Compound 2

(1) ESI-MS Signal Smooth IDG, NaN

[Graph showing mass spectrometry data]

[Chemical structure diagram]

[Graph showing NMR spectrum]

[Graph showing additional NMR spectrum]
Compound 3
Compound 5

1H NMR (500 MHz, DMSO-d6) δ ppm

Chemical Shifts:
- H1: 8.75 (br s, 1H)
- H2: 7.99 (d, J=9.6 Hz, 1H)
- H3: 7.89 (d, J=9.6 Hz, 1H)
- H4: 7.40 (d, J=8.0 Hz, 1H)
- H5: 7.35 (d, J=8.0 Hz, 1H)
- H6: 7.05 (d, J=16.0 Hz, 1H)
- H7: 6.98 (d, J=16.0 Hz, 1H)

Integrals:
- H1: 1.0
- H2: 1.0
- H3: 1.0
- H4: 1.0
- H5: 1.0
- H6: 1.0
- H7: 1.0
Compound 8

Acquisition Time: 4:24:01
Date: 19 Aug 2014

Chemical Shifts

Acquisition Time: 1:39:31
Date: 19 Aug 2014

Vertical Scale Factor: 1

Acquisition Time: 1:39:31
Date: 19 Aug 2014

Vertical Scale Factor: 1
Compound 14 continued
Compound s15

(1) Elsd Signal Smooth (80, 1x1)

Acquisition Time (sec): 4.2304
Comment: GC-054 A 155
Date: 27 Nov 2014 11:53:26

Date Start: 27 Nov 2014 11:53:26
File Name: 15104115/150104/GC-054A11501501_115151041151

Frequency (MHz): 121.175
Number: 111
Number of Transients: 15
Signal: Target

Original Points Examin: 30720
Dwell: 50.000
Points Examin: 8192
Points Sequence: jnrp

Spectrum Offset (ppm): 5.002530E-06
Spectrum Type: 1D 1H-Decoupled
Sweep Width (Hz): 8042 Hz
Temperature (degree C): 25.155

Acquisition Time (sec): 1.3601
Comment: GC-054 A 155
Date: 26 Nov 2014 12:12:16

Date Start: 26 Nov 2014 12:12:16
File Name: 15104115/150104/GC-054A11501501_115151041151

Frequency (MHz): 121.175
Number: 111
Number of Transients: 15
Signal: Target

Original Points Examin: 30720
Dwell: 50.000
Points Examin: 8192
Points Sequence: jnrp

Spectrum Offset (ppm): 5.002530E-06
Spectrum Type: 1D 1H-Decoupled
Sweep Width (Hz): 8042 Hz
Temperature (degree C): 25.155

Acquisition Time (sec): 1.3601
Comment: GC-054 A 155
Date: 26 Nov 2014 12:12:16

Date Start: 26 Nov 2014 12:12:16
File Name: 15104115/150104/GC-054A11501501_115151041151

Frequency (MHz): 121.175
Number: 111
Number of Transients: 15
Signal: Target

Original Points Examin: 30720
Dwell: 50.000
Points Examin: 8192
Points Sequence: jnrp

Spectrum Offset (ppm): 5.002530E-06
Spectrum Type: 1D 1H-Decoupled
Sweep Width (Hz): 8042 Hz
Temperature (degree C): 25.155
Compound s23

(1) ELSO Signal Number (RS, 1x1)

Acquisition Time (sec): 1.5800

Analysis Type: ELSO

Sample: Compound 23

Acquisition Time: 1.5800 sec

Retention Time: 2.08 sec

Mass: 194.11372

Temperature (deg C): 47.00

Chemical Shift ppm (ppm): 0.00000

NMR Spectra:

- Spectrum 1: Acquisition Time 1.5800 sec
- Spectrum 2: Acquisition Time 1.5800 sec
- Spectrum 3: Acquisition Time 1.5800 sec
Compound s31
### Compound s36

**Detected by:** NMR

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<th>Value</th>
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<td>Detector</td>
<td>TIC</td>
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<tr>
<td>Sample</td>
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<tr>
<td>Sample Weight (mg)</td>
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<td>Number of Transients (s)</td>
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<td>Spectrometer Type</td>
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<tr>
<td>Temperature (°C)</td>
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**Chemical Structure:**

![Chemical Structure](attachment:image1)

**Spectrum Details:**

![Spectrum](attachment:image2)

![Spectrum](attachment:image3)
**Compound s37**

**Method:** FID Detector: TIC Simul (60, 1x1)

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>Peak 1</th>
<th>Peak 2</th>
<th>Peak 3</th>
<th>Peak 4</th>
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</thead>
<tbody>
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<td>1.0</td>
<td>2.0</td>
<td>3.0</td>
<td>4.0</td>
</tr>
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</table>

**Retention Time (min):** 1.02

**Comments:**

- **Column:** DB-1500 (50 m x 0.25 mm x 0.25 mm)
- **Temperature Program:** 40°C (1 min), 4°C/min to 220°C (20 min)
- **Injection Volume:** 1.0 μL
- **Carrier Gas:** Helium
- **Flow Rate:** 1.0 mL/min
- **Split Ratio:** 1:10

---

**Additional Information:**

- **Sample Preparation:** Dissolve compound s37 in a suitable solvent and inject a 1.0 μL aliquot for analysis.
- **Chromatographic Conditions:** Standard conditions for the DB-1500 column, as specified in the GC method protocol.
- **Data Analysis:** Use peak areas to quantify the compound concentration.

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**Preparation Note:** Dissolve compound s37 in methanol (1 mg/mL) and inject a 1.0 μL aliquot for analysis.

**Retention Time (min):** 1.02

**Comments:**

- **Column:** DB-1500 (50 m x 0.25 mm x 0.25 mm)
- **Temperature Program:** 40°C (1 min), 4°C/min to 220°C (20 min)
- **Injection Volume:** 1.0 μL
- **Carrier Gas:** Helium
- **Flow Rate:** 1.0 mL/min
- **Split Ratio:** 1:10

---

**Additional Information:**

- **Sample Preparation:** Dissolve compound s37 in a suitable solvent and inject a 1.0 μL aliquot for analysis.
- **Chromatographic Conditions:** Standard conditions for the DB-1500 column, as specified in the GC method protocol.
- **Data Analysis:** Use peak areas to quantify the compound concentration.
Compound s39
Compound s40
Compound s46