Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Facile Synthesis of Photoactivatable Adenosine Analogs

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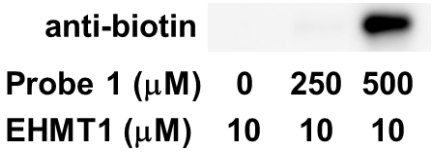
Figure S1. Photoaffinity labeling and affinity enrichment of recombinant EHMT1 using probe 1.



Synthesis of Chemical Probes

Synthesis of probe 1 (plan 1)

Synthesis of 1. To a solution of 8-bromoinosine (1 g, 2.88 mmol) in anhydrous CH_2Cl_2 (10 mL) was added DMAP (35.2 mg, 0.288 mmol). The mixture was cooled down to 0°C. To this solution was added acetic anhydride (2.72 mL, 28.8 mmol) dropwise. The reaction mixture was then allowed to warm to room temperature and stirred overnight. Reaction was quenched with ice water, aqueous layer was extracted with CH_2Cl_2, combined organic layer was washed with brine and dried over Na_2SO_4. Solvent was evaporated under reduced pressure, and the crude product was purified by silica gel column chromatography (CH_2Cl_2 with 5% methanol) to afford intermediate **1** (934 mg, 1.98 mmol, 68.7% yield) as a pale yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 2.05 (s, 3H), 2.09 (s, 3H), 2.14 (s, 3H), 4.30 (dd, *J* = 6.0, 11.6 Hz, 1H), 4.37 (d, *J* = 3.1 Hz, 1H), 4.47 (d, *J* = 11.2 Hz, 1H), 5.76 (t, *J* = 5.7 Hz, 1H), 6.08 (d, *J* = 4.4 Hz, 1H), 6.20 (d, *J* = 5.5 Hz, 1H), 8.07 (s, 1H), 12.41 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 20.37, 20.50, 20.70, 63.00, 70.33, 72.09, 80.18, 88.77, 125.82, 126.57, 145.09, 149.77, 157.44, 169.32, 169.47, 170.46. HRMS (*m/z*): calculated for $C_{16}H_{17}BrN_4O_8Na$ (M+Na): 495.0122; found: 495.0099.

Synthesis of 2. To a solution of **1** (734 mg, 1.55 mmol) in 6 mL of anhydrous DMF was added NaN_3 (403 mg, 6.20 mmol). The reaction was heated at 80°C until completion. The reaction was cooled to room temperature. Solvent was evaporated under reduced pressure. The residue was dissolved in water and extracted with CH_2Cl_2. The combined organic layer was washed with sat. $NaHCO_3$, water and brine and dried over Na_2SO_4. Solvent was evaporated under reduced pressure, and the crude product was purified by silica gel column chromatography (CH_2Cl_2 with 5% methanol) to afford intermediate **2** (406 mg, 0.93 mmol, 60.2% yield) as a yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 2.04 (s, 3H), 2.07 (s, 3H), 2.11 (s, 3H), 4.30 (m, 2H), 4.43 (dd,

J = 3.2, 11.5 Hz, 1H), 5.67 (t, *J* = 5.8 Hz, 1H), 5.93 (d, *J* = 4.8 Hz, 1H), 6.04 (t, *J* = 5.6 Hz, 1H), 8.09 (s, 1H), 13.35 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 20.37, 20.46, 20.64, 63.01, 70.32, 71.96, 79.88, 85.75, 123.20, 144.08, 145.07, 148.77, 157.64, 169.34, 169.47, 170.40. HRMS (*m/z*): calculated for $C_{16}H_{17}N_7O_8Na$ (M+Na): 458.1036; found: 458.1020.

Synthesis of 3. To a solution of **2** (406 mg, 0.93 mmol) and PyBOP (729 mg, 1.40 mmol) in 10 mL anhydrous acetonitrile was added DIPEA (325 μL, 1.87 mmol). To the reaction mixture was then added mono-*N*-Boc-1,6-diaminohexane (418 μL, 1.87 mmol) dropwise. The reaction was stirred at room temperature overnight. The reaction was quenched with water and the mixture was extracted with ethyl acetate. The combined organic layer was washed with brine and dried over Na_2SO_4. Solvent was evaporated under reduced pressure, and the crude product was purified by silica gel column chromatography (CH_2Cl_2 with 5% methanol) to afford intermediate **3** (324 mg, 0.51 mmol, 55% yield) as a yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 1.36 (m, 2H), 1.42 (s, 9H), 1.46 (stack, 6H), 2.04 (s, 3H), 2.06 (s, 3H), 2.11 (s, 3H), 3.08 (m, 2H), 3.62 (m, 2H), 4.30 (m, 2H), 4.47 (m, 2H), 5.79 (t, *J* = 5.4 Hz, 1H), 5.96 (d, *J* = 4.6 Hz, 1H), 6.13 (t, *J* = 5.6 Hz, 1H), 8.25 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 20.42, 20.48, 20.64, 26.43, 26.47, 28.41, 29.78, 30.01, 30.86, 53.38, 63.04, 70.46, 71.99, 79.82, 85.42, 144.19, 155.98, 169.38, 169.48, 170.49. HRMS (*m/z*): calculated for $C_{27}H_{39}N_9O_9Na$ (M+Na): 656.2763; found: 656.2735.

Synthesis of 4. Intermediate **3** (230 mg, 0.36 mmol) was dissolved in a mixture of CH_2Cl_2/TFA (4 mL, v/v = 9/1). The reaction mixture was stirred at room temperature for 4 h before the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography (CH_2Cl_2 with 10% methanol) to afford intermediate **4** (153 mg, 0.29 mmol, 79.5% yield) as a yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 1.36 (stack, 4H), 1.62

(stack, 4H), 2.01 (s, 3H), 2.04 (s, 3H), 2.09 (s, 3H), 2.89 (t, *J* = 7.4 Hz, 2H), 3.57 (m, 1H), 4.28 (m, 2H), 4.43 (m 1H), 5.78 (t, *J* = 5.6 Hz, 1H), 5.93 (d, *J* = 4.6 Hz, 1H), 6.13 (t, *J* = 5.5 Hz, 1H), 8.20 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 20.36, 20.45, 20.59, 25.83, 26.03, 27.24, 29.38, 30.83, 39.78, 63.03, 70.44, 71.95, 79.76, 85.38, 114.93, 117.73, 117.83, 144.11, 153.15, 169.47, 169.54, 170.57. HRMS (*m/z*): calculated for $C_{22}H_{31}N_9O_7Na$ (M+Na): 533.2346; found: 533.2341.

Synthesis of 5. To a solution of biotin (71 mg, 0.29 mmol), EDCI (55 mg, 0.29 mmol) and DMAP (53 mg, 0.43 mmol) in 2 mL anhydrous DMF was added a solution of intermediate **4** (154 mg, 0.29 mmol) in 4 mL anhydrous CH_2Cl_2. The reaction mixture was stirred at room temperature overnight. The reaction was quenched with water, the aqueous layer was extracted with CH_2Cl_2. The combined organic layer was washed with brine and dried over Na_2SO_4. Solvent was evaporated under reduced pressure, and the crude product was purified by silica gel column chromatography (CH_2Cl_2 with 10% methanol) to afford intermediate **5** (136 mg, 0.18 mmol, 62% yield) as a yellow oil. ^{1}H NMR (CD_3OD, 400 MHz) δ (ppm): 1.41 (stack, 6H), 1.51 (m, 2H), 1.66 (stack, 6H), 2.00 (s, 3H), 2.06 (s, 3H), 2.12 (s, 3H), 2.17 (t, *J* = 7.2 Hz, 2H), 2.66 (d, *J* = 12.7 Hz, 1H), 2.87 (dd, *J* = 5.0, 12.7 Hz, 1H), 3.16 (m, 3H), 3.54 (s, broad, 2H), 4.30 (stack, 3H), 4.45 (m, 2H), 5.77 (t, *J* = 5.8 Hz, 1H), 5.97 (d, *J* = 4.7 Hz, 1H), 6.14 (t, *J* = 5. 8Hz, 1H), 8.16 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 20.38, 20.44, 20.61, 25.57, 26.42, 26.52, 27.99, 28.08, 29.41, 29.57, 35.87, 39.35, 40.55, 55.64, 60.10, 61.81, 63.01, 70.42, 71.95, 79.75, 85.39, 117.73, 143.94, 152.39, 153.28, 164.02, 169.39, 169.47, 170.47, 173.07. HRMS (*m/z*): calculated for $C_{32}H_{45}N_{11}O_9SNa$ (M+Na): 782.3014; found: 782.3022.

Synthesis of probe 1. Intermediate **5** (25 mg, 0.033 mmol) was dissolved in 0.2 mL methanol. The solution was cooled down to 0°C. To the reaction mixture was added 1 mL 7N ammonia in

methanol. The reaction was stirred at 0°C overnight. Solvent was removed under reduced pressure, and the crude product was purified by silica gel column chromatography (CH_2Cl_2 with 20% methanol) to afford **probe 1** (21 mg, 0.033 mmol, quantitatively) as a yellow oil. ^{1}H NMR (CD_3OD, 400 MHz) δ (ppm): 1.41 (stack, 6H), 1.51 (m, 2H), 1.66 (stack, 6H), 2.17 (t, *J* = 7.3 Hz, 2H), 2.67 (d, *J* = 12.8 Hz, 1H), 2.88 (dd, *J* = 5.0, 12.7 Hz, 1H), 3.15 (m, 2H), 3.70 (dd, *J* = 3.0, 12.6 Hz, 1H), 3.84 (dd, *J* = 2.4, 12.6 Hz, 1H), 4.12 (m, 1H), 4.26 (dd, *J* = 4.5, 7.9 Hz, 1H), 4.30 (dd, *J* = 1.6, 5.2 Hz, 1H), 4.45 (dd, *J* = 4.9, 7.8 Hz, 1H), 5.77 (d, *J* = 7.2 Hz, 1H), 8.10 (s, 1H). ^{13}C NMR (CD_3OD, 100 MHz) δ (ppm): 27.07, 27.75, 27.86, 29.65, 29.91, 30.50, 36.96, 40.43, 41.16, 57.15, 61.75, 63.52, 64.17, 73.11, 74.24, 88.81, 90.13, 146.62, 152.57, 176.10. HRMS (*m/z*): calculated for $C_{26}H_{39}N_{11}O_6SNa$ (M+Na): 656.2697; found: 656.2706.

Synthesis of probe 2. Intermediate **5** (61 mg, 0.081 mmol) was dissolved in 1 mL 7N ammonia in methanol at -40°C. The reaction was stirred at -40°C for 2 h. Upon completion, the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography (CH_2Cl_2 with 10% methanol) to afford **probe 2** (39 mg, 0.058 mmol, 72%) as a yellow oil. ^{1}H NMR (CD_3OD, 400 MHz) δ (ppm): 1.41 (stack, 6H), 1.50 (m, 2H), 1.66 (stack, 6H), 1.98 (s, 3H), 2.17 (t, *J* = 7.3 Hz, 2H), 2.66 (d, *J* = 12.7 Hz, 1H), 2.87 (dd, *J* = 5.0, 12.8 Hz,1 H), 3.16 (m, 3H), 3.55 (s, broad, 2H), 4.11 (m, 1H), 4.26 (m, 2H), 4.44 (m, 2H), 4.52 (m, 1H), 5.05 (t, *J* = 5.3 Hz, 1H), 5.81 (d, *J* = 4.9 Hz, 1H), 8.13 (s, 1H). ^{13}C NMR (CD_3OD, 100 MHz) δ (ppm): 27.07, 27.77, 27.88, 29.66, 29.91, 30.51, 36.97, 40.45, 41.16, 57.15, 61.76, 63.53, 65.28, 72.17, 73.11, 83.56, 89.60, 153.17, 172.66, 176.11. HRMS (*m/z*): calculated for $C_{28}H_{41}N_{11}O_7SNa$ (M+Na): 698.2803; found: 698.2789.

Synthesis of probe 1 (plan 2)

Synthesis of 6. 8-Bromoinosine (500 mg, 1.45 mmol) was dissolved in a mixture of acetone

and 2,2-dimethoxypropane (25 mL, v/v = 4/1). To this solution was added *p*-TsOH (275 mg, 1.45 mmol). The reaction was stirred at room temperature overnight. The reaction was quenched with $NaHCO_3$ (121 mg, 1.45 mmol) and sat. $NaHCO_3$ solution (6 mL). The mixture wa stirred at room temperature for 1 h. The aqueous layer was extracted with ethyl acetate. The combined organic layer was washed with brine and dried over Na_2SO_4. Solvent was evaporated under reduced pressure, and the crude product was purified by silica gel column chromatography (CH_2Cl_2 with 10% methanol) to afford intermediate **6** (315 mg, 0.82 mmol, 56.3% yield) as a pale yellow oil. ^{1}H NMR ($CDCl_3$, 600 MHz) δ (ppm): 1.36 (s, 3H), 1.63 (s, 3H), 3.76 (d, *J* = 12.4 Hz, 1H), 3.91 (d, *J* = 12.4 Hz, 1H), 4.45 (s, 1H), 5.04 (d, *J* = 5.8 Hz, 1H), 5.22 (t, *J* = 5.4 Hz,1 H), 6.08 (t, *J* = 4.6 Hz, 1H), 8.35 (s, 1H), 12.96 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 25.40, 27.56, 62.99, 81.24, 82.84, 85.82, 93.26, 114.39, 126.01, 126.42, 146.07, 148.91, 157.27. HRMS (*m/z*): calculated for $C_{13}H_{16}BrN_4O_5$ (M+H): 387.0299; found: 387.0301.

Synthesis of 7. To a solution of intermediate **6** (201 mg, 0.52 mmol) in 5 mL anhydrous CH_2Cl_2 was added TEA (109 μL, 0.78 mmol) and DMAP (13 mg, 0.10 mmol). The reaction mixture was cooled down to 0°C. To the reaction mixture was added acetic anhydride (54 μL, 0.57 mmol) dropwise. The reaction was allowed to warm to room temperature and stirred overnight. The reaction was quenched with ice water. The aqueous layer was extracted with CH_2Cl_2. The combined organic layer was washed with brine and dried over Na_2SO_4. Solvent was evaporated under reduced pressure, and the crude product was purified by silica gel column chromatography (CH_2Cl_2 with 5% methanol) to afford intermediate **7** (181 mg, 0.42 mmol, 81.5% yield) as a yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 1.38 (s, 3H), 1.60 (s, 3H), 2.02 (s, 3H), 4.17 (dd, *J* = 7.2, 11.6 Hz, 1H), 4.31 (dd, *J* = 4.9, 11.6 Hz, 1H), 4.37 (m, 1H), 5.10 (dd, *J* = 4.3, 5.9 Hz, 1H), 5.52 (d, *J* = 6.4 Hz, 1H), 6.20 (s, 1H), 8.33 (s, 1H), 13.08 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 20.72, 25.38, 27.17, 63.77, 81.65, 83.65, 85.27, 91.14, 114.85, 125.54,

126.53, 145.86, 149.51, 170.48. HRMS (*m/z*): calculated for $C_{15}H_{17}BrN_4O_6Na$ (M+Na): 451.0224; found: 451.0221.

Synthesis of 8. To a solution of intermediate **7** (181 mg, 0.42 mmol) in 6 mL anhydrouse DMF was added NaN_3 (110 mg, 1.69 mmol). The reaction was heated at 80°C until completion. The reaction was cooled to room temperature. Solvent was evaporated under reduced pressure. The residue was dissolved in water and extracted with CH_2Cl_2. The combined organic layer was washed with sat. $NaHCO_3$, water and brine and dried over Na_2SO_4. Solvent was evaporated under reduced pressure, and the crude product was purified by silica gel column chromatography (CH_2Cl_2 with 5% methanol) to afford intermediate **8** (90 mg, 0.23 mmol, 54.6% yield) as a yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 1.33 (s, 3H), 1.55 (s, 3H), 1.99 (s, 3H), 4.13 (m, 1H), 4.30 (m, 2H), 4.98 (m, 1H), 5.37 (d, *J* = 6.4 Hz, 1H), 5.99 (s, 1H), 8.24 (s,1 H), 13.34 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 25.26, 27.04, 31.32, 63.78, 81.47, 83.38, 84.84, 88.36, 114.69, 122.88, 144.77, 144.84, 148.40, 157.85, 170.38. HRMS (*m/z*): calculated for $C_{15}H_{17}N_7O_6Na$ (M+Na): 414.1133; found: 414.1131.

Synthesis of 9. To a solution of **8** (129 mg, 0.33 mmol) and PyBOP (258 mg, 0.50 mmol) in 2 mL anhydrous acetonitrile was added DIPEA (115 μL, 0.66 mmol). To the reaction mixture was then added mono-*N*-Boc-1,6-diaminohexane (148 μL, 0.66 mmol) dropwise. The reaction was stirred at room temperature overnight. The reaction was quenched with water and the mixture was extracted with ethyl acetate. The combined organic layer was washed with brine and dried over Na_2SO_4. Solvent was evaporated under reduced pressure, and the crude product was purified by silica gel column chromatography (CH_2Cl_2 with 7% methanol) to afford intermediate **9** (169 mg, 0.29 mmol, 86.7% yield) as a yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 1.33 (m, 2H), 1.35 (s, 3H), 1.40 (s, 9H), 1.43 (m, 4H), 1.56 (s, 3H), 1.66 (m, 2H), 1.99 (s, 3H), 3.07 (m,

2H), 3.58 (m, 2H), 4.14 (m,1 H), 4.31 (m, 2H), 5.09 (dd, *J* = 3.4, 6.3 Hz, 1H), 5.51 (dd, *J* = 1.7, 6.4 Hz, 1H), 5.97 (d, *J* = 1.7 Hz,1 H), 8.22 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 20.69, 25.41, 26.39, 26.44, 27.13, 28.38, 29.70, 29.96, 40.39, 63.99, 78.98, 81.84, 83.30, 85.09, 88.31, 114.38, 117.86, 144.19, 152.15, 153.18, 155.95, 170.52. HRMS (*m/z*): calculated for $C_{26}H_{39}N_9O_7Na$ (M+Na): 612.2865; found: 612.2878.

Synthesis of 10. Intermediate **9** (143 mg, 0.24 mmol) was dissolved in a mixture of CH_2Cl_2/TFA (5 mL, v/v = 4/1). The reaction mixture was stirred at room temperature for 4 h before the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography (CH_2Cl_2 with 10% methanol) to afford intermediate **10** (117 mg, 0.24 mmol, 99.7% yield) as a yellow oil. ^{1}H NMR (CD_3OD, 400 MHz) δ (ppm): 1.36 (s, 3H), 1.46 (m, 4H), 1.55 (s, 3H), 1.68 (m, 4H), 1.97 (s, 3H), 2.91 (t, *J* = 7.5 Hz, 2H), 3.39 (s, 1H), 3.56 (s, broad, 2H), 4.21 (m, 2H), 4.31 (m, 1H), 5.11 (m, 1H), 5.56 (d, *J* = 6.3 Hz, 1H), 5.98 (s, 1H), 8.15 (s, 1H). ^{13}C NMR (CD_3OD, 100 MHz) δ (ppm): 20.70, 25.66, 27.28, 27.50, 27.56, 28.62, 30.50, 40.78, 65.15, 83.28, 84.69, 86.48, 89.89, 115.60, 146.01, 153.03, 154.57, 172.44. HRMS (*m/z*): calculated for $C_{21}H_{32}N_9O_5$ (M+H): 490.2521; found: 490.2504.

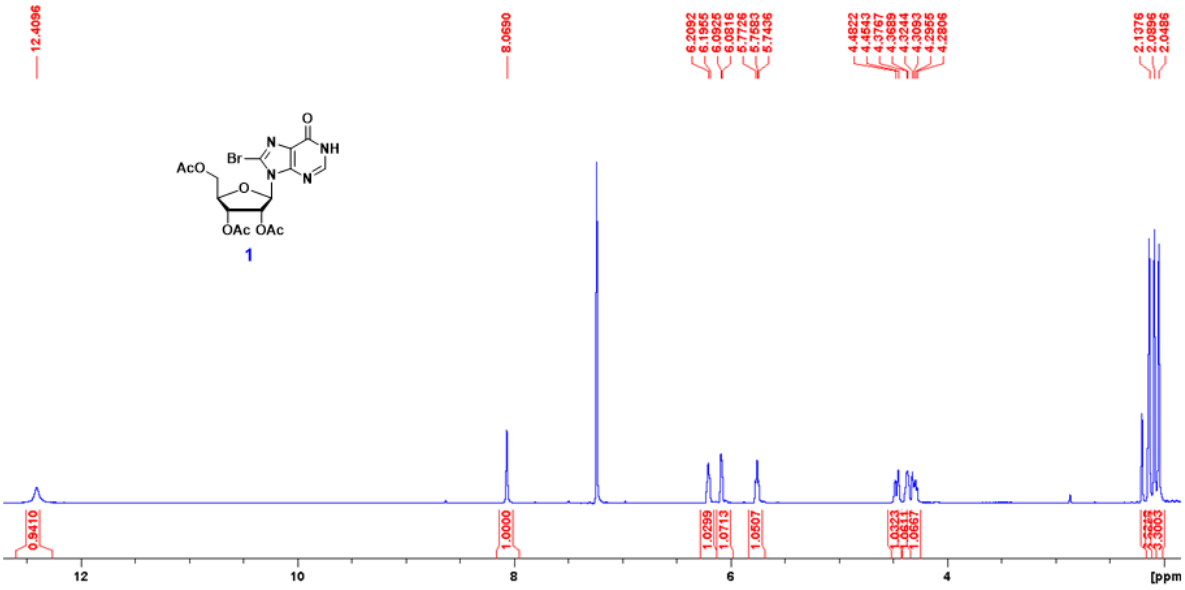
Synthesis of 11. To a solution of biotin (59 mg, 0.24 mmol), EDCI (47 mg, 0.24 mmol) and DMAP (53 mg, 0.43 mmol) in 2 mL anhydrous DMF was added a solution of intermediate **10** (119 mg, 0.24 mmol) in 4 mL anhydrous CH_2Cl_2. The reaction mixture was stirred at room temperature overnight. The reaction was quenched with water, the aqueous layer was extracted with CH_2Cl_2. The combined organic layer was washed with brine and dried over Na_2SO_4. Solvent was evaporated under reduced pressure, and the crude product was purified by silica gel column chromatography (CH_2Cl_2 with 10% methanol) to afford intermediate **11** (129 mg, 0.18 mmol, 75.5% yield) as a yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 1.36 (s, 3H0, 1.41

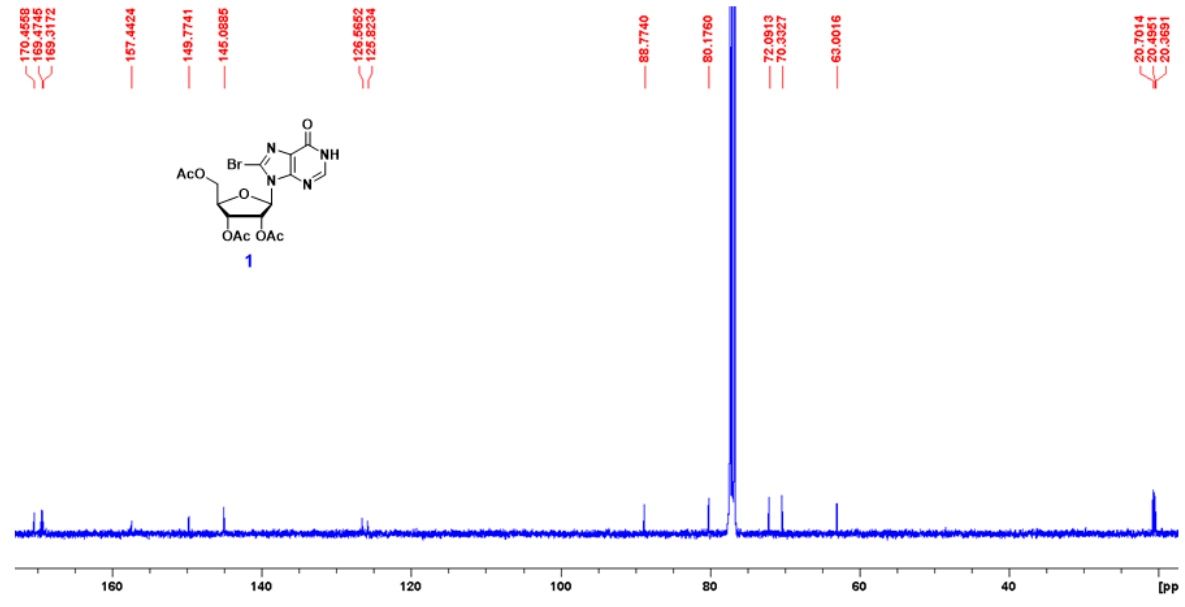
(m, 6H), 1.48 (m, 2H), 1.56 (s, 3H), 1.65 (m, 6H), 1.99 (s, 3H), 2.16 (t, *J* = 7.2 Hz, 2H), 2.68 (d, 12.7 Hz, 1H), 3.11 (m, 1H0, 3.19 (m, 2H), 3.58 (s, broad, 2H), 4.14 (m, 1H), 4.30 (m, 3H), 4.47 (m, 1H), 5.09 (m, 1H), 5.50 (d, *J* = 6.3 Hz, 1H), 5.77 (s, 1H), 5.98 (s, 1H), 6.19 (m, 1H), 6.43 (s, 1H), 8.21 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 20.72, 22.64, 25.42, 25.58, 26.40, 26.51, 27.14, 27.97, 28.04, 29.39, 29.64, 35.85, 37.04, 39.34, 40.61, 55.65, 60.08, 61.83, 63.98, 81.82, 83.29, 85.10, 88.35, 114.44, 117.75, 144.25, 152.99, 164.01, 170.55, 173.10. HRMS (*m/z*): calculated for $C_{31}H_{45}N_{11}O_7SNa$ (M+Na): 738.3116; found: 738.3080.

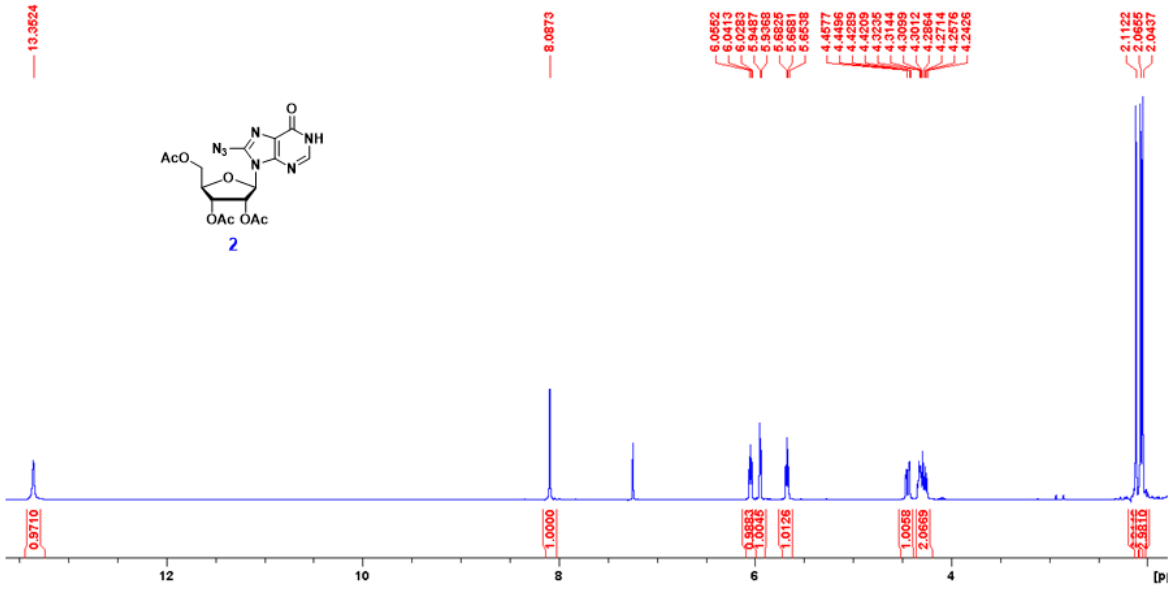
Synthesis of 12. Intermediate **11** (23 mg, 0.032 mmol) was dissolved in 1 mL 7N ammonia in methanol at -40°C. The reaction was stirred at -40°C for 2 h. Upon completion, the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography (CH_2Cl_2 with 10% methanol) to afford intermediate **12** (17 mg, 0.026 mmol, 80%) as a yellow oil. ^{1}H NMR (CD_3OD, 400 MHz) δ (ppm): 1.36 (s, 3H), 1.42 (m, 6H), 1.53 (m, 2H), 1.54 (s, 3H), 1.68 (m, 6H), 2.17 (t, *J* = 7.3 Hz, 2H), 2.67 (d, *J* = 12.7 Hz, 1H), 2.88 (dd, *J* = 5.0, 12.8 Hz, 1H), 3.56 (s, broad, 2H), 3.66 (dd, *J* = 4.7, 12.1 Hz, 1H), 3.76 (dd, *J* = 3.9, 12.1 Hz, 1H), 4.27 (m, 2H), 4.45 (m, 1H), 5.04 (dd, *J* = 2.6, 6.1 Hz, 1H), 5.38 (dd, *J* = 3.4, 6.1 Hz, 1H0, 5.93 (d, *J* = 3.4 Hz, 1H), 8.13 (s, 1H). ^{13}C NMR (CD_3OD, 100 MHz) δ (ppm): 25.73, 27.07, 27.77, 27.84, 27.87, 29.65, 29.91, 30.51, 36.96, 40.44, 41.17, 57.15, 61.76, 63.53, 63.80, 83.08, 84.35, 88.28, 91.18, 115.42, 146.03, 153.00, 176.10. HRMS (*m/z*): calculated for $C_{29}H_{43}N_{11}O_6SNa$ (M+Na): 696.3010; found: 696.2992.

Synthesis of probe 1. Intermediate **12** (17 mg, 0.025 mmol) was dissolved in 1 mL 50% TFA at 0°C. The reaction was stirred at 0°C for 4 h. The solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography (CH_2Cl_2 with 20% methanol) to afford **probe 1** (16 mg, 0.025 mmol, quantitatively) as a yellow oil.

Figure S2. NMR spectra of the probes.



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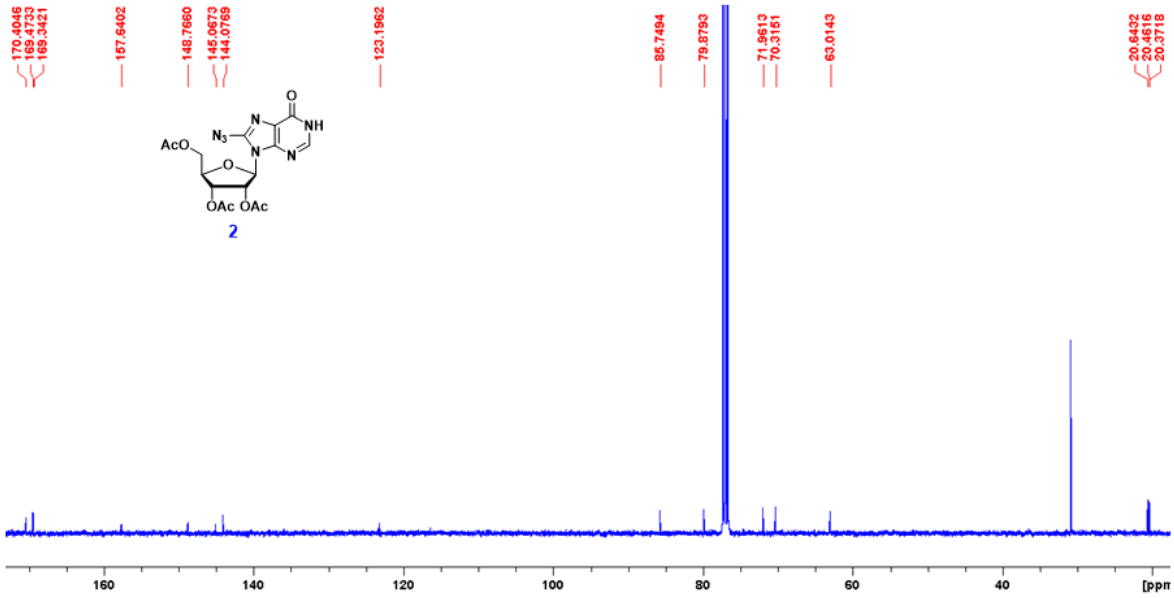
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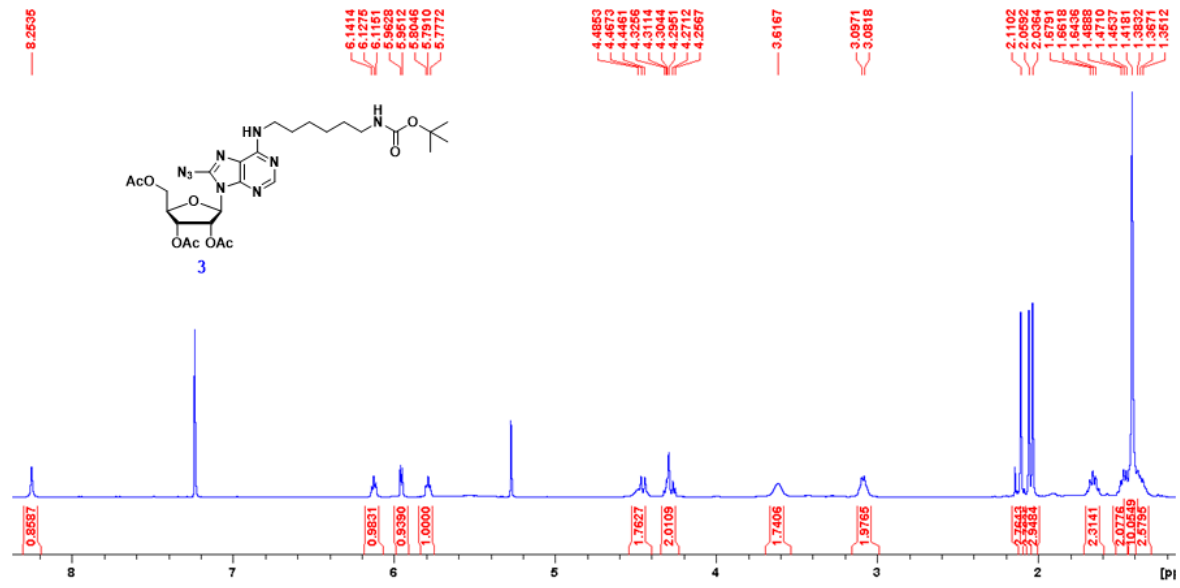
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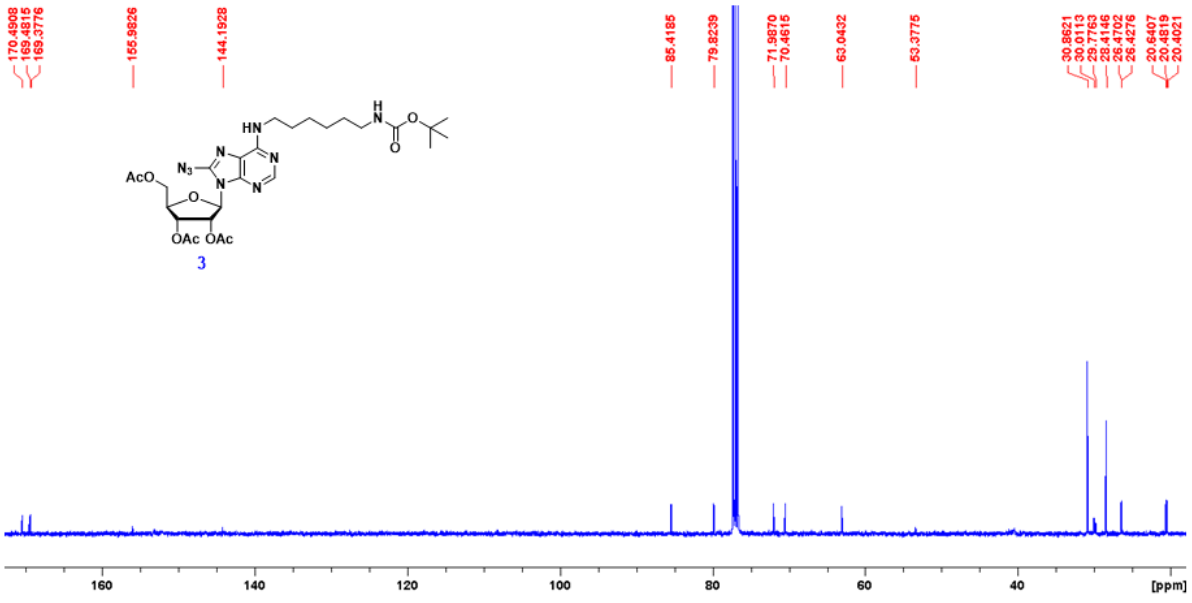
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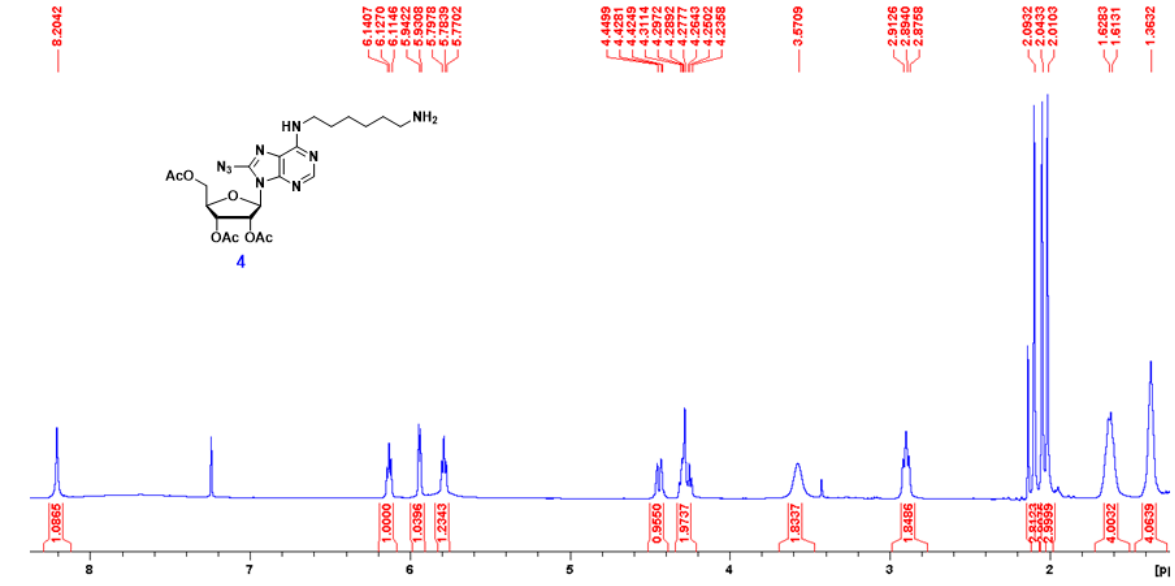
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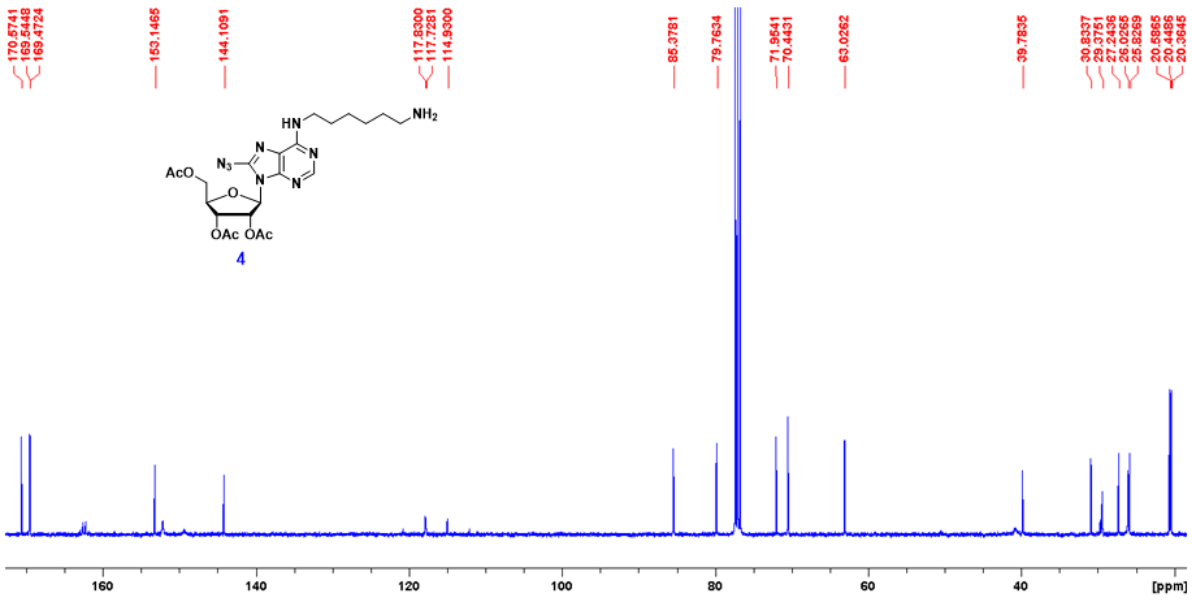
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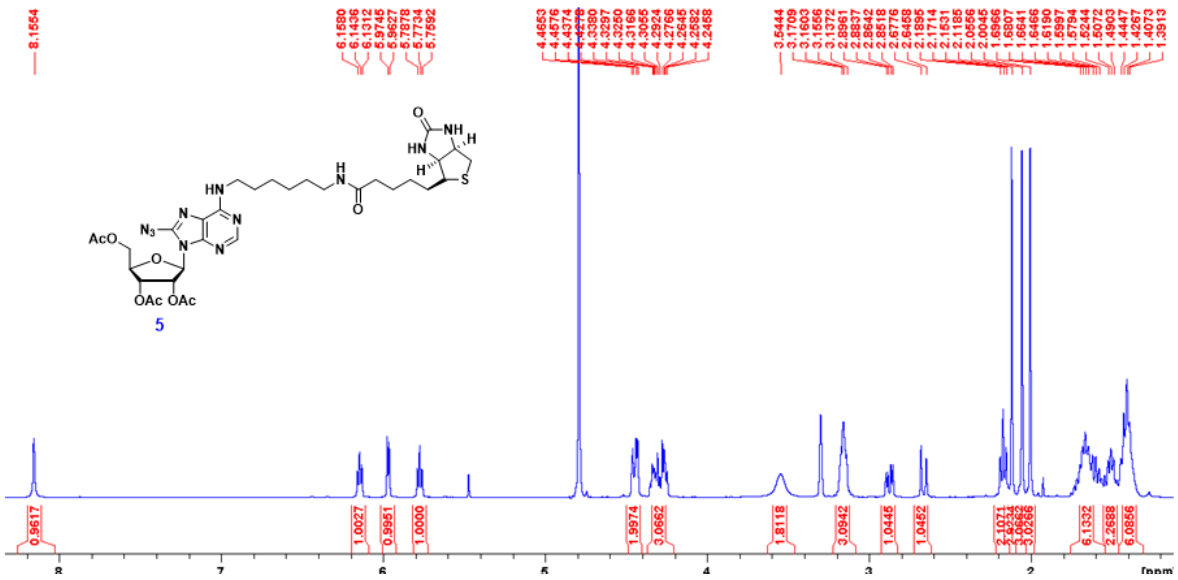
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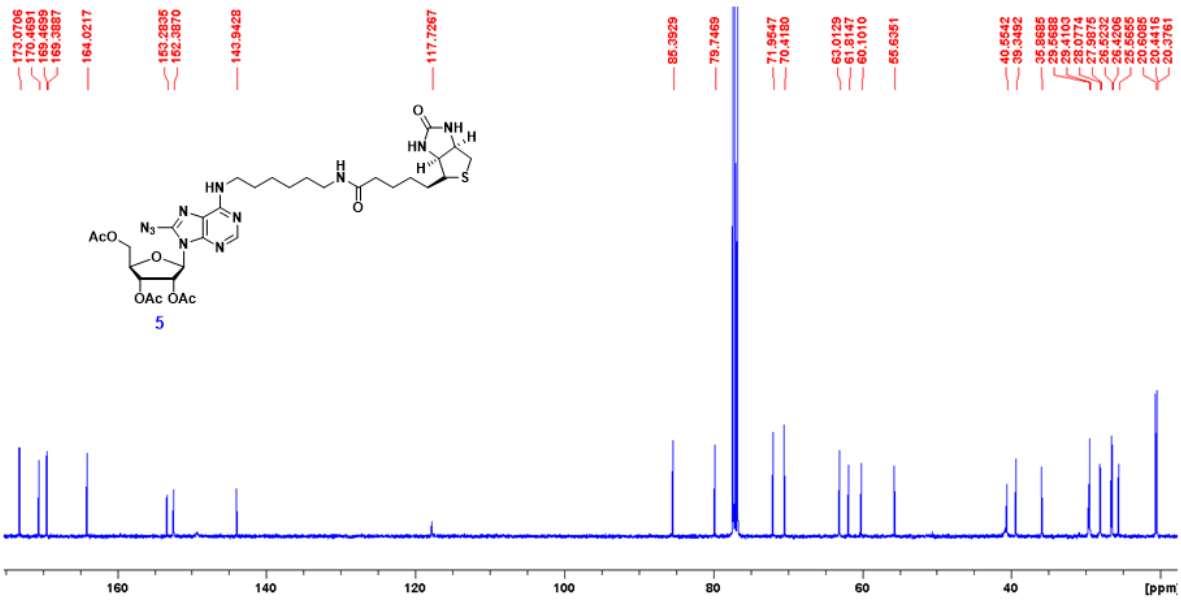
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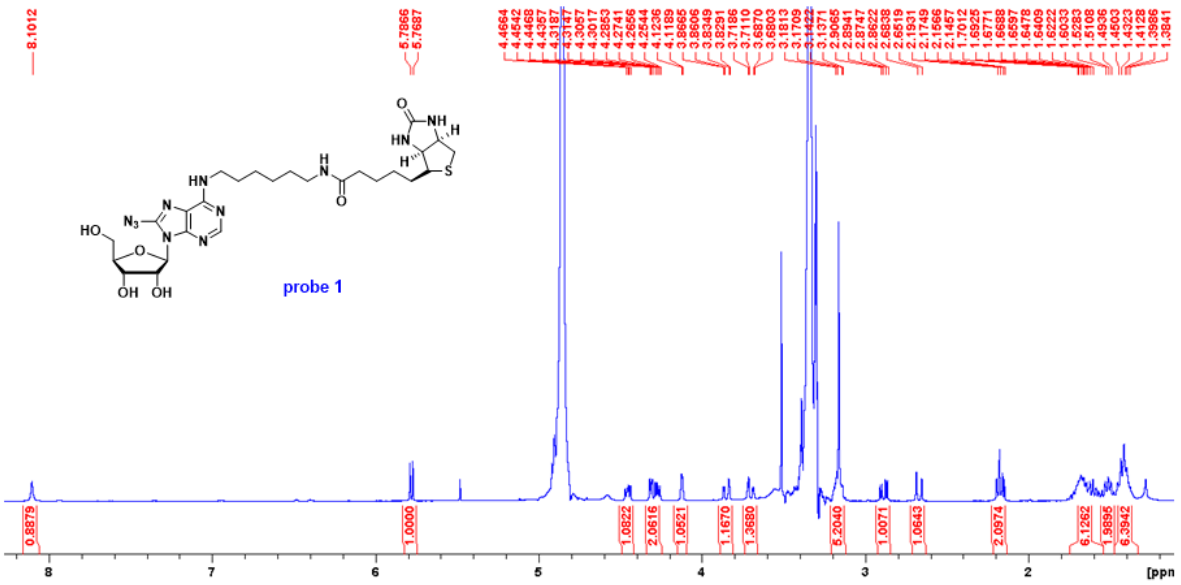
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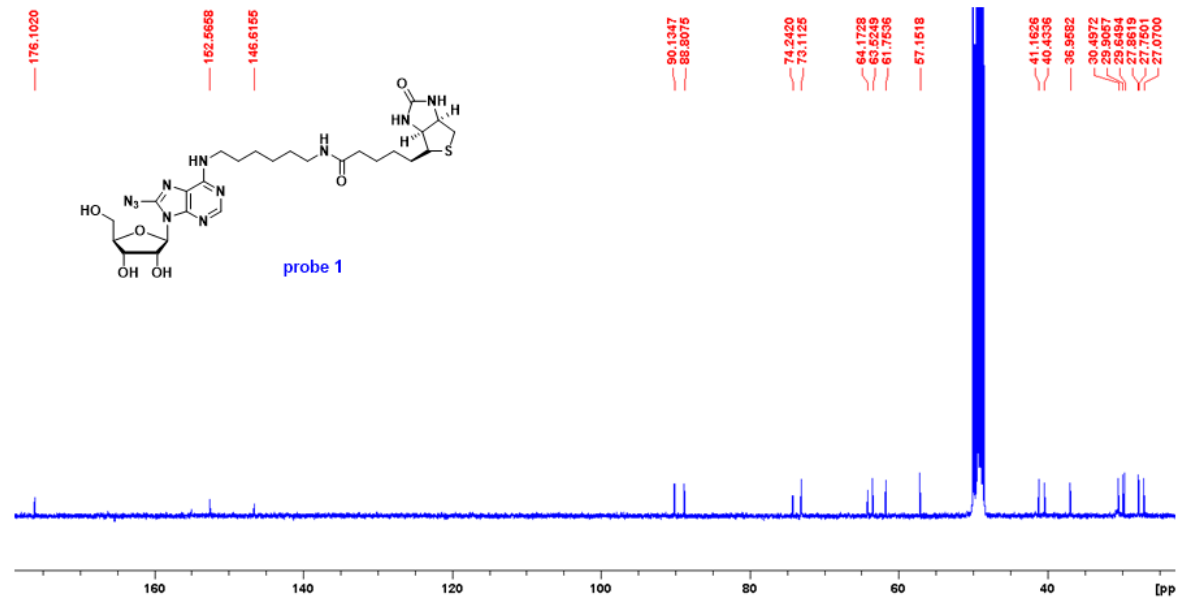
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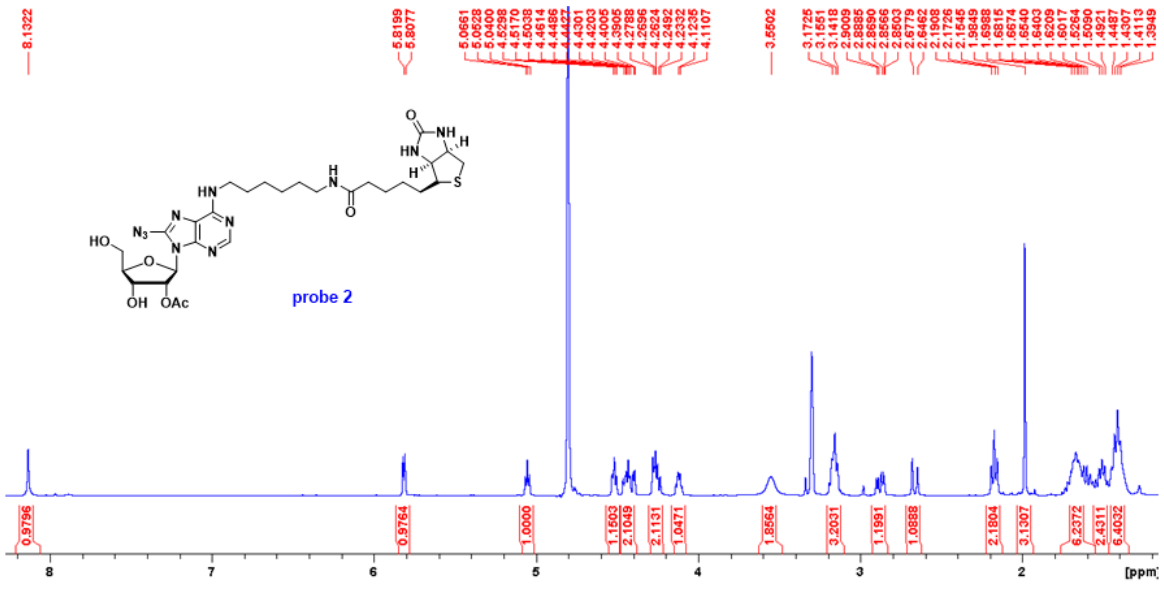
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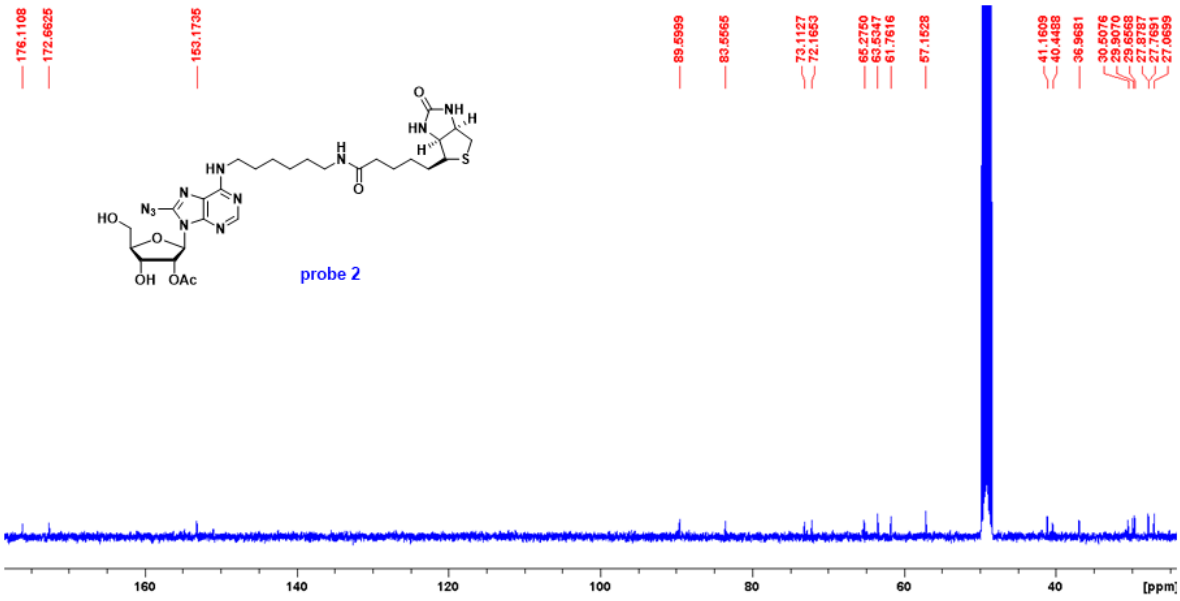
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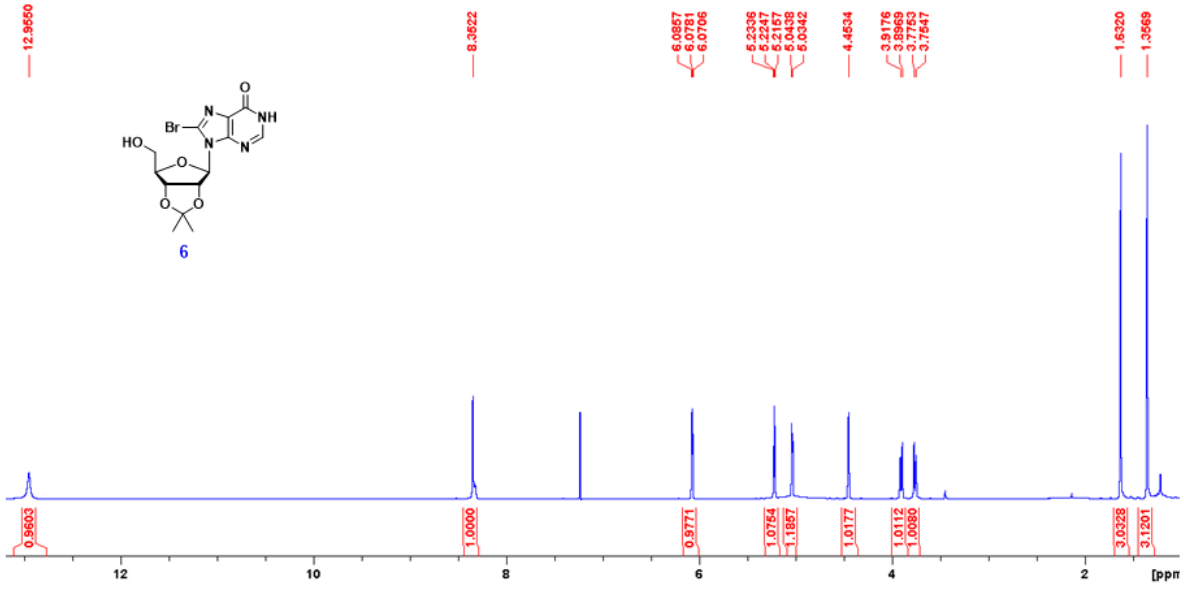
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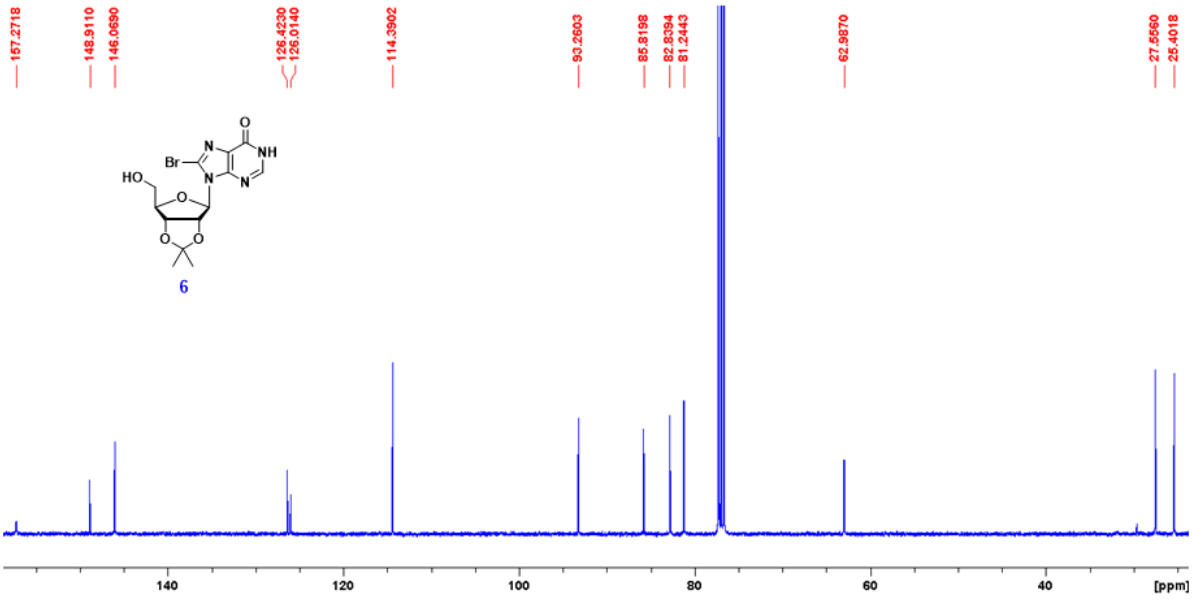
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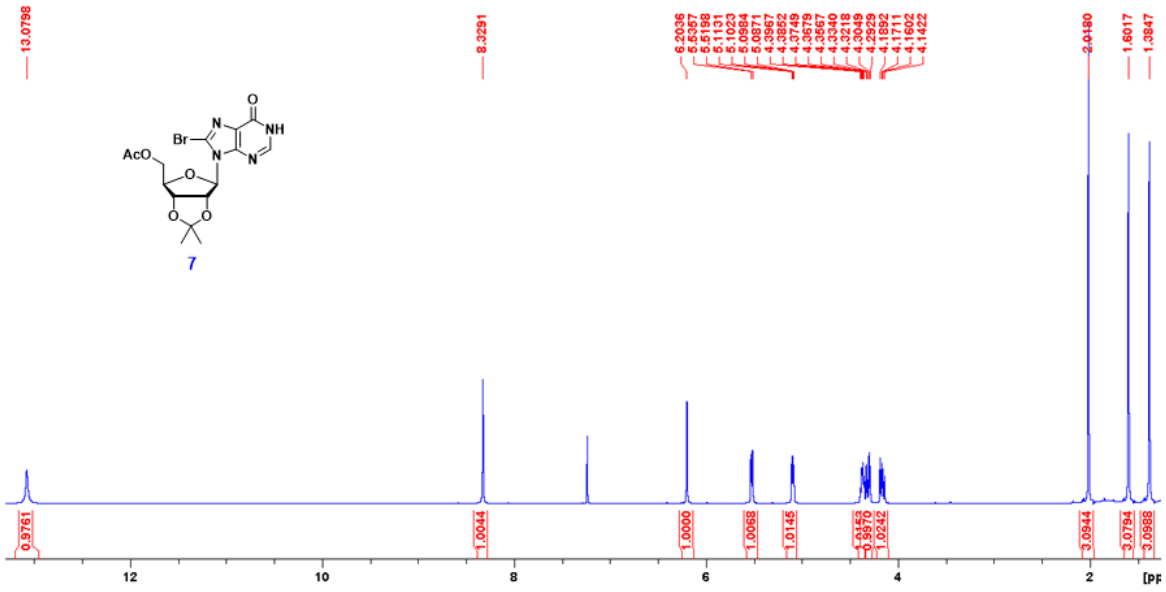
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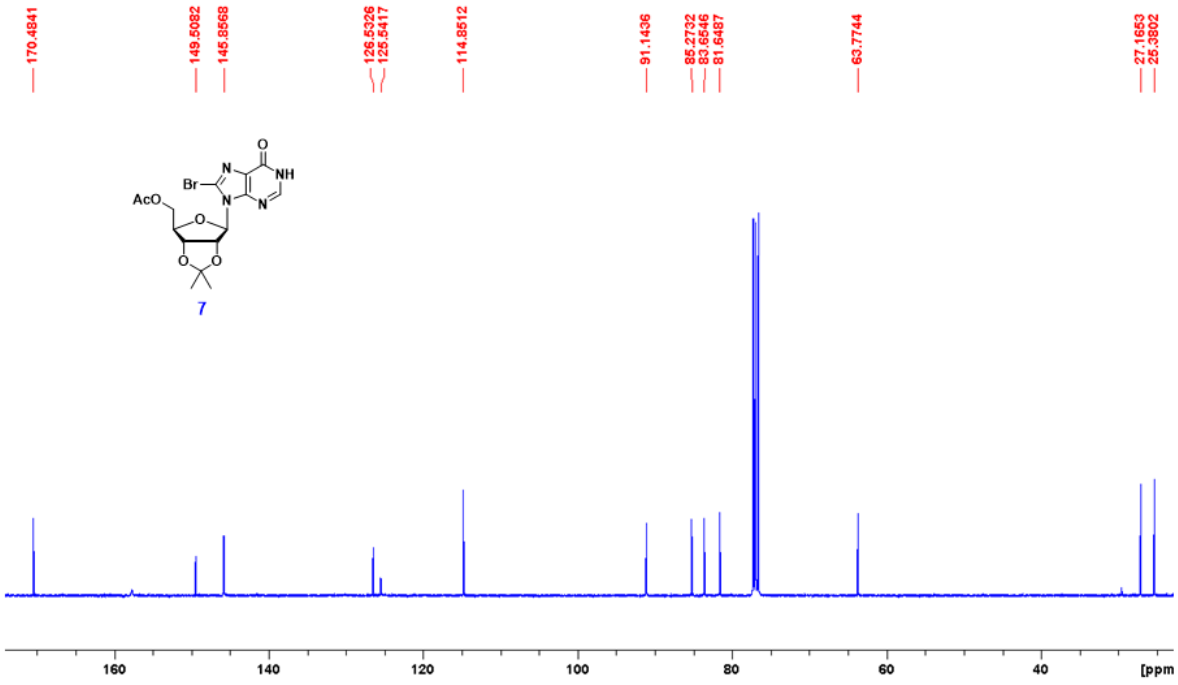
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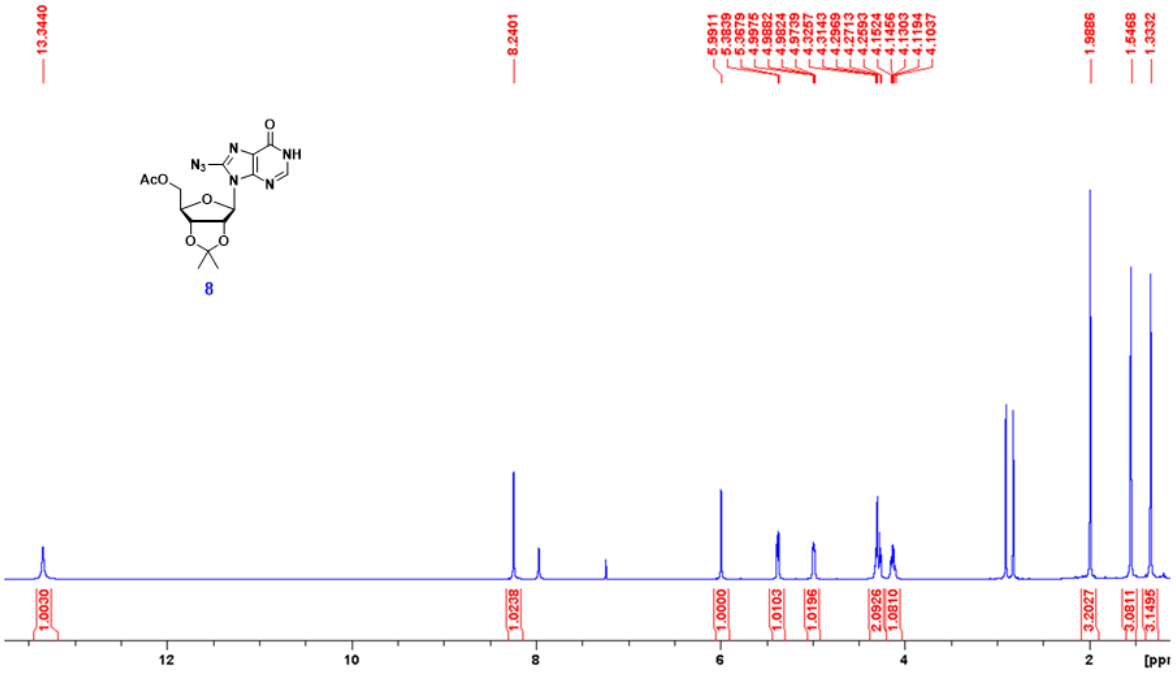
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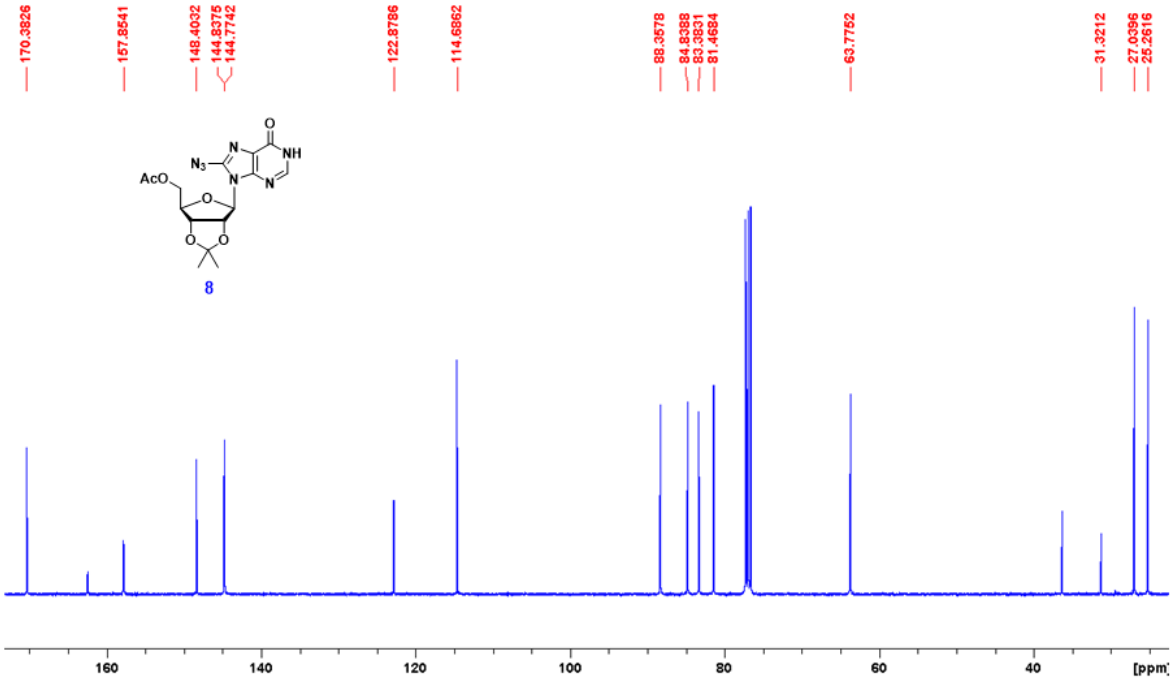
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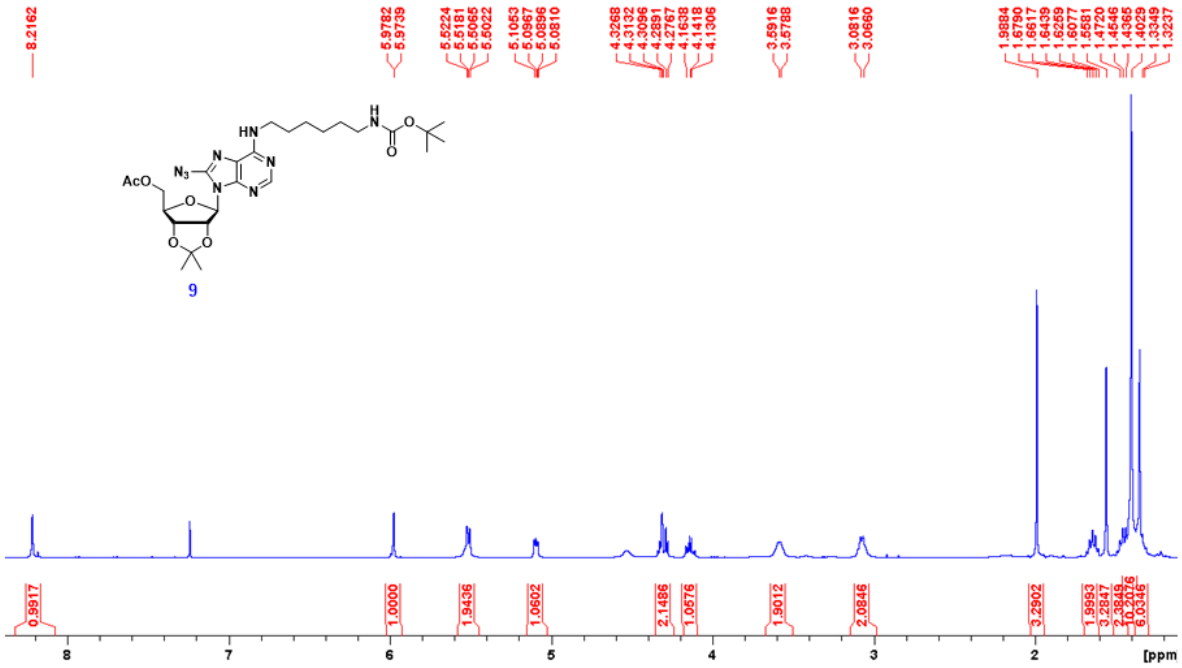
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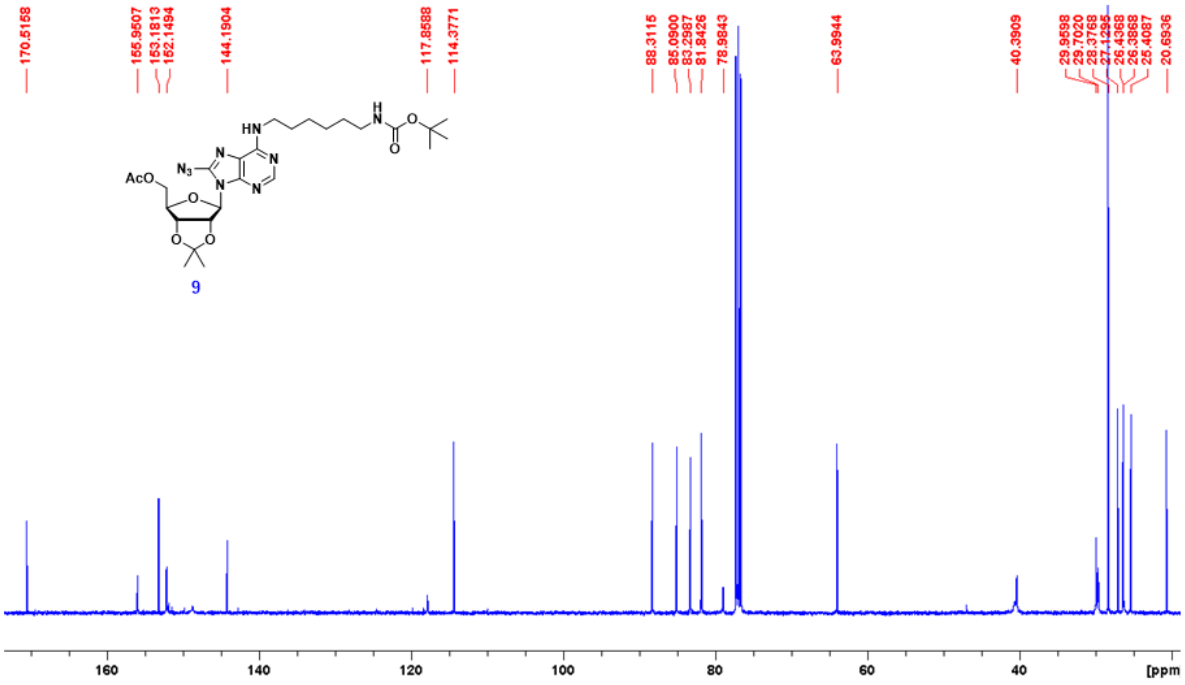
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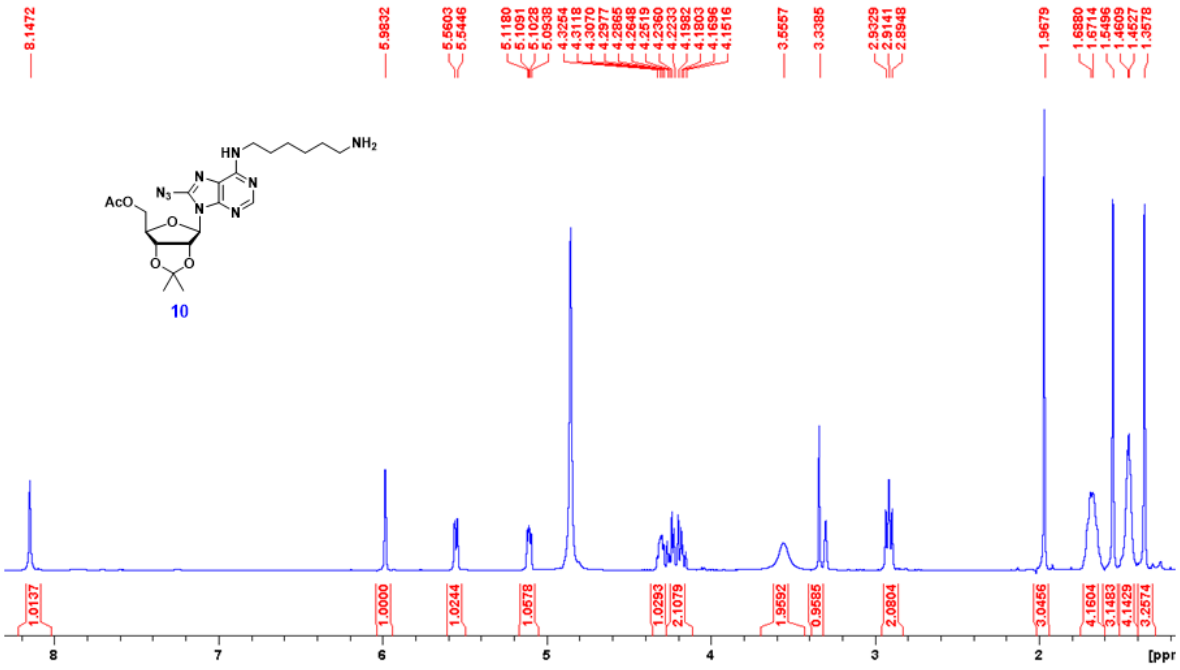
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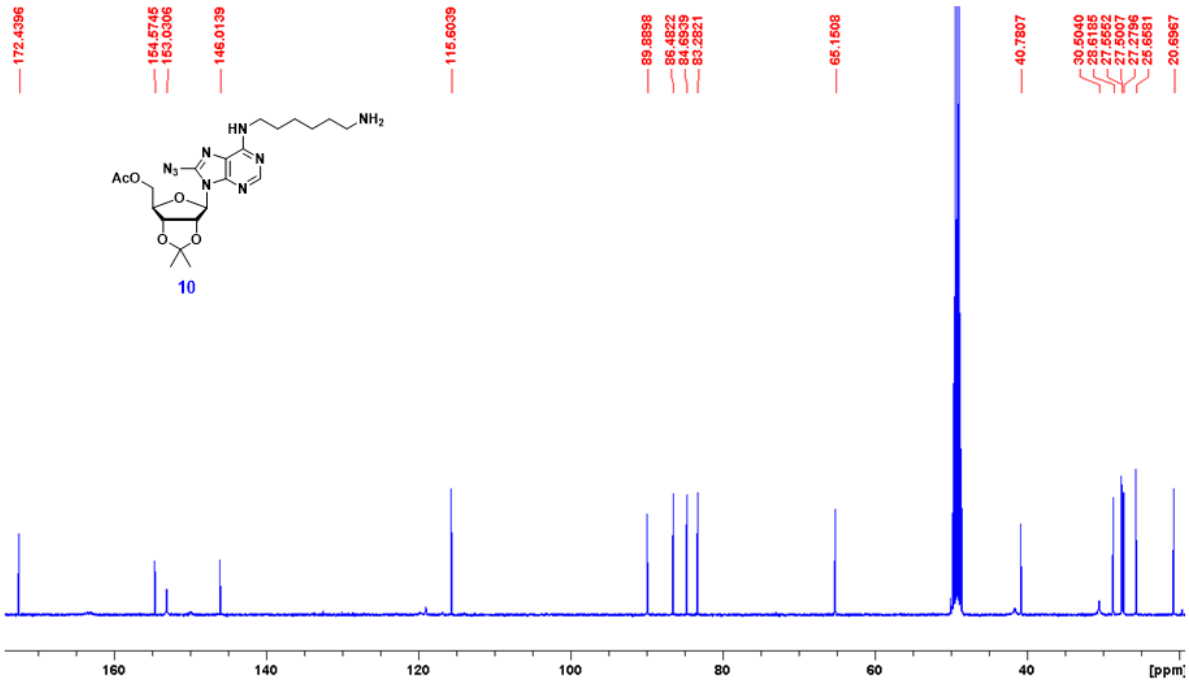
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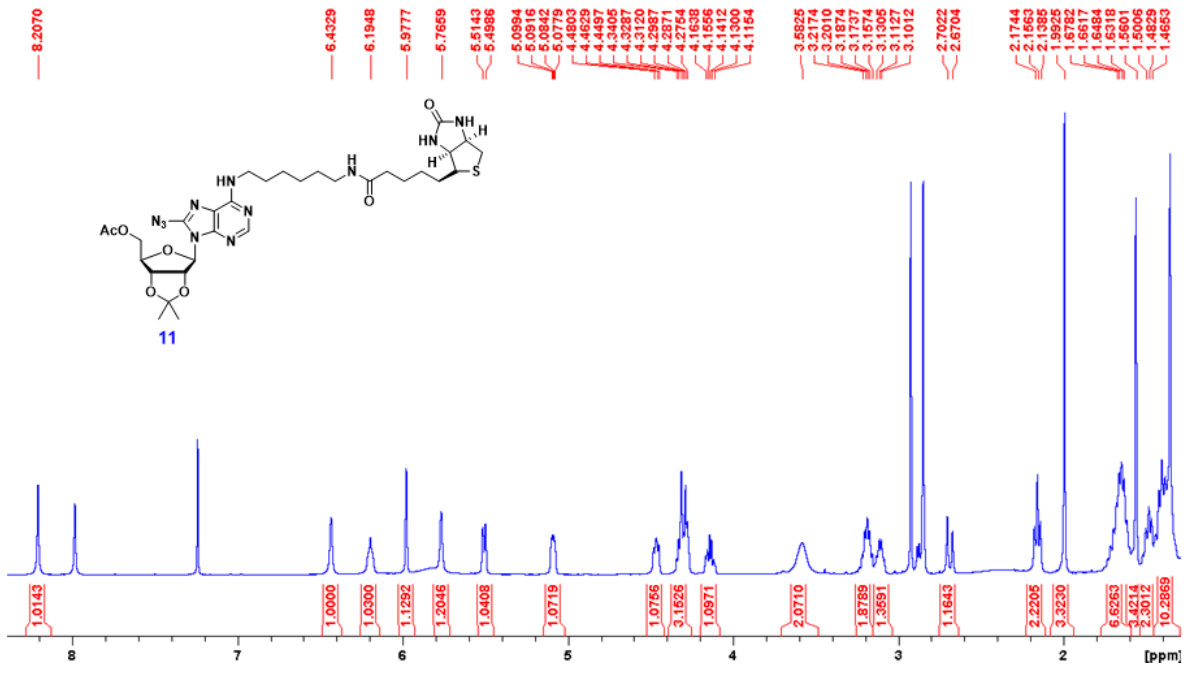
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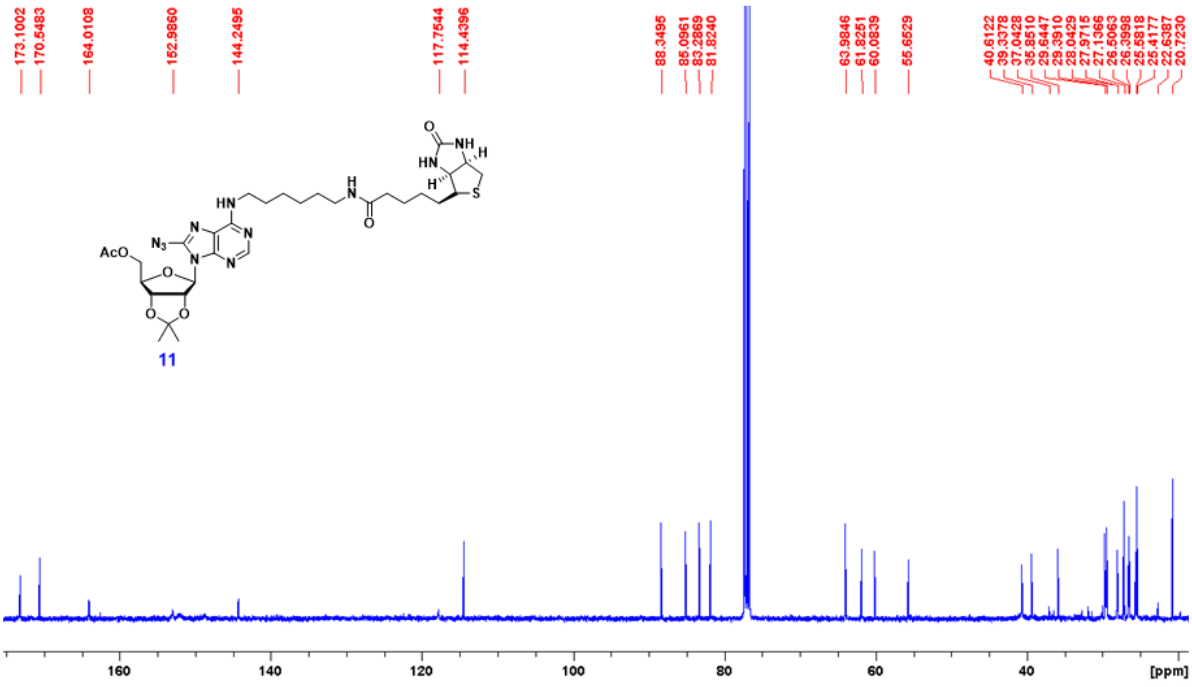
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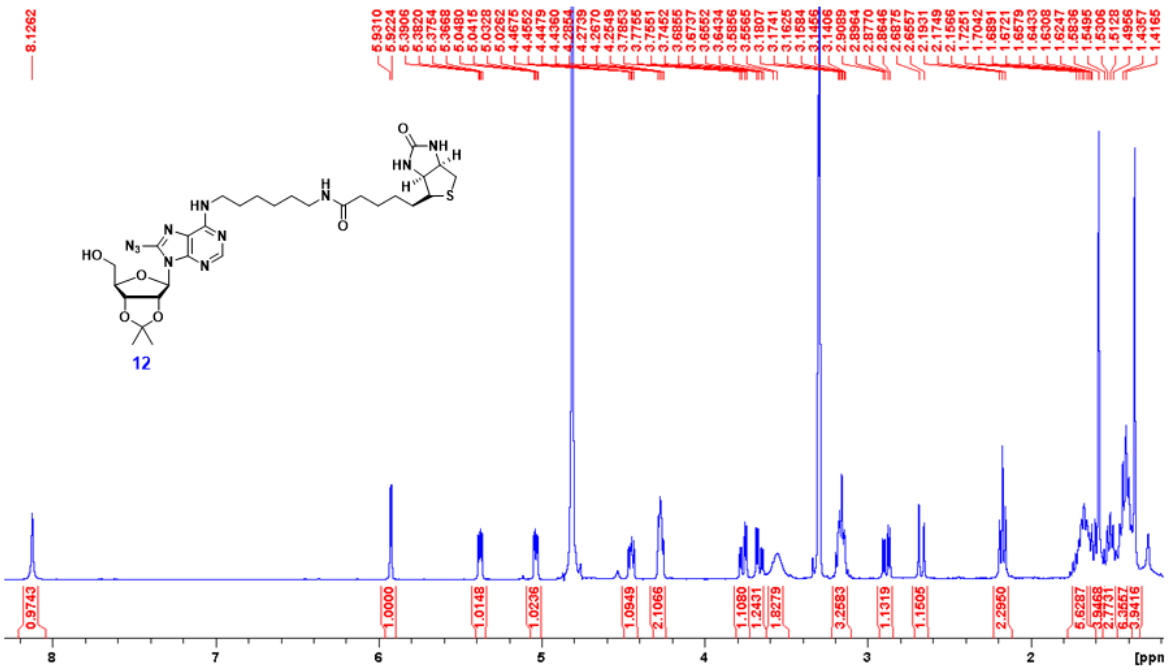
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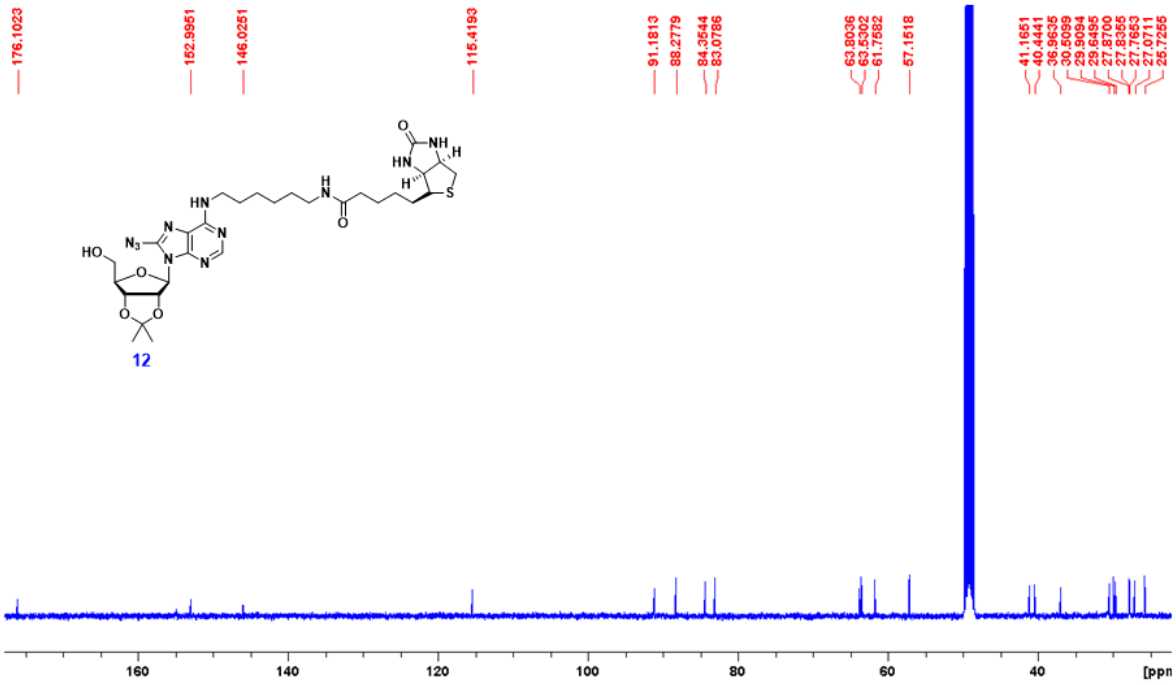
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