Supporting information

**ReACT (Redox-Activated Chemical Tagging) chemistry enables direct derivatization and fluorescent detection of S-adenosyl-L-homocysteine (SAH)**

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Figure S1. $^1$H NMR comparison of probe NapOx (top), SAH (middle), and their reaction mixture (bottom). Reaction condition: NapOx (2.0 equiv), SAH (1.0 equiv), D$_2$O/CD$_3$CN (5:3), r.t., 20 min.

Figure S2. $^1$H NMR analysis of the reaction mixtures of NapOx with different biomolecules. Reaction condition: NapOx (1.0 equiv), biomolecule (2.0 equiv), CD$_3$CN/D$_2$O (3:1), 22 °C, 10 min. For the reaction of methionine, CD$_3$CN/D$_2$O (7:3) was applied since methionine showed poor solubility in CD$_3$CN/D$_2$O (3:1).
Figure S3. $^1$H NMR analysis of the reaction mixtures of NapOx with DTT and methionine under neutral and acidic condition. For DTT reaction under neutral condition: NapOx (1.0 equiv), DTT (2.0 equiv), CD$_3$CN/D$_2$O (3:1), 22 °C, 10 min. For acidic reaction condition, 1 mM deuterated HCl solution was used to replace D$_2$O. For methionine reaction, CD$_3$CN/D$_2$O (7:3) or CD$_3$CN/1 mM deuterated HCl solution (7:3) were used to replace CD$_3$CN/D$_2$O (3:1) or CD$_3$CN/1 mM deuterated HCl solution (3:1).

1. Methods and materials

All chemicals were used as received unless otherwise stated. $^1$H NMR and $^{13}$C NMR spectra were collected on Bruker AVANCE III HD400 spectrometer. Proton chemical shifts of NMR spectra were calibrated with TMS as internals reference. HR-MS spectral data were recorded on Aglient 7250 and JEOL-JMS-T100LPAccuTOF devices. Analytical thin-layer chromatography (TLC) analysis was performed on TLC silica gel plates (0.2 ± 0.03 mm) and visualized with ultraviolet light (254 nm) to monitor reaction progression. The 96-well plate (black, flat, not treated) was purchased from Corning® (USA). Fluorescence analysis was performed on Thermo Scientific™ Varioskan™ LUX microplate reader. The analytic HPLC was run on Agilent 1260-workstation equipped with a Luna C18 column, 250 x 4.6 mm, particle size 5 μm, pore size 110 Å (Phenomenex) with a flow rate of 1 mL/min. Solvent A: H$_2$O with 0.1% trifluoroacetic acid; Solvent B: MeCN with 0.1% trifluoroacetic acid.

2. Compound Synthesis

2.1 Synthesis of oxaziridines 1a-1g
The compound 1a was synthesized following reported procedure.[1] To a mixture of ethylurea (0.62 g, 5.84 mmol) in anhydrous THF (14 mL) was added benzaldehyde (0.8 mL, 8.16 mmol) and Ti(OiPr)₄ (2.20 mL, 7.48 mmol) sequentially under N₂. The white suspension was allowed to stir overnight at r.t. The reaction mixture was dried over evaporator, and the obtained crude was dissolved in DCM (5 mL). Then this mixture was added slowly to a suspension of mCPBA (4.60 g, 75% purity, 20 mmol) in saturated K₂CO₃ aqueous solution (20 mL) and DCM (20 mL), and the resulted mixture was stirred at r.t. for 6 h. After that, the mixture was diluted with 20 mL water, and extracted with DCM for three times. The combined organic was washed with brine, and dried over anhydrous Na₂SO₄. The crude mixture was filtered, and the filtrate was concentrated under vacuum. The obtained residue was purified over silica gel chromatography (PE/EA = 4:1) to yield the desired compound 1a as a white solid (150 mg, 13% yield for two steps). ¹H NMR (400 MHz, CDCl₃) δ 7.46 (m, 5H), 6.04 (br, 1H), 5.00 (s, 1H), 3.33 (m, 2H), 1.22 (t, J = 7.2 Hz, 3H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 162.1, 132.4, 131.0, 128.6, 128.0, 79.3, 35.4, 15.2; The data are consistent with those reported in previous literature.[1]

1b was synthesized with the same procedure as compound 1a. The obtained residue was purified over Al₂O₃ column chromatography (DCM) to yield the desired compound 1b as a yellow liquid (100 mg, 17% yield for two steps). ¹H NMR (400 MHz, CDCl₃) δ 7.41 (m, 5H), 6.13 (br, 1H), 5.00 (s, 1H), 2.87 (d, J = 4.8 Hz, 3H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 162.9, 132.4, 131.0, 128.6, 128.0, 79.4, 27.0; HRMS (ESI) m/z: [M + H]+ Calcd for C₉H₁₁N₂O₂ 179.0815; found 179.0815.

1c was synthesized with the same procedure as compound 1a. The obtained residue was purified over Al₂O₃ column chromatography (PE/EA = 6:1) to yield the desired compound 1c as a white solid (102 mg, 15% yield for two steps). ¹H NMR (400 MHz, CDCl₃) δ 7.45 (m, 5H), 6.08 (br, 1H), 5.00 (s, 1H), 3.25 (m, 2H), 1.59 (m, 2H), 0.96 (t, J = 7.6 Hz, 3H). Please note that the integration of the hydrogens around δ 1.59 ppm is ca. 3.7 in supplementary NMR figure, which
is higher than 2. This is due to interference of extra H$_2$O signal at ca. 1.6 ppm. $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$) δ 162.2, 132.4, 131.0, 128.6, 128.0, 79.4, 42.1, 22.7, 11.2; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{11}$H$_{15}$N$_2$O$_2$ 207.1128; found 207.1124.

Synthesis of 1-((Prop-2-yn-1-yl)urea$^{[1]}$

\[ \text{NH}_2 \text{CH} = \text{C} \rightarrow \text{NH} \]

This compound was synthesized following reported procedure$^{[1]}$. To a solution of propargylamine (1.6 mL, 25 mmol) in aqueous HCl solution (1.0 mol, 25 mL) was added KOCN (8 g, 100 mmol). After being heated at 60 °C for 40 h, the mixture was placed in the -20 °C refrigerator to obtain a white precipitate. After vacuum filtration, the obtained solid was dissolved in MeOH (75 mL) and stirred with silica gel (10 g) for 6 h. The mixture was then filtered, and the residue was washed with MeOH. The combined filtrate was concentrated under vacuum to attain the desired urea as a white solid without further purification (1.9 g, 78%). $^1$H NMR (400 MHz, d$_6$-DMSO) δ 6.29 (t, $J$ = 6.0 Hz, 1H), 5.60 (s, 2H), 3.75 (dd, $J$ = 5.6, 2.4 Hz, 2H), 3.03 (t, $J$ = 2.4 Hz, 1H). $^{13}$C{$^1$H} NMR (101 MHz, d$_6$-DMSO) δ 158.6, 83.0, 72.9, 29.1; The data are consistent with those reported in previous literature.$^{[1]}$

![1d](image)

1d was synthesized with the same procedure as compound 1a. The obtained residue was purified over Al$_2$O$_3$ column chromatography (DCM) to yield the desired compound 1d as a yellow liquid (111 mg, 17% yield for two steps). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.45 (m, 5H), 6.52 (br, 1H), 5.04 (s, 1H), 4.07 (m, 2H), 2.30 (t, $J$ = 2.4 Hz, 1H). $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$) δ 162.0, 132.0, 131.1, 128.7, 128.0, 79.5, 78.3, 72.6, 30.2; The data are consistent with those reported in previous literature.$^{[1]}$

![1e](image)

1e was synthesized with the same procedure as compound 1a. The obtained residue was purified over Al$_2$O$_3$ column chromatography (EA) to yield the desired compound 1e as a white solid (40 mg, 4% yield for two steps). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.45 (m, 5H), 6.52 (br, 1H), 5.04 (s,
1H), 3.77 (q, \( J = 5.2 \text{ Hz} \), 2H), 3.46 (m, 2H), 2.19 (t, \( J = 5.2 \text{ Hz} \), 1H). \(^{13}\text{C}\{^1\text{H}\}) \text{ NMR (101 MHz, CDCl}_3\) \( \delta 163.1, 132.2, 131.1, 128.7, 128.0, 79.5, 61.5, 42.7; \) HRMS (ESI) \text{ m/z: [M + H]}^+ \text{ Calcd for C}_{10}H_{13}N_2O_3 209.0926; \text{ found 209.0907.}

If was synthesized with the same procedure as compound 1a. The obtained residue was purified over Al\(_2\)O\(_3\) column chromatography (PE/EA = 6:1) to yield the desired compound If as a white solid (29 mg, 6% yield for two steps). \(^1\text{H} \text{ NMR (400 MHz, CDCl}_3\) \( \delta 7.44 \text{ (m, 5H)}, 5.96 \text{ (br, 1H)}, 4.98 \text{ (s, 1H)}, 3.66 \text{ (m, 1H)}, 1.96 \text{ (m, 2H)}, 1.74 \text{ (m, 2H)}, 1.63 \text{ (m, 1H)}, 1.37 \text{ (m, 2H)}, 1.21 \text{ (m, 3H)}. \(^{13}\text{C}\{^1\text{H}\}) \text{ NMR (101 MHz, CDCl}_3\) \( \delta 161.3, 132.5, 131.0, 128.6, 128.0, 79.4, 49.4, 32.9, 32.8, 25.3, 24.7; \) The data are consistent with those reported in previous literature.[2]

1g was synthesized with the same procedure as compound 1a. The obtained residue was purified over Al\(_2\)O\(_3\) column chromatography (PE/EA = 6:1) to yield the desired compound 1g as a white solid (35 mg, 4% yield for two steps). \(^1\text{H} \text{ NMR (400 MHz, CDCl}_3\) \( \delta 7.40 \text{ (m, 10H)}, 6.36 \text{ (br, 1H)}, 5.04 \text{ (s, 1H)}, 4.47 \text{ (m, 2H)}. \(^{13}\text{C}\{^1\text{H}\}) \text{ NMR (101 MHz, CDCl}_3\) \( \delta 162.2, 137.0, 132.3, 131.1, 128.9, 128.7, 128.0, 127.8, 79.5, 44.4; \) The data are consistent with those reported in previous literature.[2]

2.2 Synthesis of compound NapOx

![NapOx](image)

The compound \textbf{NapOx} was synthesized with the same procedure as compound 1a on page S3. The obtained crude was purified over Al\(_2\)O\(_3\) chromatography with DCM as eluent to yield crude as a light yellow solid, which was further recrystallized from PE/DCM to provide the desired product \textbf{NapOx} as a white solid (140 mg, 24% yield for two steps). \(^1\text{H} \text{ NMR (400 MHz, CDCl}_3\)
δ 7.93 (s, 1H), 7.76 (d, \( J = 8.8 \) Hz, 2H), 7.43 (dd, \( J = 8.8, 1.6 \) Hz, 1H), 7.16 (m, 2H), 6.09 (br, 1H), 5.13 (s, 1H), 3.93 (s, 3H), 3.35 (m, 2H), 1.23 (t, \( J = 7.2 \) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) δ 162.2, 158.8, 136.1, 129.8, 129.0, 128.1, 127.5, 127.4, 124.1, 119.5, 105.8, 79.9, 55.4, 35.4, 14.8; HRMS (ESI) m/z: [M + H]^+ Caled for C\(_{15}\)H\(_{17}\)N\(_2\)O\(_3\) 273.1234; found 273.1230.

2.3 Synthesis of compounds 2a-2g

![Diagram of synthesis of compounds 2a-2g]

**General synthetic procedure for compounds 2a-2g:** A solution of oxaziridine 1a-1g (0.26 mmol, 2.0 equiv), SAH (0.13 mmol, 1.0 equiv) in ca. 20% MeCN aqueous solution was stirred at room temperature for approximately 1 h. The reaction mixture was washed with CH\(_2\)Cl\(_2\) for three times. Then the aqueous layer was concentrated under vacuum, and the obtained crude was purified by column chromatography over reverse silica gel to afford the target compound.

**Compound 2a** was synthesized using the procedure described above. The obtained residue was purified over reverse phase silica gel column chromatography (10% MeOH in H\(_2\)O) to yield the desired compound 2a (50 mg, 83% yield) as a white solid. \(^1\)H NMR (400 MHz, D\(_2\)O) δ [8.12] 7.98 (s, 1H), [8.06] 7.96 (s, 1H), [5.89] 5.86 (d, \( J = 5.2 \) Hz, 1H), 4.73 (q, \( J = 5.2 \) Hz, 1H), 4.38 (m, 2H), 3.70 (q, \( J = 6.8 \) Hz, 1H), 3.47 (m, 2H), 3.12 (m, 2H), [2.96] 2.82 (q, \( J = 7.2 \) Hz, 2H), 2.09 (m, 2H), [0.91] 0.78 (t, \( J = 6.8 \) Hz, 3H). \(^{13}\)C NMR (101 MHz, D\(_2\)O) δ [173.1] 173.0, [155.2] 155.2, [152.6] 152.6, [148.6] 148.4, [140.2] 140.1, [118.6] 118.6, [88.3] 88.1, 79.0, 77.8, [72.9] 72.7, [72.8] 72.5, [53.3] 52.9, 49.5, [43.4] 43.0, [24.6] 24.5, [14.4] 14.3; HRMS (ESI) m/z: [M + H]^+ Caled for C\(_{17}\)H\(_{27}\)N\(_8\)O\(_6\)S 471.1769; found 471.1780.
Compound 2b was synthesized using the procedure described above. The obtained residue was purified over reverse phase silica gel column chromatography (10% MeOH in H$_2$O) to yield the desired compound 2b (30 mg, 51% yield) as a white solid. $^1$H NMR (400 MHz, D$_2$O) $\delta$ [8.14] 8.03 (s, 1H), [8.09] 8.02 (s, 1H), [5.92] 5.90 (d, $J = 5.2$ Hz, 1H), 4.77 (m, 1H), 4.37 (m, 2H), 3.69 (q, $J = 6.4$ Hz, 1H), 3.47 (m, 2H), 3.08 (m, 2H), [2.54] 2.39 (s, 3H), 2.09 (m, 2H). $^{13}$C NMR (101 MHz, D$_2$O) $\delta$ 173.3, 168.4, [155.3] 155.3, [152.7] 152.7, [148.7] 148.5, [140.3] 140.1, [118.8] 118.7, [88.4] 88.1, 78.9, 77.8, [72.8] 72.6, [72.8], 72.5, [53.3] 52.9, 49.6, [43.5] 43.1, [24.7] 24.6; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{16}$H$_{25}$N$_8$O$_6$S 457.1612; found 457.1622.

Compound 2c was synthesized using the procedure described above. The obtained residue was purified over reverse phase silica gel column chromatography (30% MeOH in H$_2$O) to yield the desired compound 2c (28 mg, 45% yield) as a white solid. $^1$H NMR (400 MHz, D$_2$O) $\delta$ [8.19] 8.09 (s, 1H), [8.13] 8.08 (s, 1H), [5.94] 5.92 (d, $J = 5.2$ Hz, 1H), 4.78 (m, 1H), 4.38 (m, 2H), 3.65 (t, $J = 6.4$ Hz, 1H), 3.48 (m, 2H), 3.06 (m, 2H), [2.89] 2.74 (t, $J = 7.2$ Hz, 2H), 2.08 (m, 2H), [1.29] 1.11 (q, $J = 7.2$ Hz, 2H), [0.71] 0.58 (t, $J = 7.2$ Hz, 3H). $^{13}$C NMR (101 MHz, D$_2$O) $\delta$ 173.9, 167.8, 155.5, [152.8] 152.8, [148.8] 148.7, [140.4] 140.2, [118.9] 118.8, [88.3] 88.0, 79.3, 77.9, [72.9] 72.7, [72.8] 72.5, [53.4] 53.1, 49.5, [43.4] 43.1, [25.0] 24.9, [22.7] 22.6, [10.5] 10.3; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{18}$H$_{29}$N$_8$O$_6$S 485.1925; found 485.1936.
Compound 2d was synthesized using the procedure described above. The obtained residue was purified over reverse phase silica gel column chromatography (10% MeOH in H$_2$O) to yield the desired compound 2d (33 mg, 53% yield) as a white solid. $^1$H NMR (400 MHz, D$_2$O) $\delta$ [8.17] 8.07 (s, 1H), [8.12] 8.06 (s, 1H), [5.94] 5.91 (d, $J = 5.2$ Hz, 1H), 4.77 (q, $J = 5.2$ Hz, 1H), 4.40 (m, 2H), 3.72 (m, 2H), 3.61 (s, 1H), 3.50 (m, 2H), 3.13 (m, 2H), [2.45] 2.32 (t, $J = 2.4$ Hz, 1H), 2.12 (m, 2H). $^{13}$C NMR (101 MHz, D$_2$O) $\delta$ 173.2, 167.1, [155.4] 155.4, [152.8] 152.7, [148.7] 148.6, [140.4] 140.2, [118.9] 118.8, [88.4] 88.1, [81.4] 81.3, 79.0, 77.8, [72.8] 72.8, [72.8] 72.5, [71.1] 70.9, [53.2] 52.9, 49.4, [43.3] 43.0, [24.7] 24.6; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{18}$H$_{25}$N$_8$O$_6$S 481.1612; found 481.1643.

Compound 2e was synthesized using the procedure described above. The obtained residue was purified over reverse phase silica gel column chromatography (5% MeOH in H$_2$O) to yield the desired compound 2e (36 mg, 57% yield) as a white solid. $^1$H NMR (400 MHz, D$_2$O) $\delta$ [8.14] 8.02 (s, 1H), [8.09] 8.01 (s, 1H), [5.92] 5.90 (d, $J = 4.8$ Hz, 1H), 4.76 (t, $J = 5.2$ Hz, 1H), 4.38 (m, 2H), 3.71 (q, $J = 6.8$ Hz, 1H), 3.48 (m, 4H), 3.13 (m, 2H), 3.02 (m, 2H), 2.11 (m, 2H). $^{13}$C NMR (101 MHz, D$_2$O) $\delta$ 173.1, 167.5, [155.3] 155.2, [152.7] 152.6, [148.6] 148.4, [140.3] 140.1, [118.7] 118.6, [88.4] 88.1, 78.8, 77.8, [72.8] 72.6, 72.7, 60.8, 58.0, [53.2] 52.9, [49.6] 49.3, [43.4] 43.0, [24.6] 24.5; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{17}$H$_{27}$N$_8$O$_7$S 487.1718; found 487.1739.
Compound 2f was synthesized using the procedure described above. The obtained residue was purified over reverse phase silica gel column chromatography (40% MeOH in H₂O) to yield the desired compound 2f (42 mg, 69% yield) as a light yellow solid. 

$^1$H NMR (400 MHz, D₂O) δ [8.15] 8.00 (s, 1H), [8.07] 7.97 (s, 1H), [5.89] 5.86 (d, $J = 4.8$ Hz, 1H), 4.72 (br, 1H), 4.36 (m, 2H), 3.72 (t, $J = 6.4$ Hz, 1H), 3.48 (m, 2H), 3.15 (m, 2H), 3.01 (m, 1H), 2.12 (m, 2H), [1.45] 0.97 (m, 10H).

$^{13}$C NMR (101 MHz, D₂O) δ [173.0] 173.0, [166.9] 166.6, [155.3] 155.2, [152.7] 152.6, [152.7] 152.6, [148.6] 148.4, [140.2] 140.1, [118.6] 118.5, [88.2] 87.9, 79.5, 77.8, [72.9] 72.9, [53.3] 52.9, [50.0] 49.9, 49.3, [43.2] 43.0, [32.8] 32.8, [32.8] 32.6, [25.0] 24.9, [24.6] 24.5, 24.4; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{21}$H$_{33}$N$_8$O$_6$S 525.2238; found 525.2248.

Compound 2g was synthesized using the procedure described above. The obtained residue was purified over reverse phase silica gel column chromatography (30% MeOH in H₂O) to yield the desired compound 2g (30 mg, 44% yield) as a light yellow solid. 

$^1$H NMR (400 MHz, D₂O) δ [8.01] 7.96 (s, 1H), [8.09] 7.95 (s, 1H), [7.08] 6.89 (m, 5H), 5.80 (t, $J = 4.4$ Hz, 1H), 4.64 (t, $J = 5.2$ Hz, 1H), [4.48] 4.22 (t, $J = 5.2$ Hz, 1H), [4.42] 4.29 (m, 1H), 4.04 (m, 2H), 3.71 (q, $J = 6.4$ Hz, 1H), 3.46 (m, 2H), 3.10 (m, 2H), 2.12 (m, 2H).

3. Fluorescence measurement

3.1 SAH concentration measurement

A solution of NapOx in IPA (20 µL, 100 µM) and SAH in ddH₂O (20 µL, 0 - 2 mM, 2-fold dilution) was added to a mixture of IPA/ddH₂O (7:1, 160 µL) in 96-well plate, with a final concentration of 10 µM for NapOx and 0-200 µM for SAH. The mixture was incubated at 37 °C for 30 min. Then it was directly used for fluorescence measurement.

3.2 Fluorescence profiling of NapOx reaction with thiol or thioether compound

A solution of NapOx in IPA (20 µL, 2 mM) and thiol or thioether compound in 1X PBS (20 µL, 8 mM) was added to a mixture of IPA/1XPBS (7:1, 160 µL) in 96-well plate, with a final concentration of 200 µM for NapOx and 800 µM for thiol or thioether compound. The mixture was allowed to incubate at room temperature for 3 h. Then it was directly analyzed by fluorescence measurement.

3.3 NapOx selectivity under neutral or acidic condition

For the reaction performed under neutral condition, a solution of NapOx in IPA (20 µL, 100 µM) and analyte in ddH₂O (20 µL, 2 mM) was incubated in a mixture of IPA/ddH₂O (7:1, 160 µL) in 96-well plate at 37 °C for 30 min, then it was directly used for fluorescence measurement. For the reaction under acidic condition, the procedure was the same except that 1 mM HCl aqueous solution was used to replace ddH₂O.

4. HPLC experiment

Compound 1a (2.0 equiv) was mixed with SAH (1.0 equiv) in a mixture of H₂O/CH₃OH (1:1), and the mixture was allowed to incubate at room temperature for 10 min. Then, 100 µL of reaction mixture was taken, and analyzed by HPLC.
5. NMR spectra of compounds

$^1$H NMR: CDCl$_3$, 400 MHz

$^{13}$C$^1$H NMR: CDCl$_3$, 101 MHz
$^1$H NMR: CDCl$_3$, 400 MHz

$^{13}$C($^1$H) NMR: CDCl$_3$, 101 MHz
$\text{H NMR: CDCl}_3$, 400 MHz

$\text{C}^{[1]}\text{H} \text{NMR: CDCl}_3$, 101 MHz
$^1$H NMR: $d_6$-DMSO, 400 MHz

$^{13}$C($^1$H) NMR: $d_6$-DMSO, 101 MHz
$^1$H NMR: CDCl$_3$, 400 MHz

$^{13}$C($^1$H) NMR: CDCl$_3$, 101 MHz
$\text{H NMR: CDCl}_3, 400 \text{ MHz}$

$\text{C}\{^1\text{H}\} \text{ NMR: CDCl}_3, 101 \text{ MHz}$
$^1$H NMR: CDCl$_3$, 400 MHz

$^{13}$C($^1$H) NMR: CDCl$_3$, 101 MHz
$\text{H NMR: CDCl}_3, 400 \text{ MHz}$

$\text{C}^1\text{H} \text{ NMR: CDCl}_3, 101 \text{ MHz}$
$^1\text{H NMR}: \text{CDCl}_3, 400 \text{ MHz}$

$^{13}\text{C}[\text{H}] \text{NMR}: \text{CDCl}_3, 101 \text{ MHz}$
$^1$H NMR: D$_2$O, 400 MHz

$^{13}$C($^1$H) NMR: D$_2$O, 101 MHz

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$^1$H NMR: D$_2$O, 400 MHz

$^{13}$C($^1$H) NMR: D$_2$O, 101 MHz
$^{1}H$ NMR: D$_2$O, 400 MHz

$^{13}C(1)H$ NMR: D$_2$O, 101 MHz
$^1$H NMR: D$_2$O, 400 MHz

$^{13}$C($^1$H) NMR: D$_2$O, 101 MHz
$^{1}H$ NMR: $D_2O$, 400 MHz

$^{13}C(1H)$ NMR: $D_2O$, 101 MHz
$^1$H NMR: D$_2$O, 400 MHz

$^{13}$C($^1$H) NMR: D$_2$O, 101 MHz
$^1$H NMR: D$_2$O, 400 MHz

$^{13}$C($^1$H) NMR: D$_2$O, 101 MHz
6. HRMS spectra of compounds
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