

Supporting Information

One-pot Synthesis of Quinazolines via Hyrdogen-Transfer Catalysis

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Experimental section.....	S2
Characterization data of 3 , 4 , 5 , 9 and 10	S4
¹ H and ¹³ C NMR spectra of 3 , 4 , 5 , 9 and 10	S8

Experimental Section

All reactions were carried out under nitrogen. Proton and carbon magnetic resonance spectra (^1H NMR and ^{13}C NMR) were recorded using tetramethylsilane (TMS) in the solvent of CDCl_3 as the internal standard (^1H NMR: TMS at 0.00 ppm, CHCl_3 at 7.26 ppm; ^{13}C NMR: CDCl_3 at 77.4 ppm) or were recorded using tetramethylsilane (TMS) in the solvent of $\text{DMSO}-d_6$ as the internal standard (^1H NMR: TMS at 0.00 ppm, DMSO at 2.50 ppm; ^{13}C NMR: DMSO at 39.5 ppm). Melting points are uncorrected. Column chromatographic separations were carried out on ACME silica gel (200 - 300 mesh) using petroleum ether and EtOAc as eluent. All solvents were purified and dried using standard procedures.

General Methods for the Synthesis of Quinazolines between 1 and 2

1 (1 mmol), aldehyde **2** (1 mmol), styrene (4 mmol), $[\text{Cp}^*\text{IrCl}_2]_2$ (0.025 mmol) and anhydrous xylene (2 mL) were added to an oven-dried carousel tube. Then the system was degassed and filled with nitrogen. The reaction mixture was stirred and heated to reflux for 24h. After completion of the reaction, the resulting solution was cooled to room temperature, and the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 to 5:1) as the eluent to provide the desired products **4**.

Optimization of the conditions

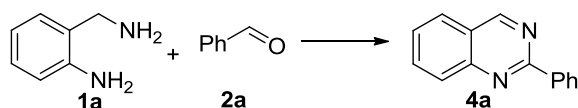


Table 1^a

	Catalyst	Additive	Acceptor	Solvent	Yield ^b
1	$[\text{Cp}^*\text{IrCl}_2]_2$	No	No	xylene	10%
2	$[\text{Cp}^*\text{IrCl}_2]_2$	No	styrene	xylene	66% ^c
3	$[\text{Cp}^*\text{IrCl}_2]_2$	No	E-crotonitrile	xylene	50% ^c
4	$[\text{Cp}^*\text{IrCl}_2]_2$	AcOH 0.2 eq.	styrene	xylene	43%
5	$[\text{Cp}^*\text{IrCl}_2]_2$	KOH 0.2 eq.	styrene	xylene	54%
6	$[\text{Cp}^*\text{IrCl}_2]_2$	<i>t</i> -BuONa 0.2 eq.	styrene	xylene	60%
7	$[\text{Cp}^*\text{IrCl}_2]_2$	K_2CO_3 0.2 eq.	styrene	xylene	46%
8	$[\text{Cp}^*\text{IrCl}_2]_2$	No	styrene	toluene	35%
9	$[\text{Cp}^*\text{IrCl}_2]_2$	No	styrene	DMF	50%
10	$[\text{Cp}^*\text{IrI}_2]_2$	No	styrene	xylene	57%
11	$\text{RuCl}_2(\text{PPh}_3)_3$	KOH 0.2 eq.	styrene	xylene	26%
12	$[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ ^d	KOH 0.2 eq.	styrene	xylene	52%
13	$[\text{Cp}^*\text{IrCl}_2]_2$	4A MS 2 eq.	styrene	xylene	51%

^a Conditions: **1a** (0.5 mmol), **2a** (0.5 mmol), catalyst (2.5 mol%), styrene (4.0 eq.) in refluxing temperature of solvent (1 mL) under N₂, 24 h. ^b H-NMR yield. ^c Isolated yield. ^d 2.5 mol% dppf was added.

Synthesis of quinazolines form alcohol **1a** and **7**

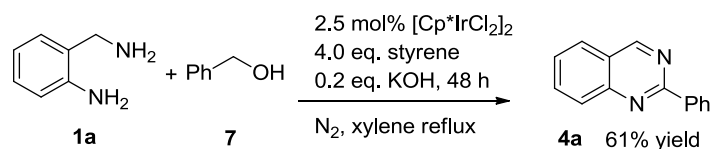


Table 2^a

	Catalyst	Additive	Acceptor	Solvent	Yield ^b
1	[Cp*IrCl ₂] ₂	No	styrene	xylene	10%
2	[Cp*IrCl ₂] ₂	KOH 0.2 eq.	styrene	xylene	61% ^c
3	[Cp*IrCl ₂] ₂	NaOH 0.2 eq.	styrene	xylene	57%
4	[Cp*IrCl ₂] ₂	<i>t</i> -BuONa 0.2 eq.	styrene	xylene	50%
5	RuCl ₂ (PPh ₃) ₃	KOH 0.2 eq.	styrene	xylene	46%
6	[Ru(<i>p</i> -cymene)Cl ₂] ₂ ^d	KOH 0.2 eq.	styrene	xylene	42%

^a Conditions: **1a** (0.5 mmol), **2a** (0.5 mmol), catalyst (2.5 mol%), acceptor (4.0 eq.), base (20 mol%) in refluxing temperature of solvent (1 mL) under N₂, 48 h. ^b H-NMR yield. ^c Isolated yield. ^d 2.5 mol% dppf was added.

2-aminobenzylamines **1a** (122 mg, 1 mmol), phenylmethanol **2** (108 mg, 1 mmol), styrene (416 mg, 4 mmol), [Cp*IrCl₂]₂ (20 mg, 0.025 mmol), KOH (11 mg, 0.2 mmol) and anhydrous xylene (2 mL) were added to an oven-dried carousel tube. Then the system was degassed and filled with nitrogen. The reaction mixture was stirred and heated to reflux for 48h. After completion of the reaction, the resulting solution was cooled to room temperature, and the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 to 5:1) as the eluent to provide the desired products **4a** (slight yellow solid, 127 mg, 61% yield).

Synthesis of 2-phenyl-4H-benzo[d][1,3]oxazine form aldehyde **2a** and **8**

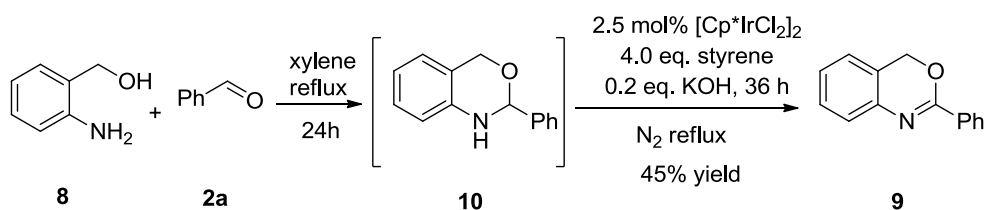


Table 3

	Catalyst	Additive	Acceptor	Solvent	Yield ^a
1	[Cp*IrCl ₂] ₂	No	Styrene 4.0 eq.	xylene	40%
2	[Cp*IrCl ₂] ₂	KOH 0.2 eq.	Styrene 4.0 eq.	xylene	45% ^b
3	[Cp*IrCl ₂] ₂	<i>t</i> -BuONa 0.2 eq.	Styrene 4.0 eq.	xylene	38%
4	[Cp*IrCl ₂] ₂	<i>p</i> -TsOH 0.2 eq.	Styrene 4.0 eq.	xylene	39%

^a H-NMR yield. ^b Isolated yield.

(2-aminophenyl) methanol **8** (123 mg, 1 mmol), benzaldehyde **2a** (106 mg, 1 mmol) and anhydrous xylene (2 mL) were added to an oven-dried carousel tube. Then the system was degassed and filled with nitrogen. The reaction mixture was stirred and heated to reflux for 24h, the reaction was cooled to room temperature, styrene (416 mg, 4 mmol), [Cp*IrCl₂]₂ (20 mg, 0.025 mmol), KOH (11 mg, 0.2 mmol) were added, the mixture was stirred and heated to reflux for 24h, the resulting solution was cooled to room temperature, and the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 to 5:1) as the eluent to provide the desired products **9** (slight yellow solid, 94 mg, 45% yield).

Characterization Data of 3, 4, 5, 9 and 10

2-phenyl-1,2,3,4-tetrahydroquinazoline (3a). White solid, mp: 102 °C - 103 °C (lit.¹ 102 °C - 105 °C). ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 7.40 (d, *J* = 8.0 Hz, 2H), 7.25 - 7.31 (m, 3H), 6.95 (t, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 8.0 Hz, 1H), 6.62 (t, *J* = 8.0 Hz, 1H), 6.47 (d, *J* = 8.0, 1H), 5.11 (s, 1H), 4.13 (d, *J* = 16, 1H), 4.10 (br, 1H), 3.86 (d, *J* = 16, 1H), 1.81 (br, 1H). ¹³C NMR (CDCl₃ - *d*₃, 100 MHz): δ 143.7, 141.6, 128.7, 128.5, 126.6, 126.2, 121.3, 118.1, 115.0, 69.6, 46.5. HRMS (ESI): [M + H]⁺: C₁₄H₁₅N₂ Calcd for 211.1235. Found: 211.1276.

2-phenylquinazoline (4a). Pale yellow solid, mp: 96 °C - 98 °C (lit.² 97 °C - 98 °C). ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 9.37 (s, 1H), 8.54 (d, *J* = 8.0, 2H), 8.00 (d, *J* = 8.0, 1H), 8.79 - 8.84 (m, 2H), 7.42 - 7.53 (m, 4H). ¹³C NMR (CDCl₃ - *d*₃, 100 MHz): δ 161.0, 160.5, 150.8, 138.0, 134.1, 130.6, 128.6, 127.2, 127.1, 123.6. HRMS (ESI): [M + H]⁺: C₁₄H₁₁N₂ Calcd for 207.0922. Found: 207.0910.

2-(3-chlorophenyl)quinazoline (4b). pale yellow solid, mp: 148 °C - 149 °C (lit.³ 148 °C - 150 °C). ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 9.46 (s, 1H), 8.63 (s, 1H), 8.49 - 8.51 (m, 1H), 8.09 (d, *J* = 8.0, 1H), 7.91 - 7.95 (m, 2H), 7.64 (t, *J* = 8.0, 1H), 7.46 - 7.48 (m, 2H). ¹³C NMR (CDCl₃ - *d*₃, 100 MHz): δ 160.5, 159.7, 150.6, 139.8, 134.7, 134.3, 130.5, 129.8, 128.7, 128.6, 127.6, 127.1, 126.6, 123.7. HRMS (ESI): [M + H]⁺: C₁₄H₁₀N₂Cl Calcd for 241.0533. Found: 241.0522.

2-(3-bromophenyl)quinazoline (4c). Yellow solid, mp: 154 °C - 156 °C (lit.³ 153 °C - 155 °C). ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 9.46 (s, 1H), 8.79 (s, 1H), 8.09 (d, *J* = 8.0, 1H), 7.90 - 7.94 (m, 2H), 7.62 - 7.65 (m, 2H), 7.40 (t, *J* = 8.0, 1H). ¹³C NMR (CDCl₃ - *d*₃, 100 MHz): δ 160.5, 159.5, 150.6,

140.0, 134.3, 133.4, 131.5, 130.1, 128.8, 127.6, 127.1, 127.0, 123.7, 122.9. HRMS (ESI): $[M + H]^+$: $C_{14}H_{10}N_2Br$ Calcd for 285.0027. Found: 241.0007.

2-(3-nitrophenyl)quinazoline (4d). Yellow solid, mp: 160 °C - 162 °C (lit.⁴ 162 °C - 163 °C). ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 9.51 (s, 1H), 9.50 (s, 1H), 8.98 (d, *J* = 8.0, 1H), 8.35 (d, *J* = 8.0, 1H), 8.14 (d, *J* = 8.0, 1H), 7.96 - 8.00 (m, 2H), 7.67 - 7.73 (m, 2H). ¹³C NMR (CDCl₃ - *d*₃, 100 MHz): δ 160.7, 158.7, 150.6, 148.5, 139.9, 134.5, 134.2, 129.5, 128.7, 127.2, 125.0, 123.9, 123.6. HRMS (ESI): $[M + H]^+$: $C_{14}H_{10}N_3O_2$ Calcd for 252.0773. Found: 252.0756.

2-(m-tolyl)quinazoline (4e). Yellow solid, mp: 97 °C - 98 °C. ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 9.44 (s, 1H), 9.40 - 9.43 (m, 2H), 8.08 (d, *J* = 8.0, 1H), 7.86 - 7.90 (m, 2H), 7.58 (t, *J* = 8.0, 1H), 7.43 (t, *J* = 8.0, 1H), 7.32 (d, *J* = 8.0, 1H), 2.48 (s, 3H). ¹³C NMR (CDCl₃ - *d*₃, 100 MHz): δ 161.2, 160.4, 150.7, 138.2, 137.9, 134.0, 131.4, 129.1, 128.6, 128.5, 127.2, 127.1, 125.8, 123.5, 21.5. HRMS (ESI): $[M + H]^+$: $C_{15}H_{13}N_2$ Calcd for 221.1079. Found: 221.1057.

2-(3-methoxyphenyl)quinazoline (4f). Pale yellow solid, mp: 89 °C - 90 °C. ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 9.46 (s, 1H), 8.23 (d, *J* = 8.0, 1H), 8.17 - 8.19 (m, 1H), 7.88 - 7.93 (m, 2H), 7.61 (t, *J* = 8.0, 1H), 7.45 (t, *J* = 8.0, 1H), 7.07 (d, *J* = 8.0, 1H), 3.95 (s, 3H). ¹³C NMR (CDCl₃ - *d*₃, 100 MHz): δ 160.8, 160.4, 160.0, 150.7, 139.5, 134.1, 129.6, 128.6, 127.3, 127.1, 123.6, 121.1, 117.2, 113.0. HRMS (ESI): $[M + H]^+$: $C_{15}H_{13}N_2O$ Calcd for 237.1028. Found: 237.1016.

2-(4-fluorophenyl)quinazoline (4g). White solid, mp: 128 °C - 130 °C (lit.² 129 °C - 130). ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 9.43 (s, 1H), 8.61 - 8.64 (m, 2H), 8.06 (d, *J* = 8.0, 1H), 7.88 - 7.92 (m, 2H), 7.59 - 7.62 (m, 1H), 7.18 - 7.22 (m, 2H). ¹³C NMR (CDCl₃ - *d*₃, 100 MHz): δ 165.9, 163.4, 160.5, 160.1, 150.7, 134.2, 130.7, 130.6, 128.5, 127.2, 127.1, 123.4, 115.6, 115.4. HRMS (ESI): $[M + H]^+$: $C_{14}H_{10}N_2F$ Calcd for 225.0828. Found: 225.0887.

2-(4-bromophenyl)quinazoline (4h). White solid, mp: 121 °C - 123 °C (lit.² 120 °C - 121 °C). ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 9.45 (s, 1H), 8.50 (d, *J* = 8.0, 2H), 8.07 (d, *J* = 8.0, 1H), 7.90 - 7.94 (m, 2H), 7.66 (d, *J* = 8.0, 2H), 7.61 - 7.65 (m, 1H), 7.59 - 7.62 (m, 1H). ¹³C NMR (CDCl₃ - *d*₃, 100 MHz): δ 160.5, 160.1, 150.7, 136.9, 134.2, 131.8, 130.1, 128.6, 127.5, 127.1, 124.4, 123.6. HRMS (ESI): $[M + H]^+$: $C_{14}H_{10}N_2Br$ Calcd for 285.0027. Found: 285.0025.

2-(4-nitrophenyl)quinazoline (4i). White solid, mp: 219 °C - 221 °C (lit.² 218 °C - 219 °C). ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 9.52 (s, 1H), 8.82 (d, *J* = 8.0, 2H), 8.37 (d, *J* = 8.0, 2H), 8.14 (d, *J* = 8.0, 1H), 7.96 - 8.00 (m, 2H), 7.69 - 7.73 (m, 1H). ¹³C NMR (CDCl₃ - *d*₃, 100 MHz): δ 160.7, 158.8, 150.6, 149.2, 143.8, 134.6, 129.4, 128.8, 128.3, 127.2, 123.8, 123.7. HRMS (ESI): $[M + H]^+$: $C_{14}H_{10}N_3O_2$ Calcd for 252.0773. Found: 272.0758.

2-(p-tolyl)quinazoline (4j). White solid, mp: 98 °C - 99 °C (lit.² 97 °C - 98). ¹H NMR (CDCl₃ - *d*₃, 400 MHz): δ 9.42 (s, 1H), 8.51 (d, *J* = 8.0, 2H), 8.05 (d, *J* = 8.0, 1H), 7.84 - 7.88 (m, 2H), 7.55 (t, *J* = 8.0,

1H), 7.33 (d, $J = 8.0$, 2H), 2.43 (s, 3H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 161.1, 160.4, 150.8, 140.8, 135.3, 134.0, 129.4, 128.5, 127.0, 123.5, 21.5. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{15}\text{H}_{13}\text{N}_2$ Calcd for 221.1079. Found: 221.1052.

2-(furan-2-yl)quinazoline (4k). Brown liquid. ^1H NMR ($\text{CDCl}_3 - d_3$, 400 MHz): δ 9.36 (s, 1H), 8.09 (d, $J = 8.0$, 1H), 7.86 - 7.90 (m, 2H), 7.69 (s, 1H), 7.57 (t, $J = 4.0$, 1H), 7.46 (d, $J = 4.0$, 1H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 160.6, 154.0, 152.4, 150.3, 145.3, 134.4, 128.3, 127.2, 123.3, 114.0, 111.2. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{12}\text{H}_9\text{N}_2\text{O}$ Calcd for 197.0715. Found: 197.0695.

2-benzylquinazoline (4l). Slight yellow solid, mp: 68 °C - 69 °C (lit.⁶ 70 - 71 °C). ^1H NMR ($\text{CDCl}_3 - d_3$, 400 MHz): δ 9.33 (s, 1H), 8.01 (d, $J = 8.0$, 1H), 7.87 - 7.89 (m, 2H), 7.58 (t, $J = 8.0$, 1H), 7.43 (d, $J = 8.0$, 2H), 7.30 (t, $J = 8.0$, 2H), 7.19 - 7.22 (m, 1H), 4.46 (s, 2H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 166.1, 160.8, 150.4, 138.5, 134.1, 129.2, 128.5, 128.1, 127.2, 127.0, 126.5, 123.1. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{15}\text{H}_{13}\text{N}_2$ Calcd for 221.1079. Found: 221.1019.

2-pentylquinazoline (4m). Pale yellow liquid. ^1H NMR ($\text{CDCl}_3 - d_3$, 400 MHz): δ 9.35 (s, 1H), 7.98 (d, $J = 8.0$, 1H), 7.85 - 7.89 (m, 2H), 7.58 (t, $J = 8.0$, 1H), 3.12 (t, $J = 8.0$, 2H), 1.89 - 1.97 (m, 2H), 1.36 - 1.45 (m, 4H), 0.91 (t, $J = 8.0$, 3H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 167.9, 160.3, 150.0, 133.9, 127.8, 127.0, 126.8, 123.0, 39.9, 31.7, 28.7, 22.5, 14.0. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{13}\text{H}_{17}\text{N}_2$ Calcd for 201.1392. Found: 201.1387.

5-fluoro-2-phenylquinazoline (4n). Pale yellow solid, mp: 100 °C - 102 °C (lit.² 101 - 102 °C). ^1H NMR ($\text{CDCl}_3 - d_3$, 400 MHz): δ 9.73 (s, 1H), 8.61 - 8.63 (m, 2H), 7.79 - 7.89 (m, 2H), 7.52 - 7.57 (m, 3H), 7.20 - 7.25 (m, 1H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 161.7, 158.2 (d, $J = 250$, 1C), 154.8, 151.5, 137.5, 134.1, 131.0, 128.6, 124.6, 114.4, 110.0. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{14}\text{H}_{10}\text{FN}_2$ Calcd for 225.0828. Found: 225.0815.

2-(4-bromophenyl)-5-fluoroquinazoline (4o). Pale yellow solid, mp: 176 °C - 177 °C. ^1H NMR ($\text{CDCl}_3 - d_3$, 400 MHz): δ 9.70 (s, 1H), 8.49 (d, $J = 8.0$, 2H), 7.82 - 7.87 (m, 2H), 7.65 (d, $J = 8.0$, 2H), 7.22 - 7.26 (m, 1H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 160.7, 158.0 (d, $J = 260$, 1C), 154.9, 151.2, 136.5, 134.2, 131.8, 130.2, 125.8, 124.5, 114.4, 111.3. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{14}\text{H}_9\text{FBrN}_2$ Calcd for 302.9933. Found: 302.9927.

5-fluoro-2-(p-tolyl)quinazoline (4p). Pale yellow solid, mp: 132 °C - 133 °C. ^1H NMR ($\text{CDCl}_3 - d_3$, 400 MHz): δ 9.71 (s, 1H), 8.51 (d, $J = 8.0$, 2H), 7.81 - 7.87 (m, 2H), 7.34 (d, $J = 8.0$, 2H), 7.19 - 7.21 (m, 1H), 2.45 (s, 3H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 161.8, 160.7, 158.2 (d, $J = 250$, 1C), 154.7, 151.5, 141.3, 134.9, 134.0, 129.4, 128.7, 124.5, 114.3, 110.7, 21.5. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{15}\text{H}_{12}\text{FN}_2$ Calcd for 239.0985. Found: 239.0989.

5-fluoro-2-pentylquinazoline (4q). Slight yellow liquid. ^1H NMR ($\text{CDCl}_3 - d_3$, 400 MHz): δ 9.52 (s, 1H), 7.67 - 7.75 (m, 2H), 7.10 - 7.14 (m, 1H), 3.04 (t, $J = 8.0$, 2H), 1.80 - 1.88 (m, 2H), 1.28 - 1.35 (m,

4H), 0.82 (t, $J = 8.0$, 3H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 168.8, 158.1 (d, $J = 250$, 1C), 154.6, 151.0, 134.0, 123.8, 113.9, 110.6, 39.9, 31.6, 28.5, 22.5, 13.9. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{13}\text{H}_{16}\text{FN}_2$ Calcd for 219.1298. Found: 219.1292.

2-((benzylamino)methyl)aniline (5). Slight yellow liquid. ^1H NMR ($\text{CDCl}_3 - d_3$, 400 MHz): δ 7.27 - 7.39 (m, 5H), 7.13 (t, $J = 8.0$ Hz, 1H), 7.06 (d, $J = 8.0$ Hz, 1H), 6.69 - 6.73 (m, 2H), 4.74 (br, 2), 3.86 (s, 2H), 3.82 (s, 2H), 1.52 (br, 1 H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 146.9, 140.2, 129.9, 128.5, 128.4, 128.1, 127.0, 123.8, 117.7, 115.7, 53.2, 52.4. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{14}\text{H}_{17}\text{N}_2$ Calcd for 213.1392. Found: 213.1377.

2-phenyl-4H-benzo[d][1,3]oxazine (9). White solid, mp: 91 °C - 92 °C (lit.² 92 °C - 93 °C). ^1H NMR ($\text{CDCl}_3 - d_3$, 400 MHz): δ 8.13 (d, $J = 8.0$, 2H), 7.41 - 7.51 (m, 3H), 7.25 - 7.34 (m, 2H), 7.16 - 7.20 (m, 1H), 7.01 (d, $J = 8.0$, 2H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 157.6, 139.7, 132.3, 131.4, 128.9, 128.2, 128.0, 126.4, 124.6, 123.7, 122.3, 66.4. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{14}\text{H}_{17}\text{N}_2$ Calcd for 213.1392. Found: 213.1377.

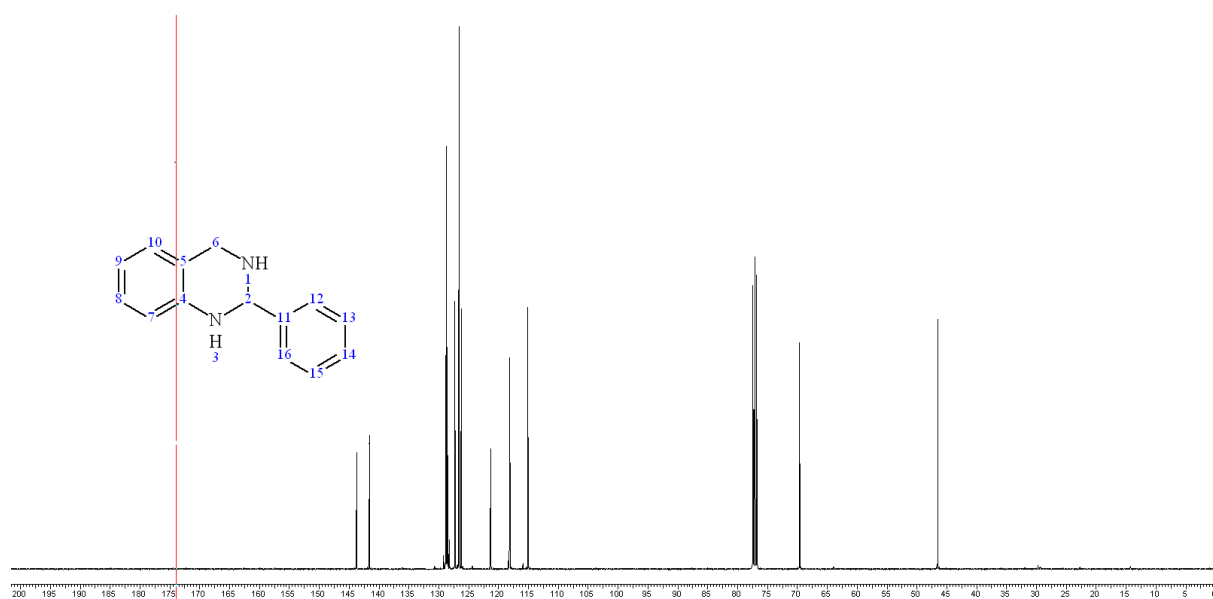
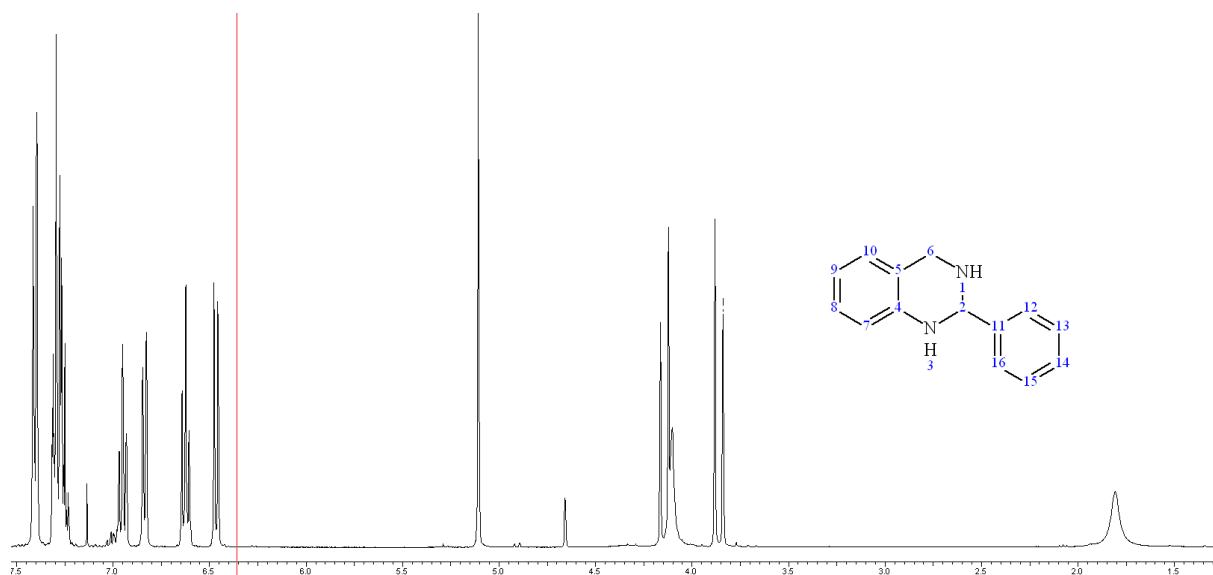
2-phenyl-2,4-dihydro-1H-benzo[d][1,3]oxazine (10). White solid, mp: 117 °C - 118 °C (lit.⁷ 116 °C - 117 °C). ^1H NMR ($\text{CDCl}_3 - d_3$, 400 MHz): δ 7.57 (d, $J = 8.0$, 2H), 7.40 - 7.44 (m, 3H), 7.11 (t, $J = 8$, 1H), 6.98 (d, $J = 8.0$, 1H), 6.85 (t, $J = 8$, 1H), 6.72 (d, $J = 8.0$, 1H), 5.59 (d, $J = 4.0$, 1H), 5.13 (d, $J = 16.0$, 1H), 4.95 (d, $J = 16.0$, 1H), 4.12 (br, 1H). ^{13}C NMR ($\text{CDCl}_3 - d_3$, 100 MHz): δ 141.6, 139.1, 129.1, 128.6, 127.4, 126.5, 125.0, 122.2, 119.8, 117.1, 85.2, 67.6. HRMS (ESI): $[\text{M} + \text{H}]^+$: $\text{C}_{14}\text{H}_{14}\text{NO}$ Calcd for 212.1075. Found: 212.1077.

Reference

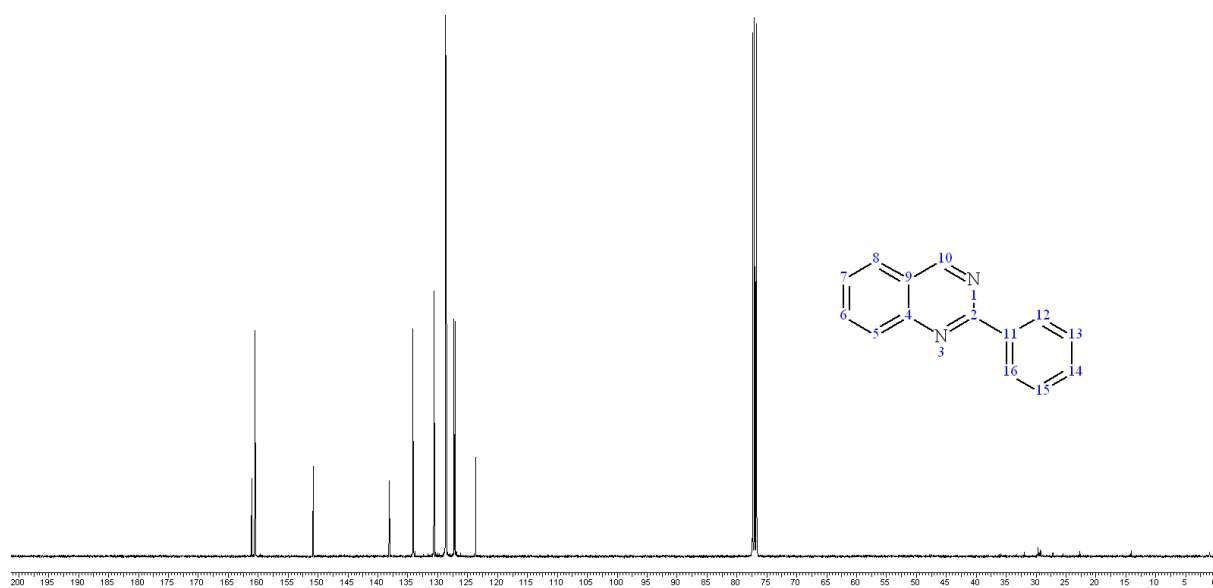
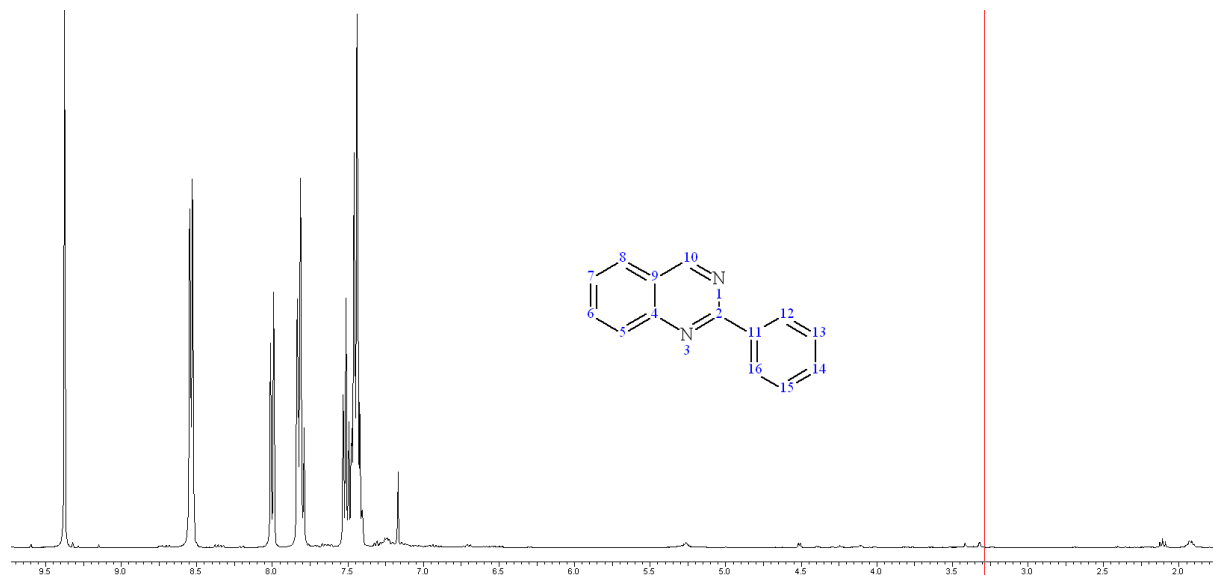
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^1H and ^{13}C NMR Spectra of 3, 4, 5, 9 and 10

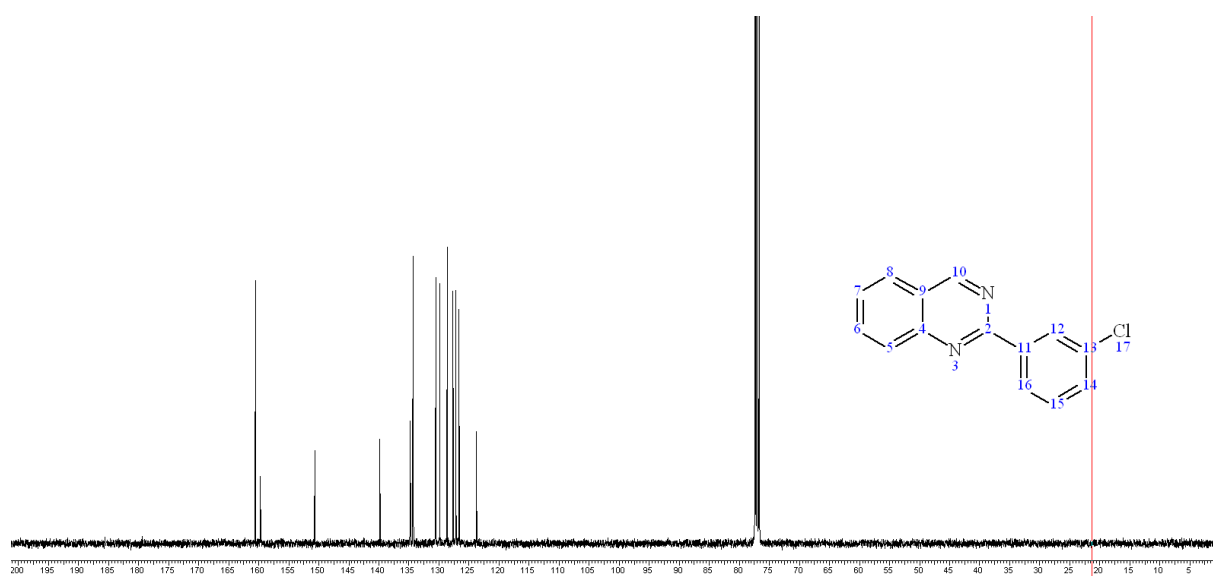
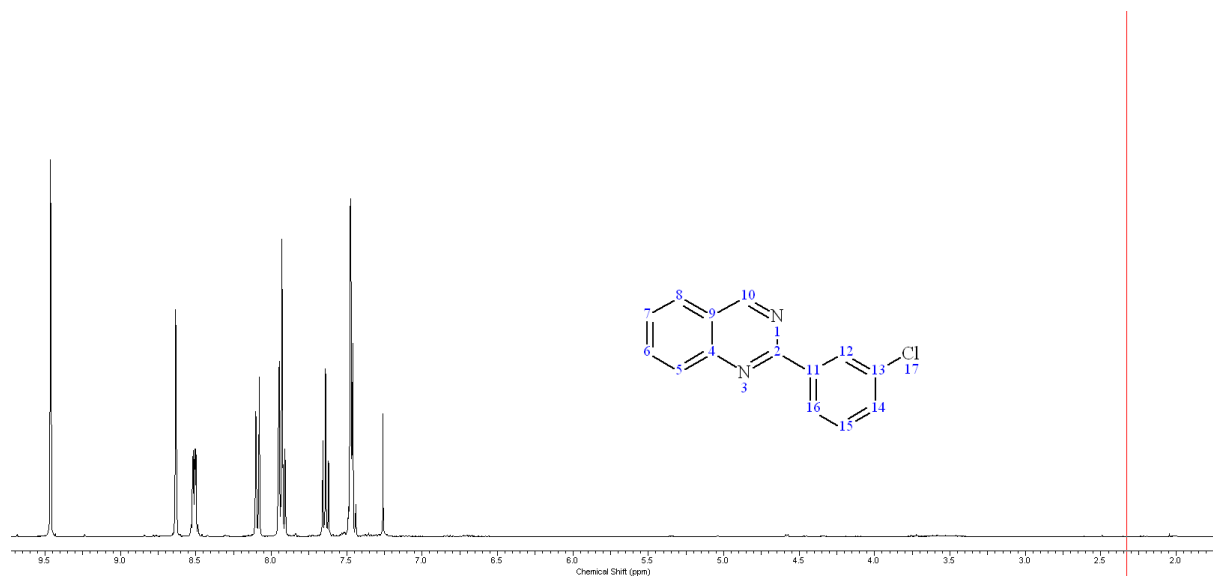
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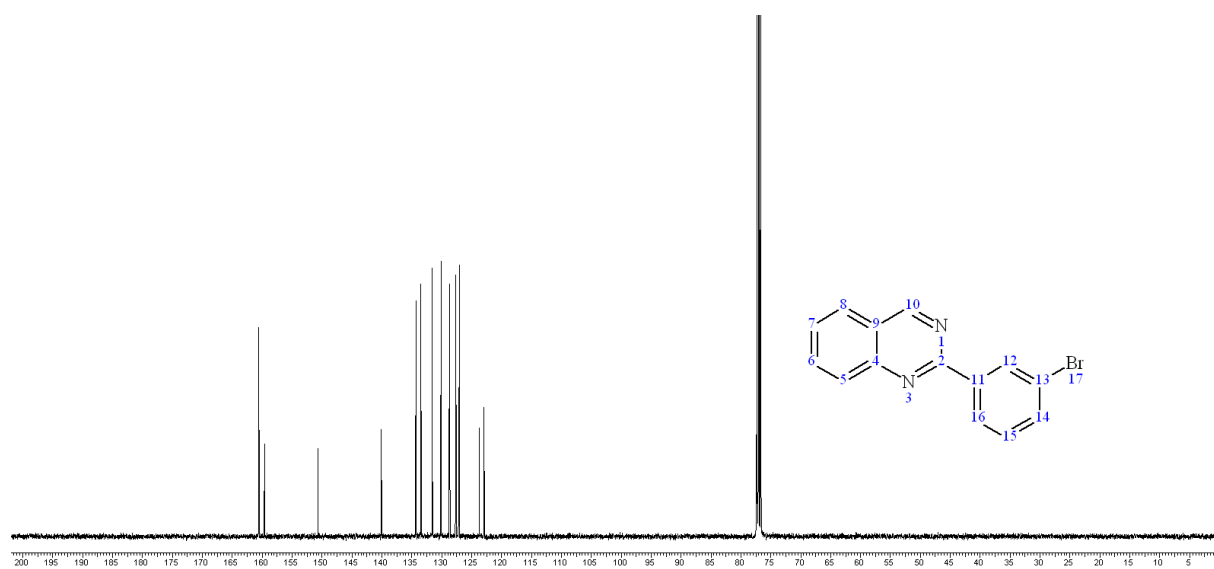
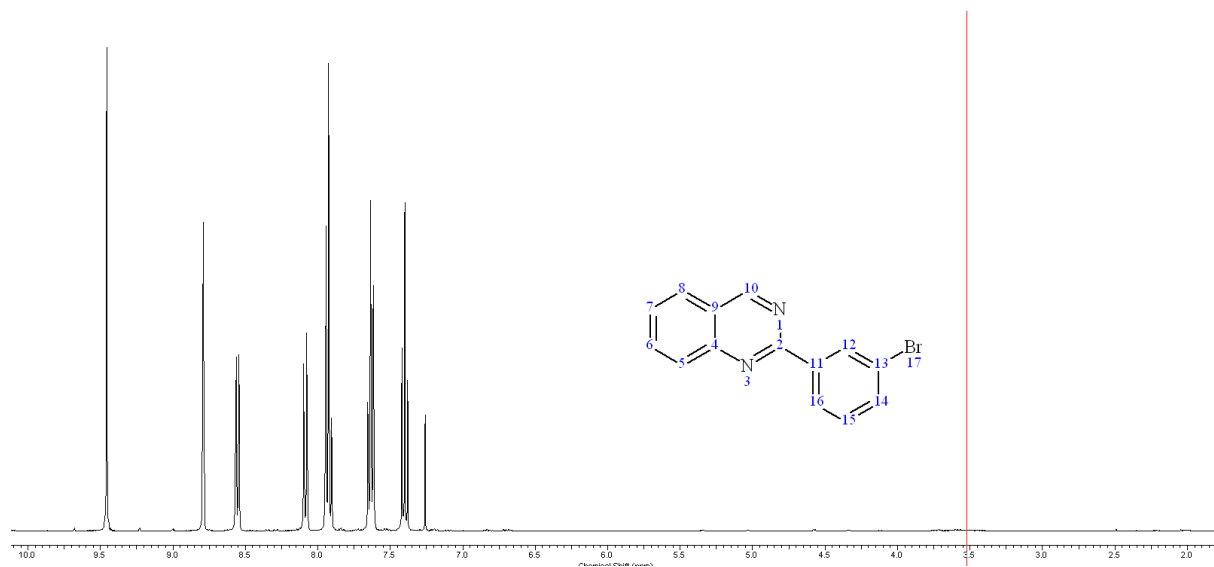
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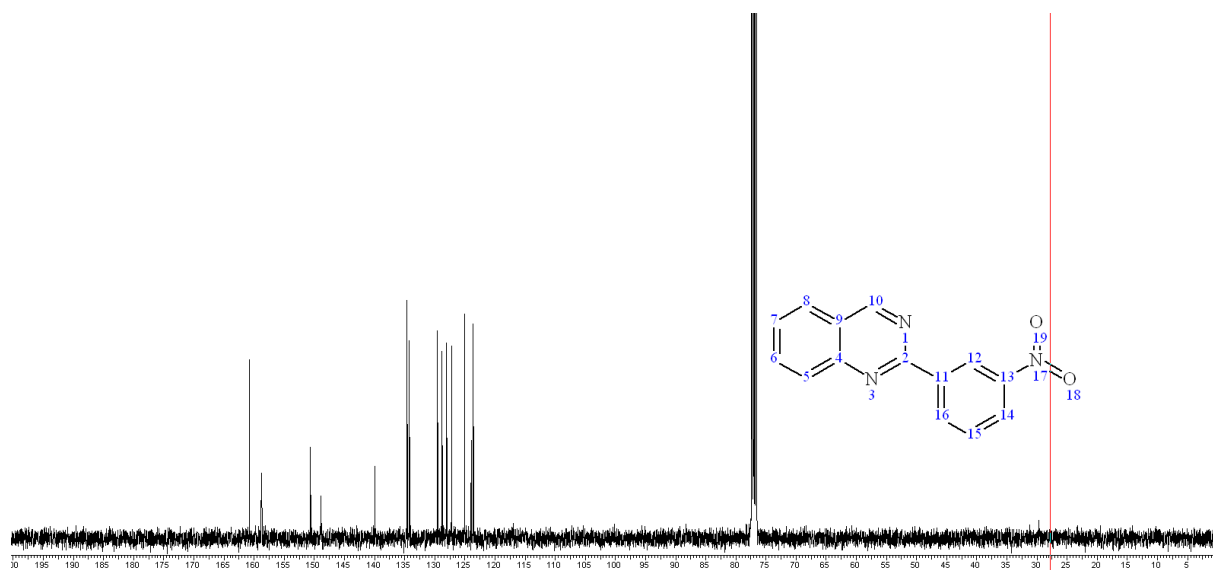
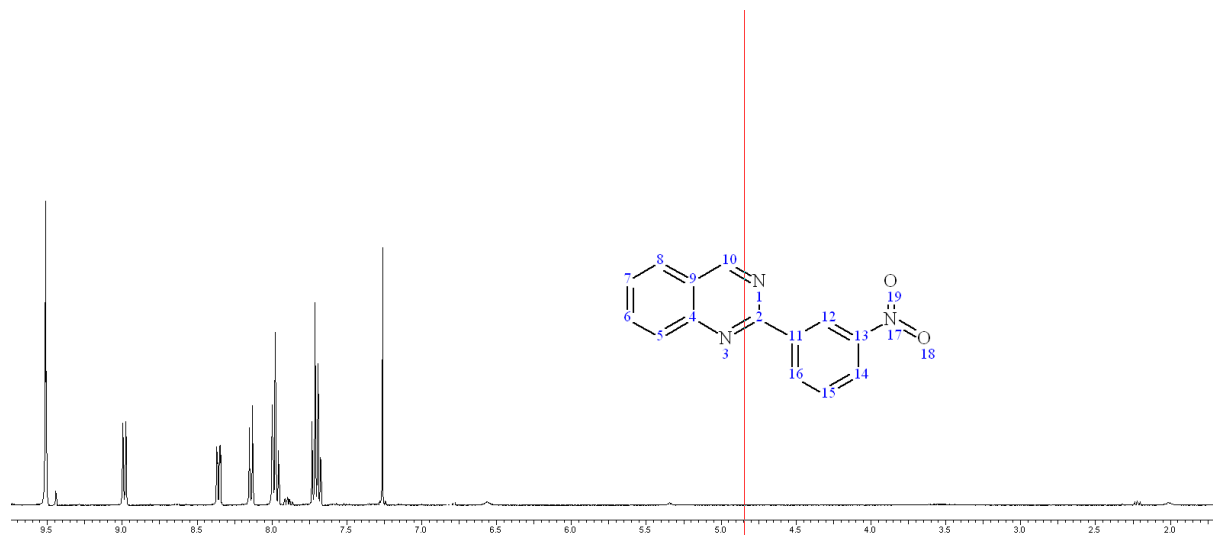
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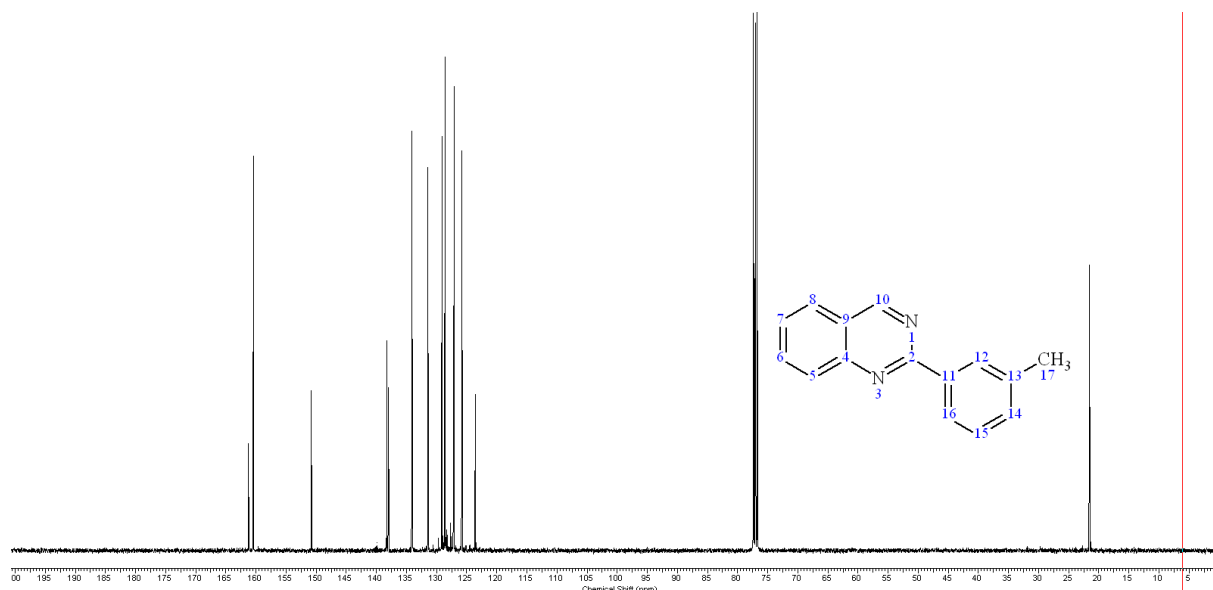
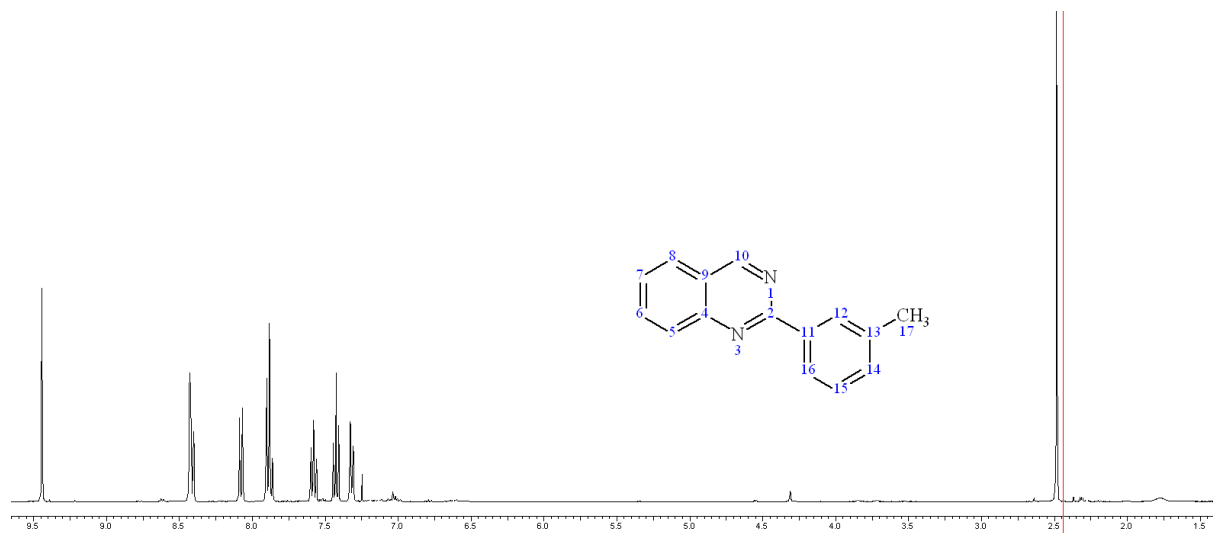
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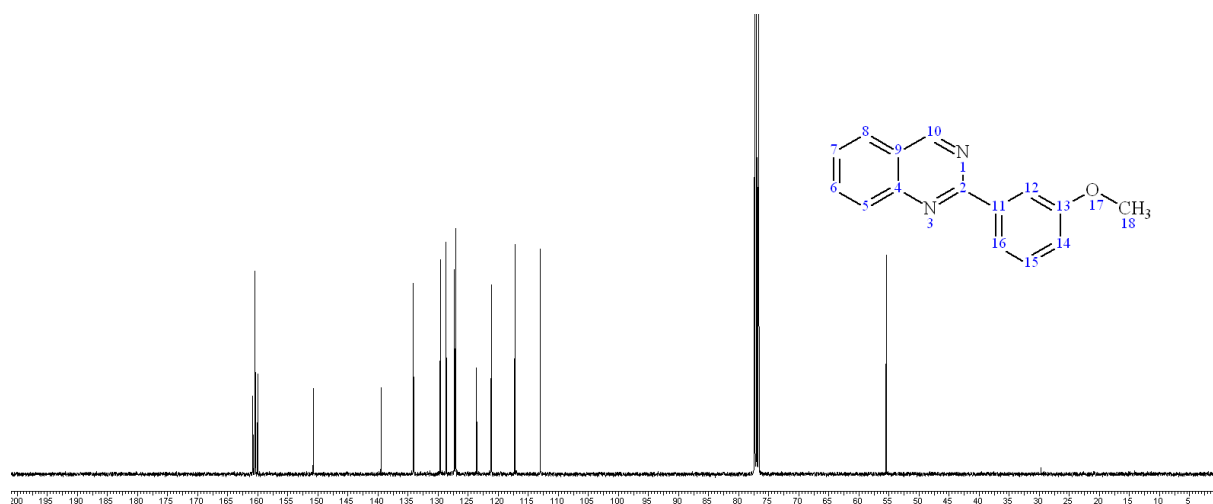
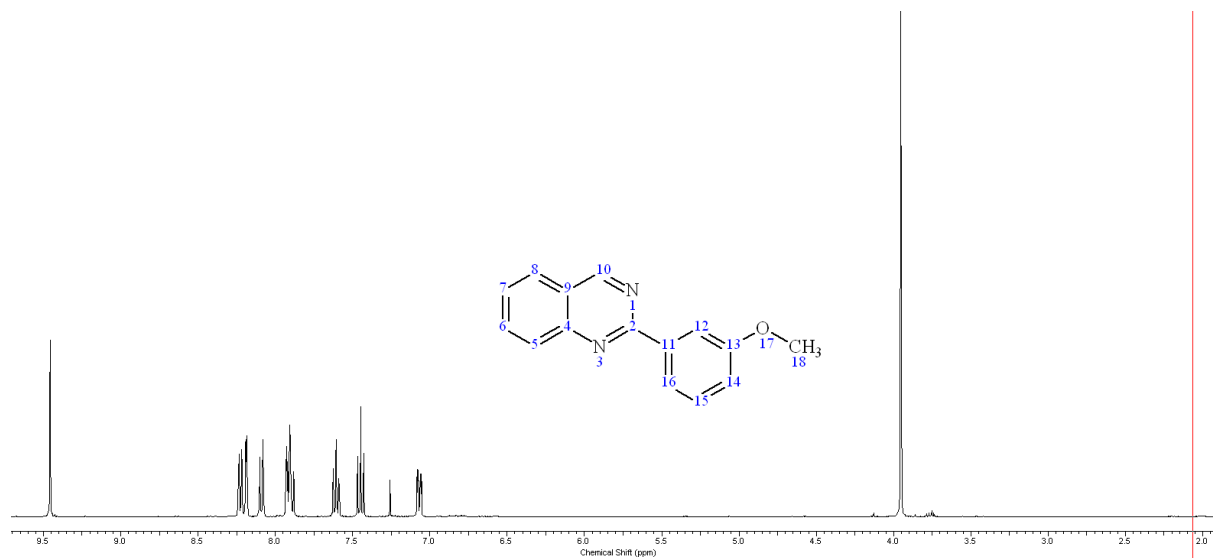
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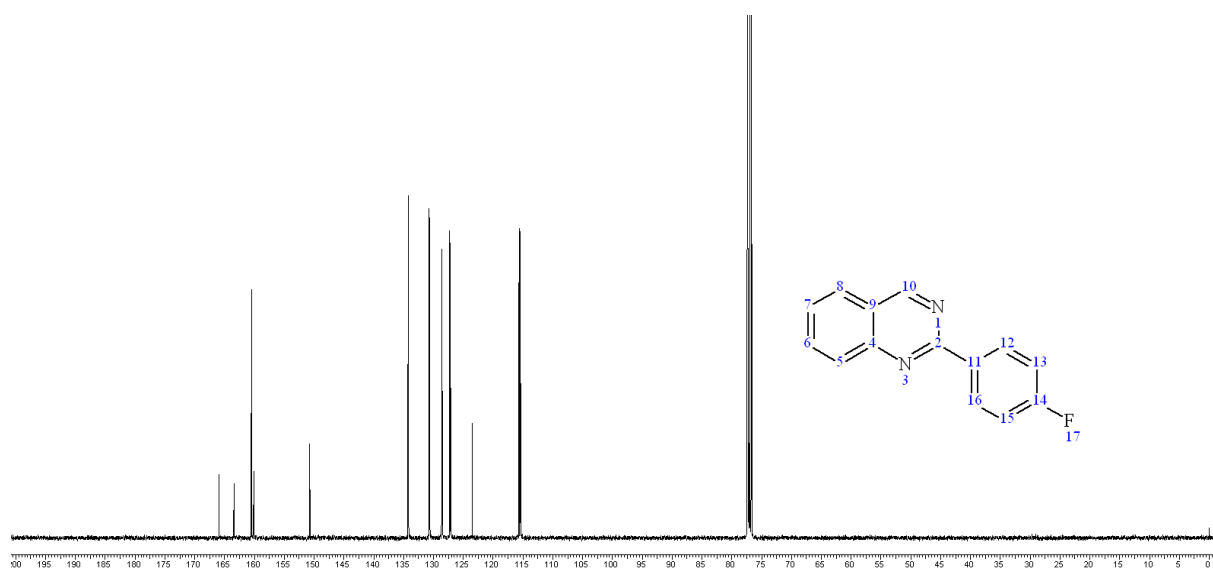
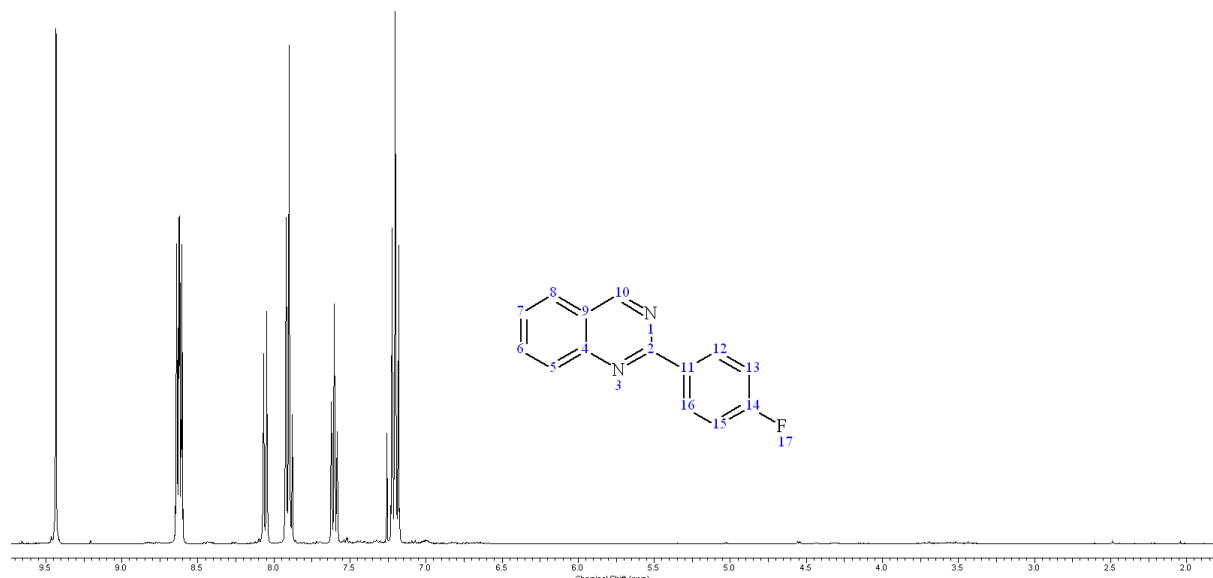
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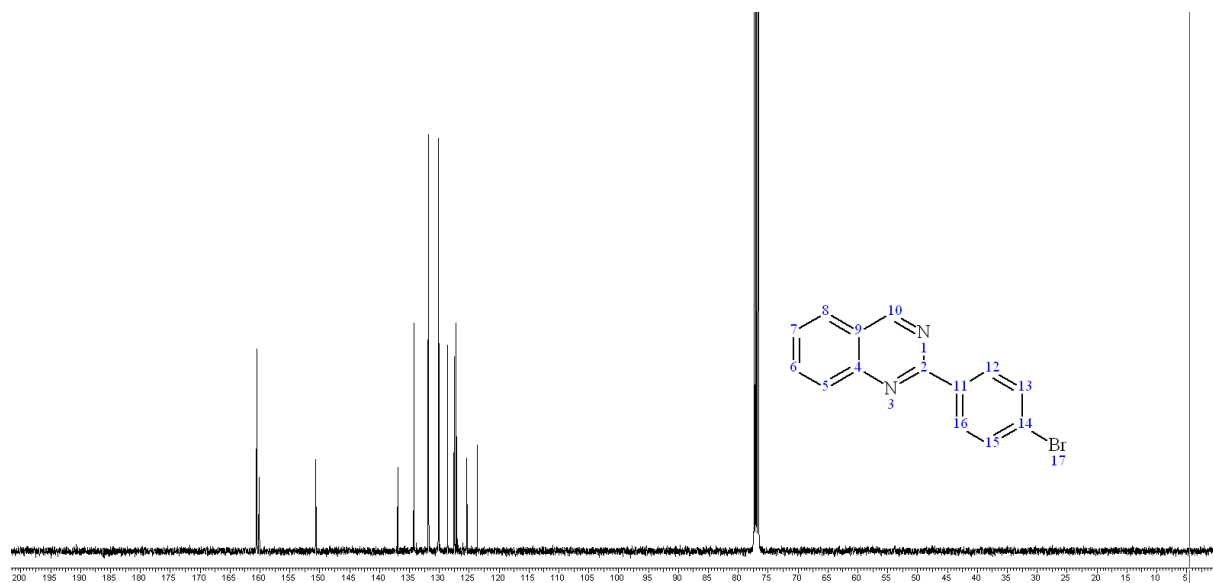
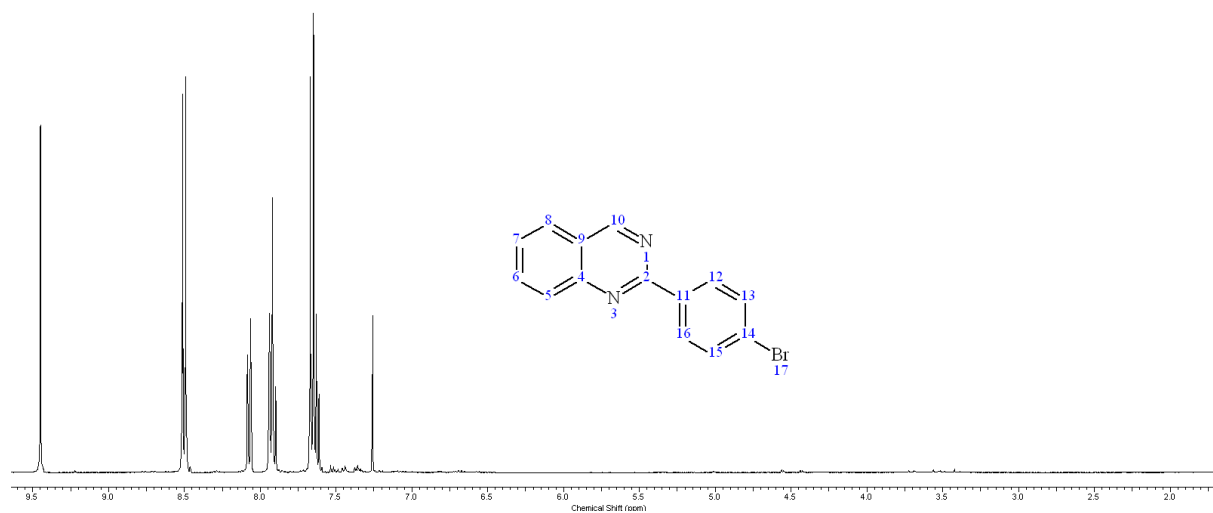
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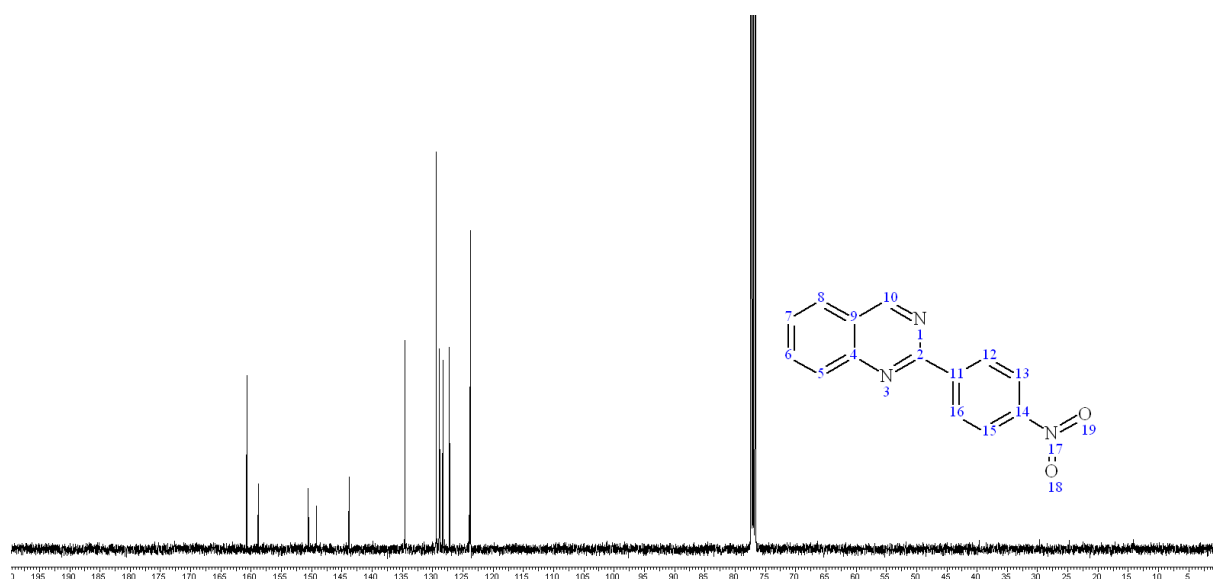
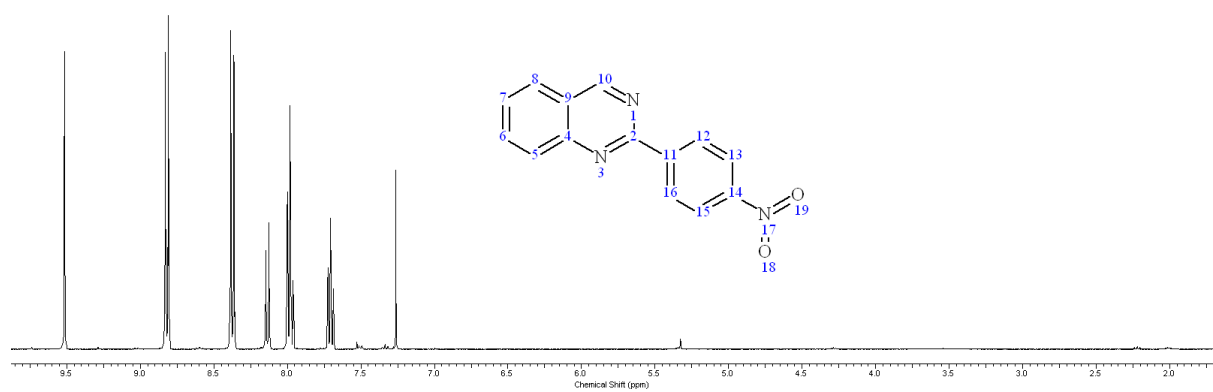
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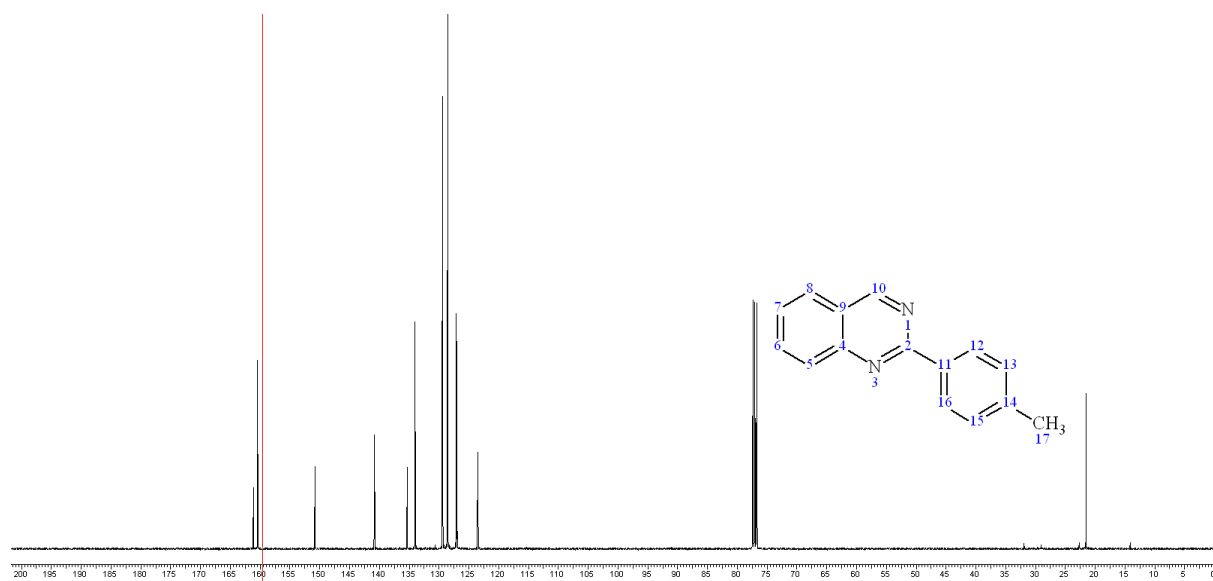
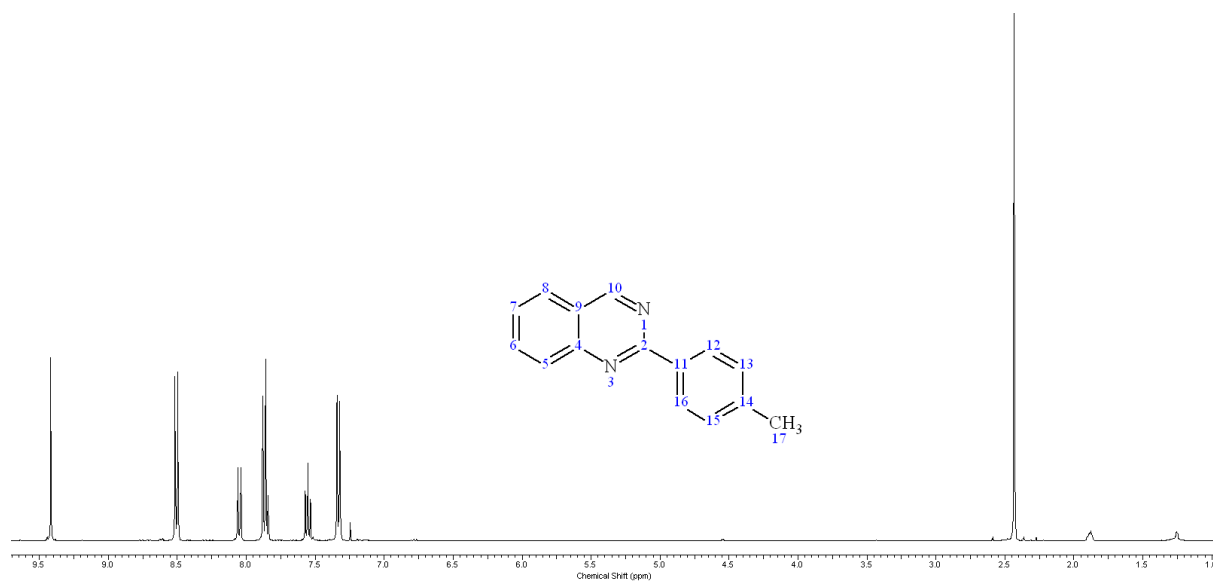
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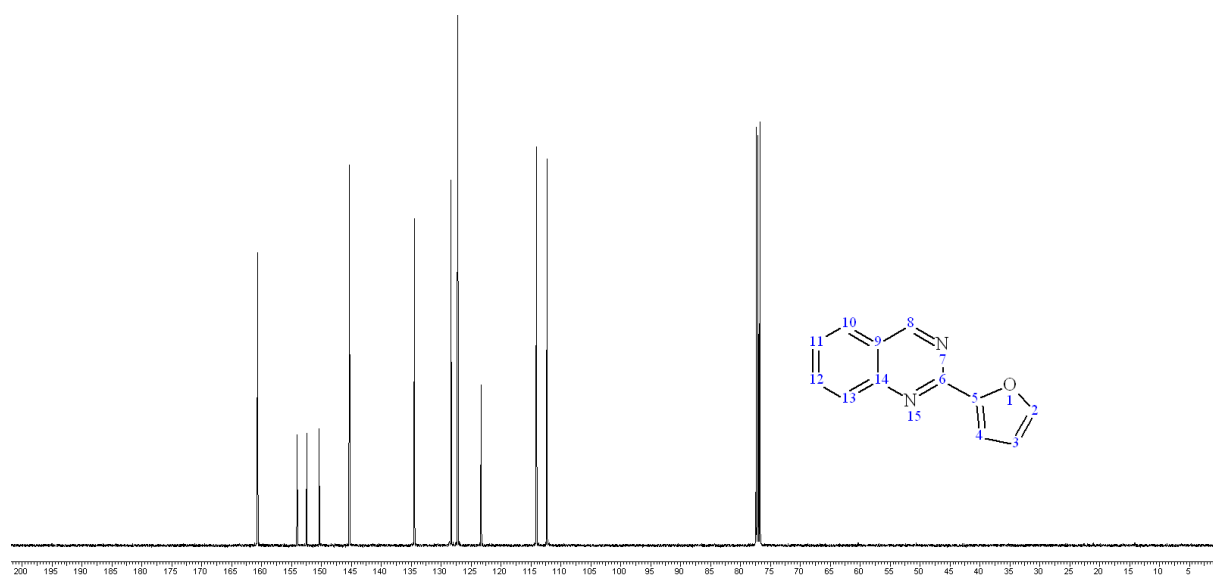
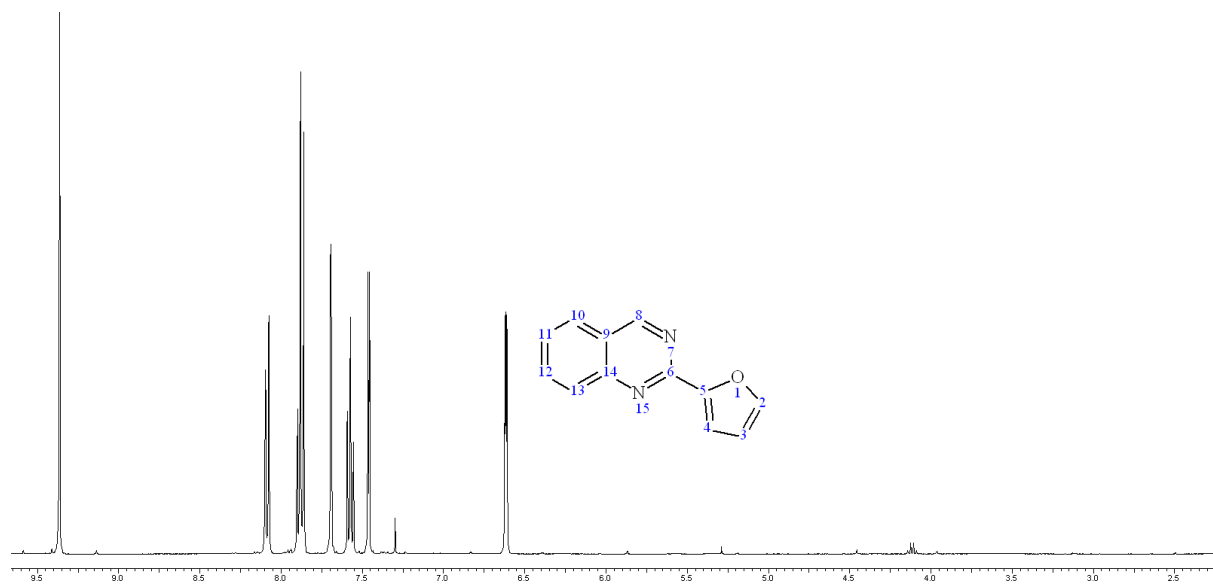
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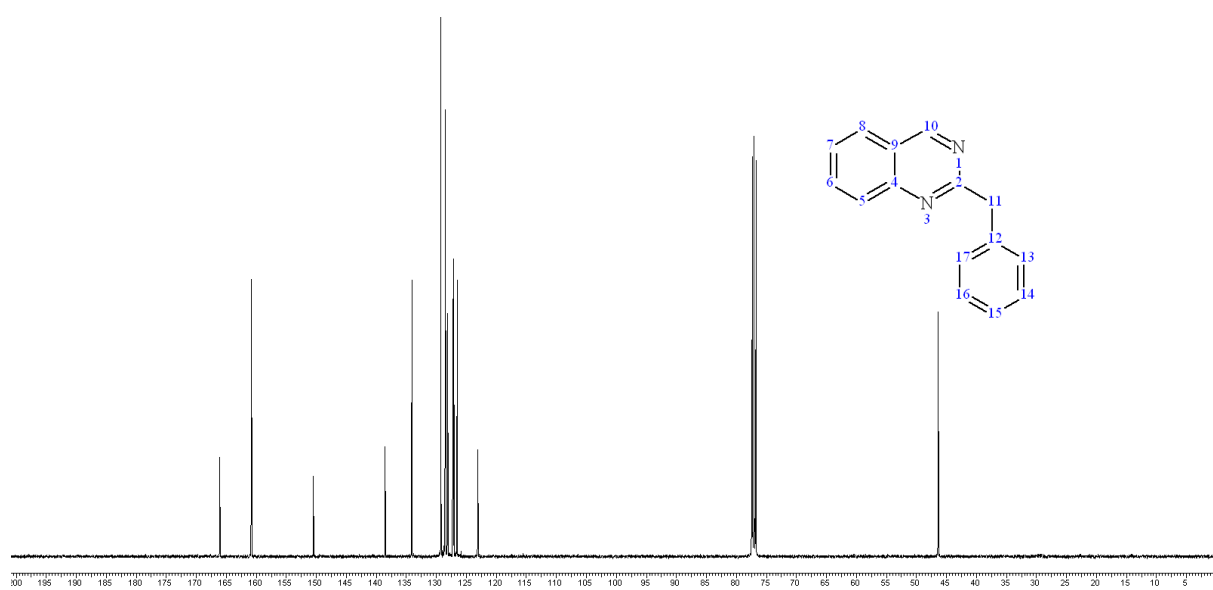
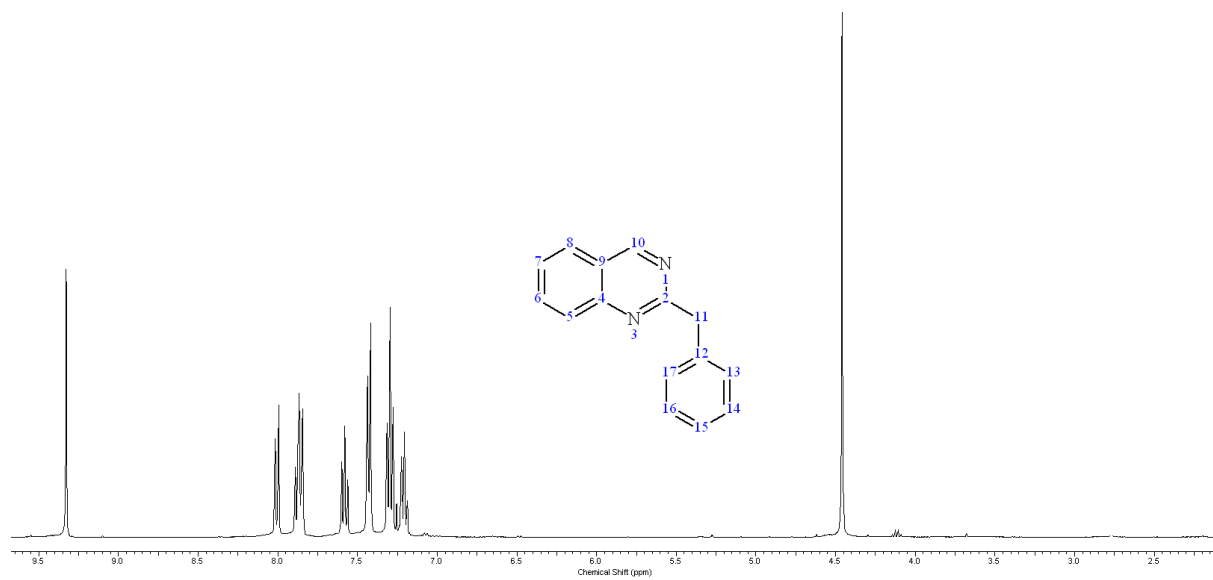
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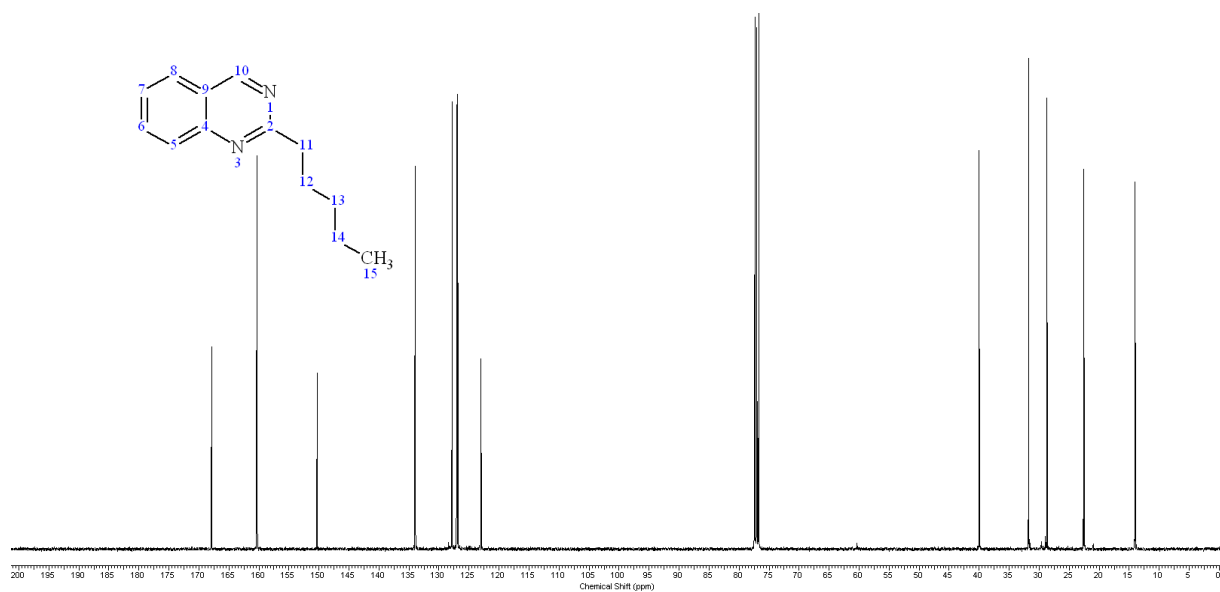
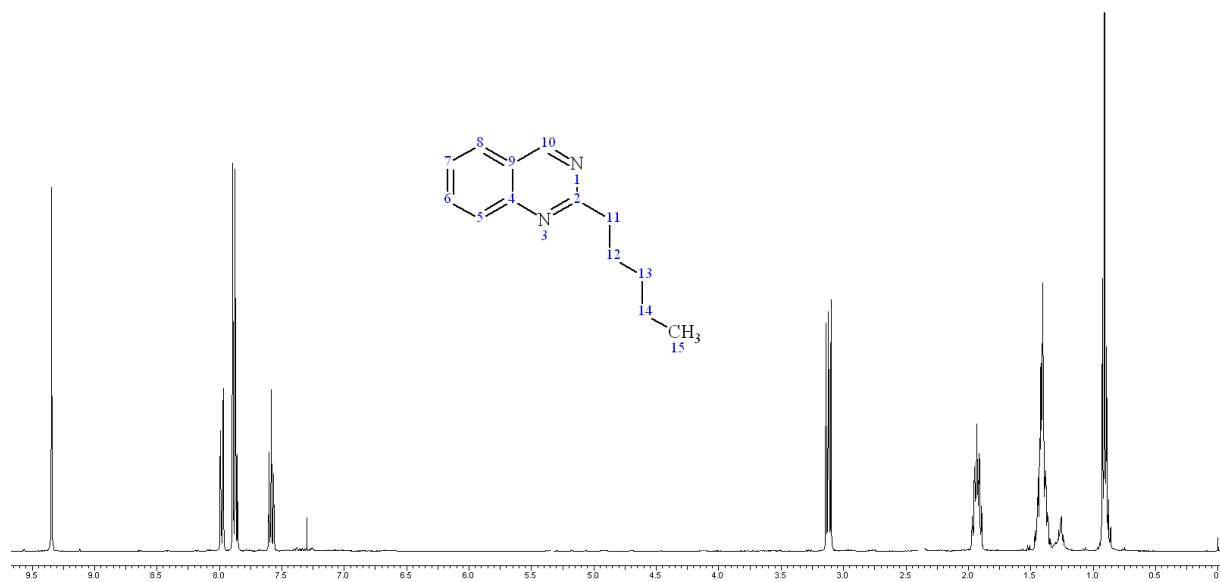
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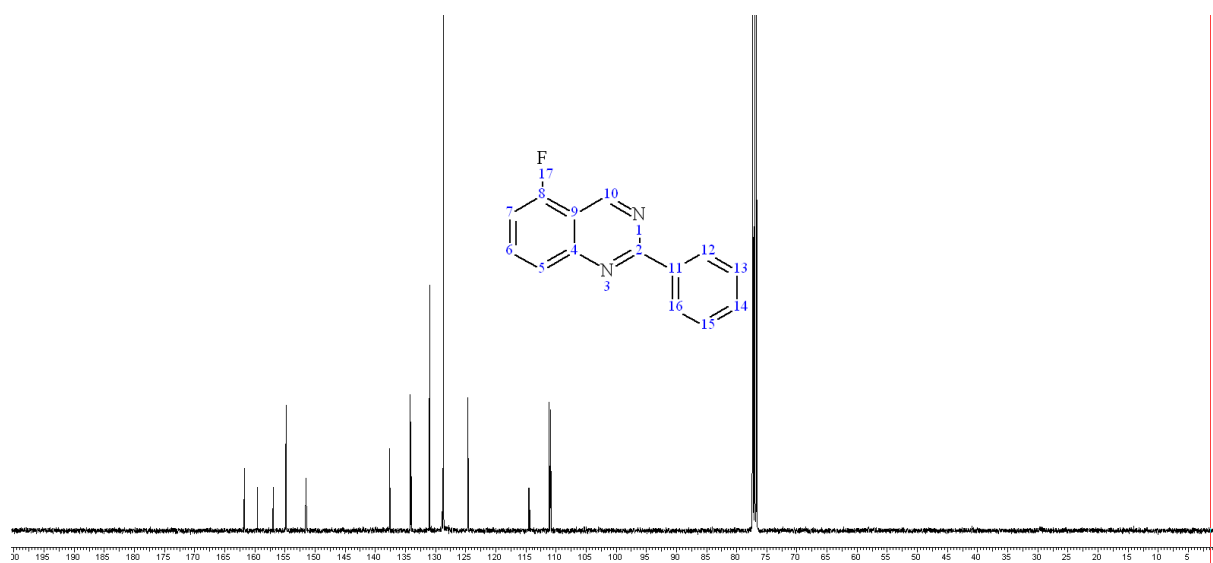
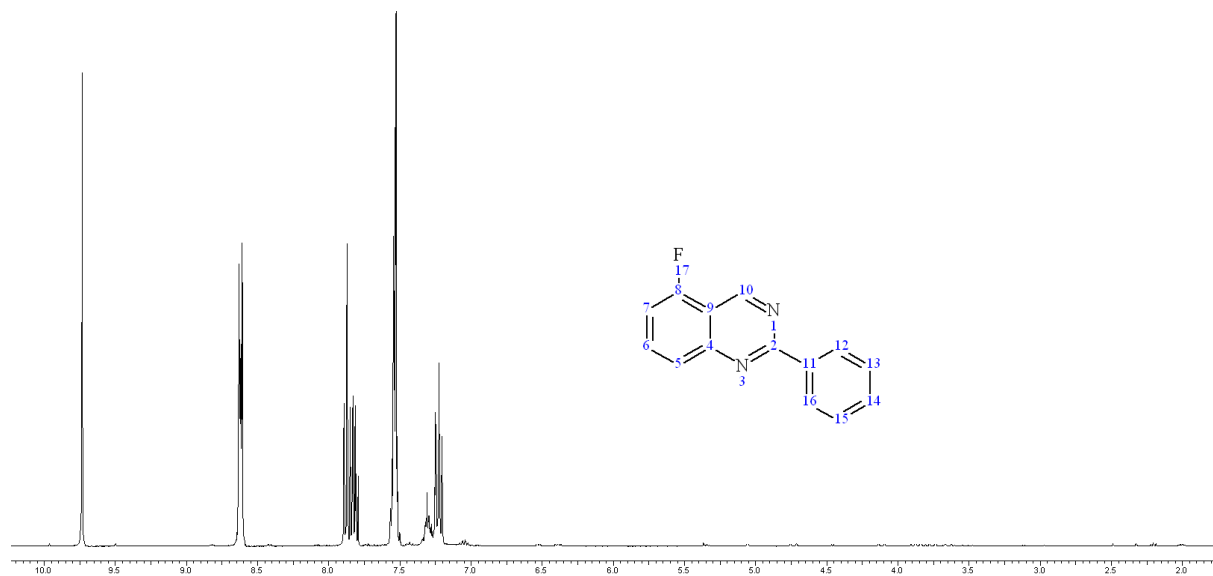
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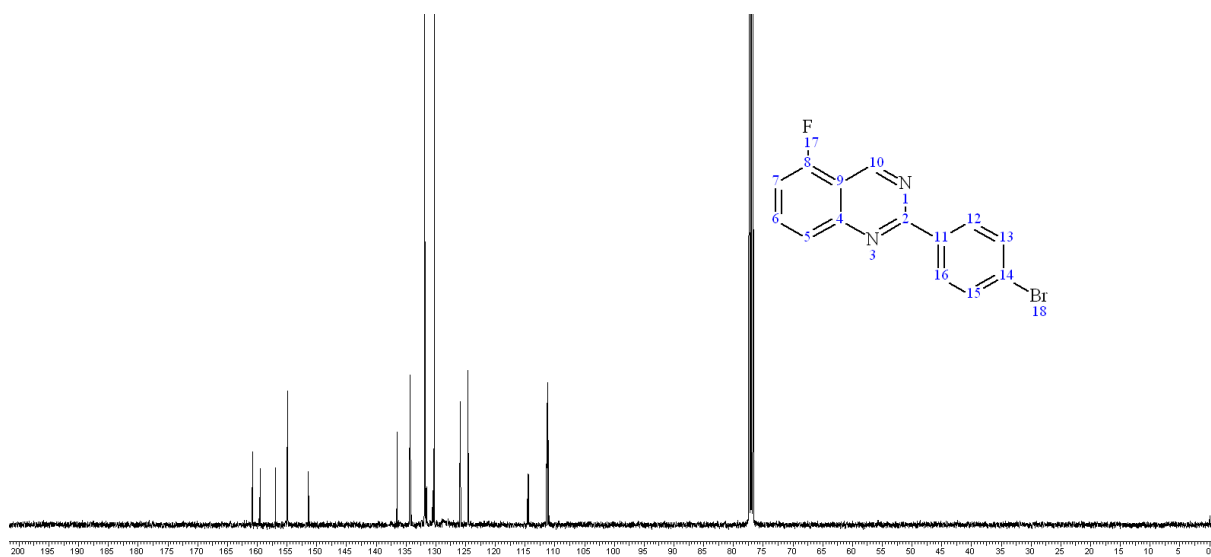
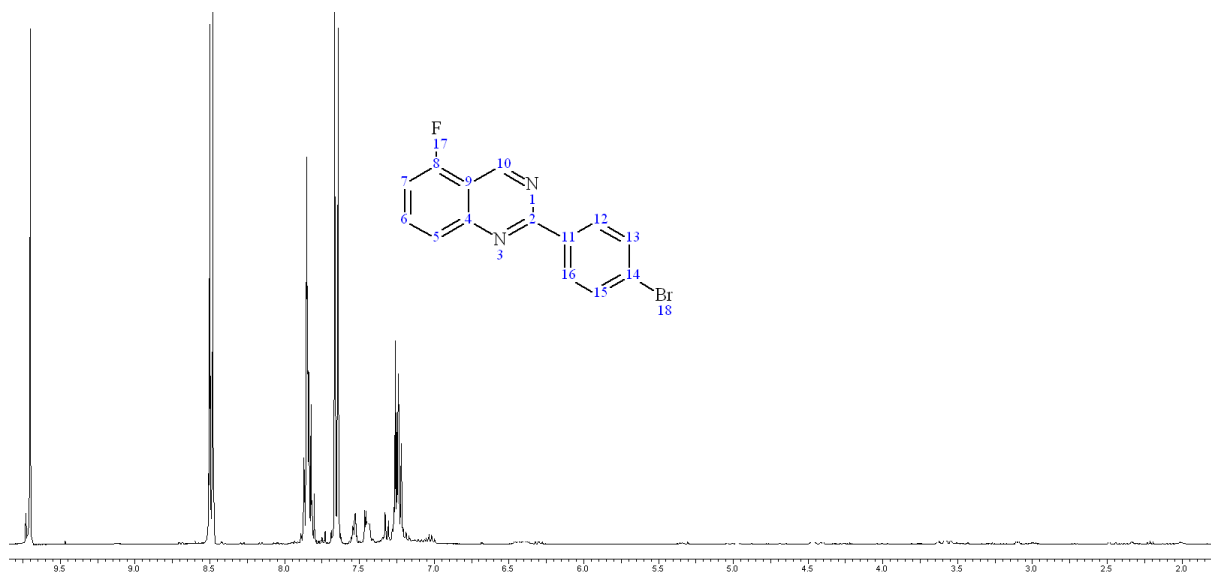
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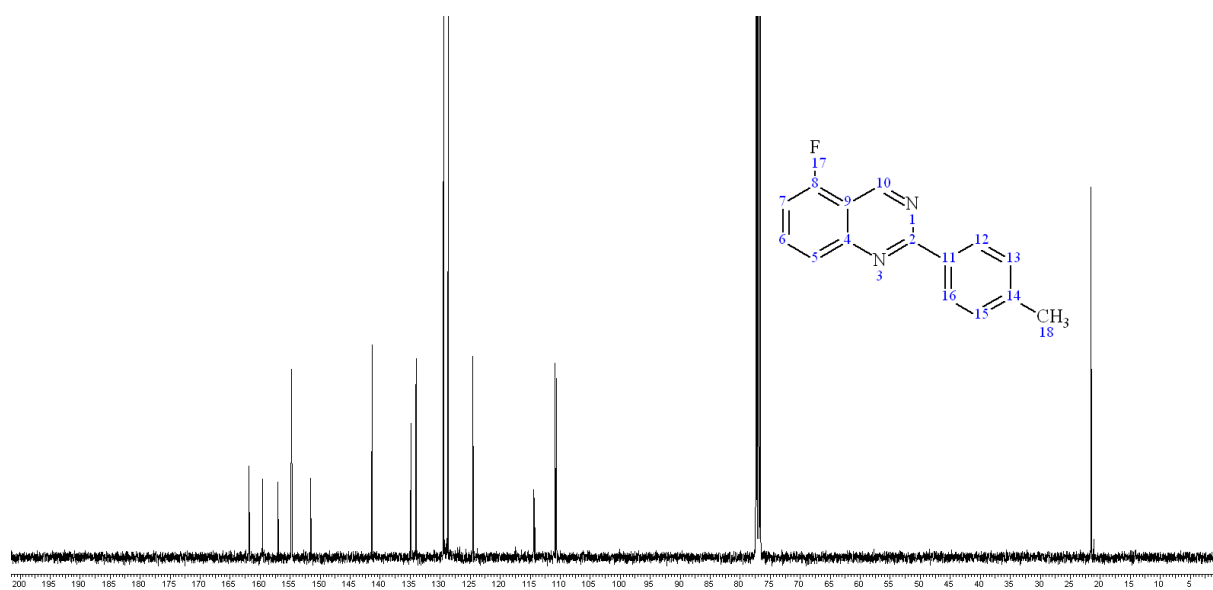
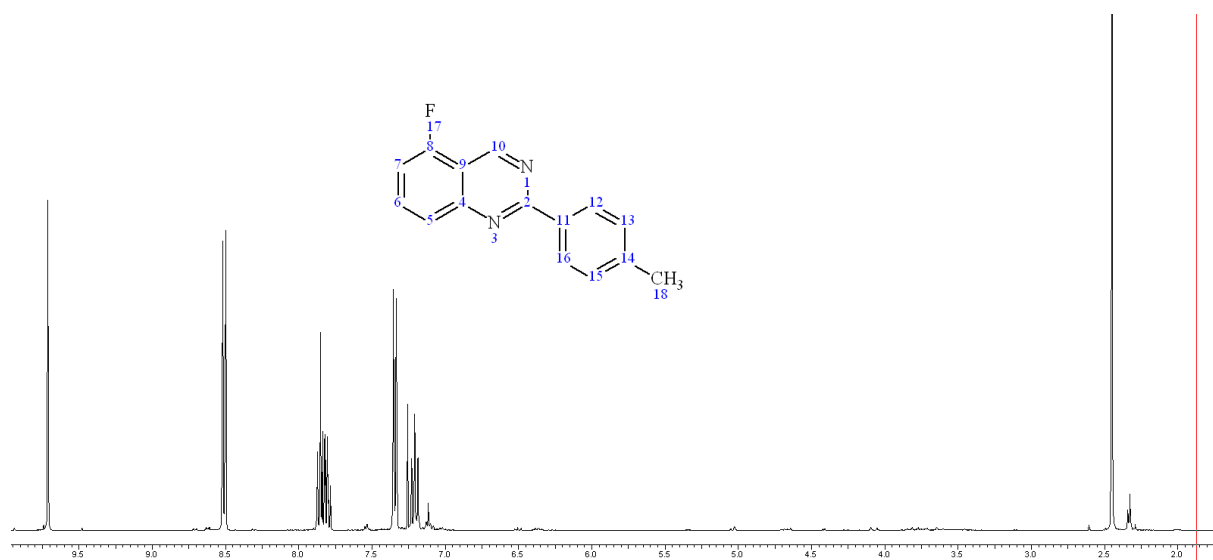
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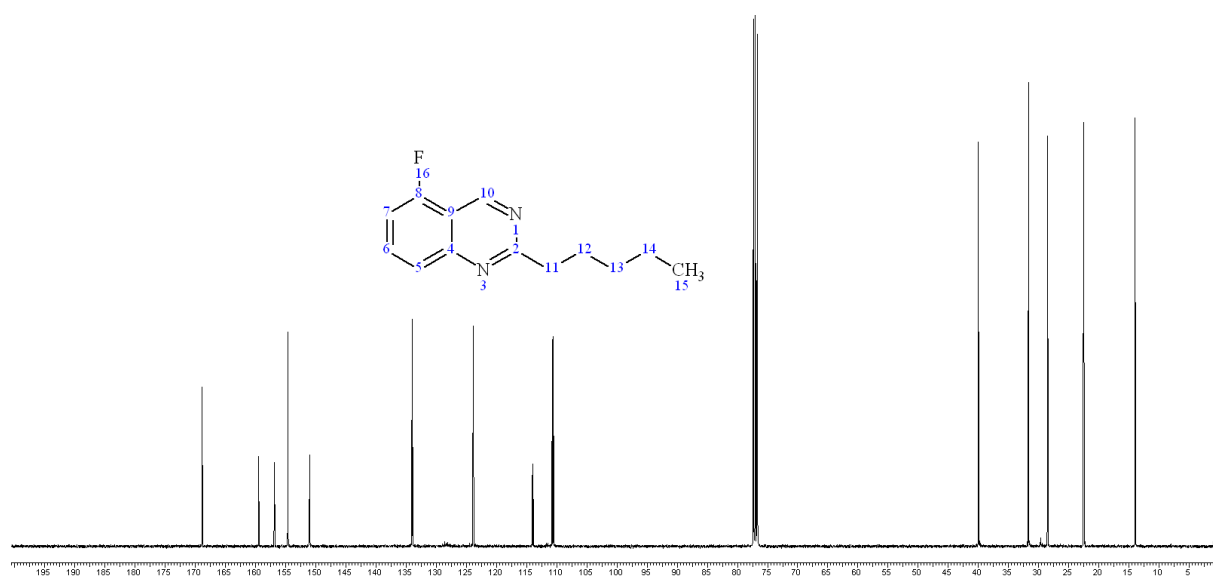
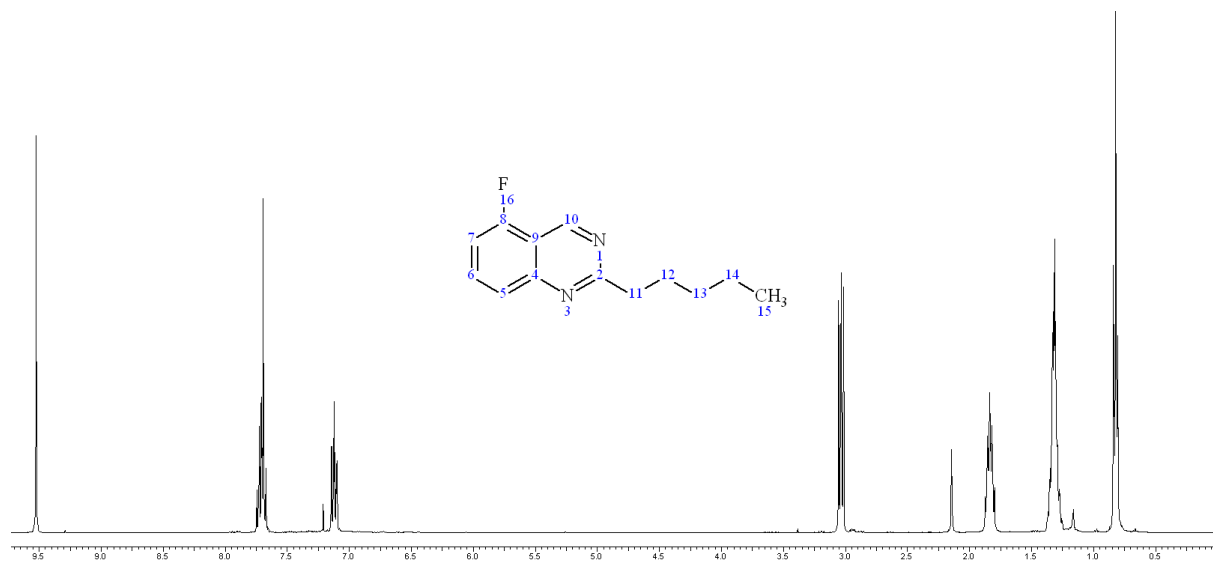
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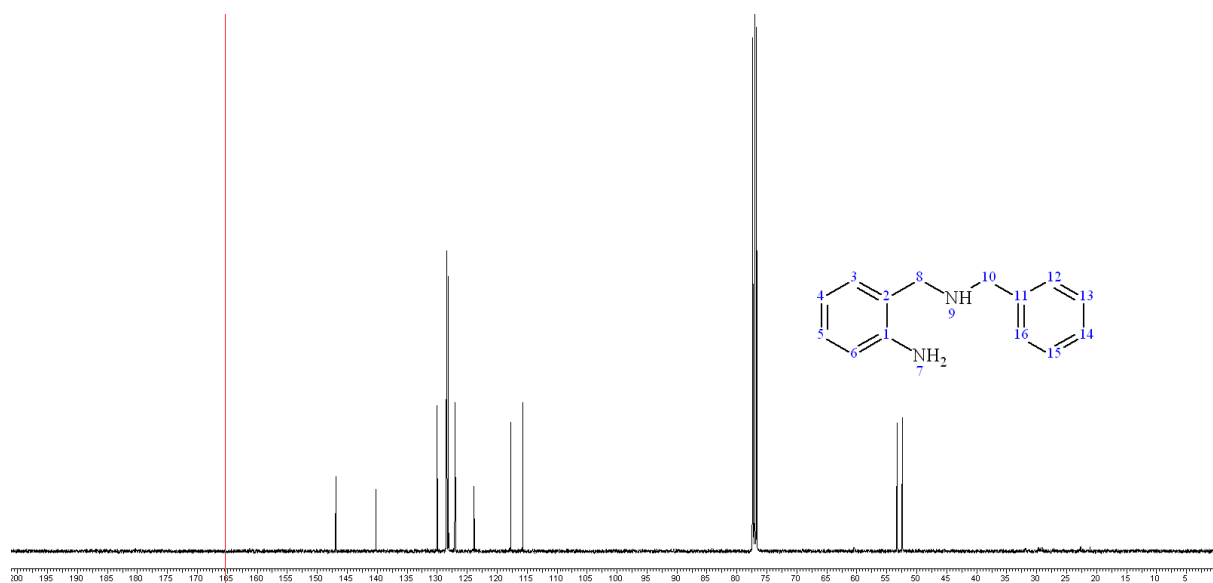
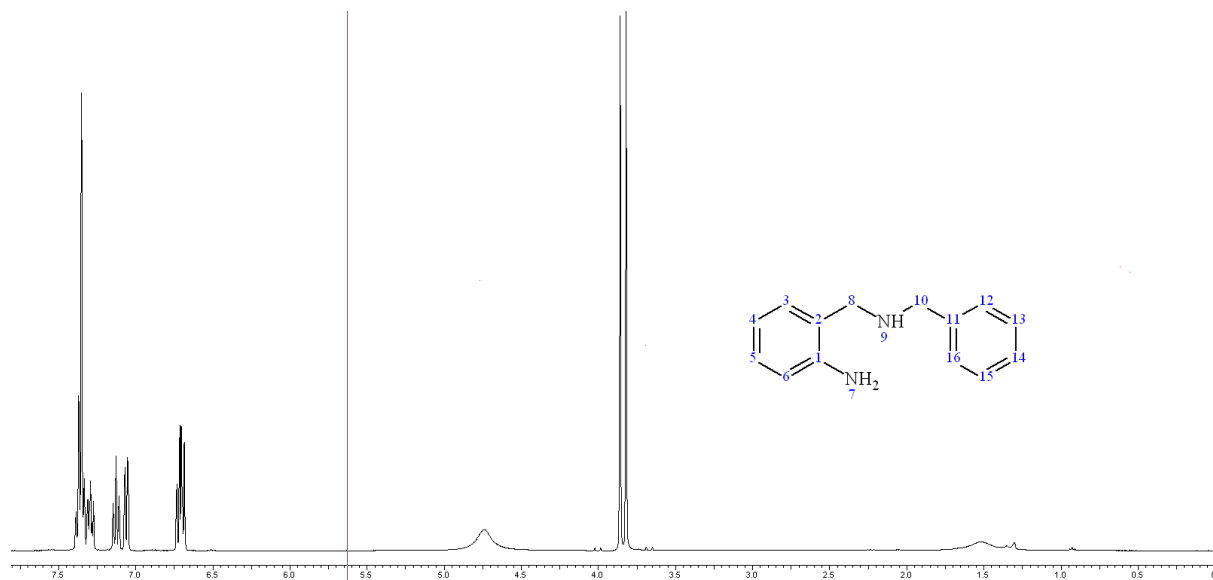
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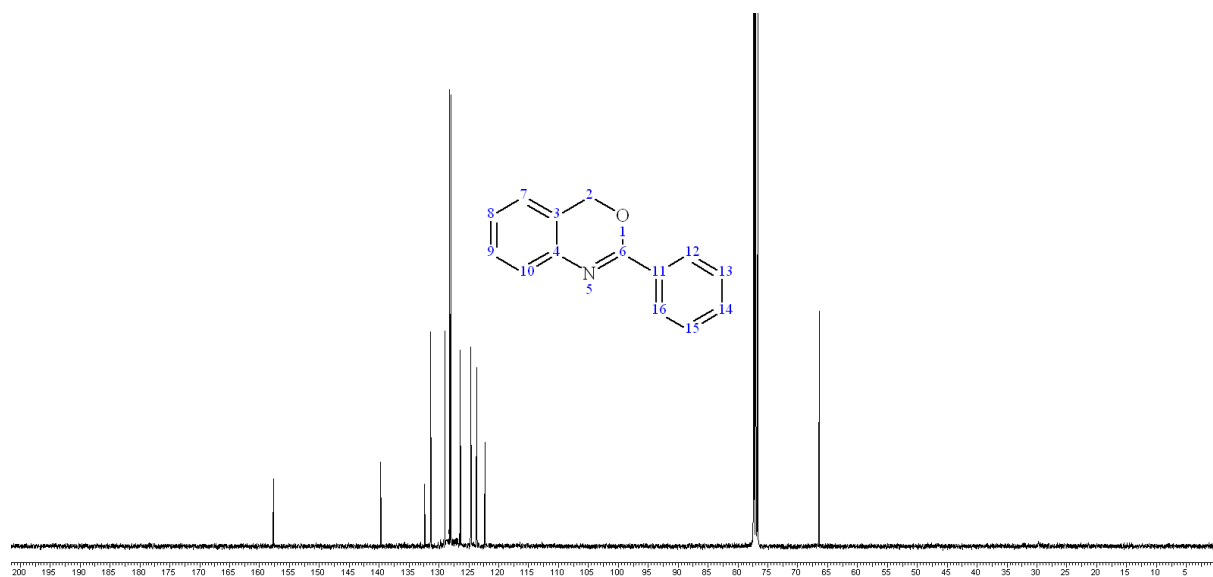
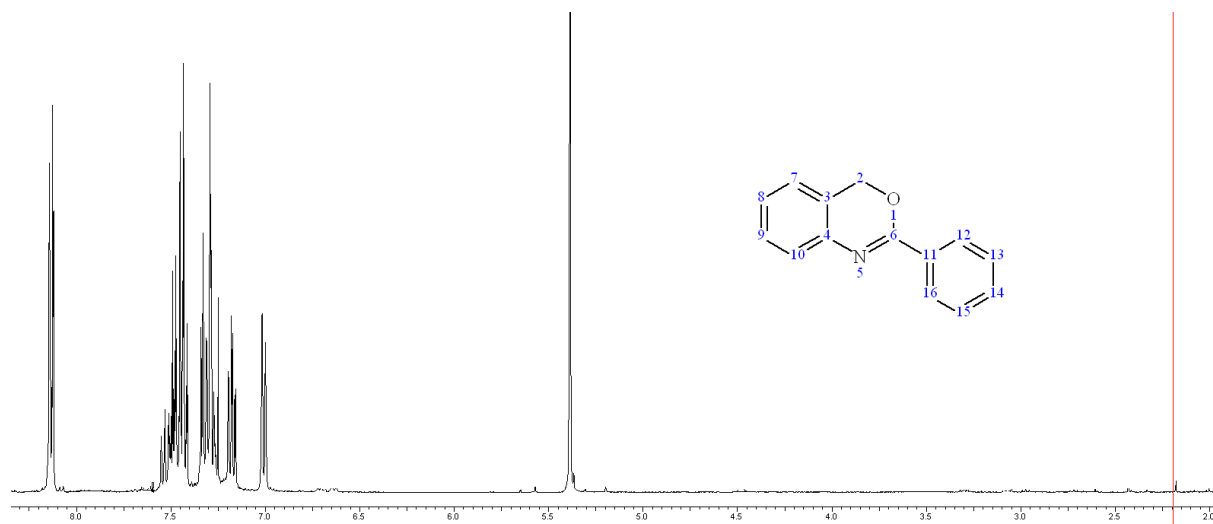
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