

Table S1. Elemental analysis of the target compounds **6a –u**.

Sample Code	M.W. g/mol	Molecular formula	Calculated CHN (%)	Found CHN (%)
6a	382.13	C ₂₃ H ₁₈ N ₄ S	C:72.22; H:4.74; N:14.65	C:71.97; H:4.66; N:14.53
6b	427.11	C ₂₃ H ₁₇ N ₅ O ₂ S	C:64.62; H:4.01; N:16.38	C:64.51; H:4.08; N:16.14
6c	407.12	C ₂₃ H ₁₇ N ₅ S	C:70.74; H:4.21; N:17.19	C:70.50; H:4.21; N:16.98
6d	416.09	C ₂₃ H ₁₇ ClN ₄ S	C:66.26; H:4.11; N:13.44	C:66.47; H:4.01; N:13.36
6e	450.05	C ₂₃ H ₁₆ Cl ₂ N ₄ S	C:61.20; H:3.57; N:12.41	C:60.93; H:3.62; N:12.17
6f	450.05	C ₂₃ H ₁₆ Cl ₂ N ₄ S	C:61.20; H:3.57; N:12.41	C:60.98; H:3.62; N:12.31
6g	396.14	C ₂₄ H ₂₀ N ₄ S	C:72.7; H:5.08; N:14.3	C:72.48; H:5.11; N:14.06
6h	416.09	C ₂₃ H ₁₇ ClN ₄ S	C:66.26; H:4.11; N:13.44	C:65.98; H:4.25; N:13.29
6i	461.07	C ₂₃ H ₁₆ ClN ₅ O ₂ S	C:59.8; H:3.49; N:15.16	C:60.07; H:3.54; N:14.86
6j	441.08	C ₂₄ H ₁₆ ClN ₅ S	C:65.23; H:3.65; N:15.85	C:65.14; H:3.87; N:15.62
6k	450.05	C ₂₃ H ₁₆ Cl ₂ N ₄ S	C:61.2; H:3.57; N:12.41	C:60.96; H:3.45; N:12.18
6l	484.01	C ₂₃ H ₁₅ Cl ₃ N ₄ S	C:56.86; H:3.11; N:11.53	C:56.71; H:3.2; N:11.36
6m	484.01	C ₂₃ H ₁₅ Cl ₃ N ₄ S	C:56.86; H:3.11; N:11.53	C:56.75; H:3.29; N:11.34
6n	430.1	C ₂₄ H ₁₉ ClN ₄ S	C:66.89; H:4.44; N:13.00	C:70.06; H:4.36; N:13.24
6o	388.17	C ₂₃ H ₂₄ N ₄ S	C:71.10; H:6.23; N:14.42	C:70.92; H:6.21; N:14.38
6p	433.16	C ₂₃ H ₂₃ N ₅ O ₂ S	C:63.72; H:5.35; N:16.15	C:63.88; H:5.43; N:16.00
6q	413.17	C ₂₄ H ₂₃ N ₅ S	C:69.71; H:5.61; N:16.94	C:69.53; H:5.85; N:16.87
6r	422.13	C ₂₃ H ₂₃ ClN ₄ S	C:65.31; H:5.48; N:13.25	C:65.25; H:5.61; N:13.16
6s	456.09	C ₂₃ H ₂₂ Cl ₂ N ₄ S	C:60.39; H:4.85; N:12.25	C:60.31; H:4.73; N:12.19
6t	456.09	C ₂₃ H ₂₂ Cl ₂ N ₄ S	C:60.39; H:4.85; N:12.25	C:60.35; H:4.69; N:11.98
6u	402.19	C ₂₄ H ₂₆ N ₄ S	C:71.61; H:6.51; N:13.92	C:71.48; H:6.67; N:14.05

PROTON DMSO {C:\Bruker\TOPSPIN} abari 10

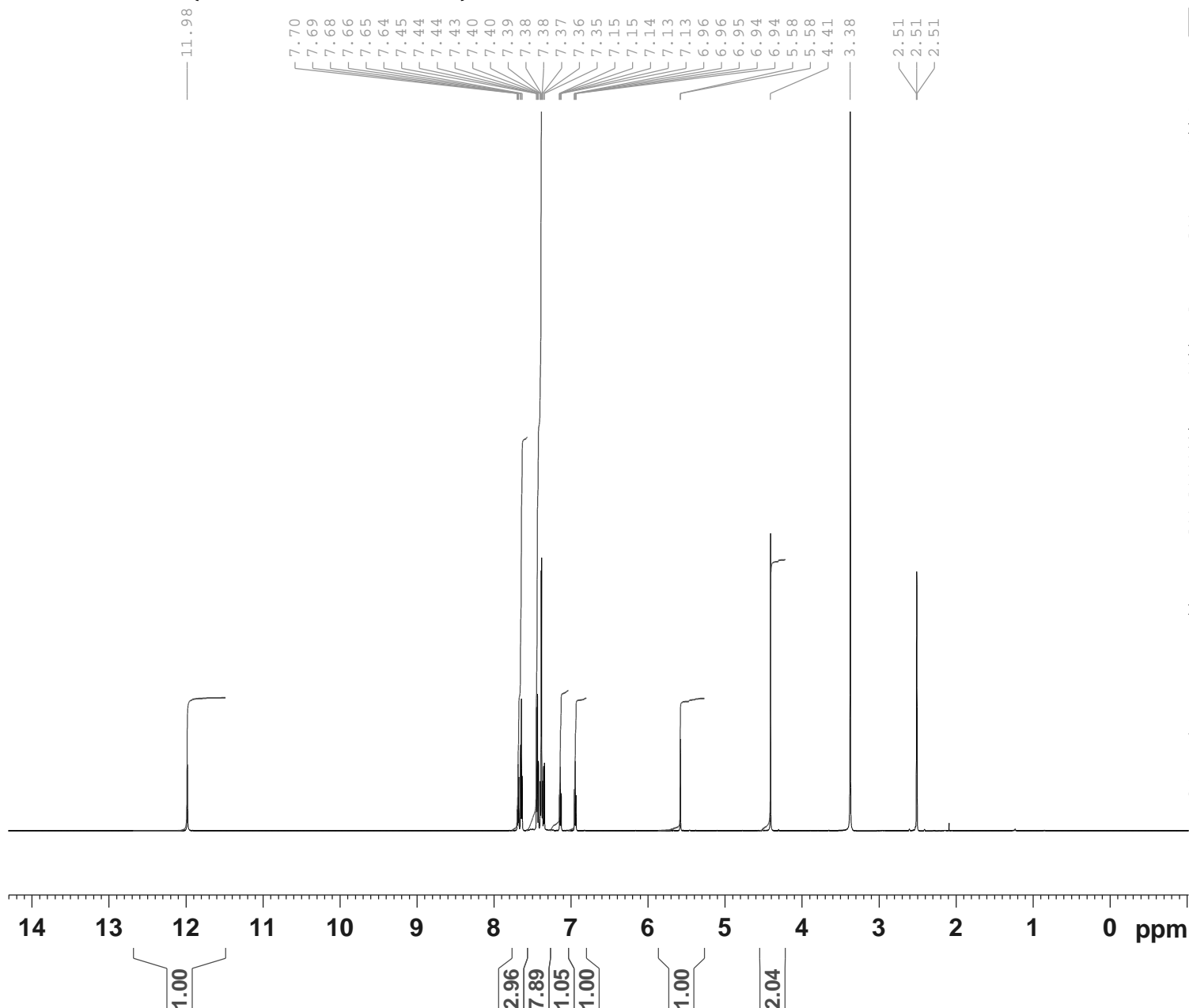


Current Data Parameters
NAME drMona-MM7
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181011
Time 10.12
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 14097.744 Hz
FIDRES 0.215115 Hz
AQ 2.3243434 sec
RG 31.35
DW 35.467 usec
DE 31.86 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 700.1743238 MHz
NUC1 1H
P1 8.00 usec
PLW1 9.64999962 W

F2 - Processing parameters
SI 65536
SF 700.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



C13CPD DMSO {C:\Bruker\TOPSPIN} abari 10



Current Data Parameters
NAME drMona-MM7
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181011
Time 11.02
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 41666.668 Hz
FIDRES 0.635783 Hz
AQ 0.7864320 sec
RG 172.3
DW 12.000 usec
DE 18.00 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 176.0754915 MHz
NUC1 13C
P1 12.00 usec
PLW1 121.00000000 W

===== CHANNEL f2 =====
SFO2 700.1728007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 65.00 usec
PLW2 9.64999962 W
PLW12 0.14618000 W
PLW13 0.06176000 W

F2 - Processing parameters
SI 32768
SF 176.0578870 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

