$^1$H NMR spectrum of compound 5a
$^{13}$C NMR spectrum of compound 5a

![NMR Spectrum Image]
Purity and HRMS of compound 5a

2. 5b: chromatogram / area
2. 5b: mass spectrum

Molecular formula: C_{18}H_{15}BrN_{2}O_{4}S
Exact mass: 449.0045
113.2589 (4+)
150.6760 (3+)
225.5101 (2+)
450.0123 (1+)
$^1$ NMR spectrum of compound 5b
$^{13}$C NMR spectrum of compound 5b
Purity and HRMS of compound 5b

4. 5d : chromatogram / area
4. 5d: mass spectrum

Molecular formula: C_{13}H_{19}N_{3}O_{5}S
Exact mass: 401.1045
101.2840 (4+)
134.7093 (3+)
201.5601 (2+)
402.1124 (1+)
$^1$NMR spectrum of compound 5c
$^{13}$C NMR spectrum of compound 5c
Purity and HRMS of compound 5c

6. 5f: chromatogram / area
6. 5f: mass spectrum

Molecular formula: C₁₆H₁₅ClF₃N₅O₄S
Exact mass: 423.0456
105.7692 (4+)
142.0230 (3+)
212.5306 (2+)
424.0534 (1+)
$^1$H NMR spectrum of compound 5d
$^{13}$C NMR spectrum of compound 5d
Purity and HRMS of compound 5d
8. 6b: mass spectrum

Molecular formula: C_{y}H_{x}Br\cdot N_{z}O_{y}S
Exact mass: 463.0201

116.7629 (4+)
153.3479 (3+)
232.5179 (2+)
464.0200 (1+)
\(^1\text{H NMR spectrum of compound 5e}\)

![Chemical Structure of Compound 5e](image)

**Bruker**

**Current Data Parameters**
- **FID**: D050_0d
- **PROC**: 1

**F2 - Acquisition Parameters**
- **NAME**: D050_0d
- **Time**: 15.00 h
- **METHOD**: D050_0d
- **NMOD**: 20000
- **TR**: 30000
- **TD**: 10000000 sec
- **F2**: 400.12 MHz
- **F1**: 16.000 sec

**F2 - Processing parameters**
- **FID**: D050_0d
- **SNR**: 10000
- **LB**: 0.20 Hz
- **GB**: 0
- **PC**: 1.00
$^{13}$C NMR spectrum of compound 5e
Purity and HRMS of compound 5e

10. 6d: chromatogram / area

peak area

chromatogram
10. 6d: mass spectrum

Molecular formula: C_{30}H_{21}N_{8}O_{5}S
Exact mass: 415.1202

104.7879 (4+)
139.3812 (3+)
208.5679 (2+)
416.1280 (1+)
$^1$H NMR spectrum of compound 5f
$^{13}$C NMR spectrum of compound 5f
Purity and HRMS of compound 5f
12. 6f: mass spectrum

Molecular formula: C$_{13}$H$_{17}$ClF$_3$N$_3$O$_4$S
Exact mass: 437.0612
110.2731 (4+)
146.6943 (3+)
219.5384 (2+)
438.0631 (1+)
$^1$H NMR spectrum of compound 5g
$^{13}$C NMR spectrum of compound 5g
Purity and HRMS of compound 5g
Molecular formula: C_{3}H_{9}BrN_{3}O_{5}

 Exact mass: 463.0201

116.7629 (4+)
153.3479 (2+)
232.5179 (2+)
464.0280 (1+)
$^{1}$H NMR spectrum of compound 5h
$^{13}$C NMR spectrum of compound 5h
Purity and HRMS of compound 5h
Molecular formula: C$_{30}$H$_{21}$N$_5$O$_9$S
Exact mass: 415.1202
104.7879 (4+)
138.3812 (3+)
208.5679 (2+)
416.1280 (1+).
$^1$H NMR spectrum of compound 5i
$^{13}$C NMR spectrum of compound 5i
Purity and HRMS of compound 5i

18. 7f: chromatogram / area

peak area

chromatogram
18. 7f : mass spectrum

Molecular formula: C_{13}H_{17}ClFNO_4S
Exact mass: 437.0612
110.2731 (4+)
146.6943 (3+)
219.5384 (2+)
438.0631 (1+)