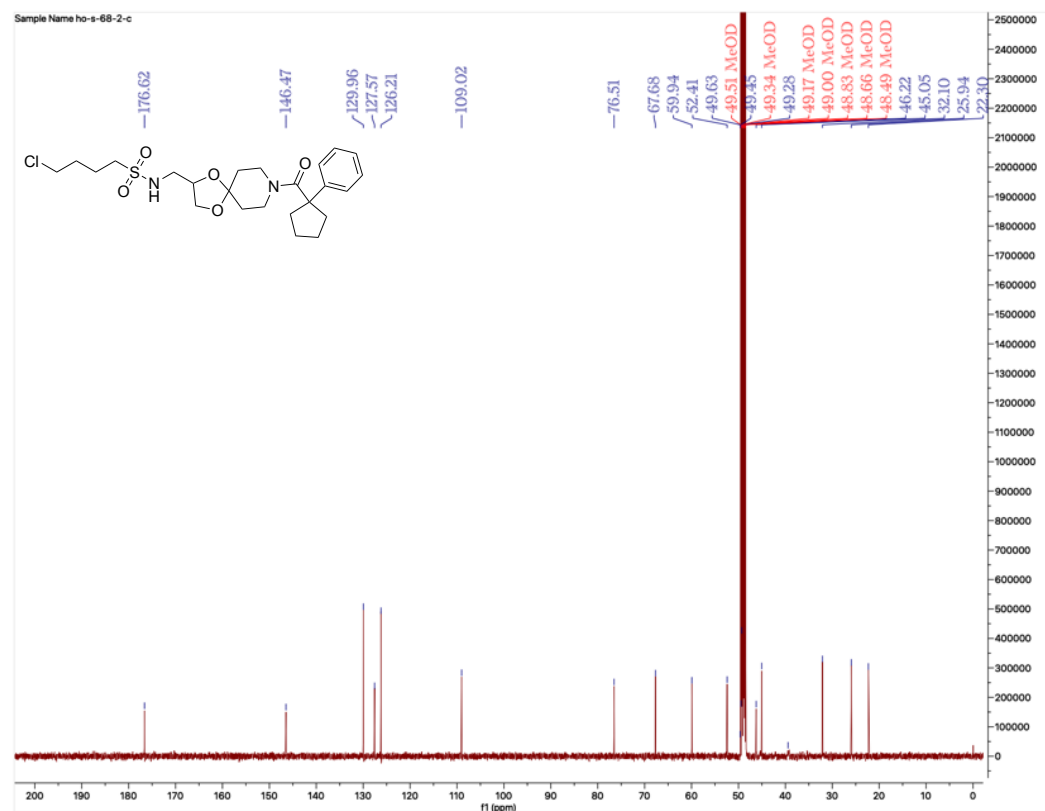


Figure S20: ^1H NMR (500 MHz, CD_3OD) for **1i**

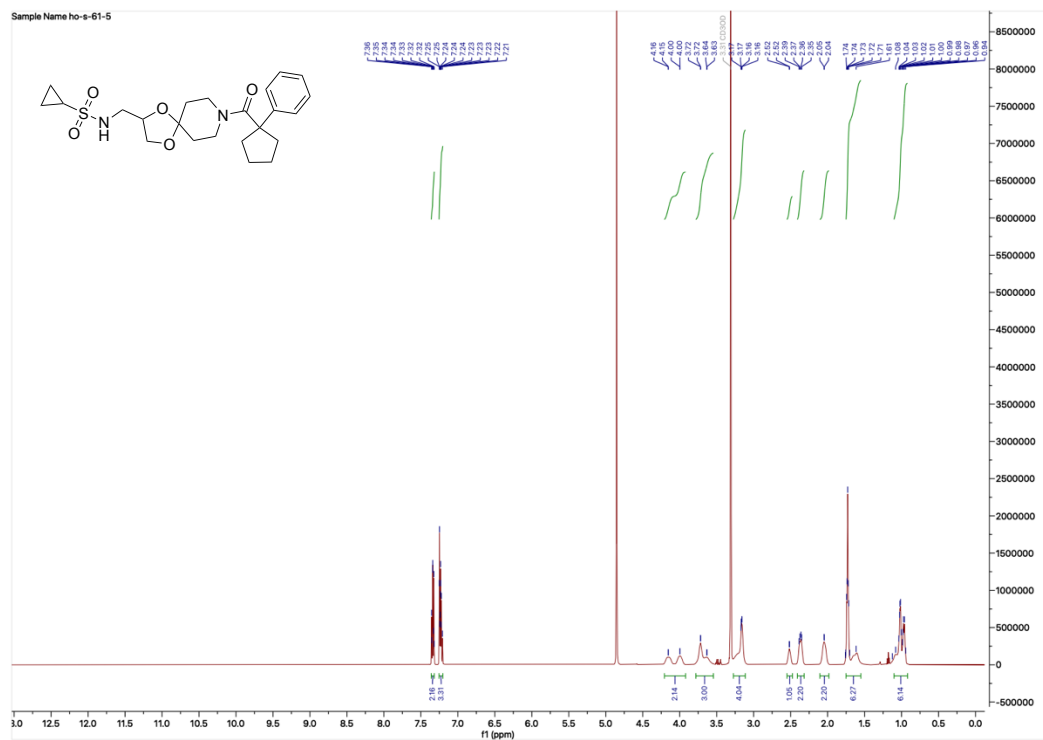
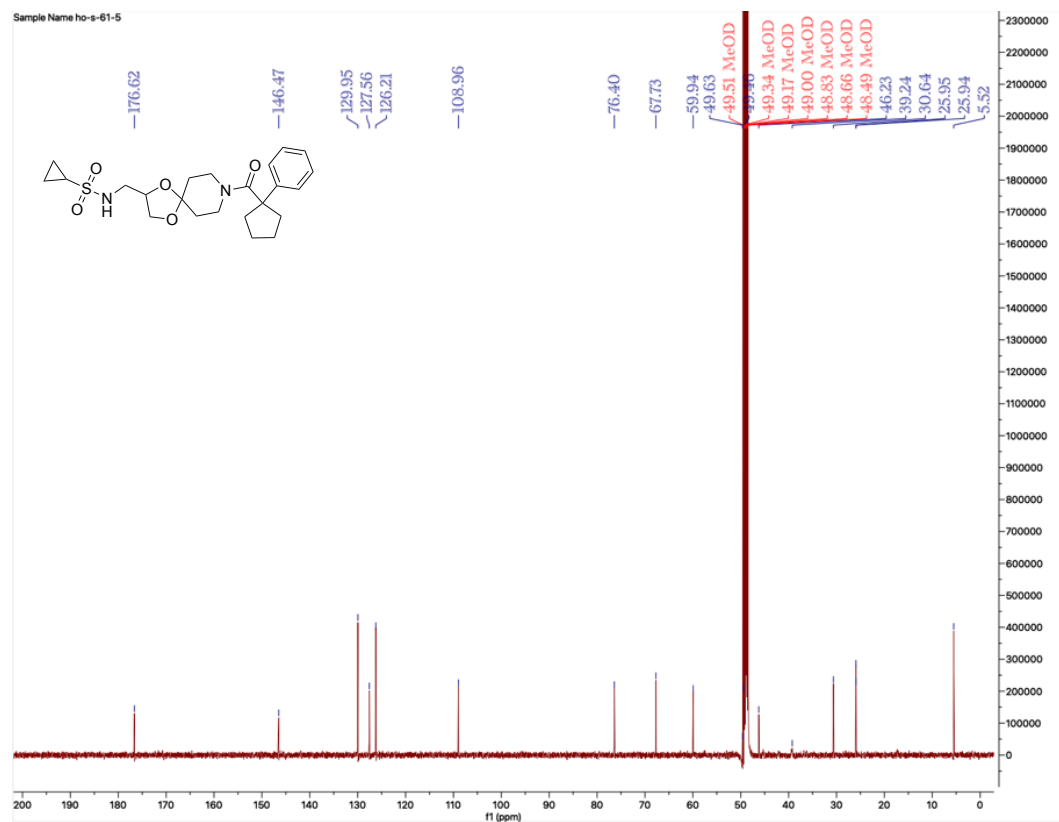


Figure S21: ^{13}C NMR (126 MHz, CD_3OD) for **1i**



Chemical structure of compound 10: O=C1N(CCC2(CCC2)C3=CC=CC=C3)CCOC1CCN(C4CC4)C5=CC=CC=C5

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (0.0 to 13.0), and the y-axis represents the intensity (0 to 1,700,000). The spectrum shows several peaks corresponding to the structure, with integration values indicated below the baseline.

Integration values (from left to right): 2.01, 2.03, 2.07, 1.96, 2.07, 2.03, 2.05, 5.96, 2.88, 2.03, 2.03.

Sample Name ho-s-66-1-c

Chemical structure of the compound (10) is shown in the top left corner. The structure is a complex molecule featuring a cyclopropane ring, a sulfonamide group, a morpholine ring, and a cyclopentanone ring.

Chemical shifts (ppm) are listed on the right side of the spectrum:

- 7.658, 7.679, 7.593, 58.24, 49.51 MeOD, 49.34 MeOD, 49.17 MeOD, 49.00 MeOD, 48.86 MeOD, 48.49 MeOD, 46.31, 45.26, 42.12, 39.24, 36.80, 35.32, 25.95, 6.25, 4.82, 4.79

Chemical shifts (ppm) are also listed on the left side of the spectrum:

- 176.61, 146.47, 129.96, 127.56, 126.20, 108.97

Sample Name ho-s61-6

Chemical structure of compound 10: C1CCC(CC1)C(=O)N2CCOC(C2)S(=O)(=O)C3CCCCC3

¹H NMR spectrum (CDCl₃) showing peaks and integration values:

Chemical Shift (ppm)	Integration
7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.17, 7.16, 7.15, 7.14, 7.13, 7.12, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24, 1.23, 1.22, 1.21, 1.20, 1.19, 1.18, 1.17, 1.16, 1.15, 1.14, 1.13, 1.12, 1.11, 1.10, 1.09, 1.08, 1.07, 1.06, 1.05, 1.04, 1.03, 1.02, 1.01, 1.00, 0.99, 0.98, 0.97, 0.96, 0.95, 0.94, 0.93, 0.92, 0.91, 0.90, 0.89, 0.88, 0.87, 0.86, 0.85, 0.84, 0.83, 0	

Sample Name ho-s61-6

Chemical structure of compound 10: C1CCC(CC1)C(=O)N2CC3OC(CS(=O)(=O)C4CCCCC4)C2O3

¹³C NMR spectrum (ppm) peaks (from left to right):

- 176.62
- 146.47
- 129.95
- 127.56
- 126.20
- 108.97
- 76.68
- 67.70
- 62.01
- 59.94
- 49.51 MeOD
- 49.45
- 49.34 MeOD
- 49.28
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 46.41
- 27.61
- 26.40
- 26.21
- 25.93

[illegible]

Sample Name ho-s-55-c

Chemical structure of compound 10: O=C1C2(CCCC2)N(C1)C3OCC(S(=O)(=O)N3)CO4

¹³C NMR spectrum (CDCl₃) showing peaks (ppm):

- 176.59
- 146.46
- 129.96
- 127.56
- 126.21
- 109.08
- 75.96
- 67.93
- 59.93
- 49.93
- 49.63
- 49.51 MeOD
- 49.45
- 49.34 MeOD
- 49.28
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 47.06
- 45.27
- 42.11
- 39.32
- 36.80
- 35.34
- 25.93
- 19.97

Figure S28: ^1H NMR (500 MHz, CD_3OD) for **1m**

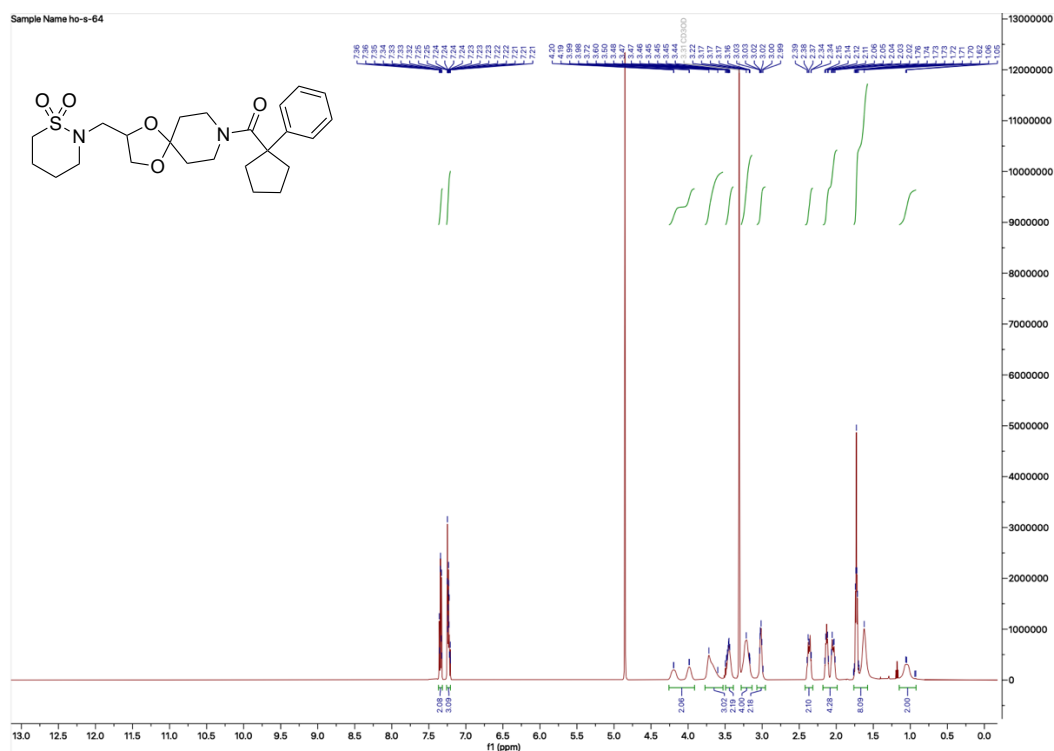
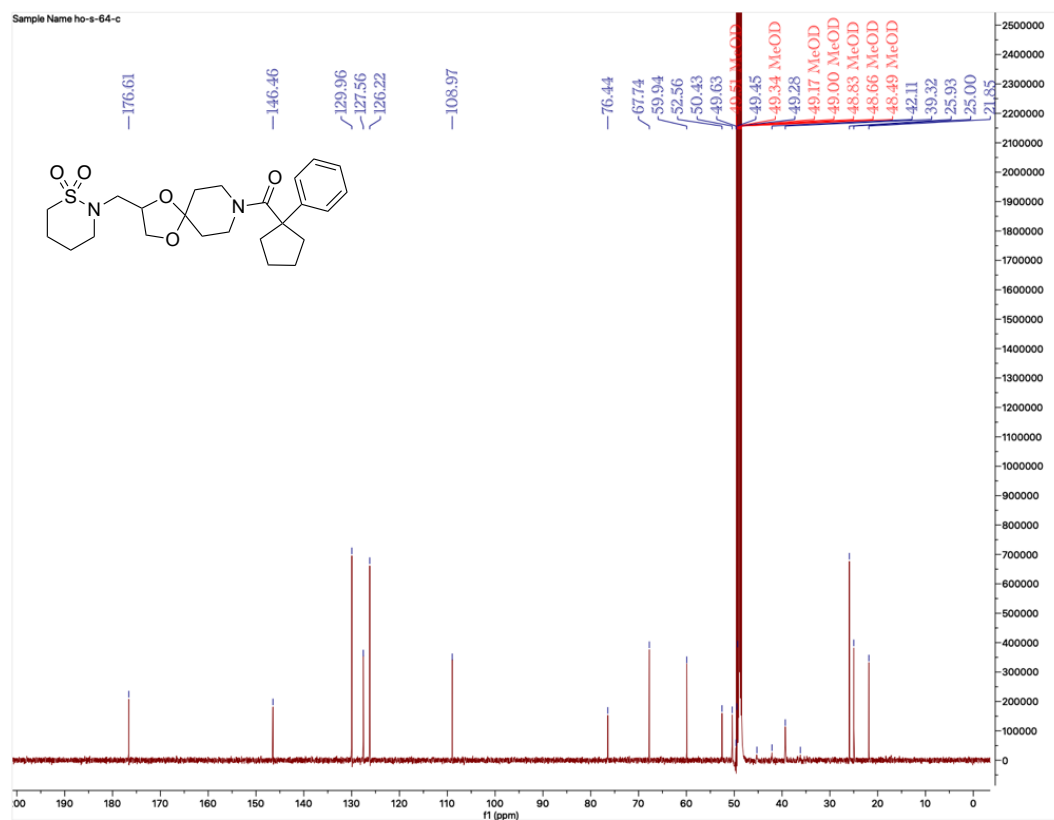


Figure S29: ^{13}C NMR (126 MHz, CD_3OD) for **1m**



[illegible]

h0-s-24-2

Chemical structure of compound 24 is shown. The ^{13}C NMR spectrum (CDCl₃) shows the following chemical shifts (ppm):

- 174.60
- 145.69
- 143.88
- 136.75
- 129.96
- 128.92
- 127.19
- 126.43
- 125.12
- 108.41
- 77.41 (CDCl₃)
- 77.16 (CDCl₃)
- 76.91 (CDCl₃)
- 74.06
- 66.36
- 60.54
- 58.65
- 38.31
- 25.36
- 21.68
- 14.35

[illegible]

Sample Name ho-s-62-3-c

Chemical structure of compound 10b is shown in the top left corner.

¹³C NMR peaks (ppm) are labeled as follows:

- 176.56
- 146.64
- 146.44
- 140.64
- 130.19
- 129.93
- 129.56
- 128.63
- 128.59
- 128.32
- 127.53
- 126.17
- 108.93
- 75.86
- 67.72
- 59.87
- 59.63
- 49.51 MeOD
- 49.45
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 46.39
- 39.29
- 25.93

Figure S34: ^1H NMR (500 MHz, CD_3OD) for **2c**

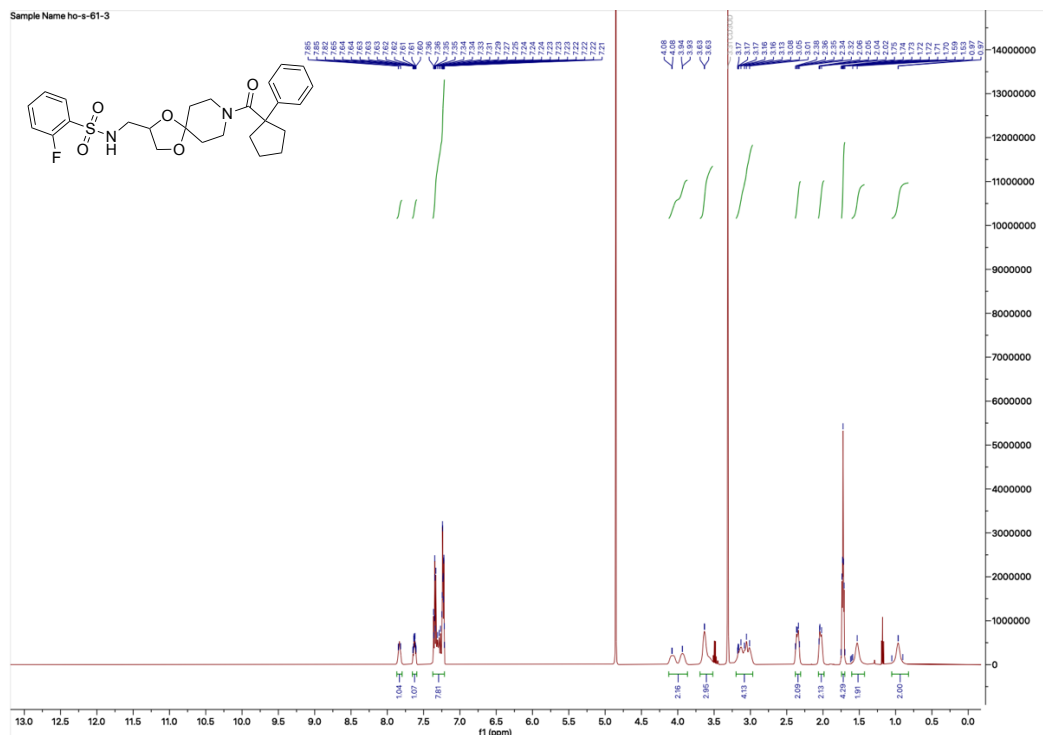


Figure S35: ^{13}C NMR (126 MHz, CD_3OD) for **2c**

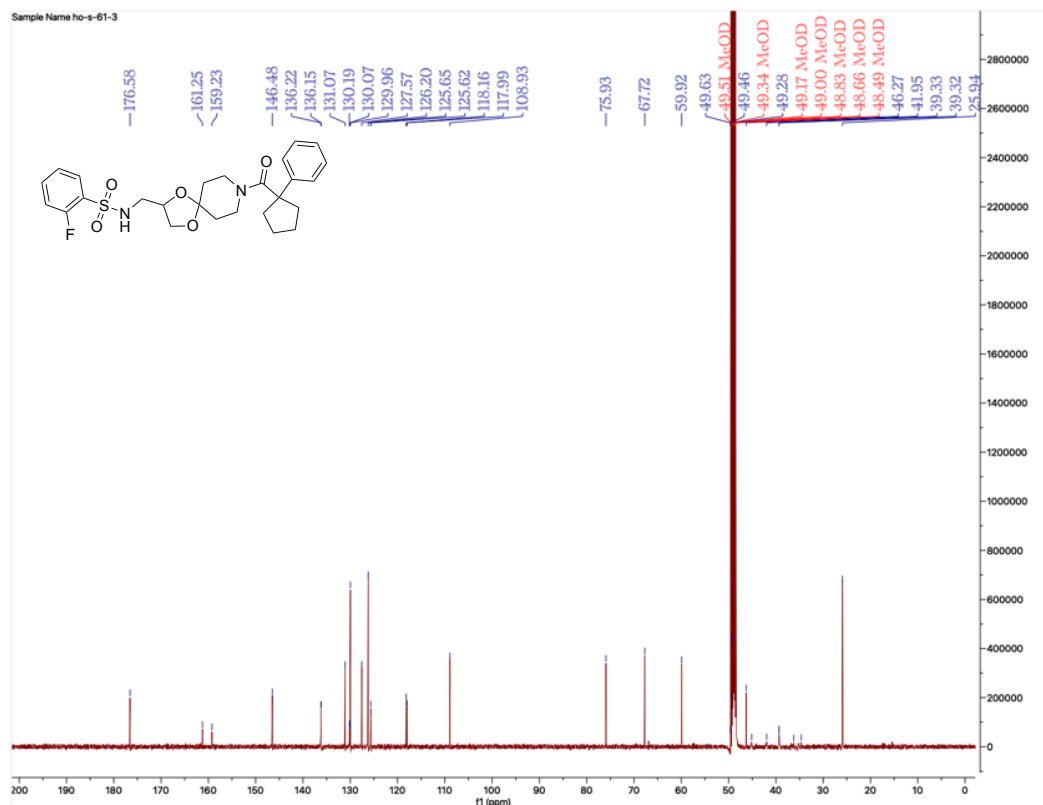


Figure S36: ^1H NMR (500 MHz, CD_3OD) for **2d**

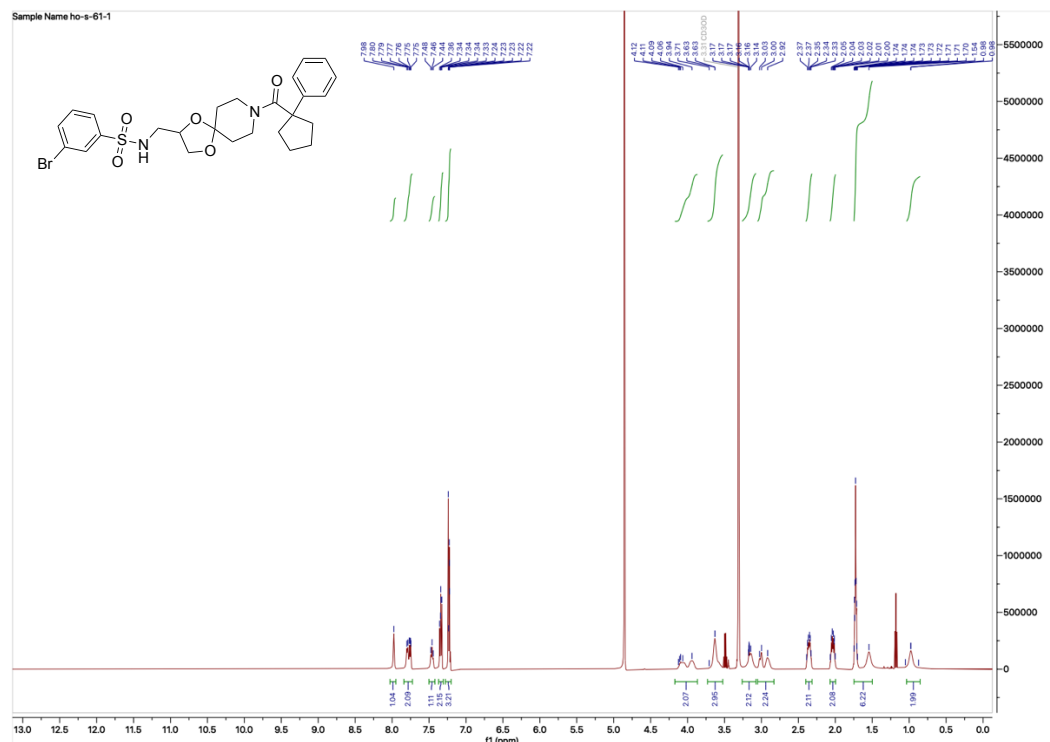


Figure S37: ^{13}C NMR (126 MHz, CD_3OD) for **2d**

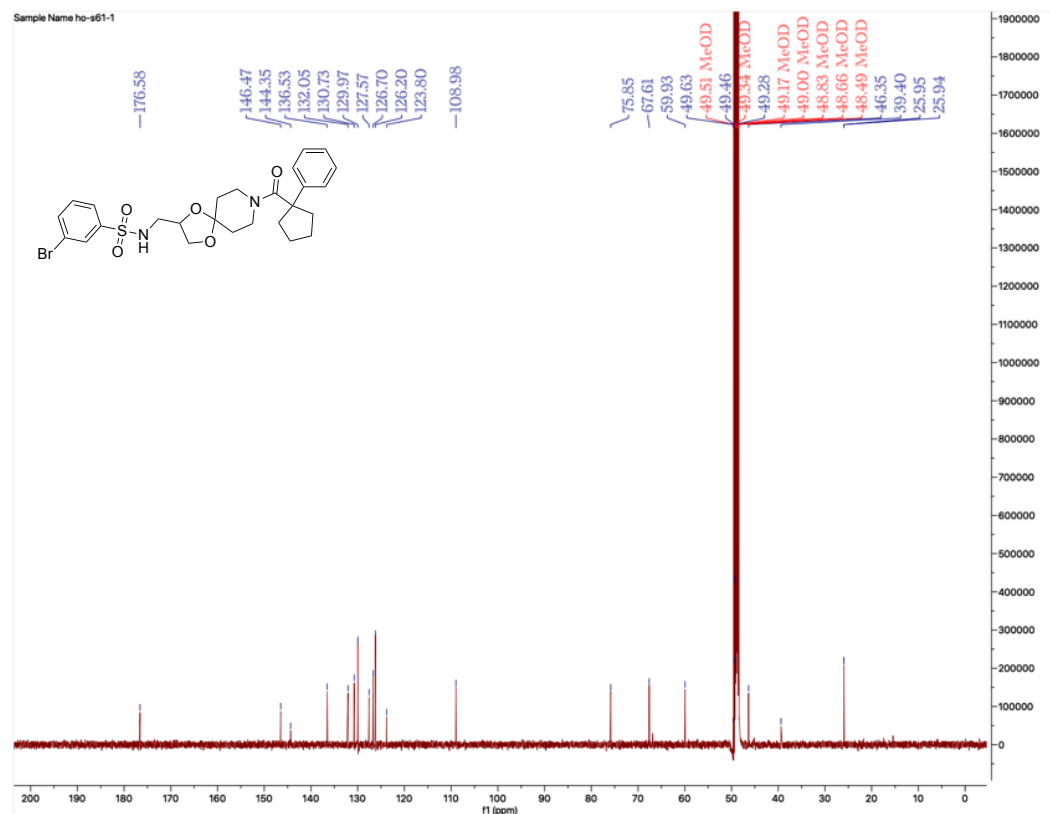


Figure S38: ^1H NMR (500 MHz, CD_3OD) for **2e**

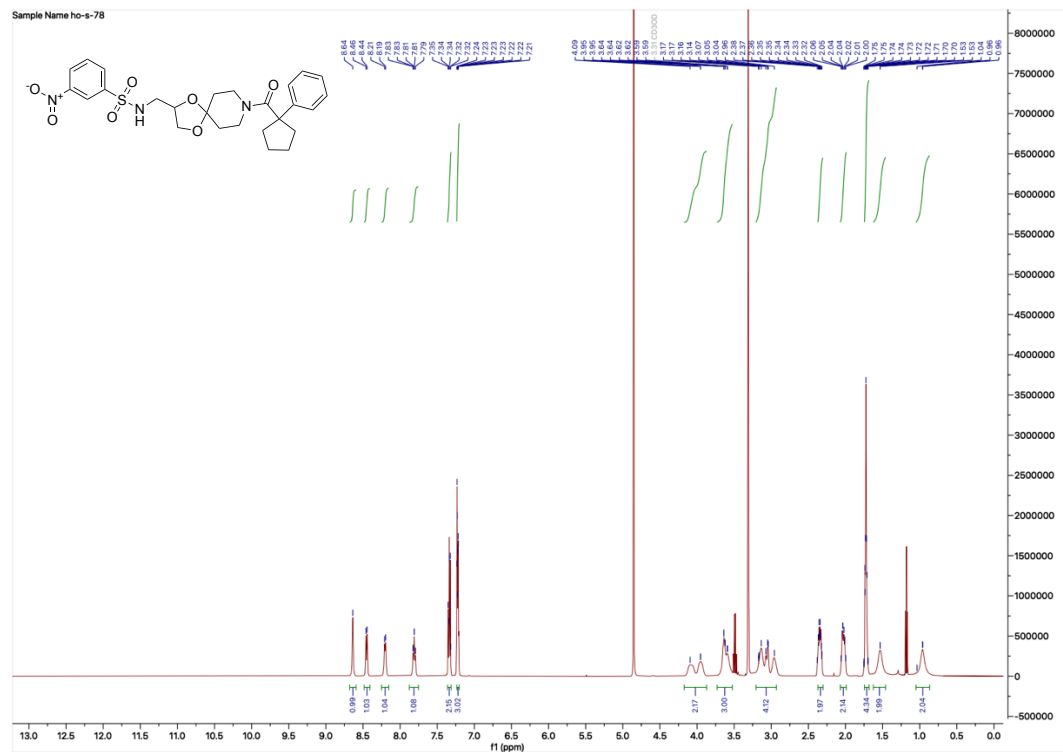
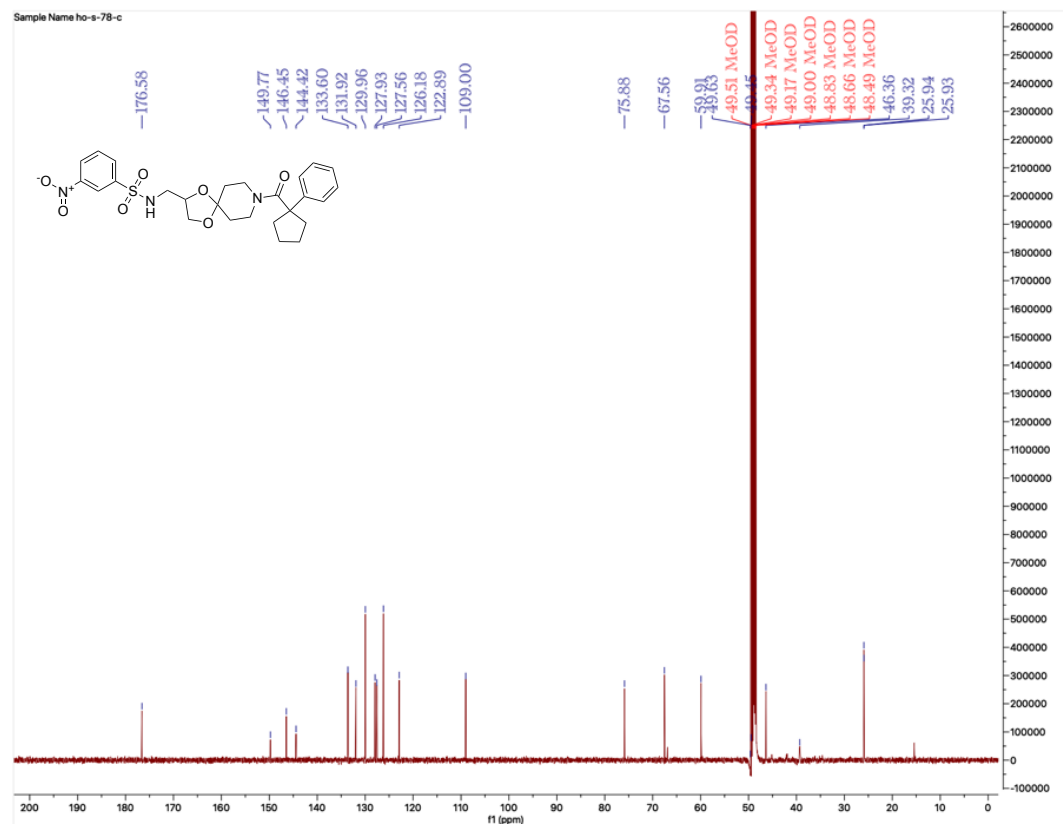


Figure S39: ^{13}C NMR (126 MHz, CD_3OD) for **2e**



[illegible]

Sample Name ho-a-62-2-c

Chemical structure of compound 10a-62-2-c is shown above the spectrum:

CN(C(=O)c1ccc(cc1)S(=O)(=O)NC2COC3CCN(C3C2)C(=O)C4CCCC4)c5ccccc5

¹H NMR spectrum (MeOD) showing chemical shifts (ppm) and integration values:

Chemical Shift (ppm)	Integration
7.5.89	75.89
6.7.66	67.66
5.9.91	59.91
4.9.63	49.63
4.9.51 MeOD	49.51
4.9.46	49.46
4.9.34 MeOD	49.34
4.9.28	49.28
4.9.17 MeOD	49.17
4.9.00 MeOD	49.00
4.8.83 MeOD	48.83
4.8.66 MeOD	48.66
4.8.49 MeOD	48.49
4.6.30	46.30
4.5.17	45.17
4.2.06	42.06
3.9.38	39.38
3.9.27	39.27
3.6.73	36.73
3.4.66	34.66
2.7.02	27.02
2.5.95	25.95
2.5.93	25.93
1.08.95	108.95
1.26.19	126.19
1.26.84	126.84
1.27.55	127.55
1.29.95	129.95
1.30.60	130.60
1.30.61	130.61
1.31.90	131.90
1.36.70	136.70
1.42.87	142.87
1.46.46	146.46
1.68.85	168.85
1.76.56	176.56

Figure S42: ^1H NMR (500 MHz, CD_3OD) for **2g**

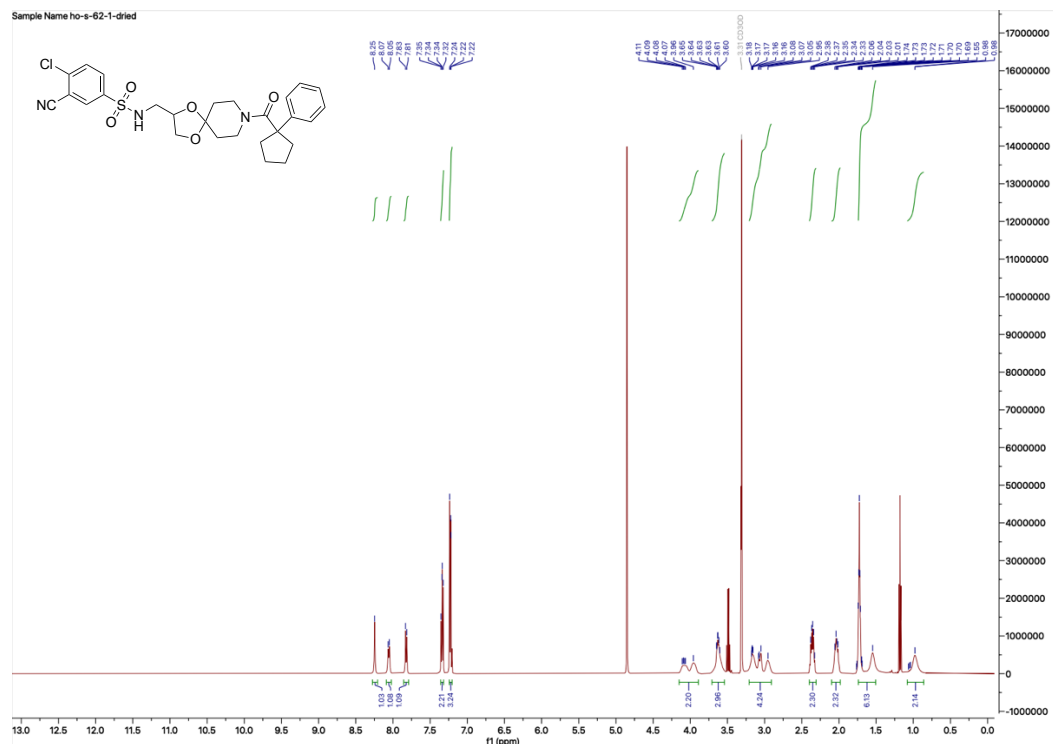
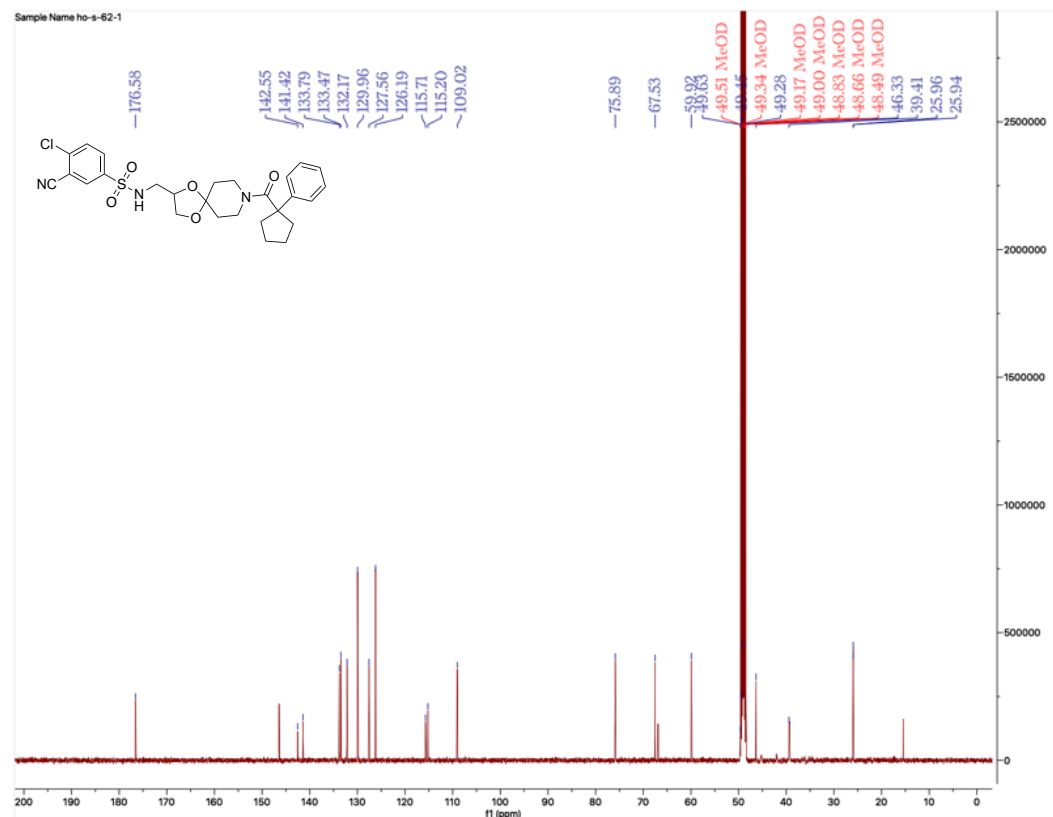


Figure S43: ^{13}C NMR (126 MHz, CD_3OD) for **2g**



Sample Name ho-s-62-5

Chemical structure of compound 10: O=[N+]([O-])c1ccc(cc1Cl)S(=O)(=O)NC[C@H]2O[C@@H]3CC[C@H]4C(=O)N(C5CCCC5)[C@H]3O2

¹H NMR spectrum (400 MHz, CDCl₃) of compound 10. The x-axis represents the chemical shift (δ) in ppm, ranging from 0.0 to 13.0. The y-axis represents the intensity. The spectrum shows several peaks, with integration values indicated below the baseline.

Chemical structure of compound 10 is shown in the top left corner.

Sample Name ho-s-62-5-c

Chemical structure of the compound (10) is shown in the top left corner. The structure is a complex molecule featuring a benzene ring with a nitro group (NO₂) and a chlorine atom (Cl). This ring is connected via a sulfonamide group (SO₂NH) to a bicyclic system consisting of a five-membered ring fused to a six-membered ring, which is further connected to a carbonyl group (C=O) and a cyclopentyl ring.

Key peaks in the spectrum are labeled with their chemical shifts (ppm):

- 176.57
- 147.70
- 146.46
- 141.60
- 139.49
- 134.35
- 129.97
- 128.89
- 127.58
- 126.67
- 126.18
- 108.99
- 76.01
- 67.61
- 59.91
- 49.51 MeOD
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 46.58
- 39.50
- 39.16
- 25.92

Figure S46: ^1H NMR (500 MHz, CD_3OD) for **2i**

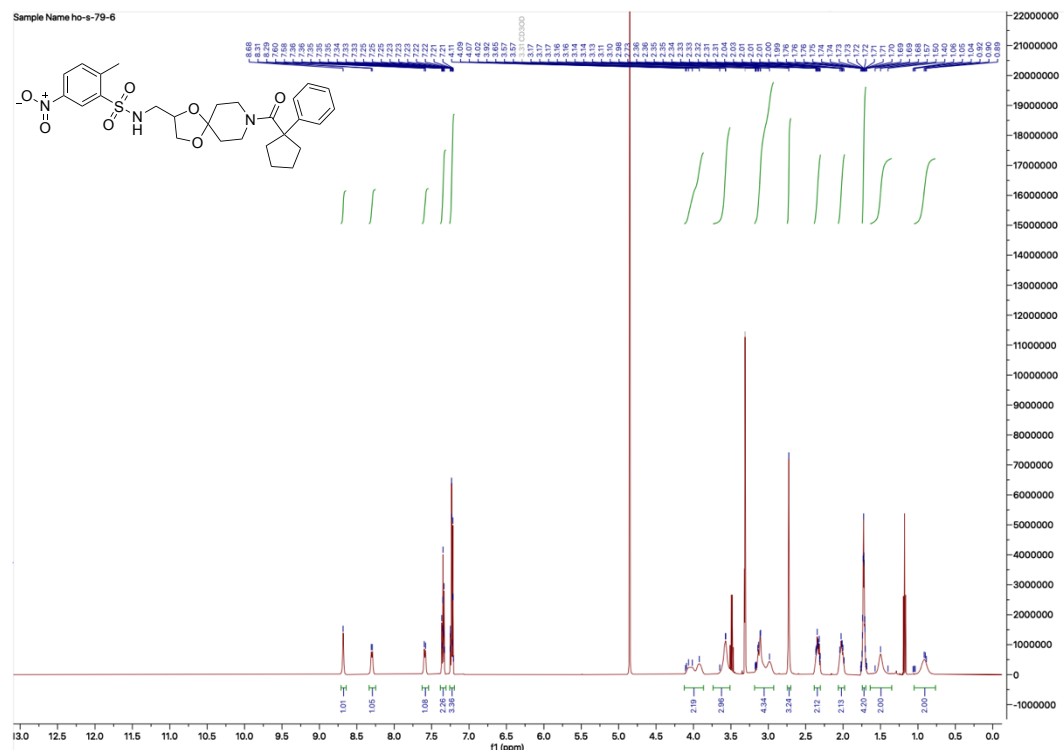


Figure S47: ^{13}C NMR (126 MHz, CD_3OD) for **2i**

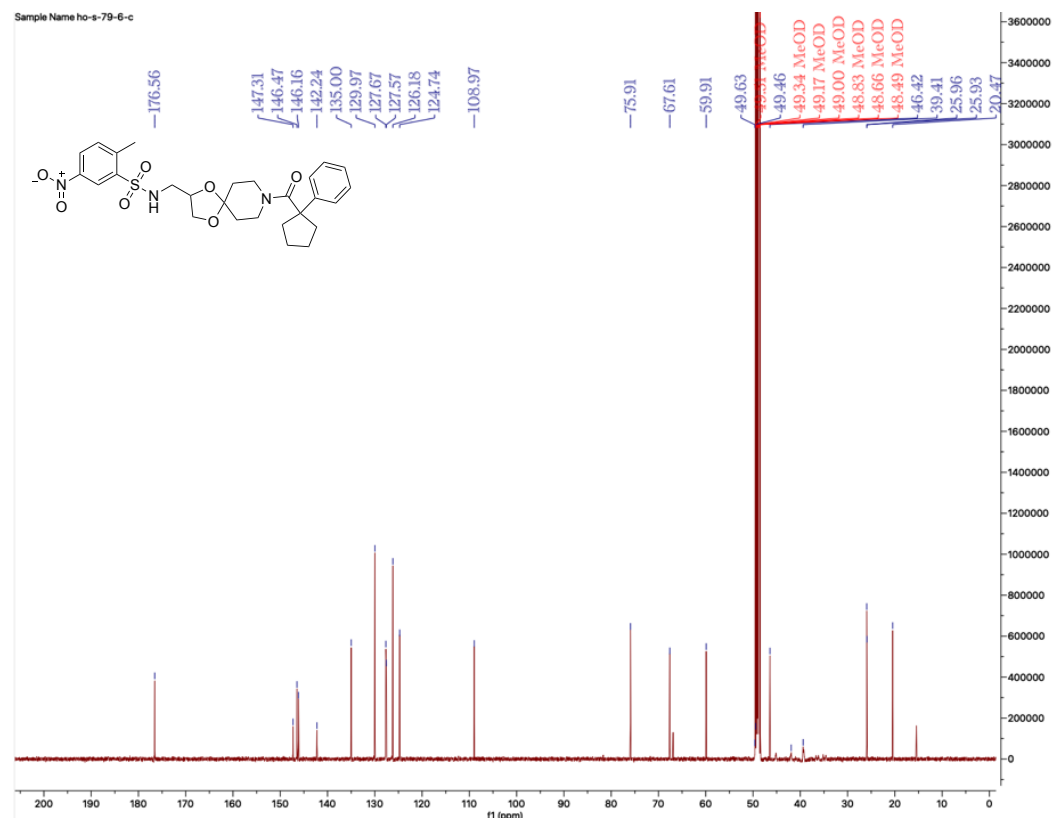


Figure S48: ^1H NMR (500 MHz, CD_3OD) for **2j**

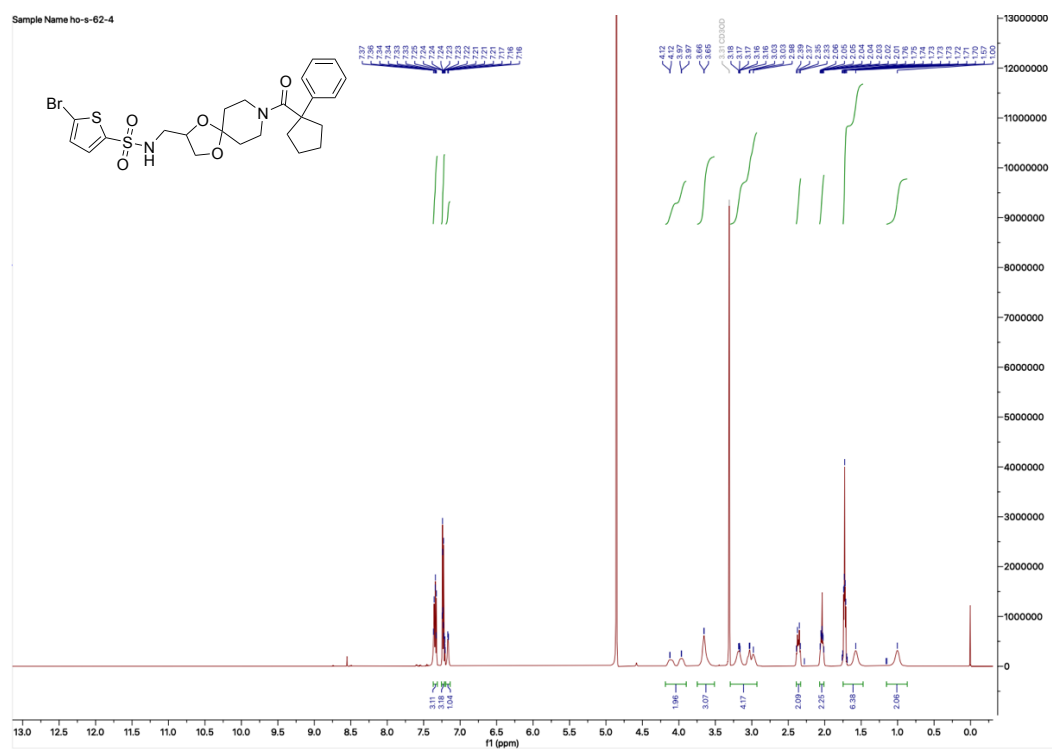


Figure S49: ^{13}C NMR (126 MHz, CD_3OD) for **2j**

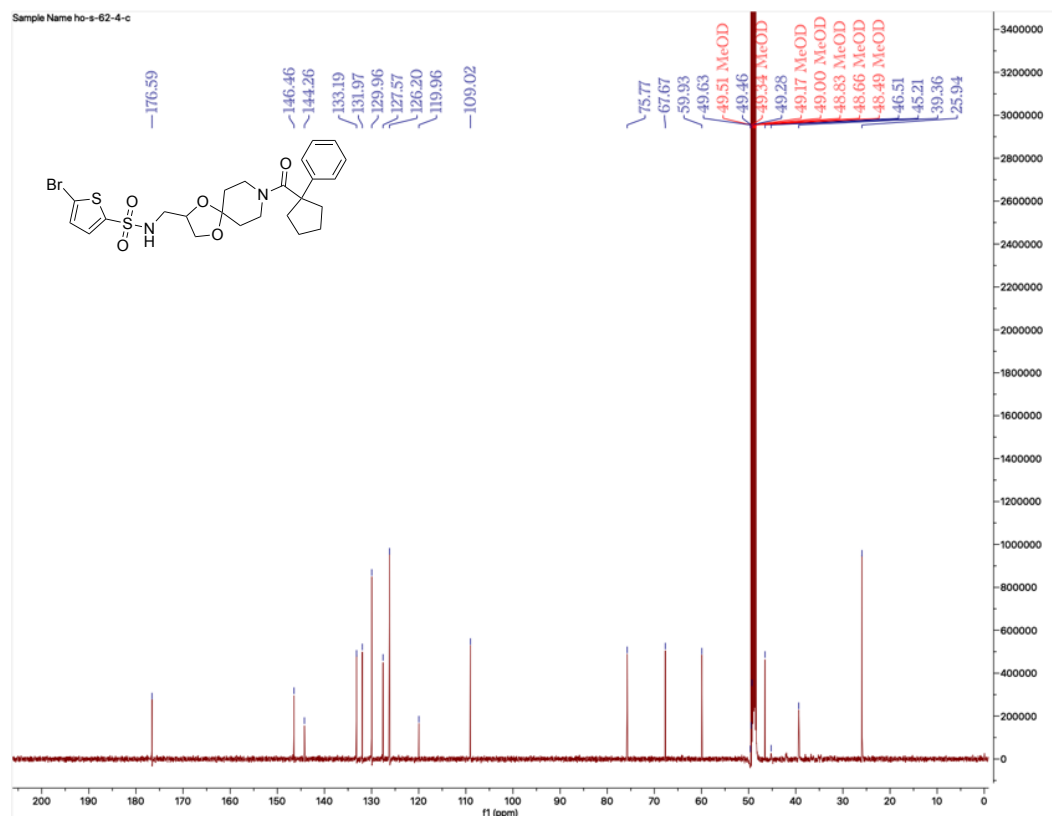


Figure S50: ^1H NMR (500 MHz, CD_3OD) for **3a**

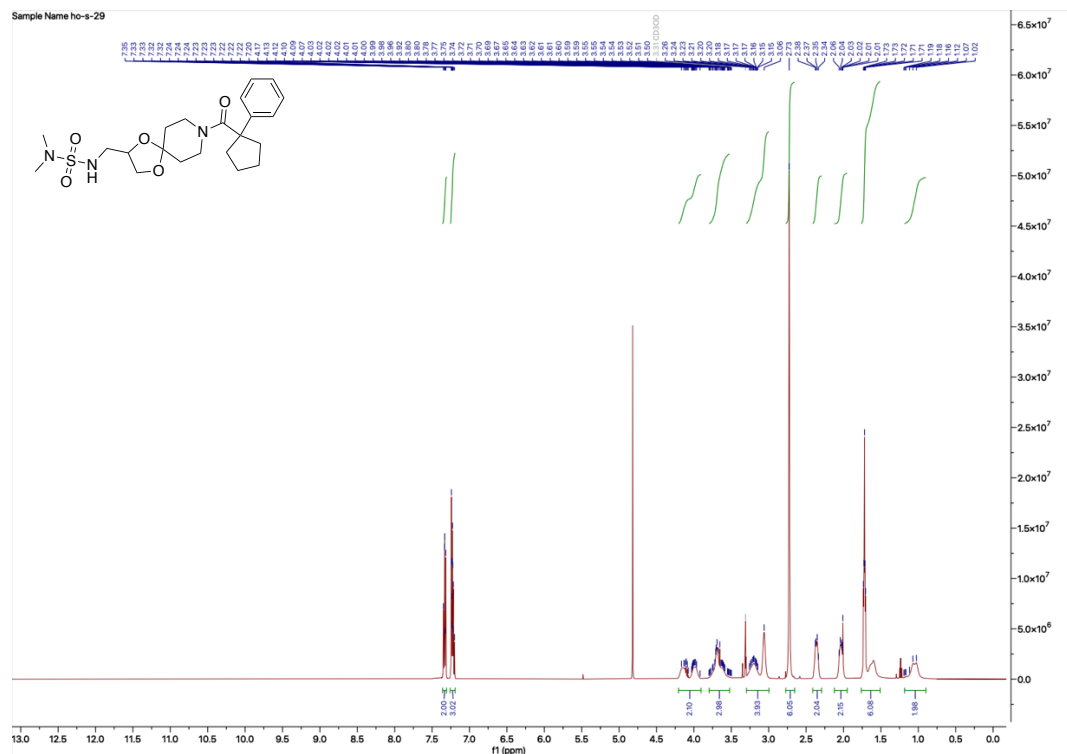


Figure S51: ^{13}C NMR (126 MHz, CD_3OD) for **3a**

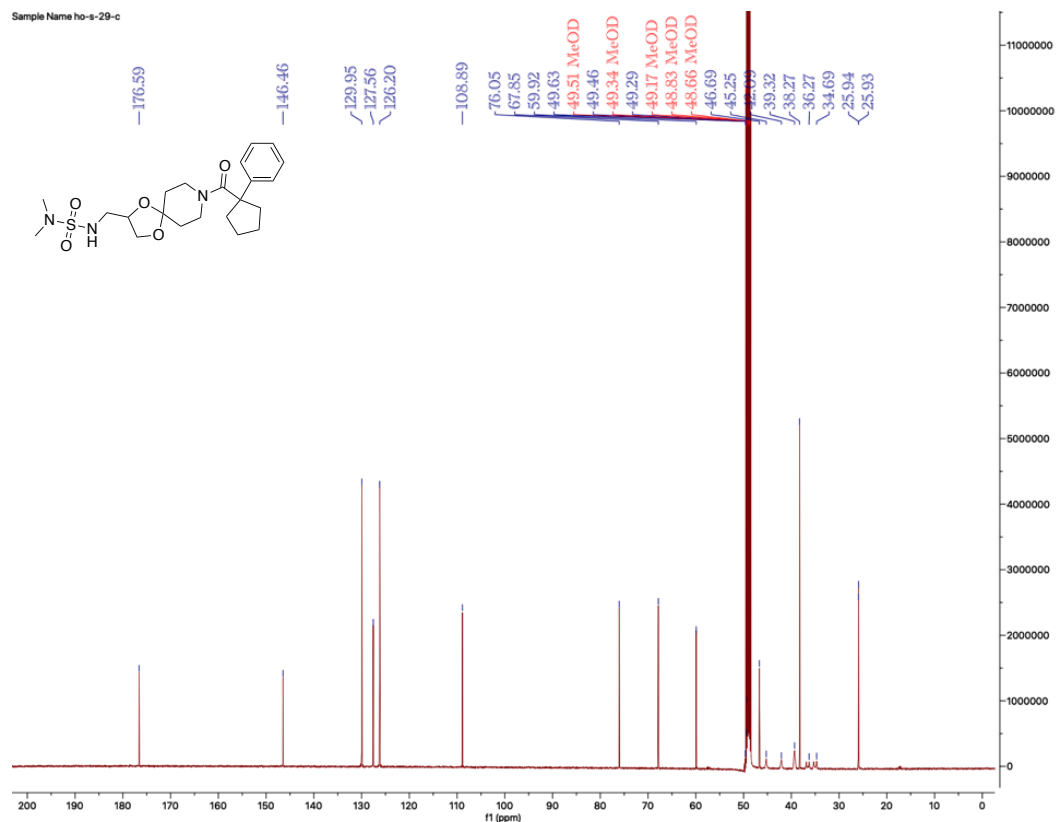


Figure S52: ^1H NMR (500 MHz, CD_3OD) for **3b**

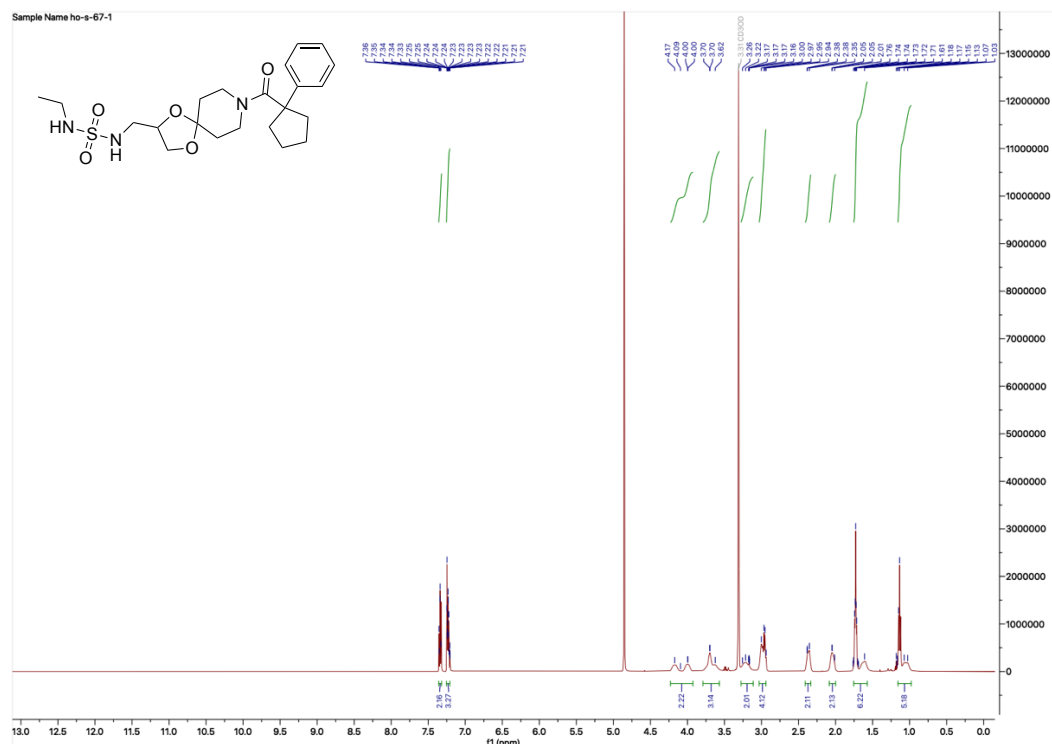


Figure S53: ^{13}C NMR (126 MHz, CD_3OD) for **3b**

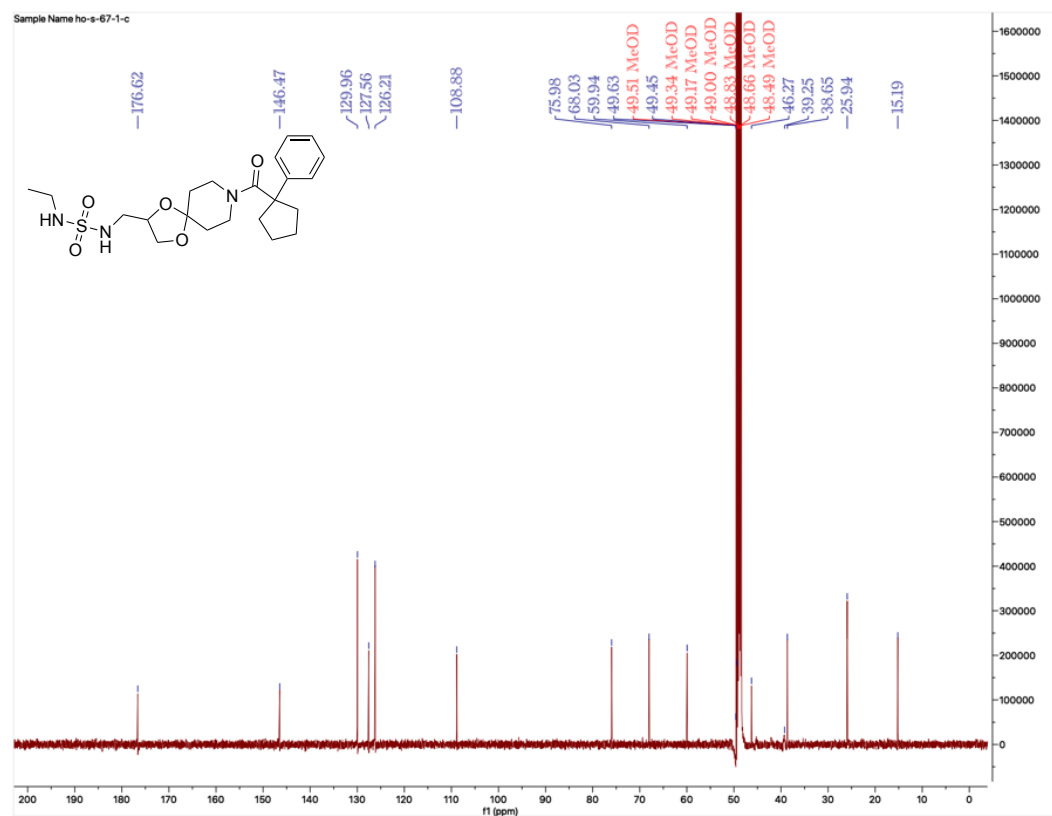


Figure S54: ^1H NMR (500 MHz, CD_3OD) for **3c**

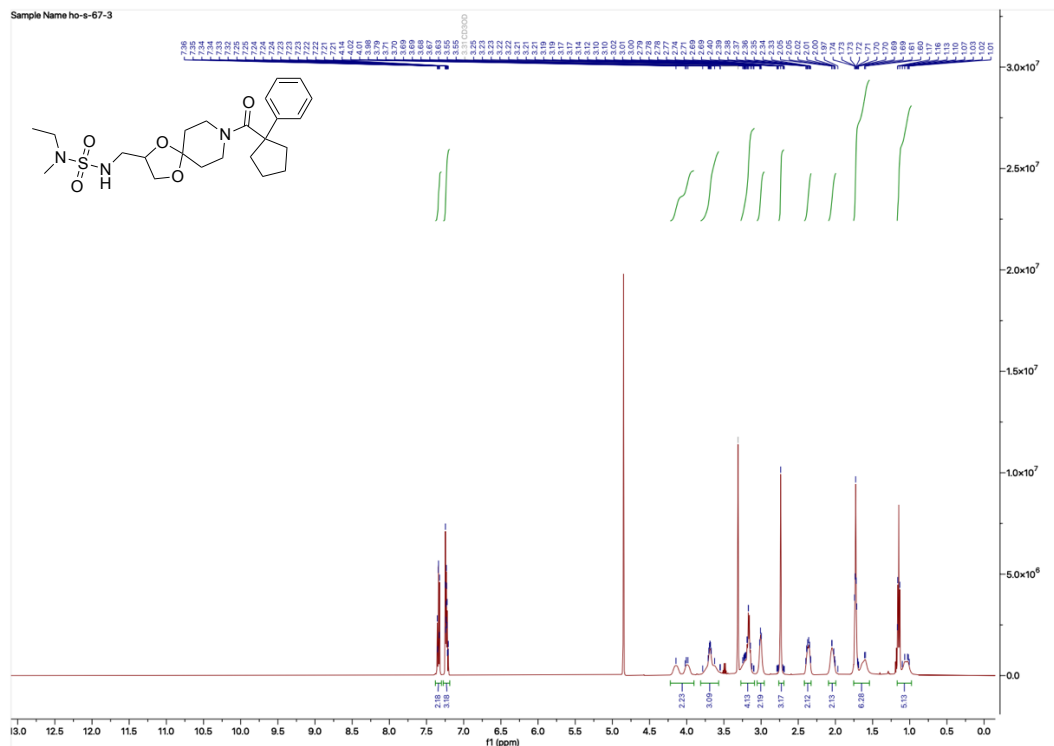


Figure S55: ^{13}C NMR (126 MHz, CD_3OD) for **3c**

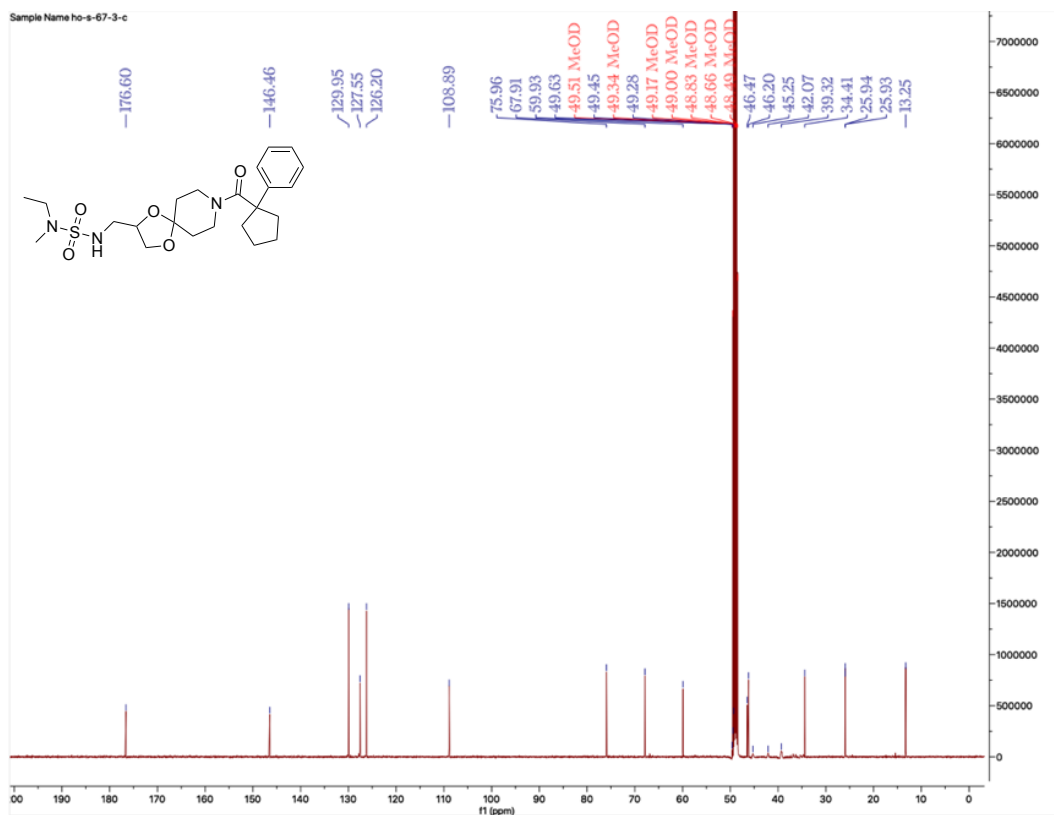


Figure S56: ^1H NMR (500 MHz, CD_3OD) for **3d**

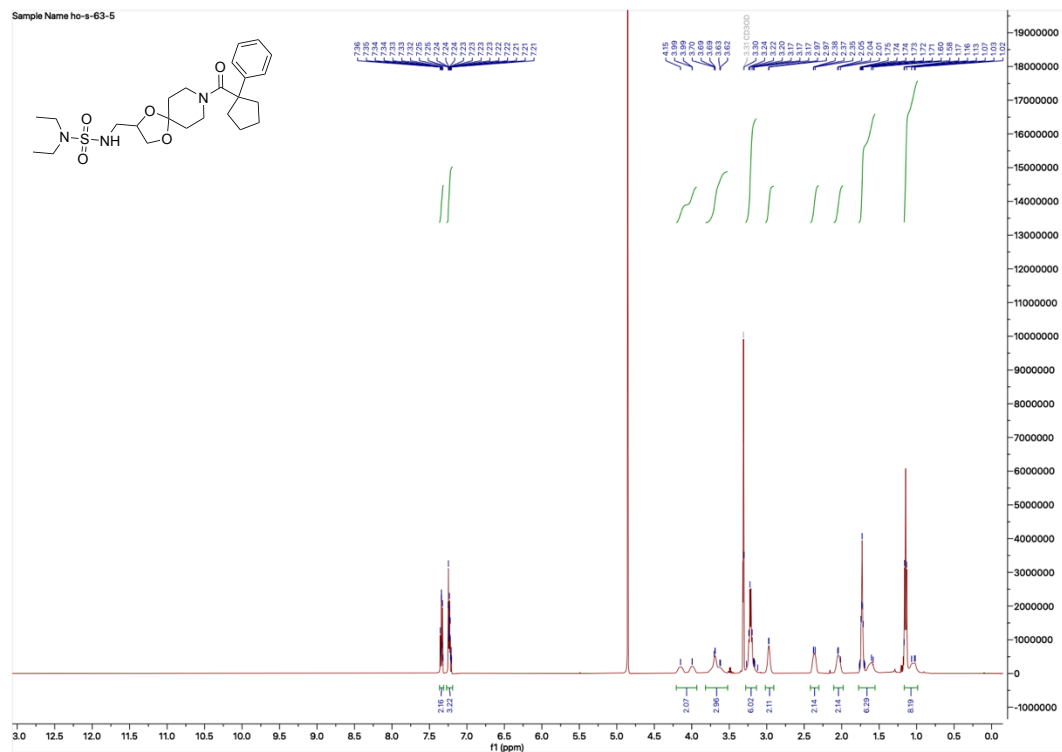


Figure S57: ^{13}C NMR (126 MHz, CD_3OD) for **3d**

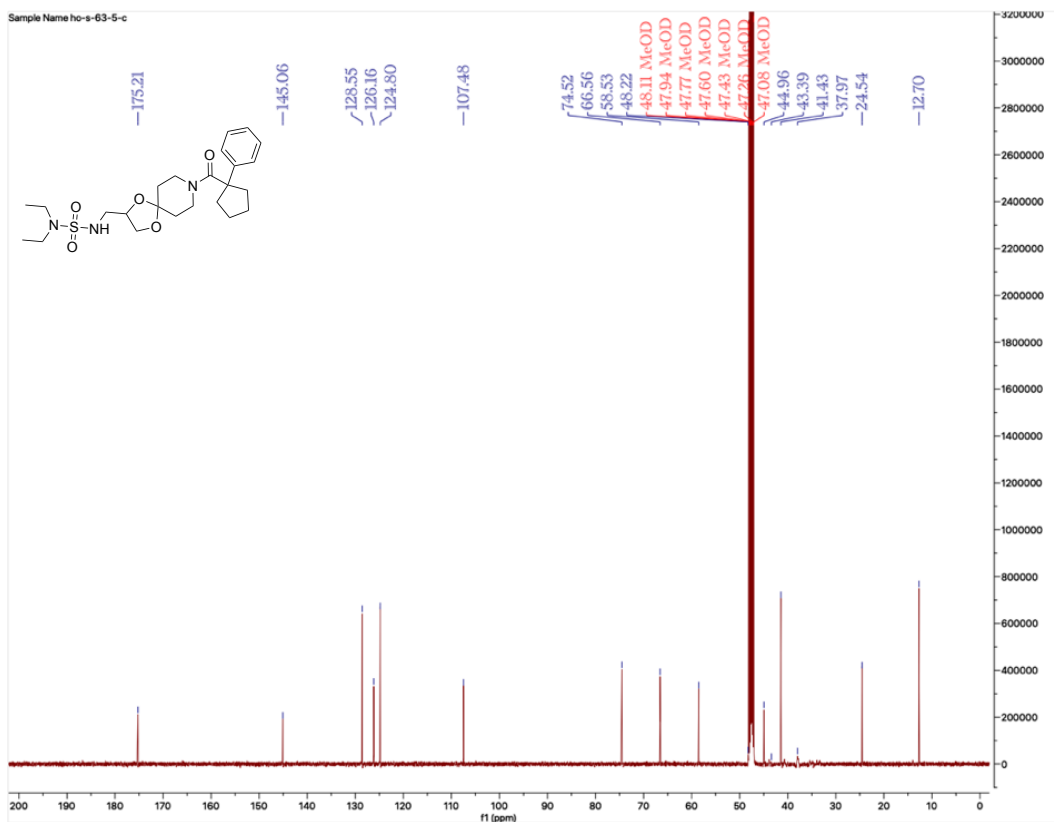


Figure S58: ^1H NMR (500 MHz, DMSO) for **3e**

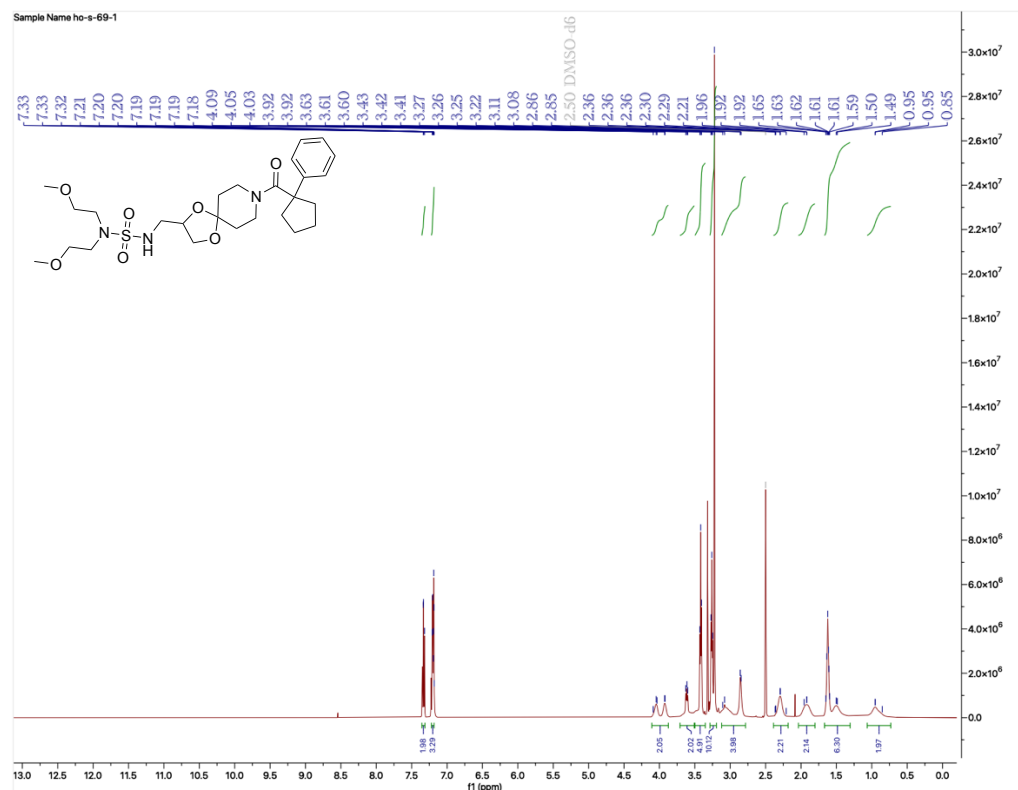
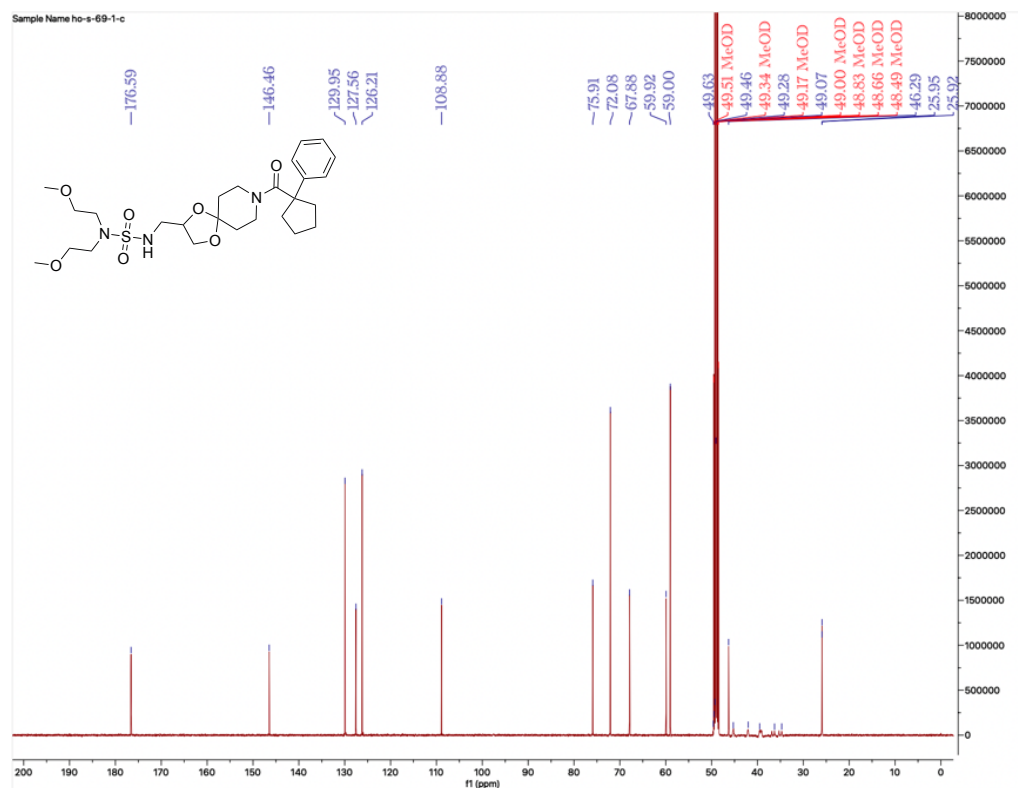


Figure S59: ^{13}C NMR (126 MHz, CD_3OD) for **3e**



Chemical structure of compound 10: CC(C)CNS(=O)(=O)NCC1OCC2(CCN(C2)C(=O)C3CCCC3)O1

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (δ), ranging from 0.0 to 13.0. The y-axis represents the intensity in arbitrary units (a.u.), ranging from 0.0 to 5.0 × 10⁷. The spectrum shows several peaks, with integration values indicated below the baseline.

Integration values (from left to right): 2.11, 2.03, 2.07, 2.07, 2.08, 1.96, 2.03, 2.03, 7.79, 2.04, 6.02.

Sample Name ho-s-67-2-c

CC(C)NS(=O)(=O)NCC1OC2CCN(C2C1=O)C3CCCC3

176.59, 146.45, 129.95, 127.56, 126.19, 108.87, 75.98, 68.01, 59.92, 51.42, 49.63, 49.51 MeOD, 49.46, 49.34 MeOD, 49.17 MeOD, 49.00 MeOD, 48.83 MeOD, 48.66 MeOD, 48.49 MeOD, 46.24, 45.26, 42.09, 39.34, 36.86, 35.31, 29.58, 25.94, 20.55

13,000,000
12,000,000
11,000,000
10,000,000
9,000,000
8,000,000
7,000,000
6,000,000
5,000,000
4,000,000
3,000,000
2,000,000
1,000,000
0

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

Figure S62: ^1H NMR (500 MHz, CD_3OD) for **3g**

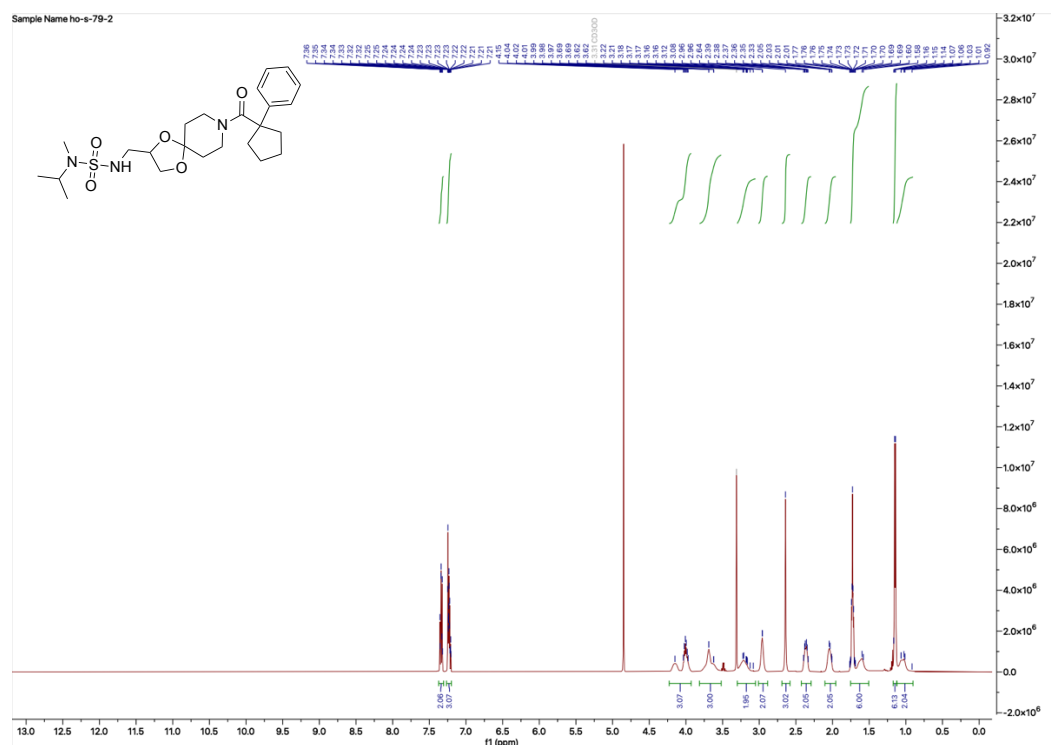


Figure S63: ^{13}C NMR (126 MHz, CD_3OD) for **3g**

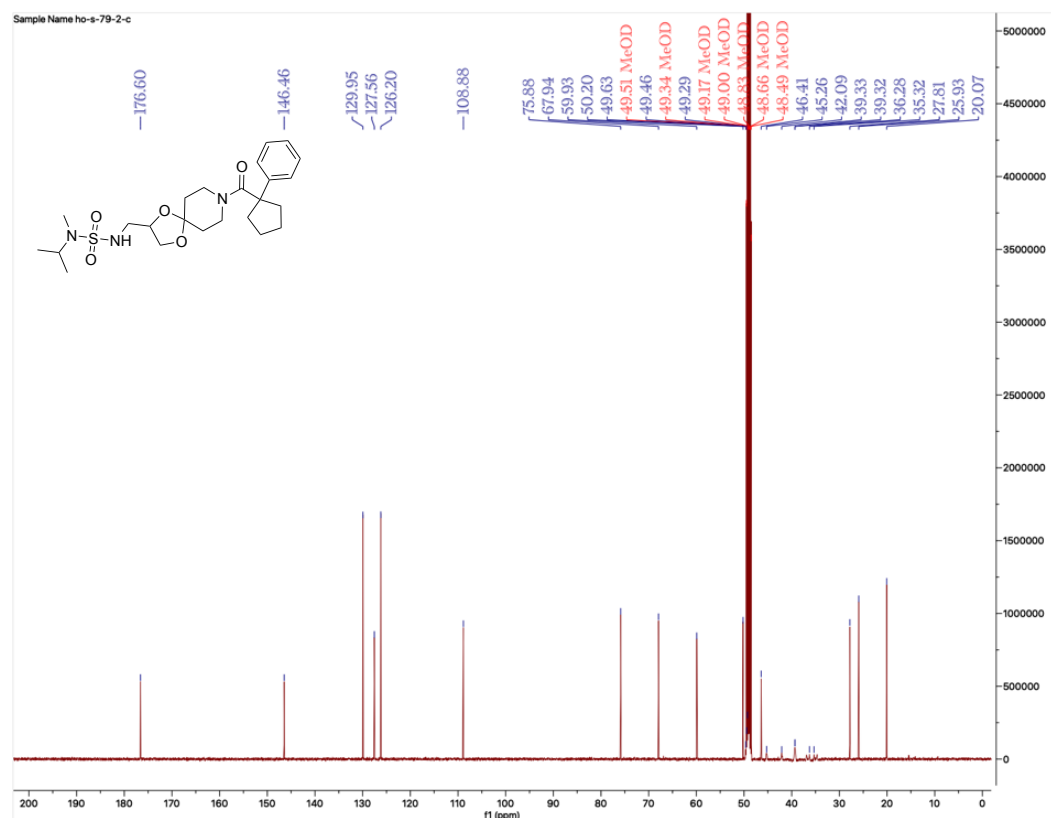


Figure S64: ^1H NMR (500 MHz, CD_3OD) for **3h**

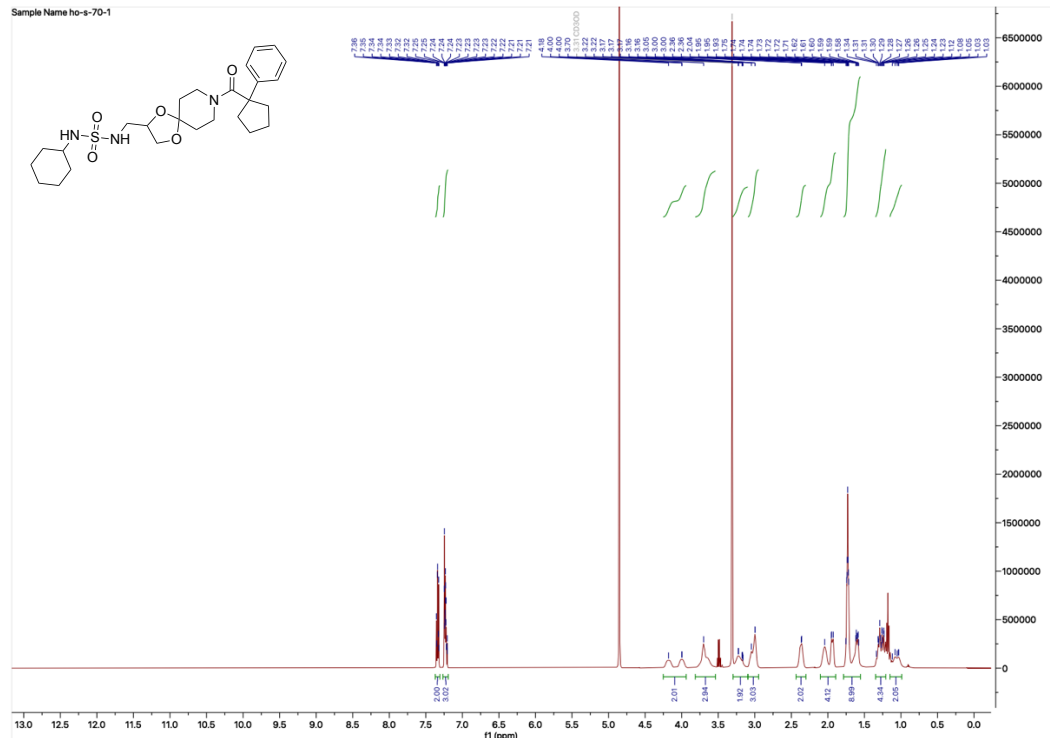
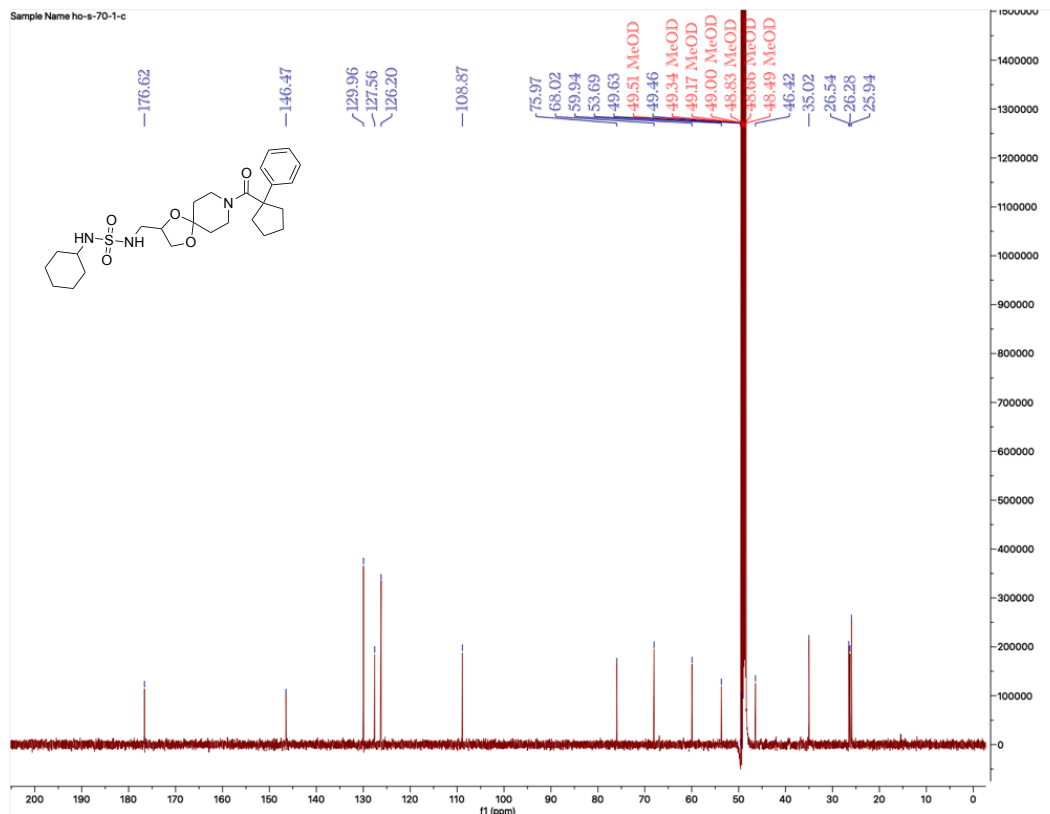


Figure S65: ^{13}C NMR (126 MHz, CD_3OD) for **3h**



[illegible]

Sample Name ho-s-66-3-c

Chemical structure of the compound (10) is shown above the spectrum.

Peak list (ppm):

- 176.61
- 146.47
- 129.96
- 127.56
- 126.21
- 108.89
- 75.88
- 67.94
- 59.94
- 58.50
- 49.63
- 49.51 MeOD
- 49.46
- 49.34 MeOD
- 49.28
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.65 MeOD
- 48.49 MeOD
- 46.42
- 31.51
- 29.26
- 27.04
- 26.52
- 25.94

[illegible]

Sample Name ho-s-63-2-c

Chemical structure of compound 1: O=C1C(C2CCCC2)N(CCC3OCC(S(=O)(=O)N4CCCC4)C3)CC1

¹H NMR (CDCl₃) peaks (ppm):

- 7.606
- 67.91
- 59.94
- 49.63
- 49.51 MeOD
- 49.46
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 46.64
- 45.33
- 39.41
- 26.47
- 25.95
- 25.93

¹³C NMR (CDCl₃) peaks (ppm):

- 176.61
- 146.47
- 129.95
- 127.56
- 126.21
- 108.90

Sample Name ho-s-63-1

Chemical structure of the compound is shown above the spectrum.

¹H NMR spectrum (400 MHz, DMSO-d₆) showing peaks from 0.0 to 13.0 ppm. The x-axis is labeled f1 (ppm). The y-axis represents intensity, ranging from 0 to 7,000,000.

Integration values (from left to right): 2.17, 3.31, 2.33, 3.11, 9.13, 2.33, 2.02, 4.35, 8.17, 1.00.

Sample Name ho-s-63-1-c

Chemical structure of the compound is shown above the spectrum:

O=S(=O)(NCC1OC2CCN(C2)C(=O)C3CCCC3)CC1

Mass Spectrum Data (m/z vs. Relative Intensity):

m/z	Relative Intensity (approx.)
176.61	100000
146.47	100000
129.95	300000
127.56	250000
126.20	300000
108.90	200000
76.03	250000
67.87	200000
59.94	200000
49.62	200000
49.51	200000
49.45	200000
49.54	1000000
49.17	200000
49.00	200000
48.83	200000
48.66	200000
48.49	200000
47.94	200000
46.65	200000
26.45	200000
25.94	200000
24.84	200000

Chemical structure of compound 10: O=S(=O)(NCC1OCC2(CCN(C2)C(=O)C3CCCC3)CC1)C1CCCCC1

¹H NMR spectrum (400 MHz, CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (δ), ranging from 13.0 to 0.0. The y-axis represents the intensity in arbitrary units, ranging from 0 to 19,000,000. The spectrum shows several peaks, with integration values indicated below the baseline.

Key peaks and integration values:

- ~8.5 ppm (broad, integration ~0.10)
- 7.4-7.5 ppm (multiplet, integration ~2.98)
- 4.7 ppm (large peak, integration ~2.98)
- 4.0-4.2 ppm (multiplet, integration ~2.19)
- 3.6-3.8 ppm (multiplet, integration ~3.07)
- 3.0-3.2 ppm (multiplet, integration ~4.24)
- 2.6-2.8 ppm (multiplet, integration ~3.32)
- 2.0-2.2 ppm (multiplet, integration ~2.18)
- 1.5-1.7 ppm (multiplet, integration ~2.15)
- 1.2-1.4 ppm (multiplet, integration ~16.18)
- 0.8-1.0 ppm (multiplet, integration ~1.96)
- 0.0 ppm (TMS, integration ~1.00)

Sample Name ho-s-79-1-c

Chemical structure of the compound (top left):

O=S1(=O)N2CCCCC2NS1CC3OC4CCN(C4)CC3C(=O)C5=CC=CC=C5

Mass spectrum data (m/z vs. Intensity):

m/z	Intensity
176.61	~400,000
146.47	~350,000
129.95	~1,200,000
127.56	~1,150,000
126.20	~600,000
108.89	~650,000
75.96	~650,000
67.97	~600,000
49.51	2,500,000
49.42	~550,000
49.17	~550,000
49.00	~550,000
48.66	~550,000
48.49	~550,000
46.29	~550,000
45.26	~550,000
42.12	~550,000
39.35	~550,000
36.28	~550,000
34.68	~550,000
30.26	~550,000
28.04	~550,000
25.95	~550,000
25.93	~550,000

Figure S74: ^1H NMR (500 MHz, CD_3OD) for **3m**

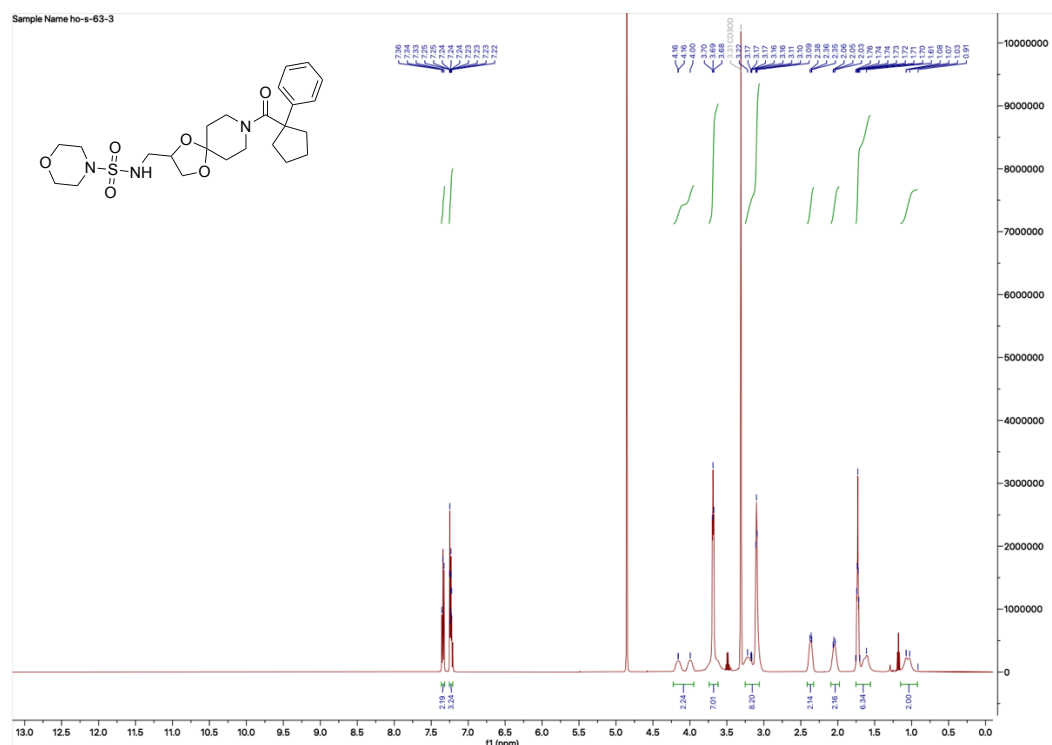


Figure S75: ^{13}C NMR (126 MHz, CD_3OD) for **3m**

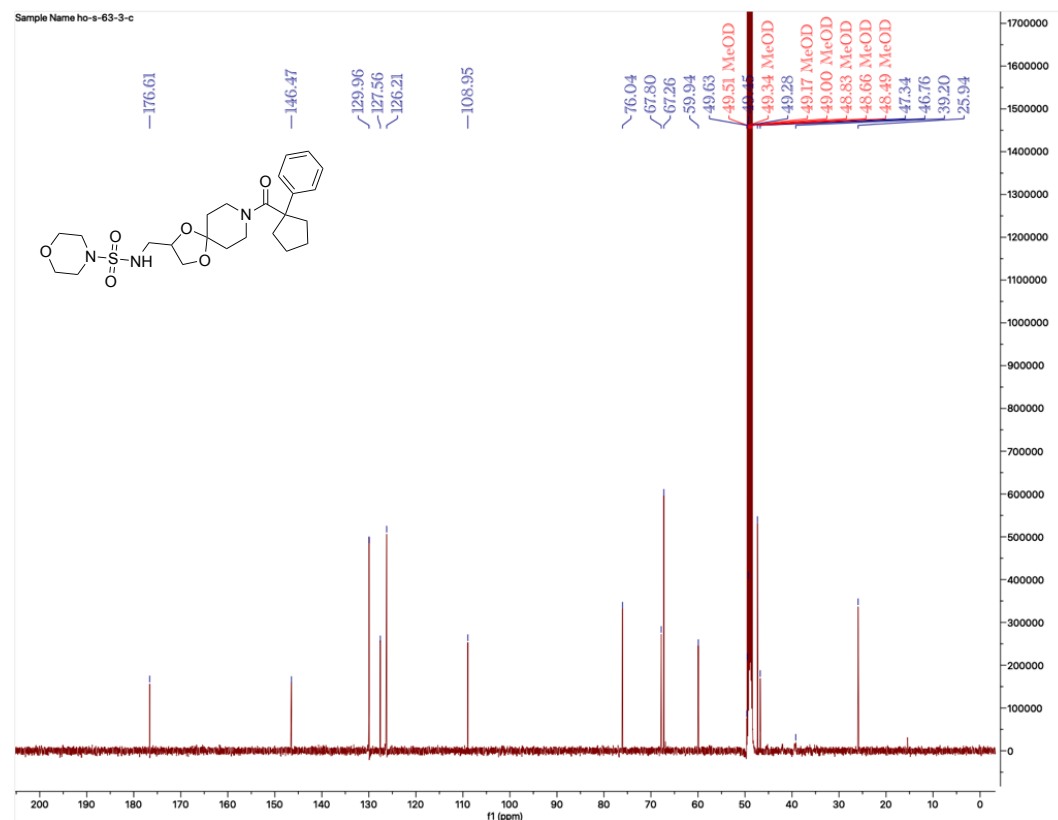


Figure S76: ^1H NMR (500 MHz, CD_3OD) for **3n**

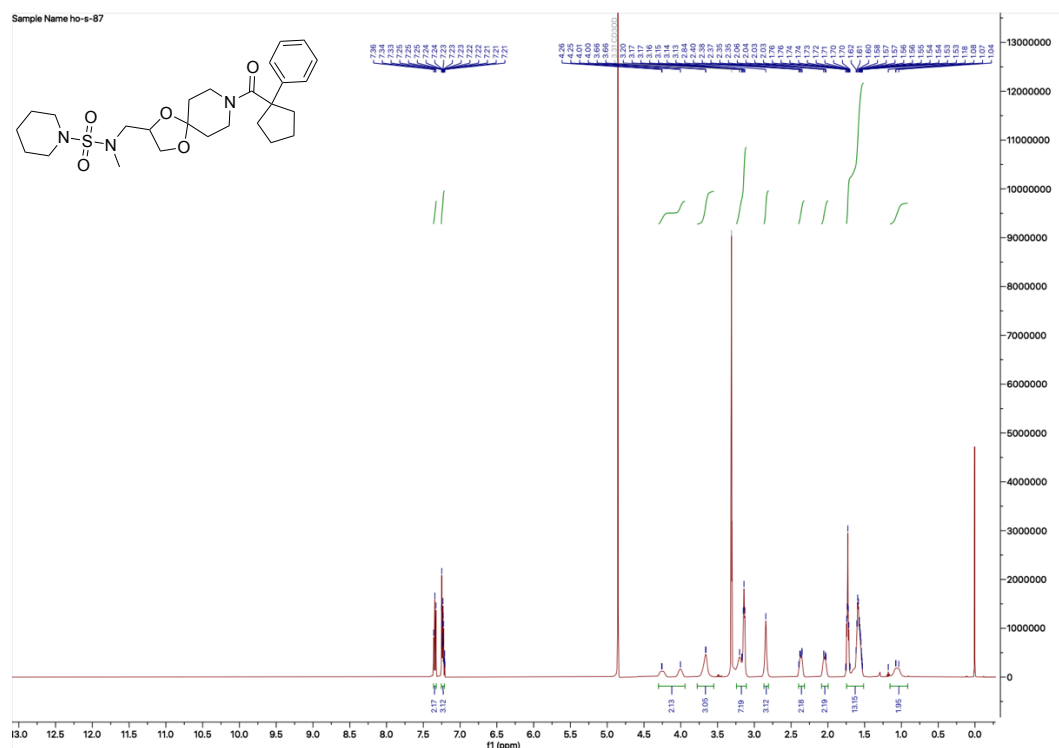


Figure S77: ^{13}C NMR (126 MHz, CD_3OD) for **3n**

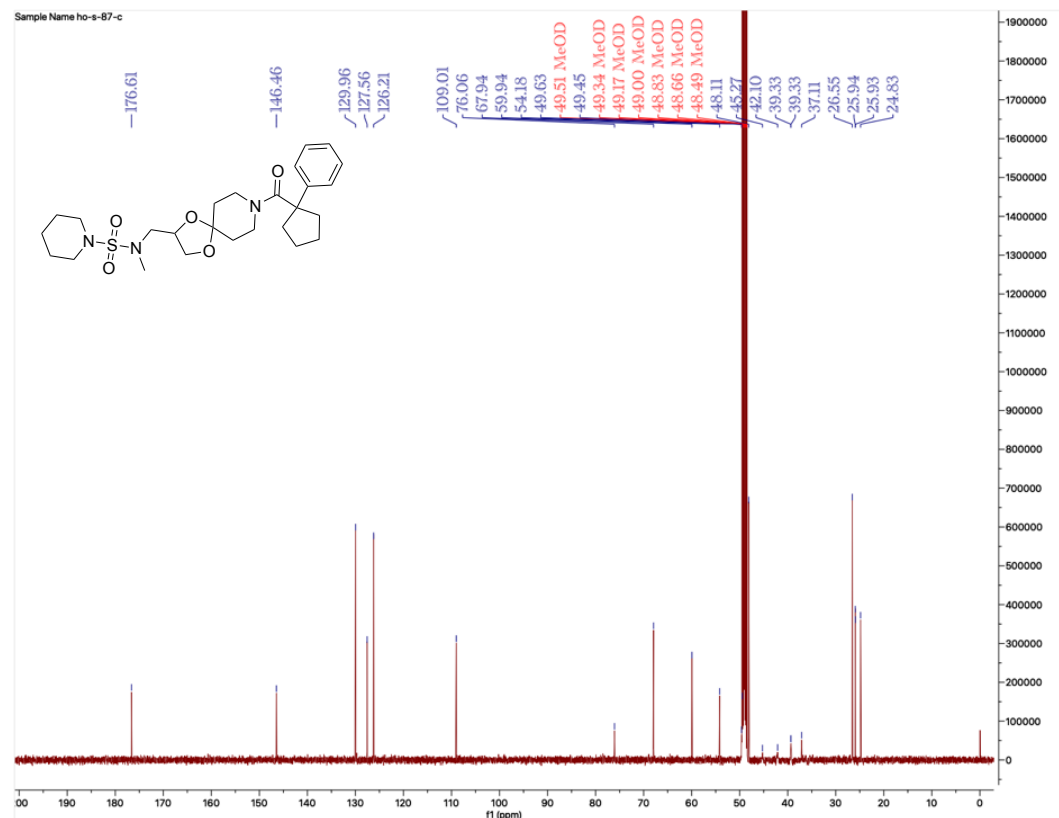


Figure S78: ^1H NMR (500 MHz, CD_3OD) for **3o**

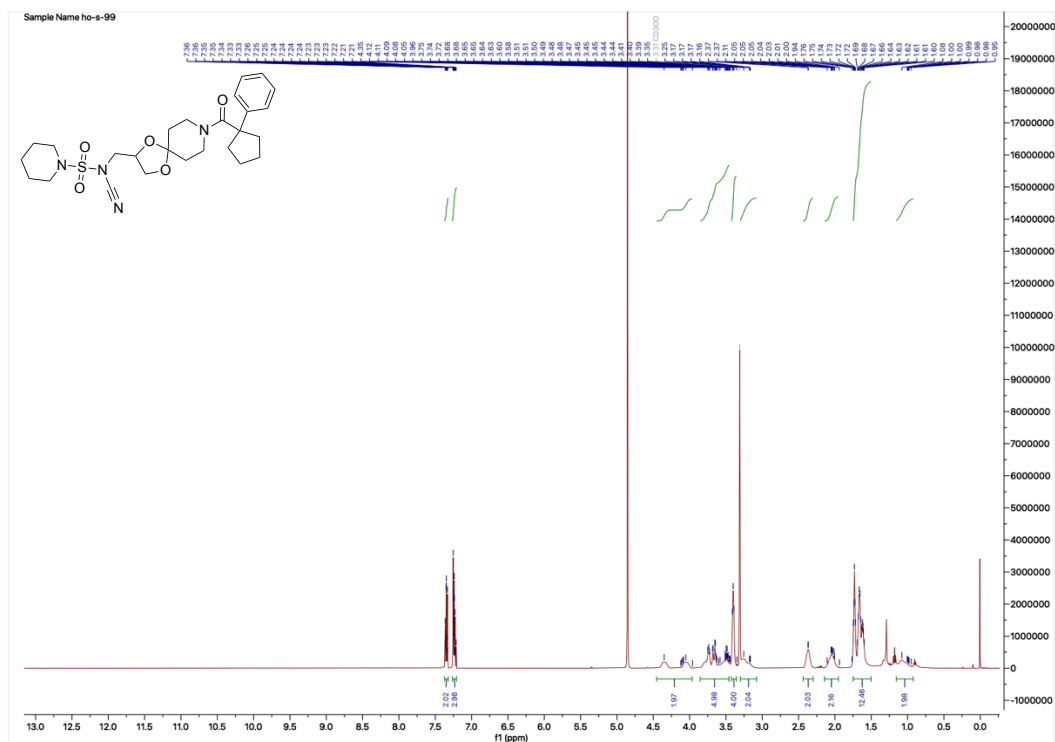


Figure S79: ^{13}C NMR (126 MHz, CD_3OD) for **3o**

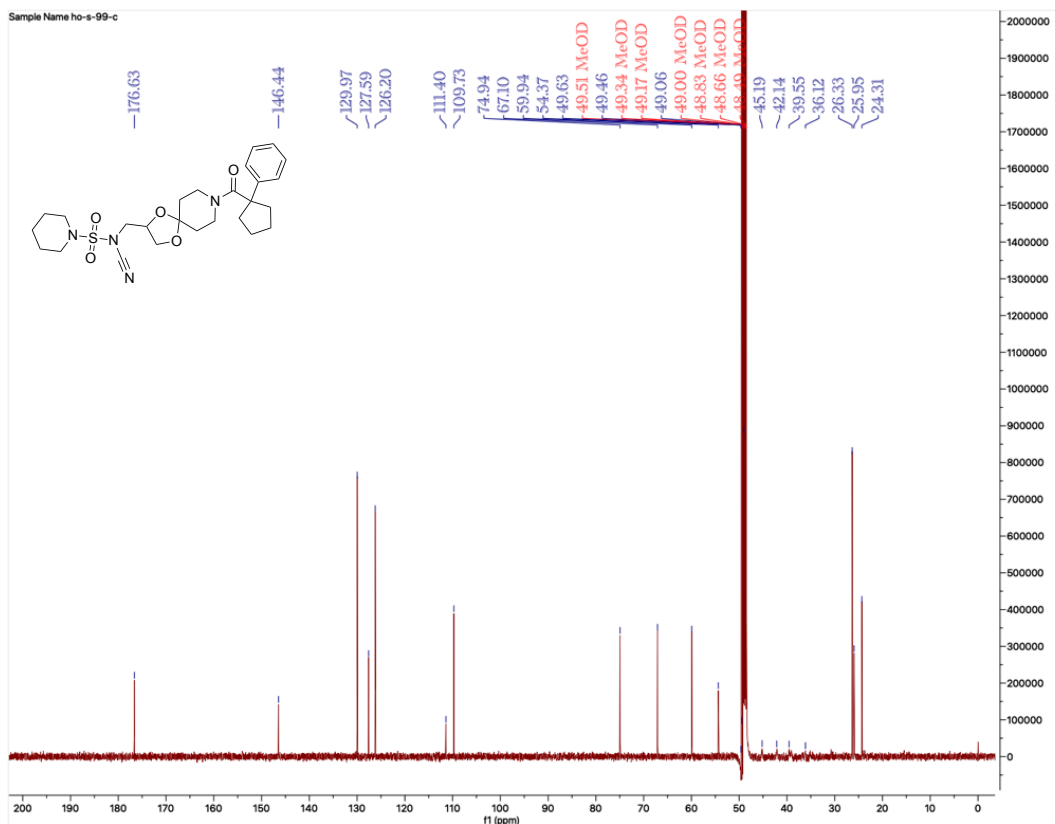


Figure S80: ^1H NMR (500 MHz, CD_3OD) for **3p**

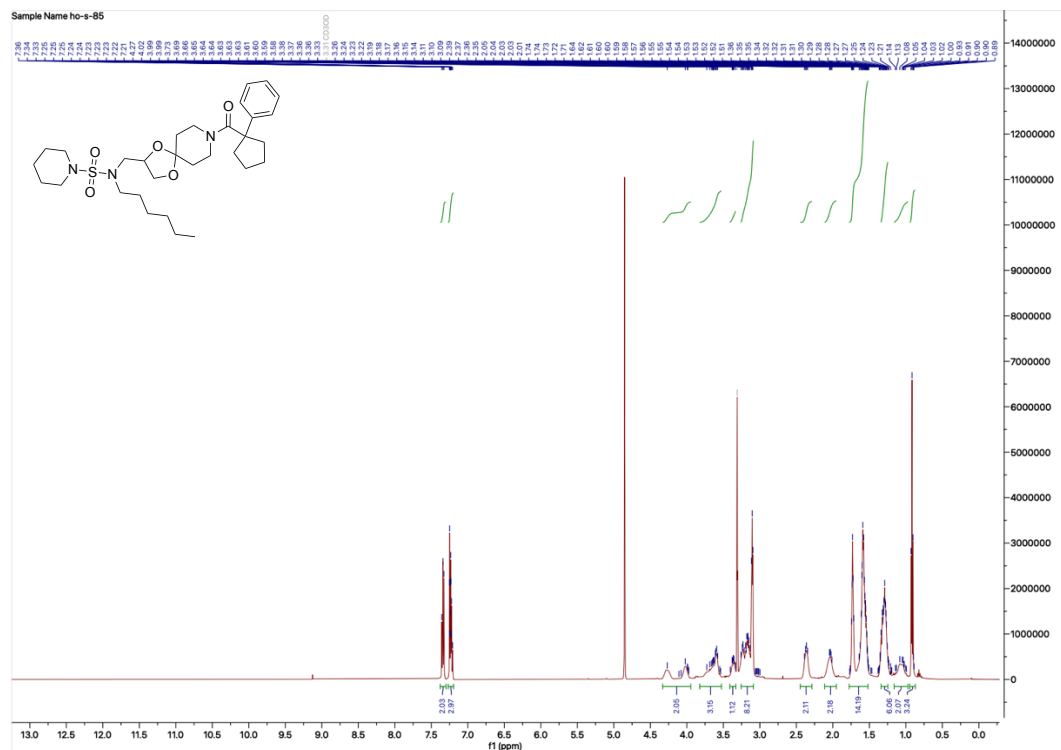
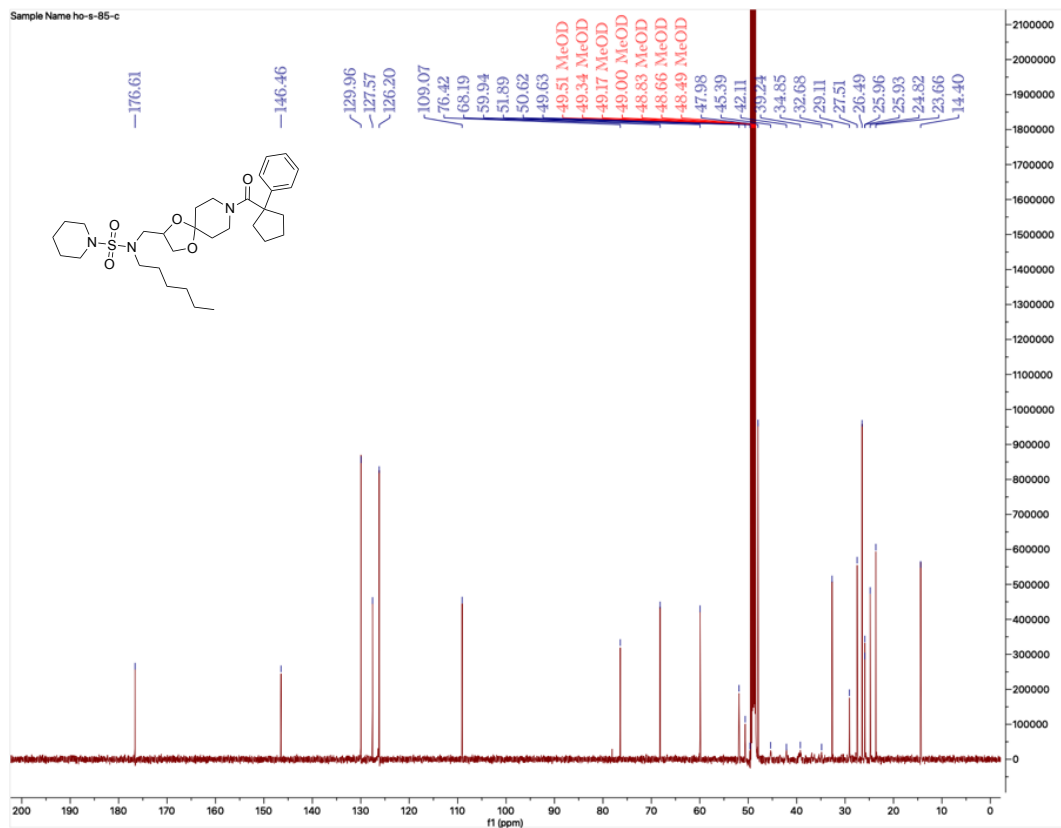


Figure S81: ^{13}C NMR (126 MHz, CD_3OD) for **3p**



Chemical structure of compound 120: CN(C)CCN(C1CCOC1C2CCOC2C(=O)C3CCCC3)C4CCCCC4=O

¹H NMR spectrum (CDCl₃) of compound 120. The x-axis represents the chemical shift in ppm (f1), ranging from 0.0 to 13.0. The y-axis represents the intensity, ranging from 0 to 2,200,000. The spectrum shows several peaks, with integration values provided below the baseline.

Integration values (from left to right): 2.22, 2.27, 1.07, 1.88, 5.12, 9.01, 6.27, 2.12, 2.01, 12.28, 2.10.

Chemical shift values (ppm): 7.36, 7.35, 7.34, 7.34, 7.33, 7.32, 7.26, 7.26, 7.25, 7.24, 7.24, 7.24, 7.23, 7.22, 7.22, 7.21, 7.21, 7.21, 3.62, 3.57, 3.51, 3.51, 3.48, 3.45, 3.45, 3.44, 3.31 (CDCl₃), 3.18, 3.17, 3.16, 3.13, 3.05, 2.66, 2.66, 1.73, 1.68, 1.63, 1.62, 1.62, 1.61, 1.60, 1.60, 1.59, 1.58, 1.57, 1.57, 1.56, 1.55, 1.55, 1.55.

[illegible]

Figure S84: ^1H NMR (500 MHz, CD_3OD) for **3r**

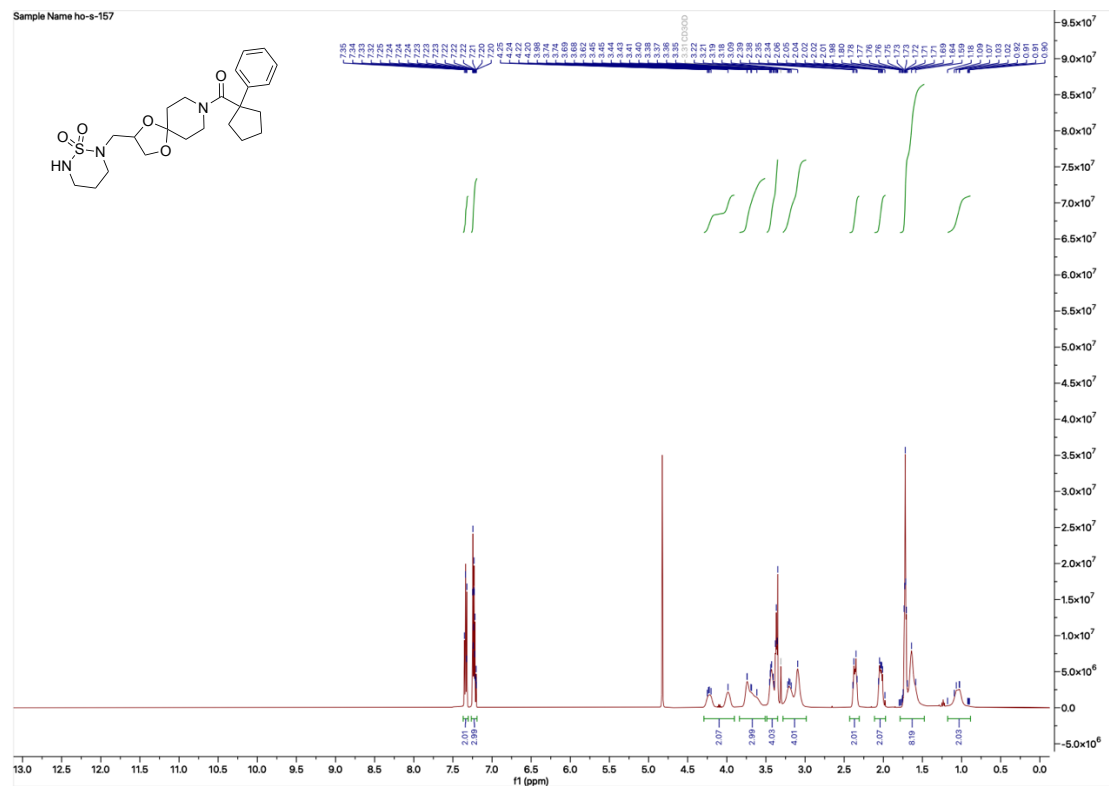


Figure S85: ^{13}C NMR (126 MHz, CD_3OD) for **3r**

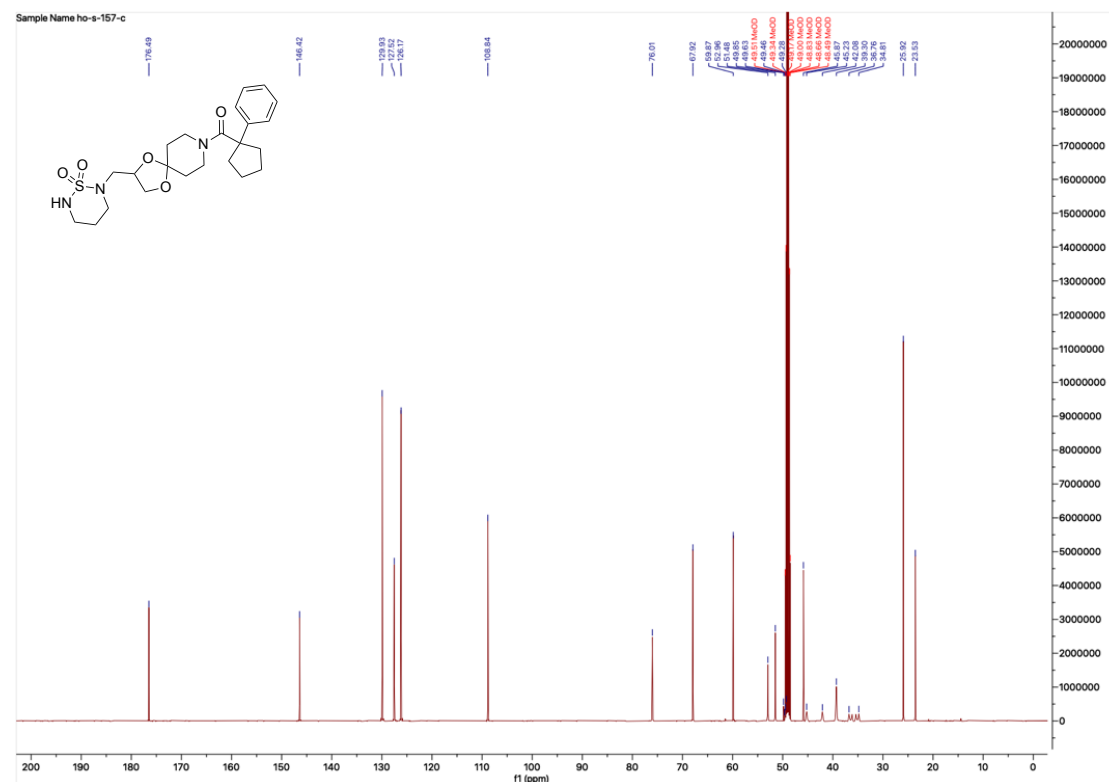


Figure S86: ^1H NMR (500 MHz, CD_3OD) for **3s**

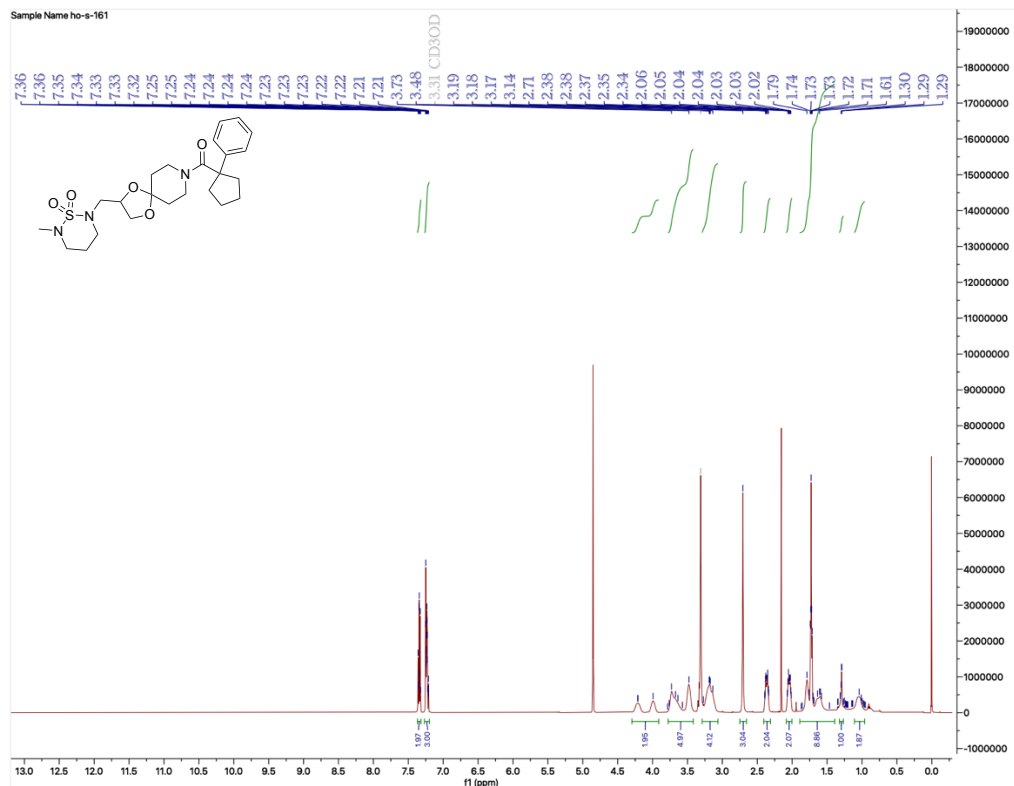


Figure S87: ^{13}C NMR (126 MHz, CD_3OD) for **3s**

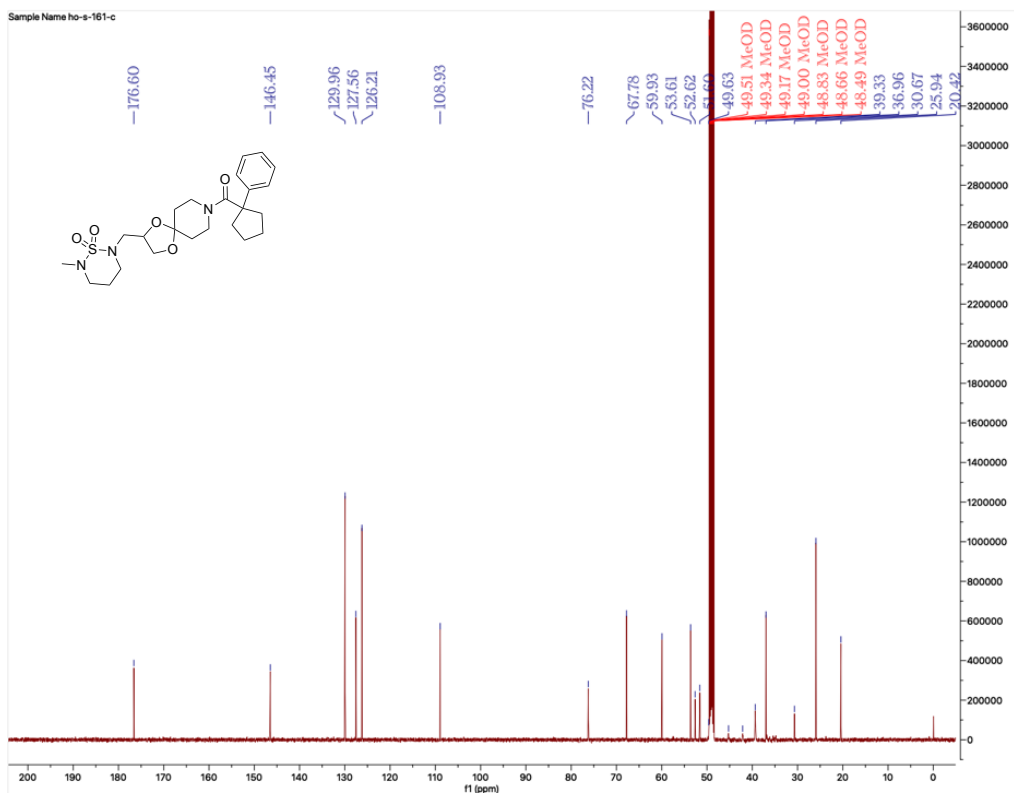


Figure S88: ^1H NMR (500 MHz, CD_3OD) for **3t**

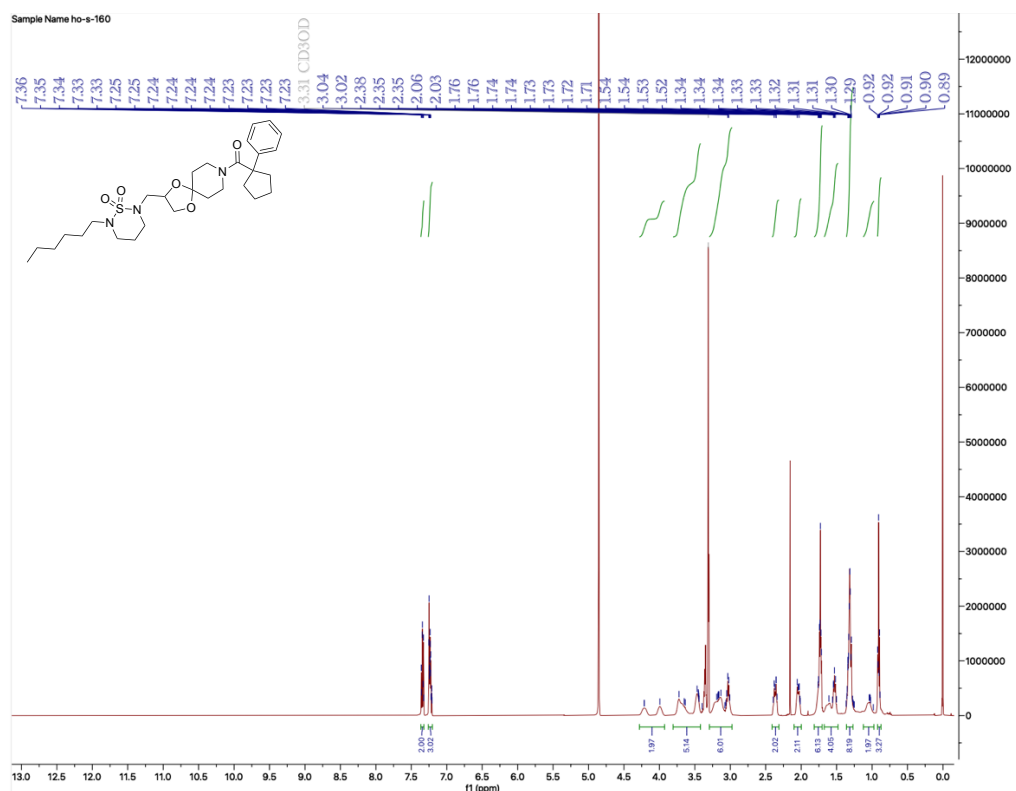


Figure S89: ^{13}C NMR (126 MHz, CD_3OD) for **3t**

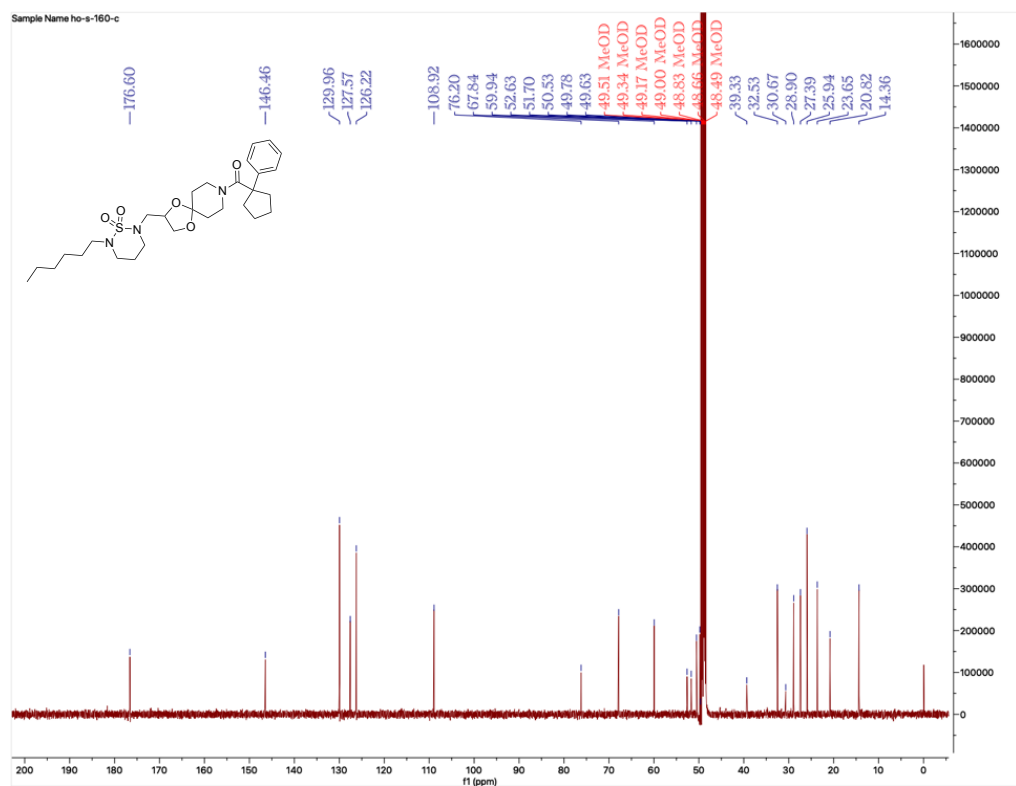


Figure S90: ^1H NMR (500 MHz, CD_3OD) for **4a**

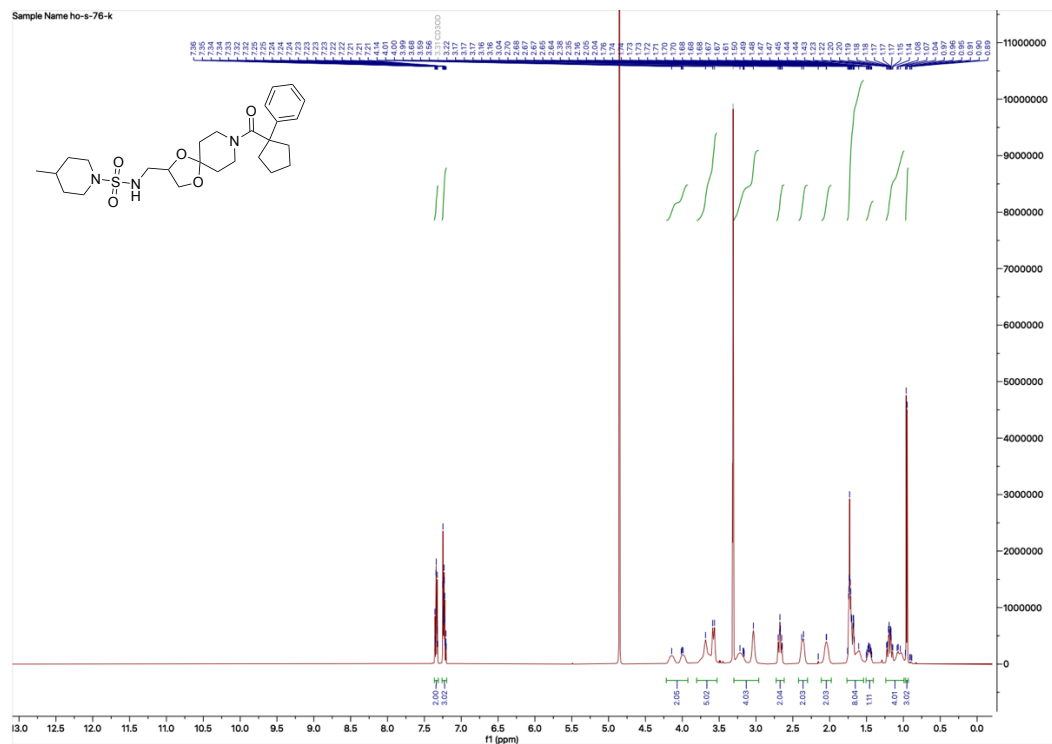
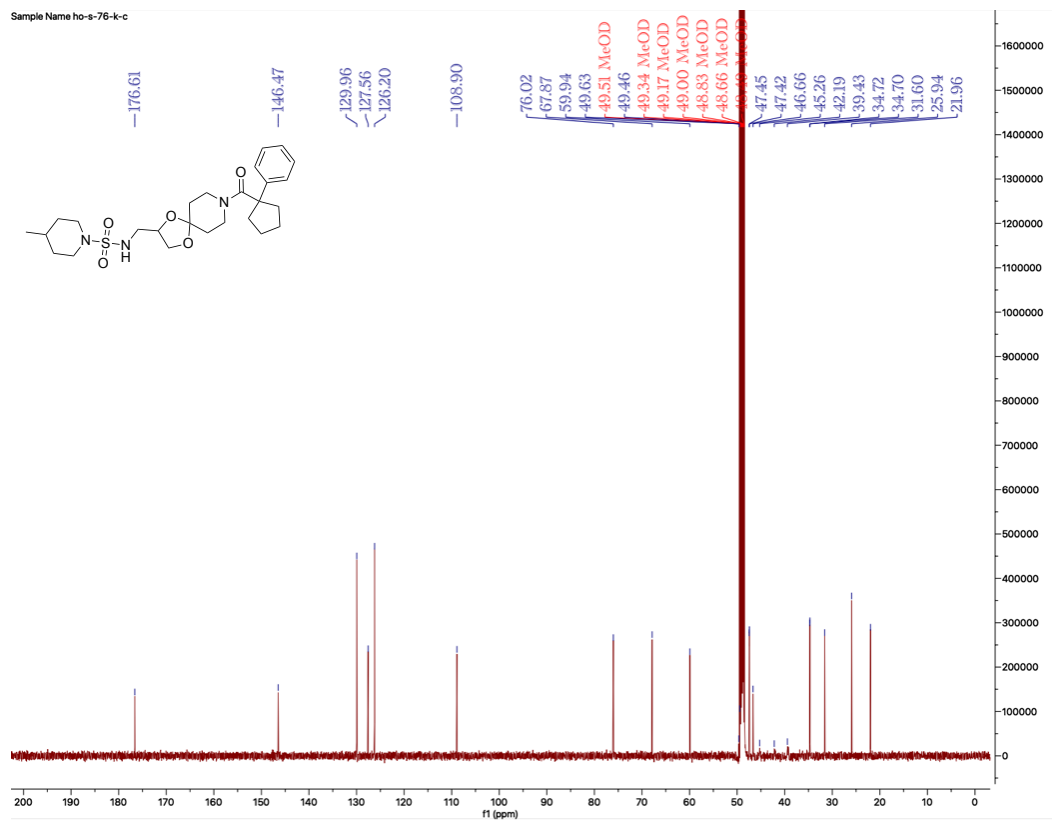


Figure S91: ^{13}C NMR (126 MHz, CD_3OD) for **4a**



Sample Name ho-s-79-3-c

Chemical structure: N#CC1CCN(S(=O)(=O)NC2C3OC4C(C2)NCC5C(C4)C(=O)C6=CC=CC=C6C5)CC1

13C NMR spectrum (f1 (ppm) vs intensity):

Chemical shifts (ppm):

- 176.62
- 146.47
- 129.96
- 127.56
- 126.21
- 122.31
- 108.96
- 75.98
- 67.80
- 59.94
- 49.62
- 49.51 MeOD
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 46.68
- 45.29
- 39.20
- 29.25
- 26.64
- 25.94

Figure S94: ^1H NMR (400 MHz, DMSO) for **4c**

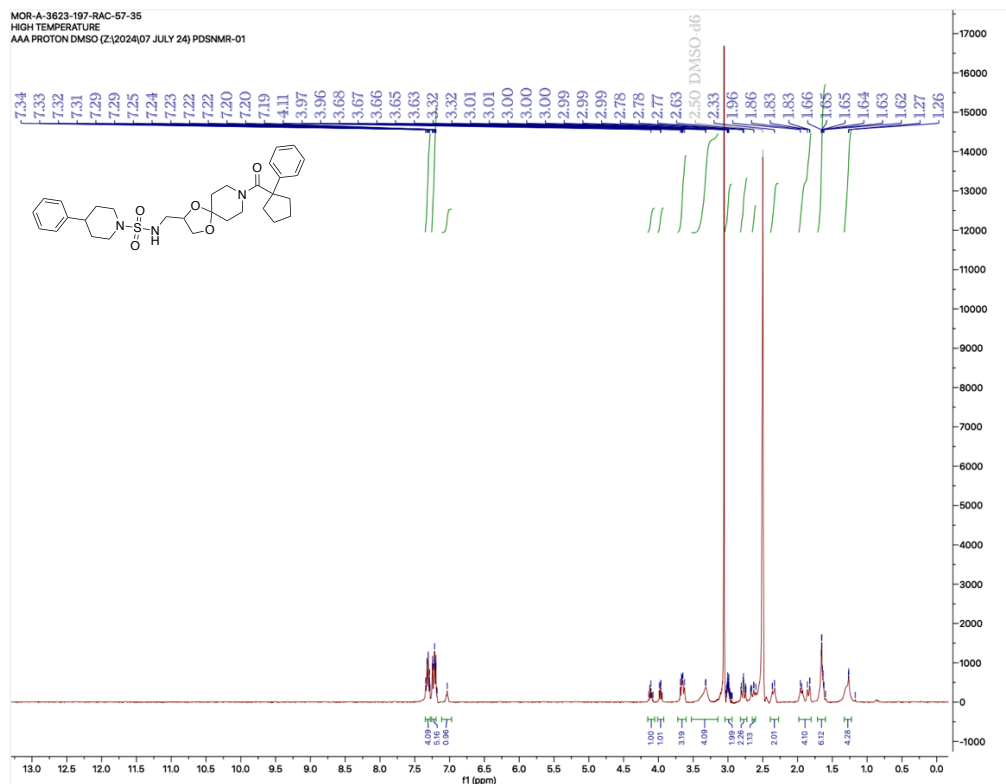
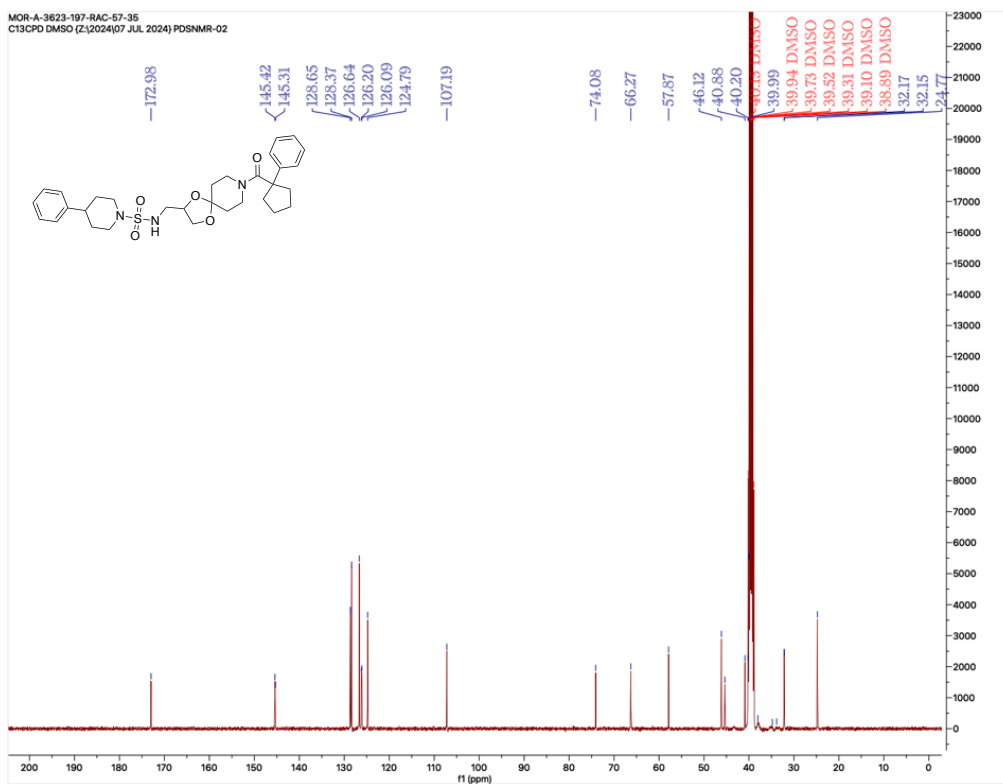


Figure S95: ^{13}C NMR (101 MHz, DMSO) for **4c**



Sample Name ho-s-79-5

Chemical structure of compound 10b is shown above the spectrum.

¹H NMR spectrum (CDCl₃) of compound 10b. The x-axis represents the chemical shift (ppm) from 13.0 to 0.0. The y-axis represents the intensity (arbitrary units) from 0 to 11,000,000. The spectrum shows several peaks, with integration values indicated below the baseline and chemical shift values (ppm) listed above the peaks.

Integration values (from left to right): 2.11, 3.14, 2.12, 3.06, 2.12, 2.11, 8.32, 1.96.

Chemical shift values (ppm) (from left to right): 7.286, 7.285, 7.284, 7.283, 7.282, 7.281, 7.280, 7.279, 7.278, 7.277, 7.276, 7.275, 7.274, 7.273, 7.272, 7.271, 7.270, 7.269, 7.268, 7.267, 7.266, 7.265, 7.264, 7.263, 7.262, 7.261, 7.260, 7.259, 7.258, 7.257, 7.256, 7.255, 7.254, 7.253, 7.252, 7.251, 7.250, 7.249, 7.248, 7.247, 7.246, 7.245, 7.244, 7.243, 7.242, 7.241, 7.240, 7.239, 7.238, 7.237, 7.236, 7.235, 7.234, 7.233, 7.232, 7.231, 7.230, 7.229, 7.228, 7.227, 7.226, 7.225, 7.224, 7.223, 7.222, 7.221, 7.220, 7.219, 7.218, 7.217, 7.216, 7.215, 7.214, 7.213, 7.212, 7.211, 7.210, 7.209, 7.208, 7.207, 7.206, 7.205, 7.204, 7.203, 7.202, 7.201, 7.200, 7.199, 7.198, 7.197, 7.196, 7.195, 7.194, 7.193, 7.192, 7.191, 7.190, 7.189, 7.188, 7.187, 7.186, 7.185, 7.184, 7.183, 7.182, 7.181, 7.180, 7.179, 7.178, 7.177, 7.176, 7.175, 7.174, 7.173, 7.172, 7.171, 7.170, 7.169, 7.168, 7.167, 7.166, 7.165, 7.164, 7.163, 7.162, 7.161, 7.160, 7.159, 7.158, 7.157, 7.156, 7.155, 7.154, 7.153, 7.152, 7.151, 7.150, 7.149, 7.148, 7.147, 7.146, 7.145, 7.144, 7.143, 7.142, 7.141, 7.140, 7.139, 7.138, 7.137, 7.136, 7.135, 7.134, 7.133, 7.132, 7.131, 7.130, 7.129, 7.128, 7.127, 7.126, 7.125, 7.124, 7.123, 7.122, 7.121, 7.120, 7.119, 7.118, 7.117, 7.116, 7.115, 7.114, 7.113, 7.112, 7.111, 7.110, 7.109, 7.108, 7.107, 7.106, 7.105, 7.104, 7.103, 7.102, 7.101, 7.100, 7.099, 7.098, 7.097, 7.096, 7.095, 7.094, 7.093, 7.092, 7.091, 7.090, 7.089, 7.088, 7.087, 7.086, 7.085, 7.084, 7.083, 7.082, 7.081, 7.080, 7.079, 7.078, 7.077, 7.076, 7.075, 7.074, 7.073, 7.072, 7.071, 7.070, 7.069, 7.068, 7.067, 7.066, 7.065, 7.064, 7.063, 7.062, 7.061, 7.060, 7.059, 7.058, 7.057, 7.056, 7.055, 7.054, 7.053, 7.052, 7.051, 7.050, 7.049, 7.048, 7.047, 7.046, 7.045, 7.044, 7.043, 7.042, 7.041, 7.040, 7.039, 7.038, 7.037, 7.036, 7.035, 7.034, 7.033, 7.032, 7.031, 7.030, 7.029, 7.028, 7.027, 7.026, 7.025, 7.024, 7.023, 7.022, 7.021, 7.020, 7.019, 7.018, 7.017, 7.016, 7.015, 7.014, 7.013, 7.012, 7.011, 7.010, 7.009, 7.008, 7.007, 7.006, 7.005, 7.004, 7.003, 7.002, 7.001, 7.000, 6.999, 6.998, 6.997, 6.996, 6.995, 6.994, 6.993, 6.992, 6.991, 6.990, 6.989, 6.988, 6.987, 6.986, 6.985, 6.984, 6.983, 6.982, 6.981, 6.980, 6.979, 6.978, 6.977, 6.976, 6.975, 6.974, 6.973, 6.972, 6.971, 6.970, 6.969, 6.968, 6.967, 6.966, 6.965, 6.964, 6.963, 6.962, 6.961, 6.960, 6.959, 6.958, 6.957, 6.956, 6.955, 6.954, 6.953, 6.952, 6.951, 6.950, 6.949, 6.948, 6.947, 6.946, 6.945, 6.944, 6.943, 6.942, 6.941, 6.940, 6.939, 6.938, 6.937, 6.936, 6.935, 6.934, 6.933, 6.932, 6.931, 6.930, 6.929, 6.928, 6.927, 6.926, 6.925, 6.924, 6.923, 6.922, 6.921, 6.920, 6.919, 6.918, 6.917, 6.916, 6.915, 6.914, 6.913, 6.912, 6.911, 6.910, 6.909, 6.908, 6.907, 6.906, 6.905, 6.904, 6.903, 6.902, 6.901, 6.900, 6.899, 6.898, 6.897, 6.896, 6.895, 6.894, 6.893, 6.892, 6.891, 6.890, 6.889, 6.888, 6.887, 6.886, 6.885, 6.884, 6.883, 6.882, 6.881, 6.880, 6.879, 6.878, 6.877, 6.876, 6.875, 6.874, 6.873, 6.872, 6.871, 6.870, 6.869, 6.868, 6.867, 6.866, 6.865, 6.864, 6.863, 6.862, 6.861, 6.860, 6.859, 6.858, 6.857, 6.856, 6.855, 6.854, 6.853, 6.852, 6.851, 6.850, 6.849, 6.848, 6.847, 6.846, 6.845, 6.844, 6.843, 6.842, 6.841, 6.840, 6.839, 6.838, 6.837, 6.836, 6.835, 6.834, 6.833, 6.832, 6.831, 6.830, 6.829, 6.828, 6.827, 6.826, 6.825, 6.824, 6.823, 6.822, 6.821, 6.820, 6.819, 6.818, 6.817, 6.816, 6.815, 6.814, 6.813, 6.812, 6.811, 6.810, 6.809, 6.808, 6.807, 6.806, 6.805, 6.804, 6.803, 6.802, 6.801, 6.800, 6.799, 6.798, 6.797, 6.796, 6.795, 6.794, 6.793, 6.792, 6.791, 6.790, 6.789, 6.788, 6.787, 6.786, 6.785, 6.784, 6.783, 6.782, 6.781, 6.780, 6.779, 6.778, 6.777, 6.776, 6.775, 6.774, 6.773, 6.772, 6.771, 6.770, 6.769, 6.768, 6.767, 6.766, 6.765, 6.764, 6.763, 6.762, 6.761, 6.760

Sample Name ho-s-79-5-c

Chemical structure of the compound (10) is shown above the spectrum.

Peak list (ppm):

- 176.62
- 146.46
- 129.96
- 127.56
- 126.20
- 122.53
- 120.60
- 118.67
- 108.96
- 75.85
- 67.81
- 59.94
- 52.32
- 52.06
- 51.81
- 49.63
- 49.51 MeOD
- 49.45
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 46.57
- 46.08
- 45.22
- 42.02
- 32.93
- 32.75
- 32.56
- 25.94
- 22.87
- 22.84
- 22.80

Figure S98: ^1H NMR (500 MHz, CD_3OD) for **5a**

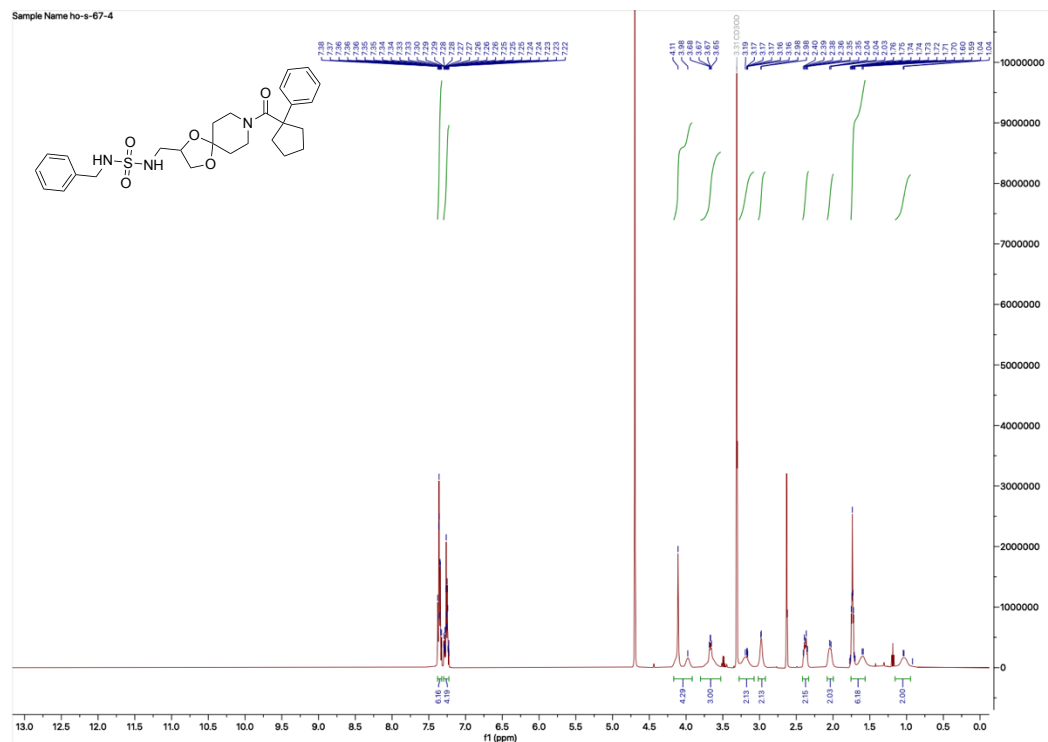
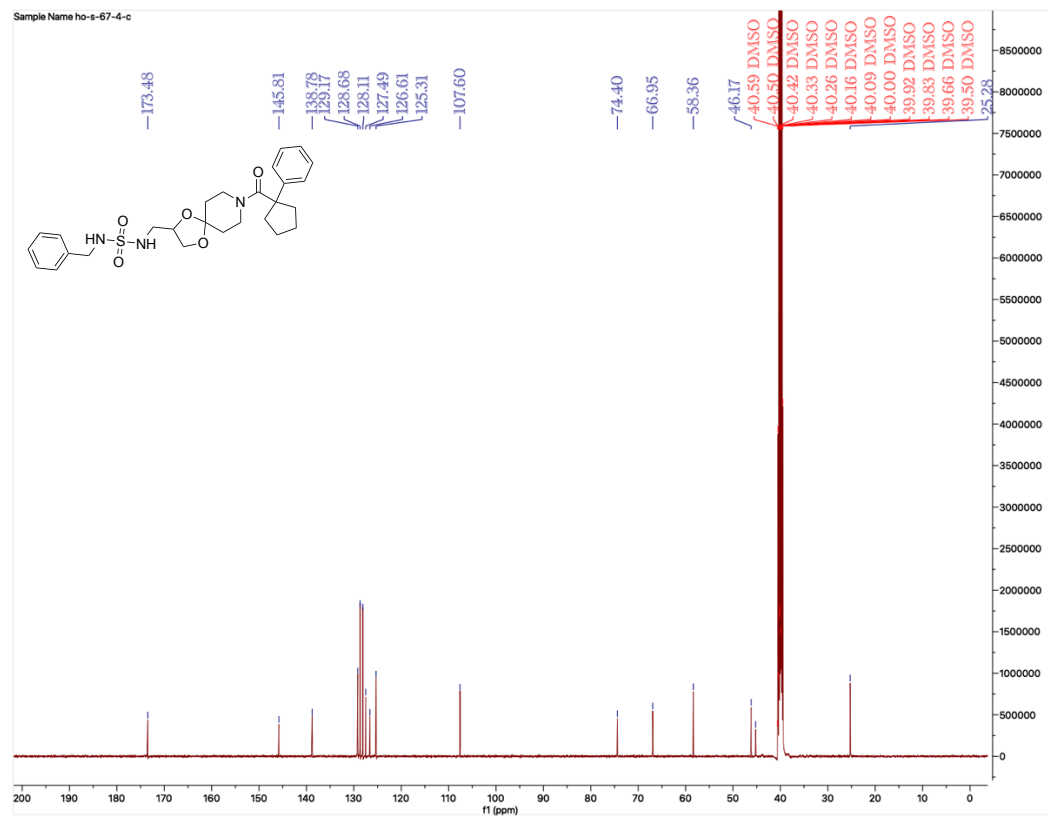


Figure S99: ^{13}C NMR (126 MHz, DMSO) for **5a**



Chemical structure of compound 66-2: CN(C)S(=O)(=O)NC1OCCN(C1C(=O)C2CCCC2)C3=CC=CC=C3

¹H NMR spectrum (400 MHz, CDCl₃) showing peaks from 0.0 to 13.0 ppm. The x-axis is labeled 'F1 (ppm)' and the y-axis is labeled 'Intensity'. Integration values are shown below the baseline.

Chemical Shift (ppm)	Integration
7.36	2.00
4.25	3.00
4.03	4.24
3.99	3.00
3.95	4.24
3.91	3.00
3.87	4.24
3.83	3.00
3.79	4.24
3.75	3.00
3.71	4.24
3.67	3.00
3.63	4.24
3.59	3.00
3.55	4.24
3.51	3.00
3.47	4.24
3.43	3.00
3.39	4.24
3.35	3.00
3.31	4.24
3.27	3.00
3.23	4.24
3.19	3.00
3.15	4.24
3.11	3.00
3.07	4.24
3.03	3.00
2.99	4.24
2.95	3.00
2.91	4.24
2.87	3.00
2.83	4.24
2.79	3.00
2.75	4.24
2.71	3.00
2.67	4.24
2.63	3.00
2.59	4.24
2.55	3.00
2.51	4.24
2.47	3.00
2.43	4.24
2.39	3.00
2.35	4.24
2.31	3.00
2.27	4.24
2.23	3.00
2.19	4.24
2.15	3.00
2.11	4.24
2.07	3.00
2.03	4.24
1.99	3.00
1.95	4.24
1.91	3.00
1.87	4.24
1.83	3.00
1.79	4.24
1.75	3.00
1.71	4.24
1.67	3.00
1.63	4.24
1.59	3.00
1.55	4.24
1.51	3.00
1.47	4.24
1.43	3.00
1.39	4.24
1.35	3.00
1.31	4.24
1.27	3.00
1.23	4.24
1.19	3.00
1.15	4.24
1.11	3.00
1.07	4.24
1.03	3.00
0.99	4.24
0.95	3.00
0.91	4.24
0.87	3.00
0.83	4.24
0.79	3.00
0.75	4.24
0.71	3.00
0.67	4.24
0.63	3.00
0.59	4.24
0.55	3.00
0.51	4.24
0.47	3.00
0.43	4.24
0.39	3.00
0.35	4.24
0.31	3.00
0.27	4.24
0.23	3.00
0.19	4.24
0.15	3.00
0.11	4.24
0.07	3.00
0.03	4.24
0.00	3.00

Sample Name ho-s-66-2-c

Chemical structure of compound 10: CN(C)S(=O)(=O)NC1COC2(CCN(C2C(=O)C3CCCC3)C1)O

Peak assignments (ppm):

- 176.60
- 146.46
- 138.07
- 129.95
- 129.64
- 129.46
- 128.79
- 127.56
- 126.20
- 108.93
- 75.99
- 67.88
- 59.93
- 55.17
- 49.63
- 49.51 MeOD
- 49.46
- 49.34 MeOD
- 49.28
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 46.54
- 46.39
- 42.02
- 39.31
- 39.26
- 36.86
- 35.31
- 34.81
- 25.94

MOR-A-3772-08B-RAC-57-24
D2O EXCHANGE
HIGH TEMPERATURE
AAA PROTON DMSO (Z:)2024/06 JUN 24) PDSNMR-01

Chemical structure of compound 57-24 (MOR-A-3772-08B-RAC-57-24) is shown as an inset. The structure is a complex molecule featuring a benzene ring, a sulfonamide group, a cyclic ether, and a carbonyl group.

The ^1H NMR spectrum (DMSO- d_6) shows the following chemical shifts (ppm) and integration values:

Chemical Shift (ppm)	Integration
7.34	2.28
7.33	2.96
7.32	
7.30	
7.21	
7.20	
7.20	
7.20	
7.19	
7.18	
7.18	
4.27	
4.26	
3.29	
3.23	
3.23	
3.23	
3.09	
3.08	
3.07	
2.93	
2.92	
2.91	
2.91	
2.91	
2.91	
2.91	
2.50	
2.50	
1.94	
1.65	
1.64	
1.63	
1.62	
1.62	
1.62	
1.24	
1.24	
1.00	
0.99	
0.98	
0.98	
0.98	
0.97	
0.96	

MOR-A-3772-086-RAC-57-24
C13CPD DMSO (Z:[2024]07 JUL 2024) PDSNMR-02

Chemical structure of compound 57-24 is shown. The structure is a complex molecule featuring a benzene ring, a sulfonamide group, a morpholine ring, and a cyclopentyl group.

¹³C NMR spectrum (DMSO-d₆) showing chemical shifts (ppm) for compound 57-24. The spectrum displays peaks corresponding to the structure, with labeled values including 173.00, 145.34, 137.44, 128.68, 128.37, 128.03, 127.33, 126.12, 124.83, 107.21, 73.98, 66.33, 57.89, 49.91, 44.98, 43.39, 41.58, 40.16 DMSO, 39.95 DMSO, 39.74 DMSO, 39.53 DMSO, 39.33 DMSO, 39.12 DMSO, 38.91 DMSO, 34.87, 24.79, and 12.82.

Figure S104: ^1H NMR (400 MHz, DMSO) for **5d**

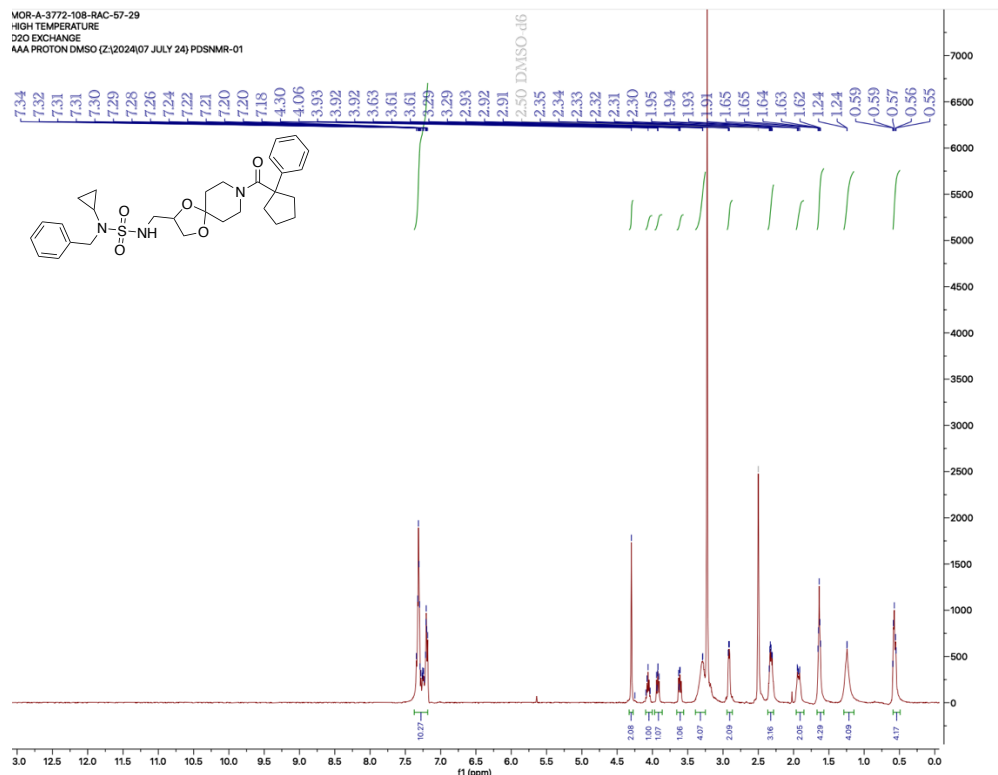


Figure S105: ^{13}C NMR (101 MHz, DMSO) for **5d**

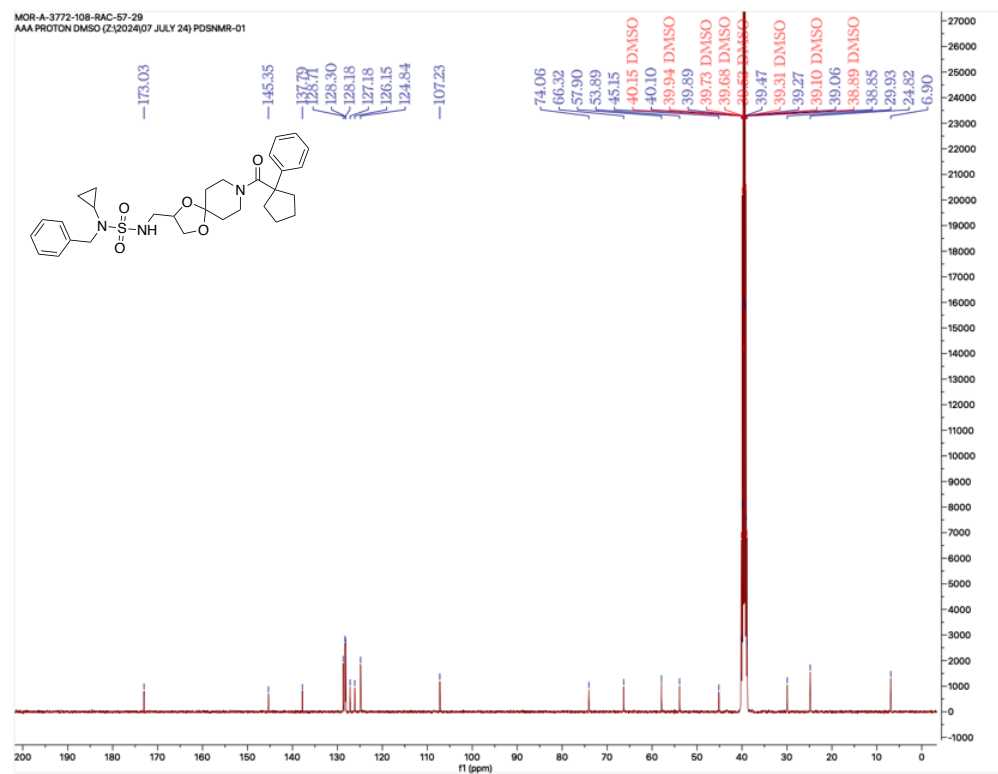


Figure S106: ^1H NMR (500 MHz, CD_3OD) for **5e**

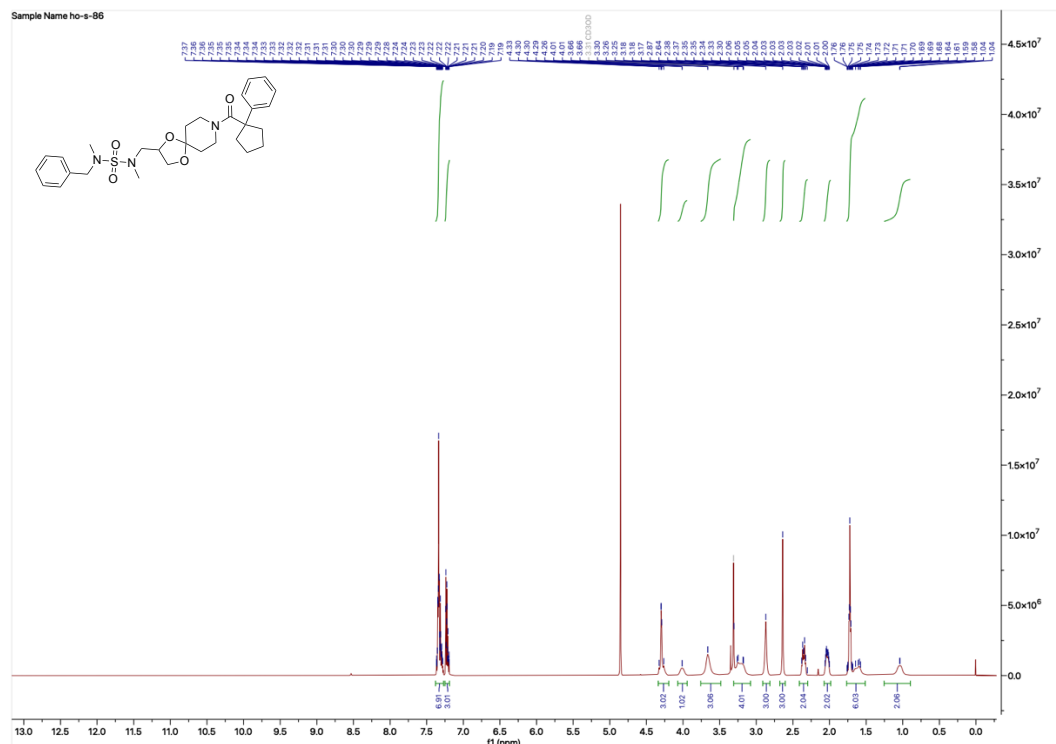


Figure S107: ^{13}C NMR (126 MHz, CD_3OD) for **5e**

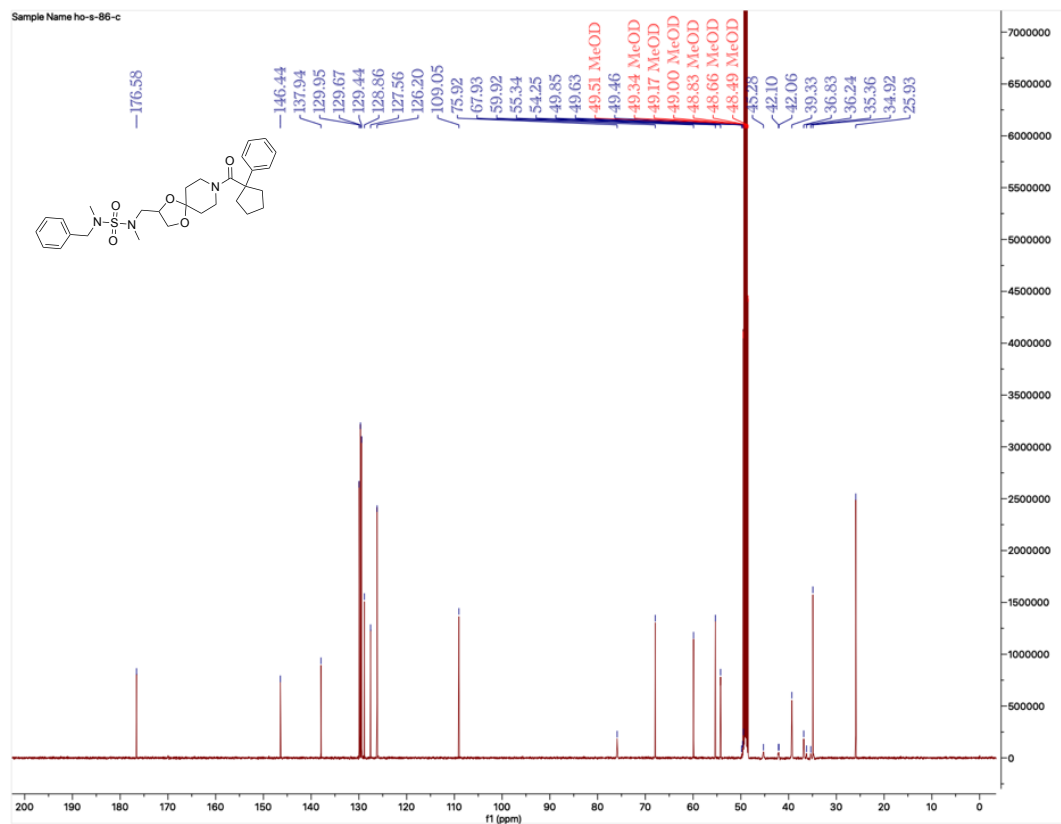


Figure S108: ^1H NMR (500 MHz, CD_3OD) for **5f**

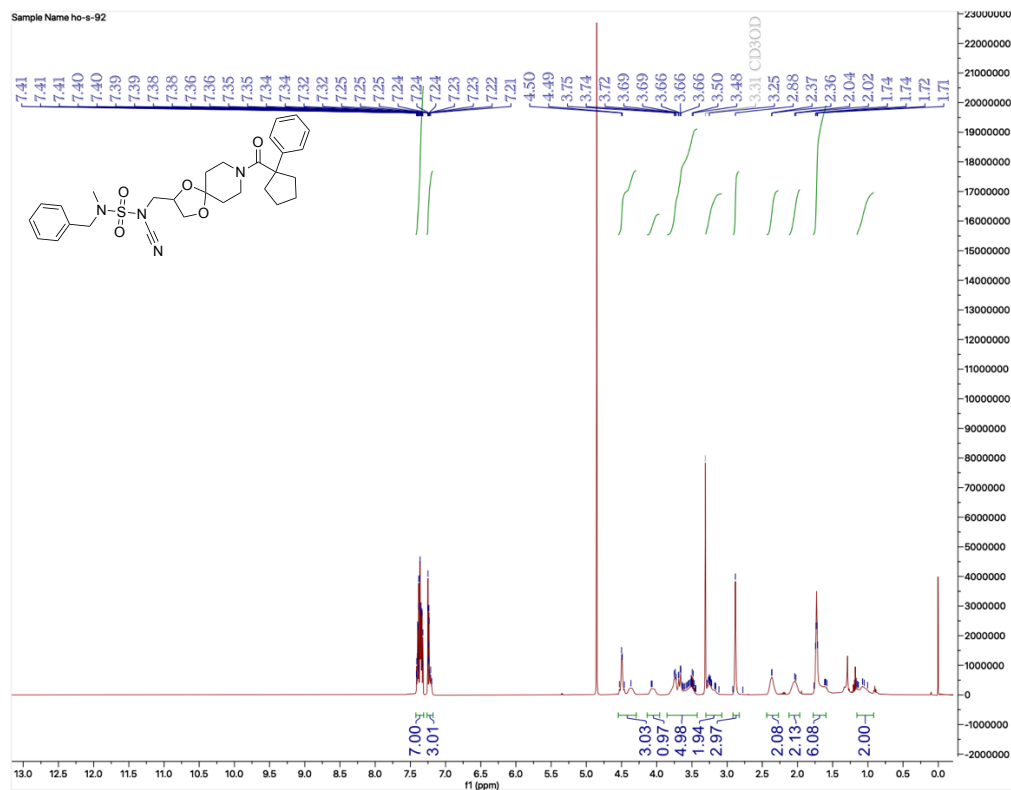
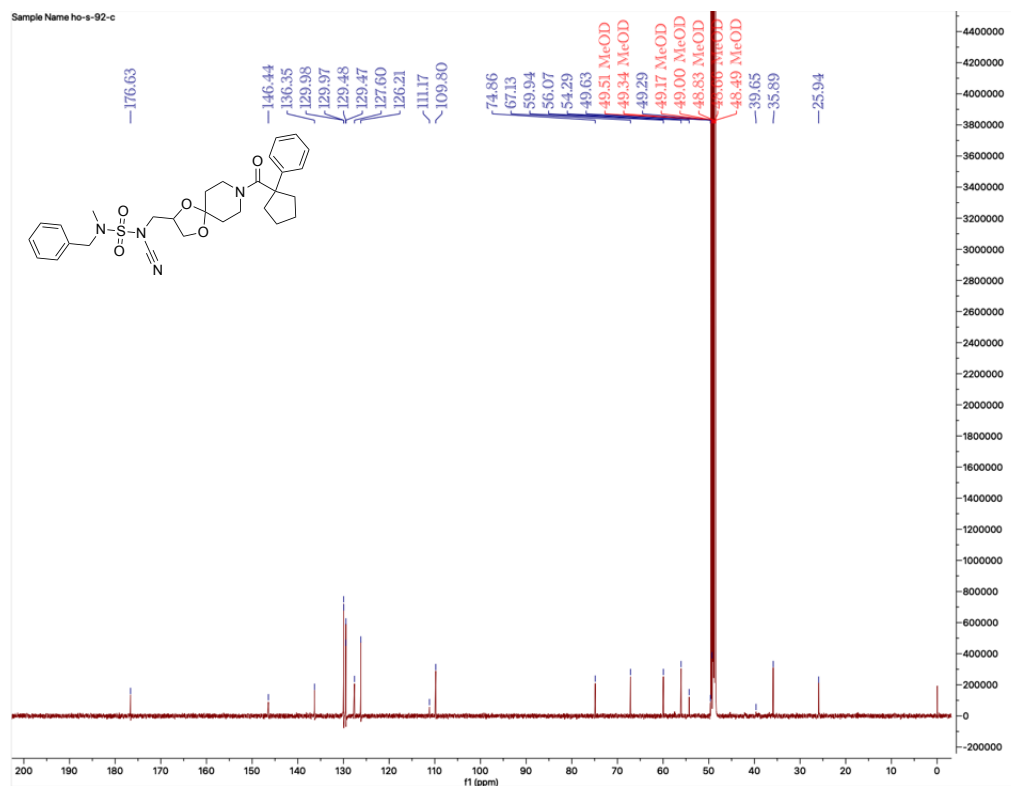


Figure S109: ^{13}C NMR (126 MHz, CD_3OD) for **5f**



Sample Name ho-s-84

Chemical structure of compound 10 is shown in the top left corner. The structure is a complex molecule featuring a sulfonamide group, a tetrahydropyran ring, and a cyclopentyl group.

The ^1H NMR spectrum displays chemical shifts (ppm) on the x-axis, ranging from 13.0 to 0.0. The y-axis represents intensity, with a scale from 2.0×10^6 to 3.0×10^7 . The spectrum shows several sharp peaks, with integration values indicated below the baseline. Key peaks are observed in the aromatic region (7.0-7.5 ppm), a large solvent peak at 5.0 ppm, and multiple peaks in the aliphatic region (1.0-4.0 ppm).

Integration values (from left to right): 2.06, 3.06, 3.19, 1.12, 3.00, 1.19, 5.00, 3.11, 2.18, 2.15, 6.30, 6.11, 2.13, 1.04, 1.02, 1.00, 0.99, 0.98, 0.97.

Sample Name ho-s-84-c

Chemical structure of the compound (ho-s-84-c) is shown above the spectrum. The structure is a complex molecule featuring a sulfonamide group, a morpholine ring, and a cyclohexane ring.

Mass spectrum data (m/z vs. Relative Intensity):

m/z	Relative Intensity (approx.)
176.58	400,000
146.44	1,000,000
138.01	500,000
129.95	500,000
129.67	1,800,000
129.48	1,800,000
128.85	1,200,000
127.56	1,200,000
126.19	1,200,000
109.11	800,000
76.20	100,000
68.18	100,000
59.92	100,000
55.29	100,000
51.88	100,000
50.43	100,000
49.63	100,000
49.51 MeOD	4,400,000
49.46	100,000
49.34 MeOD	100,000
49.17 MeOD	100,000
49.00 MeOD	100,000
48.83 MeOD	100,000
48.66 MeOD	100,000
48.49 MeOD	100,000
45.31	100,000
39.35	100,000
39.32	100,000
36.29	100,000
34.88	100,000
32.68	100,000
29.00	100,000
27.55	100,000
25.96	100,000
25.93	100,000
23.67	100,000
14.41	100,000

Sample Name: ho-s-104

Chemical structure of 104: CN(C)CCN(S(=O)(=O)Cc1ccccc1)CC2OCCN(C2)C(=O)C3CCCC3

¹H NMR spectrum (CDCl₃) showing peaks (ppm):

- 7.37, 7.36, 7.35, 7.35, 7.34, 7.33, 7.33, 7.32, 7.32, 7.31, 7.31, 7.30, 7.30, 7.30, 7.30, 7.29, 7.24, 7.24, 7.24, 7.22, 7.22, 7.21, 7.21, 7.20, 7.20, 7.19, 4.30, 4.30, 3.59, 3.57, 3.56, 3.47, 3.45, 3.45, 3.44, 3.44, 3.31 (CDCl₃), 3.17, 3.17, 2.67, 2.65, 2.64, 2.62, 2.35, 2.33, 2.28, 2.01, 1.74, 1.73, 1.72, 1.71

Integration values: 2.00, 1.99, 3.00, 1.02, 6.28, 3.37, 4.89, 7.98, 2.28, 6.38, 1.97

Sample Name ho-s-104-c

Chemical structure of compound 104c is shown above the spectrum.

Key peaks (ppm) labeled on the spectrum:

- 175.18
- 145.05
- 136.52
- 128.56
- 128.30
- 128.11
- 127.51
- 126.17
- 124.81
- 74.95
- 66.66
- 58.52
- 56.77
- 53.95
- 48.11 MeOD
- 48.06
- 47.94 MeOD
- 47.77 MeOD
- 47.60 MeOD
- 47.43 MeOD
- 47.26 MeOD
- 46.39
- 44.26
- 33.52
- 24.53

Figure S114: ^1H NMR (500 MHz, CD_3OD) for **5i**

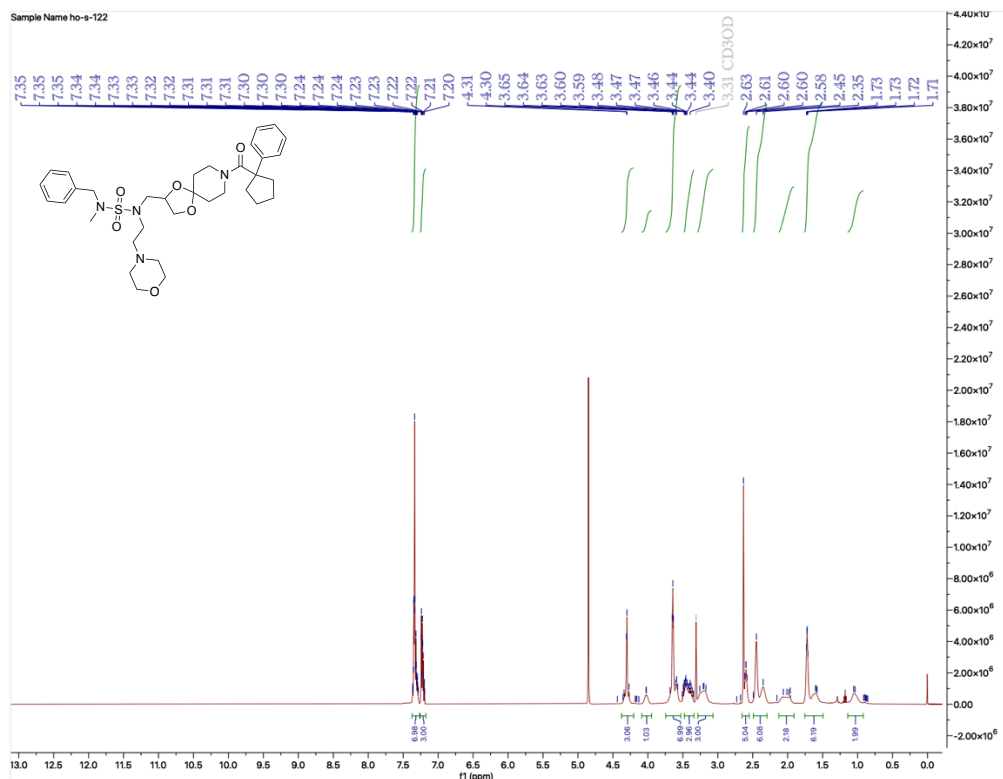
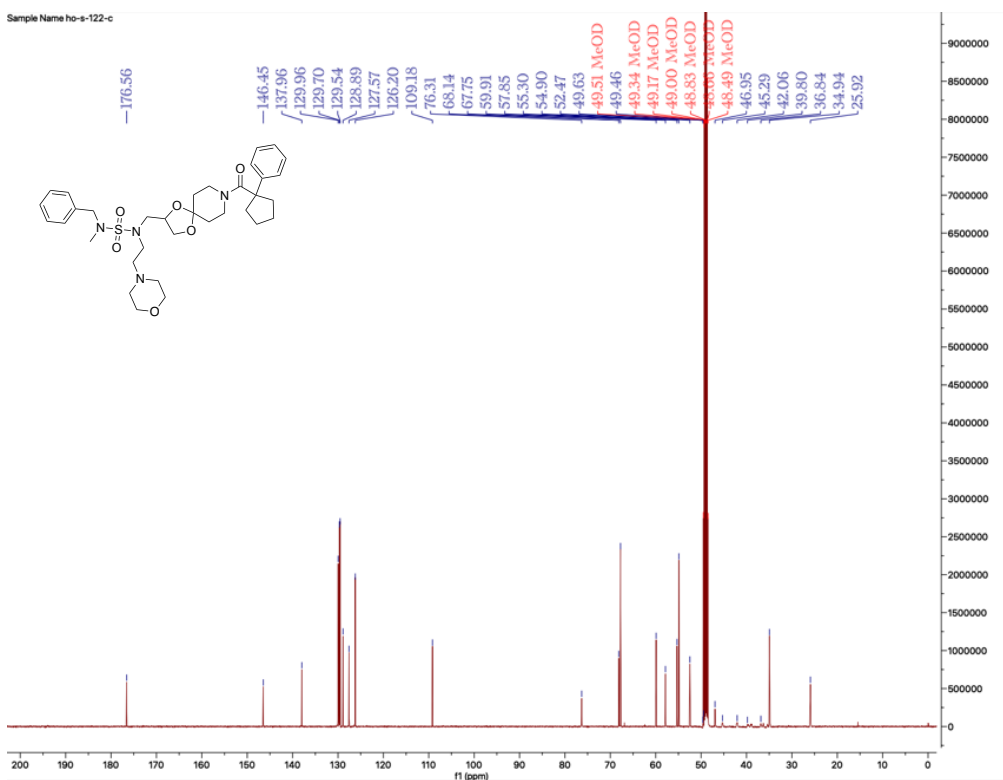


Figure S115: ^{13}C NMR (126 MHz, CD_3OD) for **5i**



Sample Name ho-s124

Chemical structure of compound 10:

CN(C)C(=O)N(S(=O)(=O)Cc1ccccc1)CC2OCCN(C2)C(=O)C3CCCC3

¹H NMR spectrum (400 MHz, CDCl₃) showing chemical shifts (ppm) and integration values:

Chemical Shift (ppm)	Integration
7.26	2.22
7.25	1.01
7.24	
7.23	
7.22	
7.21	
7.20	
7.19	
7.18	
7.17	
7.16	
7.15	
7.14	
7.13	
7.12	
7.11	
7.10	
7.09	
7.08	
7.07	
7.06	
7.05	
7.04	
7.03	
7.02	
7.01	
7.00	
6.99	
6.98	
6.97	
6.96	
6.95	
6.94	
6.93	
6.92	
6.91	
6.90	
6.89	
6.88	
6.87	
6.86	
6.85	
6.84	
6.83	
6.82	
6.81	
6.80	
6.79	
6.78	
6.77	
6.76	
6.75	
6.74	
6.73	
6.72	
6.71	
6.70	
6.69	
6.68	
6.67	
6.66	
6.65	
6.64	
6.63	
6.62	
6.61	
6.60	
6.59	
6.58	
6.57	
6.56	
6.55	
6.54	
6.53	
6.52	
6.51	
6.50	
6.49	
6.48	
6.47	
6.46	
6.45	
6.44	
6.43	
6.42	
6.41	
6.40	
6.39	
6.38	
6.37	
6.36	
6.35	
6.34	
6.33	
6.32	
6.31	
6.30	
6.29	
6.28	
6.27	
6.26	
6.25	
6.24	
6.23	
6.22	
6.21	
6.20	
6.19	
6.18	
6.17	
6.16	
6.15	
6.14	
6.13	
6.12	
6.11	
6.10	
6.09	
6.08	
6.07	
6.06	
6.05	
6.04	
6.03	
6.02	
6.01	
6.00	
5.99	
5.98	
5.97	
5.96	
5.95	
5.94	
5.93	
5.92	
5.91	
5.90	
5.89	
5.88	
5.87	
5.86	
5.85	
5.84	
5.83	
5.82	
5.81	
5.80	
5.79	
5.78	
5.77	
5.76	
5.75	
5.74	
5.73	
5.72	
5.71	
5.70	
5.69	
5.68	
5.67	
5.66	
5.65	
5.64	
5.63	
5.62	
5.61	
5.60	
5.59	
5.58	
5.57	
5.56	
5.55	
5.54	
5.53	
5.52	
5.51	
5.50	
5.49	
5.48	
5.47	
5.46	
5.45	
5.44	
5.43	
5.42	
5.41	
5.40	
5.39	
5.38	
5.37	
5.36	
5.35	
5.34	
5.33	
5.32	
5.31	
5.30	
5.29	
5.28	
5.27	
5.26	
5.25	
5.24	
5.23	
5.22	
5.21	
5.20	
5.19	
5.18	
5.17	
5.16	
5.15	
5.14	
5.13	
5.12	
5.11	
5.10	
5.09	
5.08	
5.07	
5.06	
5.05	
5.04	
5.03	
5.02	
5.01	
5.00</	

Sample Name ho-s-124-c

Chemical structure of compound 124c is shown above the spectrum:

CN(C)C(=O)N(CS(=O)(=O)Cc1ccccc1)CC2OC3CCN(C(=O)C4CCCC4)CC23

¹H NMR spectrum (MeOD) showing chemical shifts (ppm) and integration values:

Chemical Shift (ppm)	Integration
7.4527	1.00
7.4849	1.00
7.4866	1.00
7.4883	1.00
7.4900	1.00
7.4917	1.00
7.4934	1.00
7.4951	1.00
7.4968	1.00
7.4985	1.00
7.4999	1.00
7.5012	1.00
7.5025	1.00
7.5038	1.00
7.5051	1.00
7.5064	1.00
7.5077	1.00
7.5090	1.00
7.5103	1.00
7.5116	1.00
7.5129	1.00
7.5142	1.00
7.5155	1.00
7.5168	1.00
7.5181	1.00
7.5194	1.00
7.5207	1.00
7.5220	1.00
7.5233	1.00
7.5246	1.00
7.5259	1.00
7.5272	1.00
7.5285	1.00
7.5298	1.00
7.5311	1.00
7.5324	1.00
7.5337	1.00
7.5350	1.00
7.5363	1.00
7.5376	1.00
7.5389	1.00
7.5402	1.00
7.5415	1.00
7.5428	1.00
7.5441	1.00
7.5454	1.00
7.5467	1.00
7.5480	1.00
7.5493	1.00
7.5506	1.00
7.5519	1.00
7.5532	1.00
7.5545	1.00
7.5558	1.00
7.5571	1.00
7.5584	1.00
7.5597	1.00
7.5610	1.00
7.5623	1.00
7.5636	1.00
7.5649	1.00
7.5662	1.00
7.5675	1.00
7.5688	1.00
7.5701	1.00
7.5714	1.00
7.5727	1.00
7.5740	1.00
7.5753	1.00
7.5766	1.00
7.5779	1.00
7.5792	1.00
7.5805	1.00
7.5818	1.00
7.5831	1.00
7.5844	1.00
7.5857	1.00
7.5870	1.00
7.5883	1.00
7.5896	1.00
7.5909	1.00
7.5922	1.00
7.5935	1.00
7.5948	1.00
7.5961	1.00
7.5974	1.00
7.5987	1.00
7.5999	1.00
7.6012	1.00
7.6025	1.00
7.6038	1.00
7.6051	1.00
7.6064	1.00
7.6077	1.00
7.6090	1.00
7.6103	1.00
7.6116	1.00
7.6129	1.00
7.6142	1.00
7.6155	1.00
7.6168	1.00
7.6181	1.00
7.6194	1.00
7.6207	1.00
7.6220	1.00
7.6233	1.00
7.6246	1.00
7.6259	1.00
7.6272	1.00
7.6285	1.00
7.6298	1.00
7.6311	1.00
7.6324	1.00
7.6337	1.00
7.6350	1.00
7.6363	1.00
7.6376	1.00
7.6389	1.00
7.6402	1.00
7.6415	1.00
7.6428	1.00
7.6441	1.00
7.6454	1.00
7.6467	1.00
7.6480	1.00
7.6493	1.00
7.6506	1.00
7.6519	1.00
7.6532	1.00
7.6545	1.00
7.6558	1.00
7.6571	1.00
7.6584	1.00
7.6597	1.00
7.6610	1.00
7.6623	1.00
7.6636	1.00
7.6649	1.00
7.6662	1.00
7.6675	1.00
7.6688	1.00
7.6701	1.00
7.6714	1.00
7.6727	1.00
7.6740	1.00
7.6753	1.00
7.6766	1.00
7.6779	1.00
7.6792	1.00
7.6805	1.00
7.6818	1.00
7.6831	1.00
7.6844	1.00
7.6857	1.00
7.6870	1.00
7.6883	1.00
7.6896	1.00
7.6909	1.00
7.6922	1.00
7.6935	1.00
7.6948	1.00
7.6961</	

Sample Name ho-s-146

Chemical structure of compound 146 is shown in the top left corner.

¹H NMR spectrum (CD₃OD) showing peaks from 0 to 7.35 ppm. The x-axis is labeled "f1 (ppm)" and the y-axis is labeled "Intensity".

Peak list (ppm): 7.35, 7.35, 7.35, 7.35, 7.34, 7.33, 7.33, 7.32, 7.31, 7.30, 7.29, 7.29, 7.28, 7.25, 7.24, 7.24, 7.23, 7.23, 7.22, 7.22, 7.21, 4.31, 4.19, 4.16, 3.62, 3.60, 3.59, 3.39, 3.35, 3.34, 3.32, 3.31, 3.31 CD₃OD, 2.67, 2.35, 1.99, 1.97, 1.96, 1.96, 1.87, 1.86, 1.84, 1.84, 1.73, 1.72.

Integration values (from left to right): 2.22, 2.22, 6.36, 1.05, 4.00, 5.00, 2.00, 3.20, 2.17, 4.18, 2.18, 0.15, 1.97.

Sample Name ho-s-146-c

Chemical structure of compound 146c is shown. The structure is a complex molecule featuring a benzyl group, a sulfonamide, a pyrrolidine ring, a morpholine ring, and a cyclopentyl group.

¹³C NMR spectrum (f1 (ppm)) showing peaks at the following chemical shifts (ppm):

- 176.58
- 168.87
- 146.45
- 138.12
- 129.96
- 129.63
- 129.49
- 128.79
- 127.57
- 126.21
- 109.08
- 76.55
- 68.10
- 59.95
- 55.32
- 52.69
- 49.63
- 49.51 MeOD
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 47.24
- 46.86
- 45.31
- 42.04
- 35.00
- 27.13
- 25.89
- 25.03
- 0.04

Figure S120: ^1H NMR (500 MHz, CD_3OD) for **5I**

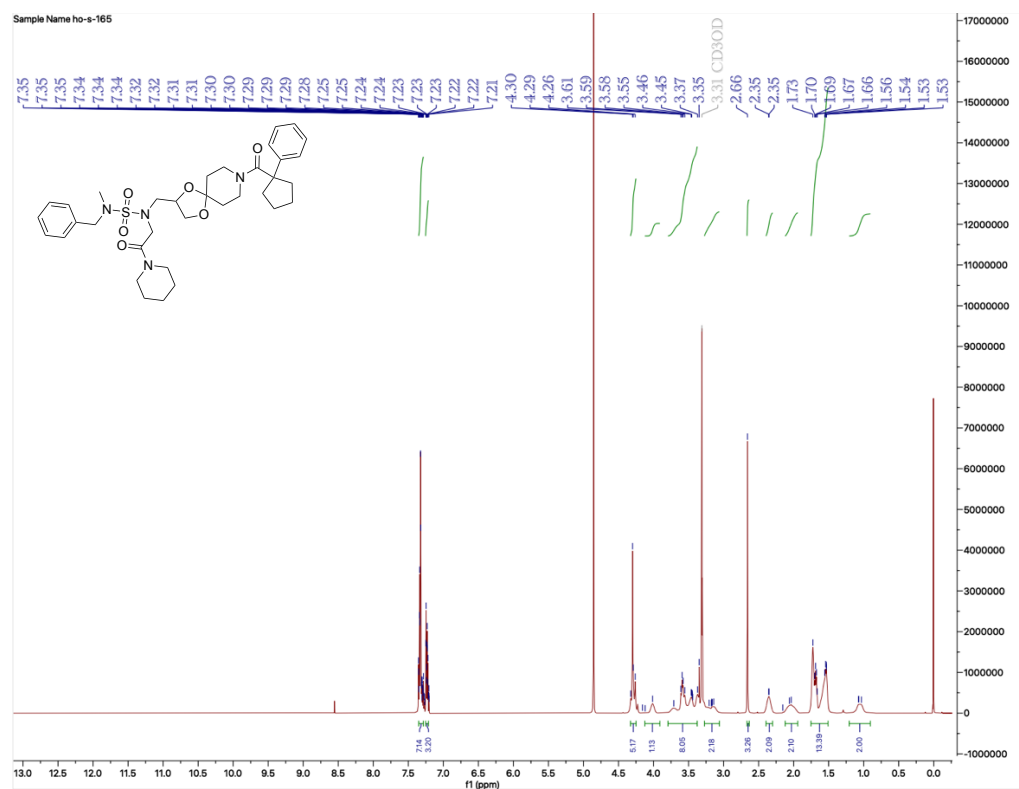


Figure S121: ^{13}C NMR (126 MHz, CD_3OD) for **5I**

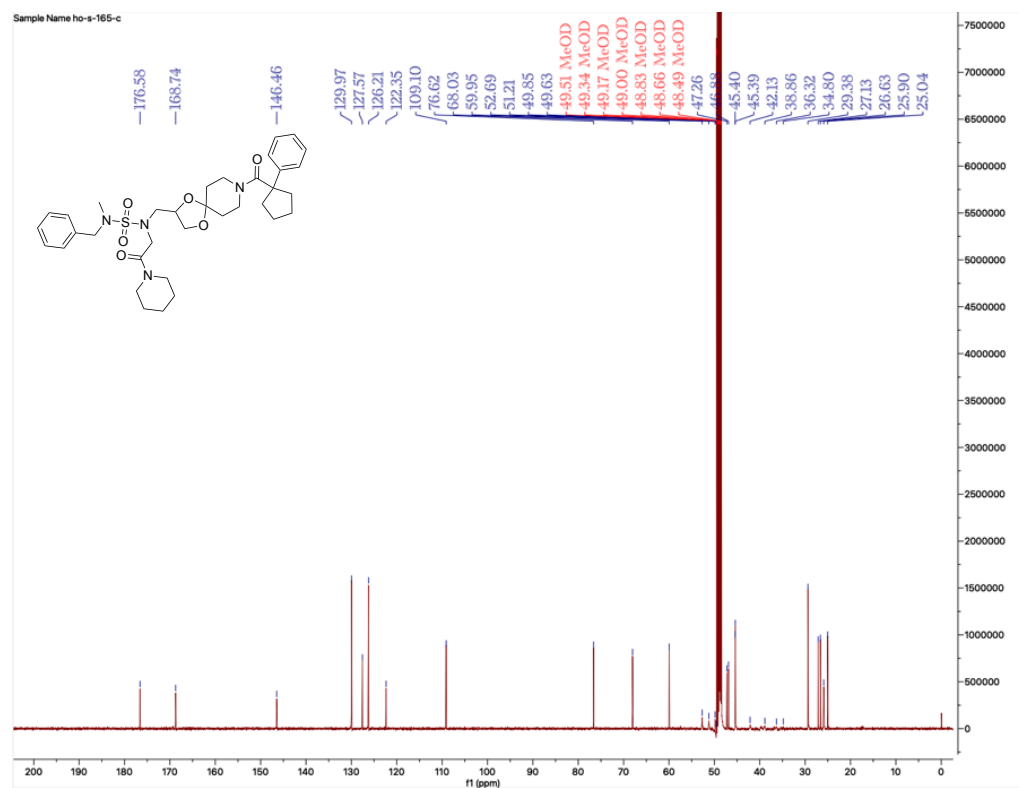


Figure S122: ^1H NMR (500 MHz, CD_3OD) for **5m**

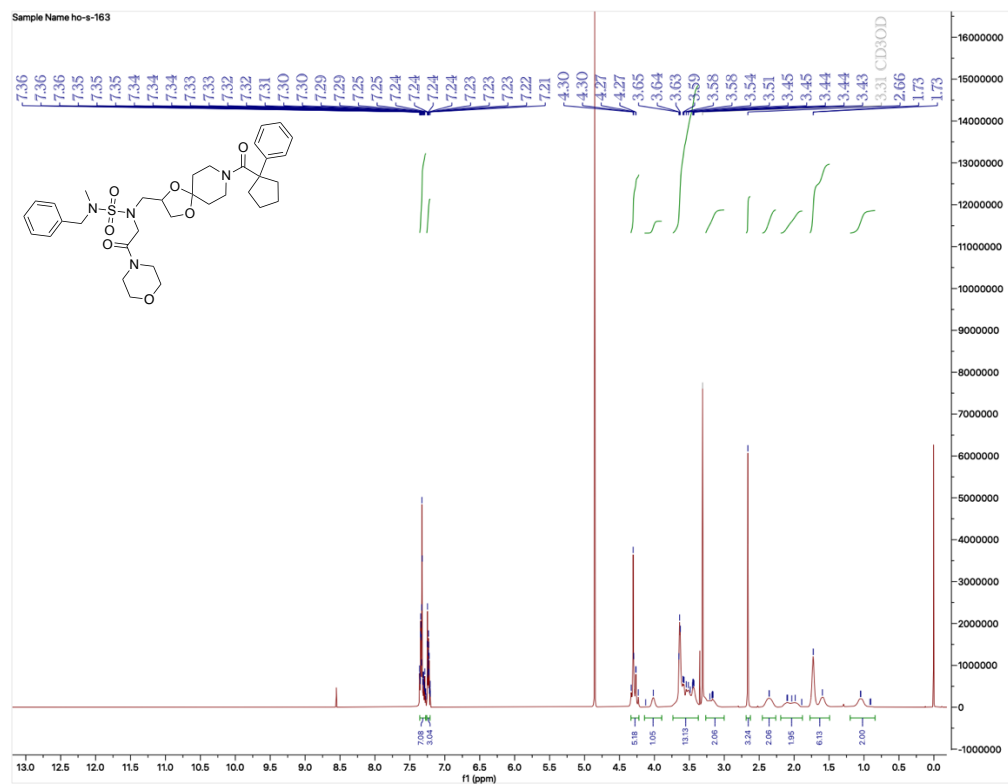
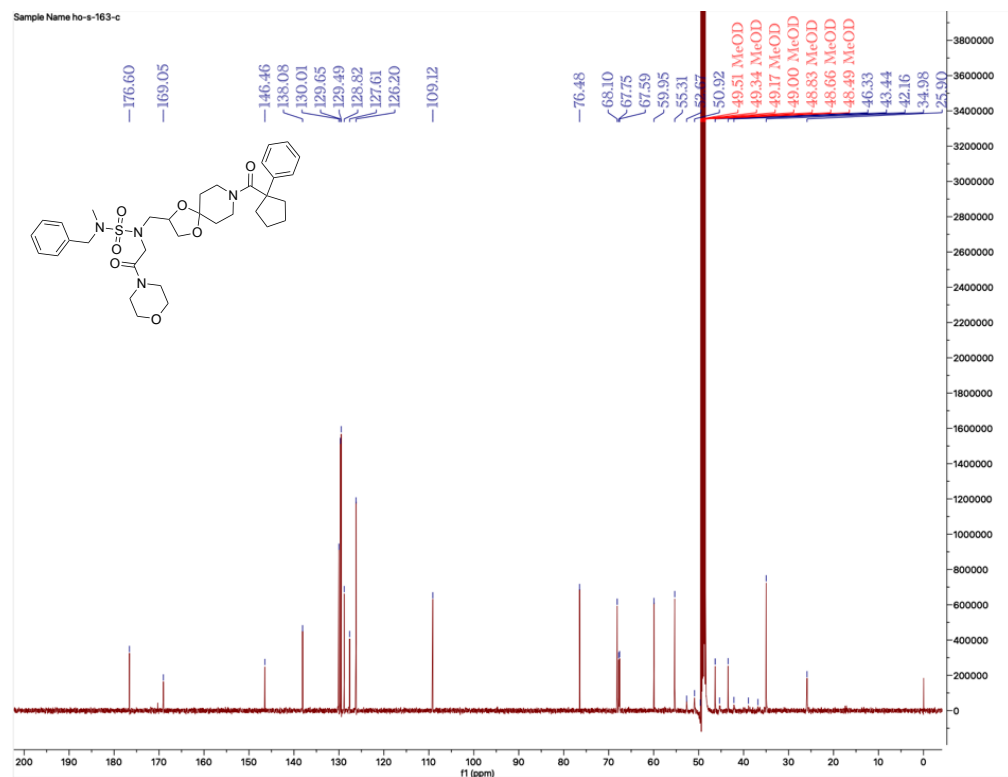


Figure S123: ^{13}C NMR (126 MHz, CD_3OD) for **5m**



Sample Name ho-s-116

Chemical structure of the compound is shown above the spectrum.

Chemical shift (ppm) values (from left to right): 12.99, 12.97, 12.95, 12.93, 12.91, 12.89, 12.87, 12.85, 12.83, 12.81, 12.79, 12.77, 12.75, 12.73, 12.71, 12.69, 12.67, 12.65, 12.63, 12.61, 12.59, 12.57, 12.55, 12.53, 12.51, 12.49, 12.47, 12.45, 12.43, 12.41, 12.39, 12.37, 12.35, 12.33, 12.31, 12.29, 12.27, 12.25, 12.23, 12.21, 12.19, 12.17, 12.15, 12.13, 12.11, 12.09, 12.07, 12.05, 12.03, 12.01, 11.99, 11.97, 11.95, 11.93, 11.91, 11.89, 11.87, 11.85, 11.83, 11.81, 11.79, 11.77, 11.75, 11.73, 11.71, 11.69, 11.67, 11.65, 11.63, 11.61, 11.59, 11.57, 11.55, 11.53, 11.51, 11.49, 11.47, 11.45, 11.43, 11.41, 11.39, 11.37, 11.35, 11.33, 11.31, 11.29, 11.27, 11.25, 11.23, 11.21, 11.19, 11.17, 11.15, 11.13, 11.11, 11.09, 11.07, 11.05, 11.03, 11.01, 10.99, 10.97, 10.95, 10.93, 10.91, 10.89, 10.87, 10.85, 10.83, 10.81, 10.79, 10.77, 10.75, 10.73, 10.71, 10.69, 10.67, 10.65, 10.63, 10.61, 10.59, 10.57, 10.55, 10.53, 10.51, 10.49, 10.47, 10.45, 10.43, 10.41, 10.39, 10.37, 10.35, 10.33, 10.31, 10.29, 10.27, 10.25, 10.23, 10.21, 10.19, 10.17, 10.15, 10.13, 10.11, 10.09, 10.07, 10.05, 10.03, 10.01, 9.99, 9.97, 9.95, 9.93, 9.91, 9.89, 9.87, 9.85, 9.83, 9.81, 9.79, 9.77, 9.75, 9.73, 9.71, 9.69, 9.67, 9.65, 9.63, 9.61, 9.59, 9.57, 9.55, 9.53, 9.51, 9.49, 9.47, 9.45, 9.43, 9.41, 9.39, 9.37, 9.35, 9.33, 9.31, 9.29, 9.27, 9.25, 9.23, 9.21, 9.19, 9.17, 9.15, 9.13, 9.11, 9.09, 9.07, 9.05, 9.03, 9.01, 8.99, 8.97, 8.95, 8.93, 8.91, 8.89, 8.87, 8.85, 8.83, 8.81, 8.79, 8.77, 8.75, 8.73, 8.71, 8.69, 8.67, 8.65, 8.63, 8.61, 8.59, 8.57, 8.55, 8.53, 8.51, 8.49, 8.47, 8.45, 8.43, 8.41, 8.39, 8.37, 8.35, 8.33, 8.31, 8.29, 8.27, 8.25, 8.23, 8.21, 8.19, 8.17, 8.15, 8.13, 8.11, 8.09, 8.07, 8.05, 8.03, 8.01, 7.99, 7.97, 7.95, 7.93, 7.91, 7.89, 7.87, 7.85, 7.83, 7.81, 7.79, 7.77, 7.75, 7.73, 7.71, 7.69, 7.67, 7.65, 7.63, 7.61, 7.59, 7.57, 7.55, 7.53, 7.51, 7.49, 7.47, 7.45, 7.43, 7.41, 7.39, 7.37, 7.35, 7.33, 7.31, 7.29, 7.27, 7.25, 7.23, 7.21, 7.19, 7.17, 7.15, 7.13, 7.11, 7.09, 7.07, 7.05, 7.03, 7.01, 6.99, 6.97, 6.95, 6.93, 6.91, 6.89, 6.87, 6.85, 6.83, 6.81, 6.79, 6.77, 6.75, 6.73, 6.71, 6.69, 6.67, 6.65, 6.63, 6.61, 6.59, 6.57, 6.55, 6.53, 6.51, 6.49, 6.47, 6.45, 6.43, 6.41, 6.39, 6.37, 6.35, 6.33, 6.31, 6.29, 6.27, 6.25, 6.23, 6.21, 6.19, 6.17, 6.15, 6.13, 6.11, 6.09, 6.07, 6.05, 6.03, 6.01, 5.99, 5.97, 5.95, 5.93, 5.91, 5.89, 5.87, 5.85, 5.83, 5.81, 5.79, 5.77, 5.75, 5.73, 5.71, 5.69, 5.67, 5.65, 5.63, 5.61, 5.59, 5.57, 5.55, 5.53, 5.51, 5.49, 5.47, 5.45, 5.43, 5.41, 5.39, 5.37, 5.35, 5.33, 5.31, 5.29, 5.27, 5.25, 5.23, 5.21, 5.19, 5.17, 5.15, 5.13, 5.11, 5.09, 5.07, 5.05, 5.03, 5.01, 4.99, 4.97, 4.95, 4.93, 4.91, 4.89, 4.87, 4.85, 4.83, 4.81, 4.79, 4.77, 4.75, 4.73, 4.71, 4.69, 4.67, 4.65, 4.63, 4.61, 4.59, 4.57, 4.55, 4.53, 4.51, 4.49, 4.47, 4.45, 4.43, 4.41, 4.39, 4.37, 4.35, 4.33, 4.31, 4.29, 4.27, 4.25, 4.23, 4.21, 4.19, 4.17, 4.15, 4.13, 4.11, 4.09, 4.07, 4.05, 4.03, 4.01, 3.99, 3.97, 3.95, 3.93, 3.91, 3.89, 3.87, 3.85, 3.83, 3.81, 3.79, 3.77, 3.75, 3.73, 3.71, 3.69, 3.67, 3.65, 3.63, 3.61, 3.59, 3.57, 3.55, 3.53, 3.51, 3.49, 3.47, 3.45, 3.43, 3.41, 3.39, 3.37, 3.35, 3.33, 3.31, 3.29, 3.27, 3.25, 3.23, 3.21, 3.19, 3.17, 3.15, 3.13, 3.11, 3.09, 3.07, 3.05, 3.03, 3.01, 2.99, 2.97, 2.95, 2.93, 2.91, 2.89, 2.87, 2.85, 2.83, 2.81, 2.79, 2.77, 2.75, 2.73, 2.71, 2.69, 2.67, 2.65, 2.63, 2.61, 2.59, 2.57, 2.55, 2.53, 2.51, 2.49, 2.47, 2.45, 2.43, 2.41, 2.39, 2.37, 2.35, 2.33, 2.31, 2.29, 2.27, 2.25, 2.23, 2.21, 2.19, 2.17, 2.15, 2.13, 2.11, 2.09, 2.07, 2.05, 2.03, 2.01, 1.99, 1.97, 1.95, 1.93, 1.91, 1.89, 1.87, 1.85, 1.83, 1.81, 1.79, 1.77, 1.75, 1.73, 1.71, 1.69, 1.67, 1.65, 1.63, 1.61, 1.59, 1.57, 1.55, 1.53, 1.51, 1.49, 1.47, 1.45, 1.43, 1.41, 1.39, 1.37, 1.35, 1.33, 1.31, 1.29, 1.27, 1.25, 1.23, 1.21, 1.19, 1.17, 1.15, 1.13, 1.11, 1.09, 1.07, 1.05, 1.03, 1.01, 0.99, 0.97, 0.95, 0.93, 0

Sample Name ho-a-116-c

Chemical structure of compound 116c is shown. The structure is a complex molecule with a sulfonamide group, a bicyclic ether, and a benzylidene-protected amine.

¹³C NMR spectrum (MeOD) showing chemical shifts (ppm) on the x-axis and intensity on the y-axis. The spectrum displays several peaks, with the following chemical shifts labeled:

- 176.60
- 146.48
- 129.95
- 127.55
- 126.20
- 106.78
- 82.90
- 81.15
- 59.92
- 49.51 MeOD
- 49.45
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 47.91
- 44.02
- 26.66
- 26.49
- 25.95
- 24.86

CC1(C)OC(=O)N1CC2(CCN(C2)C3CCCC3)C(=O)N4CCCC4

¹H NMR spectrum (CD₃OD) of compound 10. The x-axis represents the chemical shift in ppm (δ), ranging from 0.0 to 13.0. The y-axis represents the intensity, ranging from 0.0 to 6.0 × 10⁷. The spectrum shows several peaks, with the most prominent ones in the aromatic region (7.0–7.4 ppm) and the aliphatic region (1.0–2.0 ppm). A large solvent peak is visible at 3.31 ppm. Integration values are provided below the baseline.

Chemical Shift (ppm)	Integration
7.36	2.01
7.35	3.00
7.34	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	
7.36	
7.35	
7.34	
7.32	
7.25	
7.24	
7.23	
7.22	
7.22	
7.37	

Sample Name ho-s-128-c

Chemical structure of compound ho-s-128-c is shown above the spectra.

¹H NMR spectrum (top) is recorded in MeOD. The x-axis represents chemical shift in ppm, ranging from 0 to 10. The y-axis represents intensity, ranging from 0 to 7,500,000. The spectrum shows several sharp peaks, with the most intense peak at approximately 4.9 ppm.

¹³C NMR spectrum (bottom) is recorded in CDCl₃. The x-axis represents chemical shift in ppm, ranging from 0 to 200. The y-axis represents intensity, ranging from 0 to 7,500,000. The spectrum shows several sharp peaks, with the most intense peak at approximately 176.57 ppm.

Peak list for ¹H NMR (ppm): 8.292, 8.112, 59.90, 49.51 MeOD, 49.34 MeOD, 49.17 MeOD, 49.00 MeOD, 48.83 MeOD, 48.49 MeOD, 45.25, 45.24, 44.07, 41.98, 39.32, 38.47, 36.59, 29.26, 26.63, 25.95, 23.26.

Peak list for ¹³C NMR (ppm): 176.57, 146.48, 129.95, 127.55, 122.30, 106.85.

Figure S128: ^1H NMR (400 MHz, CD_3OD) for **6c**

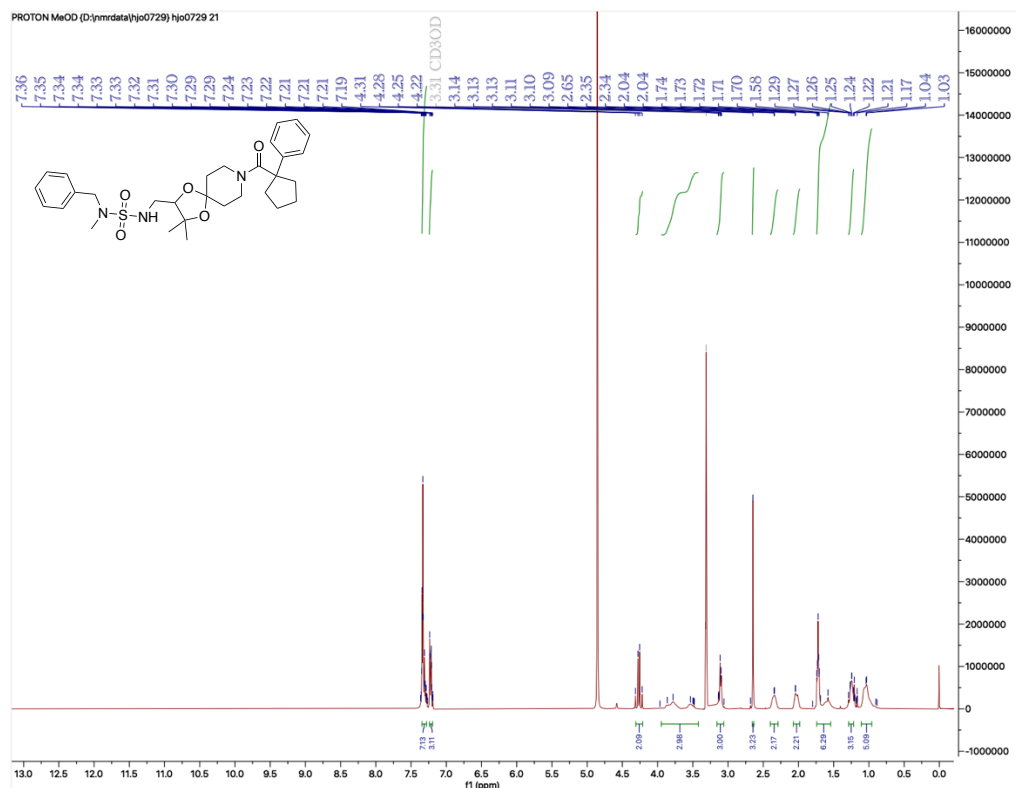


Figure S129: ^{13}C NMR (126 MHz, CD_3OD) for **6c**

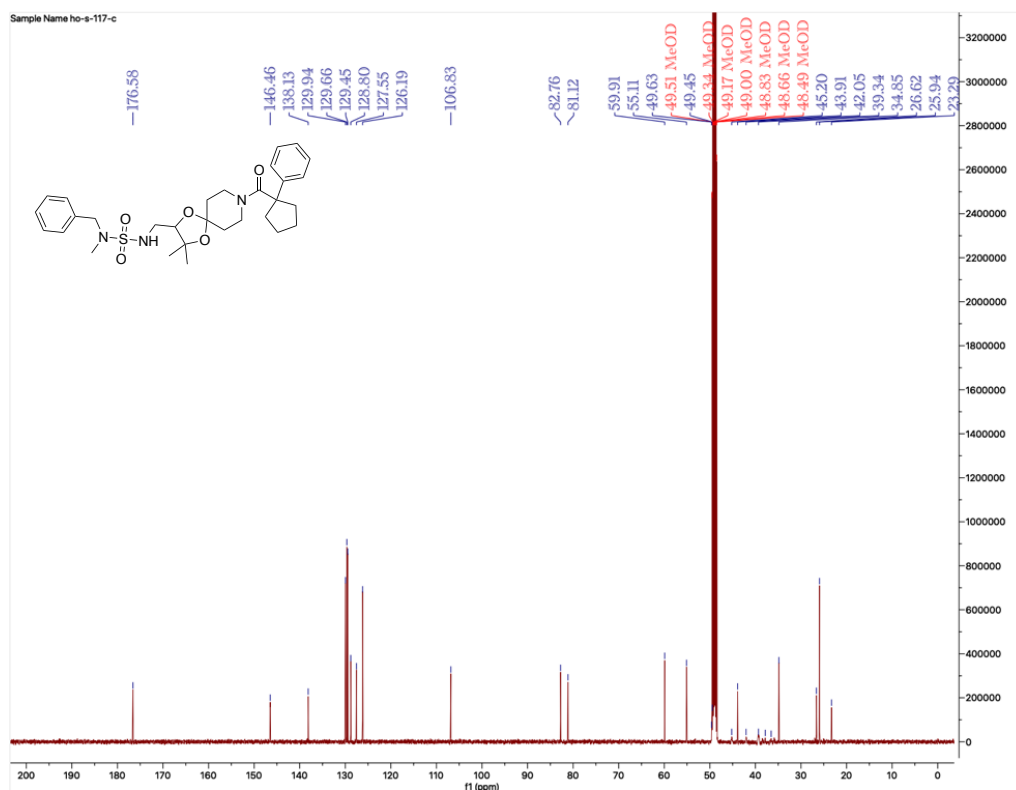


Figure S130: ^1H NMR (500 MHz, CD_3OD) for **6d**

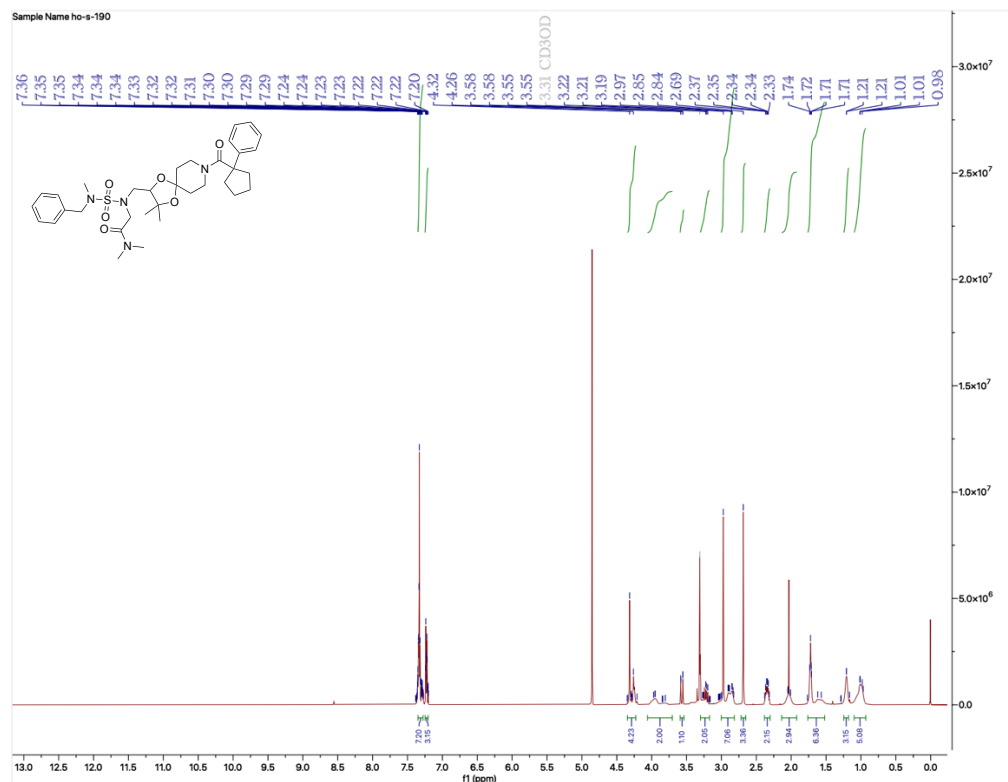
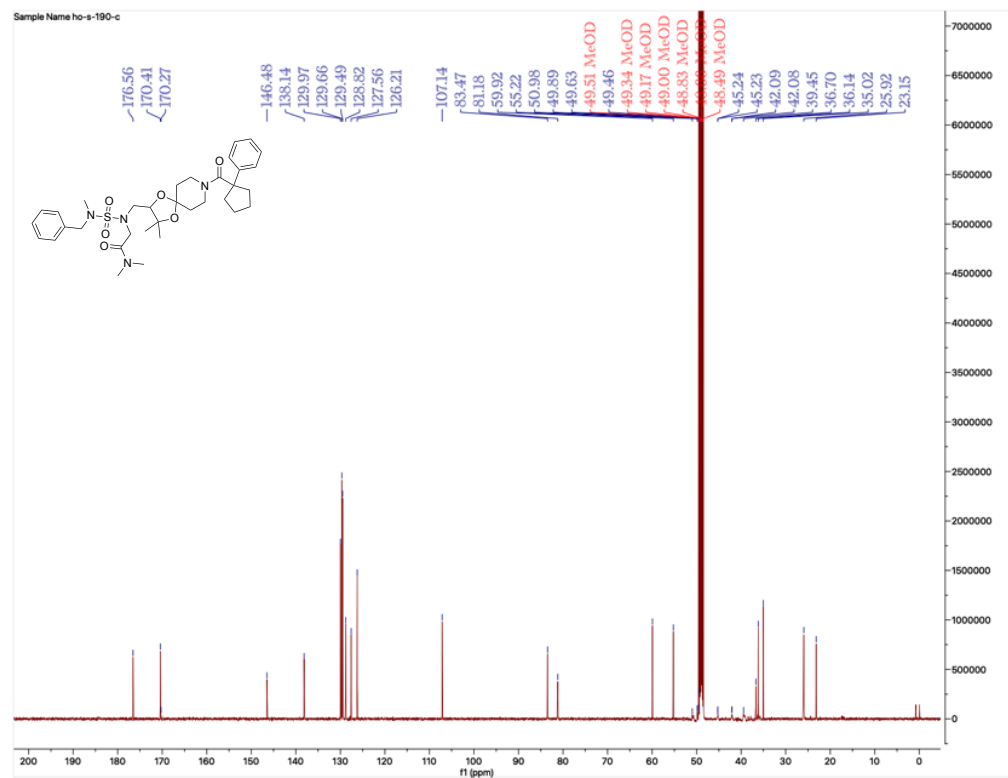


Figure S131: ^{13}C NMR (126 MHz, CD_3OD) for **6d**



Sample Name ho-s-134

Chemical structure of the compound (ho-s-134) is shown in the top left corner. The structure is a complex molecule featuring a sulfonamide group, a cyclic ether, and a cyclopentanone moiety.

The ^1H NMR spectrum displays the following chemical shifts (ppm) and integrations:

Chemical Shift (ppm)	Integration
7.23	2.28
7.03	3.3
4.83	2.06
3.53	4.17
3.23	5.02
2.13	2.36
1.93	4.13
1.63	6.81
1.23	3.11
1.03	5.0

Sample Name ho-s-134-c

Chemical structure of compound 134c is shown. The spectrum displays peaks corresponding to the structure, with labeled chemical shifts (ppm):

- 176.60
- 146.47
- 129.96
- 127.57
- 126.20
- 106.89
- 83.54
- 81.35
- 59.93
- 51.75
- 49.63
- 49.51 MeOD
- 49.46
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.49 MeOD
- 45.20
- 42.17
- 26.34
- 25.94
- 25.04
- 23.26
- 21.96

Figure S134: ^1H NMR (500 MHz, CD_3OD) for **7a**

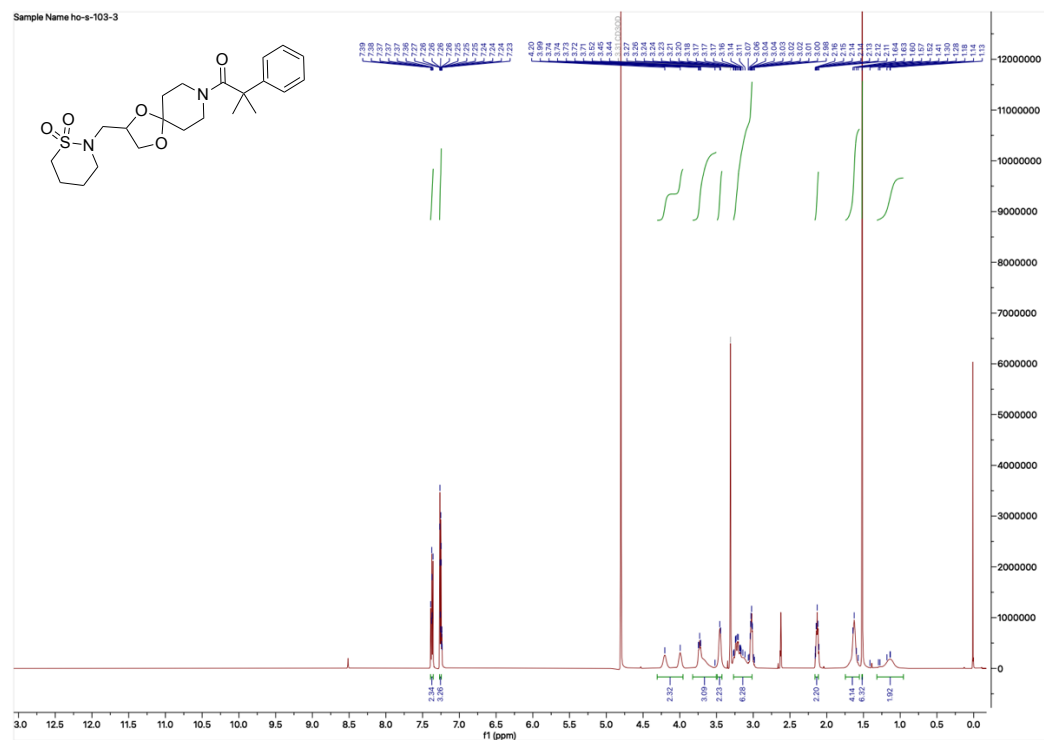


Figure S135: ^{13}C NMR (126 MHz, CD_3OD) for **7a**

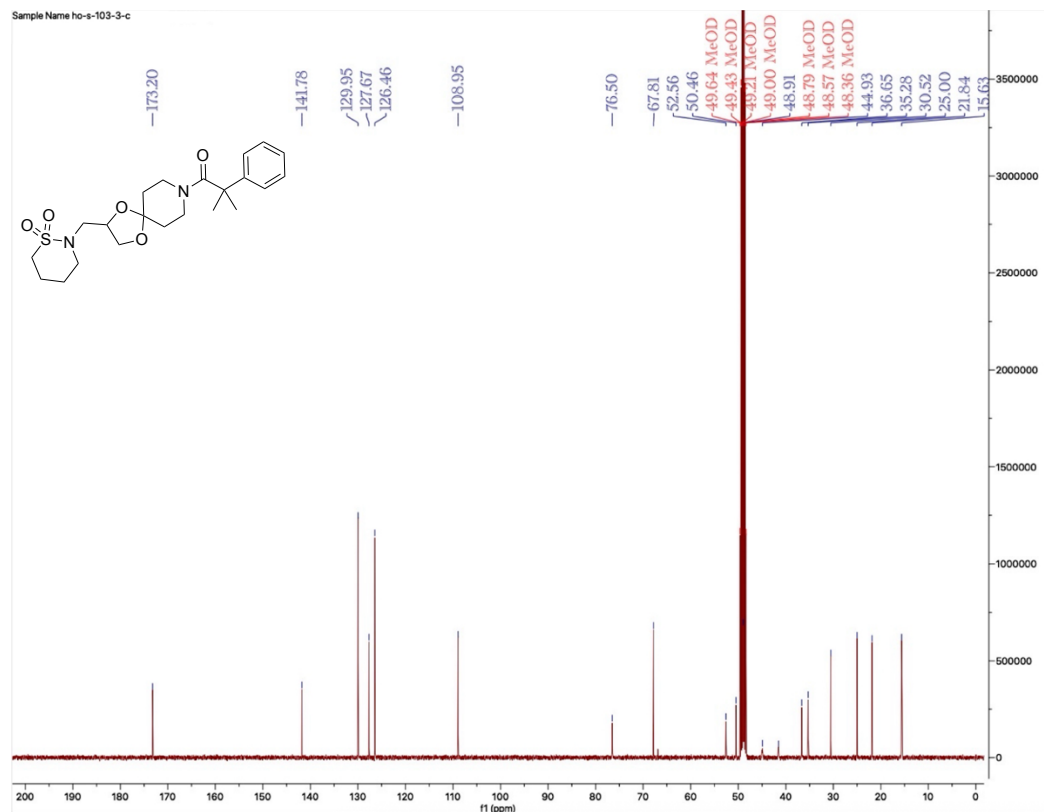


Figure S136: ^1H NMR (400 MHz, CD_3OD) for **7b**

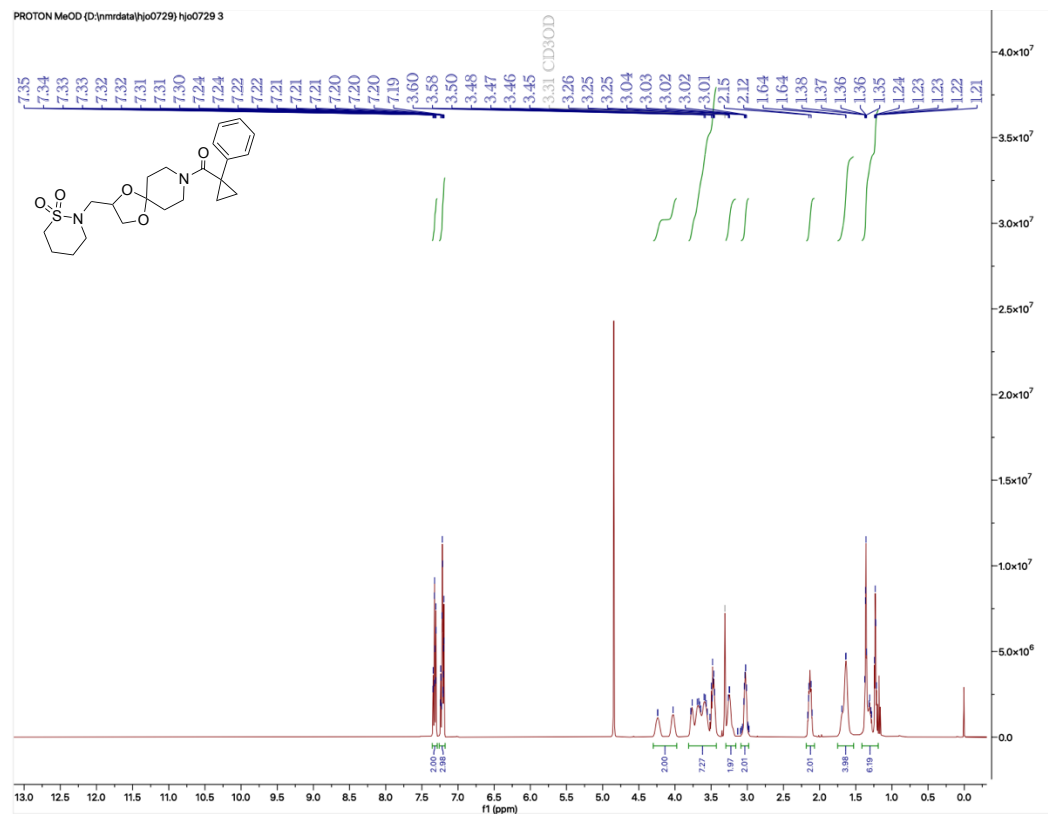


Figure S137: ^{13}C NMR (126 MHz, CD_3OD) for **7b**

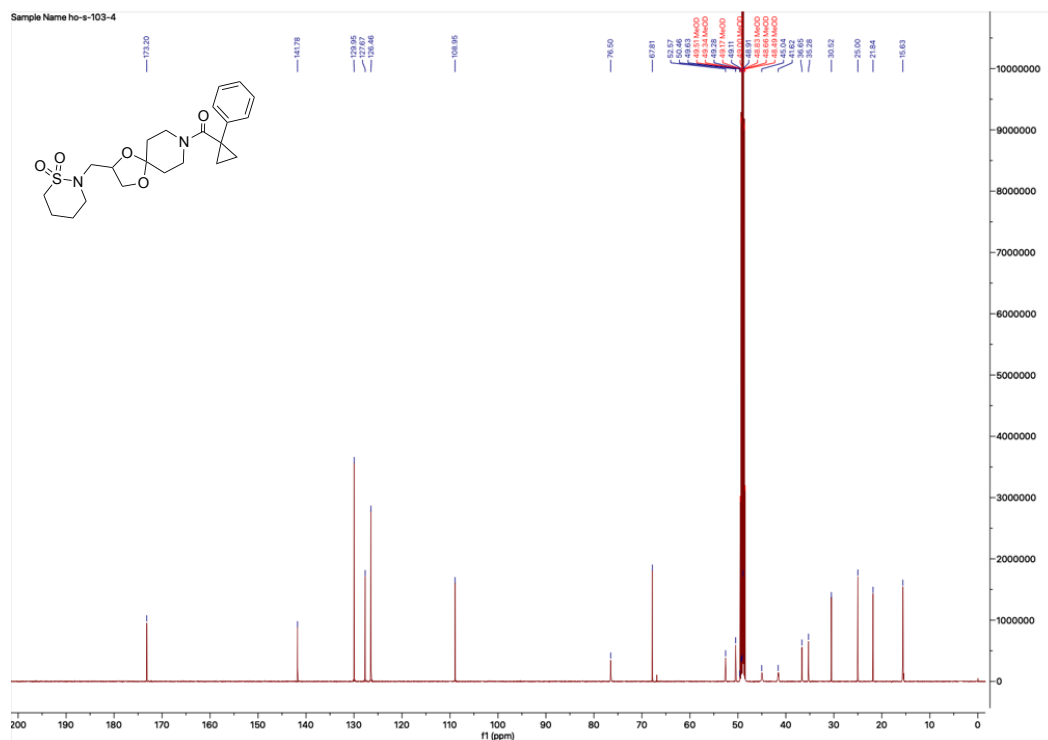


Figure S138: ^1H NMR (400 MHz, CD_3OD) for **7c**

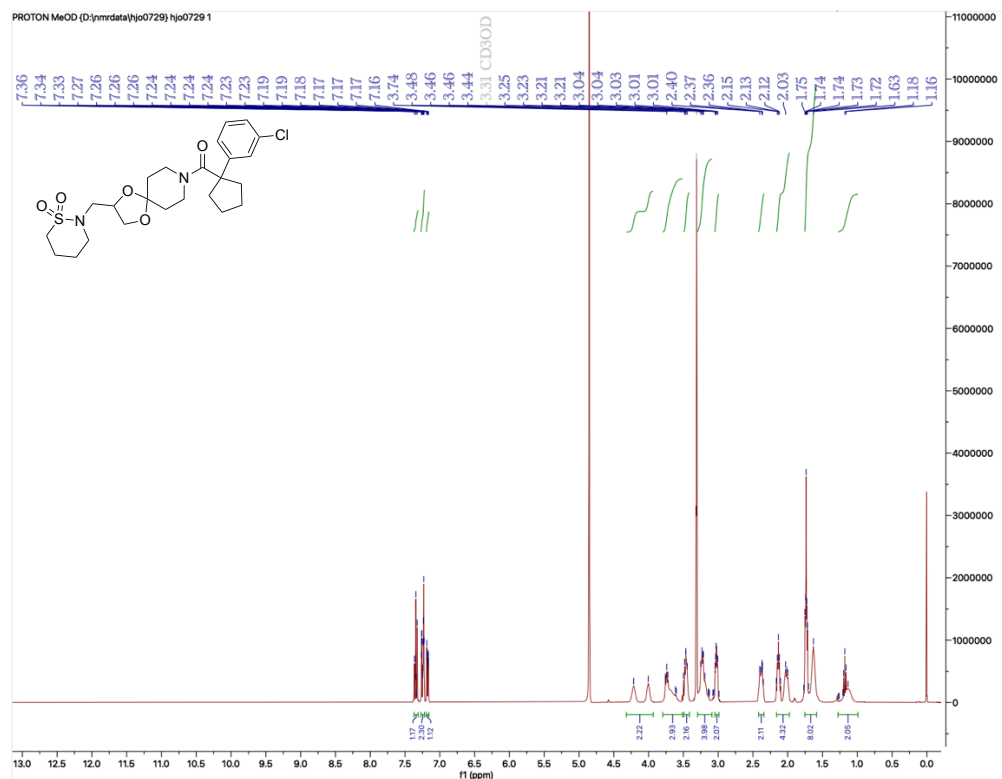
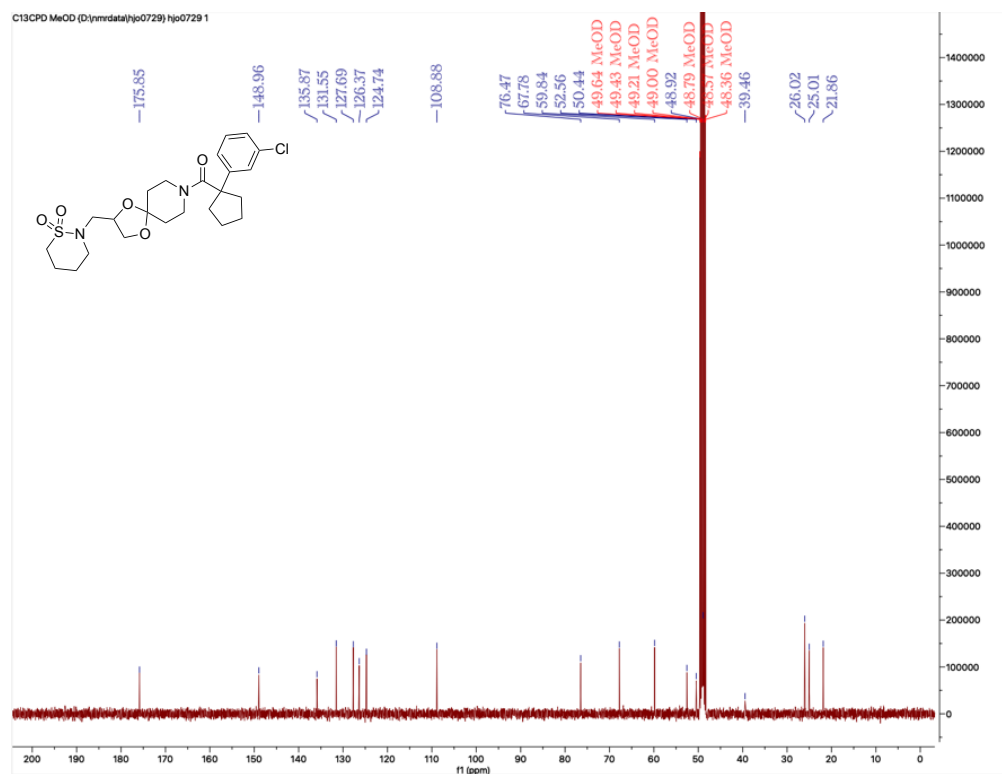


Figure S139: ^{13}C NMR (126 MHz, CD_3OD) for **7c**



Sample Name ho-s-103-2

Chemical structure of compound 103-2: Clc1ccc(cc1)C(=O)N2CCOC(C2)C3CCCC3S(=O)(=O)N3CCCCC3

¹H NMR spectrum (CDCl₃) showing chemical shifts (ppm) and integration values:

Chemical Shift (ppm)	Integration
7.36	2.21
7.35	2.22
7.34	2.21
7.34	2.22
7.25	2.21
7.24	2.22
7.23	2.21
7.22	2.22
4.21	2.21
4.00	2.22
3.76	2.21
3.75	2.22
3.74	2.21
3.72	2.22
3.45	2.21
3.45	2.22
3.44	2.21
3.44	2.22
3.31	2.21
3.31	2.22
3.24	2.21
3.22	2.22
3.21	2.21
3.20	2.22
3.19	2.21
3.04	2.22
3.03	2.21
3.03	2.22
3.02	2.21
3.01	2.22
2.39	2.21
2.38	2.22
2.37	2.21
2.35	2.22
2.16	2.21
2.15	2.22
2.13	2.21
2.12	2.22
2.12	2.21
2.11	2.22
2.01	2.21
1.74	2.22
1.73	2.21
1.73	2.22
1.72	2.21
1.71	2.22
1.70	2.21
1.63	2.22

C13CPD MeOD (D:\pmrdata\hjo0729) hjo0729 2

O=S1(=O)CCN(C1)C2OCC3(C2)CCN(C3)C(=O)C4(C)CCCC4c5ccc(Cl)cc5

Chemical structure of the compound is shown. The structure is a complex molecule featuring a sulfonamide group, a morpholine ring, a piperidine ring, and a cyclopentyl ring, all connected by various linkages. A chlorine atom is attached to the piperidine ring.

¹³C NMR spectrum (MeOD) showing chemical shifts (ppm) on the x-axis (0 to 200) and intensity on the y-axis (0 to 1,700,000). The spectrum displays several peaks corresponding to the carbon atoms in the molecule.

Chemical shifts (ppm) labeled on the spectrum:

- 176.05
- 145.34
- 133.32
- 129.98
- 127.99
- 108.91
- 76.48
- 67.76
- 59.57
- 52.58
- 50.41
- 49.64 MeOD
- 49.33 MeOD
- 49.21 MeOD
- 49.00 MeOD
- 48.92
- 48.79 MeOD
- 48.57 MeOD
- 48.36 MeOD
- 39.42
- 25.93
- 25.90
- 25.00
- 21.85

Figure S142: ^1H NMR (500 MHz, CD_3OD) for **R-3a**

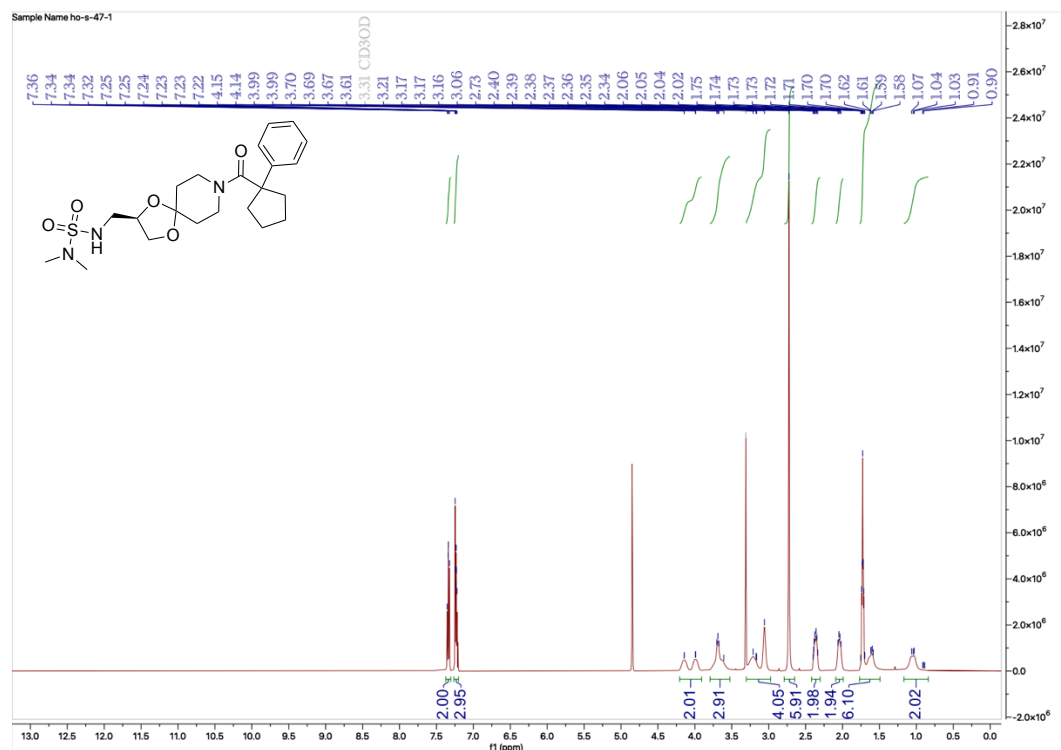
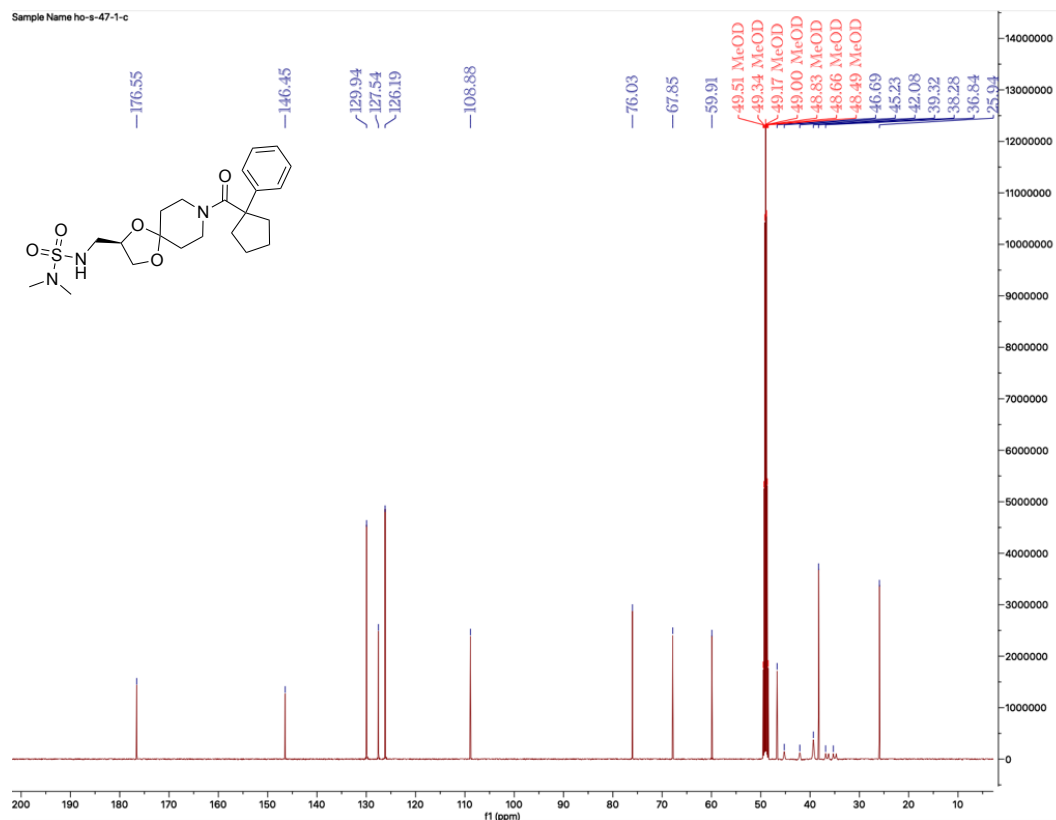


Figure S143: ^{13}C NMR (126 MHz, CD_3OD) for **R-3a**



Sample Name 10b-s-47-2

Chemical structure: CN(C)S(=O)(=O)N[C@H]1CCOC1C2CCN(C2C(=O)C3CCCC3)C4CCCC4

¹H NMR spectrum (CDCl₃) showing peaks from 0 to 13 ppm. The x-axis is labeled (f1 (ppm)) and the y-axis is labeled intensity. Integration values are shown below the baseline.

Peak list (ppm): 7.386, 7.344, 7.322, 7.286, 7.264, 7.238, 7.222, 4.844, 4.800, 4.756, 4.712, 4.668, 4.624, 4.580, 4.536, 4.492, 4.448, 4.404, 4.360, 4.316, 4.272, 4.228, 4.184, 4.140, 4.096, 4.052, 4.008, 3.964, 3.920, 3.876, 3.832, 3.788, 3.744, 3.700, 3.656, 3.612, 3.568, 3.524, 3.480, 3.436, 3.392, 3.348, 3.304, 3.260, 3.216, 3.172, 3.128, 3.084, 3.040, 3.000, 2.956, 2.912, 2.868, 2.824, 2.780, 2.736, 2.692, 2.648, 2.604, 2.560, 2.516, 2.472, 2.428, 2.384, 2.340, 2.296, 2.252, 2.208, 2.164, 2.120, 2.076, 2.032, 1.988, 1.944, 1.900, 1.856, 1.812, 1.768, 1.724, 1.680, 1.636, 1.592, 1.548, 1.504, 1.460, 1.416, 1.372, 1.328, 1.284, 1.240, 1.196, 1.152, 1.108, 1.064, 1.020, 0.976, 0.932, 0.888, 0.844, 0.800, 0.756, 0.712, 0.668, 0.624, 0.580, 0.536, 0.492, 0.448, 0.404, 0.360, 0.316, 0.272, 0.228, 0.184, 0.140, 0.096, 0.052, 0.008.

Integration values: 2.13, 3.11, 2.08, 2.80, 4.21, 6.31, 2.50, 2.61, 6.10, 1.05.

Sample Name ho-s-47-2

CN(C)C(=O)N[C@@H]1COC2(CCN(C2)C(=O)C3CCCC3C1)c4ccccc4

176.61, 146.47, 129.95, 127.56, 126.21, 108.90, 76.06, 67.86, 66.91, 59.94, 49.63, 49.51 MeOD, 49.46, 49.34 MeOD, 49.29, 49.17 MeOD, 49.00 MeOD, 48.83 MeOD, 48.66 MeOD, 48.49 MeOD, 46.70, 39.36, 38.27, 25.94

176.61, 146.47, 129.95, 127.56, 126.21, 108.90, 76.06, 67.86, 66.91, 59.94, 49.63, 49.51 MeOD, 49.46, 49.34 MeOD, 49.29, 49.17 MeOD, 49.00 MeOD, 48.83 MeOD, 48.66 MeOD, 48.49 MeOD, 46.70, 39.36, 38.27, 25.94

Sample Name ho-s-110

Chemical structure of the compound is shown above the spectrum.

Peak list (ppm):

- 7.286, 7.285, 7.284, 7.282, 7.281, 7.280, 7.279, 7.278, 7.277, 7.276, 7.275, 7.274, 7.273, 7.272, 7.271, 7.270, 7.269, 7.268, 7.267, 7.266, 7.265, 7.264, 7.263, 7.262, 7.261, 7.260, 7.259, 7.258, 7.257, 7.256, 7.255, 7.254, 7.253, 7.252, 7.251, 7.250, 7.249, 7.248, 7.247, 7.246, 7.245, 7.244, 7.243, 7.242, 7.241, 7.240, 7.239, 7.238, 7.237, 7.236, 7.235, 7.234, 7.233, 7.232, 7.231, 7.230, 7.229, 7.228, 7.227, 7.226, 7.225, 7.224, 7.223, 7.222, 7.221, 7.220, 7.219, 7.218, 7.217, 7.216, 7.215, 7.214, 7.213, 7.212, 7.211, 7.210, 7.209, 7.208, 7.207, 7.206, 7.205, 7.204, 7.203, 7.202, 7.201, 7.200, 7.199, 7.198, 7.197, 7.196, 7.195, 7.194, 7.193, 7.192, 7.191, 7.190, 7.189, 7.188, 7.187, 7.186, 7.185, 7.184, 7.183, 7.182, 7.181, 7.180, 7.179, 7.178, 7.177, 7.176, 7.175, 7.174, 7.173, 7.172, 7.171, 7.170, 7.169, 7.168, 7.167, 7.166, 7.165, 7.164, 7.163, 7.162, 7.161, 7.160, 7.159, 7.158, 7.157, 7.156, 7.155, 7.154, 7.153, 7.152, 7.151, 7.150, 7.149, 7.148, 7.147, 7.146, 7.145, 7.144, 7.143, 7.142, 7.141, 7.140, 7.139, 7.138, 7.137, 7.136, 7.135, 7.134, 7.133, 7.132, 7.131, 7.130, 7.129, 7.128, 7.127, 7.126, 7.125, 7.124, 7.123, 7.122, 7.121, 7.120, 7.119, 7.118, 7.117, 7.116, 7.115, 7.114, 7.113, 7.112, 7.111, 7.110, 7.109, 7.108, 7.107, 7.106, 7.105, 7.104, 7.103, 7.102, 7.101, 7.100, 7.099, 7.098, 7.097, 7.096, 7.095, 7.094, 7.093, 7.092, 7.091, 7.090, 7.089, 7.088, 7.087, 7.086, 7.085, 7.084, 7.083, 7.082, 7.081, 7.080, 7.079, 7.078, 7.077, 7.076, 7.075, 7.074, 7.073, 7.072, 7.071, 7.070, 7.069, 7.068, 7.067, 7.066, 7.065, 7.064, 7.063, 7.062, 7.061, 7.060, 7.059, 7.058, 7.057, 7.056, 7.055, 7.054, 7.053, 7.052, 7.051, 7.050, 7.049, 7.048, 7.047, 7.046, 7.045, 7.044, 7.043, 7.042, 7.041, 7.040, 7.039, 7.038, 7.037, 7.036, 7.035, 7.034, 7.033, 7.032, 7.031, 7.030, 7.029, 7.028, 7.027, 7.026, 7.025, 7.024, 7.023, 7.022, 7.021, 7.020, 7.019, 7.018, 7.017, 7.016, 7.015, 7.014, 7.013, 7.012, 7.011, 7.010, 7.009, 7.008, 7.007, 7.006, 7.005, 7.004, 7.003, 7.002, 7.001, 7.000, 6.999, 6.998, 6.997, 6.996, 6.995, 6.994, 6.993, 6.992, 6.991, 6.990, 6.989, 6.988, 6.987, 6.986, 6.985, 6.984, 6.983, 6.982, 6.981, 6.980, 6.979, 6.978, 6.977, 6.976, 6.975, 6.974, 6.973, 6.972, 6.971, 6.970, 6.969, 6.968, 6.967, 6.966, 6.965, 6.964, 6.963, 6.962, 6.961, 6.960, 6.959, 6.958, 6.957, 6.956, 6.955, 6.954, 6.953, 6.952, 6.951, 6.950, 6.949, 6.948, 6.947, 6.946, 6.945, 6.944, 6.943, 6.942, 6.941, 6.940, 6.939, 6.938, 6.937, 6.936, 6.935, 6.934, 6.933, 6.932, 6.931, 6.930, 6.929, 6.928, 6.927, 6.926, 6.925, 6.924, 6.923, 6.922, 6.921, 6.920, 6.919, 6.918, 6.917, 6.916, 6.915, 6.914, 6.913, 6.912, 6.911, 6.910, 6.909, 6.908, 6.907, 6.906, 6.905, 6.904, 6.903, 6.902, 6.901, 6.900, 6.899, 6.898, 6.897, 6.896, 6.895, 6.894, 6.893, 6.892, 6.891, 6.890, 6.889, 6.888, 6.887, 6.886, 6.885, 6.884, 6.883, 6.882, 6.881, 6.880, 6.879, 6.878, 6.877, 6.876, 6.875, 6.874, 6.873, 6.872, 6.871, 6.870, 6.869, 6.868, 6.867, 6.866, 6.865, 6.864, 6.863, 6.862, 6.861, 6.860, 6.859, 6.858, 6.857, 6.856, 6.855, 6.854, 6.853, 6.852, 6.851, 6.850, 6.849, 6.848, 6.847, 6.846, 6.845, 6.844, 6.843, 6.842, 6.841, 6.840, 6.839, 6.838, 6.837, 6.836, 6.835, 6.834, 6.833, 6.832, 6.831, 6.830, 6.829, 6.828, 6.827, 6.826, 6.825, 6.824, 6.823, 6.822, 6.821, 6.820, 6.819, 6.818, 6.817, 6.816, 6.815, 6.814, 6.813, 6.812, 6.811, 6.810, 6.809, 6.808, 6.807, 6.806, 6.805, 6.804, 6.803, 6.802, 6.801, 6.800, 6.799, 6.798, 6.797, 6.796, 6.795, 6.794, 6.793, 6.792, 6.791, 6.790, 6.789, 6.788, 6.787, 6.786, 6.785, 6.784, 6.783, 6.782, 6.781, 6.780, 6.779, 6.778, 6.777, 6.776, 6.775, 6.774, 6.773, 6.772, 6.771, 6.770, 6.769, 6.768, 6.767, 6.766, 6.765, 6.764, 6.763, 6.762, 6.761, 6.760, 6.759, 6.758, 6.757, 6.756, 6.755, 6.754, 6.753, 6.752, 6.751, 6.750, 6.749, 6.748, 6.747, 6.746, 6.745, 6.744, 6.743, 6.742, 6.741, 6.740, 6.739, 6.738, 6.737, 6.736, 6.735, 6.734, 6.733, 6.732, 6.731, 6.730, 6.729, 6.728, 6.727, 6.726, 6

Sample Name ho-s-110-c

O=S(=O)(N[C@@H]1CCOC12CCN(C2)C(=O)C3CCCC3C3=CC=CC=C3)N4CCCCC4

Chemical structure of the compound is shown. The structure is a complex molecule featuring a sulfonamide group, a morpholine ring, and a cyclopentyl ring, with a chiral center indicated by a wedge bond.

13C NMR spectrum (f1 (ppm)) showing chemical shifts (ppm) and integrations:

Chemical Shift (ppm)	Integration
176.50	
146.44	
129.93	
127.53	
126.17	
109.02	
108.86	
75.98	
67.85	
59.88	
49.51 MeOD	
49.34 MeOD	
49.17 MeOD	
49.00 MeOD	
48.83 MeOD	
48.66 MeOD	
48.49 MeOD	
47.91	
46.64	
43.20	
42.10	
39.42	
30.69	
26.42	
25.94	
24.81	

Figure S148: ^1H NMR (500 MHz, CD_3OD) for **R-3k**

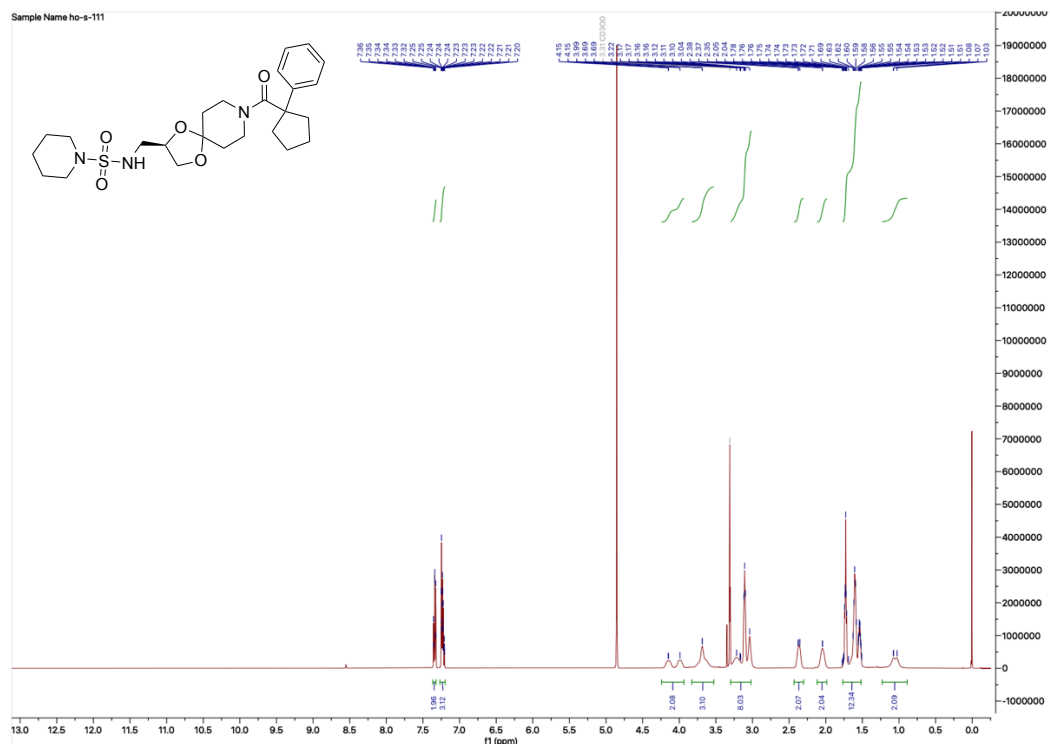
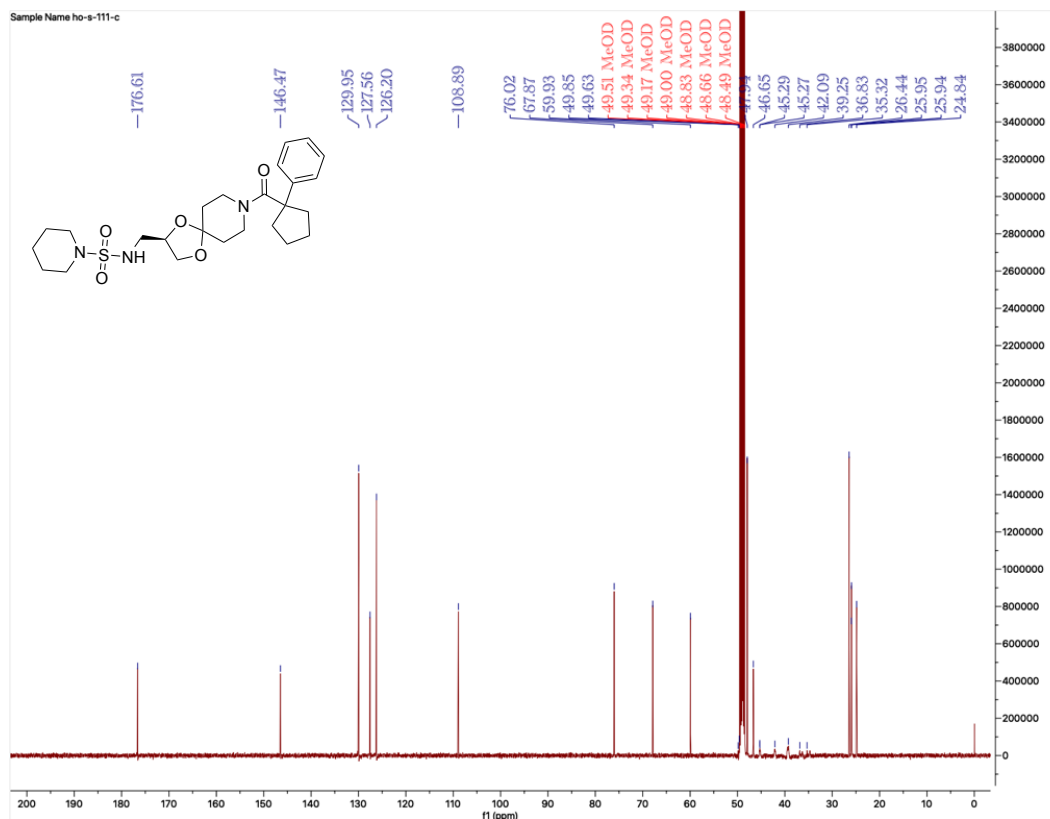


Figure S149: ^{13}C NMR (126 MHz, CD_3OD) for **R-3k**



Sample Name ho-s-105-2-c

Chemical structure of compound 105-2-c is shown above the spectrum.

Key peaks in the spectrum are labeled with their chemical shifts (ppm):

- 176.61
- 146.45
- 129.96
- 127.56
- 126.22
- 108.97
- 76.44
- 67.74
- 59.94
- 52.56
- 50.43
- 49.63
- 49.51 MeOD
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.91
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 45.29
- 42.07
- 39.33
- 34.81
- 25.93
- 25.00
- 21.84

[illegible]

Sample Name ho-s-106-c

Chemical structure of compound 106c is shown. The structure is a complex molecule featuring a sulfonamide group, a morpholine ring, and a cyclopentyl ketone moiety.

¹³C NMR spectrum (MeOD) showing chemical shifts (ppm) for compound 106c. The spectrum displays several peaks, with the following labeled chemical shifts (ppm):

- 176.61
- 146.45
- 129.96
- 127.56
- 126.22
- 108.97
- 76.44
- 67.74
- 59.94
- 52.56
- 50.43
- 49.63
- 49.51 MeOD
- 49.46
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.91
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 39.32
- 25.00
- 21.84

Chemical structure of compound 10b is shown in the top left corner. The structure is a cyclohexane ring substituted with a nitrile group (NC) and a sulfonamide group (N(SO₂NH-CH₂-CH₂-O-CH₂-CH₂-N-C(=O)-C₆H₅)).

The ¹H NMR spectrum (CDCl₃) shows the following peaks and integrations:

- Peak at ~7.3 ppm (NH, integration ~1.00)
- Peak at ~3.5 ppm (CH₂-O, integration ~2.00)
- Peak at ~2.5 ppm (CH₂-CH₂, integration ~2.00)
- Peak at ~1.5 ppm (CH₂-CH₂, integration ~2.00)
- Peak at ~1.0 ppm (CH₂-CH₂, integration ~1.00)

Sample Name ho-s-118-c

Chemical structure of compound 118c is shown in the top left. The structure is a complex molecule featuring a 4-cyanopiperidine ring connected via a sulfonamide group to a 1,3-dioxolane ring, which is further connected to a 1,4-dioxane ring. The 1,4-dioxane ring is substituted with a benzylidene group and a cyclopentylidene group.

The ^{13}C NMR spectrum (MeOD) shows the following chemical shifts (ppm):

- 176.61
- 146.47
- 129.96
- 127.56
- 126.21
- 122.31
- 108.96
- 75.98
- 67.80
- 59.93
- 49.63
- 49.51 MeOD
- 49.46
- 49.34 MeOD
- 49.17 MeOD
- 49.00 MeOD
- 48.83 MeOD
- 48.66 MeOD
- 48.49 MeOD
- 46.68
- 45.29
- 39.23
- 29.25
- 26.64
- 25.94

Figure S156: ^1H NMR (500 MHz, CD_3OD) for **R-4b**

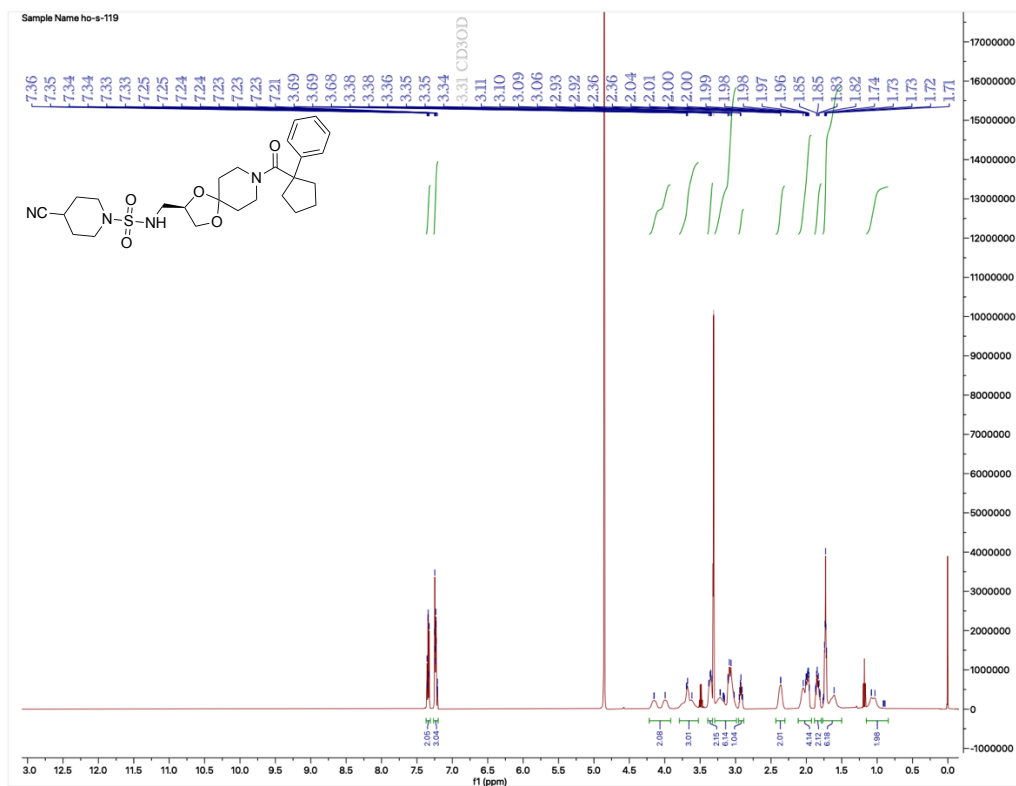


Figure S157: ^{13}C NMR (126 MHz, CD_3OD) for **R-4b**

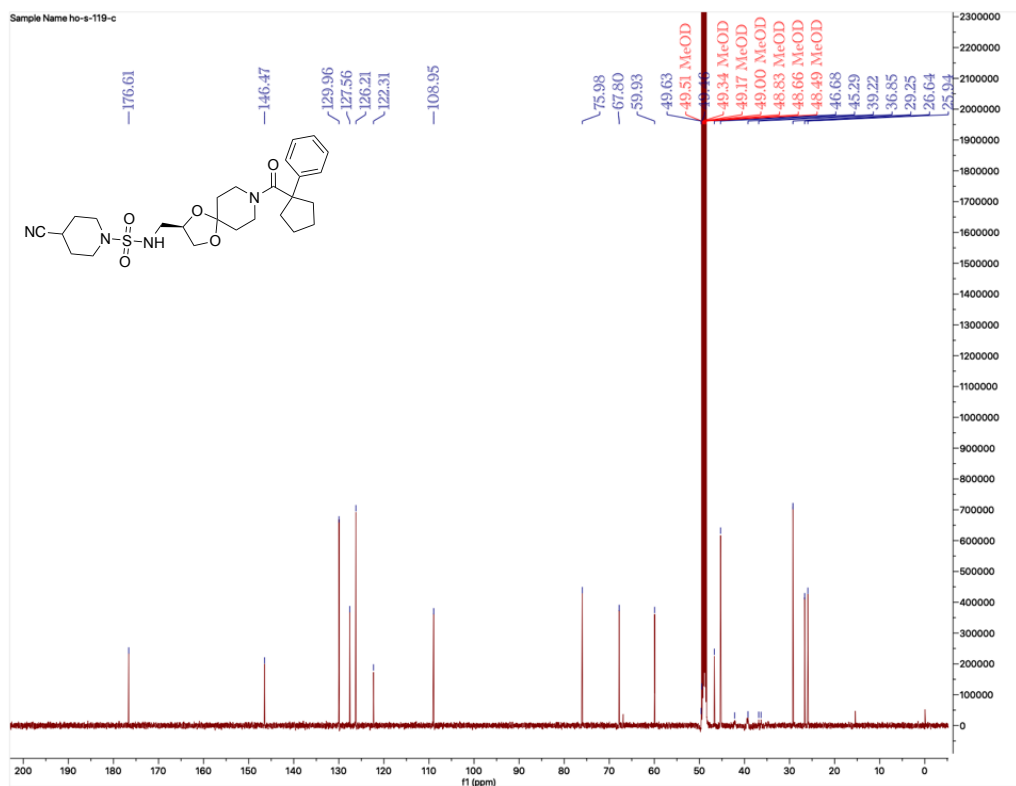


Figure S158: ^1H NMR (500 MHz, CD_3OD) for **S-5b**

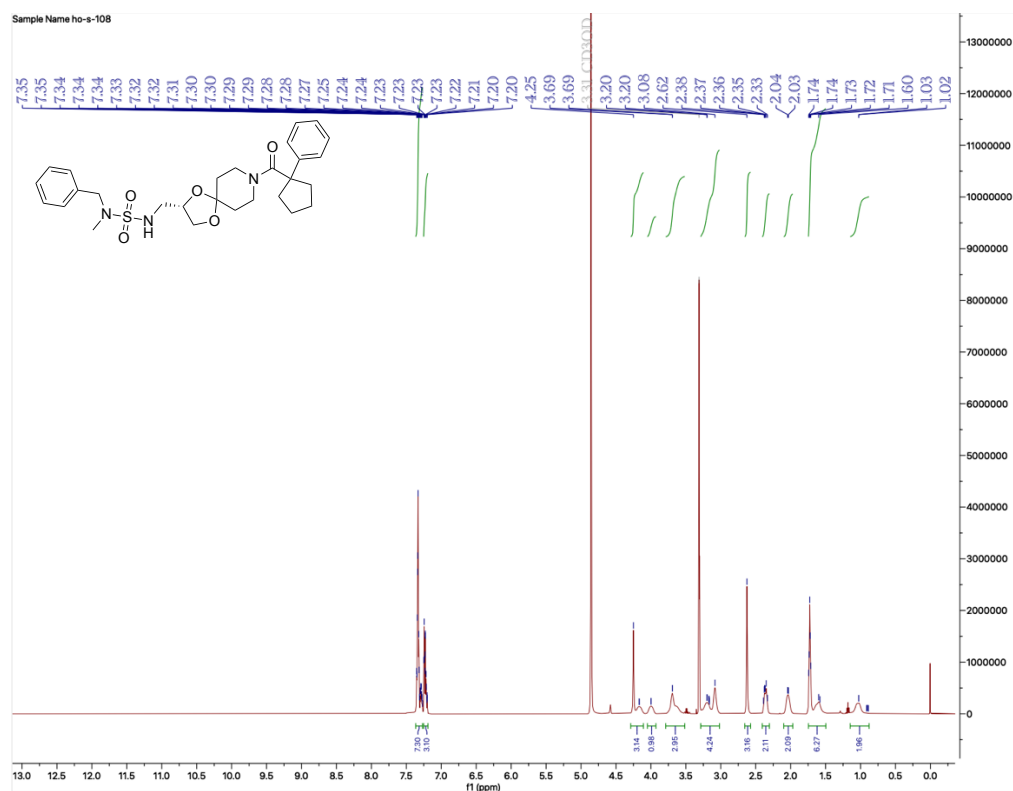


Figure S159: ^{13}C NMR (126 MHz, CD_3OD) for **S-5b**

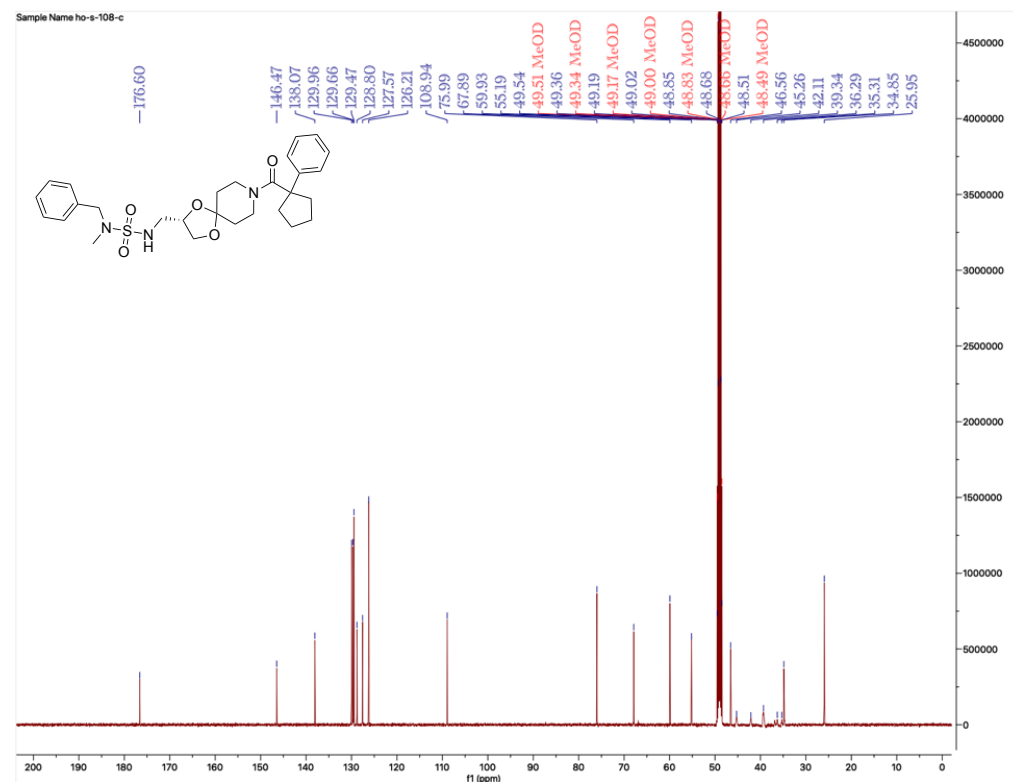


Figure S160: ^1H NMR (500 MHz, CD_3OD) for **R-5b**

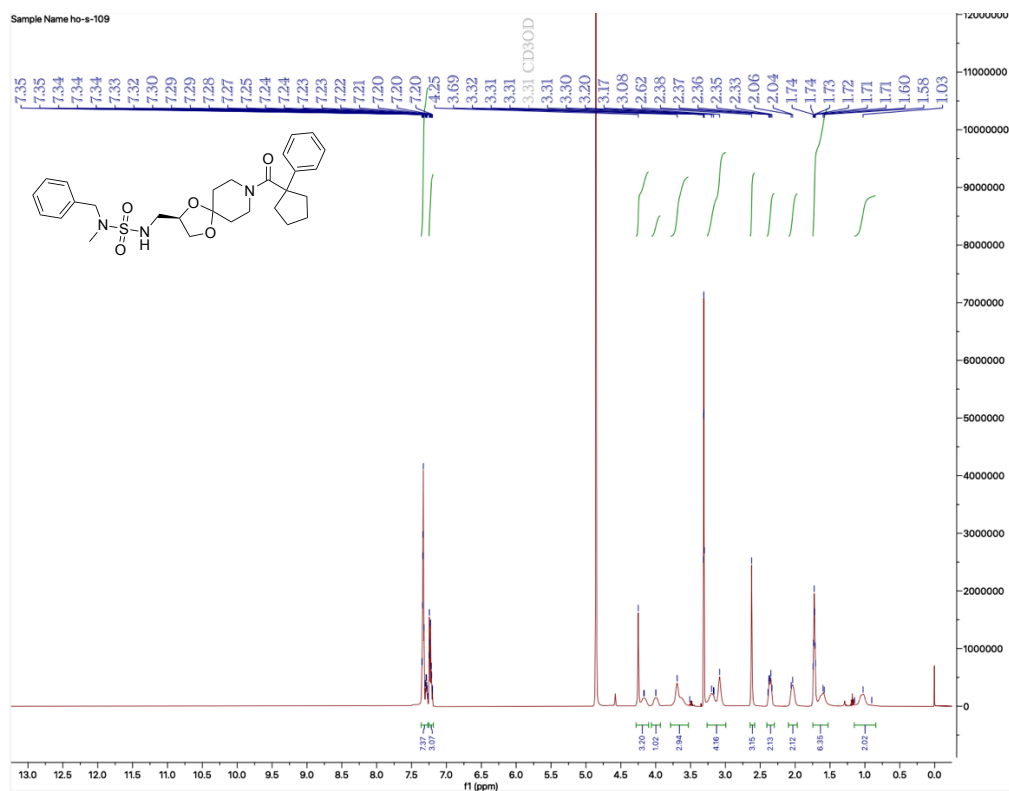
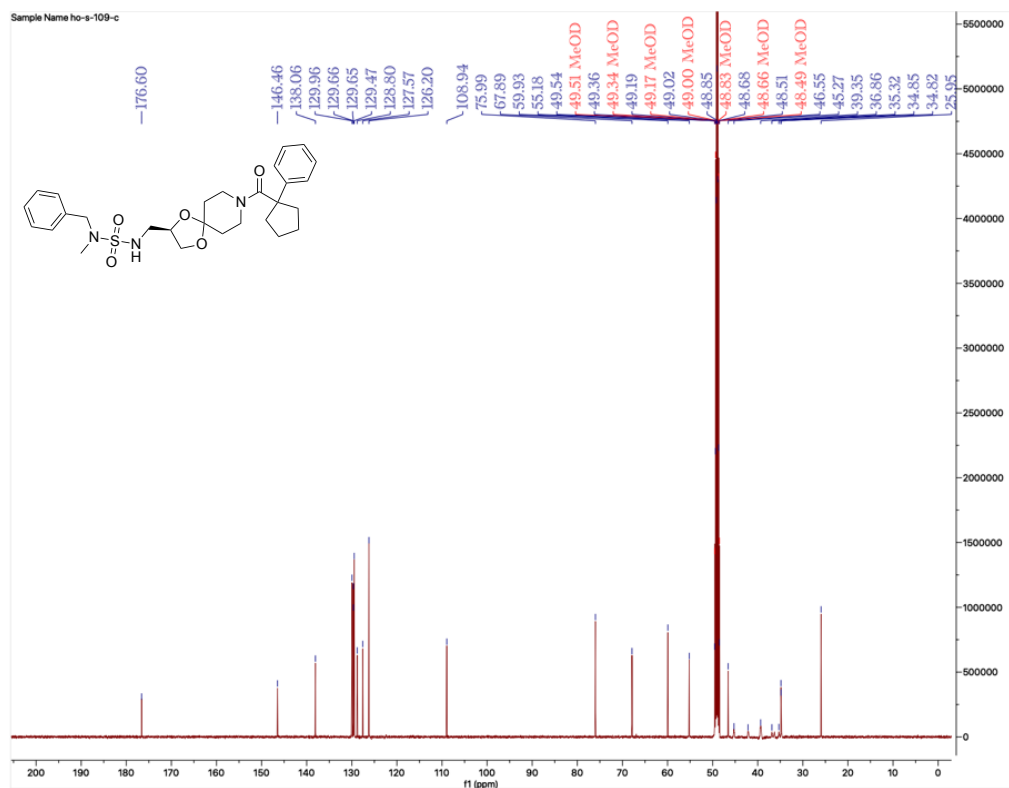
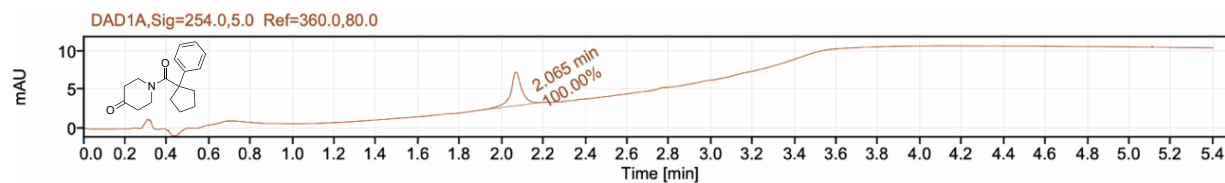


Figure S161: ^{13}C NMR (126 MHz, CD_3OD) for **R-5b**



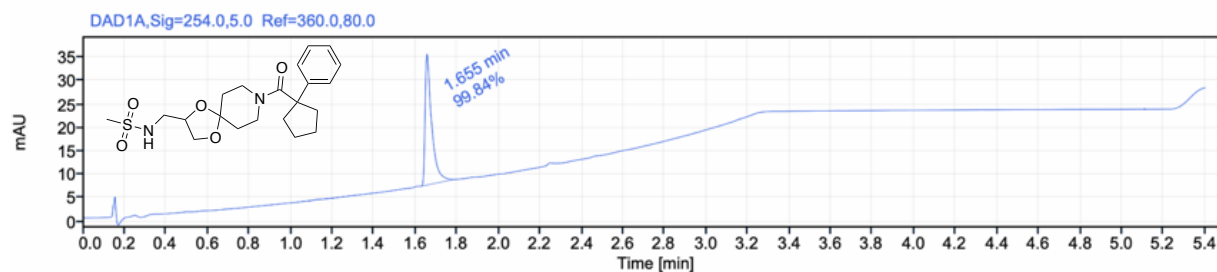
HPLC analyses

Figure S162: HPLC trace of intermediate II



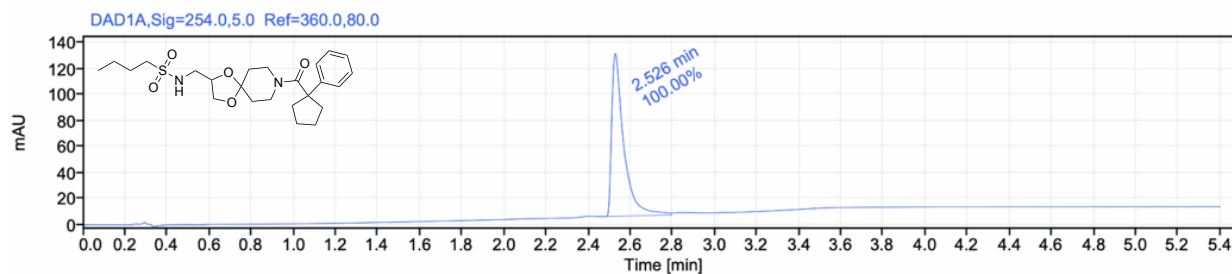
Signal Name	DAD1A			
RT (min)	Signal description	Area	Area%	
2.065	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	16.1	100.00	

Figure S163: HPLC trace of 1a



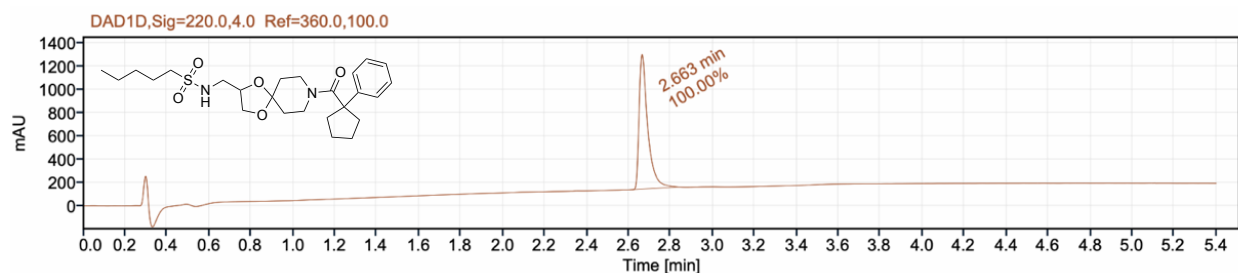
Signal Name	DAD1A			
RT (min)	Signal description	Area	Area%	
2.129	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	317.8	100.00	

Figure S164: HPLC trace of 1b



Signal Name	DAD1A			
RT (min)	Signal description	Area	Area%	
2.526	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	500.6	100.00	

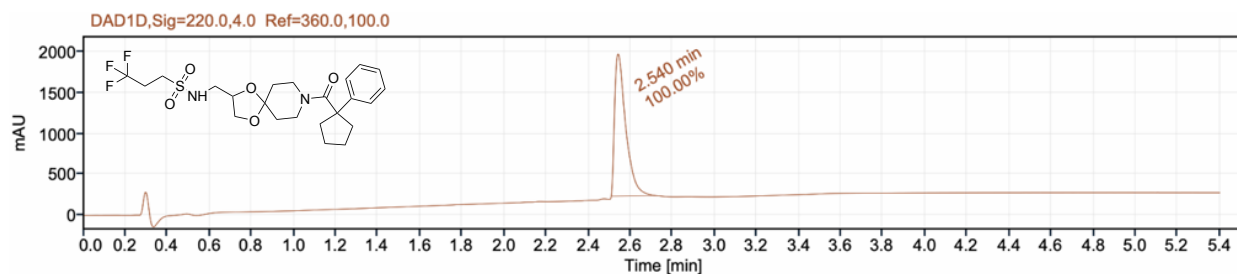
Figure S165: HPLC trace of 1c



Signal Name DAD1D

RT (min)	Signal description	Area	Area%
2.663	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	3334.8	100.00

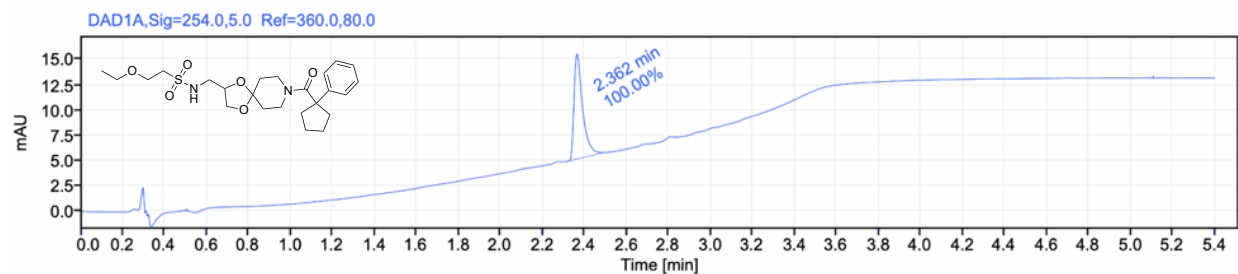
Figure S166: HPLC trace of 1d



Signal Name DAD1D

RT (min)	Signal description	Area	Area%
2.540	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	6403.3	100.00

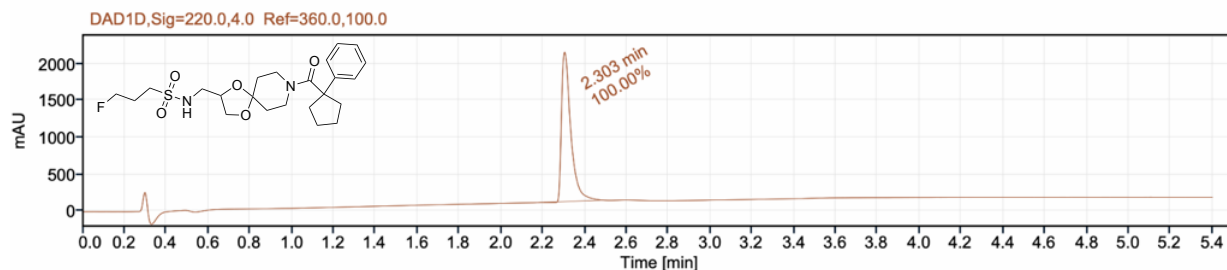
Figure S167: HPLC trace of 1e



Signal Name DAD1A

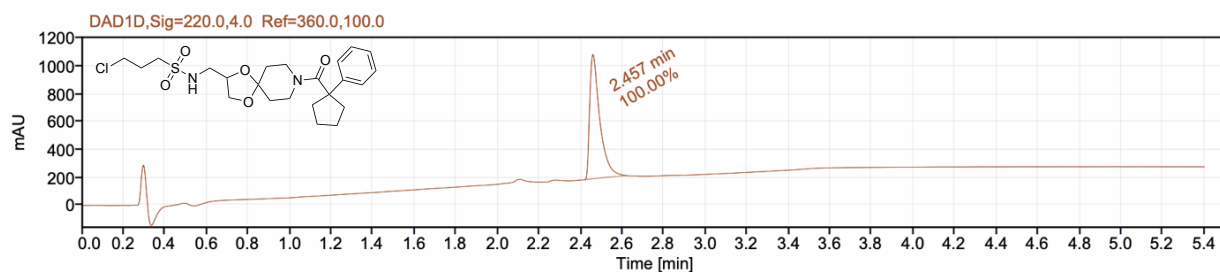
RT (min)	Signal description	Area	Area%
2.362	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	29.3	100.00

Figure S168: HPLC trace of 1f



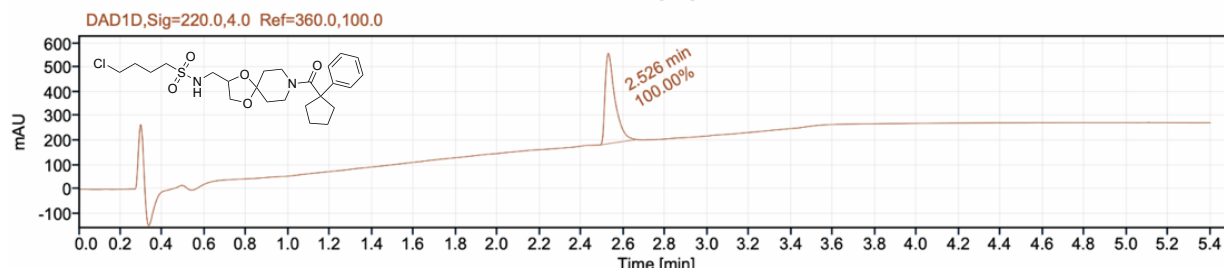
Signal Name		DAD1D		
RT (min)	Signal description	Area	Area%	
2.303	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	6260.8	100.00	

Figure S169: HPLC trace of 1g



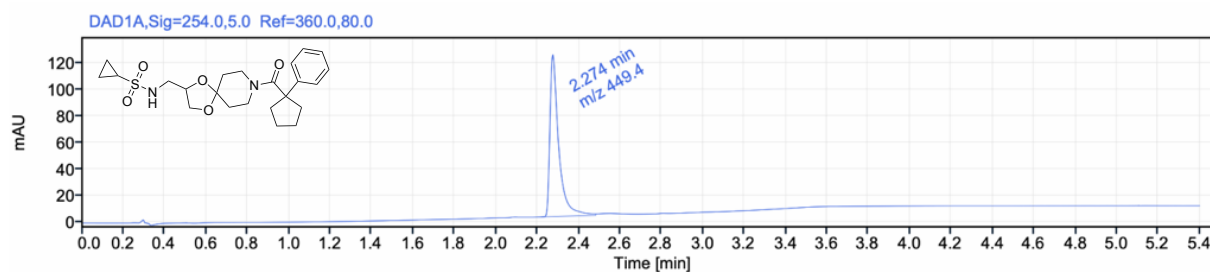
Signal Name		DAD1D		
RT (min)	Signal description	Area	Area%	
2.457	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	3014.5	100.00	

Figure S170: HPLC trace of 1h



Signal Name		DAD1D		
RT (min)	Signal description	Area	Area%	
2.526	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	1222.3	100.00	

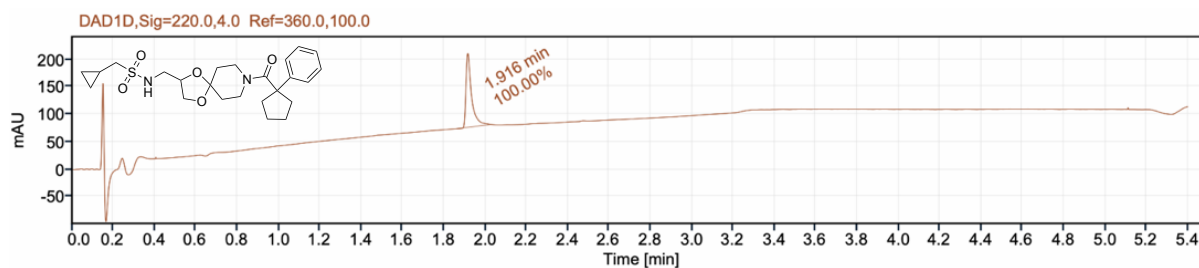
Figure S171: HPLC trace of 1i



Signal Name DAD1A

RT (min)	Signal description	Area	Area%
2.274	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	361.1	100.00

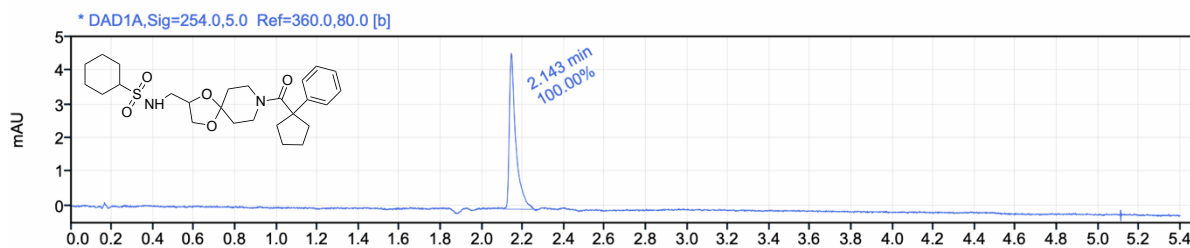
Figure S172: HPLC trace of 1j



Signal Name DAD1D

RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
1.916	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			251.7	100.00

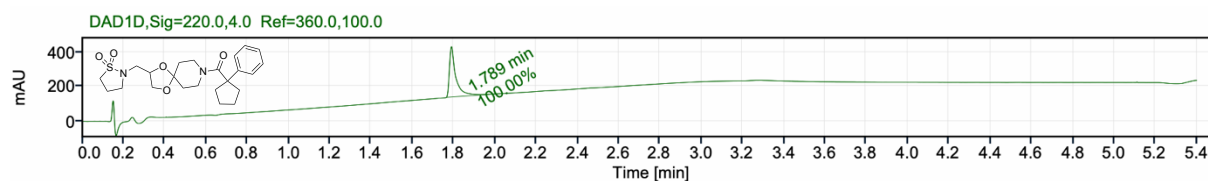
Figure S173: HPLC trace of 1k



Signal Name DAD1A

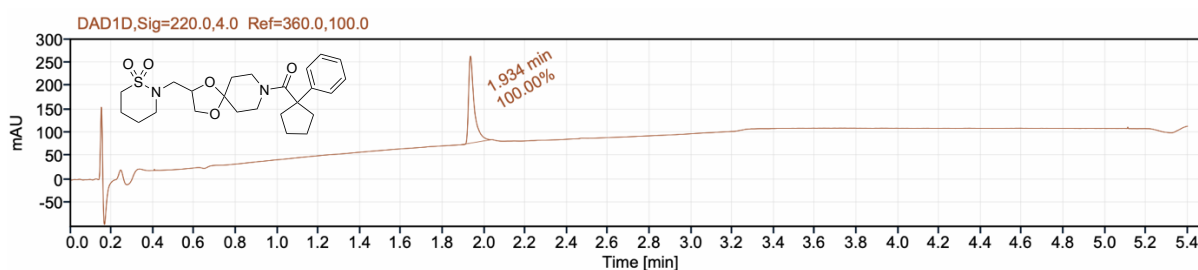
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
2.143	* DAD1A,Sig=254.0,5.0 Ref=360.0,80.0 [b]			10.1	100.00

Figure S174: HPLC trace of 1l



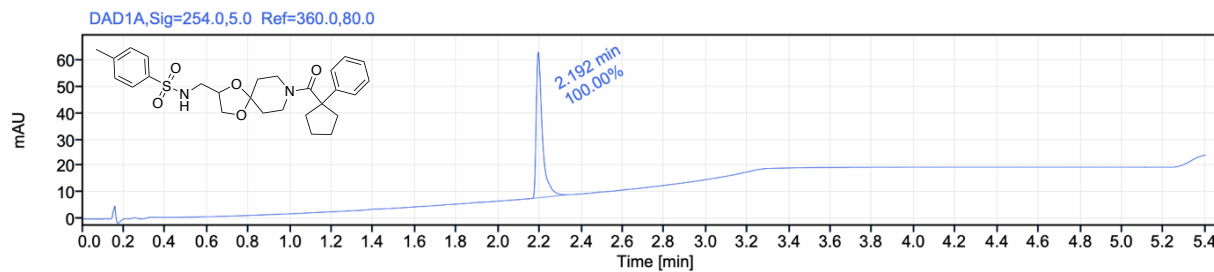
Signal Name		DAD1D					
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%		
1.789	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			620.9	100.00		

Figure S175: HPLC trace of 1m



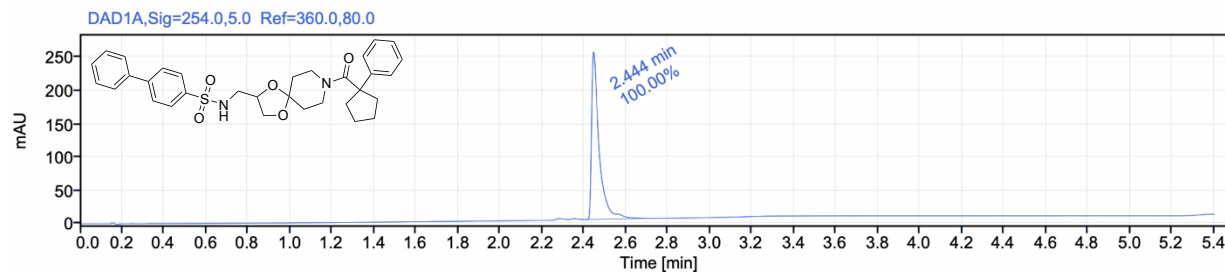
Signal Name		DAD1D					
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%		
1.934	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			349.2	100.00		

Figure S176: HPLC trace of 2a



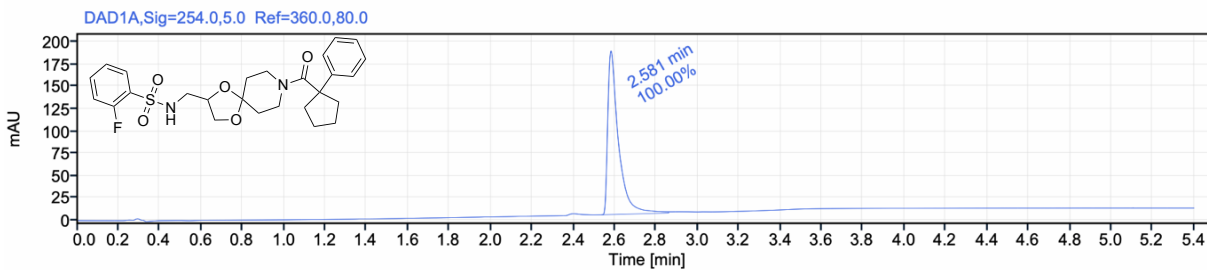
Signal Name		DAD1A					
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%		
2.192	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0			113.2	100.00		

Figure S177: HPLC trace of 2b



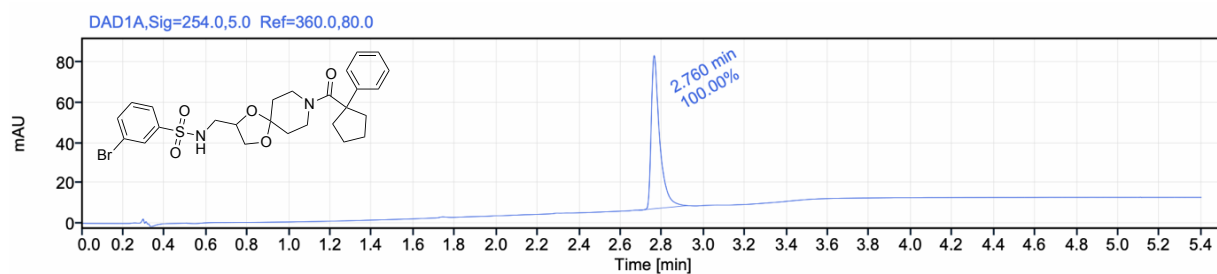
Signal Name		DAD1A					
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%		
2.444	DAD1A, Sig=254.0,5.0 Ref=360.0,80.0			645.5	100.00		

Figure S178: HPLC trace of 2c



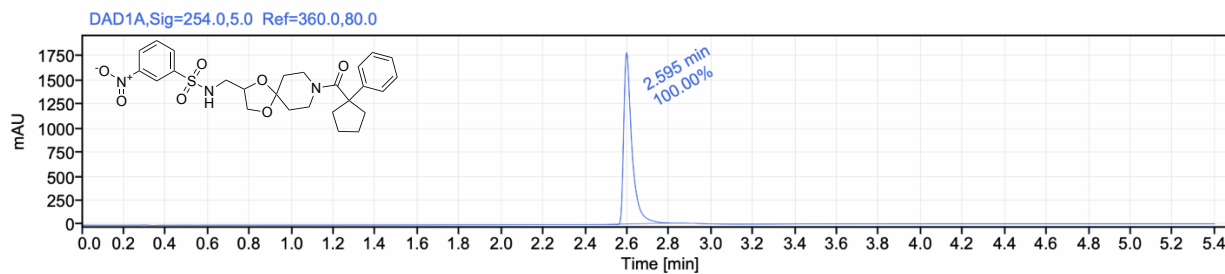
Signal Name		DAD1A			
RT (min)	Signal description	Area	Area%		
2.581	DAD1A, Sig=254.0,5.0 Ref=360.0,80.0	662.8	100.00		

Figure S179: HPLC trace of 2d



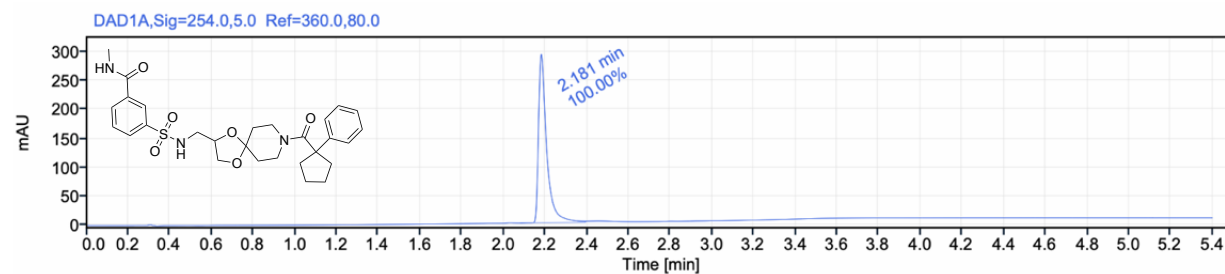
Signal Name		DAD1A			
RT (min)	Signal description	Area	Area%		
2.760	DAD1A, Sig=254.0,5.0 Ref=360.0,80.0	217.4	100.00		

Figure S180: HPLC trace of 2e



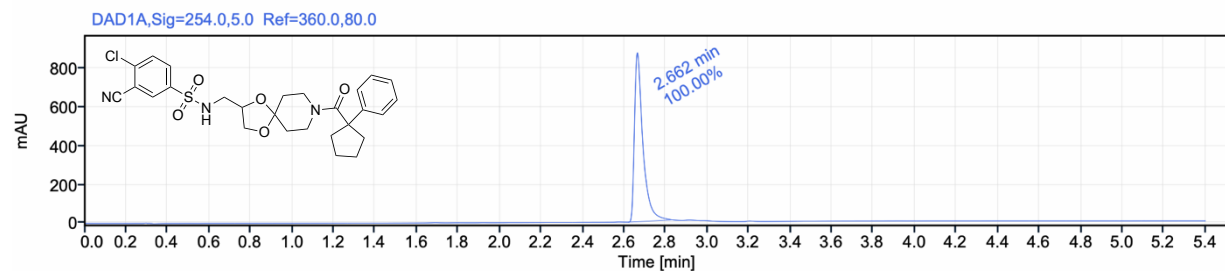
Signal Name		DAD1A	
RT (min)	Signal description	Area	Area%
2.595	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	4839.8	100.00

Figure S181: HPLC trace of 2f



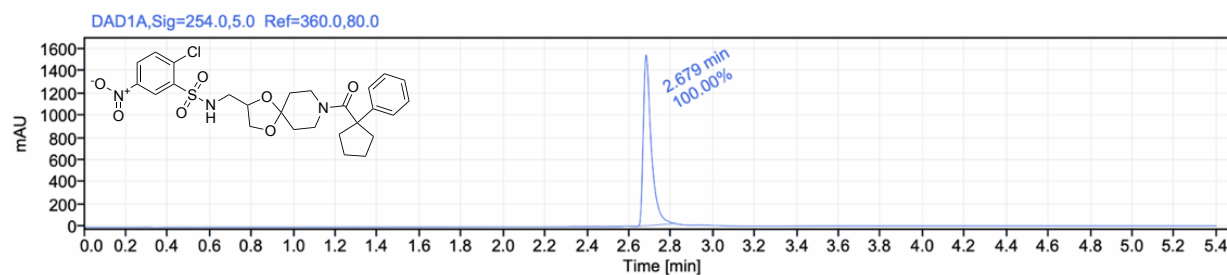
Signal Name		DAD1A	
RT (min)	Signal description	Area	Area%
2.181	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	799.2	100.00

Figure S182: HPLC trace of 2g



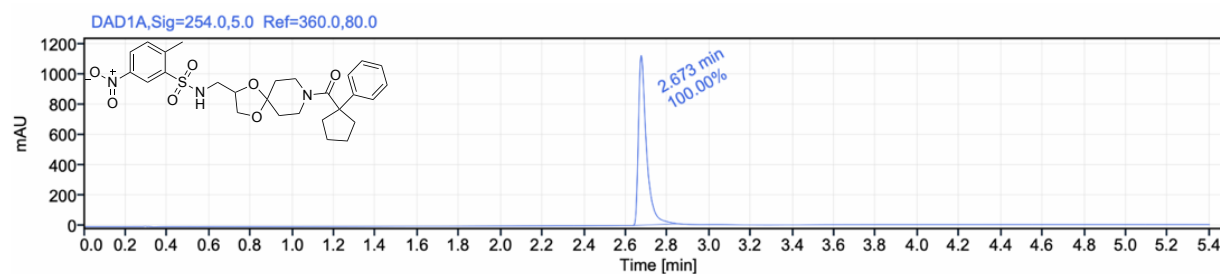
Signal Name		DAD1A	
RT (min)	Signal description	Area	Area%
2.662	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	2470.1	100.00

Figure S183: HPLC trace of 2h



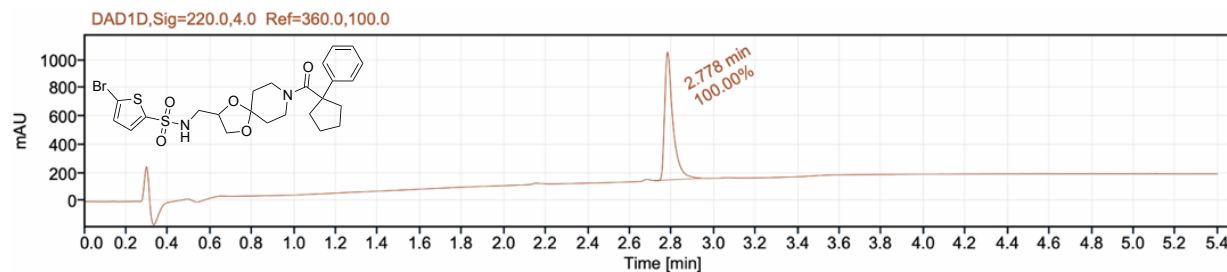
Signal Name	DAD1A		
RT (min)	Signal description	Area	Area%
2.679	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	4066.0	100.00

Figure S184: HPLC trace of 2i



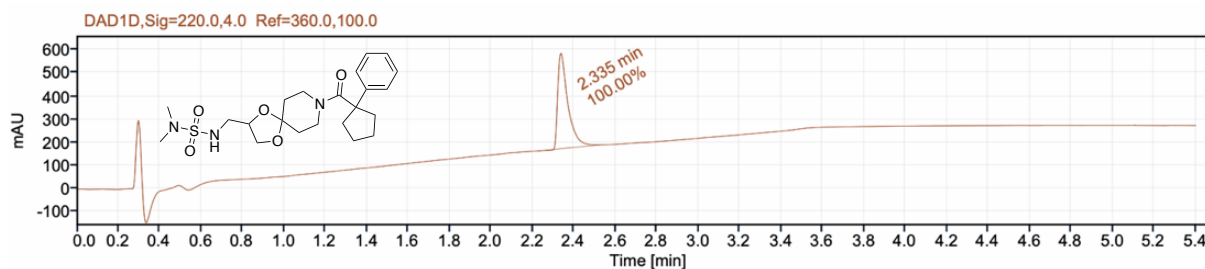
Signal Name	DAD1A		
RT (min)	Signal description	Area	Area%
2.673	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	3008.6	100.00

Figure S185: HPLC trace of 2j



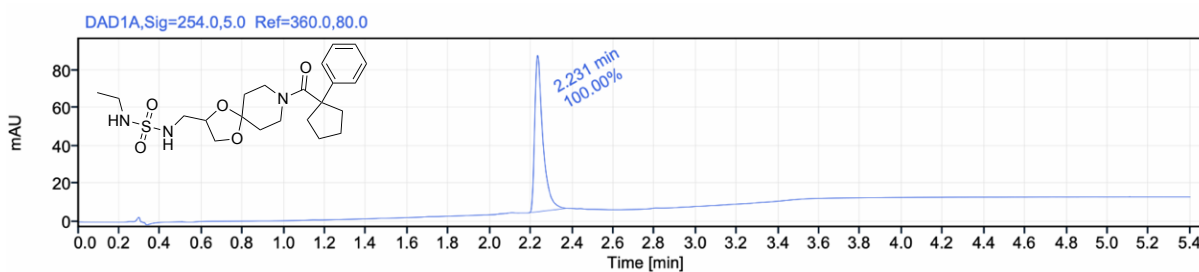
Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.778	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	2491.2	100.00

Figure S186: HPLC trace of 3a



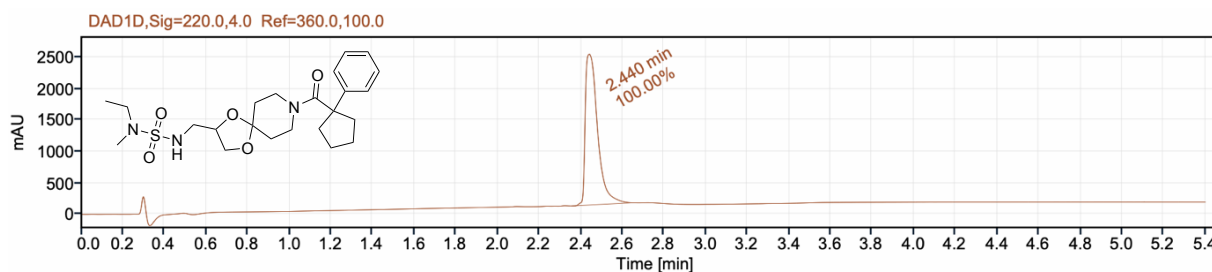
Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.335	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	1402.7	100.00

Figure S187: HPLC trace of 3b



Signal Name	DAD1A		
RT (min)	Signal description	Area	Area%
2.231	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	227.7	100.00

Figure S188: HPLC trace of 3c



Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.440	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	9865.8	100.00

Figure S189: HPLC trace of 3d

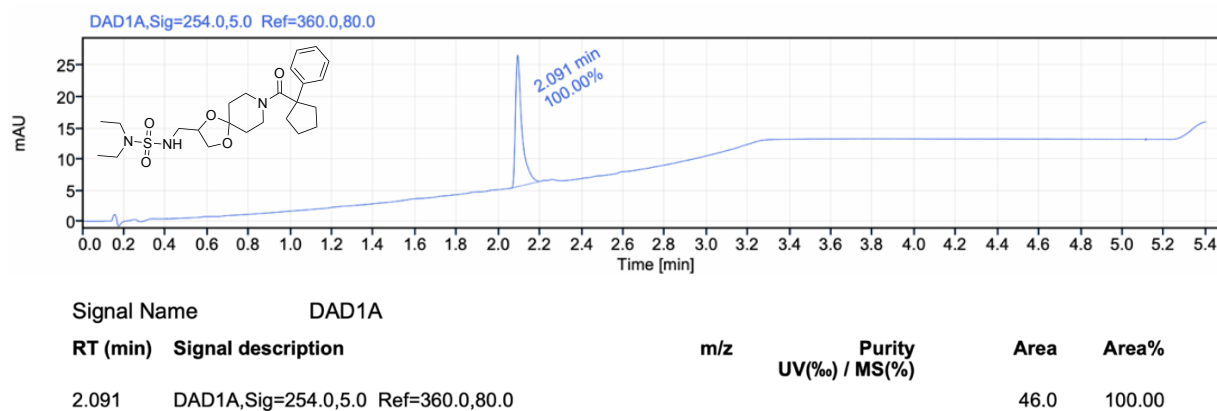


Figure S190: HPLC trace of 3e

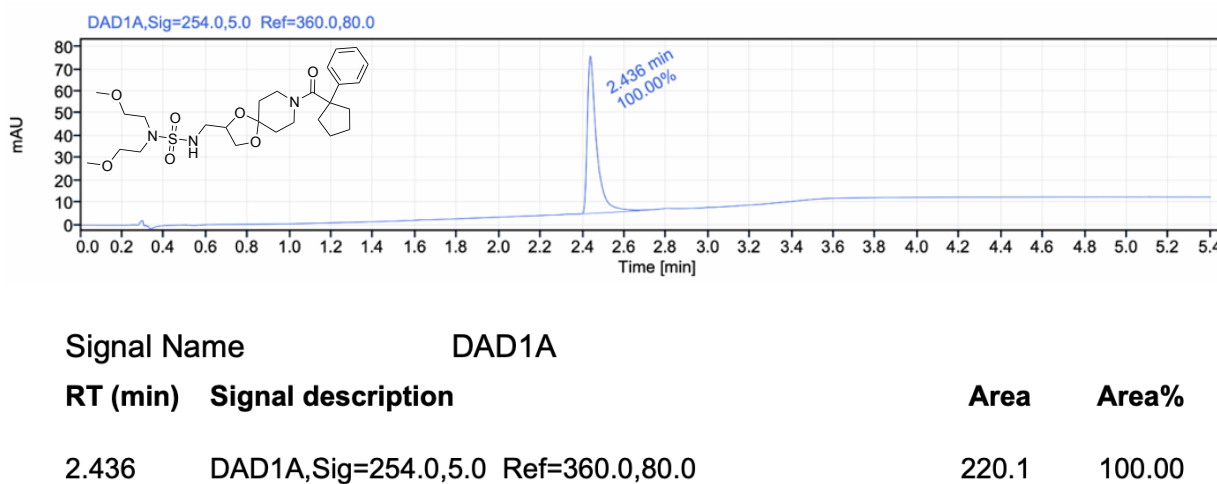


Figure S191: HPLC trace of 3f

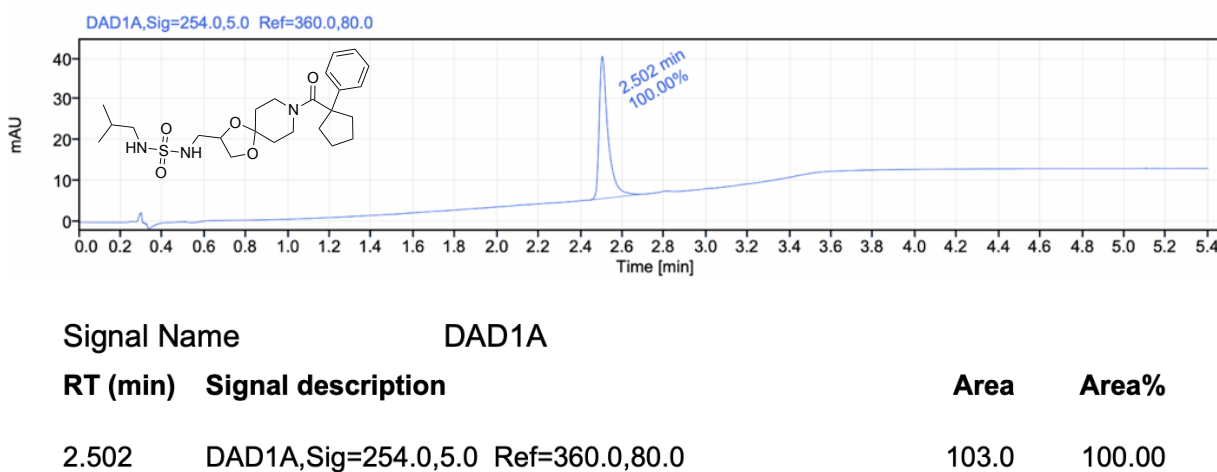
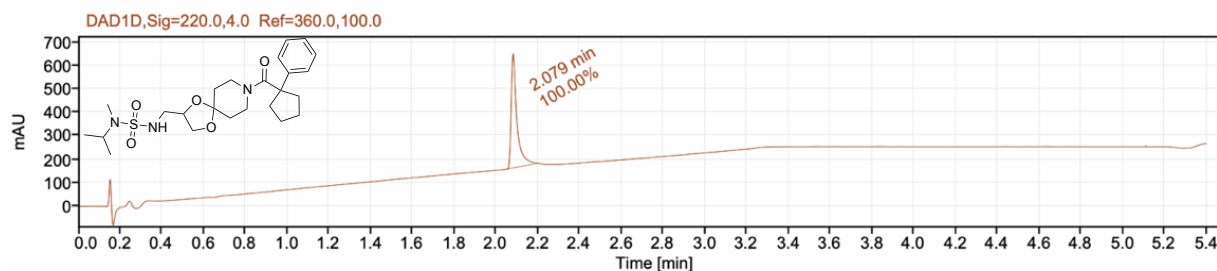


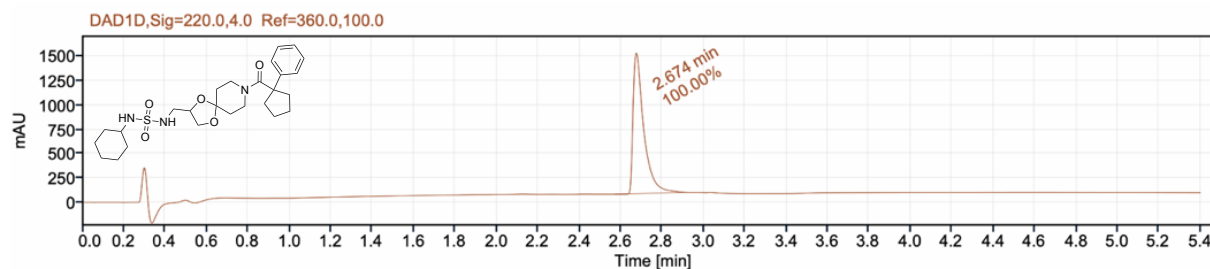
Figure S192: HPLC trace of 3g



Signal Name DAD1D

RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
2.079	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			924.6	100.00

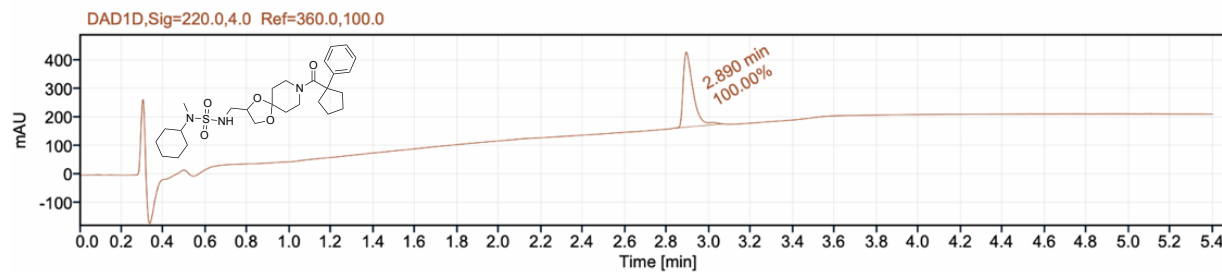
Figure S193: HPLC trace of 3h



Signal Name DAD1D

RT (min)	Signal description	Area	Area%
2.674	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	5219.9	100.00

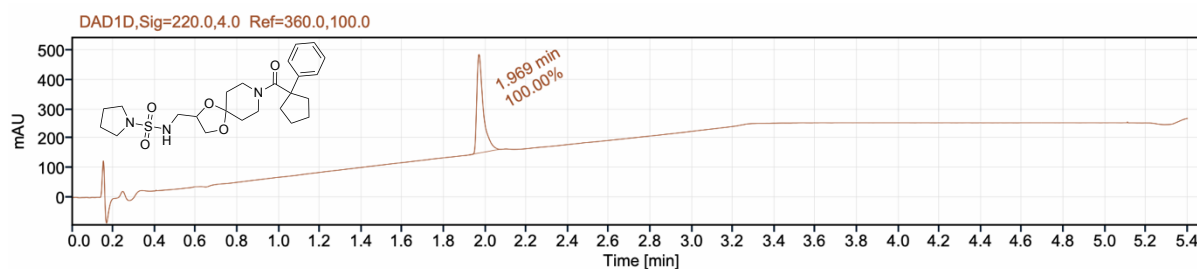
Figure S194: HPLC trace of 3i



Signal Name DAD1D

RT (min)	Signal description	Area	Area%
2.890	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	857.1	100.00

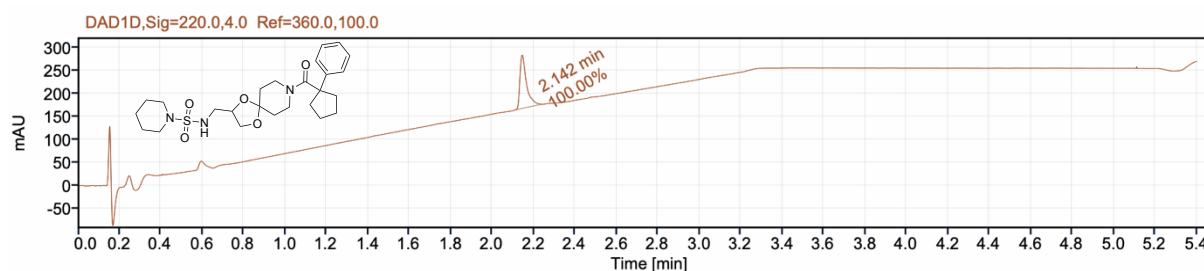
Figure S195: HPLC trace of 3j



Signal Name DAD1D

RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
1.969	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			731.3	100.00

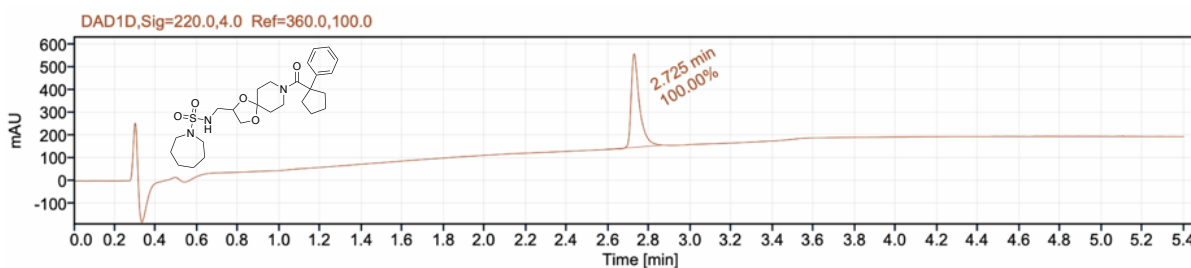
Figure S196: HPLC trace of 3k



Signal Name DAD1D

RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
2.142	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			256.6	100.00

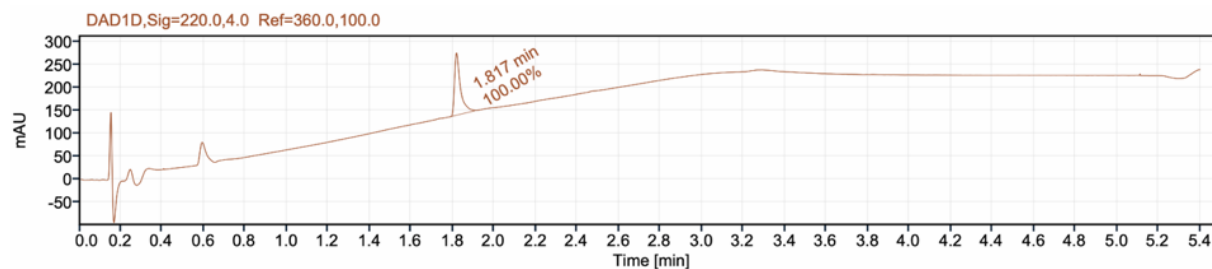
Figure S197: HPLC trace of 3l



Signal Name DAD1D

RT (min)	Signal description	Area	Area%
2.725	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	1144.6	100.00

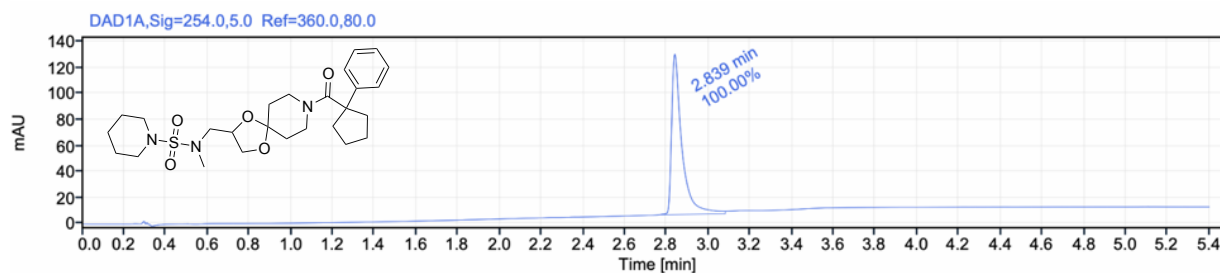
Figure S198: HPLC trace of 3m



Signal Name DAD1D

RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
1.817	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			270.5	100.00

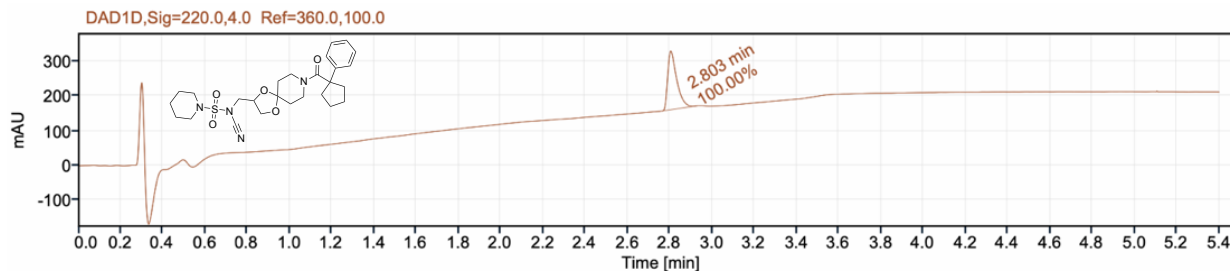
Figure S199: HPLC trace of 3n



Signal Name DAD1A

RT (min)	Signal description	Area	Area%
2.839	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	424.4	100.00

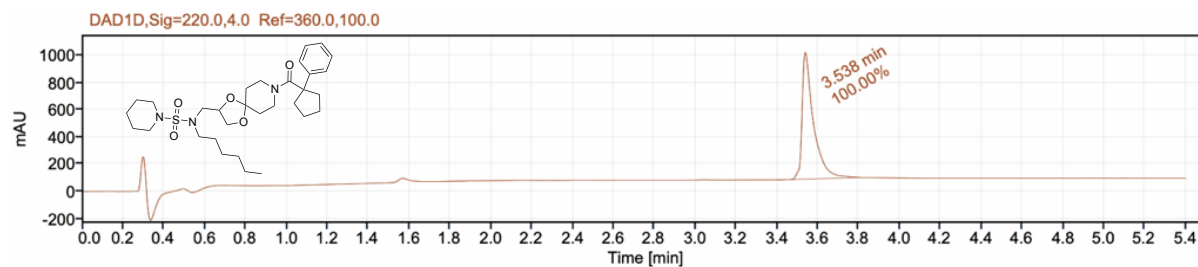
Figure S200: HPLC trace of 3o



Signal Name DAD1D

RT (min)	Signal description	Area	Area%
2.803	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	502.8	100.00

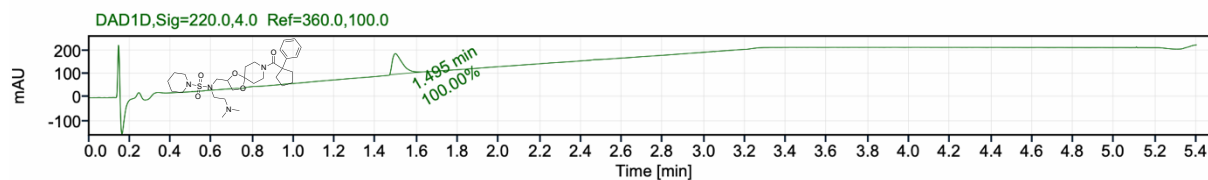
Figure S201: HPLC trace of 3p



Signal Name DAD1D

RT (min)	Signal description	Area	Area%
3.538	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	3617.1	100.00

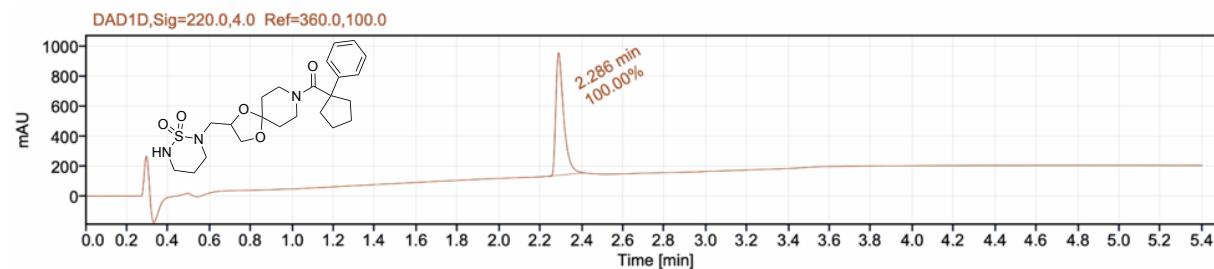
Figure S202: HPLC trace of 3q



Signal Name DAD1D

RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
1.495	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			306.9	100.00

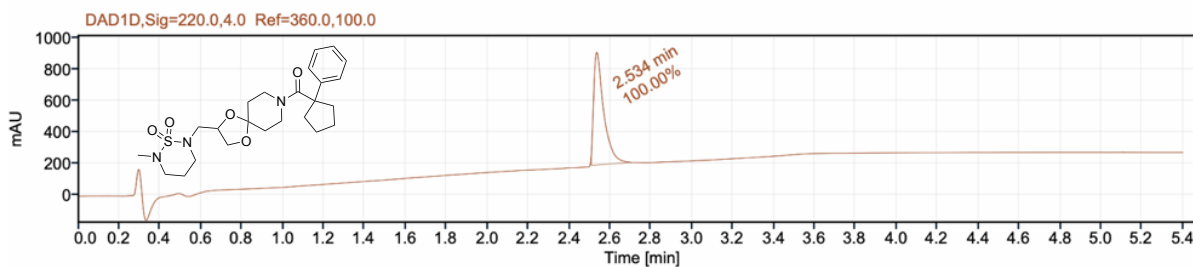
Figure S203: HPLC trace of 3r



Signal Name DAD1D

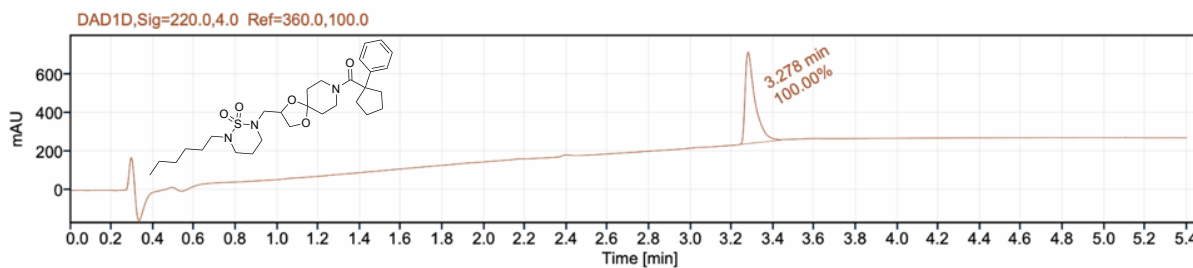
RT (min)	Signal description	Area	Area%
2.286	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	2156.1	100.00

Figure S204: HPLC trace of 3s



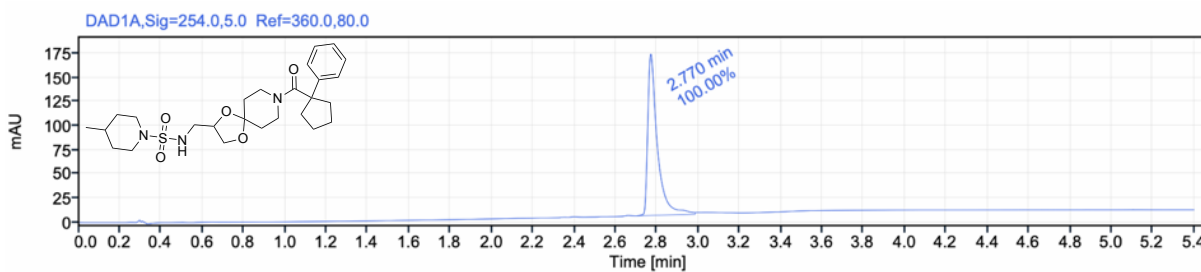
Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.534	DAD1D, Sig=220.0, 4.0 Ref=360.0, 100.0	2451.8	100.00

Figure S205: HPLC trace of 3t



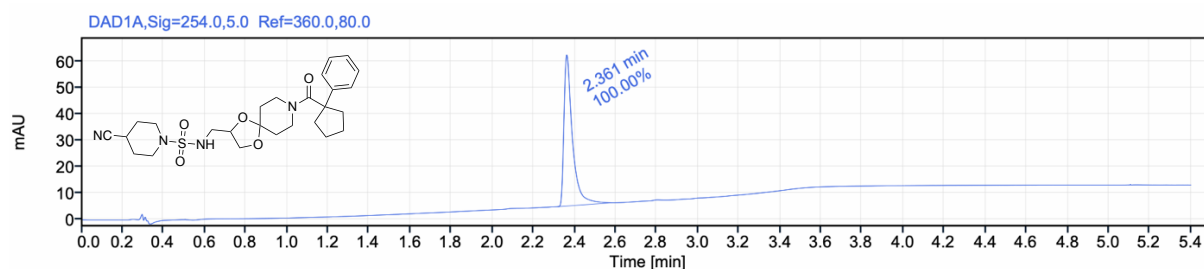
Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
3.278	DAD1D, Sig=220.0, 4.0 Ref=360.0, 100.0	1575.4	100.00

Figure S206: HPLC trace of 4a



Signal Name	DAD1A		
RT (min)	Signal description	Area	Area%
2.770	DAD1A, Sig=254.0, 5.0 Ref=360.0, 80.0	543.1	100.00

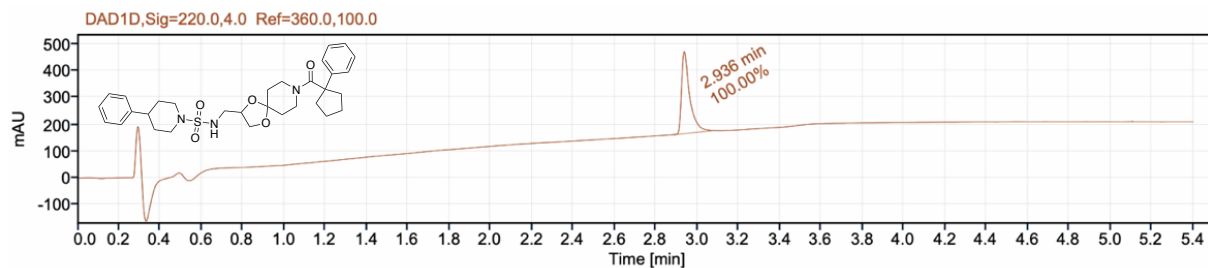
Figure S207: HPLC trace of 4b



Signal Name DAD1A

RT (min)	Signal description	Area	Area%
2.361	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	164.9	100.00

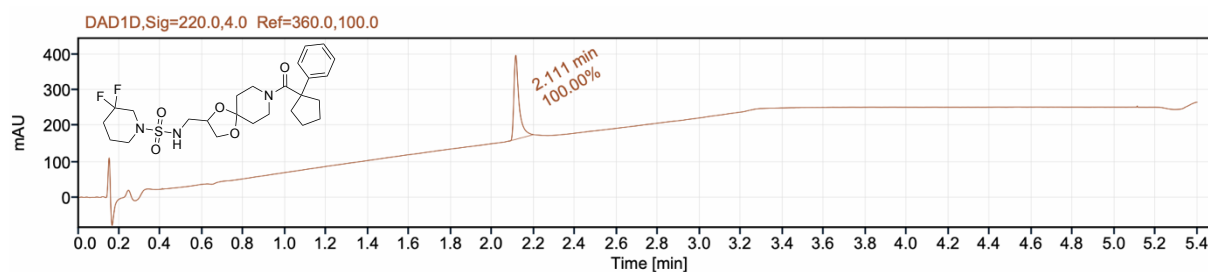
Figure S208: HPLC trace of 4c



Signal Name DAD1D

RT (min)	Signal description	Area	Area%
2.936	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	852.2	100.00

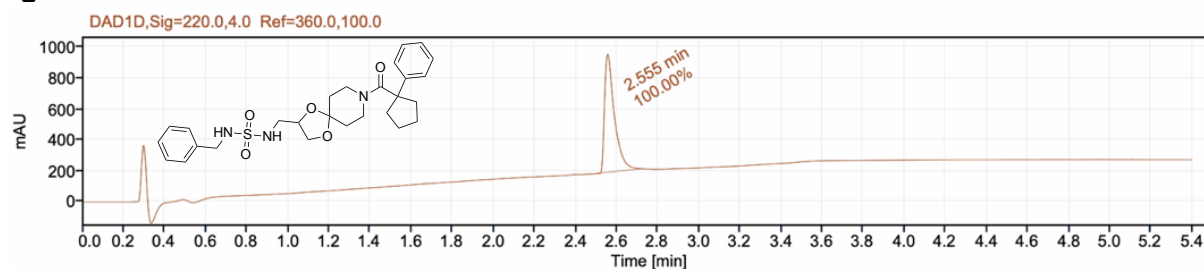
Figure S209: HPLC trace of 4d



Signal Name DAD1D

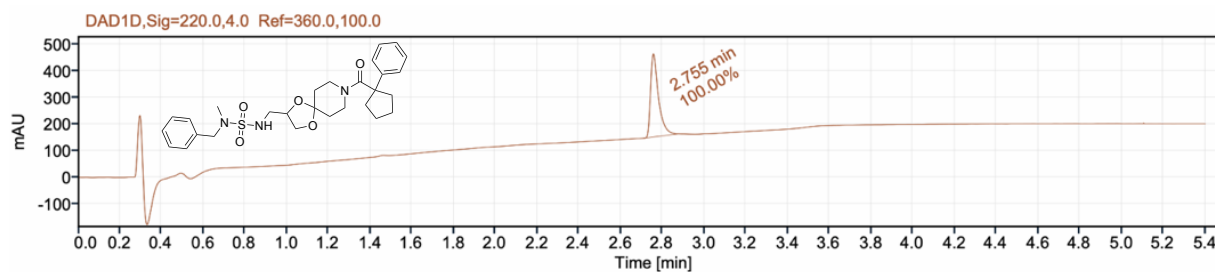
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
2.111	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			410.3	100.00

Figure S210: HPLC trace of 5a



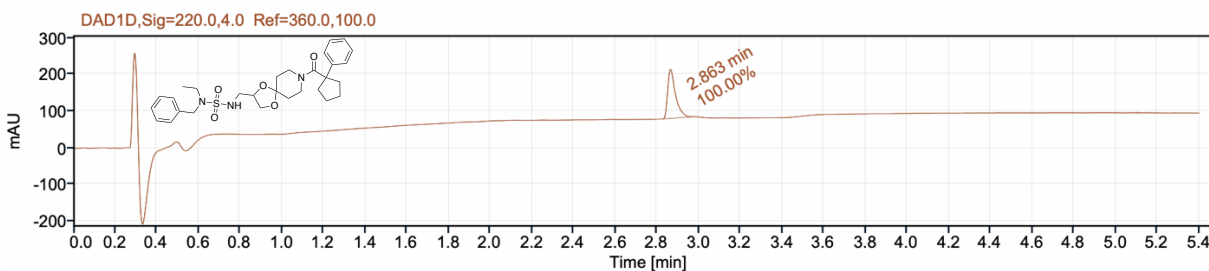
Signal Name		DAD1D	
RT (min)	Signal description	Area	Area%
2.555	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	2538.9	100.00

Figure S211: HPLC trace of 5b



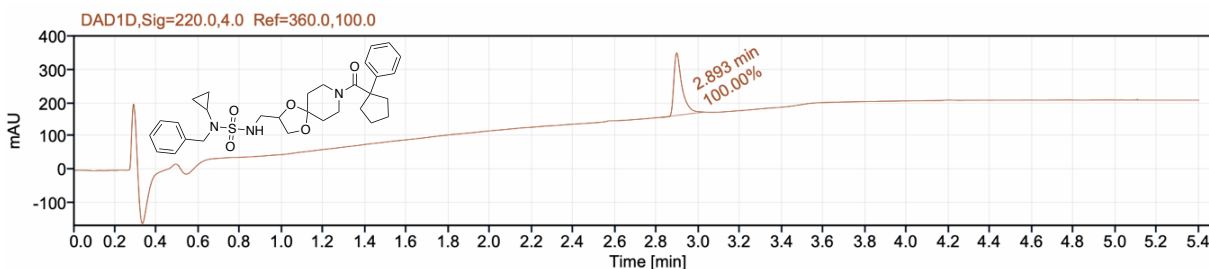
Signal Name		DAD1D	
RT (min)	Signal description	Area	Area%
2.755	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	830.4	100.00

Figure S212: HPLC trace of 5c



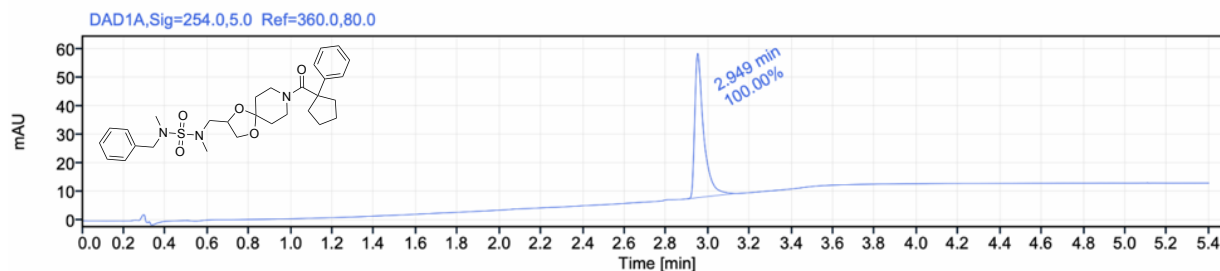
Signal Name		DAD1D	
RT (min)	Signal description	Area	Area%
2.863	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	347.3	100.00

Figure S213: HPLC trace of 5d



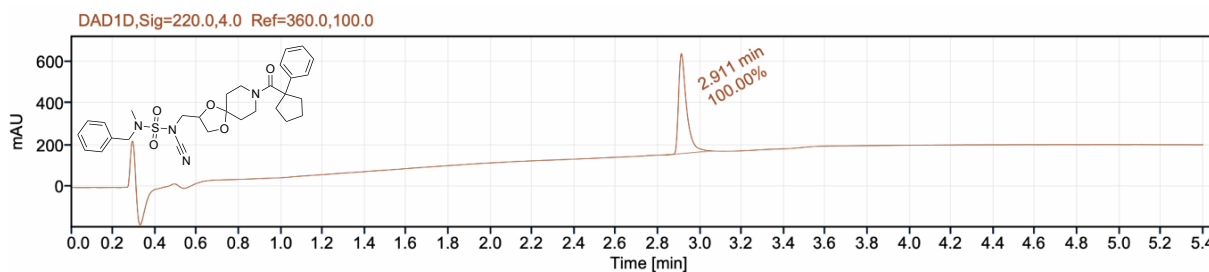
Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.893	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	506.1	100.00

Figure S214: HPLC trace of 5e



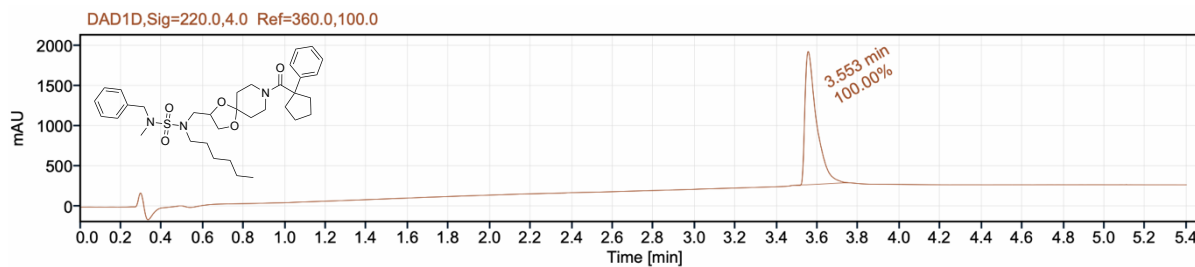
Signal Name	DAD1A		
RT (min)	Signal description	Area	Area%
2.949	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	148.9	100.00

Figure S215: HPLC trace of 5f



Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.911	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	1262.4	100.00

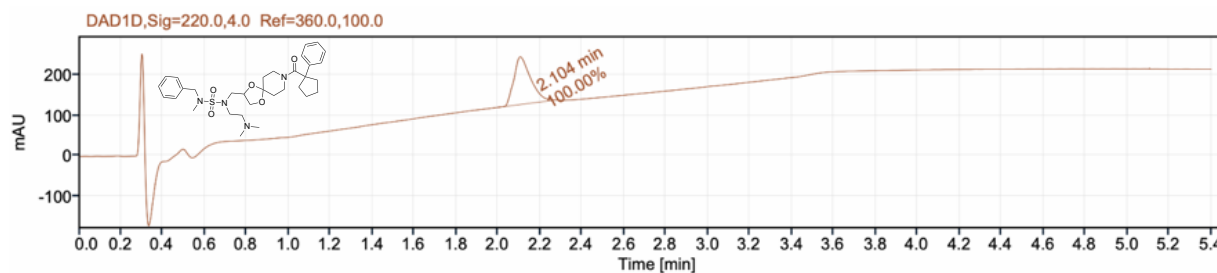
Figure S216: HPLC trace of 5g



Signal Name DAD1D

RT (min)	Signal description	Area	Area%
3.553	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	6452.7	100.00

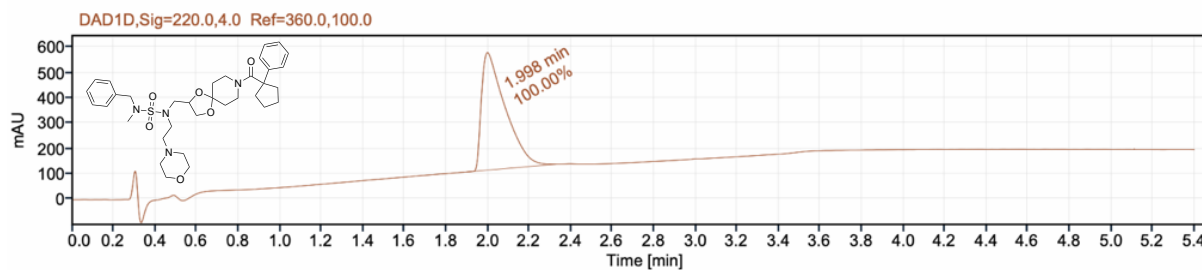
Figure S217: HPLC trace of 5h



Signal Name DAD1D

RT (min)	Signal description	Area	Area%
2.104	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	646.6	100.00

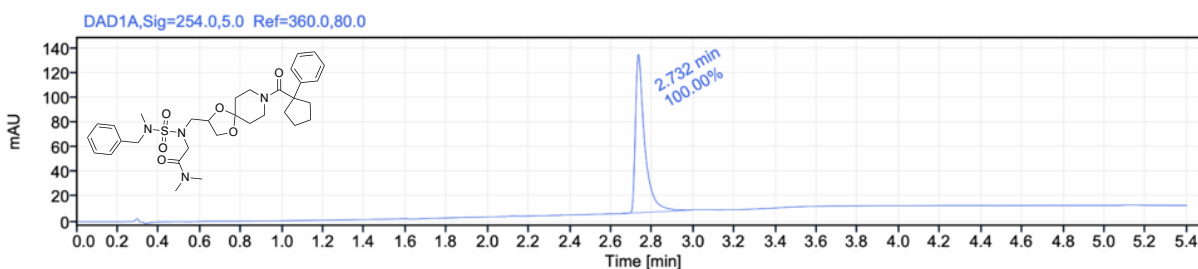
Figure S218: HPLC trace of 5i



Signal Name DAD1D

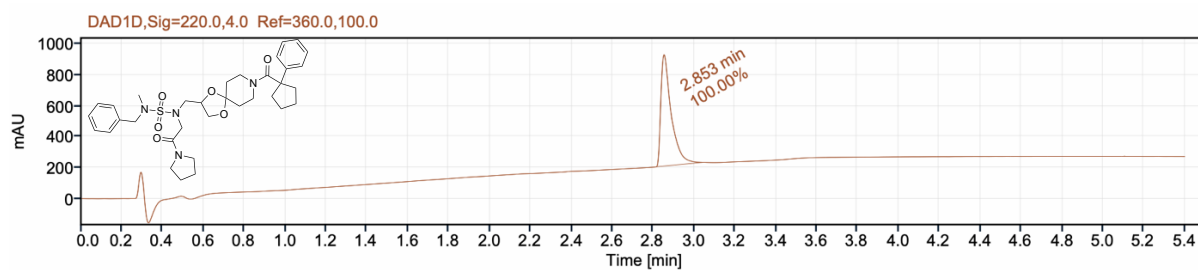
RT (min)	Signal description	Area	Area%
1.998	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	3678.6	100.00

Figure S219: HPLC trace of 5j



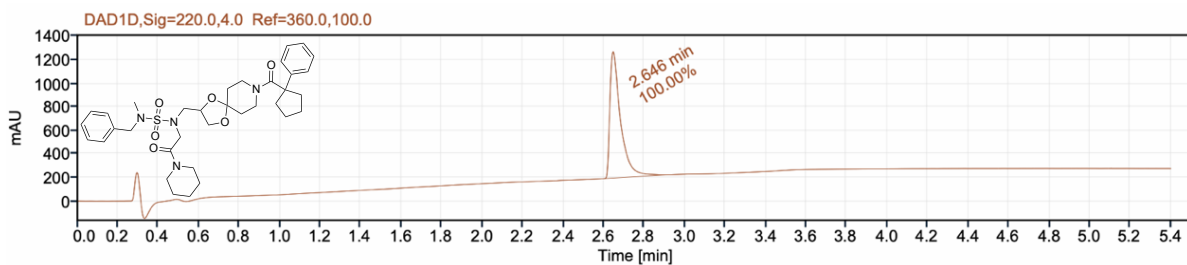
Signal Name	DAD1A		
RT (min)	Signal description	Area	Area%
2.732	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	403.3	100.00

Figure S220: HPLC trace of 5k



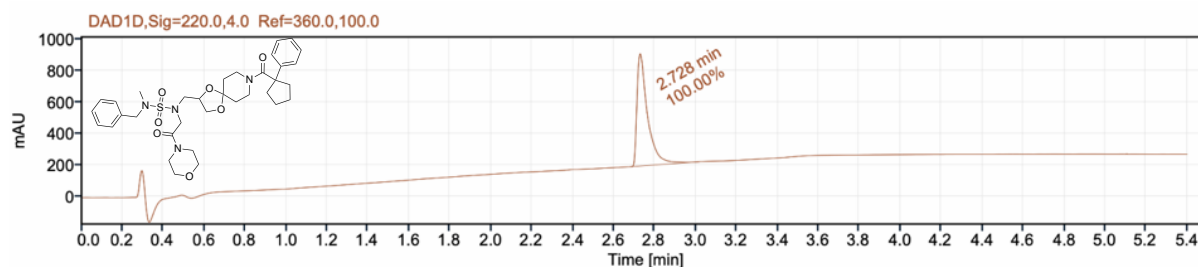
Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.853	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	2549.0	100.00

Figure S221: HPLC trace of 5l



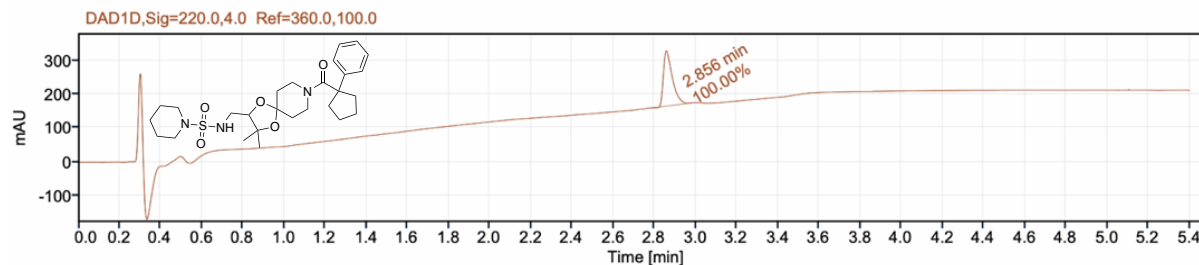
Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.646	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	3916.9	100.00

Figure S222: HPLC trace of 5m



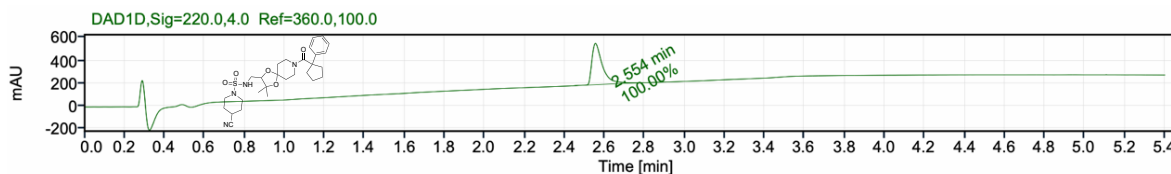
Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.728	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	2560.2	100.00

Figure S223: HPLC trace of 6a



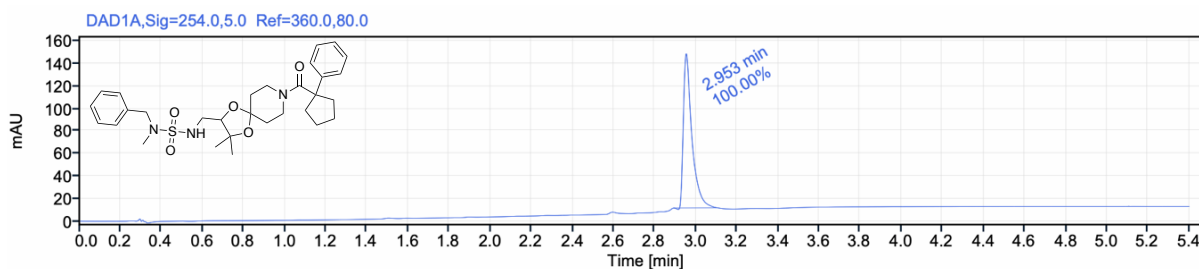
Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.856	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	492.3	100.00

Figure S224: HPLC trace of 6b



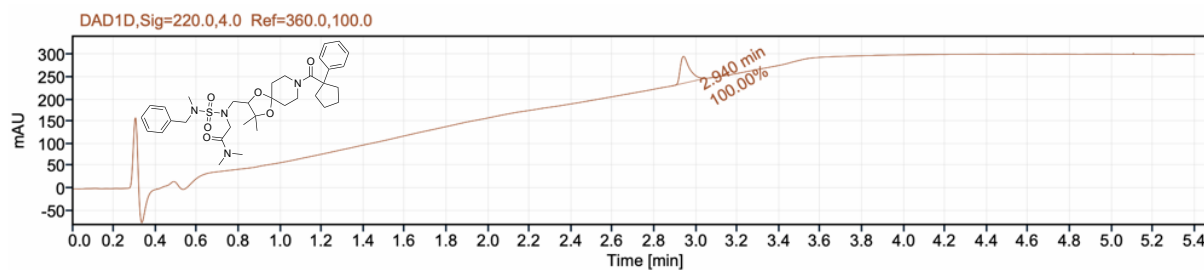
Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.554	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	1327.0	100.00

Figure S225: HPLC trace of 6c



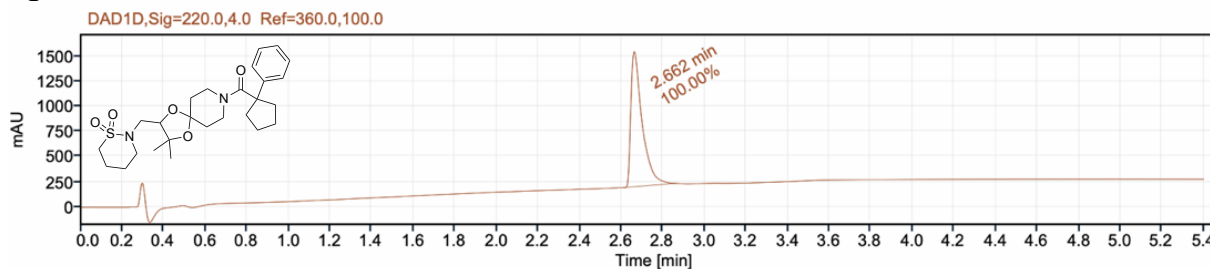
Signal Name		DAD1A		
RT (min)	Signal description	Area	Area%	
2.953	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	396.2	100.00	

Figure S226: HPLC trace of 6d



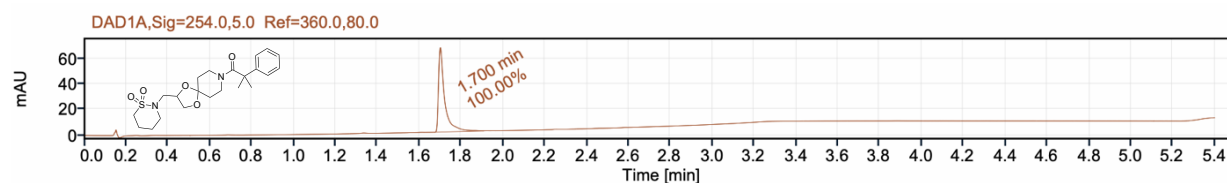
Signal Name		DAD1D		
RT (min)	Signal description	Area	Area%	
2.940	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	190.6	100.00	

Figure S227: HPLC trace of 6e



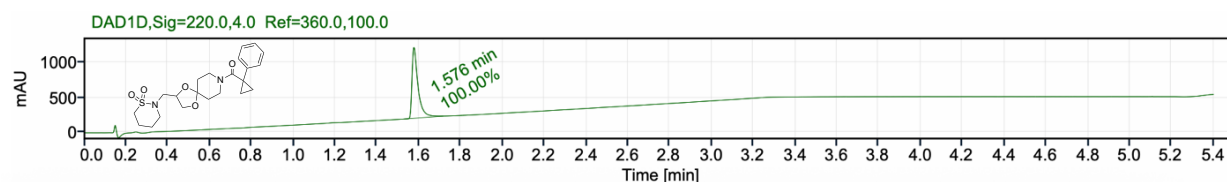
Signal Name		DAD1D		
RT (min)	Signal description	Area	Area%	
2.662	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	5074.7	100.00	

Figure S228: HPLC trace of 7a



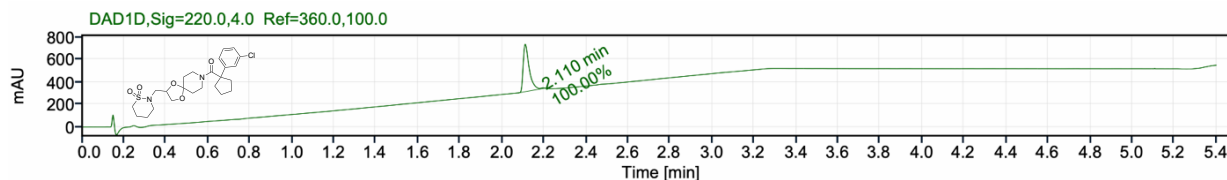
Signal Name		DAD1A			
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
1.700	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0			137.6	100.00

Figure S229: HPLC trace of 7b



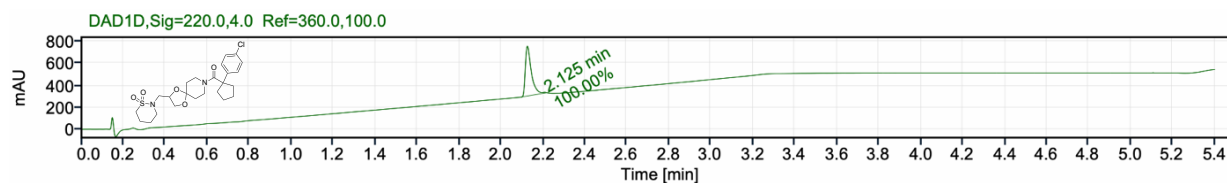
Signal Name		DAD1D			
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
1.576	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			2029.8	100.00

Figure S230: HPLC trace of 7c



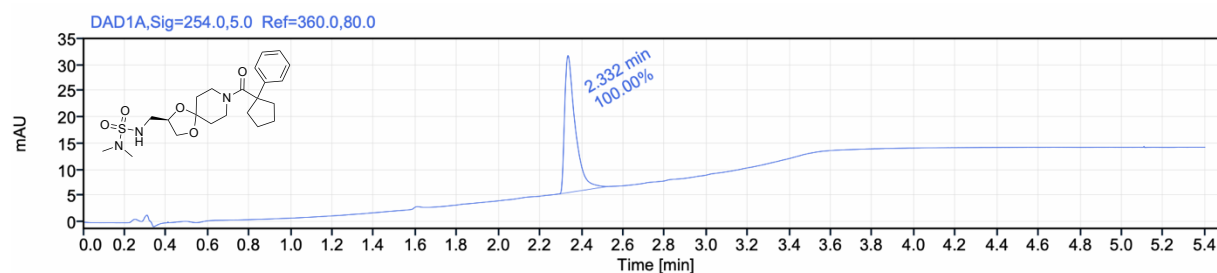
Signal Name		DAD1D			
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
2.110	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			840.7	100.00

Figure S231: HPLC trace of 7d



Signal Name		DAD1D			
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
2.125	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			908.6	100.00

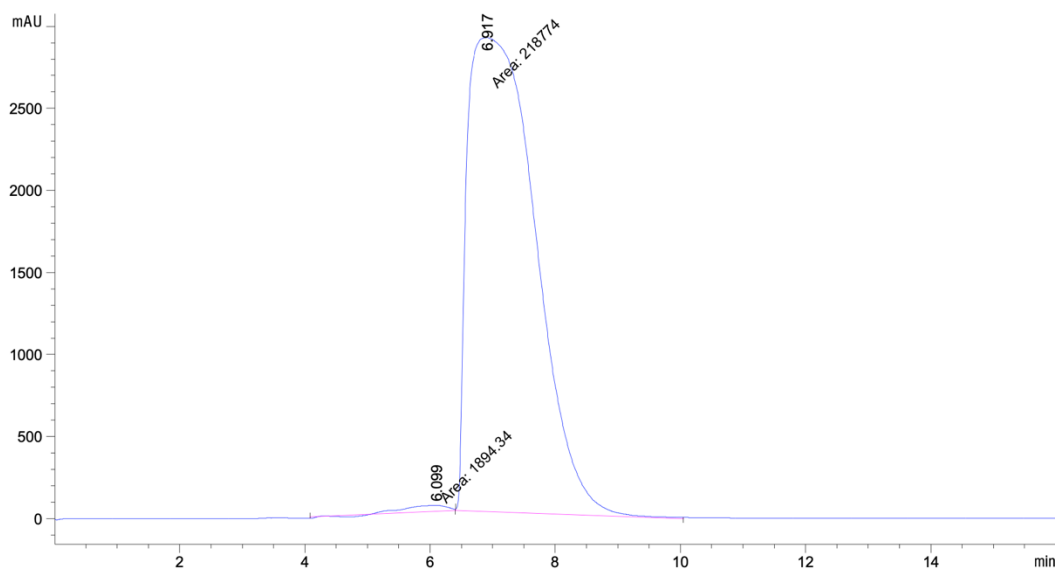
Figure S232: HPLC trace of **R-3a**



Signal Name DAD1A

RT (min)	Signal description	Area	Area%
2.332	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	93.2	100.00

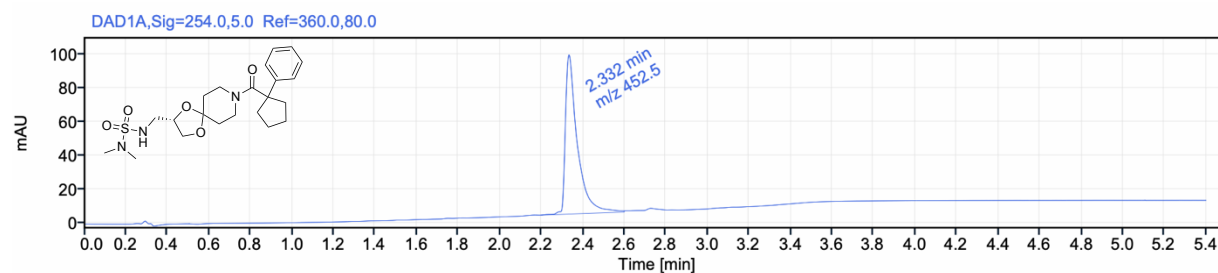
Figure S233: Chiral HPLC trace of **R-3a**



Signal 1: DAD1 B, Sig=220,4 Ref=off

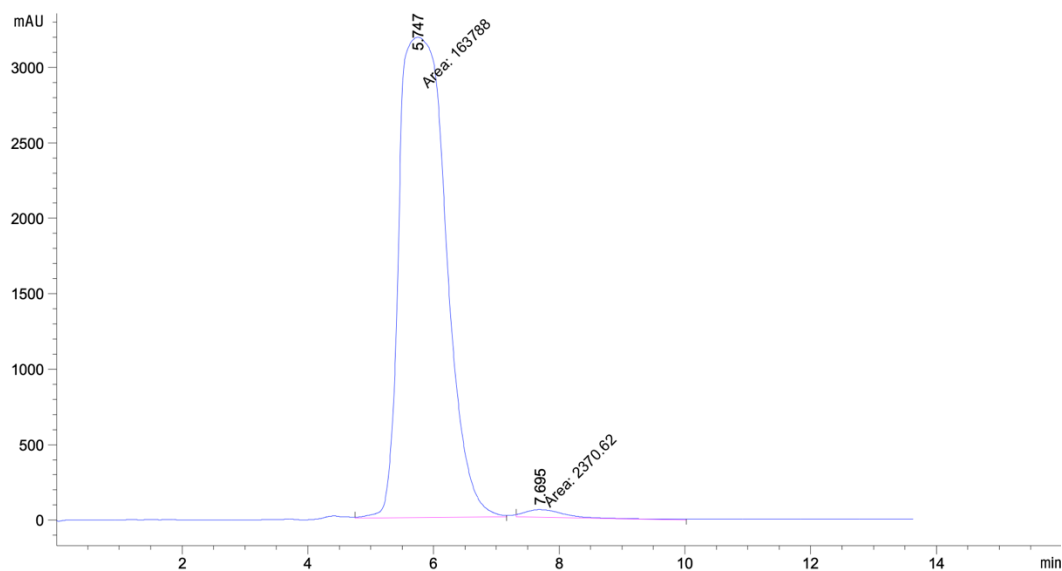
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.099	MM	0.8779	1894.33691	35.96227	0.8585
2	6.917	MM	1.2621	2.18774e5	2889.12842	99.1415

Figure S234: HPLC trace of **S-3a**



Signal Name		DAD1A	
RT (min)	Signal description	Area	Area%
2.332	DAD1A,Sig=254.0,5.0 Ref=360.0,80.0	376.5	100.00

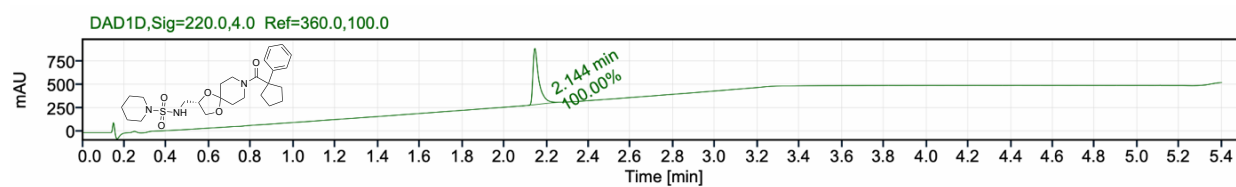
Figure S235: Chiral HPLC trace of **S-3a**



Signal 1: DAD1 B, Sig=220,4 Ref=off

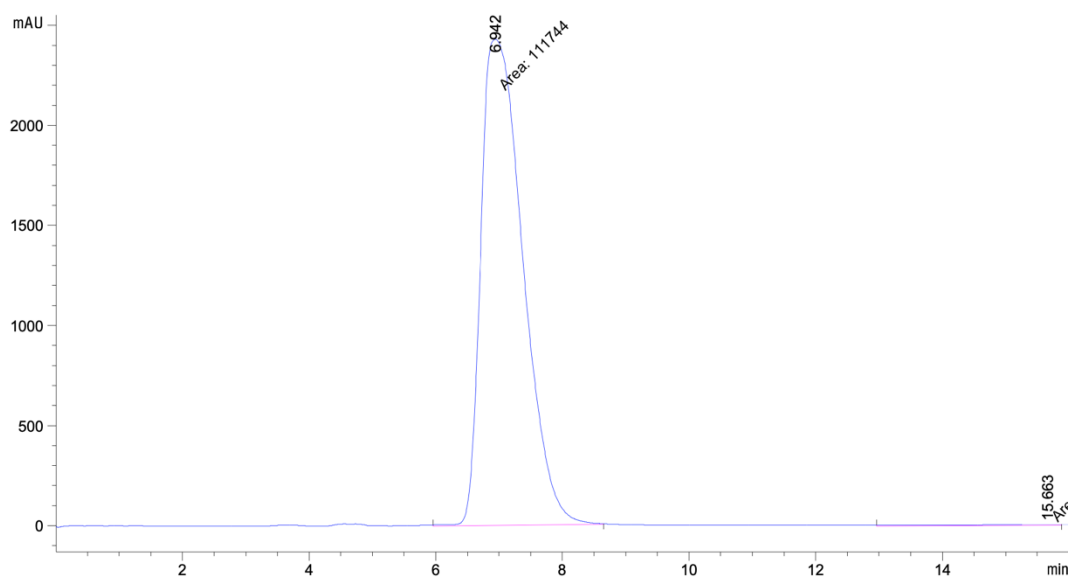
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.747	MM	0.8578	1.63788e5	3182.13818	98.5733
2	7.695	MM	0.7726	2370.61914	51.13731	1.4267

Figure S236: HPLC trace of S-3k



Signal Name	DAD1D	m/z	Purity UV(%) / MS(%)	Area	Area%
RT (min)	Signal description				
2.144	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			1172.1	100.00

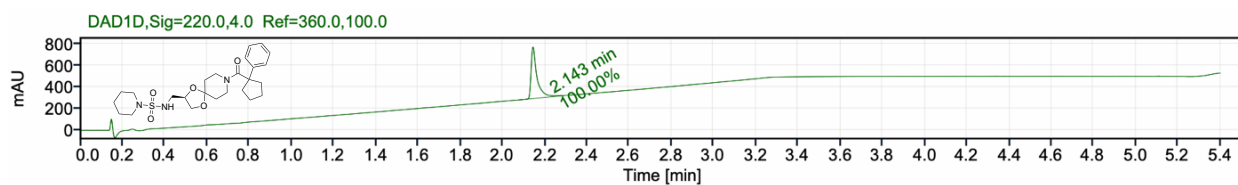
Figure S237: Chiral HPLC trace of S-3k



Signal 1: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.942	MM	0.7668	1.11744e5	2428.92163	99.4461
2	15.663	MM	2.2899	622.38013	4.52995	0.5539

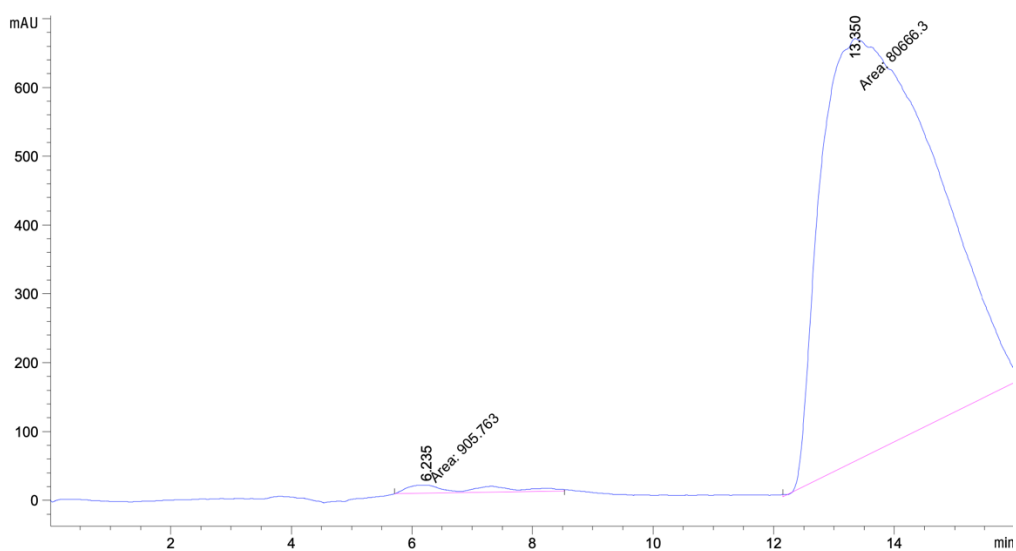
Figure S238: HPLC trace of **R-3k**



Signal Name DAD1D

RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
2.143	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0			935.2	100.00

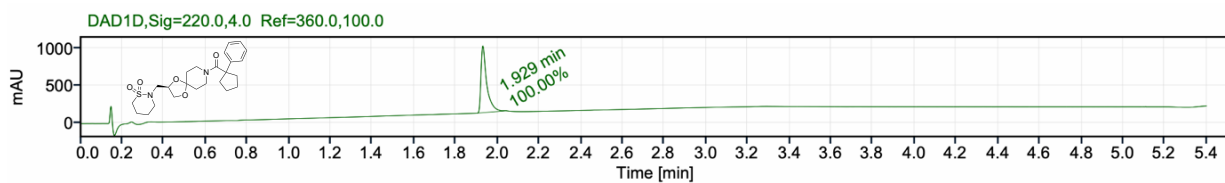
Figure S239: Chiral HPLC trace of **R-3k**



Signal 1: DAD1 B, Sig=220,4 Ref=off

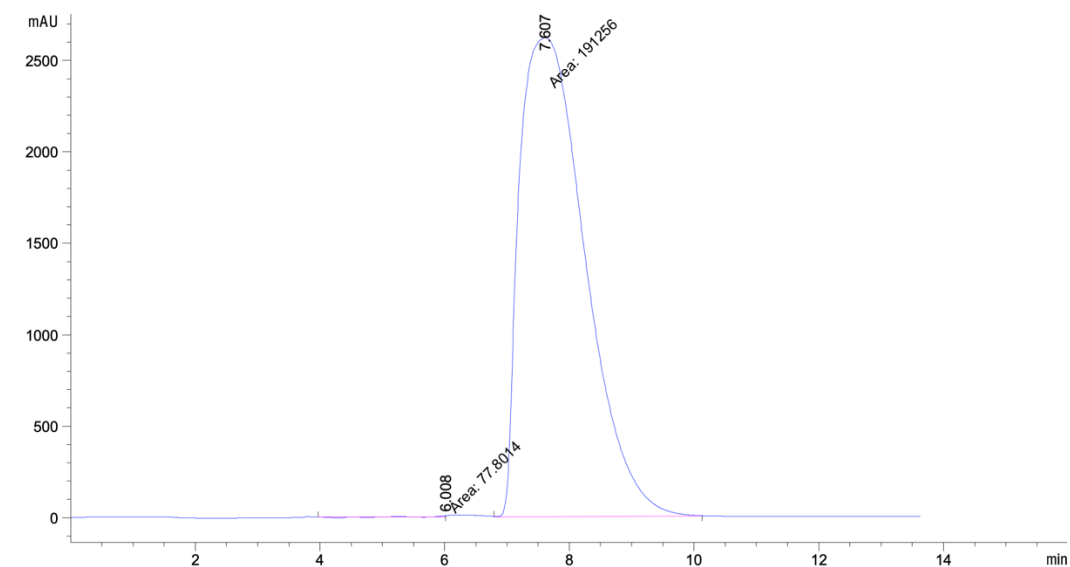
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.235	MM	1.2822	905.76251	11.77319	1.1104
2	13.350	MM	2.1888	8.06663e4	614.22253	98.8896

Figure S240: HPLC trace of **R-1m**



Signal Name		DAD1D			
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
1.929	DAD1D, Sig=220.0, 4.0 Ref=360.0, 100.0			1687.6	100.00

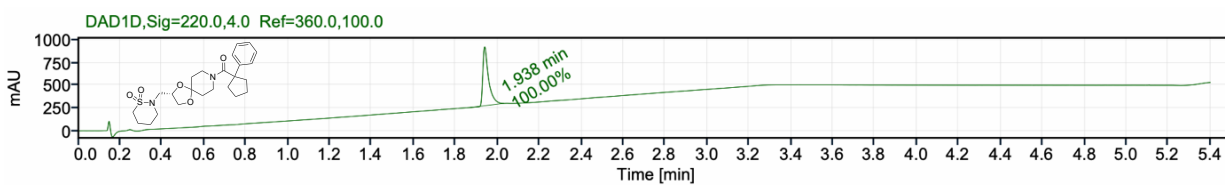
Figure S241: Chiral HPLC trace of **R-1m**



Signal 1: DAD1 B, Sig=220,4 Ref=off

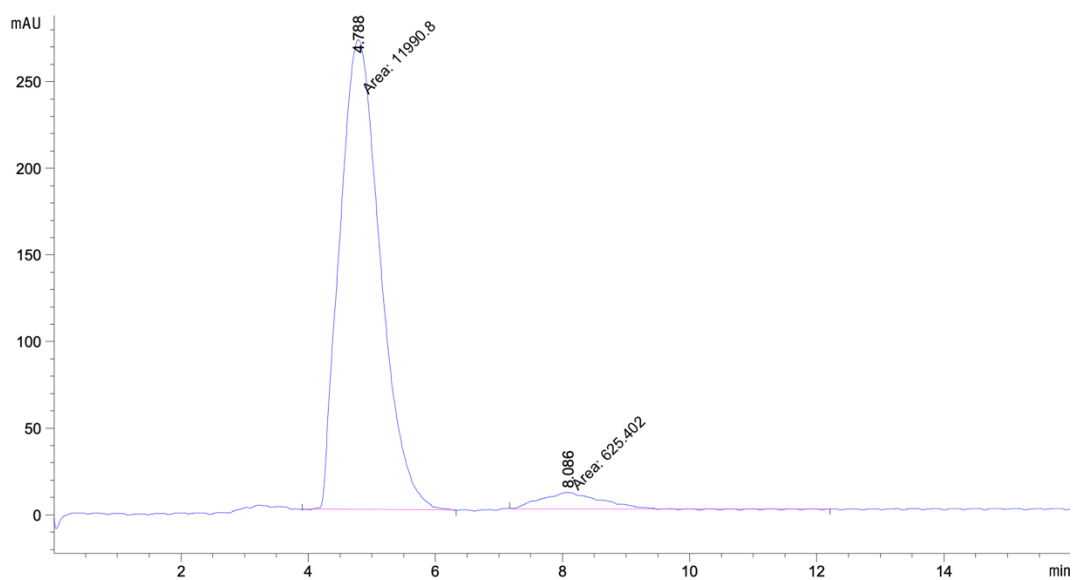
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.008	MM	0.2028	77.80135	6.39372	0.0407
2	7.607	MM	1.2168	1.91256e5	2619.55542	99.9593

Figure S242: HPLC trace of S-1m



Signal Name		DAD1D					
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%		
1.938	DAD1D, Sig=220.0, 4.0 Ref=360.0, 100.0			1227.3	100.00		

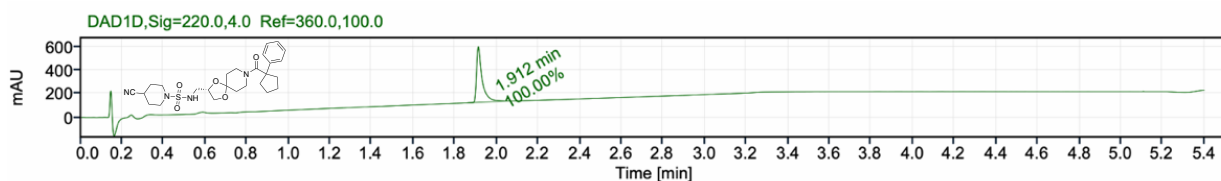
Figure S243: Chiral HPLC trace of S-1m



Signal 1: DAD1 B, Sig=220,4 Ref=off

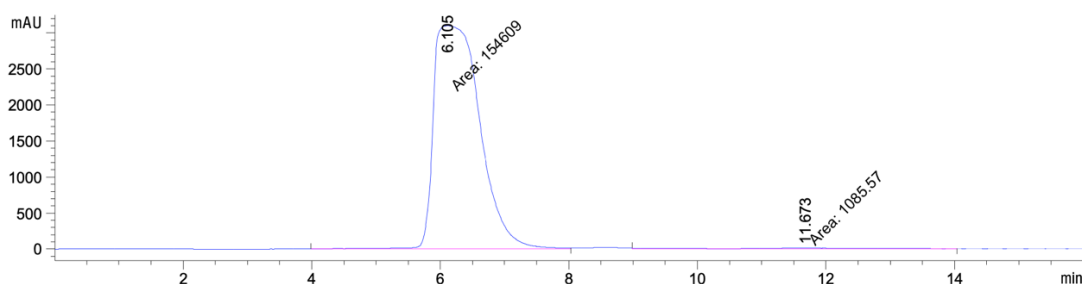
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.788	MM	0.7373	1.19908e4	271.06897	95.0429
2	8.086	MM	1.0977	625.40216	9.49558	4.9571

Figure S244: HPLC trace of S-4b



Signal Name		DAD1D					
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%		
1.912	DAD1D, Sig=220.0,4.0 Ref=360.0,100.0			888.6	100.00		

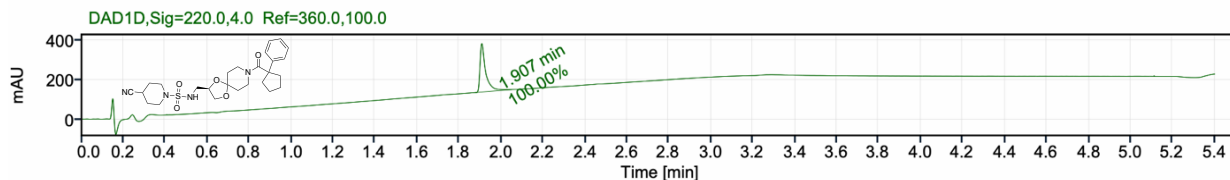
Figure S245: Chiral HPLC trace of S-4b



Signal 2: DAD1 B, Sig=220,4 Ref=off

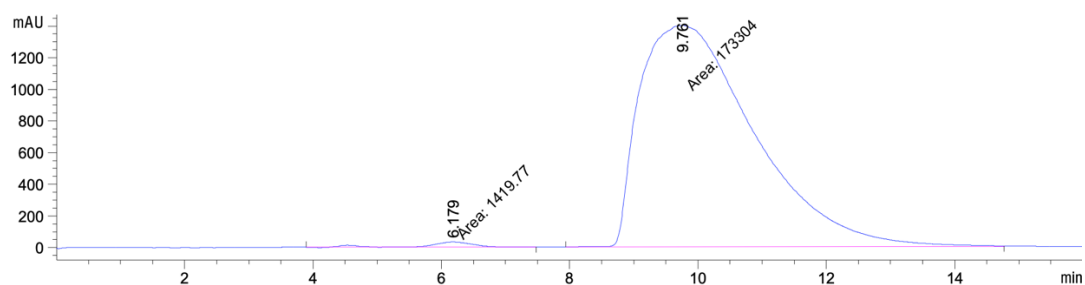
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.105	MM	0.8332	1.54609e5	3092.85156	99.3028
2	11.673	MM	1.9753	1085.57361	9.15960	0.6972

Figure S246: HPLC trace of R-4b



Signal Name		DAD1D					
RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%		
1.907	DAD1D, Sig=220.0,4.0 Ref=360.0,100.0			467.8	100.00		

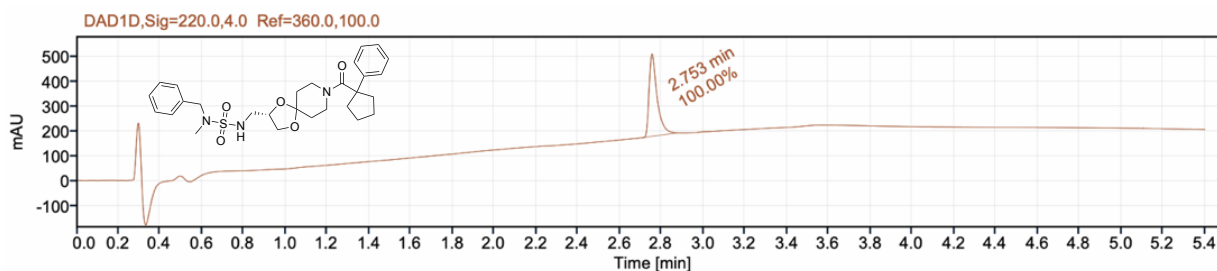
Figure S247: Chiral HPLC trace of **R-4b**



Signal 2: DAD1 B, Sig=220,4 Ref=off

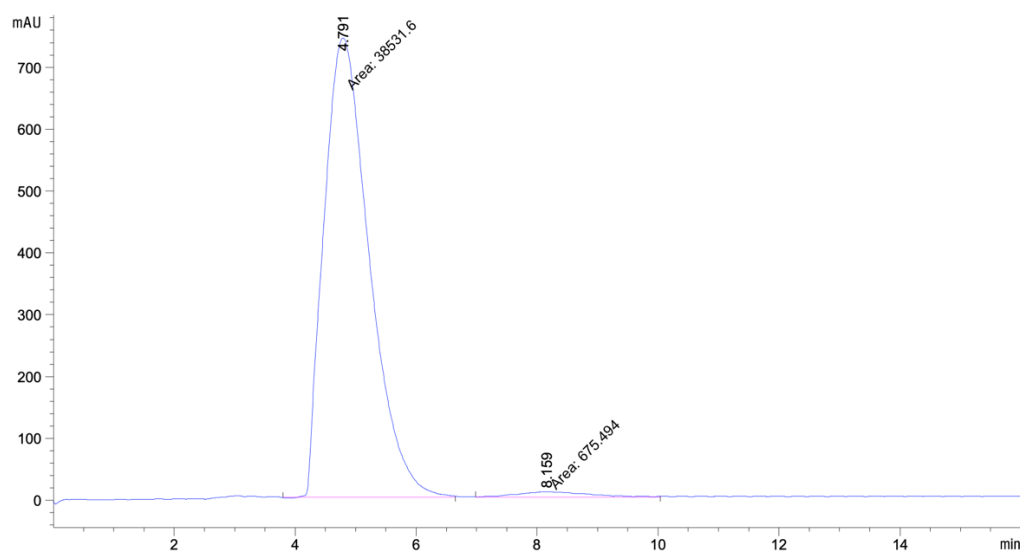
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.179	MM	0.7478	1419.77014	31.64187	0.8126
2	9.761	MM	2.0644	1.73304e5	1399.15979	99.1874

Figure S248: HPLC trace of **S-5b**



Signal Name	DAD1D		
RT (min)	Signal description	Area	Area%
2.753	DAD1D,Sig=220.0,4.0 Ref=360.0,100.0	882.0	100.00

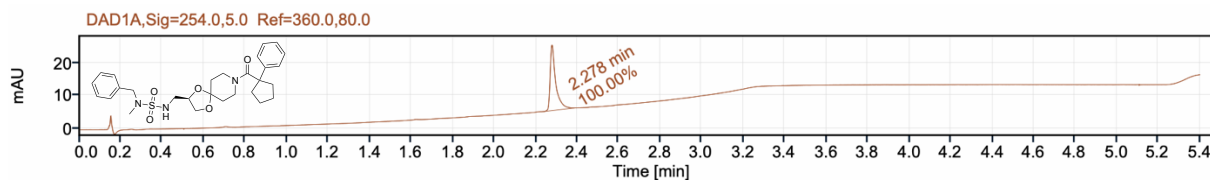
Figure S249: Chiral HPLC trace of **S-5b**



Signal 1: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.791	MM	0.8655	3.85316e4	741.98560	98.2771
2	8.159	MM	1.3044	675.49414	8.63099	1.7229

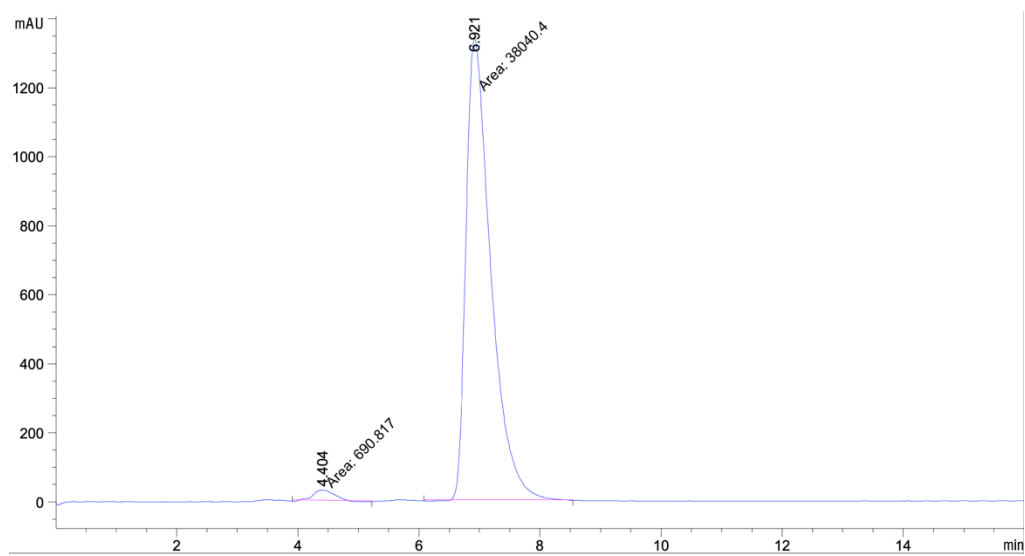
Figure S250: HPLC trace of **R-5b**



Signal Name DAD1A

RT (min)	Signal description	m/z	Purity UV(%) / MS(%)	Area	Area%
2.278	DAD1A, Sig=254.0,5.0 Ref=360.0,80.0			36.6	100.00

Figure S251: Chiral HPLC trace of **R-5b**



Signal 1: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.404	MM	0.3981	690.81689	28.92428	1.7836
2	6.921	MM	0.4747	3.80404e4	1335.53735	98.2164