Supplementary Information

Synthesis and Evaluation of Duocarmycin and CC-1065 Analogues Containing Modifications in the Subunit Linking Amide

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N^2-[(5,6,7-Trimethoxyindol-2-yl)thiocarbonyl]-1,2,9,9a-tetrahydrocyclopropa[*c*]benz[*e*]indol-4-one (7). A solution of **8** (7 mg, 0.012 mmol, 1 equiv) in CH_3CN (0.12 mL) was treated with DBU (5.6 mg, 0.037 mmol, 3 equiv), and the reaction mixture was stirred at 25 °C for 45 min. PTLC (50% EtOAc/hexanes) afforded **7** (2 mg, 30%) as a yellow semi-solid: ^{1}H NMR (acetone-d_6, 500 MHz) δ 10.30 (br s, 1H, NH), 8.04 (d, J = 7.8 Hz, 1H, C5-H), 7.60 (t, J = 7.8 Hz, 1H, C6-H), 7.42 (t, J = 7.8 Hz, 1H, C7-H), 7.22 (d, J = 7.8 Hz, 1H, C8-H), 6.99 (d, J = 2.2 Hz, 1H, C3′-H), 6.87 (s, 1H, C4′-H), 5.83 (s, 1H, C3-H), 4.64 (dd, J = 4.9, 12.0 Hz, 1H, C1-*H*H), 4.33 (d, J = 12.0 Hz, 1H, C1-H*H*), 3.96 (s, 3H, OCH_3), 3.86 (s, 3H, OCH_3), 3.84 (s, 3H, OCH_3), 3.12 (dt, J = 4.9, 5.2, 7.8 Hz, 1H, C9a-H), 2.13 (t, J = 4.9 Hz, 1H, C9-*H*H), 2.00 (dd, J = 4.9, 7.8 Hz, 1H, C9-H*H*); ^{13}C NMR (acetone-d_6, 125 MHz) δ 192.2, 184.5, 161.7, 151.6, 142.2, 141.7, 140.1, 138.1, 133.4, 133.0, 128.4, 127.3, 127.0, 124.5, 123.1, 112.4, 108.1, 99.0, 61.5, 60.5, 56.5, 34.1, 32.4, 28.9, 25.9; IR (film) ν_{max} 3298, 2937, 1732, 1615, 1372, 1299, 1272, 1236, 1112, 1047, 997, 778 cm^{-1}; UV (pH 3 buffer) λ_{max} 366 nm (ε 15270), UV (CH_3OH) λ_{max} 365 nm (ε 14730); FABHRMS (NBA/NaI) *m/z* 447.1391 (M^+ + H, $C_{25}H_{22}N_2O_4S$ requires 447.1379).

(+)-(8a*R*,9b*S*)-7: yellow semi-solid: $[\alpha]_D^{23}$ +580 (*c* 0.0005, EtOAc).

(−)-(8a*S*,9b*R*)-7: yellow semi-solid: $[\alpha]_D^{23}$ −576 (*c* 0.0005, EtOAc).

5-(Benzyloxy)-1-(chloromethyl)-3-[(5,6,7-trimethoxyindol-2-yl)carbonyl]-1,2-dihydro-3*H*-benz[*e*]indole (12). A sample of **10** (40 mg, 0.095 mmol, 1 equiv) was treated with 3 M HCl–EtOAc (2 mL) at 24 °C for 30 min. The solvent was removed in vacuo to afford the crude amine salt **11** (quantitative). The salt was dissolved in DMF (1 mL) and treated sequentially with $NaHCO_3$ (40 mg, 0.473 mmol, 5 equiv), 5,6,7-trimethoxyindole-2-carboxylic acid (36 mg, 0.142 mmol, 1.5 equiv) and EDCI (54 mg, 0.283 mmol, 3 equiv) and the suspension was stirred at 24 °C for 22 h. The mixture was diluted with H_2O (1.5 mL) and extracted with EtOAc (3 × 3 mL). The organic layer was washed with 1 N aqueous HCl (1 × 3 mL), saturated aqueous $NaHCO_3$ (1 × 3 mL) and saturated aqueous NaCl (1 × 5 mL), dried (Na_2SO_4), filtered and concentrated in vacuo. Flash chromatography (0.8 × 10 cm SiO_2, 0–40% EtOAc/hexane gradient elution) afforded **12** (28 mg, 53%) as a green solid: mp 93–95 °C dec; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.40 (br s, 1H, C1′-H), 8.34 (d, J = 8.4 Hz, 1H, C5-H), 8.18 (s, 1H, C3-H), 7.71 (d, J = 8.4 Hz, 1H, C8-H), 7.33–7.56 (m, 7H, C6-H, C7-H, C4-OCH_2ArH), 7.01 (d, J = 2.2 Hz, 1H, C3′-H), 6.87 (s, 1H, C4′-H), 5.33 (d, J = 11.5 Hz, 1H, C4-OC*H*HAr), 5.27 (d, J = 11.5 Hz, 1H, C4-OCH*H*Ar), 4.79 (d, J = 10.5 Hz, 1H, C2-*H*H), 4.66 (ap t, J = 9.5 Hz, 1H, C2-H*H*), 4.07–4.15 (m, 1H, C1-H), 4.07 (s, 3H, OCH_3), 3.95–3.99 (m, 1H, C*H*H-Cl), 3.94 (s, 3H, OCH_3), 3.91 (s, 3H, OCH_3), 3.46 (ap t, J = 10.5 Hz, 1H, CH*H*-Cl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.4, 155.8, 150.1, 142.1, 140.6, 138.8, 136.7, 129.8, 129.7, 128.6 (2), 128.0, 127.8, 127.5 (2), 125.5, 124.0, 123.7, 123.6, 122.1, 116.2, 106.5, 98.3, 97.6,

70.3, 61.5, 61.1, 56.2, 55.4, 46.0, 43.1; IR (film) ν_{max} 1617, 1577, 1491, 1458, 1405, 1311, 1268, 1232 cm^{-1}; FABHRMS (NBA/CsI) *m/z* 689.0802 (M^+ + Cs, $C_{32}H_{29}ClN_2O_5$ requires 689.0819).

5-(Benzyloxy)-1-(chloromethyl)-3-[(5,6,7-trimethoxyindol-2-yl)thiocarbonyl]-1,2-dihydro-3*H*-benz[*e*]indole (13). A solution of **12** (42 mg, 0.076 mmol, 1 equiv) in benzene (0.8 mL) was treated with Lawesson's reagent (23 mg, 0.057 mmol, 0.75 equiv) and warmed to 80 °C for 1.5 h. The solvent was removed in vacuo. Flash chromatography (1 × 10 cm SiO_2, 0–25% EtOAc/hexane gradient elution) afforded **13** (38 mg, 88%) as a yellow solid: mp 135–137 °C dec; ^1H NMR ($CDCl_3$, 400 MHz) δ 9.26 (br s, 1H, C1′-H), 8.29 (d, *J* = 8.2 Hz, 1H, C6-H), 7.73 (d, *J* = 8.2 Hz, 1H, C9-H), 7.56 (t, *J* = 7.8 Hz, 1H, C7-H), 7.44 (t, *J* = 7.8 Hz, 1H, C8-H), 7.23–7.33 (m, 6H, C4-H, C4-OCH_2ArH), 6.75 (d, *J* = 1.9 Hz, 1H, C3′-H), 6.73 (s, 1H, C4′-H), 4.94–4.96 (br d, 1H, C4-OC*H*HAr), 4.83–4.89 (br d, 1H, C4-OCH*H*Ar), 4.87 (d, *J* = 12.2 Hz, 1H, C2-*H*H), 4.76 (dd, *J* = 7.8, 12.2 Hz, 1H, C2-H*H*), 4.10 (s, 3H, OCH_3), 3.91–3.97 (m, 2H, C1-H, C*H*H-Cl), 3.92 (s, 3H, OCH_3), 3.87 (s, 3H, OCH_3), 3.62 (ap t, *J* = 10.8 Hz, 1H, CH*H*-Cl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 185.1, 154.7, 150.3, 142.1, 140.5, 138.9, 136.3, 135.7, 130.0, 128.6, 128.5, 128.2, 128.1, 127.2, 126.7, 125.1, 124.2, 123.8, 123.4, 122.5, 120.9, 104.7, 98.3, 97.4, 70.5, 63.3, 61.6, 61.5, 61.2, 56.2, 45.7, 41.5, 29.7; IR (film) ν_{max} 2938, 1581, 1461, 1402, 1320, 1230, 1119 cm^{-1}; FABHRMS (NBA/NaI) *m/z* 573.1631 (M^+ + H, $C_{32}H_{30}ClN_2O_4S$ requires 573.1615).

5-(Benzyloxy)-1-(chloromethyl)-3-[(5,6,7-trimethoxyindol-2-yl)iminocarbonyl]-1,2-dihydro-3*H*-benz[*e*]indole (14). A suspension of **13** (25 mg, 0.044 mmol, 1 equiv) in CH_3CN (0.5 mL) was treated with CH_3I (62 mg, 0.437 mmol, 10 equiv) and stirred at 24 °C for 24 h. The solvent was removed in vacuo and resuspended in THF (1 mL). The suspension was cooled (–78 °C) and treated with ammonia(g) under a stream of nitrogen. The solution was allowed to warm to 24 °C over a 20 h period and the solvent removed in vacuo. Flash chromatography (0.5 × 15 cm SiO_2, 0–10% CH_3OH/CH_2Cl_2 gradient elution) afforded **14** (23 mg, 95%) as a pale yellow solid: mp 161–164 °C dec; ^1H NMR (DMSO-d_6, 400 MHz) δ 9.89 (br s, 1H, NH), 8.10 (d, *J* = 8.4 Hz, 1H, C6-H), 7.98 (d, *J* = 8.4 Hz, 1H, C9-H), 7.64 (t, *J* = 7.7 Hz, 1H, C7-H), 7.48 (t, *J* = 7.7 Hz, 1H, C8-H), 7.27–7.35 (m, 3H, C4-OCH_2ArH), 7.05–7.11 (m, 4H, C4-OCH_2ArH, C3′-H, C4′-H), 5.48 (br s, 1H, C4-H), 4.59 (ap t, *J* = 9.7 Hz, 1H, C2-*H*H), 4.25–4.36 (m, 4H, C4-OCH_2Ar, C2-H*H*, C1-H), 4.02–4.13 (m, 2H, CH_2Cl), 3.86 (s, 3H, OCH_3), 3.83 (s, 3H, OCH_3), 3.69 (s, 3H, OCH_3); ^1H NMR (CD_3OD, 500 MHz) δ 8.16 (d, *J* = 8.3 Hz, 1H, C6-H), 7.87 (d, *J* = 8.3 Hz, 1H, C9-H), 7.60 (t, *J* = 7.5 Hz, 1H, C7-H), 7.43 (t, *J* = 7.5 Hz, 1H, C8-H), 7.24–7.31 (m, 3H, C4-OCH_2ArH), 7.01–7.08 (m, 4H, C4-OCH_2ArH, C3′-H, C4′-H), 5.34 (br s, 1H, C4-H), 4.54 (dd, *J* = 8.3, 11.6 Hz, 1H, C2-*H*H), 4.46 (d, *J* = 11.6 Hz, 1H, C2-H*H*), 4.34 (d, *J* = 12.2 Hz, 1H, C5-OC*H*HAr), 4.30 (d, *J* = 12.2 Hz, 1H, C5-OCH*H*Ar), 4.19–4.23 (m, 1H, C1-H), 4.10 (dd, *J* = 3.1, 11.1 Hz, 1H, C*H*H-Cl), 3.95 (d, *J* = 11.1 Hz, 1H, CH*H*-Cl), 3.92 (s, 3H, OCH_3), 3.89 (s, 3H, OCH_3), 3.77 (s, 3H, OCH_3); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 154.4, 153.9, 150.0, 140.2, 139.5, 138.9, 135.9, 133.0, 129.6, 128.6 (2), 128.5, 128.4, 128.1, 126.8 (2), 125.1, 123.5, 122.9, 122.8, 122.5, 119.7, 97.9, 95.7, 69.3, 61.1, 61.0, 56.1, 55.0, 46.3, 40.8, the remaining signal was not detected and is believed to overlap with 154.4; IR (film) ν_{max} 3500, 2934, 1578, 1458, 1406, 1317, 1219, 1121 cm^{-1}; FABHRMS (NBA/CsI) *m/z* 556.2015 (M^+ + H, $C_{32}H_{30}ClN_3O_4$ requires 556.2003).

1-(Chloromethyl)-3-[(5,6,7-trimethoxyindol-2-yl)iminocarbonyl]-1,2-dihydro-3*H*-benz[*e*]indole (9). A suspension of **14** (1.7 mg, 0.003 mmol, 1 equiv) in CH_3OH (0.5 mL) and a catalytic amount of Pd–C (10%) was stirred at 24 °C for 6 h under H_2 (1 atm). The suspension was filtered (Celite) and the solvent was removed in vacuo to afford crude **9** (1.4 mg, 100%) as a pale

yellow solid: mp 155–158 °C dec; ^{1}H NMR (CD_3OD, 500 MHz) δ 8.15 (d, J = 8.3 Hz, 1H, C6-H), 7.86 (d, J = 8.3 Hz, 1H, C9-H), 7.82–7.90 (br s, 1H, C4-H), 7.59 (t, J = 7.7 Hz, 1H, C7-H), 7.42 (t, J = 7.7 Hz, 1H, C8-H), 7.21 (br s, 1H, C3′-H), 7.01 (s, 1H, C4′-H), 4.66 (dd, J = 8.5, 11.0 Hz, 1H, C2-*H*H), 4.45 (d, J = 11.0 Hz, 1H, C2-H*H*), 4.19–4.26 (m, 1H, C1-H), 4.21 (dd, J = 3.2, 10.9 Hz, 1H, C*H*H-Cl), 4.03 (d, J = 10.9 Hz, 1H, CH*H*-Cl), 3.95 (s, 3H, OCH_3), 3.89 (s, 6H, OCH_3); ^{1}H NMR (acetone-d_6, 400 MHz) δ 11.90 (br s, 1H, OH), 10.10 (br s, 1H, NH), 8.22 (d, J = 8.1 Hz, 1H, C6-H), 7.90 (d, J = 8.1 Hz, 1H, C9-H), 7.59 (t, J = 7.6 Hz, 1H, C7-H), 7.46 (t, J = 7.6 Hz, 1H, C8-H), 7.28 (s, 1H, C4′-H), 6.92 (s, 1H, C4-H), 6.90 (br s, 1H, C3′-H), 4.93 (dd, J = 8.5, 11.3 Hz, 1H, C2-*H*H), 4.57 (d, J = 11.3 Hz, 1H, C2-H*H*), 4.20–4.24 (m, 1H, C1-H), 4.09–4.12 (m, 1H, C*H*H-Cl), 3.99–4.01 (m, 1H, CH*H*-Cl), 3.97 (s, 3H, OCH_3), 3.88 (s, 3H, OCH_3), 3.85 (s, 3H, OCH_3); ^{13}C NMR (acetone-d_6, 100 MHz) δ 156.0, 155.1, 151.7, 142.7, 140.4, 140.3, 131.4, 129.9, 129.5, 129.1, 125.6, 124.8, 124.5, 124.2, 124.0, 120.1, 113.0, 99.2, 98.6, 61.6, 61.5, 60.4, 56.5, 47.0, 42.5; IR (film) ν_{max} 3182, 1679, 1584, 1463, 1403, 1317, 1220, 1121 cm^{-1}; FABHRMS (NBA/NaI) m/z 466.1550 (M^+ + H, $C_{25}H_{25}ClN_3O_4$ requires 466.1534).

Alternatively, a suspension of **8** (12.0 mg, 0.025 mmol, 1 equiv) in CH_3CN (0.25 mL) was treated with CH_3I (54 mg, 0.373 mmol, 15 equiv) and stirred at 24 °C for 24 h. The solvent was removed in vacuo and resuspended in THF (1 mL). The suspension was cooled (−78 °C) and treated with ammonia(g) under a stream of nitrogen. The solution was allowed to warm to 24 °C over a 20 h period and the solvent removed in vacuo. PTLC (4% MeOH/CH_2Cl_2) afforded **9** (10.1 mg, 91%) as a pale yellow solid.

Alternatively, a solution of **14** (18 mg, 0.032 mmol, 1 equiv) in TFA (1.6 mL, 0.02 M) was warmed to 70 °C for 0.5 h. The solvent was removed in vacuo. PTLC (4% MeOH/CH_2Cl_2) afforded **9** (12 mg, 80%) as a pale yellow solid.

(−)-(8a*R*,9b*S*)-9: pale yellow solid: $[\alpha]_D^{23}$ −76 (*c* 0.007, CH_3OH).

(+)-(8a*S*,9b*R*)-9: pale yellow solid: $[\alpha]_D^{23}$ +72 (*c* 0.002, CH_3OH).

***N*^{2}-[(5,6,7-Trimethoxyindol-2-yl)iminocarbonyl]-1,2,9,9a-tetrahydrocyclopropa[*c*]benz[*e*]indol-4-one (6).** A solution of **9** (12.0 mg, 0.026 mmol, 1 equiv) in CH_3CN (0.43 mL) was treated with DBU (11.8 mg, 0.077 mmol, 3 equiv), and the reaction mixture was stirred at 25 °C for 45 min. The reaction mixture was concentrated in vacuo. PTLC (4% CH_3OH/CH_2Cl_2) afforded **6** (3.8 mg, 34%) as a pale yellow solid: mp 140–142 °C dec; ^{1}H NMR (acetone-d_6, 500 MHz) δ 10.51 (br s, 1H, NH), 8.99 (br s, 1H, NH), 8.00 (d, J = 7.6 Hz, 1H, C5-H), 7.51 (t, J = 7.6 Hz, 1H, C6-H), 7.34 (t, J = 7.6 Hz, 1H, C7-H), 7.12 (d, J = 7.6 Hz, 1H, C8-H), 6.88 (s, 1H, C4′-H), 6.74 (d, J = 1.5 Hz, 1H, C3′-H), 5.37 (s, 1H, C3-H), 4.43 (dd, J = 5.1, 11.2 Hz, 1H, C1-*H*H), 3.95 (d, J = 11.2 Hz, 1H, C1-H*H*), 3.93 (s, 3H, OCH_3), 3.84 (s, 3H, OCH_3), 3.80 (s, 3H, OCH_3), 3.04 (dt, J = 4.9, 5.1, 7.8 Hz, 1H, C9a-H), 1.93 (t, J = 4.9 Hz, 1H, C9-*H*H), 1.80 (dd, J = 4.9, 7.8 Hz, 1H, C9-H*H*); ^{13}C NMR (acetone-d_6, 125 MHz) δ 184.0, 163.8, 151.1, 141.7, 140.9, 140.2, 133.8, 132.4, 132.3, 132.2, 126.9, 126.8, 126.7, 124.5, 122.8, 106.7, 106.1, 98.9, 61.5, 56.6, 55.4, 34.3, 24.9, the two remaining peaks were not observed and are believed to be obscured by the solvent peak at 30 ppm; IR (film) ν_{max} 3284, 2936, 1698, 1614, 1562, 1463, 1410, 1317, 1242, 1196, 1121, 1104 cm^{-1}; UV (CH_3OH) λ_{max} 306 nm (ε 15700); FABHRMS (NBA/NaI) m/z 452.1574 (M^+ + Na, $C_{25}H_{23}N_3O_4$ requires 452.1586).

(+)-(8a*R*,9b*S*)-6: pale yellow solid: $[\alpha]_D^{23}$ +30 (*c* 0.0002, CH_3OH).

(−)-(8a*S*,9b*R*)-6: pale yellow solid: $[\alpha]_D^{23}$ −30 (*c* 0.0002, CH_3OH).

Addition of CH_3OH to 6. *Acid-catalyzed*: A cooled solution (0 ºC) of **6** (5.0 mg, 0.012

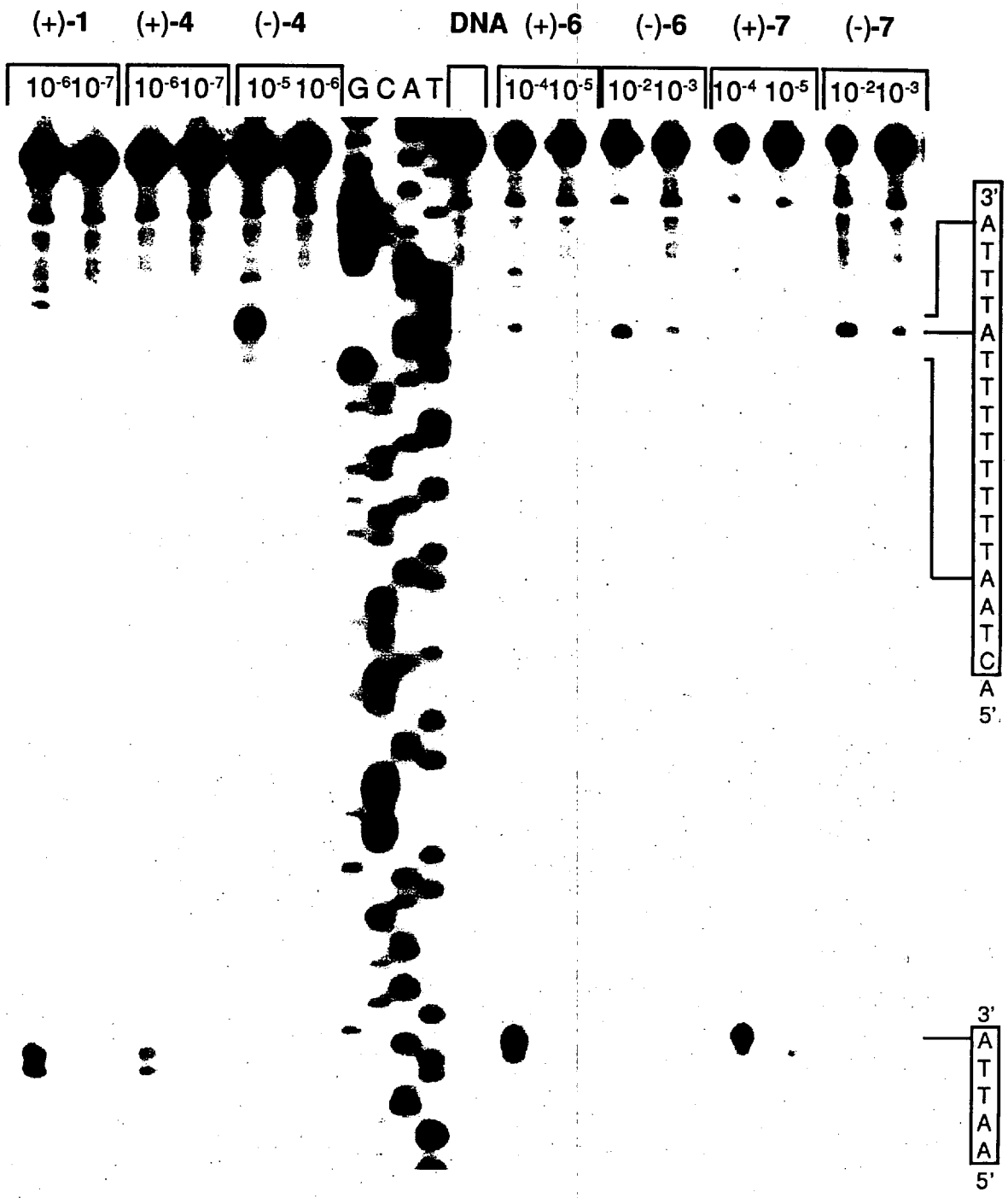
mmol, 1 equiv) in CH_3OH (1.2 mL) was treated with CF_3SO_3H (0.14 mL, 0.011 M in CH_3OH, 0.24 equiv). The solution was allowed to warm to 24 °C, stirred for 72 h and the solvent was removed in vacuo. PTLC (8% CH_3OH/CH_2Cl_2) afforded **15** (2.0 mg, 87%) as a light tan solid identical in all respects with authentic material.

Uncatalyzed: A solution of **6** (3.2 mg, 0.007 mmol) in CH_3OH (0.4 mL) was treated with H_2O (0.4 mL) and stirred (25 °C, 60 h). The solvent was removed in vacuo. PTLC (5% CH_3OH/CH_2Cl_2) afforded **15** (1.4 mg, 95%) as a tan solid and **16** (1.4 mg, 71%) as a tan solid. For **16**: mp 78–81 °C dec; ^{1}H NMR (acetone-d_6, 400 MHz) δ 10.40 (br s, 1H), 8.43 (br s, 1H), 6.89 (s, 2H), 3.97 (s, 3H), 3.84 (s, 3H), 3.83 (s, 3H), 3.82 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 150.9, 140.8, 140.1, 130.7, 126.9, 124.6, 105.2, 98.8, 61.4, 56.5, 55.6, 52.9 ppm, the remaining signal was not detected and is believed to overlap with the peak at 150.9; IR (film) ν_{max} 3315, 2937, 2360, 1639, 1631, 1440, 1366, 1311, 1110 cm^{-1}; FABHRMS (NBA/NaI) *m/z* 265.1190 ($M^+ + H$, $C_{13}H_{17}N_2O_4$ requires 265.1188).

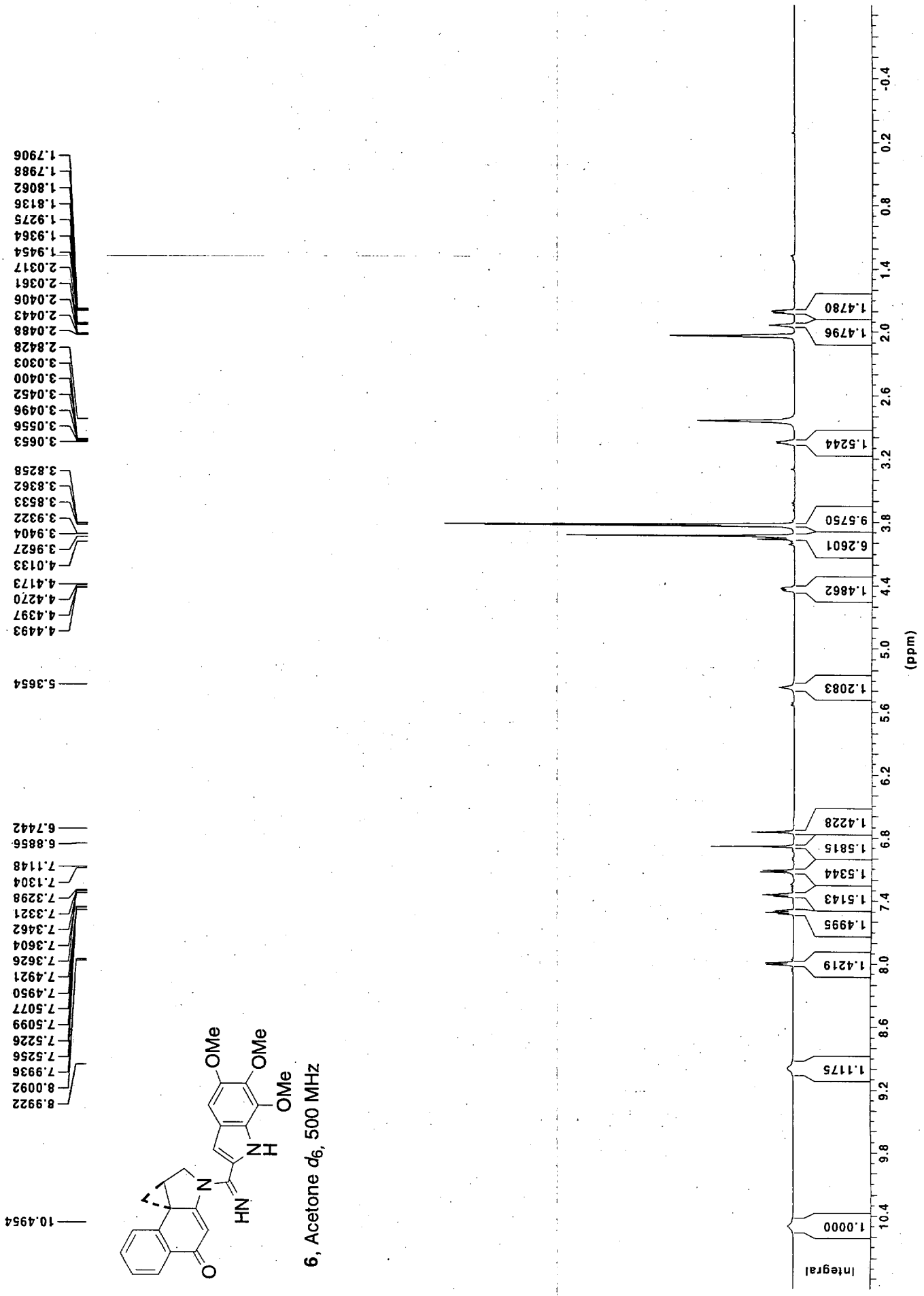
Solvolysis Reactivity. A sample of **4** (0.05 mg) was dissolved in CH_3OH (1.5 mL) and mixed with pH 3 aqueous buffer (1.5 mL). The pH 3 buffer contained 4:1:20 (v/v/v) 0.1 M citric acid, 0.2 M Na_2HPO_4, and H_2O, respectively. The solution was sealed and kept at 25 °C protected from light. The UV spectra was measured at hourly time intervals during the first 6–12 h, every day for the next week. The decrease in the long wavelength absorption at 360 nm (pH 3) was monitored. The solvolysis rate constant and the half-life were calculated from data recorded at the long wavelength from the least-squared treatment (r = 0.99) of the slope of the plot of time versed $\ln[(A_f - A_i)/(A_f - A)]$.

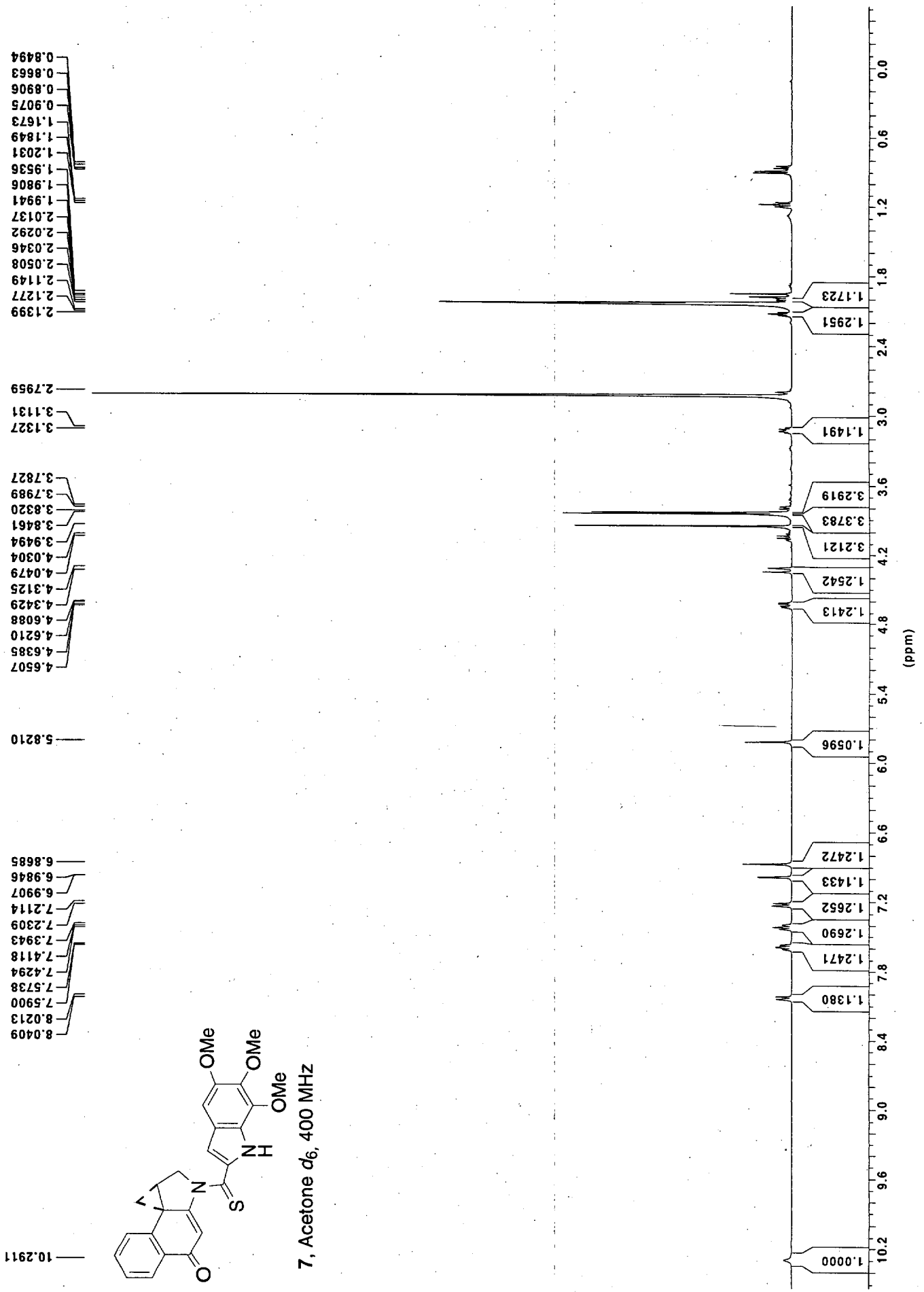
Similarly, **6** (0.05 mg) was dissolved in CH_3OH (1.5 mL) and mixed with pH 3 aqueous buffer (1.5 mL). The solution was sealed and kept at 25 °C protected from light. The UV spectra was measured at regular time intervals as described above. The increase in the long wavelength absorption at 314 nm (pH 3) was monitored. The solvolysis rate constant and the half-life were determined as detailed above (r = 0.99).

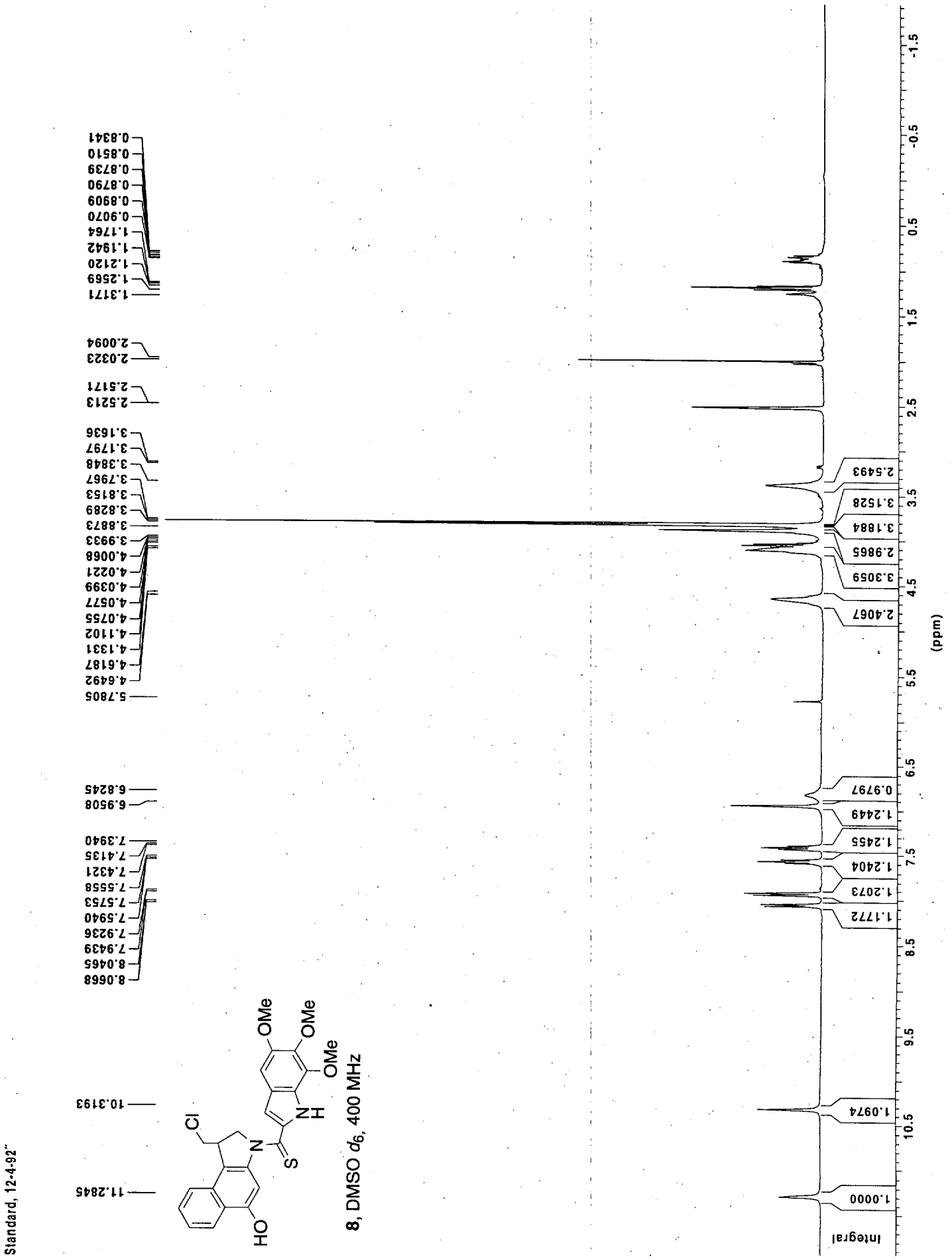
Similarly, **7** (0.05 mg) was dissolved in CH_3OH (1.5 mL) and mixed with pH 3 aqueous buffer (1.5 mL). The solution was sealed and kept at 25 °C protected from light. The UV spectra was measured at regular time intervals as described above. The decrease in the long wavelength absorption at 366 nm (pH 3) was monitored. The solvolysis rate constant and the half-life were determined as detailed above (r = 0.99).

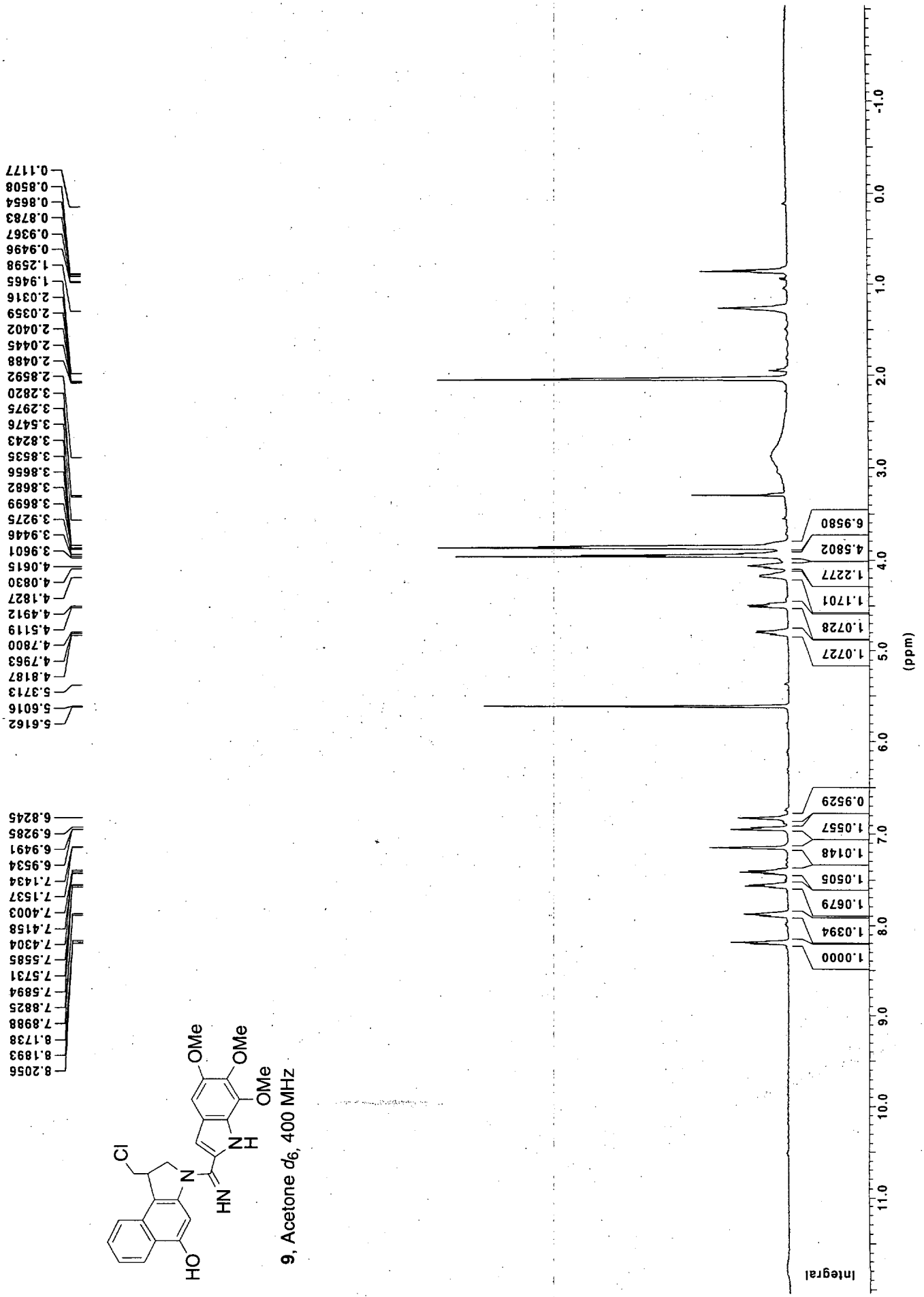


Supporting Information Figure. Thermally induced strand cleavage of w794 DNA (144 bp nucleotide no. 5238-138) after DNA-agent incubation with (+)-**1**, (+)- and (–)-**4**, **6**, **7** (25 °C, 24 h), removal of unbound agent by EtOH precipitation and 30 min thermolysis (100 °C) followed by denaturing 8% PAGE and autoradiography. Lanes 1 and 2, (+)-**1** (25 °C, 1×10^{-6} to 1×10^{-7} M); lanes 3 and 4, (+)-**4** (25 °C, 1×10^{-6} to 1×10^{-7} M); lanes 5, (–)-**4** (25 °C, 1×10^{-5} M); lanes 6–9, Sanger G, C, A and T sequencing standards; lane 10, control DNA; lanes 11–13, (+)-**7** (25 °C, 1×10^{-4} to 1×10^{-6} M); lanes 14–16, (–)-**7** (25 °C, 1×10^{-2} to 1×10^{-4} M); lanes 17–19, (+)-**6** (25 °C, 1×10^{-4} to 1×10^{-6} M); lanes 20–22, (–)-**6** (25 °C, 1×10^{-2} to 1×10^{-4} M).

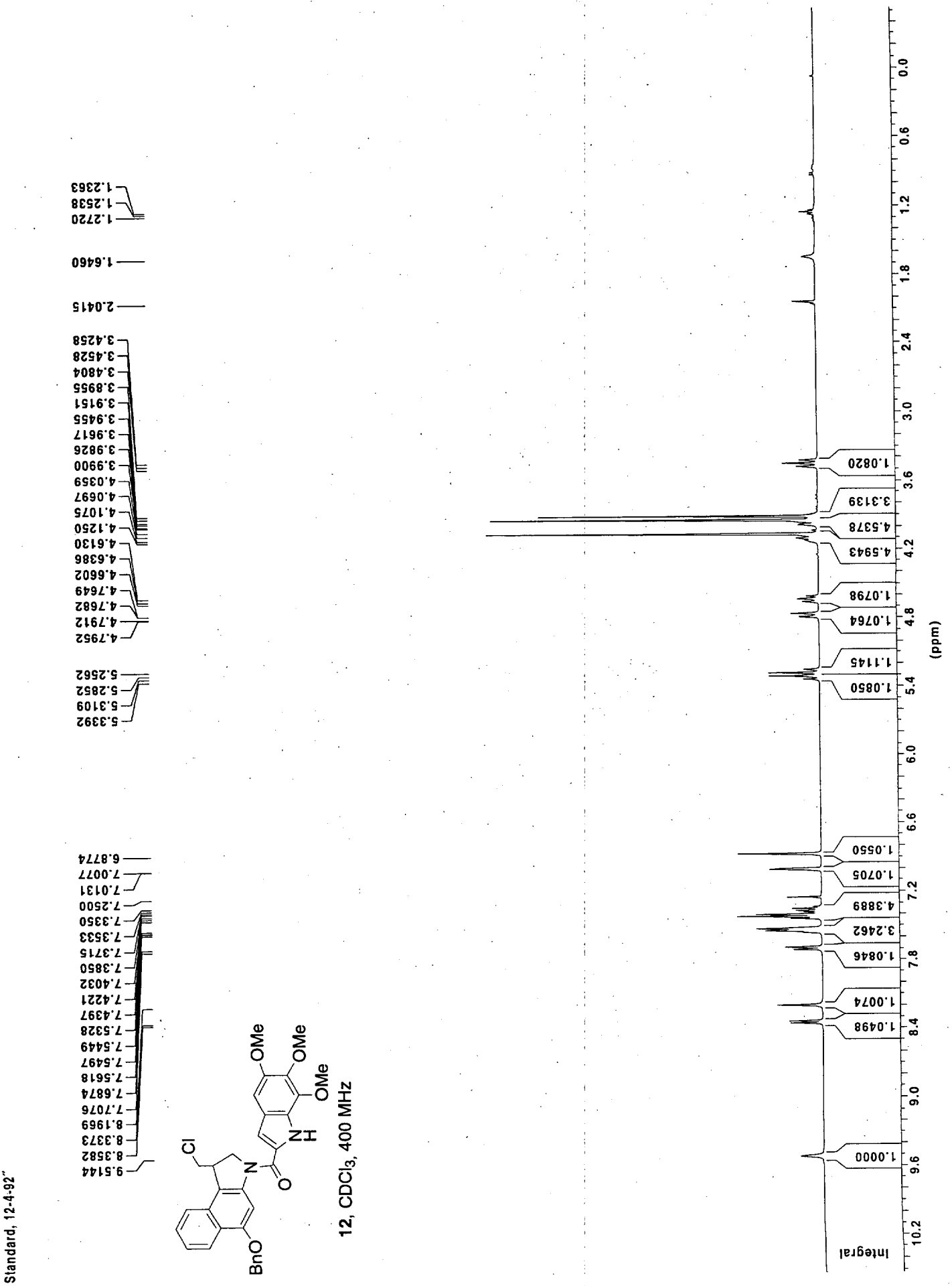


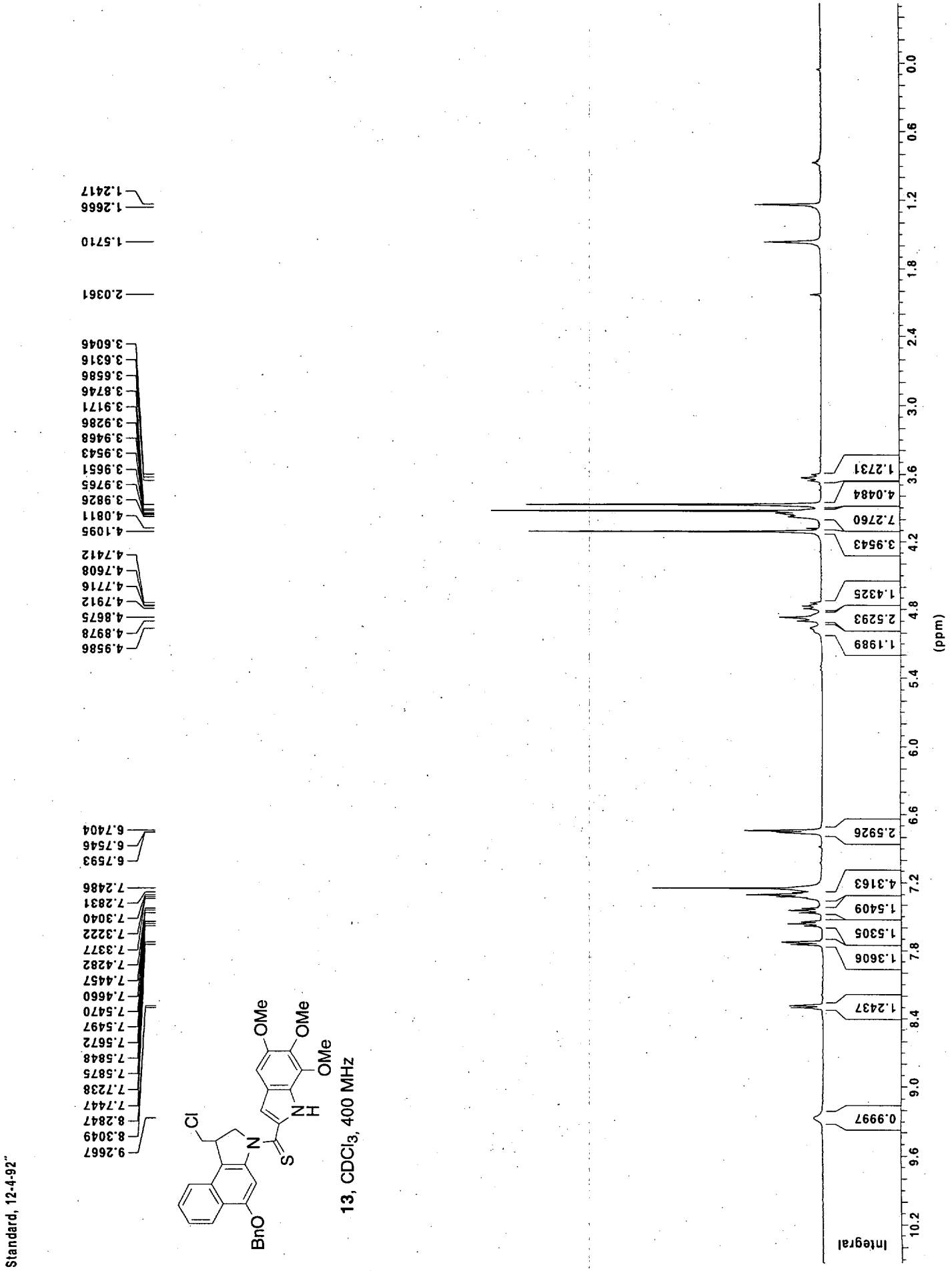


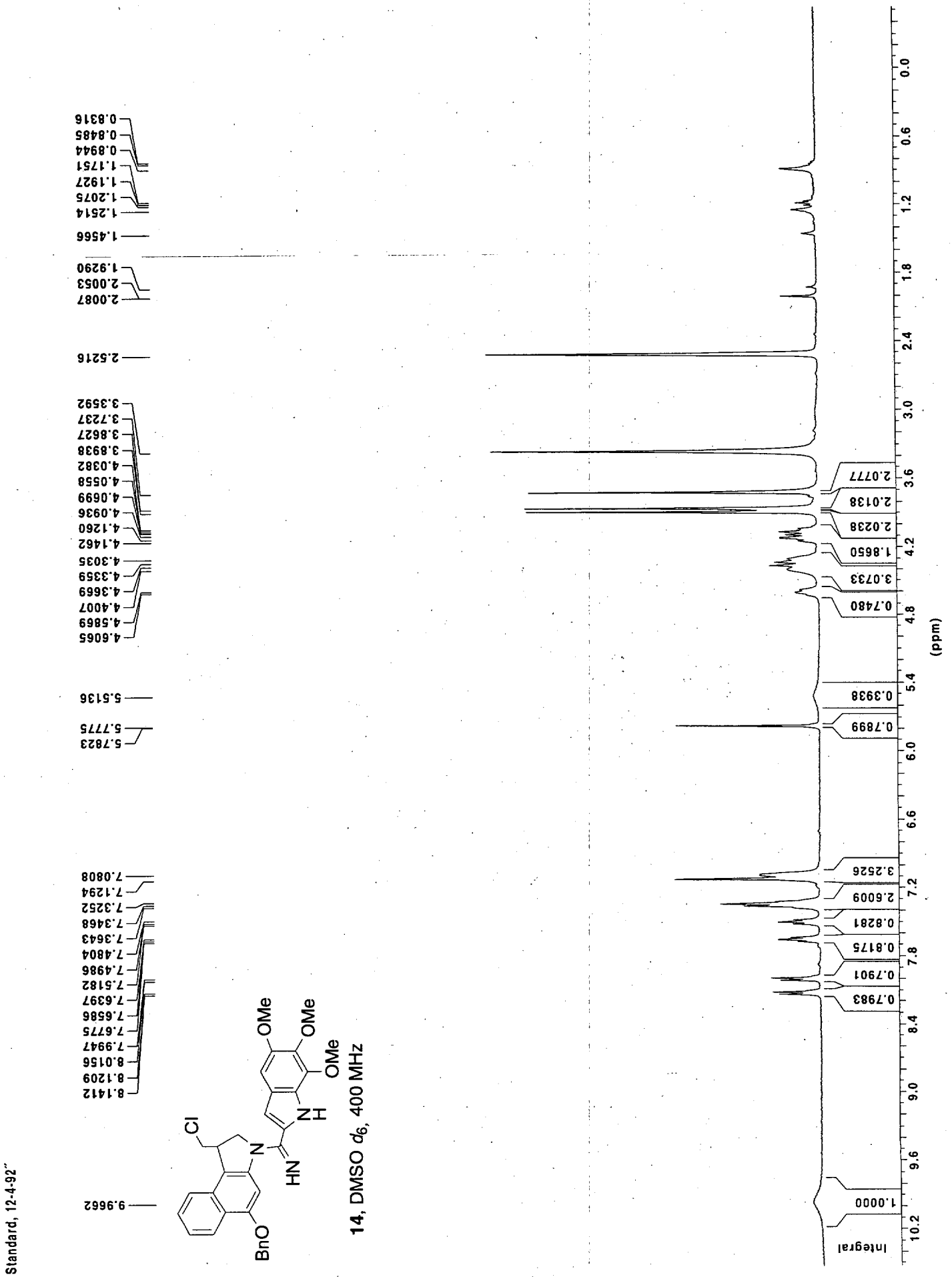


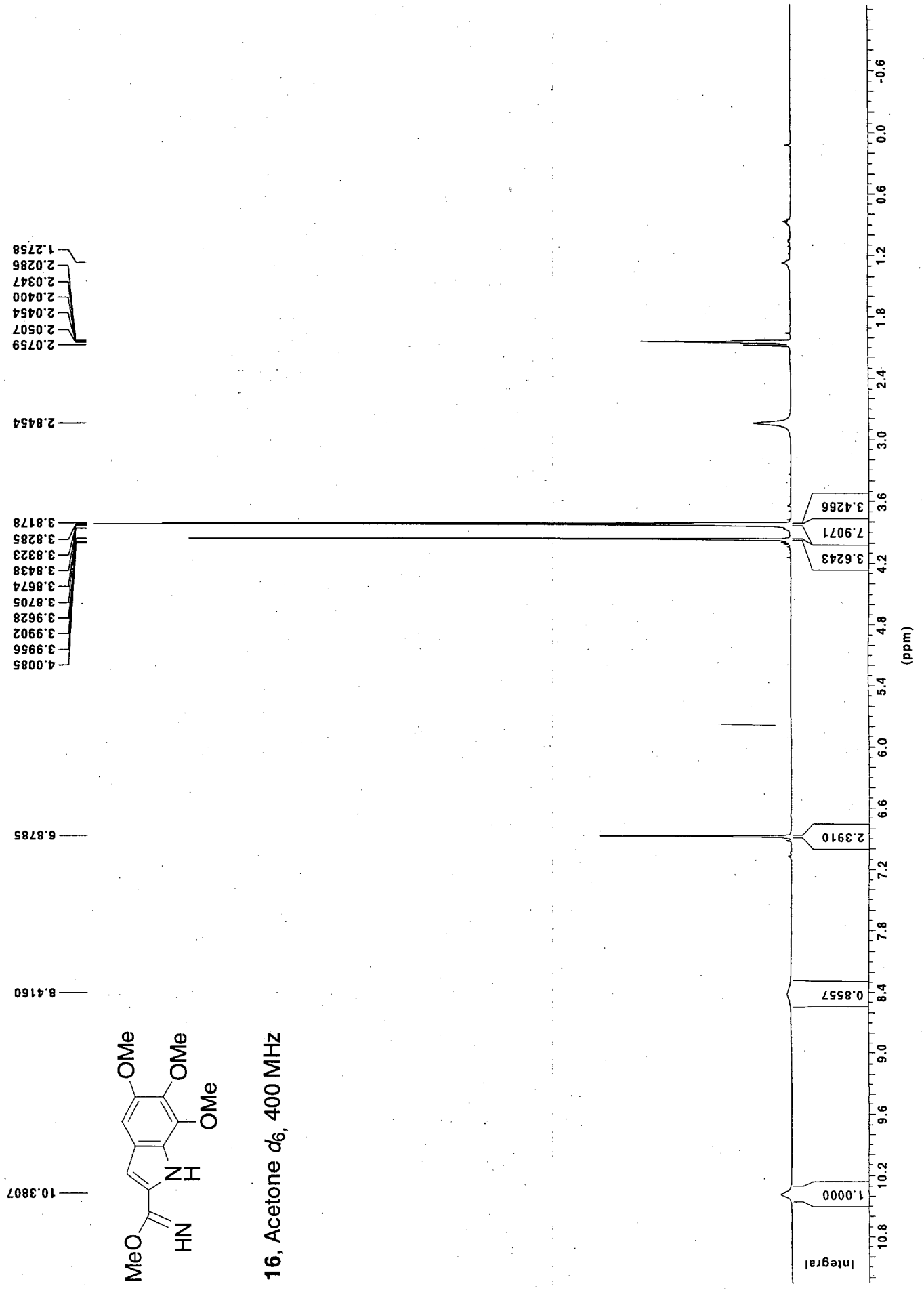


9, Acetone d_6, 400 MHz








OMe
OMe
OMe
N
H
NH
MeO
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6.8785
4.0085
3.9956
3.9902
3.9628
3.8705
3.8674
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3.8323
3.8285
3.8178
2.8454
2.0759
2.0507
2.0454
2.0400
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3.6243
2.3910
0.8557
1.0000
Integral
(ppm)