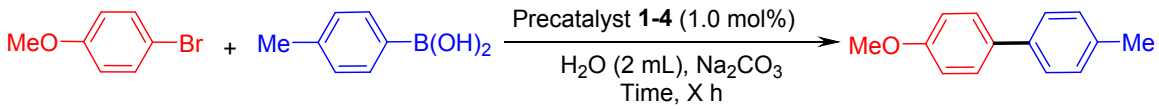
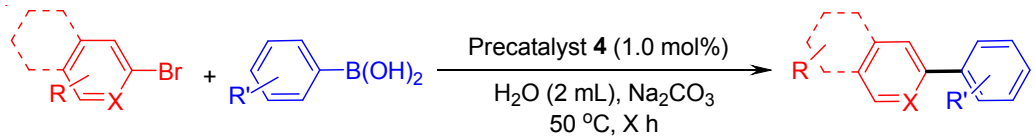
Table 1: **Initial screening in Suzuki-Miyaura cross-coupling of (hetero)aryl halides** [a,b]

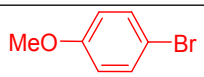
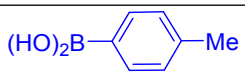
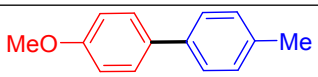
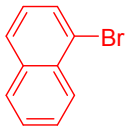
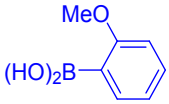
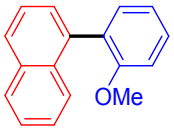
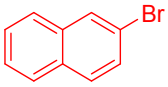
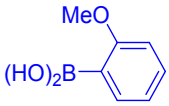
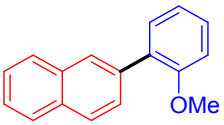
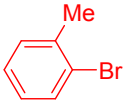
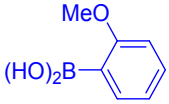
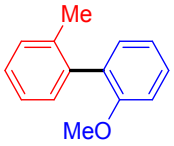
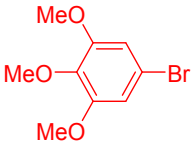
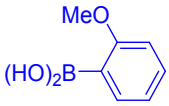
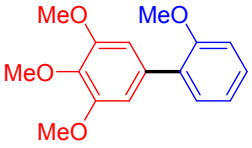
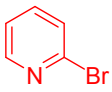
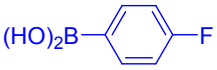
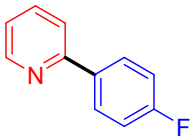
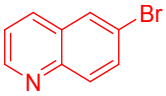
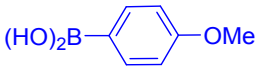
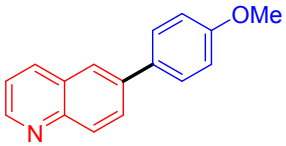
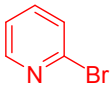
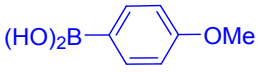
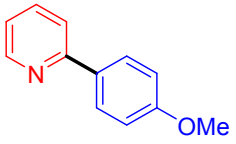
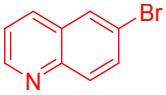
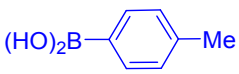
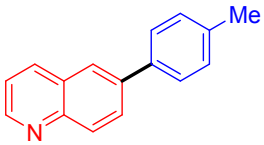


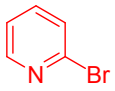
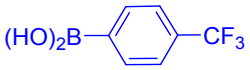
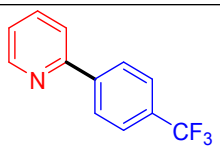
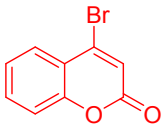
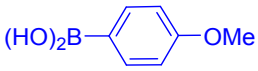
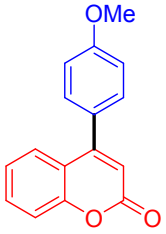
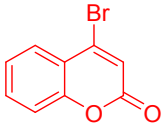
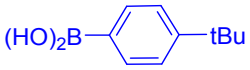
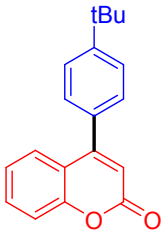
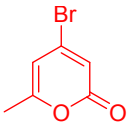
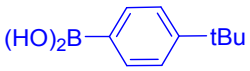
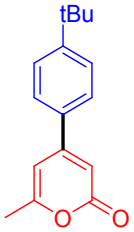
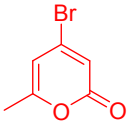
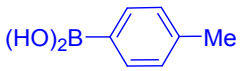
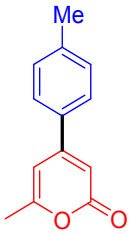
S. No.	*Pd-Complexes*	*Temp °C*	*Time (h)*	*Yield%*
1	$Pd(OAc)_2/PPh_3$	r.t.	3.0	15
2	Pd_2dba_3/PPh_3	r.t.	3.0	19
3	$Pd(OAc)_2$/X-Phos	r.t.	3.0	29
4	$Pd(OAc)_2$/TPA	r.t.	3.0	43
5	**1**	r.t.	3.0	52
6	**2**	r.t.	3.0	48
7	**3**	r.t.	3.0	37
8	**4**	**r.t.**	**3.0**	**65**
9	$[PdCl_2(PPh_3)_2]$	r.t.	3.0	0
10	$[Pd(C_6H_5CN)_2Cl_2]$	r.t.	3.0	0
11	Hermann Beller	r.t.	3.0	0
12	Combiphos	r.t.	3.0	0
13	$[PdCl_2(TPA)_2]$	r.t.	3.0	41
14	$[PdBr_2(TPA)_2]$	r.t.	3.0	57
15	$[PdI_2(TPA)_2]$	r.t.	3.0	23
16	**4**	**50**	**0.5**	**97**
17	**4**	50	2.0	89[c]
18	**4**	50	6.0	58[d]
19	**4**	50	24.0	18[e]
20	**4**	r.t.	3.0	94[f]

[a] Aryl boronic acid (1.0 mmol), **aryl bromide** (1.0 mmol), **Catalyst** (1.0 mol%), 2 mL H_2O, Na_2CO_3 (2.0 mmol). [b] Yields are isolated yields and an average of two runs. [c] **Catalyst** concentration (0.5 mol%- TON: 178). [d] Catalyst concentration (0.1 mol%- TON: 580). [e] **Catalyst** concentration (0.05 mol%- TON: 900). [f] Instead of 4-Bromoanisole, 4-Iodoanisole was employed as the substrate.

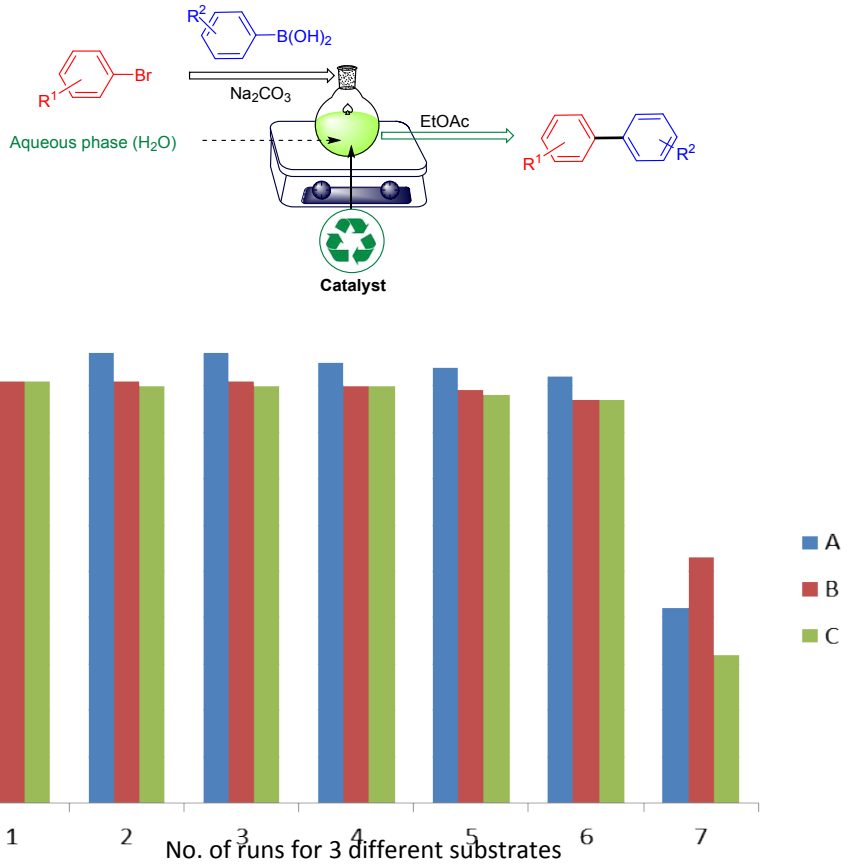
Table 2: **Scope study for Suzuki-Miyaura cross-coupling of (hetero)aryl halides** [a,b]



S. No.	*Aryl halide*	*Aryl Boronic Acid*	*Product*	*Time h*	*Yield%*
1				0.5	97
2				2.0	91
3				2.0	84
4				2.0	80
5				3.0	93
6				0.5	91
7				2.0	88
8				0.5	96
9				2.0	69

10				0.5	87
11				0.5	85
12				0.5	89
13				0.5	97
14				0.5	85

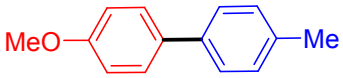
[a] Aryl boronic acid (1.0 mmol), aryl bromide (1.0 mmol), Catalyst (1.0 mol%), 2 mL H_2O, Na_2CO_3 (2.0 mmol). [b] Isolated yields.



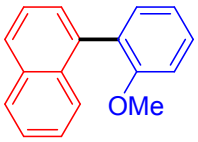
Scheme 2: Recycling studies for precatalyst **4**.

Representative procedure for Suzuki-Miyaura cross-coupling of aryl (heteroaryl)bromides:

A solution of precatalyst **4** (0.01 mmol, 1.0 mol%) in degassed H_2O (2.0 mL) was stirred for 5 min at ambient temperature under N_2. Then, 4-bromoanisole(187 mg, 1.0 mmol) was added via syringe and the solution stirred for 5 min. Thereafter, 4-methylphenyl boronic acid (136 mg, 1.1 mmol) was added along with Na_2CO_3 (2.0 mmol), and the resulting solution was stirred at 50 °C for 0.5 h. At ambient temperature, more H_2O (10 mL) was added and the organic products were extracted with EtOAc (3 x 10 mL). The combined organic layers were concentrated *in vacuo* and the remaining residue was purified by column chromatography (*n*-hexane/EtOAc: 200/1) to yield **4-Methoxy-4'-biphenyl** (97%) as a colorless solid.

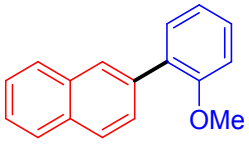


4-Methoxy-4'-methylbiphenyl: ^{1}H-NMR(300 MHz, $CDCl_3$): δ = 7.43 (d, J = 8.2 Hz, 2H), 7.42 (d, J = 8.3 Hz, 2H), 7.19 (d, J = 7.9 Hz, 2H), 7.00- 6.87 (m, 2H), 3.87 (s, 3H), 2.35 (s, 3H). ^{13}C-NMR(75 MHz, $CDCl_3$): δ = 158.7, 137.8, 136.3, 133.7, 129.4, 127.9, 126.6, 114.1, 55.3, 21.0. MS (EI) *m/z* (relative intensity) 198 (100) [M^+].The spectral data were in accordance with those reported in the literature.

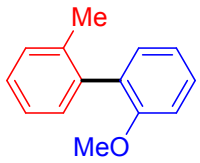


1-(2′-Methoxyphenyl)naphthalene: ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.87 (t, J = 7.5 Hz, 2H), 7.59 (d, J = 8.2 Hz, 1H), 7.53-7-48 (m, 1H), 7.50-7.34 (m, 4H), 7.29-7.26 (m, 1H), 7.12-7.01 (m, 2H), 3.69 (s, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 157.2, 136.9, 133.4, 132.0, 131.9, 129.5, 128.9, 128.0, 127.6, 127.2, 126.4, 125.6, 125.5, 125.3, 120.5, 110.9, 55.5. MS (EI), *m/z* (relative

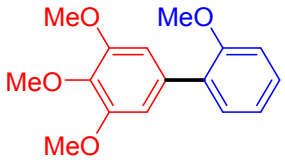
intensity) 234 (100) [M^+].The spectral data were in accordance with those reported in the literature.



2-(2′-Methoxyphenyl)naphthalene: ^{1}H-NMR(300 MHz, $CDCl_3$): δ = 7.96 (s, 1H), 7.91–7.82 (m, 3H), 7.70-7.65 (m,1H), 7.50–7.32 (m, 4H), 7.11-7.00 (m, 2H), 3.83 (s, 3H). ^{13}C-NMR(75 MHz, $CDCl_3$): δ = 156.7, 136.2, 133.4, 132.4, 131.1, 130.7, 128.8, 128.1, 128.0, 127.9, 127.1, 125.9, 125.8, 120.9, 111.3, 55.6. MS (EI) *m/z* (relative intensity) 234 (94) [M^+].The spectral data were in accordance with those reported in the literature.

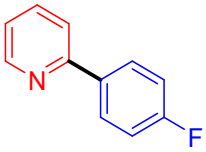


2-Methoxy-2′-methylbipheyl:^{1}H-NMR(300 MHz, $CDCl_3$): δ = 7.417-36 (m, 1H), 7.35–7.20 (m, 5H), 7.08-7.02 (m,1H), 7.03 (d, J = 8.2 Hz, 1H), 3.82 (s, 3H), 2.22 (s, 3H). ^{13}C-NMR(75 MHz, $CDCl_3$): δ = 156.4, 138.5, 136.7, 130.9, 130.8, 129.9, 129.4, 128.4, 127.2, 125.3, 120.3, 110.6, 55.4, 20.0. MS (EI) *m/z* (relative intensity) 198 (100) [M^+].The spectral data were in accordance with those reported in the literature.

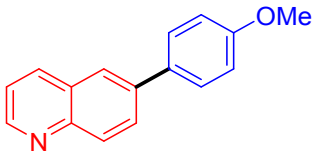


2-Methoxy-3′,4′,5′-trimethoxybiphenyl: ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.32-7.26 (m, 2H), 7.04-6.91 (m, 2H), 6.76 (s, 2H), 3.87 (s, 3H), 3.85 (s, 6H), 3.84 (s, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 156.2, 152.7, 137.0, 134.0, 130.7, 130.5, 128.6, 120.8, 111.2, 106.8, 60.8, 56.1,

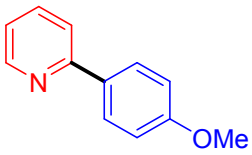
55.6. MS (EI), *m/z* (relative intensity) 274 (100) [M^+].The spectral data were in accordance with those reported in the literature.



2-(4-Fluorophenyl)pyridine: ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.67-8.61 (m, 1H), 8.03–7.93 (m, 2H), 7.77–7.62 (m, 2H), 7.24 – 7.10 (m, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 163.4, 156.4, 149.6, 136.8, 135.5, 128.6, 122.0, 120.2, 115.6. MS (EI) *m/z* (relative intensity) 173 (100) [M^+].The spectral data were in accordance with those reported in the literature.

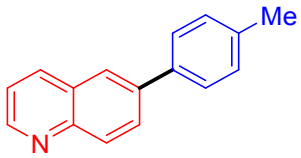


6-(4′-Methoxyphenyl)quinoline: ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.89-8.84 (m, 1H), 8.18-8.12 (m, 2H), 7.96-7.92 (m, 2H), 7.66 (d, J = 8.1 Hz, 2H), 7.41-7.37 (m, 1H), 7.02 (d, J = 8.1 Hz, 2H), 3.86 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 159.5, 150.0, 147.4, 138.9, 136.1, 132.7, 129.7, 129.0, 128.5, 128.4, 124.6, 121.4, 114.4, 55.4. MS (EI), *m/z* (relative intensity) 235 (100) [M^+].The spectral data were in accordance with those reported in the literature.

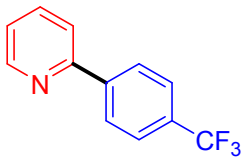


2-(4-Methoxyphenyl)pyridine: ^{1}H-NMR(300 MHz, $CDCl_3$): δ = 8.63-8.58 (m, 1H), 7.93 (d, J = 8.5 Hz, 2H), 7.73–7.61 (m, 2H), 7.14 (m, 1H), 6.98 (d, J = 8.5 Hz, 2H), 3.84 (s, 3H). ^{13}C-NMR(75 MHz, $CDCl_3$): δ = 160.6, 157.3, 149.7, 136.8, 132.2, 128.3, 121.5, 119.9, 114.3, 55.5.

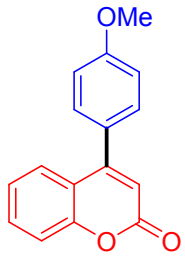
MS (EI) *m/z* (relative intensity) 185 (100) [M^+].The spectral data were in accordance with those reported in the literature.



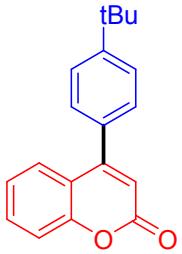
6-(4′-Methylphenyl)quinoline: ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.90-8.85 (m, 1H), 8.18-8.14 (m, 2H), 7.98-7.95 (m, 2H), 7.60 (d, J = 8.1 Hz, 2H), 7.41-7.37 (m, 1H), 7.29 (d, J = 8.1 Hz, 2H), 2.41 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 150.1, 147.5, 139.1, 137.6, 137.3, 136.1, 129.7, 129.6, 129.1, 128.4, 127.2, 125.0, 121.3, 21.1. MS (EI), *m/z* (relative intensity) 219 (100) [M^+].The spectral data were in accordance with those reported in the literature.



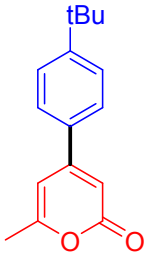
2-{4-(Trifluoromethyl)phenyl}pyridine: ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.80–8.66 (m, 1H), 8.11 (d, J = 8.2 Hz, 2H), 7.87–7.65 (m, 4H), 7.30-7.27 (m, 1H).^{13}C NMR (75 MHz, $CDCl_3$): δ = 155.8, 149.9, 142.6, 136.8, 130.9, 127.1, 125.6, 124.2, 122.9, 120.8.MS (EI) *m/z*(relative intensity) 223 (100) [M^+].The spectral data were in accordance with those reported in the literature.



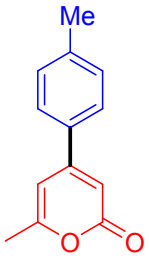
4-(4-Methoxyphenyl)-*2H*-benzopyran-2-one:^{1}H NMR (300 MHz, $CDCl_3$) δ 3.80 (s, 3H), 6.30 (s, 1H), 7.05 (d, J = 9.0 Hz, 2H), 7.21-7.27 (m, 1H), 7.38-7.44 (m, 3H), 7.51-7.58 (m, 2H); ^{13}C NMR (75 MHz) δ 161.0, 160.9, 155.4, 154.3, 131.9, 130.1, 127.5, 126.0, 124.1, 119.2, 117.4, 114.6, 114.4, 55.5. MS (EI) *m/z* (relative intensity) 253 (100, M + H^+).The spectral data were in accordance with those reported in the literature.



4-(4-*tert*Butylphenyl)-*2H*-benzopyran-2-one: M.p. 112-113 ^{o}C.^{1}H NMR (300 MHz, $CDCl_3$) δ 1.30 (s, 9H), 6.30 (s, 1H), 7.13-7.18 (m, 1H), 7.31-7.38 (m, 3H), 7.44-7.57 (m, 4H); ^{13}C NMR (75 MHz) δ 161.0, 155.7, 154.2, 153.1, 132.3, 130.1, 128.3, 127.2, 126.0, 124.1, 119.1, 117.3, 114.9, 34.5, 31.3. MS (EI) *m/z* (relative intensity) 278 (100, M^+).The spectral data were in accordance with those reported in the literature.



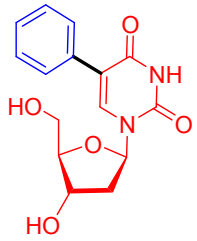
4-(4-*tert*Butylphenyl)-6-methyl-2-pyranone: ^{1}H NMR (500 MHz, $CDCl_3$) 7.70 (d, J = 7.4 Hz, 2H), 7.49 (d, J = 7.4 Hz, 2H, 6.69 (s, 1H), 6.44 (s, 1H), 2.26 (s, 3H), 1.28 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) 162.8, 162.6, 154.8, 154.1, 132.3, 127.1, 126.3, 106.6, 103.1, 35.0, 31.3, 20.0; MS (EI) *m/z* (relative intensity) 242 (100, M^+);The spectral data were in accordance with those reported in the literature.



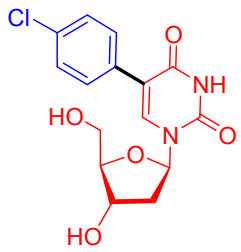
4-(4-Methylphenyl)-6-methyl-2-pyranone: ^{1}H NMR (500 MHz, $CDCl_3$): 7.68 (d, J = 7.9 Hz, 2H), 7.30 (d, J = 7.9 Hz, 2H), 6.70 (s, 1H), 6.44 (s, 1H), 2.34 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 162.9, 162.6, 154.8, 141.3, 132.2, 130.1, 127.3, 106.4, 103.0, 21.3, 20.0; MS (EI) *m/z* (relative intensity) 200 (100, M^+);The spectral data were in accordance with those reported in the literature.

General procedure for Recycling studies of aryl bromides with aryl boronic acids using precatalyst: A solution of precatalyst **4** (0.01 mmol, 1.0 mol%) in degassed H_2O (2.0 mL) was stirred for 5 min at ambient temperature under N_2. Then, 4-bromoanisole(187 mg, 1.0 mmol) was added via syringe and the solution stirred for 5 min. Thereafter, 4-methylphenyl boronic acid (136 mg, 1.1 mmol) was added along with Na_2CO_3 (2.0 mmol), and the resulting solution was stirred at 50 °C for 0.5 h. At ambient temperature, the organic products were extracted with EtOAc (2 x 10 mL). The catalytic aqueous layer was recharged with substrates, base and the reaction was again continued for the reported time at 50 ^{o}C.

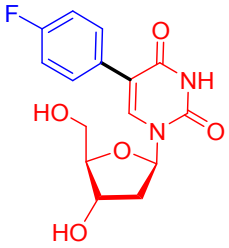
General procedure for Suzuki-Miyaura cross-coupling of 5-iodo-2′-deoxyuridine with aryl boronic acids: A solution of precatalyst **3** (0.005 mmol, 1.0 mol%) in degassed H_2O (1.0 mL) was stirred for 5 min at ambient temperature under N_2. Then, 5-iodo-2′-deoxyuridine (177 mg, 0.5 mmol) was added and the solution stirred for 5 min at 80 °C. Thereafter, phenyl boronic acid (90 mg, 0.75 mmol) was added along with Et_3N (1.0 mmol) and degassed water (2.0 mL). The resulting solution was then stirred at 80 °C for 6.0 h. After the completion of reaction the solvent was removed under vacuo and the resultant residue obtained was purified using column chromatography in CH_2Cl_2: MeOH solvent system (96:4) to afford the desired product as a white solid.



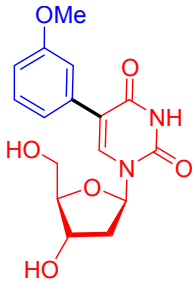
5-Phenyl-2′-deoxyuridine: White solid. ^{1}H (400 MHz, DMSO-d_6) 11.53 (s, 1H), 8.18 (s, 1H), 7.55 (d, 2H, J = 7.4 Hz), 7.38–7.27 (m, 3H), 6.27 (t, 1H, J = 6.5 Hz), 5.24 (d, 1H, J = 4.0 Hz), 5.14 (t, 1H, J = 4.5 Hz), 4.31 (s, 1H), 3.82 (d, 1H, J = 2.8 Hz), 3.65–3.56 (m, 2H), 2.29–2.12 (m, 2H). ^{13}C (101 MHz, DMSO-d_6) 162.4, 150.3, 138.3, 133.5, 128.4, 128.2, 127.5, 113.7, 87.8, 84.7, 70.5, 61.2, 40.1. MS (ESI): m/z = 305 [M + H^+], 327 [M + Na^+]. The spectral data were in accordance with those reported in the literature.



5-(4-Chlorophenyl)-2´-deoxyuridine: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.56 (s, 1H), 8.27 (s, 1H), 7.59 (dd, 2H, J = 8.7, 5.2 Hz), 7.43 (dd, 2H, J = 8.8, 5.4 Hz), 6.22 (t, 1H, J = 6.5 Hz), 5.26 (d, 1H, J = 4.0 Hz), 5.14 (t, 1H, J = 4.5 Hz), 4.29-4.27 (m, 1H), 3.82 (q, 1H, J = 3.1 Hz), 3.65-3.56 (m, 2H), 2.28-2.13 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.3, 150.1, 132.4, 132.0, 129.8, 128.4, 112.4, 87.7, 84.8, 70.3, 61.0, 40.1. MS (ESI): m/z = 339 [M + H^+], 361 [M + Na^+].

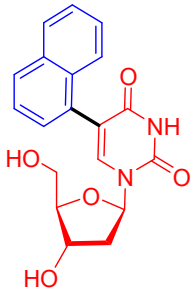


5-(4-Fluorophenyl)-2´-deoxyuridine: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.53 (s, 1H), 8.20 (s, 1H), 7.58 (dd, 2H, J = 8.4, 5.1 Hz), 7.20 (dd, 2H, J = 8.7, 5.3 Hz), 6.23 (t, 1H, J = 6.5 Hz), 5.26 (d, 1H, J = 4.1 Hz), 5.12 (t, 1H, J = 4.4 Hz), 4.31-4.26 (m, 1H), 3.81 (q, 1H, J = 3.1 Hz), 3.62-3.58 (m, 2H), 2.27-2.13 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.7, 161.8 (d, 1C, $J_{C\text{-}F}$ = 185.4 Hz), 150.0, 138.1, 129.7 (d, 2C, $J_{C\text{-}F}$ = 7.9 Hz), 129.2 (d, 1C, $J_{C\text{-}F}$ = 3.4 Hz), 115.0 (d, 2C, J_{CF} = 21.2 Hz), 112.5, 87.6, 84.5, 70.2, 60.9, 40.0. MS (ESI): m/z = 323 [M + H^+], 345 [M + Na^+].

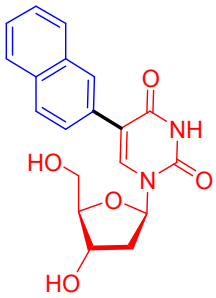


5-(3-Methoxyphenyl)-2´-deoxyuridine: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.51 (s, 1H), 8.21 (s, 1H), 7.27 (t, 1H, J = 7.9 Hz), 7.15 (s, 1H), 7.12 (d, 1H, J = 7.9 Hz), 6.88 (dd, 1H, J = 6.9, 2.2

Hz), 6.24 (t, 1H, J = 6.4 Hz), 5.27 (d, 1H, J = 4.1 Hz), 5.12 (t, 1H, J = 4.3 Hz), 4.30-4.27 (m, 1H), 3.83-3.81 (m, 1H), 3.76 (s, 3H), 3.60 (ddd, 2H, J = 24.3, 12.0, 3.1 Hz), 2.27-2.13 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.1, 159.1, 150.0, 138.3, 134.0, 129.2, 120.2, 113.5, 113.5, 112.8, 87.6, 84.6, 70.3, 61.0, 55.0, 40.1. MS (ESI): m/z = 335 [M + H^+], 357 [M + Na^+].

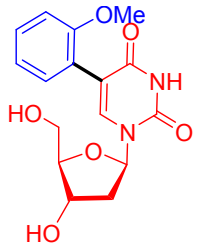


5-(1-Naphthyl)-2´-deoxyuridine: White solid. NMR ^{1}H (400 MHz, DMSO-d_6) δ = 11.57 (s, 1H), 8.03 (s, 1H), 7.96–7.93 (m, 2H), 7.73 (d, 1H, J = 8.0 Hz), 7.54-7.46 (m, 3H), 7.40-7.38 (m, 1H), 6.28 (t, 1H, J = 6.2 Hz), 5.24 (d, 1H, J = 2.1 Hz), 4.85-4.83 (m, 1H), 3.77 (d, 1H, J = 2.6 Hz), 3.48-3.45 (m, 1H), 2.27–2.15 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) d = 162.6, 150.5, 139.5, 133.2, 132.1, 131.4, 128.4, 128.2, 126.1, 125.9, 125.5, 113.7, 87.5, 84.4, 70.4, 61.0, 40.1. MS (ESI): m/z = 355 [M + H^+], 377 [M + Na^+].

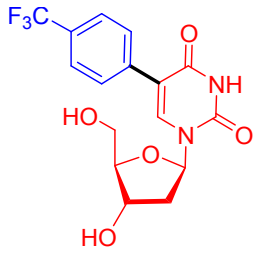


5-(2-Naphthyl)-2´-deoxyuridine: White solid. NMR ^{1}H (400 MHz, DMSO-d_6) δ = 11.59 (s, 1H), 8.37 (s, 1H), 8.14 (s, 1H), 7.93–7.88 (m, 3H), 7.71-7.68 (m, 1H), 7.54-7.48 (m, 2H), 6.27 (t, 1H, J = 6.2 Hz), 5.28 (d, 1H, J = 1.9 Hz), 5.19-5.17 (m, 1H), 4.32 (s, 1H), 3.84 (d, 1H, J = 2.8 Hz), 3.67-3.58 (m, 2H), 2.33–2.15 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) d = 162.4, 150.0, 138.6, 132.9, 132.1, 130.9, 128.1, 127.4, 126.5, 126.3, 126.2, 126.1, 113.3, 87.5, 84.6, 70.1, 60.9,

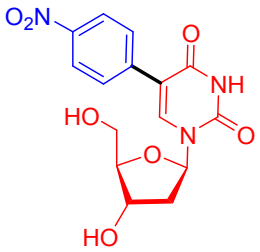
40.1. MS (ESI): m/z = 355 [M + H^+], 377 [M + Na^+]. The spectral data were in accordance with those reported in the literature.



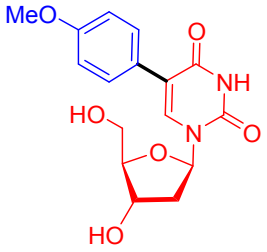
5-(2-Methoxyphenyl)-2´-deoxyuridine: White solid. NMR 1H (400MHz, DMSO-d6) d = 11.39 (s, 1H), 7.91 (s, 1H), 7.26 (t, 1H, *J* = 7.6 Hz), 7.20 (dd, 1H, *J* = 7.1, 0.9 Hz), 7.01 (d, 1H, *J* = 8.2 Hz), 6.92 (t, 1H, *J* = 7.2 Hz), 6.23 (t, 1H, *J* = 7.2 Hz), 5.22 (s, 2H), 4.89 (s, 1H), 4.22 (s, 1H), 3.70 (s, 3H), 3.50 (d, 2H, *J* = 2.0 Hz), 3.32 (s, 2H), 2.17–2.11 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d6) d = 161.9, 157.2, 150.3, 139.0, 131.3, 129.2, 121.9, 120.1, 111.4, 87.5, 84.2, 70.6, 61.3, 55.4, 40.1. MS (ESI): m/z = 335 [M + H^+], 357 [M + Na^+]. The spectral data were in accordance with those reported in the literature.



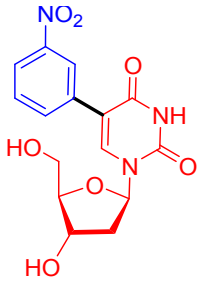
5-(4-Trifluorophenyl)-2´-deoxyuridine: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.61 (s, 1H), 8.40 (s, 1H), 7.81-7.78 (m, 2H), 7.72-7.70 (m, 2H), 6.24-6.20 (m, 1H), 5.27-5.15 (m, 2H), 4.31-4.29 (m, 1H), 3.83-3.81 (m, 1H), 3.67-3.57 (m, 2H), 2.30-2.15 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ . MS (ESI): m/z = 373 [M + H^+], 395 [M + Na^+].



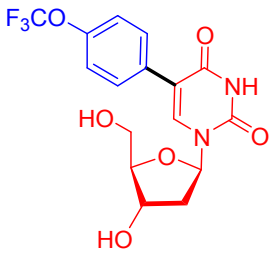
5-(4-Nitrophenyl)-2´-deoxyuridine: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.68 (s, 1H), 8.53-8.49 (m, 1H), 8.23-8.17 (m, 2H), 7.91-7.88 (m, 2H), 6.22-6.20 (m, 1H), 5.27-5.22 (m, 2H), 4.31 (s, 1H), 3.83-3.81 (m, 1H), 3.66-3.63 (m, 2H), 2.27-2.21 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ MS (ESI): m/z = 350 [M + H^+], 372 [M + Na^+].



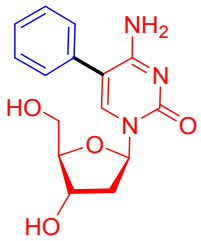
5-(4-Methoxyphenyl)-2´-deoxyuridine: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.45 (s, 1H), 8.10 (s, 1H), 7.48 (d, J = 7.9 Hz, 2H), 6.92 (d, J = 7.8 Hz, 2H), 5.25-5.23 (m, 1H), 5.10-5.08 (m, 1H), 4.30-4.27 (m, 1H), 3.81-3.79 (m, 1H), 3.76 (s, 3H), 3.76-3.55 (m, 2H), 2.26-2.11 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ . MS (ESI): m/z = 335 [M + H^+], 357 [M + Na^+].



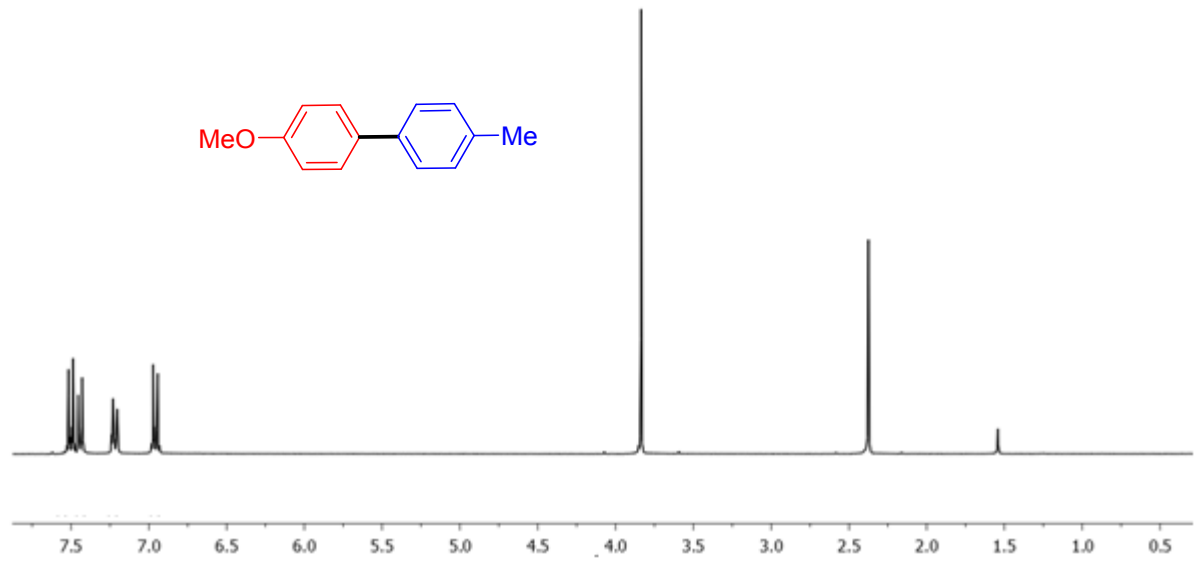
5-(3-Nitrophenyl)-2´-deoxyuridine: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.67 (s, 1H), 8.52-8.46 (m, 2H), 8.17-8.14 (m, 1H), 7.99-7.97 (m, 1H), 7.68-7.64 (m, 1H), 6.23-6.20 (m, 1H), 5.28-5.17 (m, 2H), 4.31 (s, 1H), 3.84-3.82 (m, 1H), 3.67-3.58 (m, 2H), 2.30-2.16 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ . MS (ESI): m/z = 350 [M + H^+], 372 [M + Na^+].



5-(4-Trifluoromethoxyphenyl)-2´-deoxyuridine: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.57 (s, 1H), 8.28 (s, 1H), 7.68-7.66 (m, 2H), 7.37-7.35 (m, 2H), 6.24-6.21 (m, 1H), 5.26-5.12 (m, 2H), 4.30-4.28 (m, 1H), 3.83-3.81 (m, 1H), 3.67-3.56 (m, 2H), 2.29-2.13 (m, 2H) . ^{13}C NMR (100 MHz, DMSO-d_6) δ . MS (ESI): m/z = 389 [M + H^+], 411 [M + Na^+].



5-Phenyl-2´-deoxycytidine: ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.88 (s, 1H), 7.42-7.33 (m, 6H), 6.44 (s, 1H), 6.20 (t, J = 6.2 Hz, 1H), 5.21-5.19 (m, 1H), 4.96 (s, 1H), 4.22 (s, 1H), 3.77 (s, 1H), 3.54-3.51 (m, 2H), 2.13-2.05 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.1, 154.3, 140.2, 133.7, 129.0, 128.8, 127.6, 107. 7, 87.3, 85.1, 70.1, 61.0, 40.5. MS (ESI): m/z = 304 [M + H^+], 326 [M + Na^+].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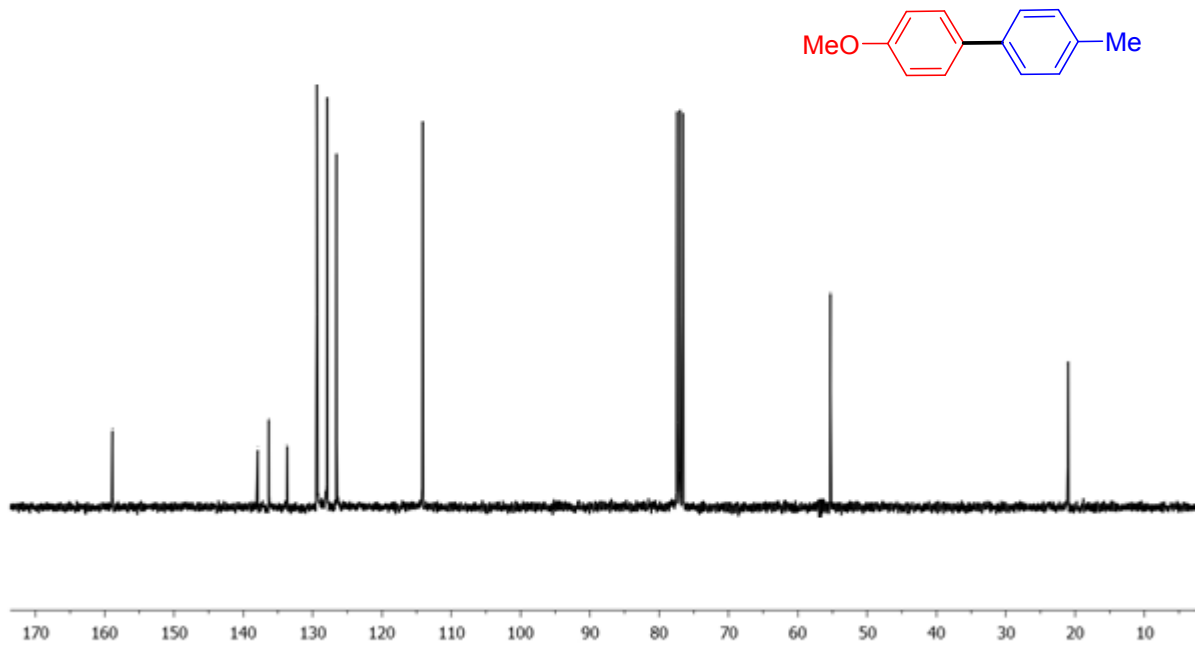
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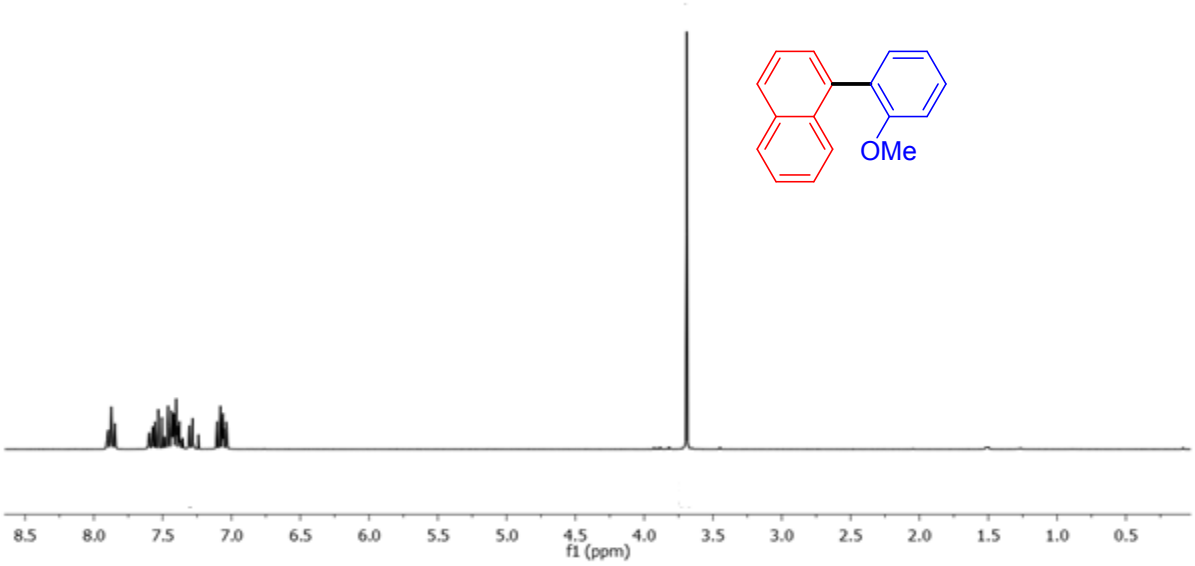
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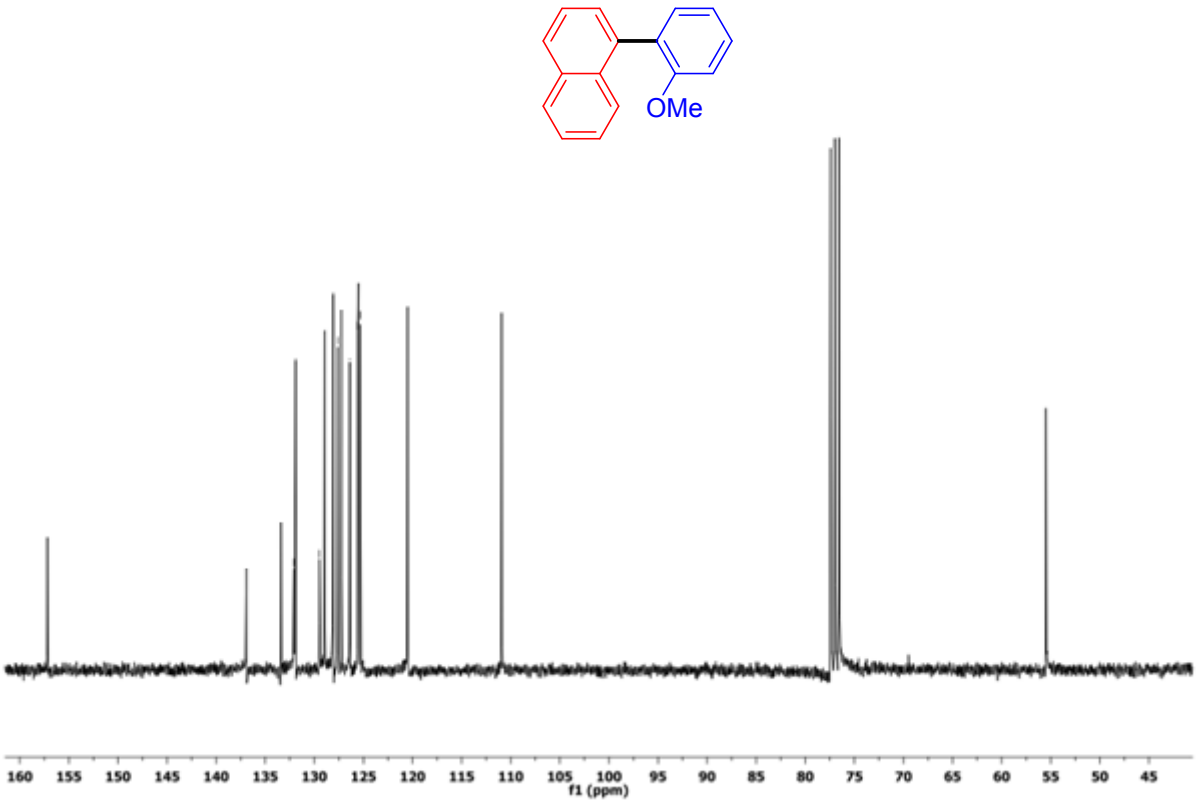
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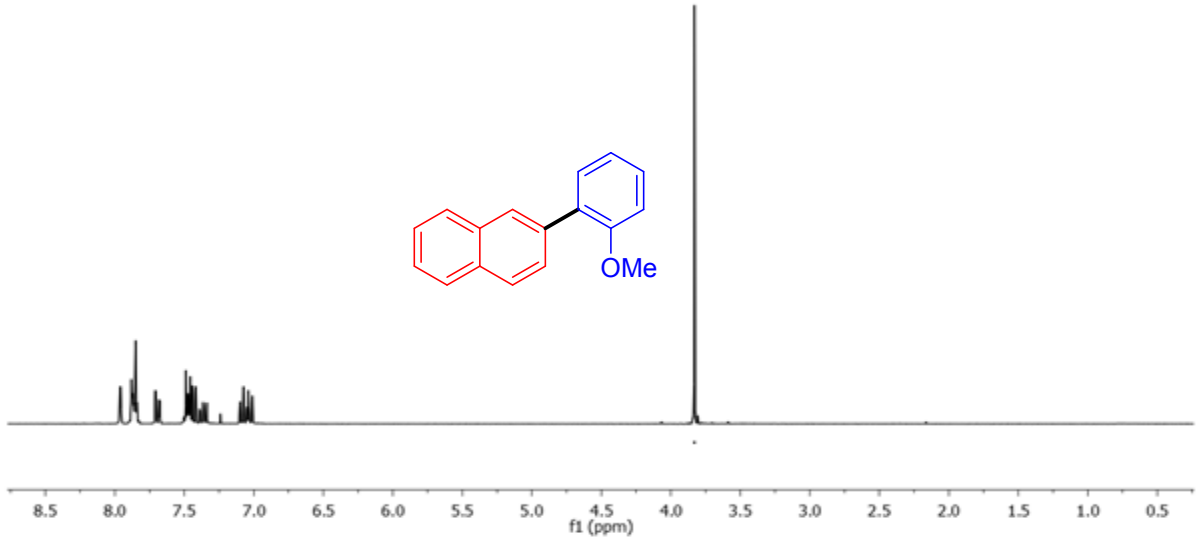
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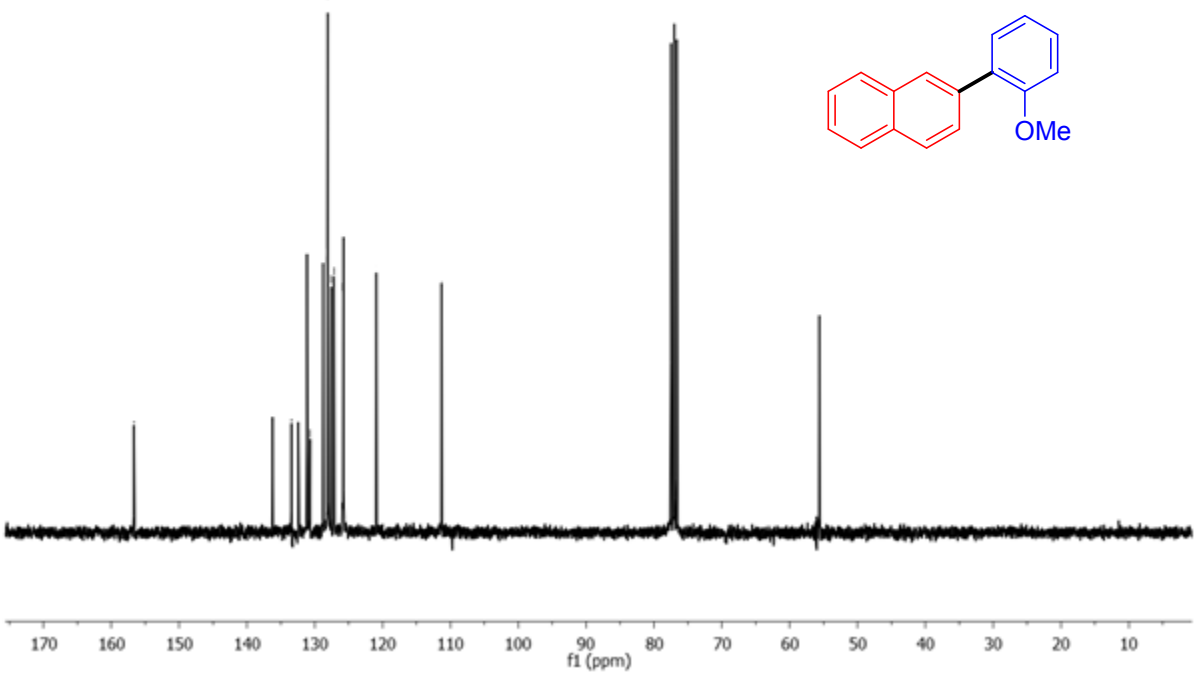
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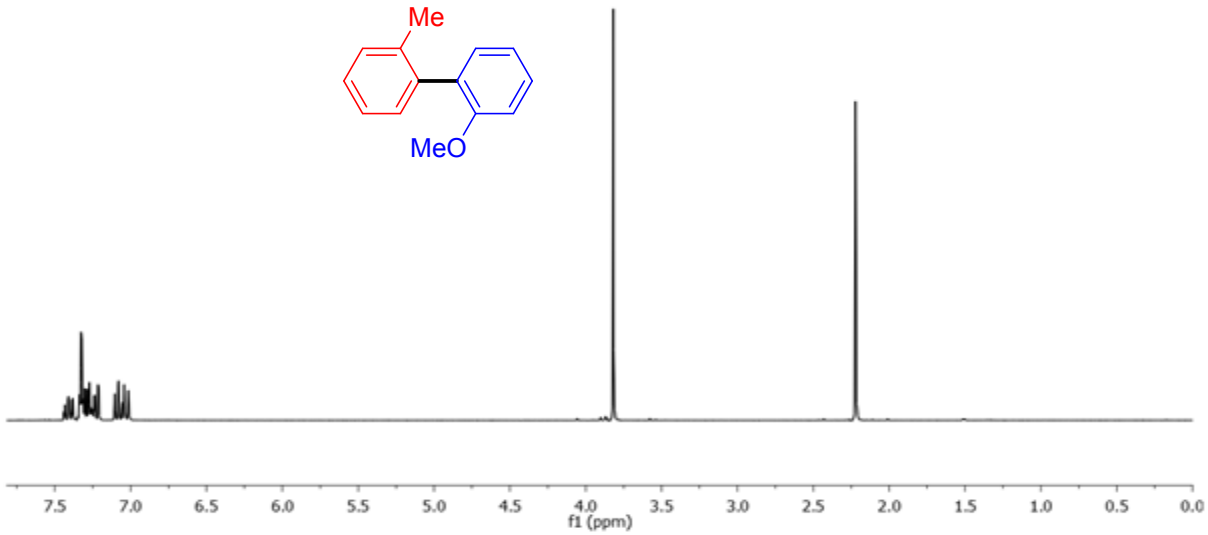
f1 (ppm)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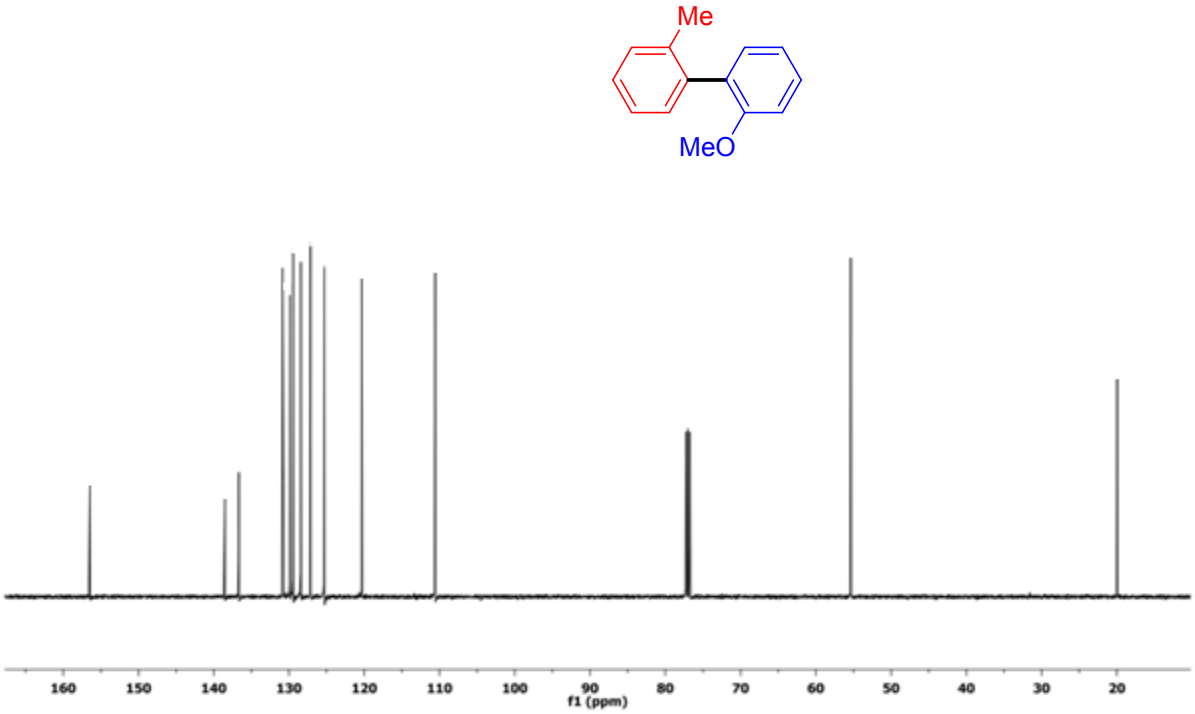
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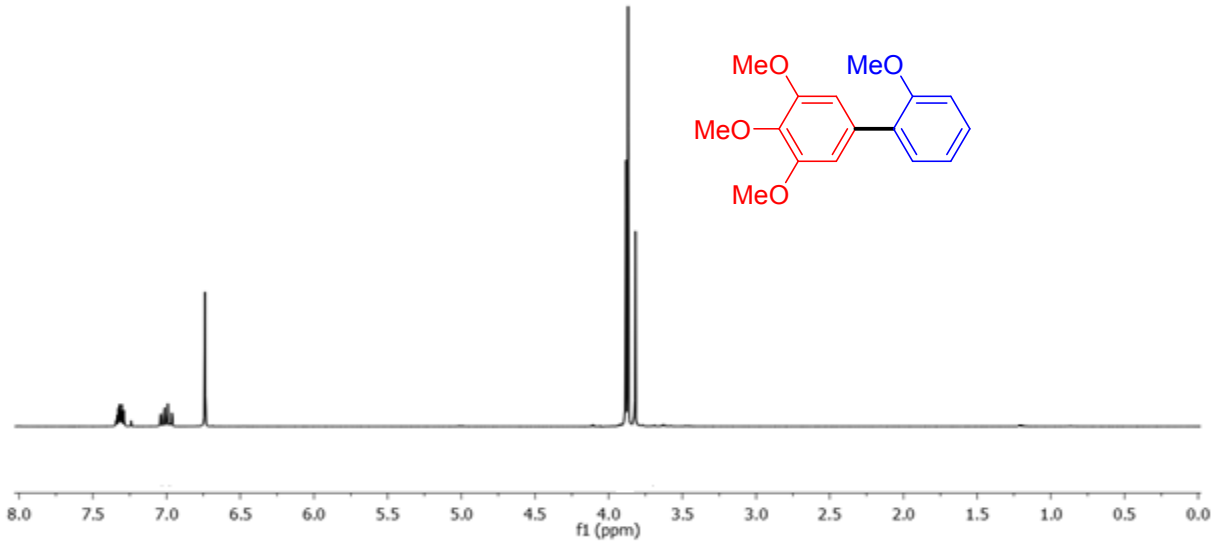
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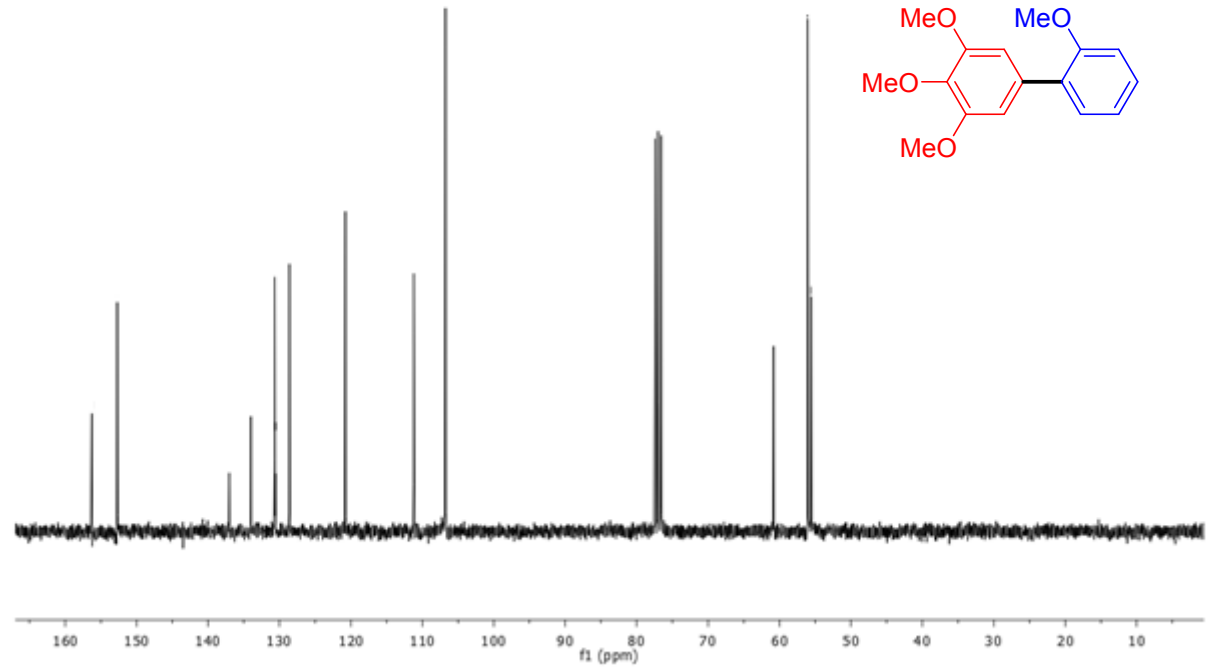
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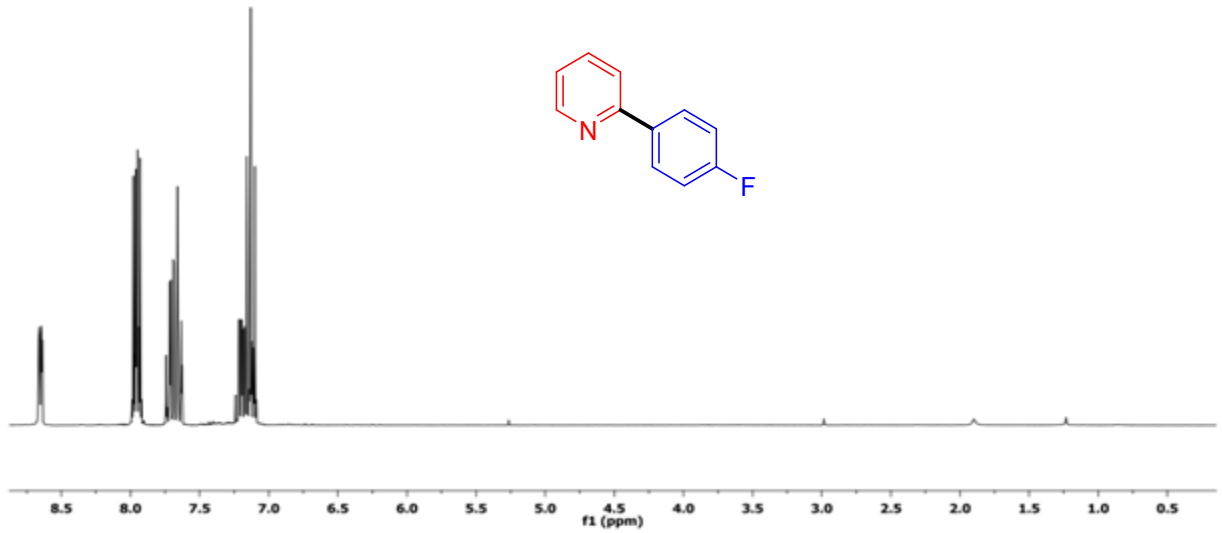
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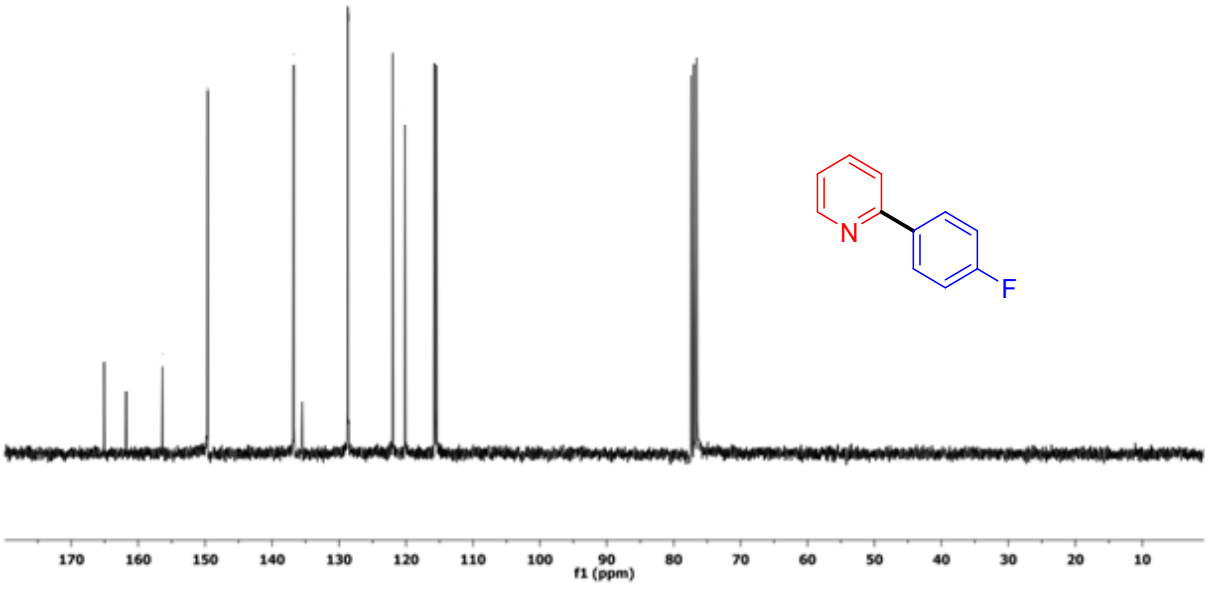
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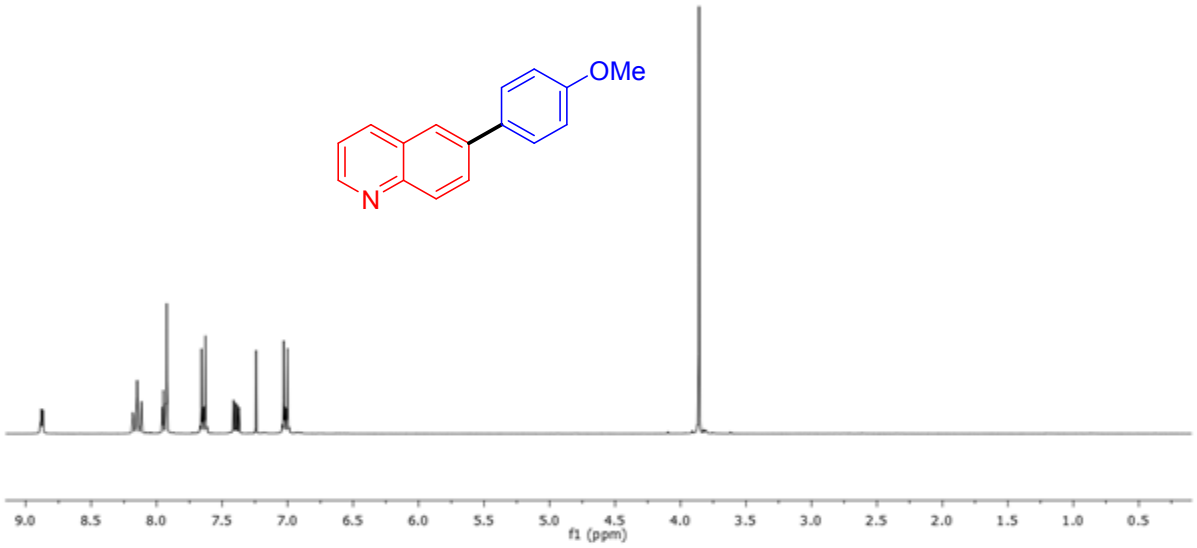
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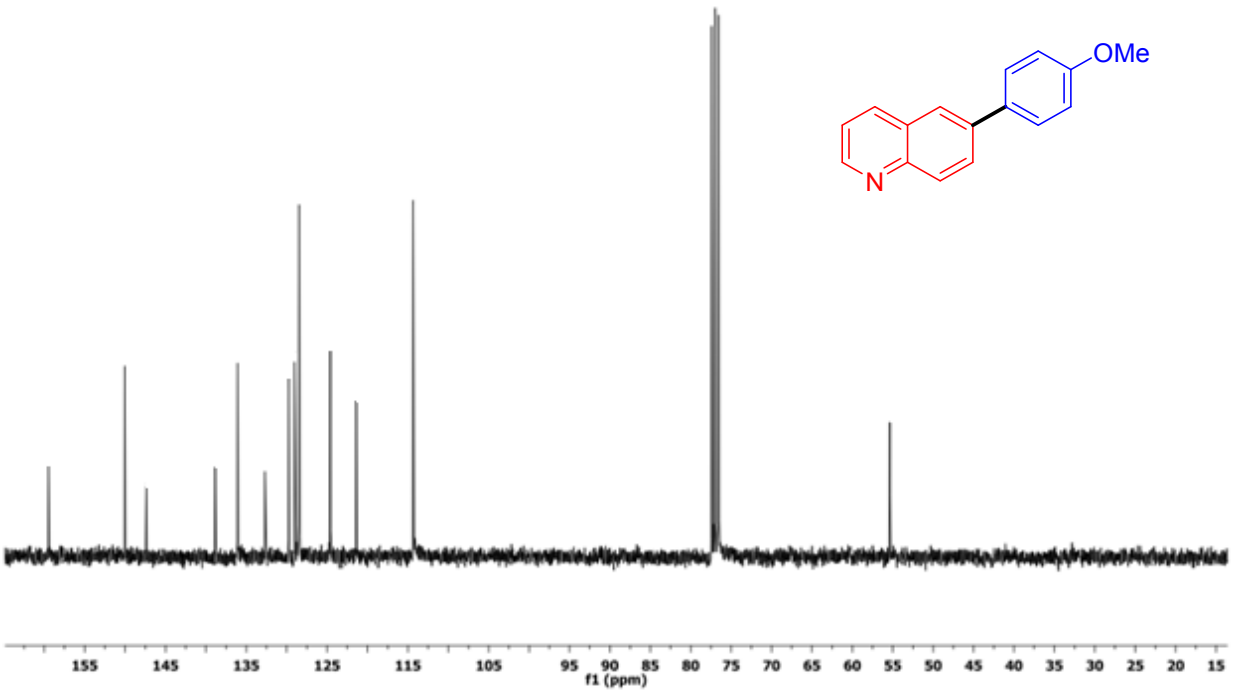
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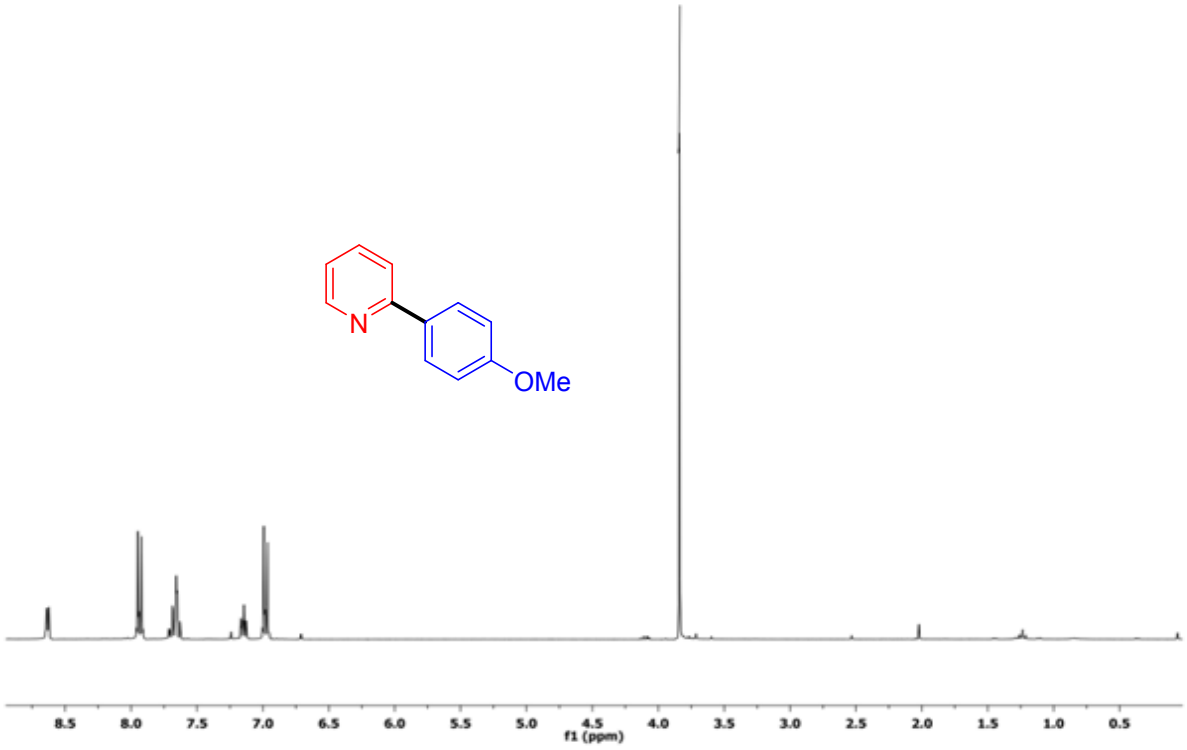
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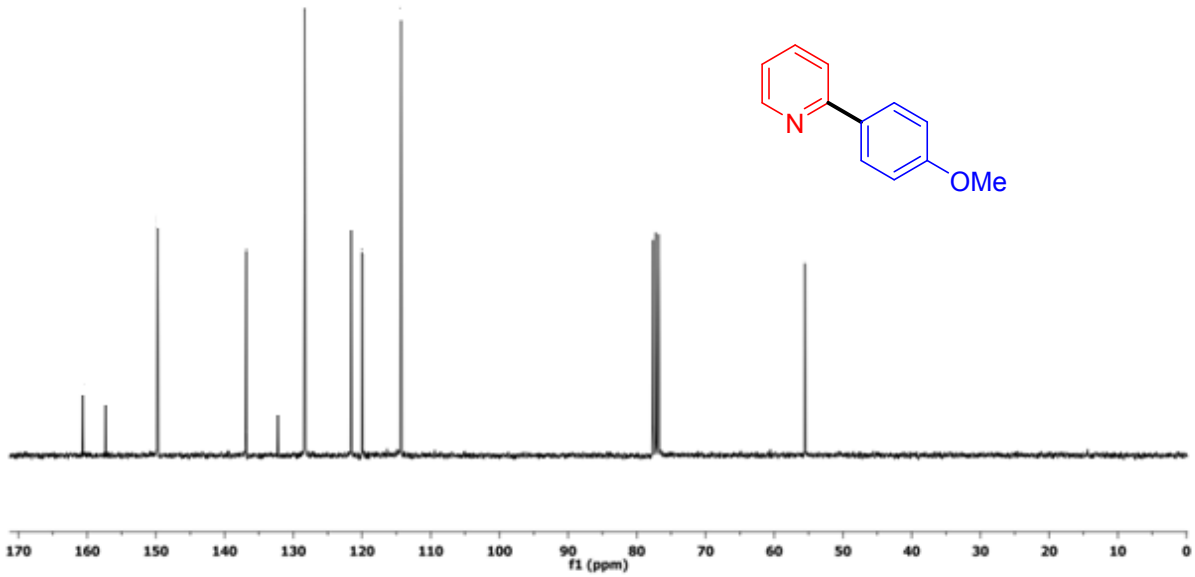
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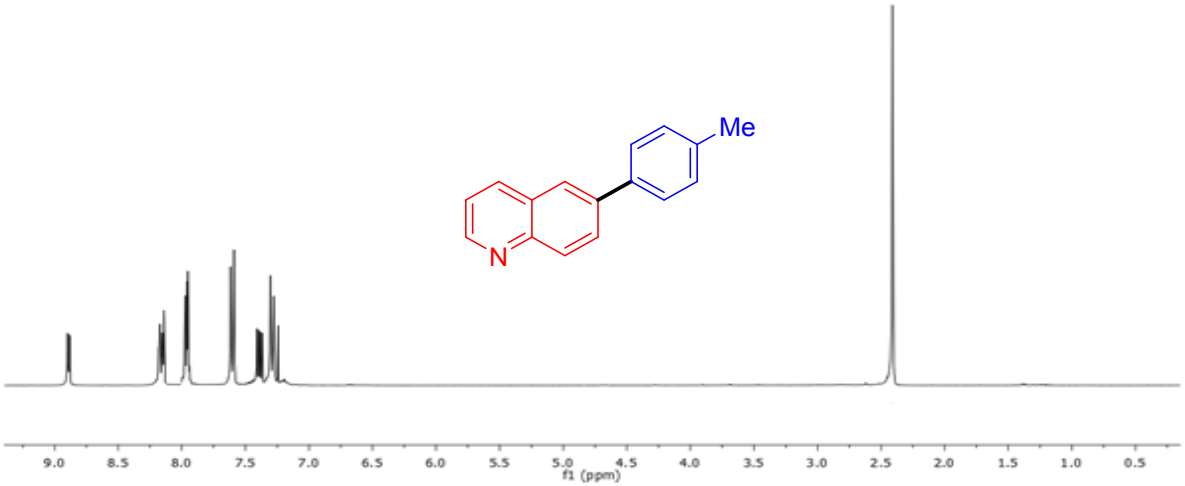
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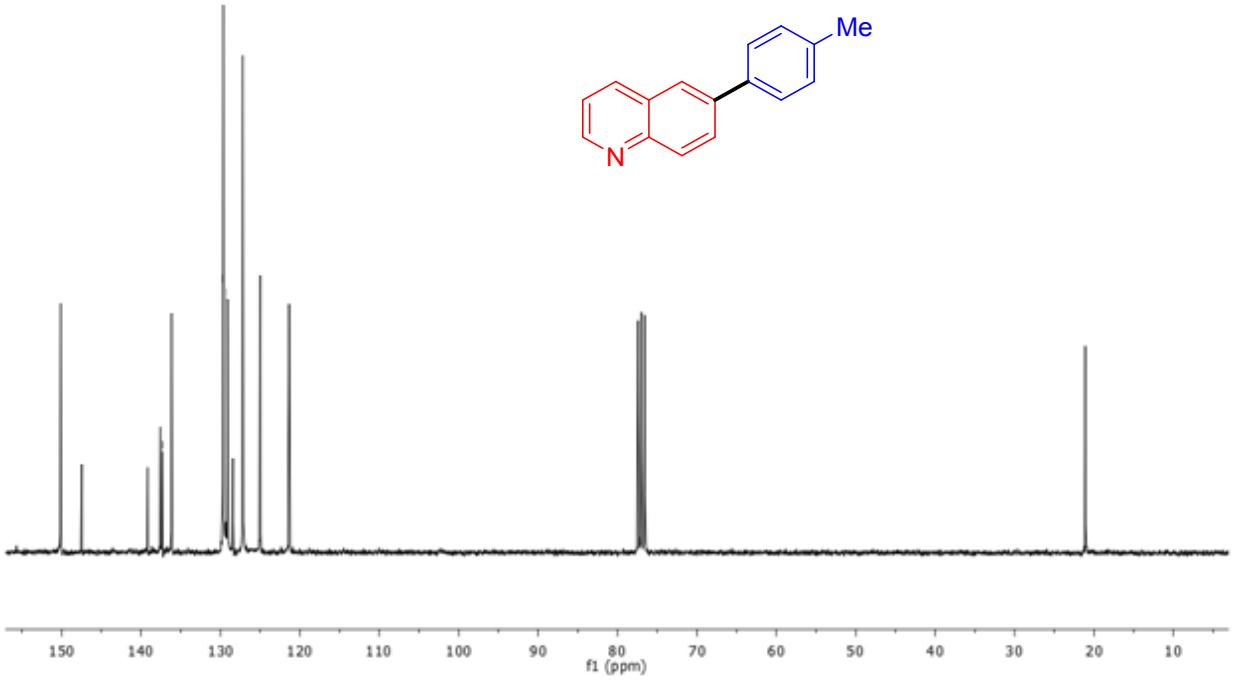
f1 (ppm)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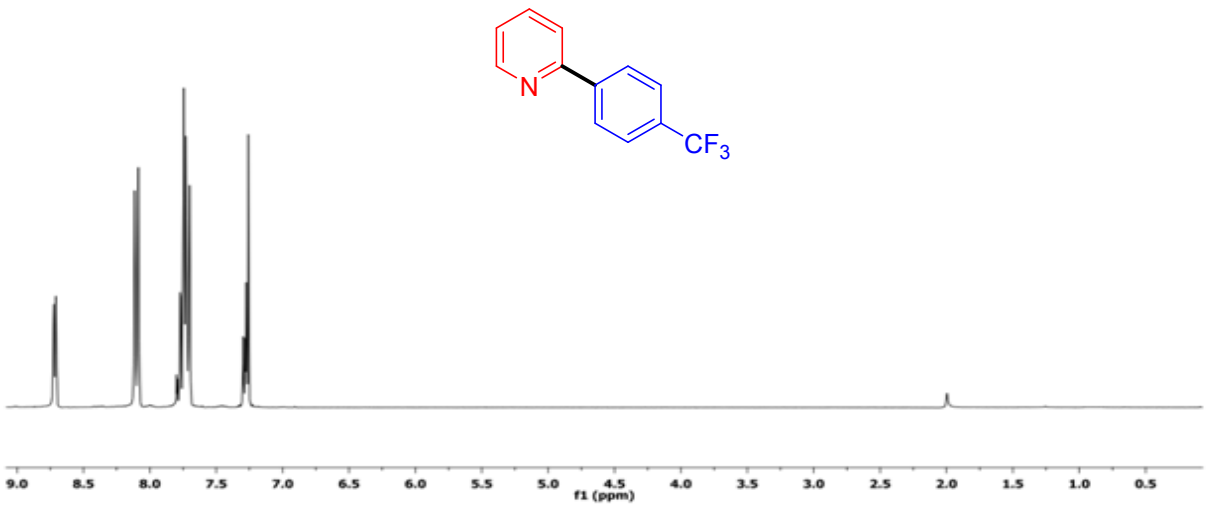
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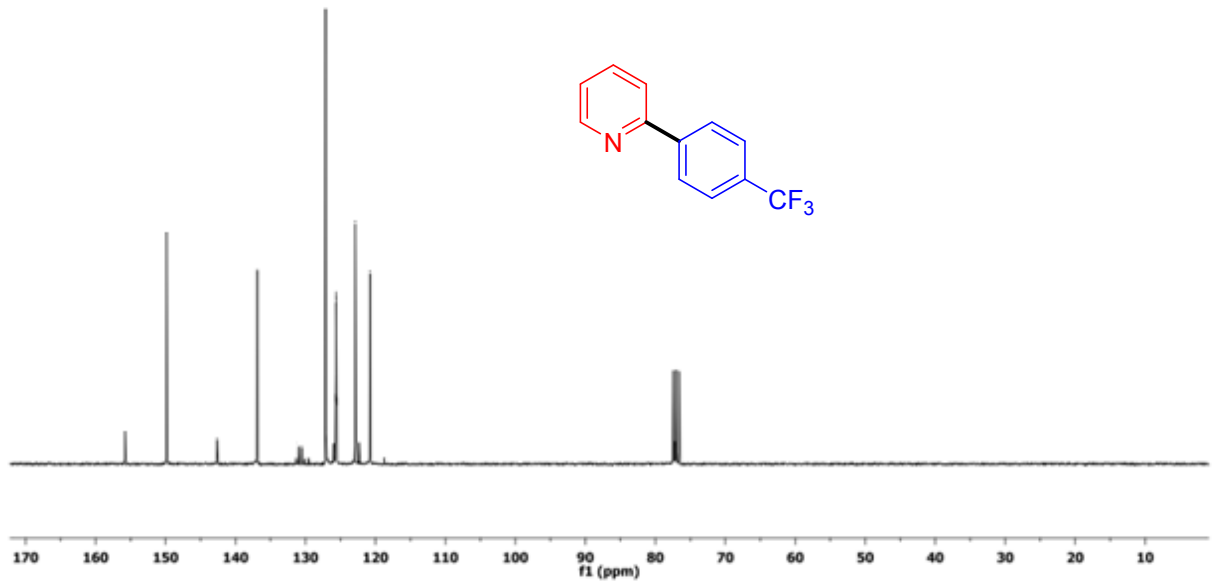
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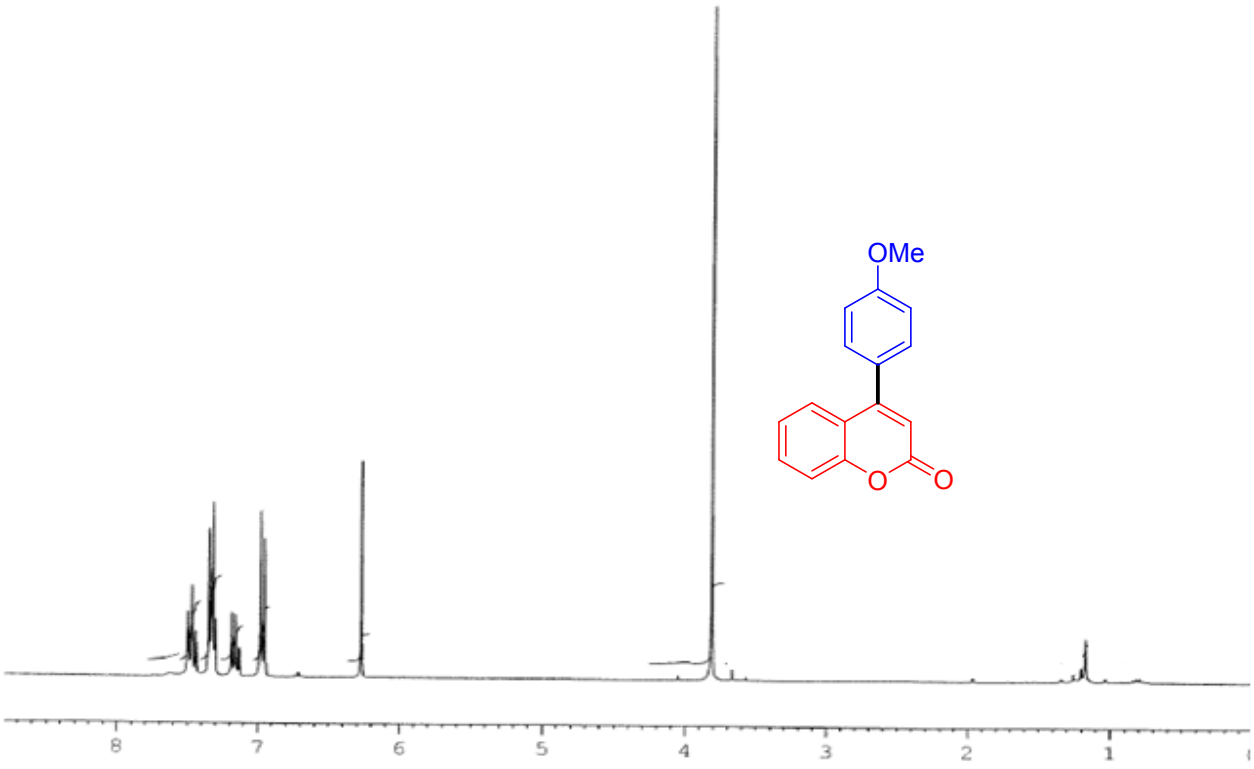
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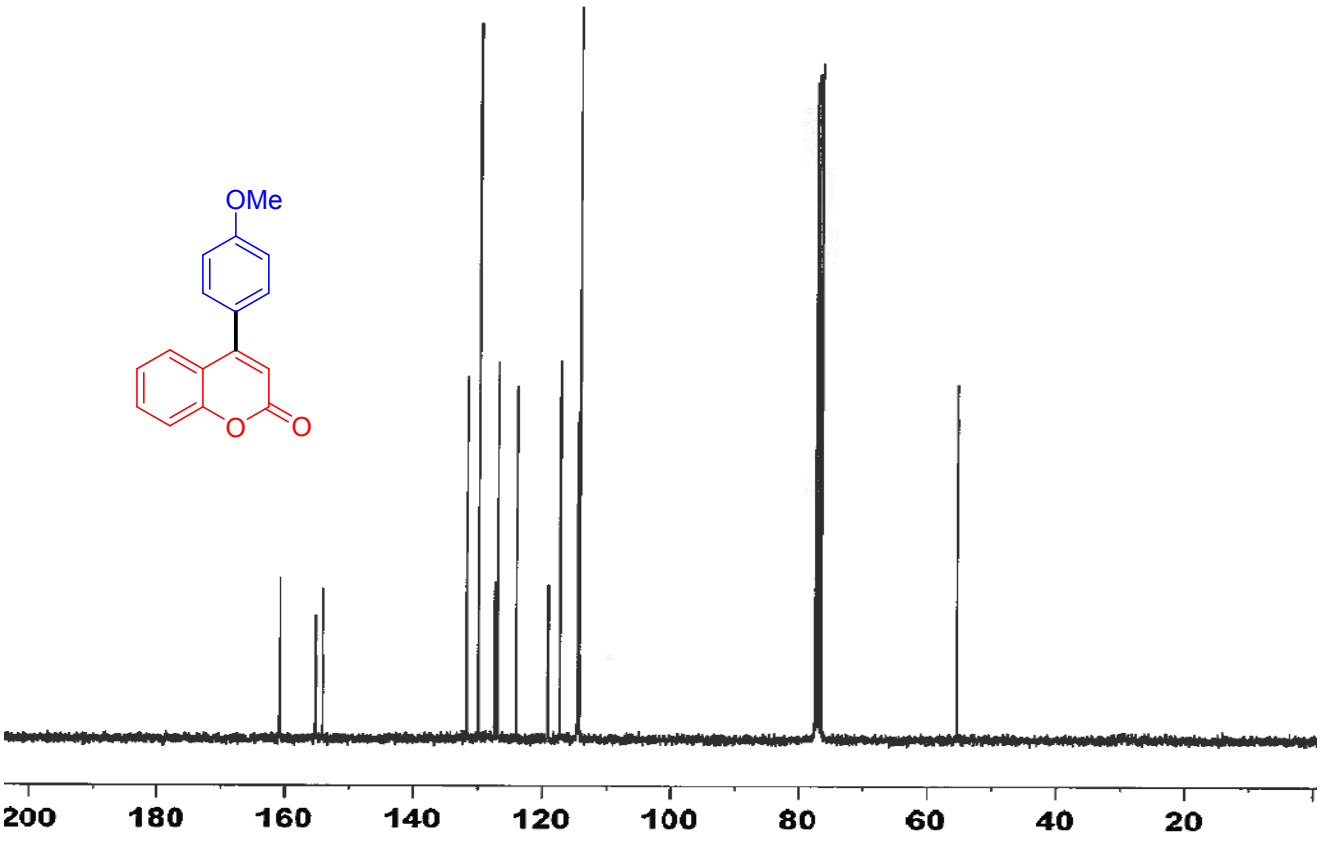
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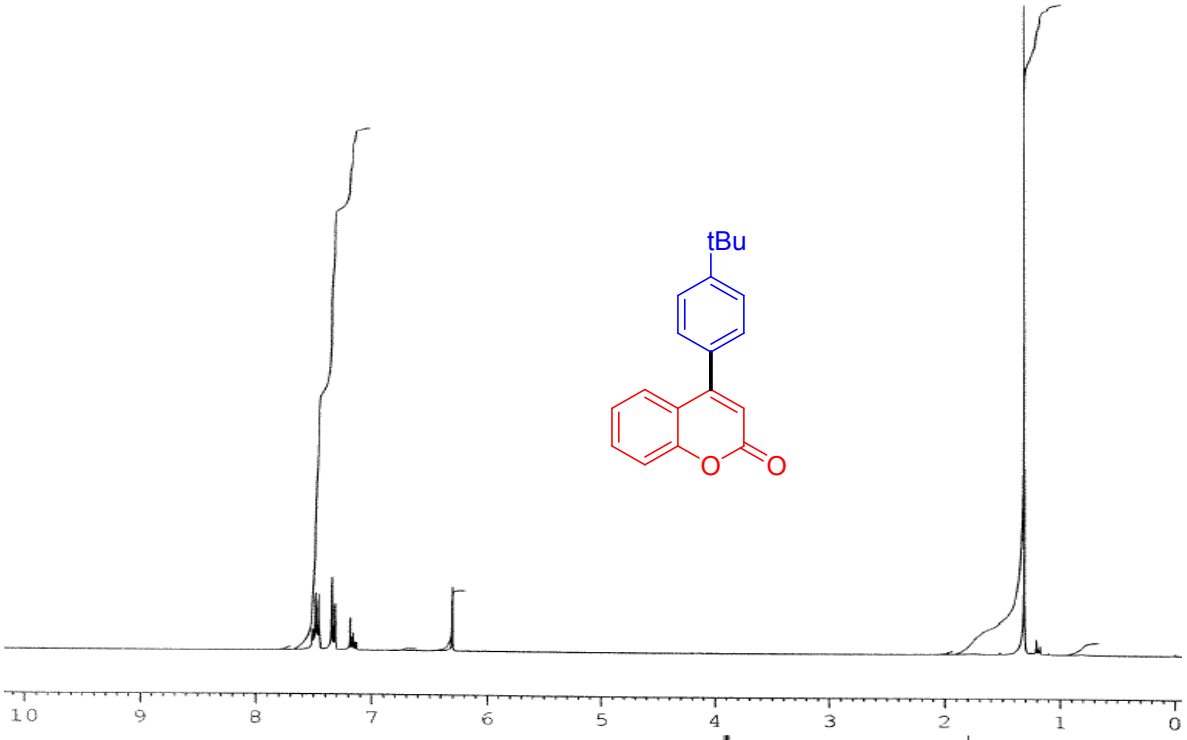
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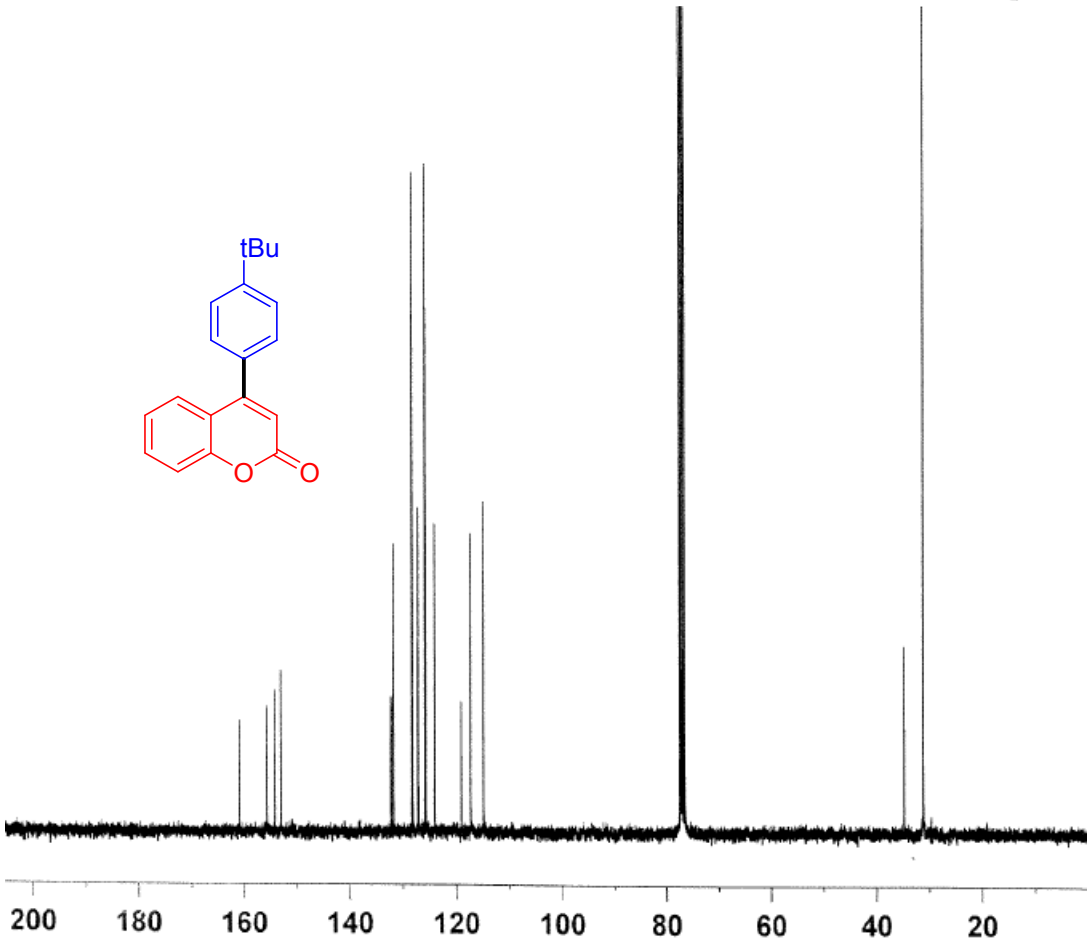
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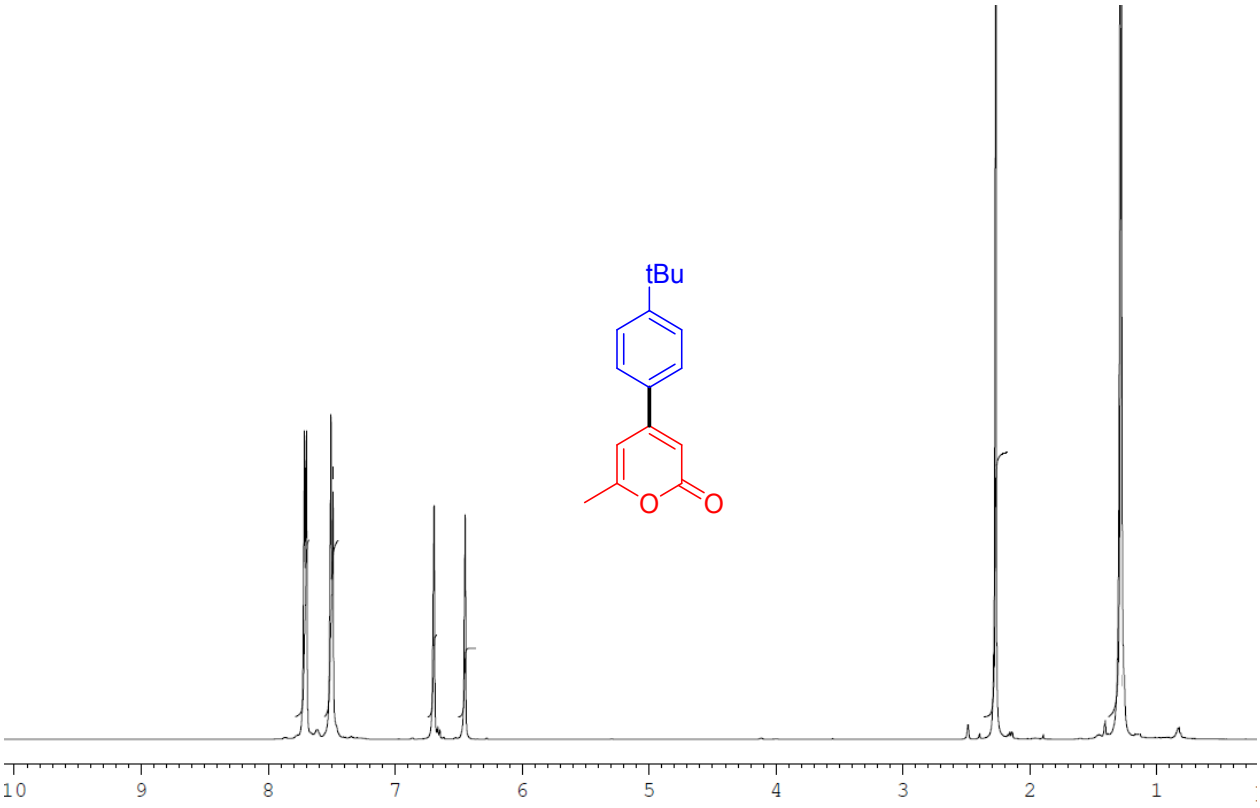
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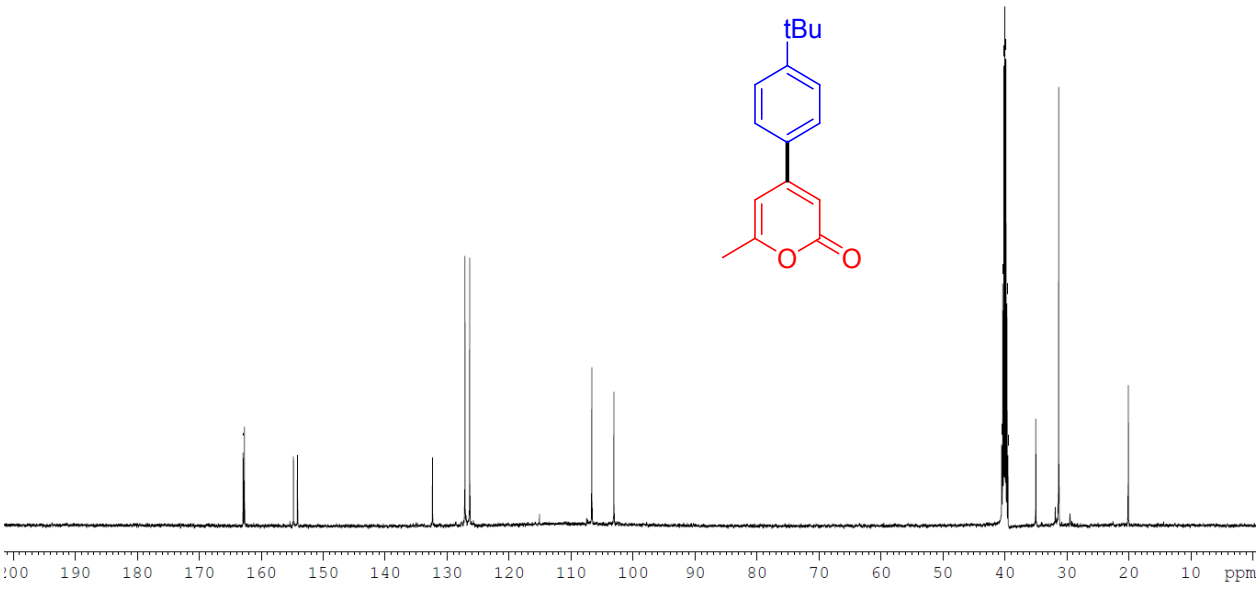
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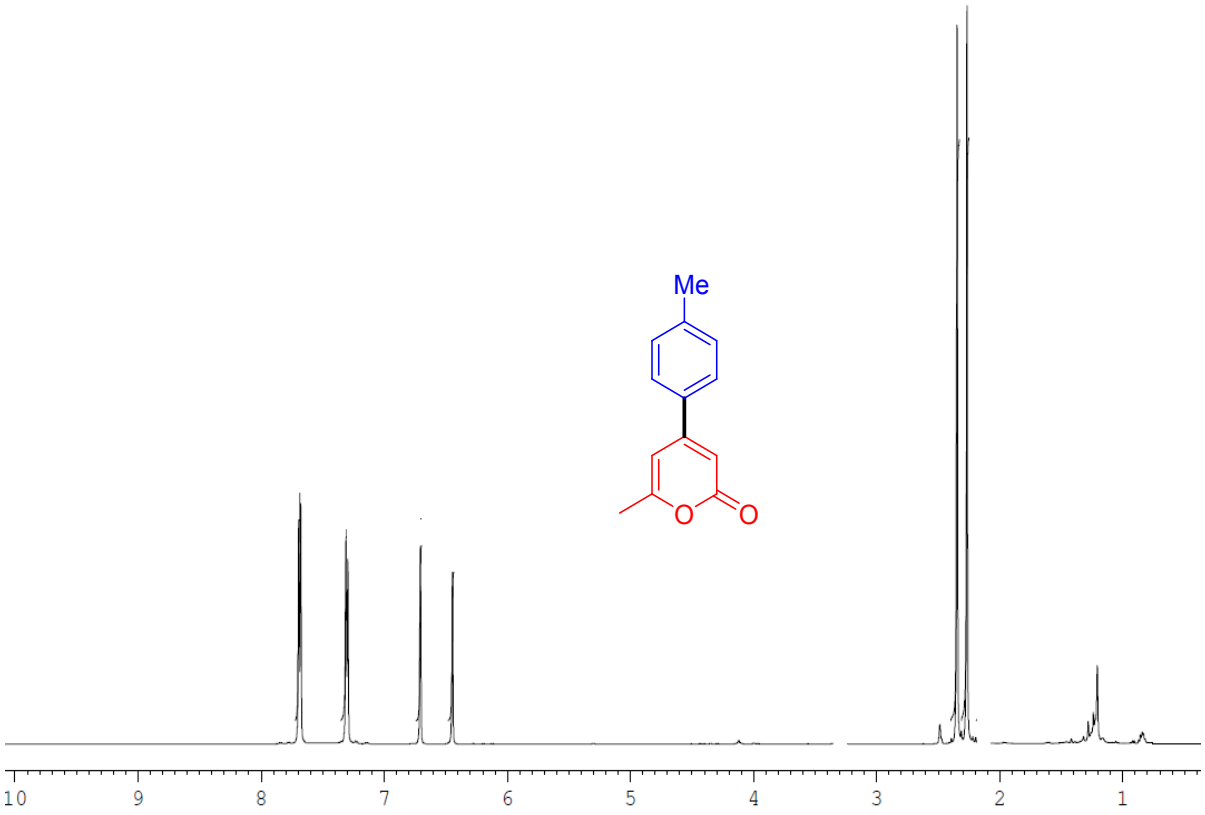
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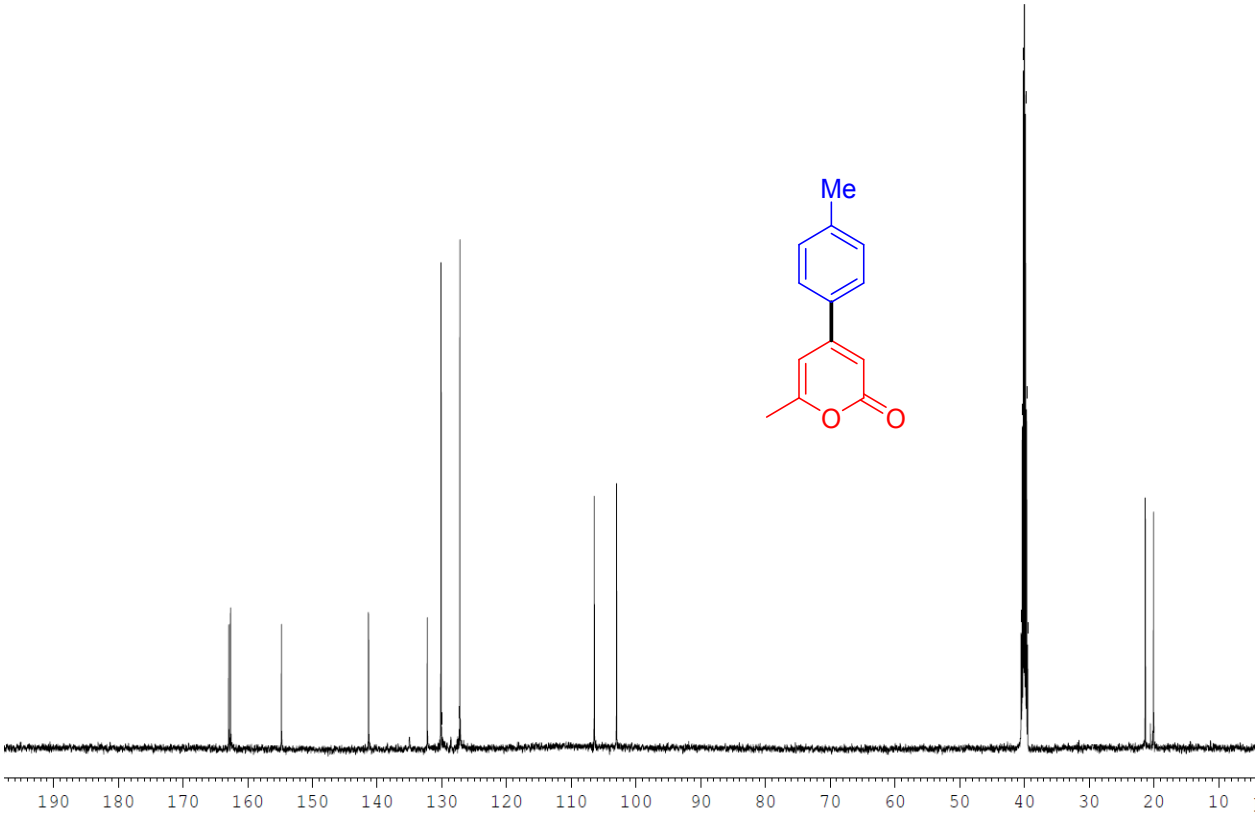
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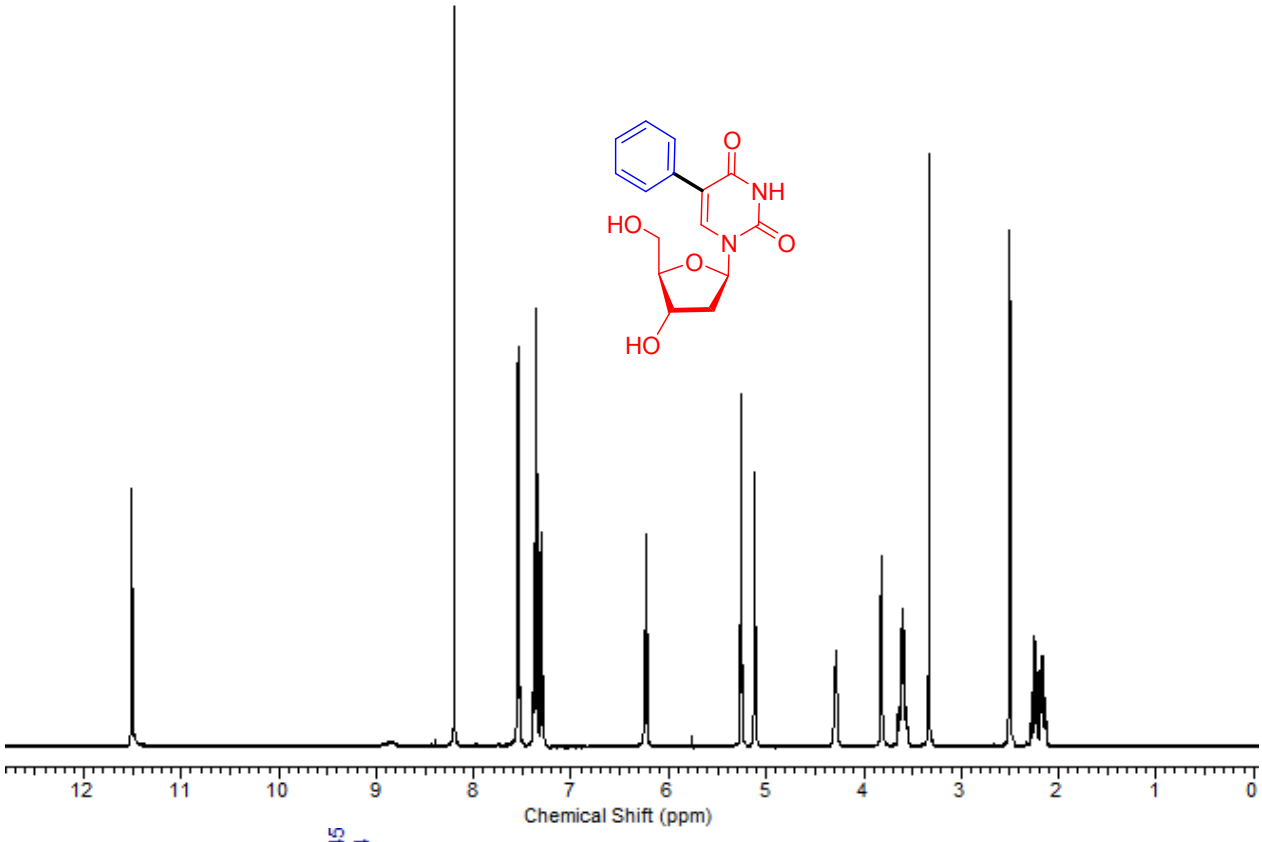
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HO
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4
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1
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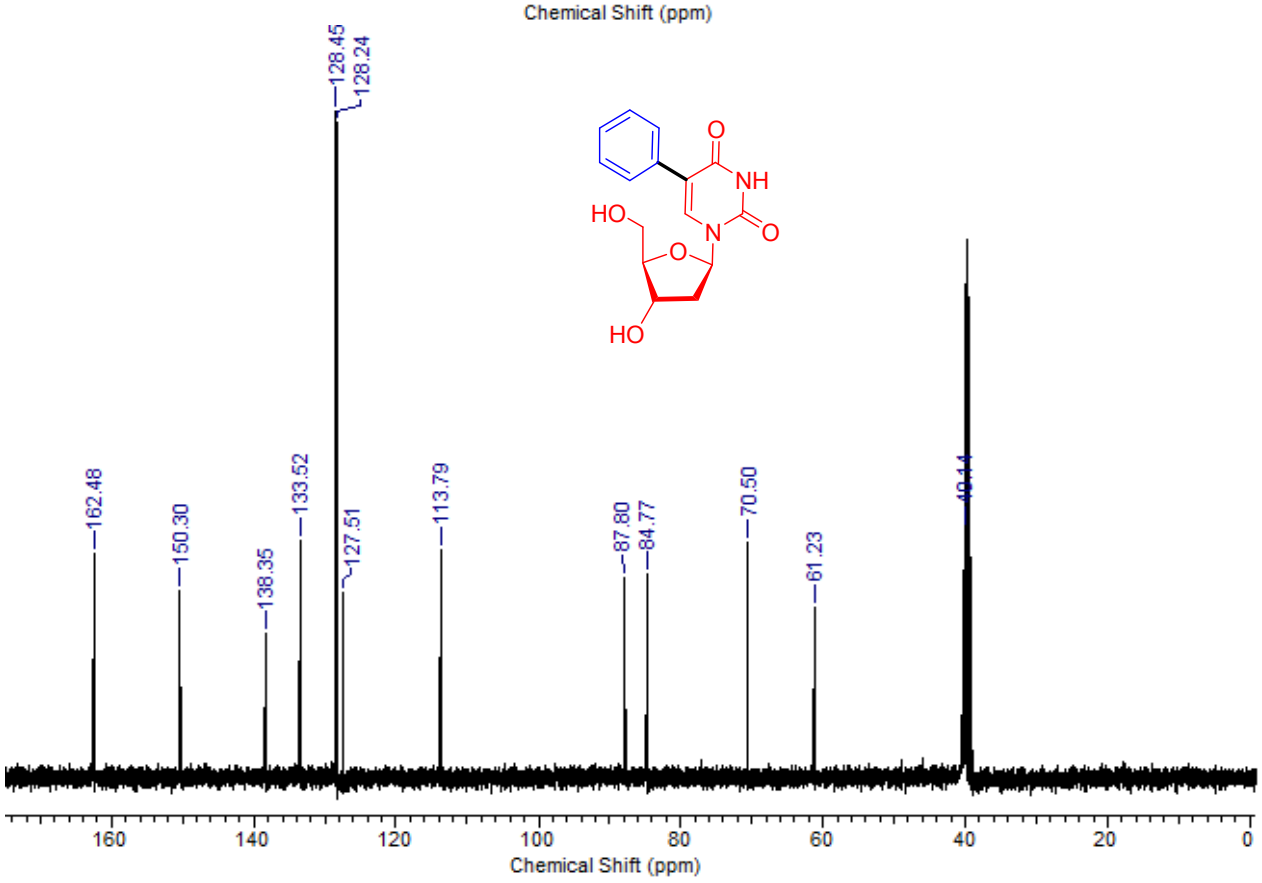
Chemical Shift (ppm)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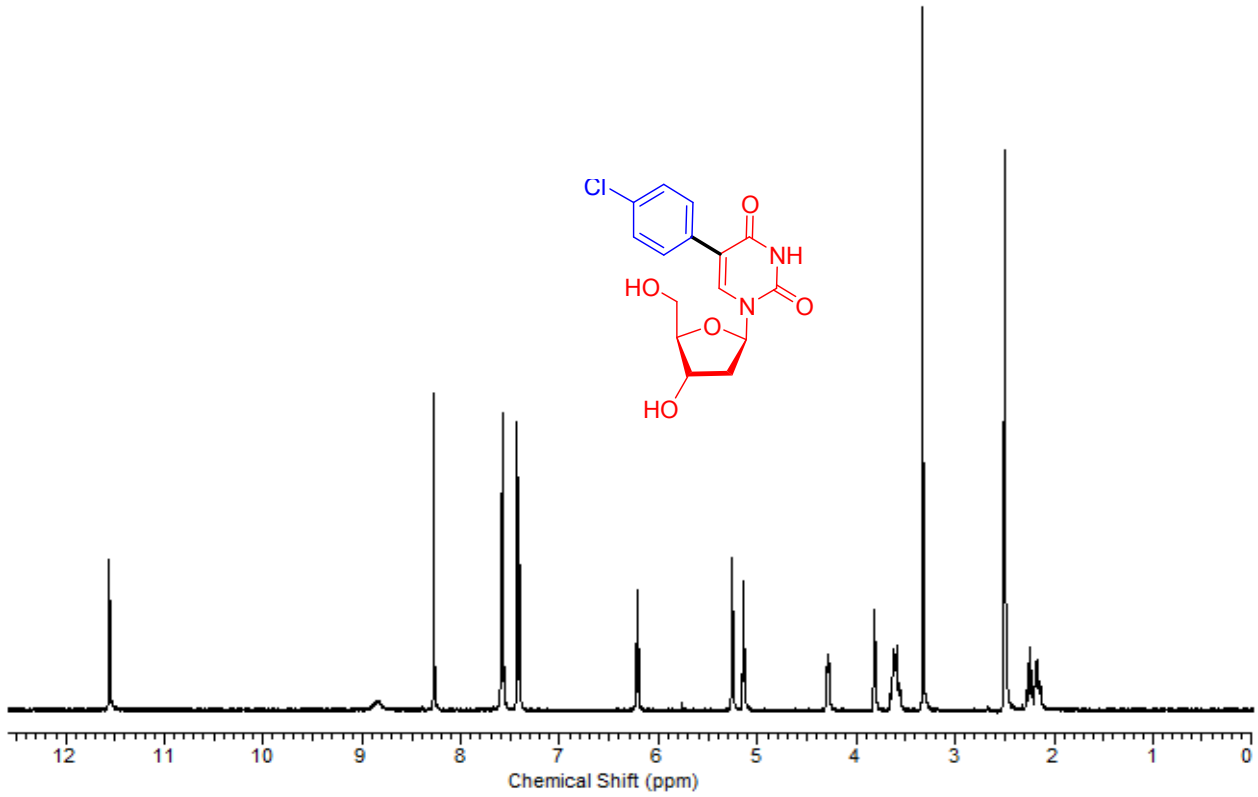
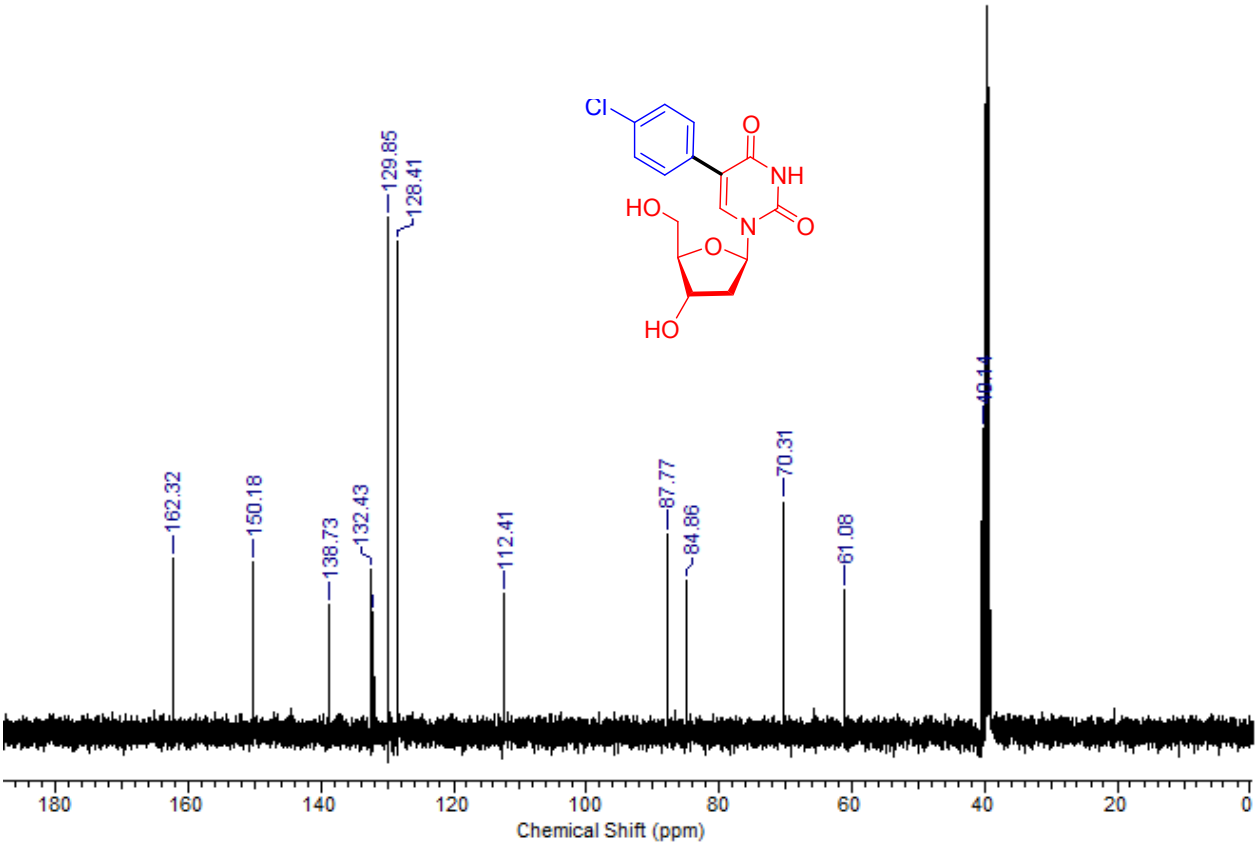
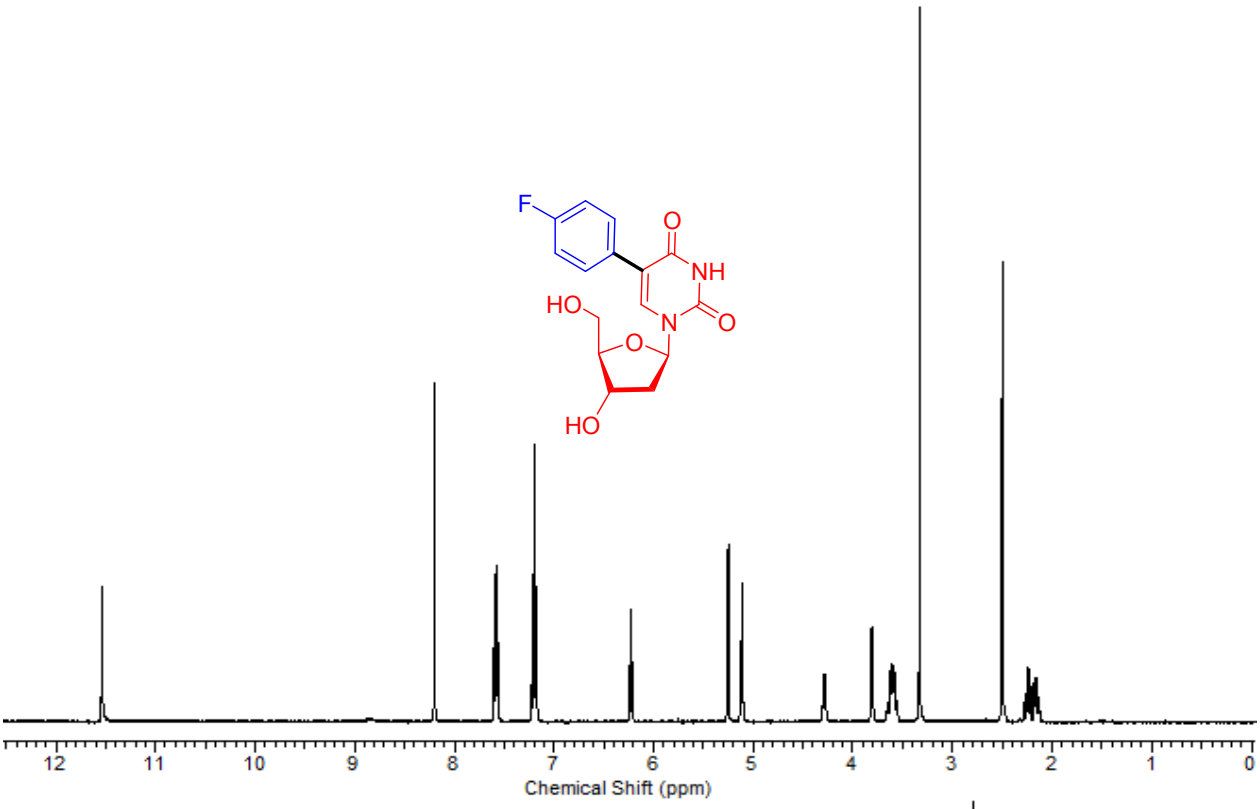
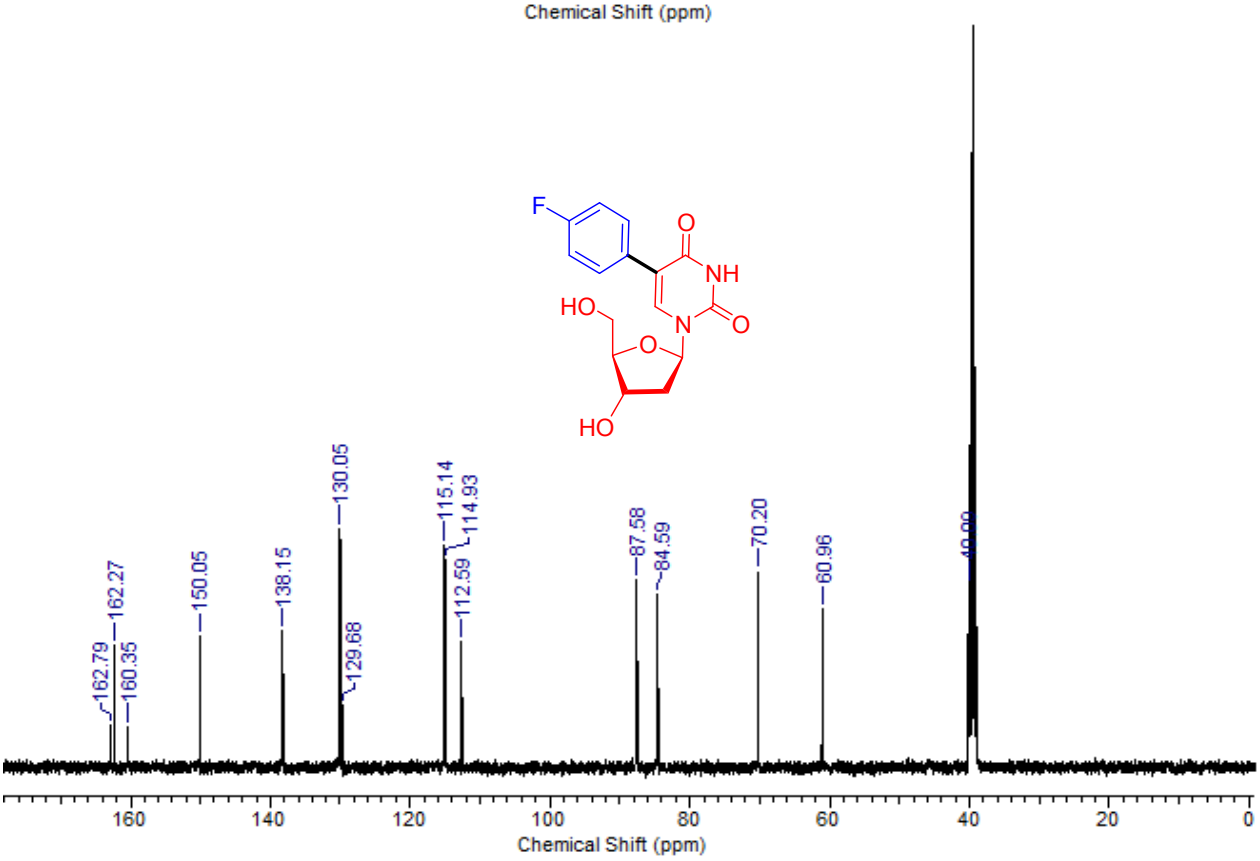
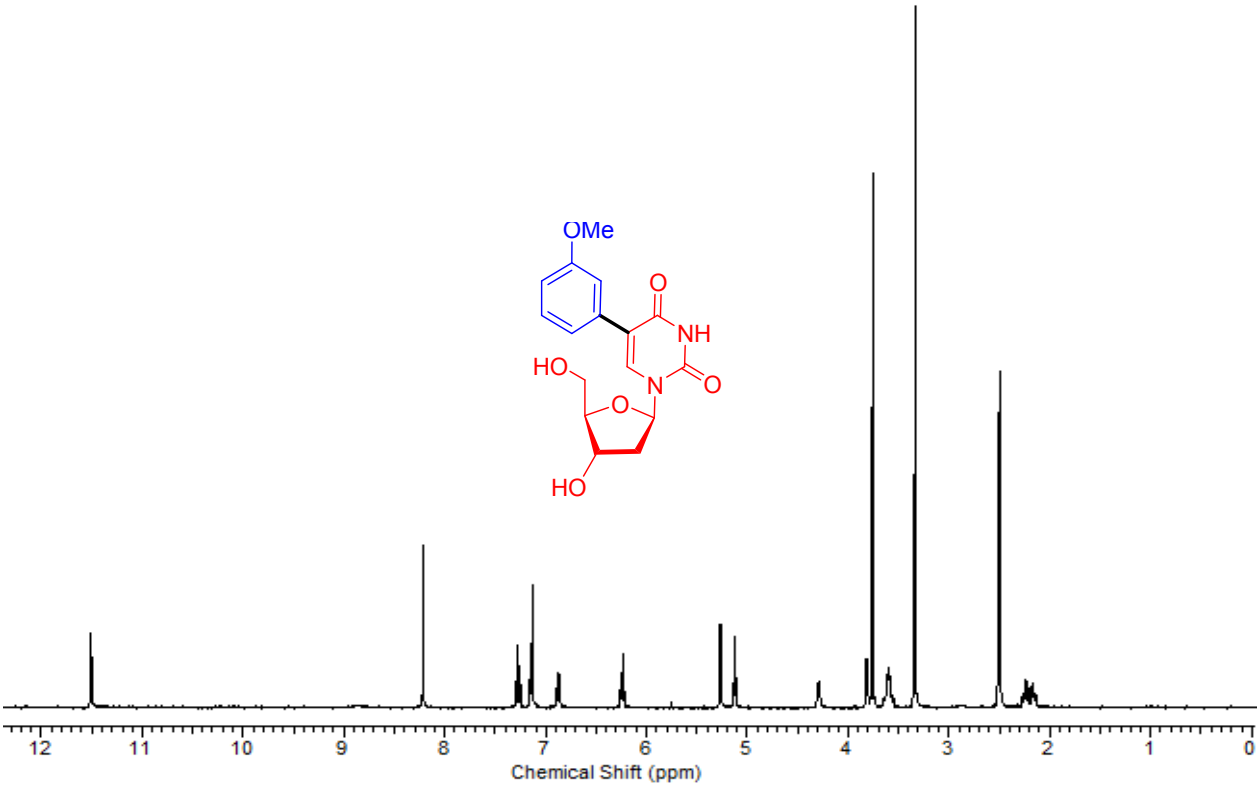
40
20
0
Chemical Shift (ppm)

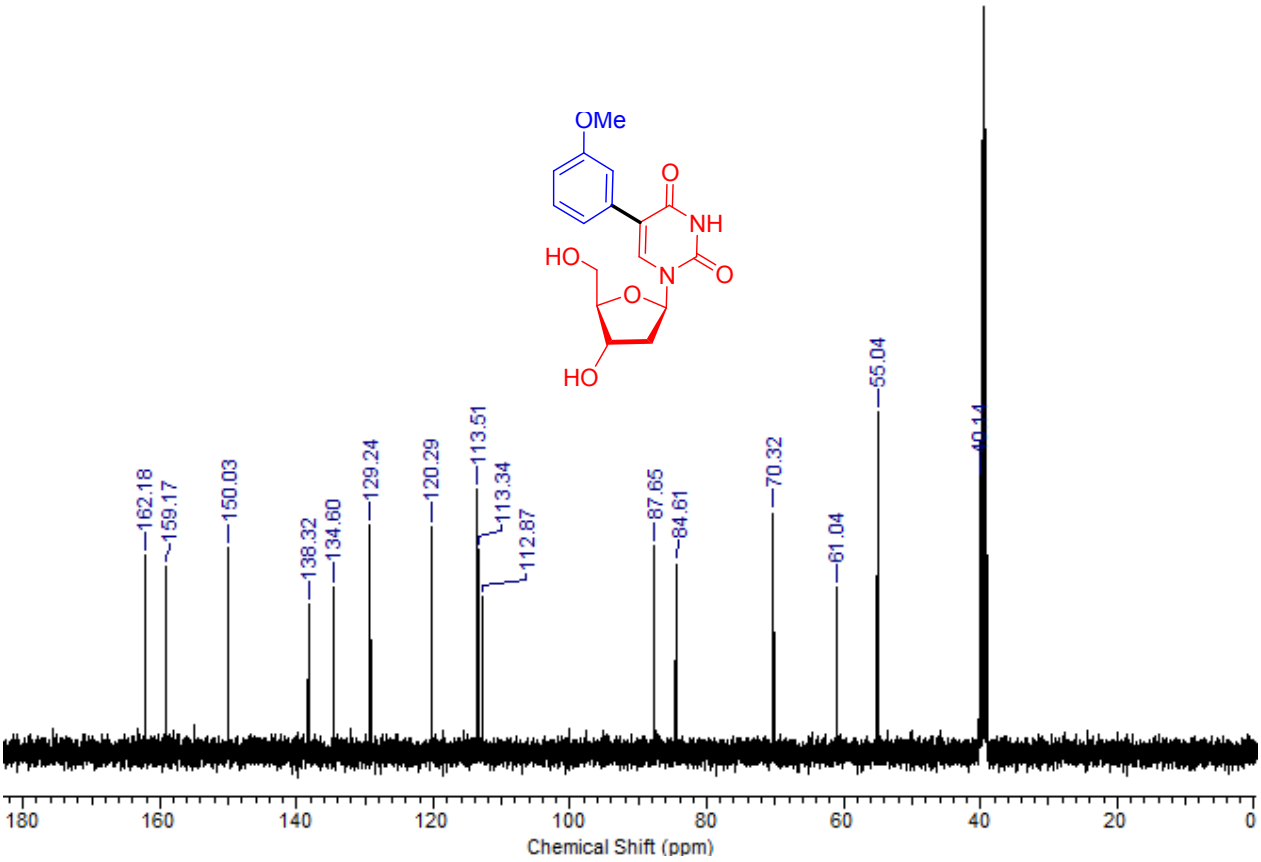

Cl
O
NH
N
O
HO
O
HO
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

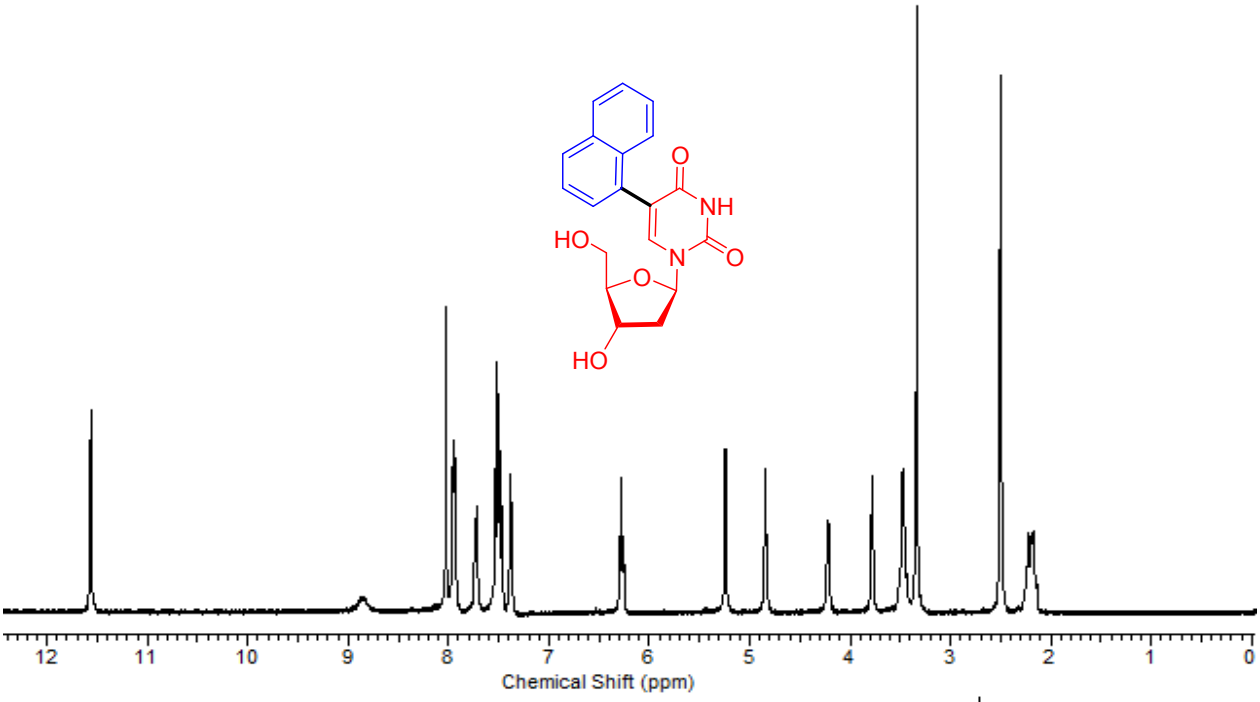

Cl
O
NH
N
O
HO
O
HO
129.85
128.41
162.32
150.18
138.73
132.43
112.41
87.77
84.86
70.31
61.08
49.14
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

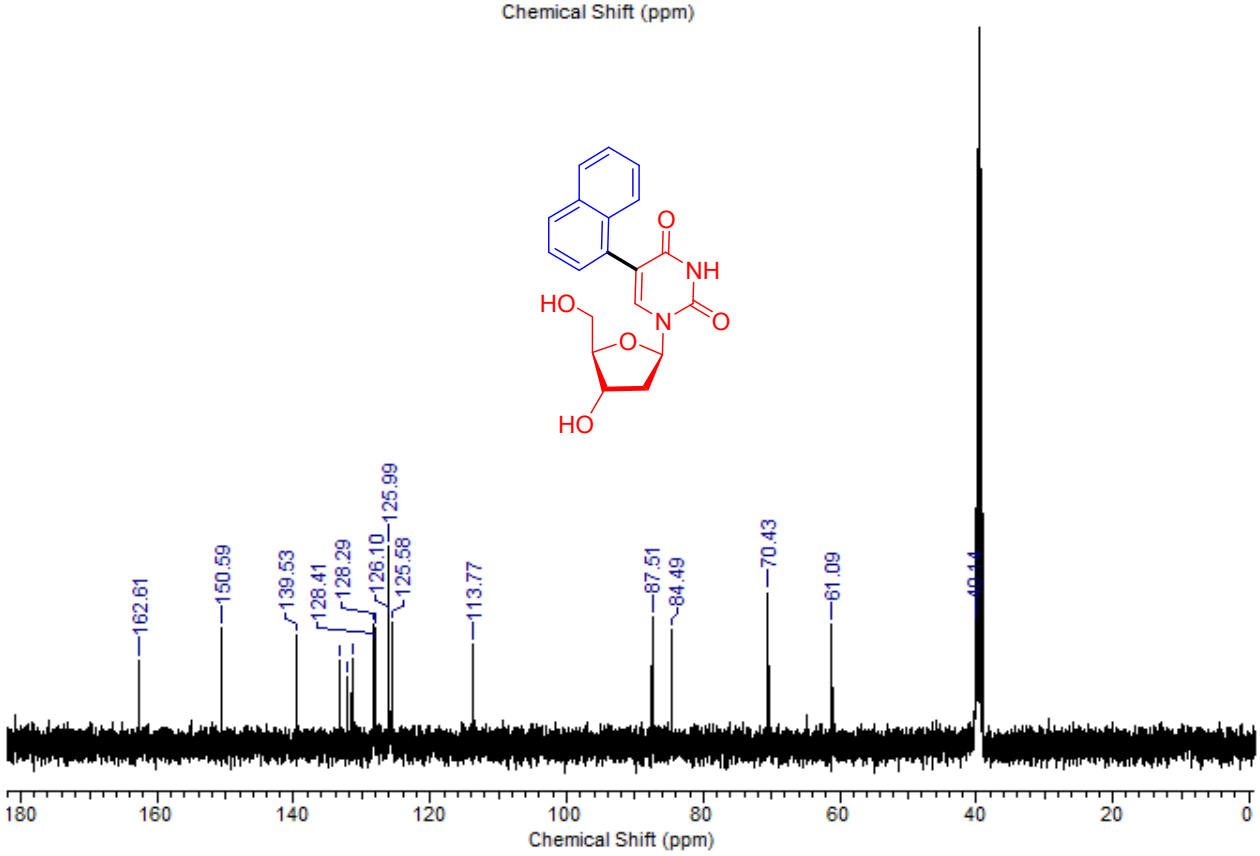

F
O
NH
HO
N
O
O
HO
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

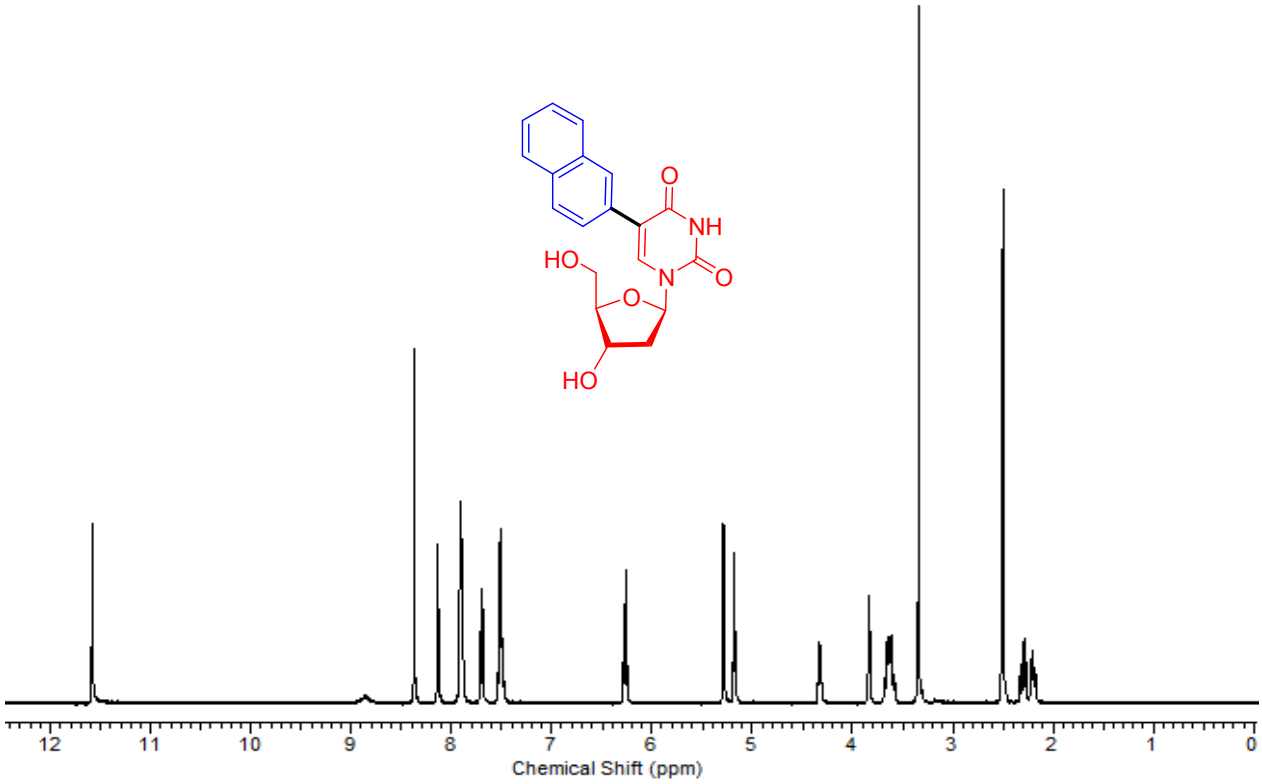

F
O
NH
HO
N
O
O
HO
162.79
162.27
160.35
150.05
138.15
130.05
129.68
115.14
114.93
112.59
87.58
84.59
70.20
60.96
40.00
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

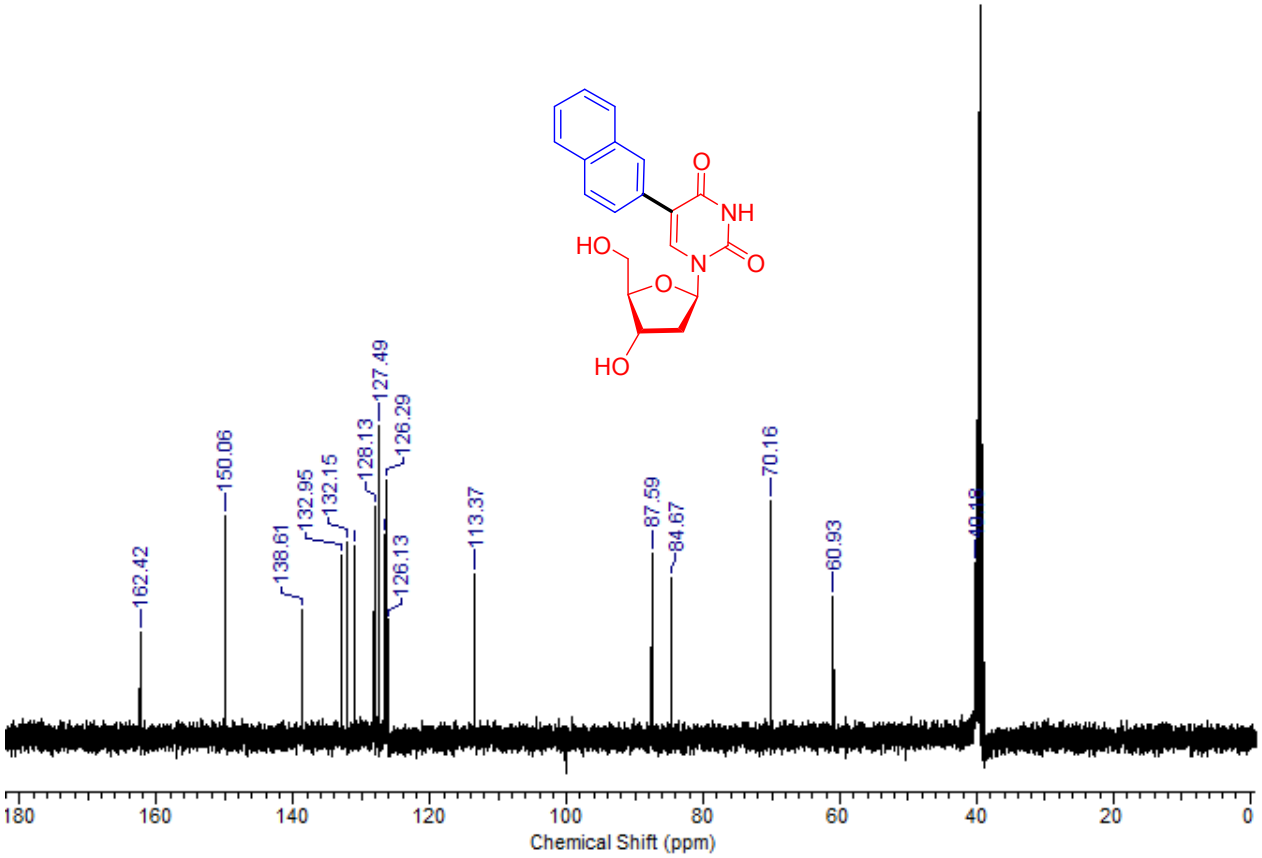

OMe
O
NH
HO
N
O
O
HO
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

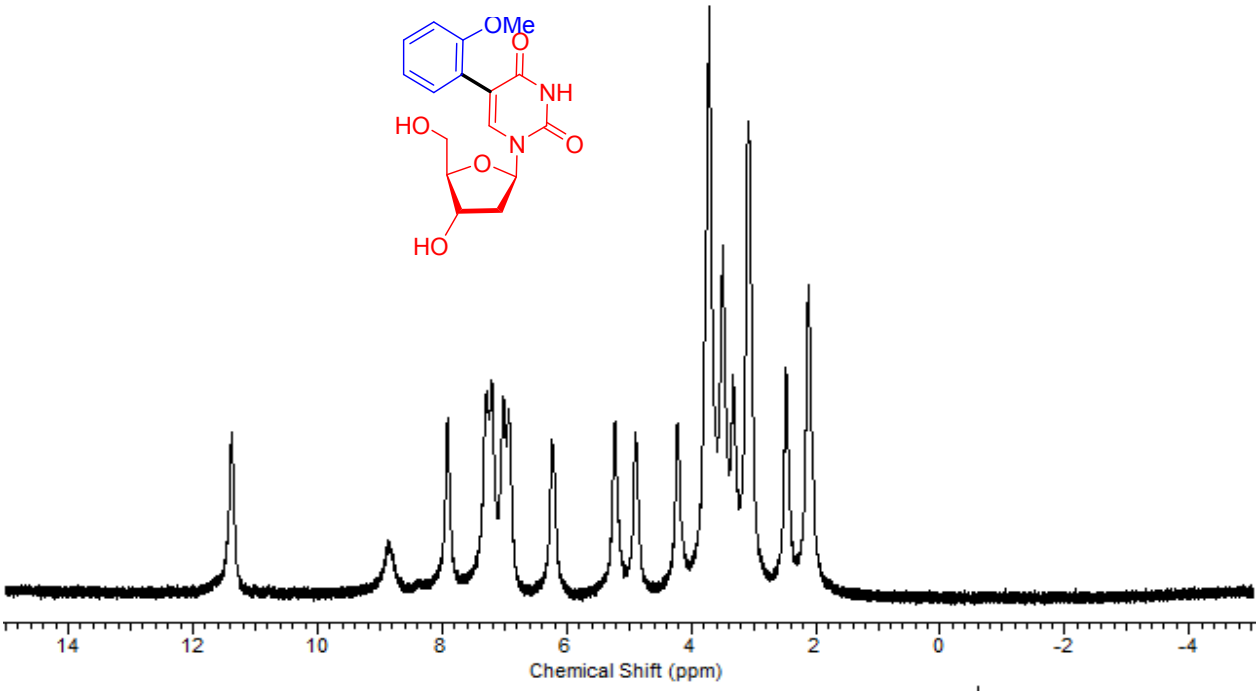

OMe
O
NH
HO
N
O
O
HO
162.18
159.17
150.03
138.32
134.60
129.24
120.29
113.51
113.34
112.87
87.65
84.61
70.32
61.04
55.04
40.14
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

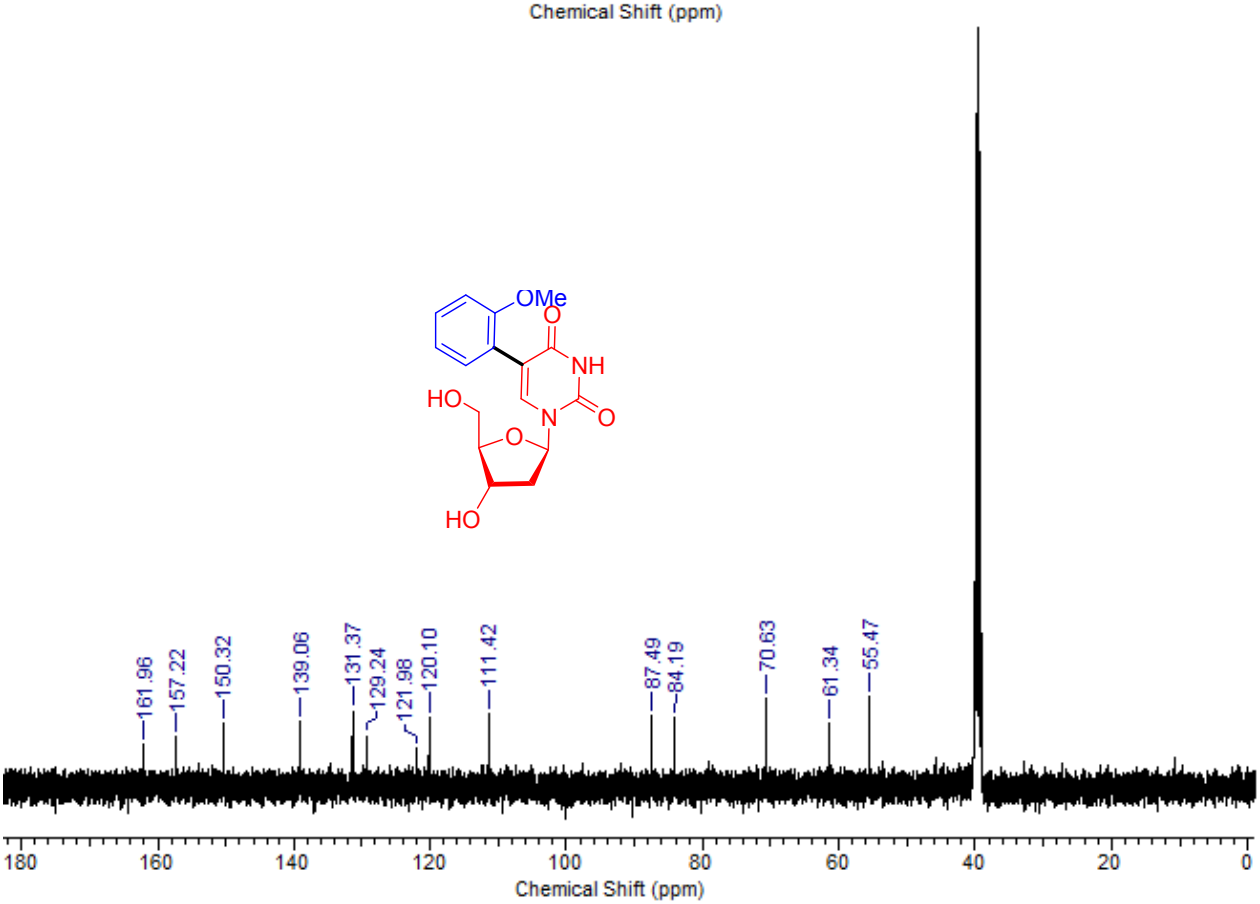

O
NH
HO
N
O
O
HO
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

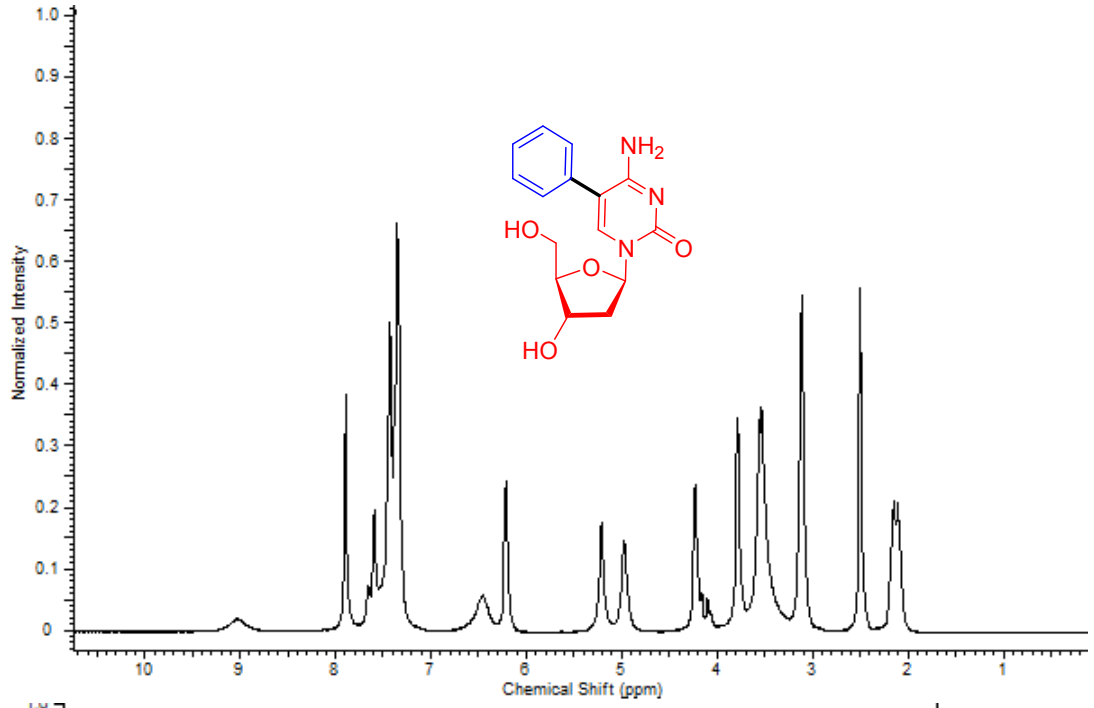

O
NH
HO
N
O
O
HO
162.61
150.59
139.53
128.41
128.29
126.10
125.99
125.58
113.77
87.51
84.49
70.43
61.09
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

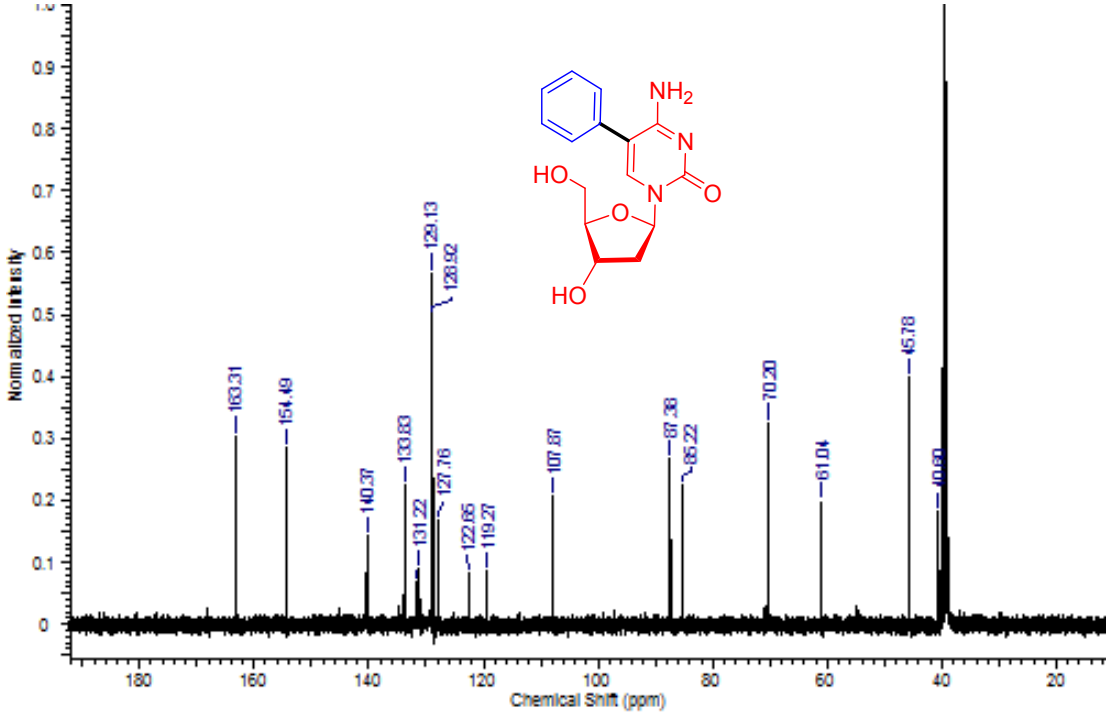

O
NH
HO
N
O
O
HO
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

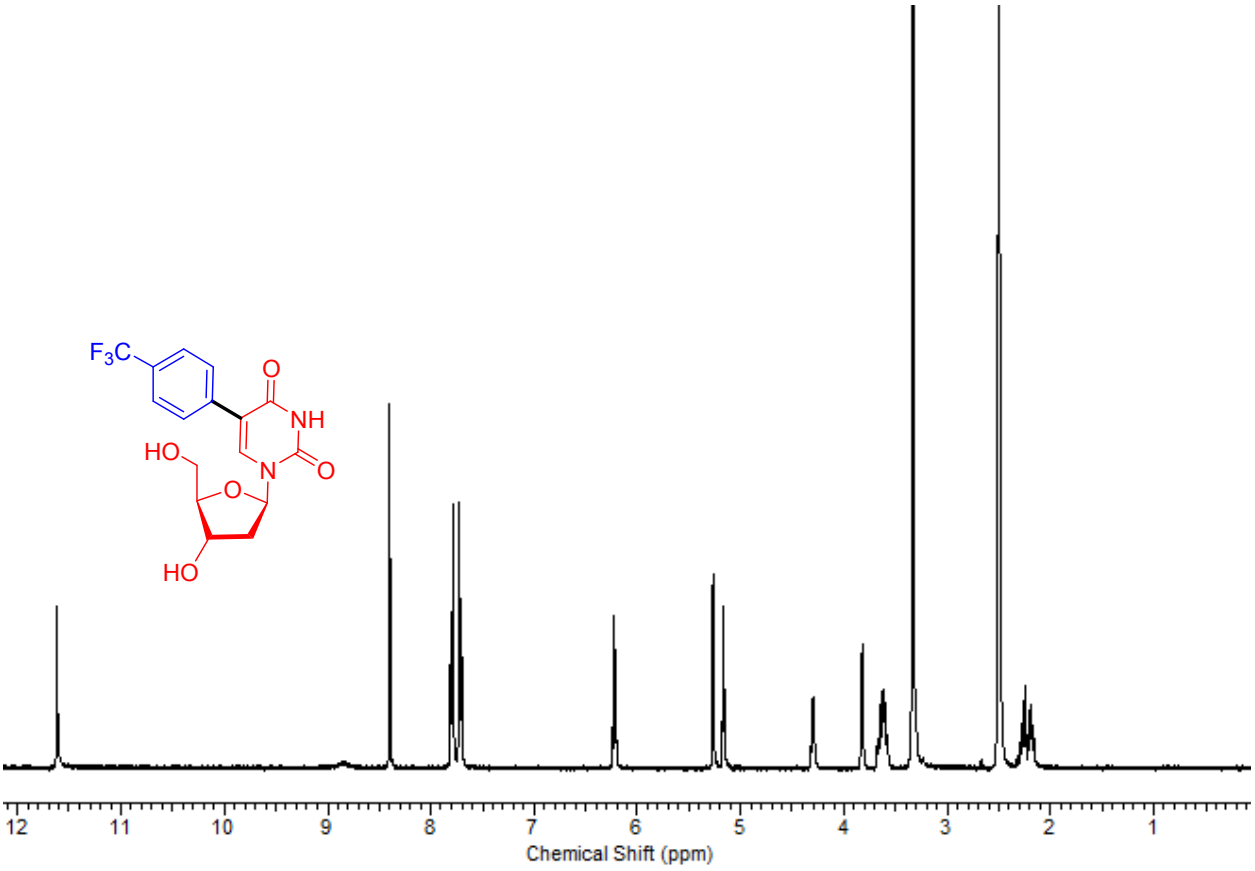

O
NH
HO
N
O
O
HO
162.42
150.06
138.61
132.95
132.15
128.13
127.49
126.29
126.13
113.37
87.59
84.67
70.16
60.93
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

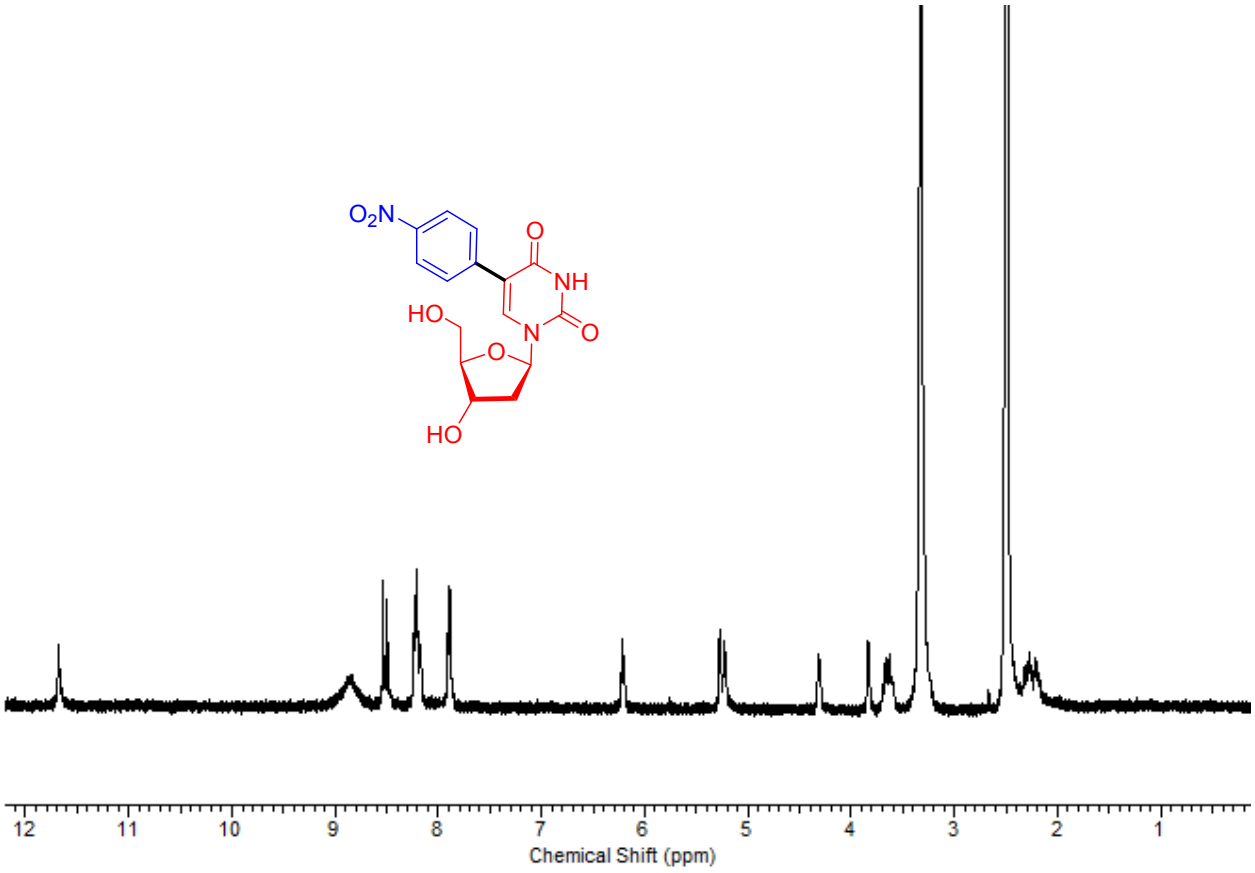

OMe
O
NH
HO
N
O
O
HO
14
12
10
8
6
4
2
0
-2
-4
Chemical Shift (ppm)

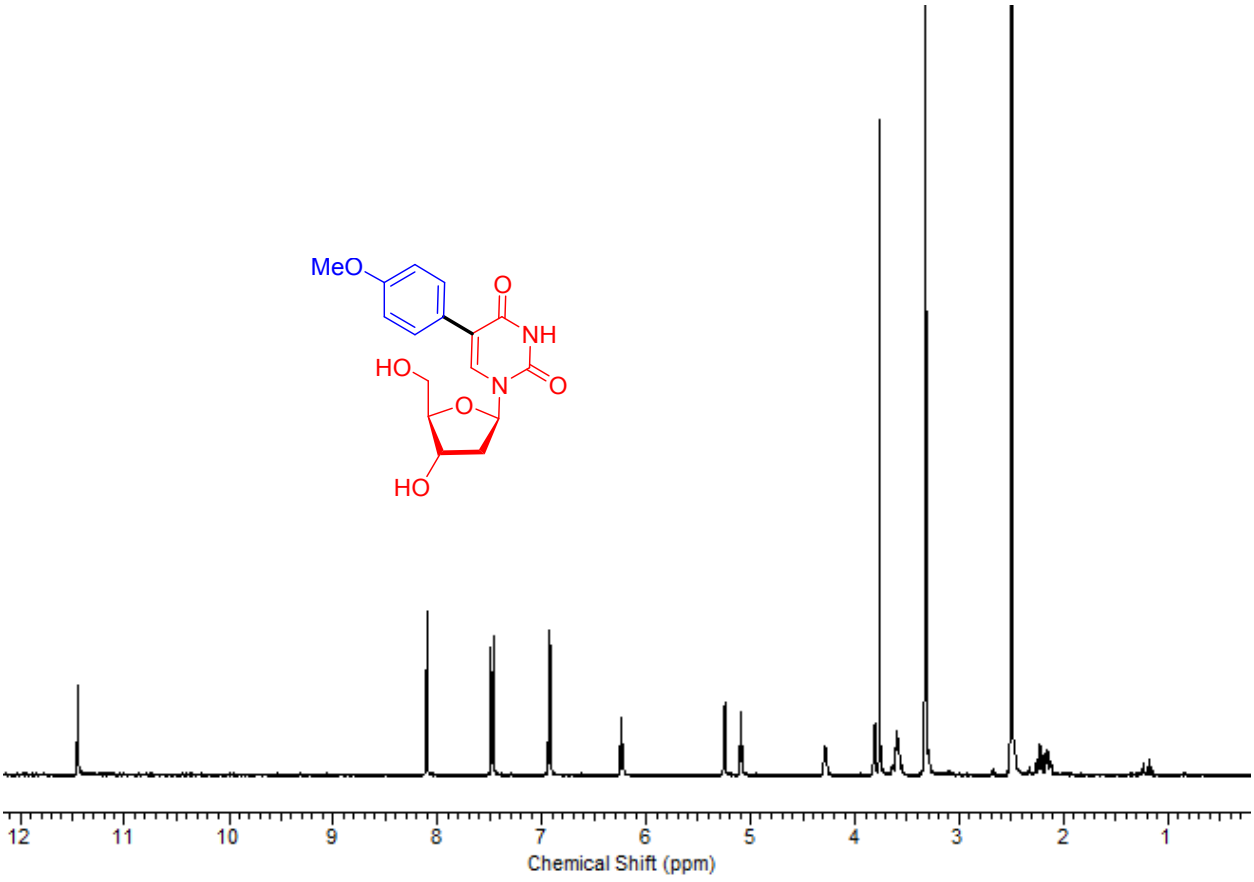

OMe
O
NH
HO
N
O
O
HO
161.96
157.22
150.32
139.06
131.37
129.24
121.98
120.10
111.42
87.49
84.19
70.63
61.34
55.47
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

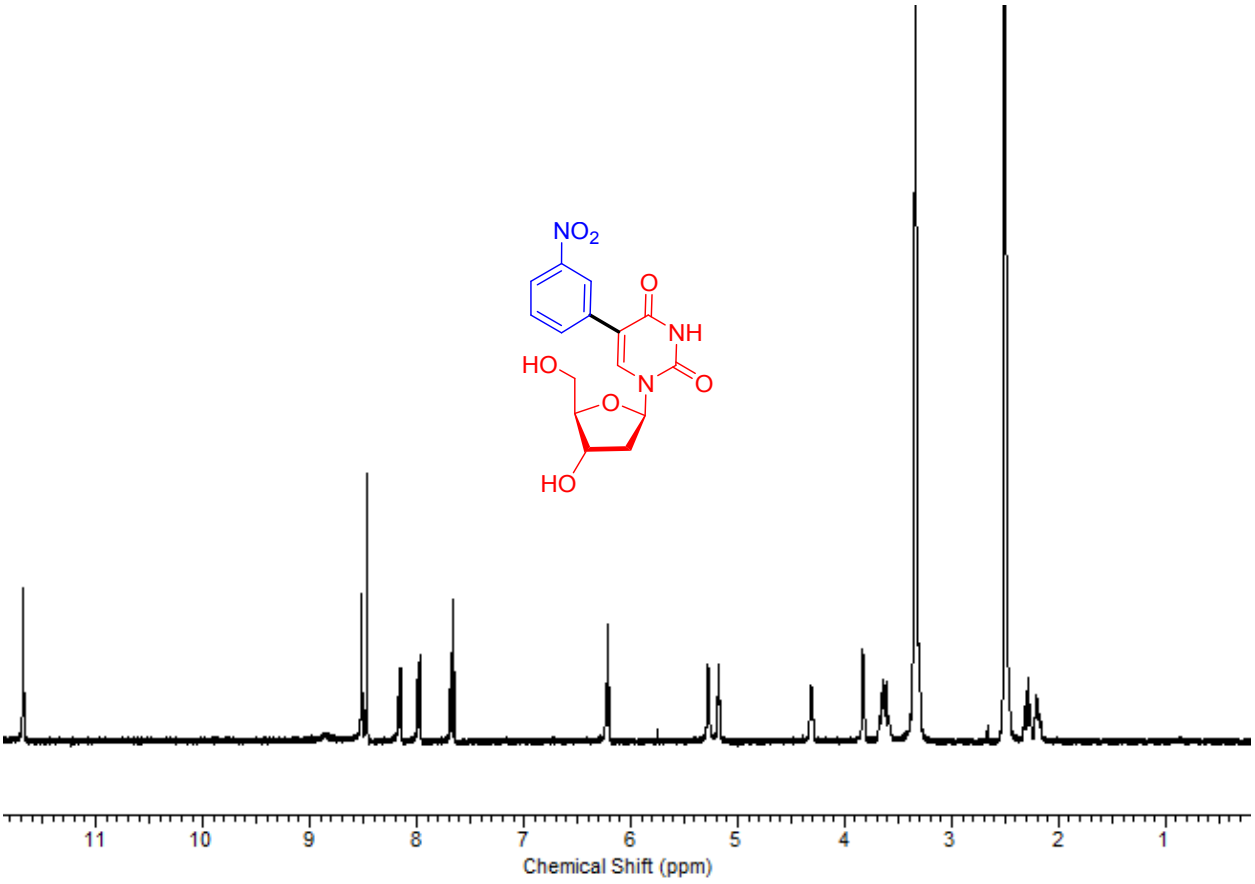

Normalized Intensity
Chemical Shift (ppm)
NH2
N
HO
N
O
O
HO

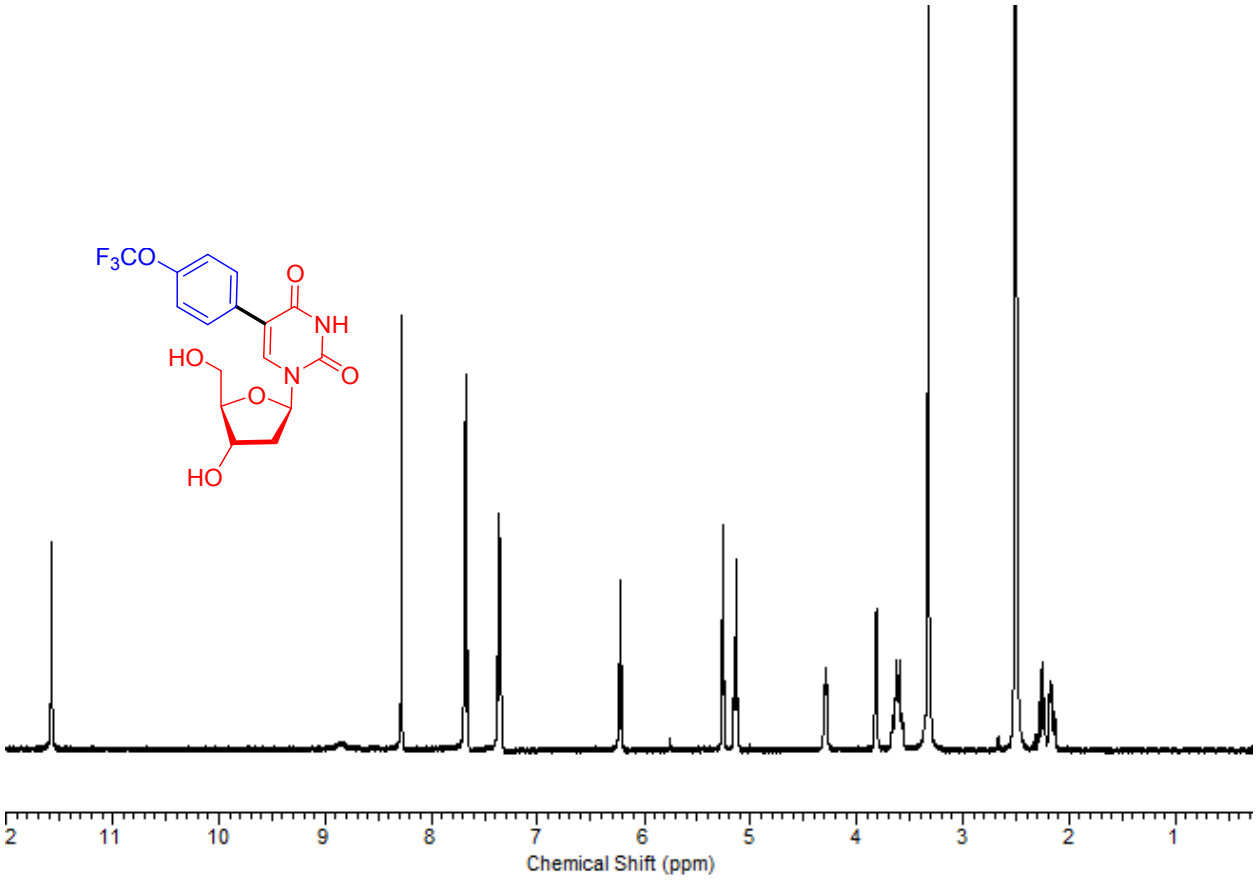

Normalized Intensity
Chemical Shift (ppm)
NH2
N
HO
N
O
O
HO
163.31
154.49
140.37
133.83
131.22
129.13
128.92
127.76
122.85
119.27
107.87
87.38
85.22
70.20
61.04
45.78
40.80

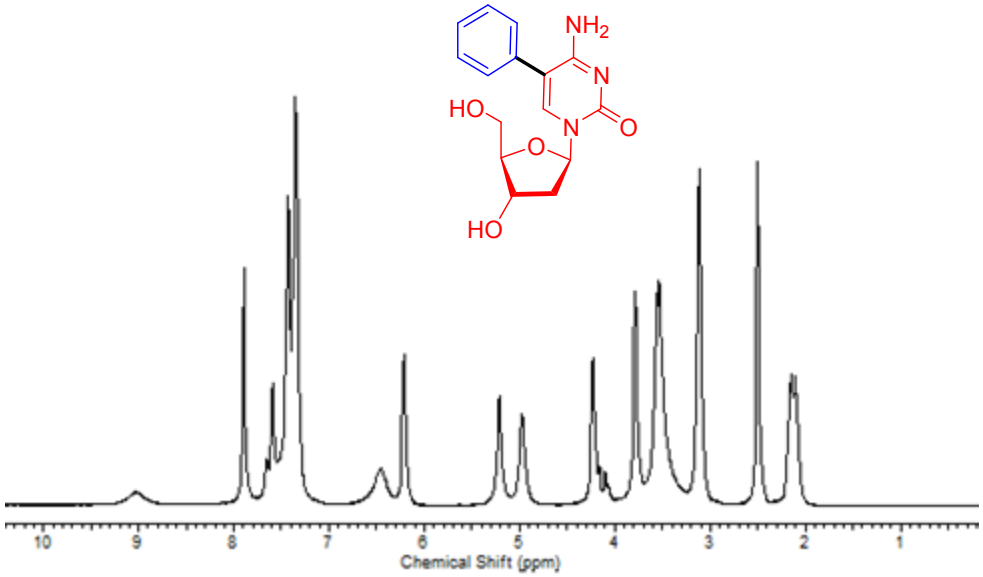

F3C
O
NH
HO
N
O
O
HO
12
11
10
9
8
7
6
5
4
3
2
1
Chemical Shift (ppm)

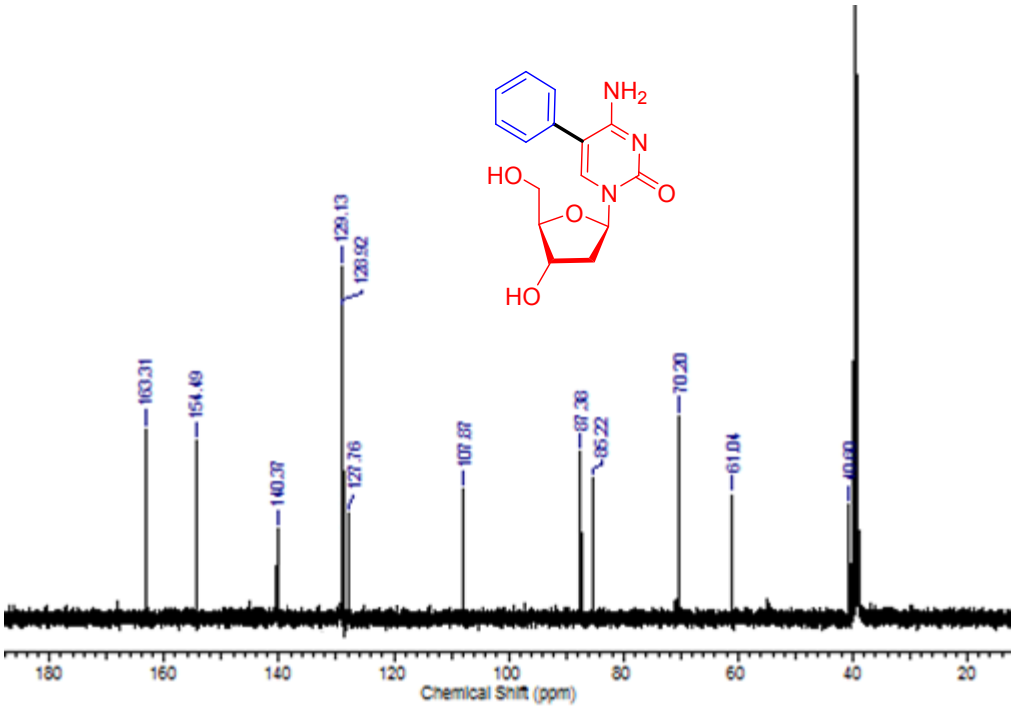

O2N
O
NH
HO
N
O
O
HO
12
11
10
9
8
7
6
5
4
3
2
1
Chemical Shift (ppm)


MeO
O
NH
HO
N
O
O
HO
12
11
10
9
8
7
6
5
4
3
2
1
Chemical Shift (ppm)


NO2
O
NH
HO
N
O
O
HO
11
10
9
8
7
6
5
4
3
2
1
Chemical Shift (ppm)


F3CO
O
NH
HO
N
O
O
HO
2
11
10
9
8
7
6
5
4
3
2
1
Chemical Shift (ppm)


NH2
N
HO
N
O
O
HO
10
9
8
7
6
5
4
3
2
1
Chemical Shift (ppm)


NH2
N
HO
N
O
O
HO
163.31
154.49
140.37
129.13
128.92
127.76
107.87
87.36
85.22
70.20
61.04
40.60
180
160
140
120
100
80
60
40
20
Chemical Shift (ppm)