SUPPORTING INFORMATION

Palladium(II)-catalyzed direct O-alkenylation of 2-arylquinazolinones with *N*-tosylhydrazones: an efficient route to O-alkenylquinazolines

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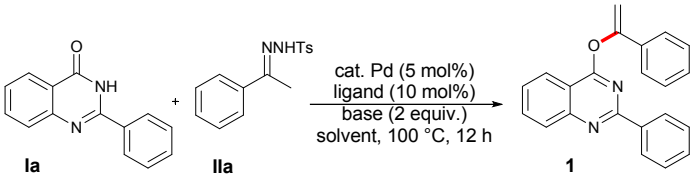
1.1 General Experimental Details:

Reactions were carried out in oven dried round-bottomed flasks. All solvents and reagents were used, as received from the suppliers. TLC was performed on Merck Kiesel gel 60, F_{254} plates with the layer thickness of 0.25 mm. Column chromatography was performed on silica gel (100-200 mesh) using a gradient of ethyl acetate and hexane as mobile phase. Melting points were determined on a Fisher John's melting point apparatus and are uncorrected. IR spectra were recorded on a Bruker Alpha Spectrometer FT-IR system. ^{1}H NMR spectral data were collected at 300, 400, 500 & 600 MHz, while ^{13}C NMR were recorded at 100, 125 and 150 MHz. ^{1}H NMR spectral data are given as chemical shifts in ppm followed by multiplicity (s- singlet; d- doublet; dd- doublet of doublet; t- triplet; q- quartet; m- multiplet), number of protons and coupling constants. ^{13}C NMR chemical shifts are expressed in ppm. The mass spectral analyses were carried out using Electrospray Ionization (ESI) techniques. Mass spectra were obtained on a Shimadzu LCMS-2020 mass spectrometer. HRMS (ESI) spectral data were collected using Q-star & ORBITRAP High Resolution Mass Spectrometer.

1.2 Optimization of reaction conditions.[a]



entry	catalyst/ligand	base	solvent	yield (%)[b]
1	$Pd(OAc)_2$/none	K_2CO_3	1,4-dioxane	0
2[c]	$Pd(OAc)_2$/none	Cs_2CO_3	1,4-dioxane	0
3	$Pd(OAc)_2$/PPh_3	Cs_2CO_3	1,4-dioxane	67
4	$Pd(OAc)_2$/PPh_3	K_2CO_3	1,4-dioxane	33
5	$Pd(OAc)_2$/PPh_3	KO^{t}Bu	1,4-dioxane	21
6	$Pd(OAc)_2$/PPh_3	LiO^{t}Bu	1,4-dioxane	27
7	$Pd(OAc)_2$/PPh_3	K_3PO_4	1,4-dioxane	52
8	$Pd(OAc)_2$/PCy_3[d]	Cs_2CO_3	1,4-dioxane	41
9	$Pd(OAc)_2$/Dppp[d]	Cs_2CO_3	1,4-dioxane	31
10	$Pd(OAc)_2$/Bpy[d]	Cs_2CO_3	1,4-dioxane	35
11	$Pd(OAc)_2$/Phen[d]	Cs_2CO_3	1,4-dioxane	43

12	$Pd(OAc)_2$/Dmphen[d]	Cs_2CO_3	1,4-dioxane	28
13	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	DCE	30
14	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	toluene	38
15	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	DMF	51
16	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	DMAc	0
17	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	DMSO	0
18	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	MeOH	0
19	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	*t*-AmOH	90
20	$Pd(OAc)_2(PPh_3)_2$/none	Cs_2CO_3	*t*-AmOH	65
21	$PdCl_2/PPh_3$	Cs_2CO_3	*t*-AmOH	41
22	$PdCl_2(MeCN)_2/PPh_3$	Cs_2CO_3	*t*-AmOH	20
23	$PdCl_2(PhCN)_2/PPh_3$	Cs_2CO_3	*t*-AmOH	13
24	$Pd(TFA)_2/PPh_3$	Cs_2CO_3	*t*-AmOH	0
25[e]	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	*t*-AmOH	90
26[f]	**$Pd(OAc)_2/PPh_3$**	**Cs_2CO_3**	***t*-AmOH**	**90**
27[g]	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	*t*-AmOH	44
28[h]	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	*t*-AmOH	10
29	$Pd_2(dba)_3/PPh_3$	Cs_2CO_3	*t*-AmOH	17
30	$Pd(PPh_3)_4$/none	Cs_2CO_3	*t*-AmOH	21
31	none/PPh_3	Cs_2CO_3	*t*-AmOH	0
32	$Pd(OAc)_2/PPh_3$	none	*t*-AmOH	0
33[i]	$Pd(OAc)_2/PPh_3$	Cs_2CO_3	*t*-AmOH	90
34[j]	$Pd(OAc)_2(PPh_3)_2$/none	Cs_2CO_3	*t*-AmOH	41

[a]Unless specified, the reaction was carried out with **Ia** (0.5 mmol) , **IIa** (0.5 mmol), catalyst (5 mol%), ligand (10 mol%), base (2 equiv.) in a solvent (3 mL) at 100 °C for 12 h, in open air. [b]Isolated yield (average of two runs). [c]TBAI (20 mol%) was used. [d]PCy_3 = tricyclohexylphosphine, Dppp = 1,3-bis(diphenylphosphino)propane, Bpy = 2,2′-bipyridyl, Phen = 1,10-phenanthroline, Dmphen = 2,9-dimethyl-1,10-phenanthroline. [e]At 80 °C. [f]$Pd(OAc)_2$ (2.5 mol%), PPh_3 (5 mol%), Cs_2CO_3 (1 equiv.) at 80 °C. [g]$Pd(OAc)_2$ (1 mol%), PPh_3 (2 mol%), Cs_2CO_3 (1 equiv.) at 80 °C. [h]Under N_2. [i]Under O_2 (balloon). [j]$CuCl_2$ (2 equiv.) was used.

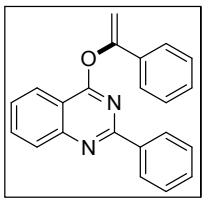
1.3 General Experimental Procedure for Synthesis of Derivatives (1-30).

A mixture of quinazolinone (**Ia**, 0.5 mmol, 1.0 equiv.), *N*-tosylhydrazone (**IIa**, 0.5 mmol, 1.0 equiv.), Cs_2CO_3 (0.5 mmol, 1.0 equiv.), $Pd(OAc)_2$ (2.8 mg, 2.5 mol%), PPh_3 (6.5 mg, 5 mol%), and *tert*-amyl alcohol (3.0 mL) were added to a round-bottomed flask. The reaction mixture was stirred in open air at 80 °C and the progress of the reaction was monitored by

TLC. After completion of the reaction, the mixture was cooled to room temperature. The reaction mixture was partitioned between ethyl acetate (25.0 mL) and water (25.0 mL) in a separatory funnel. The organic layer was washed with water, and brine, dried over anhydrous Na_2SO_4 (s) and concentrated under vacuum. The residue was purified by column chromatography using a gradient of hexane and ethyl acetate as the eluent system to afford the pure products.

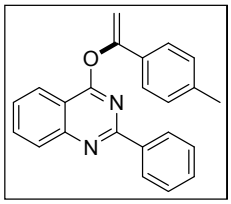
1.4 Analytical data

2-Phenyl-4-((1-phenylvinyl)oxy)quinazoline (1).



Yield: 90% (145 mg); pale yellow solid; mp: 163–165 °C; IR (neat): ν_{max} = 3063, 3028, 2923, 2853, 1718, 1622, 1575, 1557, 1490, 1349, 1264, 1068, 946, 757, 696 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.37 (d, *J* = 8.1 Hz, 1H), 8.31 (d, *J* = 3.6 Hz, 2H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.83 (t, *J* = 7.6 Hz, 1H), 7.57 (dd, *J* = 18.6, 7.4 Hz, 3H), 7.38 (d, *J* = 2.3 Hz, 2H), 7.31 – 7.27 (m, 4H), 5.60 (d, *J* = 1.3 Hz, 1H), 5.28 (d, *J* = 1.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.1, 160.0, 155.2, 152.5, 137.6, 135.0, 133.8, 130.4, 128.7, 128.4, 128.2, 128.1, 127.8, 126.7, 125.2, 123.3, 114.8, 101.9; MS (ESI): *m/z*: 325 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{17}ON_2$: 325.13354 $[M+H]^+$; found: 325.13318.

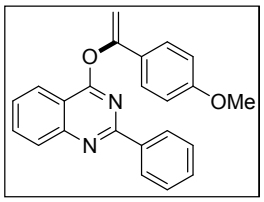
2-Phenyl-4-((1-(*p*-tolyl)vinyl)oxy)quinazoline (2).



Yield: 91% (153 mg); white solid; mp: 173–175 °C; IR (neat): ν_{max} = 3062, 3028, 2923, 2853, 1735, 1621, 1575, 1557, 1488, 1457, 1387, 1348, 1261, 1066, 945, 770, 709 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.39 (dd, *J* = 8.2, 0.8 Hz, 1H), 8.32 (dd, *J* = 6.6, 3.3 Hz, 2H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.89 – 7.86 (m, 1H), 7.62 – 7.59 (m, 1H), 7.49 (d, *J* = 8.2 Hz, 2H), 7.41 – 7.39 (m, 3H), 7.12 (d, *J* = 8.0 Hz, 2H), 5.56 (d, *J* = 2.0 Hz, 1H), 5.23 (d, *J* = 2.0 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR (125

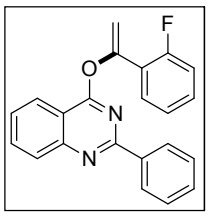
MHz, $CDCl_3$): δ 166.2, 160.0, 155.3, 152.5, 138.7, 137.7, 133.8, 132.2, 130.4, 129.1, 128.4, 128.2, 128.1, 126.7, 125.2, 123.4, 114.9, 101.1, 21.2; MS (ESI): *m/z*: 339 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{23}H_{19}ON_2$: 339.14919 $[M+H]^+$; found: 339.14858.

4-((1-(4-Methoxyphenyl)vinyl)oxy)-2-phenylquinazoline (3).



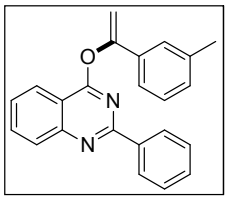
Yield: 86% (152 mg); white solid; mp: 198–200 °C; IR (neat): ν_{max} = 3064, 2922, 2851, 1713, 1611, 1513, 1451, 1243, 1029, 829, 708 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.06 (d, *J* = 8.0 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.42 (d, *J* = 7.8 Hz, 2H), 7.40 – 7.37 (m, 3H), 7.31 (dd, *J* = 12.2, 3.4 Hz, 2H), 7.24 (d, *J* = 1.0 Hz, 1H), 6.89 (d, *J* = 8.6 Hz, 2H), 5.47 (s, 1H), 5.23 (s, 1H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 159.2, 159.0, 158.1, 149.3, 139.8, 136.1, 133.8, 132.7, 130.5, 129.9, 129.5, 128.4, 128.2, 127.5, 126.6, 113.8, 111.5, 55.2; MS (ESI): *m/z*: 355 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{23}H_{19}O_2N_2$: 355.14410 $[M+H]^+$; found: 355.14339.

4-((1-(2-Fluorophenyl)vinyl)oxy)-2-phenylquinazoline (4).



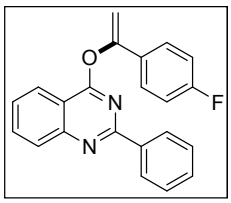
Yield: 82% (140 mg); colorless solid; mp: 129–130 °C; IR (neat): ν_{max} = 3066, 2919, 2850, 1730, 1621, 1575, 1558, 1489, 1455, 1253, 1159, 762, 709 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6): δ 8.40 (d, *J* = 7.9 Hz, 1H), 8.23 (d, *J* = 6.7 Hz, 2H), 8.06 – 8.02 (m, 2H), 7.78 – 7.76 (m, 1H), 7.63 – 7.61 (m, 1H), 7.51 – 7.45 (m, 3H), 7.39 – 7.36 (m, 1H), 7.28 (dd, *J* = 11.5, 8.4 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 5.72 (s, 1H), 5.61 (d, *J* = 1.2 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6): δ 165.4, 159.9, 158.5, 158.3, 151.7, 149.2, 136.7, 134.9, 131.0, 130.8 (d, *J* = 8.6 Hz), 128.6, 128.4 (d, *J* = 2.0 Hz), 127.8, 127.8, 124.7, 123.4, 122.6 (d, *J* = 11.5 Hz), 116.3 (d, *J* = 22.1 Hz), 114.1, 107.4 (d, *J* = 6.3 Hz); MS (ESI): *m/z*: 343 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{16}FN_2O$: 343.12412 $[M+H]^+$; found: 343.12311.

2-Phenyl-4-((1-(*m*-tolyl)vinyl)oxy)quinazoline (5).



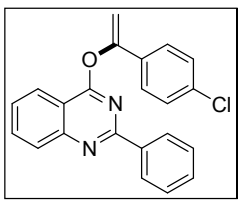
Yield: 85% (143 mg); white solid; mp: 161–163 °C; IR (neat): ν_{max} = 2918, 2850, 1726, 1622, 1575, 1557, 1461, 1384, 1349, 1269, 785, 768, 706 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.39 (dd, *J* = 8.2, 0.8 Hz, 1H), 8.32 (dd, *J* = 6.7, 3.0 Hz, 2H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.90 – 7.85 (m, 1H), 7.63 – 7.59 (m, 1H), 7.43 – 7.39 (m, 4H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.10 (d, *J* = 8.4 Hz, 2H), 5.58 (d, *J* = 2.0 Hz, 1H), 5.25 (d, *J* = 2.0 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.2, 160.0, 155.5, 152.5, 138.0, 137.7, 135.1, 133.8, 130.4, 129.5, 128.5, 128.3, 128.2, 128.1, 126.7, 126.0, 123.4, 122.5, 114.9, 101.8, 22.6; MS (ESI): *m/z*: 339 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{23}H_{19}N_2O$: 339.14919 $[M+H]^+$; found: 339.14843.

4-((1-(4-Fluorophenyl)vinyl)oxy)-2-phenylquinazoline (6).



Yield: 92% (157 mg); pale yellow solid; mp: 178–180 °C; IR (neat): ν_{max} = 3065, 2923, 2853, 1718, 1600, 1575, 1507, 1449, 1261, 837, 770, 710 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.36 (d, *J* = 8.1 Hz, 1H), 8.32 (d, *J* = 3.8 Hz, 2H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.88 – 7.85 (m, 1H), 7.61 – 7.56 (m, 2H), 7.41 (dd, *J* = 7.1, 5.2 Hz, 2H), 7.06 – 7.02 (m, 2H), 6.99 – 6.96 (m, 2H), 5.54 (d, *J* = 1.9 Hz, 1H), 5.26 (d, *J* = 1.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.0, 164.1, 159.9, 154.4, 152.5, 137.6, 133.9, 130.5, 129.3, 128.4, 128.3, 127.2, 127.1, 126.8, 123.3, 115.4 (d, *J* = 21.8 Hz), 114.8, 101.8; MS (ESI): *m/z*: 343 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{16}FN_2O$: 343.12412 $[M+H]^+$; found: 343.12447.

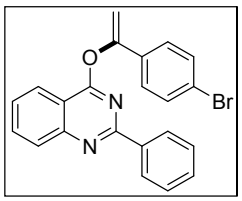
4-((1-(4-Chlorophenyl)vinyl)oxy)-2-phenylquinazoline (7).



Yield: 89% (159 mg); pale yellow solid; mp: 200–202 °C; IR (neat): ν_{max} = 2922, 2852, 1690, 1623, 1575, 1556, 1490, 1460, 1259, 1214, 1092, 829, 754, 668 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, *J* = 8.1 Hz, 1H), 8.31 (d, *J* = 4.7 Hz, 2H), 8.03 (d, *J* = 8.6 Hz, 1H), 7.89 – 7.83 (m, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.43 – 7.39 (m, 2H), 7.28 (d, *J* = 8.5 Hz, 2H), 5.59 (d, *J* =

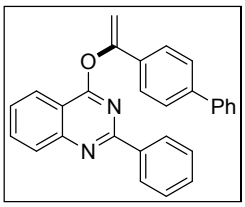
1.8 Hz, 1H), 5.30 (d, *J* = 1.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.0, 159.9, 154.2, 152.5, 137.5, 134.5, 133.9, 133.6, 130.5, 128.7, 128.3, 128.3, 127.8, 126.8, 126.5, 123.2, 114.7, 102.5; MS (ESI): *m/z*: 359 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{16}ClN_2O$: 359.09457 $[M+H]^+$; found: 359.09500.

4-((1-(4-Bromophenyl)vinyl)oxy)-2-phenylquinazoline (8).



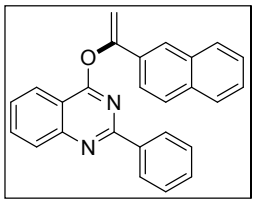
Yield: 87% (175 mg); yellow solid; mp: 138–140 °C; IR (neat): ν_{max} = 3019, 2923, 2853, 1688, 1623, 1575, 1557, 1487, 1262, 1214, 830, 748, 667 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.36 (d, *J* = 8.1 Hz, 1H), 8.32 – 8.30 (m, 2H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.90 – 7.87 (m, 1H), 7.63 – 7.55 (m, 2H), 7.46 (d, *J* = 4.8 Hz, 3H), 7.41 (dd, *J* = 5.4, 1.7 Hz, 3H), 5.61 (d, *J* = 2.2 Hz, 1H), 5.30 (d, *J* = 2.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.0, 159.9, 154.3, 152.5, 137.5, 134.1, 134.0, 131.6, 130.5, 129.0, 128.4, 128.3, 128.2, 126.8, 123.2, 122.8, 114.7, 102.6; MS (ESI): *m/z*: 405 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{16}BrN_2O$: 403.04405 $[M+H]^+$; found: 403.04403.

4-((1-([1,1'-Biphenyl]-4-yl)vinyl)oxy)-2-phenylquinazoline (9).



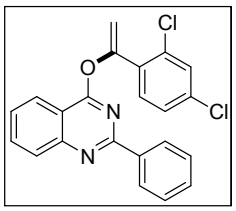
Yield: 73% (146 mg); white solid; mp: 139–141 °C; IR (neat): ν_{max} = 3056, 3028, 2923, 2853, 1680, 1603, 1551, 1517, 1486, 1447, 1267, 1218, 839, 765, 696 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.40 (d, *J* = 8.1 Hz, 1H), 8.34 (dd, *J* = 5.8, 3.7 Hz, 2H), 8.11 – 8.08 (m, 1H), 8.05 – 8.00 (m, 1H), 7.87 (t, *J* = 7.6 Hz, 1H), 7.67 (dd, *J* = 8.3, 2.6 Hz, 2H), 7.61 – 7.53 (m, 5H), 7.44 – 7.37 (m, 3H), 7.34 – 7.29 (m, 2H), 5.66 (d, *J* = 2.3 Hz, 1H), 5.30 (d, *J* = 2.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.1, 160.0, 154.9, 152.5, 141.4, 140.6, 137.6, 133.8, 130.4, 129.6, 128.7, 128.4, 128.1, 127.2, 127.1, 127.0, 126.9, 126.5, 125.6, 123.3, 114.8, 101.9; MS (ESI): *m/z*: 401 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{28}H_{21}N_2O$: 401.16484 $[M+H]^+$; found: 401.16440.

4-((1-(Naphthalen-2-yl)vinyl)oxy)-2-phenylquinazoline (10).



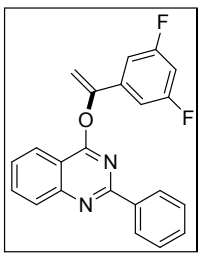
Yield: 69% (129 mg); yellow solid; mp: 135–137 °C; IR (neat): ν_{max} = 3056, 2924, 2853, 1716, 1678, 1623, 1599, 1573, 1488, 1449, 1270, 817, 772, 709 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.45 (d, *J* = 7.9 Hz, 1H), 8.30 (dd, *J* = 3.3, 1.8 Hz, 2H), 8.11 (d, *J* = 6.7 Hz, 1H), 8.05 – 8.01 (m, 2H), 7.89 – 7.75 (m, 4H), 7.63 – 7.58 (m, 1H), 7.46 – 7.40 (m, 2H), 7.34 (d, *J* = 5.5 Hz, 2H), 7.21 (s, 1H), 5.75 (s, 1H), 5.37 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.2, 160.0, 155.2, 152.5, 137.6, 133.9, 130.4, 129.6, 128.4, 128.3, 128.2, 127.7, 127.5, 126.8, 126.3, 126.1, 126.0, 124.9, 124.3, 124.0, 123.4, 123.1, 114.9, 102.4; MS (ESI): *m/z*: 375 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{26}H_{19}ON_2$: 375.14919 $[M+H]^+$; found: 375.14935.

4-((1-(2,4-Dichlorophenyl)vinyl)oxy)-2-phenylquinazoline (11).



Yield: 82% (161 mg); yellow solid; mp: 155–156 °C; IR (neat): ν_{max} = 3066, 2923, 2852, 1723, 1621, 1575, 1559, 1489, 1271, 822, 771, 708, 680 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.50 (dd, *J* = 5.6, 1.7 Hz, 1H), 8.37 (dd, *J* = 3.4, 1.8 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.85 – 7.80 (m, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.58 – 7.52 (m, 2H), 7.48 – 7.42 (m, 2H), 7.36 (dd, *J* = 6.7, 2.1 Hz, 1H), 7.25 – 7.17 (m, 2H), 5.57 (d, *J* = 1.5 Hz, 1H), 5.46 (d, *J* = 1.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.3, 159.7, 152.4, 151.8, 134.8, 133.9, 133.1, 130.5, 129.6, 128.4, 128.2, 128.0, 127.6, 127.4, 127.2, 126.9, 126.4, 123.5, 115.1, 107.4; MS (ESI): *m/z*: 393 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{15}Cl_2N_2O$: 393.0556 $[M+H]^+$; found: 393.0547.

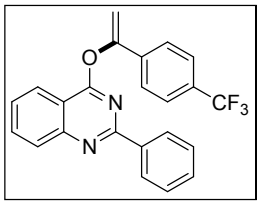
4-((1-(3,5-Difluorophenyl)vinyl)oxy)-2-phenylquinazoline (12).



Yield: 89% (160 mg); light yellow solid; mp: 140–142 °C; IR (neat): ν_{max} = 3067, 2923, 2852, 1740, 1621, 1589, 1557, 1488, 1384, 1347, 1317, 1263, 1211, 1118, 987, 860, 771, 706 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.35 (d, *J* = 8.4 Hz, 1H), 8.32 (dd, *J* = 6.5, 2.8 Hz, 2H), 8.18 (d, *J* = 7.5 Hz, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.90 (t, *J* = 7.6 Hz, 1H), 7.63 (dd, *J* = 14.4, 7.0 Hz, 1H), 7.52 (t, *J* =

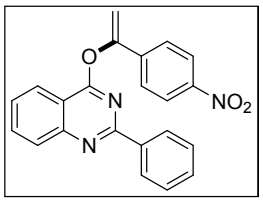
7.7 Hz, 1H), 7.43 (d, *J* = 2.2 Hz, 1H), 7.12 (d, *J* = 6.4 Hz, 2H), 6.79 – 6.72 (m, 1H), 5.65 (d, *J* = 2.1 Hz, 1H), 5.38 (d, *J* = 2.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 164.3 (d, *J* = 12.8 Hz), 161.8 (d, *J* = 13.0 Hz), 159.8, 152.6, 137.4, 134.1, 130.6, 130.1, 128.7, 128.3, 128.2, 127.0, 123.2, 114.6, 108.4 (d, *J* = 7.5 Hz), 108.1, 104.1; MS (ESI): *m/z*: 361 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{15}F_2N_2O$: 361.1147 $[M+H]^+$; found: 361.1141.

2-Phenyl-4-((1-(4-(trifluoromethyl)phenyl)vinyl)oxy)quinazoline (13).



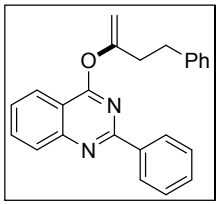
Yield: 78% (153 mg); white solid; mp: 173–175 °C; IR (neat): ν_{max} = 3066, 2923, 2852, 1739, 1621, 1576, 1489, 1265, 770, 708 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.37 (d, *J* = 8.0 Hz, 1H), 8.27 (d, *J* = 7.9 Hz, 2H), 8.04 (d, *J* = 8.3 Hz, 2H), 7.90 – 7.87 (m, 1H), 7.71 (d, *J* = 8.3 Hz, 2H), 7.63 – 7.60 (m, 1H), 7.58 (d, *J* = 8.4 Hz, 2H) 7.39 (d, *J* = 6.6 Hz, 2H), 5.70 (d, *J* = 2.2 Hz, 1H), 5.40 (d, *J* = 2.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.9, 159.8, 154.0, 152.5, 138.6, 137.4, 134.1, 130.6, 130.1, 128.7, 128.5, 128.3, 128.3, 128.2, 126.9, 125.5, 123.2, 114.7, 104.1; MS (ESI): *m/z*: 393 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{23}H_{16}ON_2F_3$: 393.12092 $[M+H]^+$; found: 393.12127.

4-((1-(4-Nitrophenyl)vinyl)oxy)-2-phenylquinazoline (14).



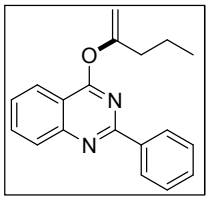
Yield: 68% (125 mg); yellow solid; mp: 152–153 °C; IR (neat): ν_{max} = 2922, 2852, 1726, 1594, 1518, 1343, 1219, 970, 854, 772, 686 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 – 8.17 (m, 2H), 8.14 (d, *J* = 8.9 Hz, 1H), 7.61 (d, *J* = 8.8 Hz, 1H), 7.50 (t, *J* = 9.2 Hz, 2H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.34 (d, *J* = 8.7 Hz, 1H), 7.23 – 7.18 (m, 4H), 7.09 (dd, *J* = 12.2, 4.1 Hz, 1H), 5.60 (s, 1H), 5.53 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 155.3, 151.9, 148.2, 144.0, 138.2, 137.2, 133.2, 131.0, 129.5, 129.1, 128.9, 128.6, 127.9, 126.9, 123.4, 116.5, 102.7; MS (ESI): *m/z*: 370 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{16}N_3O_3$: 370.11862 $[M+H]^+$; found: 370.11768.

2-Phenyl-4-((4-phenylbut-1-en-2-yl)oxy)quinazoline (15).



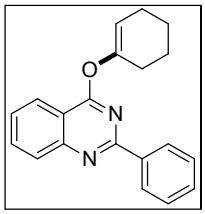
Yield: 71% (125 mg); white solid; mp: 182–183 °C; IR (neat): ν_{max} = 3063, 3026, 2922, 2853, 1735, 1621, 1574, 1558, 1492, 1216, 754, 700 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 8.54 (dd, *J* = 6.9, 2.9 Hz, 2H), 8.20 – 8.14 (m, 1H), 8.05 – 7.97 (m, 1H), 7.85 – 7.80 (m, 1H), 7.58 – 7.52 (m, 1H), 7.50 (dd, *J* = 4.9, 1.4 Hz, 3H), 7.27 (dd, *J* = 2.7, 1.4 Hz, 2H), 7.24 – 7.17 (m, 3H), 5.03 (d, *J* = 1.5 Hz, 1H), 4.95 (d, *J* = 0.6 Hz, 1H), 2.88 – 2.79 (m, 2H), 2.77 – 2.69 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.4, 160.0, 157.5, 151.9, 141.6, 138.2, 133.3, 132.7, 130.3, 129.4, 128.3, 128.2, 127.9, 126.1, 125.8, 123.5, 115.5, 101.6, 37.8, 31.9; MS (ESI): *m/z*: 353 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{24}H_{21}N_2O$: 353.16484 $[M+H]^+$; found: 353.16525.

4-(Pent-1-en-2-yloxy)-2-phenylquinazoline (16).



Yield: 68% (98 mg); pale yellow solid; mp: 191–192 °C; IR (neat): ν_{max} = 3065, 2959, 2929, 1717, 1620, 1572, 1558, 1491, 1445, 1219, 771, 708, 681 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.57 (dd, *J* = 7.2, 1.1 Hz, 2H), 8.17 (dd, *J* = 8.1, 0.6 Hz, 1H), 8.04 (d, *J* = 7.4 Hz, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.82 – 7.78 (m, 1H), 7.54 – 7.48 (m, 2H), 7.43 (t, *J* = 7.7 Hz, 1H), 5.01 (s, 1H), 4.93 (s, 1H), 2.56 (t, *J* = 7.5 Hz, 2H), 1.78 – 1.71 (m, 2H), 0.99 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.5, 160.0, 151.8, 138.3, 133.2, 130.3, 129.4, 128.4, 128.2, 127.8, 126.1, 123.5, 115.6, 100.9, 38.2, 19.8, 14.0; MS (ESI): *m/z*: 291 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{19}H_{19}N_2O$: 291.14919 $[M+H]^+$; found: 291.14825.

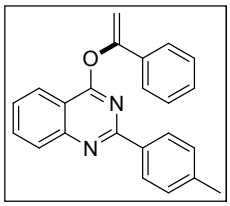
4-(Cyclohex-1-en-1-yloxy)-2-phenylquinazoline (17).



Yield: 66% (99 mg); white solid; mp: 199–201 °C; IR (neat): ν_{max} = 3064, 3028, 2924, 2853, 1715, 1619, 1572, 1557, 1490, 1448, 1416, 1274, 769, 709, 683 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.56 (dd, *J* = 7.9, 1.8 Hz, 2H), 8.18 (dd, *J* = 8.2, 0.9 Hz, 1H), 8.05 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.82 – 7.77 (m, 1H), 7.52 – 7.48 (m, 2H), 7.45 – 7.40 (m, 1H), 5.62 – 5.56 (m, 1H), 2.42 –

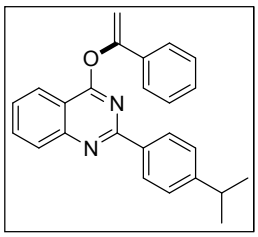
2.38 (m, 2H), 2.36 – 2.32 (m, 2H), 1.93 – 1.85 (m, 2H), 1.82 – 1.73 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.2, 160.1, 151.9, 138.3, 133.2, 132.6, 130.3, 129.5, 128.3, 128.2, 127.8, 126.1, 123.6, 115.7, 31.4, 29.6, 25.6, 23.7; MS (ESI): *m/z*: 303 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{20}H_{19}N_2O$: 303.14919 $[M+H]^+$; found: 303.14864.

4-((1-Phenylvinyl)oxy)-2-(*p*-tolyl)quinazoline (18).



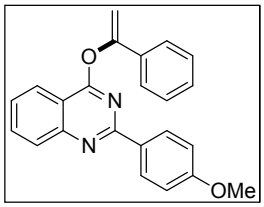
Yield: 82% (138 mg); light yellow solid; mp: 173–175 °C; IR (neat): ν_{max} = 3060, 3028, 2922, 2853, 1612, 1574, 1554, 1489, 1453, 1384, 1260, 766, 695 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.37 (d, *J* = 8.1 Hz, 1H), 8.19 (d, *J* = 8.1 Hz, 2H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.87 – 7.83 (m, 1H), 7.61 – 7.56 (m, 3H), 7.33 – 7.27 (m, 3H), 7.19 (d, *J* = 8.0 Hz, 2H), 5.60 (d, *J* = 1.9 Hz, 1H), 5.28 (d, *J* = 1.9 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.0, 160.1, 155.3, 152.5, 140.6, 135.1, 133.7, 129.0, 128.6, 128.4, 128.0, 127.7, 126.5, 126.2, 125.3, 123.3, 114.8, 101.8, 21.4; MS (ESI): *m/z*: 339 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{23}H_{19}ON_2$: 339.14919 $[M+H]^+$; found: 339.14882.

2-(4-Isopropylphenyl)-4-((1-phenylvinyl)oxy)quinazoline (19).



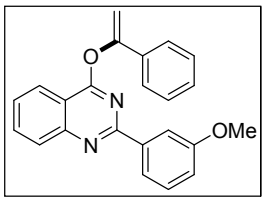
Yield: 86% (157 mg); white solid; mp: 175–177 °C; IR (neat): ν_{max} = 3062, 2959, 2922, 2852, 1605, 1575, 1555, 1489, 1453, 1384, 1347, 1261, 772, 698 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, *J* = 8.1 Hz, 1H), 8.23 (dd, *J* = 8.0, 3.8 Hz, 2H), 8.01 (d, *J* = 8.3 Hz, 1H), 7.82 (t, *J* = 7.7 Hz, 1H), 7.60 (d, *J* = 7.3 Hz, 2H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.30 – 7.23 (m, 4H), 7.20 – 7.11 (m, 1H), 5.59 (d, *J* = 2.0 Hz, 1H), 5.27 (d, *J* = 2.0 Hz, 1H), 2.96 – 2.86 (m, 1H), 1.24 (dd, *J* = 6.9, 2.2 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.0, 160.1, 155.2, 152.5, 151.5, 135.4, 135.1, 133.7, 128.6, 128.5, 128.4, 128.0, 127.0, 126.3, 125.2, 123.3, 114.7, 101.8, 34.0, 23.8; MS (ESI): *m/z*: 367 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{25}H_{23}N_2O$: 367.18049 $[M+H]^+$; found: 367.17921.

2-(4-Methoxyphenyl)-4-((1-phenylvinyl)oxy)quinazoline (20).



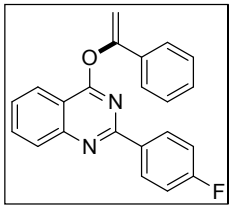
Yield: 86% (152 mg); light brown solid; mp: 177–178 °C; IR (neat): ν_{max} = 3019, 2925, 1605, 1572, 1552, 1515, 1452, 1349, 1215, 907, 748, 667 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.36 (dd, *J* = 8.1, 0.7 Hz, 1H), 8.26 (d, *J* = 8.9 Hz, 2H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.87 – 7.83 (m, 1H), 7.61 – 7.55 (m, 3H), 7.34 – 7.28 (m, 3H), 6.90 (d, *J* = 8.9 Hz, 2H), 5.60 (d, *J* = 2.0 Hz, 1H), 5.28 (d, *J* = 2.0 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.0, 161.7, 159.8, 155.3, 135.1, 133.8, 130.1, 129.1, 128.7, 128.4, 127.8, 127.5, 126.3, 125.2, 123.4, 114.6, 113.6, 101.9, 55.3; MS (ESI): *m/z*: 355 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{23}H_{19}O_2N_2$: 355.14410 $[M+H]^+$; found: 355.14349.

2-(3-Methoxyphenyl)-4-((1-phenylvinyl)oxy)quinazoline (21).



Yield: 80% (141 mg); yellow solid; mp: 178–180 °C; IR (neat): ν_{max} = 3063, 3001, 2929, 2836, 1599, 1575, 1559, 1491, 1457, 1345, 1256, 768, 689 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.38 (dd, *J* = 8.1, 0.8 Hz, 1H), 8.02 (t, *J* = 7.0 Hz, 1H), 7.94 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.84 – 7.82 (m, 1H), 7.61 – 7.57 (m, 2H), 7.42 (d, *J* = 7.2 Hz, 2H), 7.38 (d, *J* = 1.8 Hz, 1H), 7.31 – 7.27 (m, 2H), 7.16 – 7.14 (m, 1H), 6.97 – 6.94 (m, 1H), 5.60 (d, *J* = 2.0 Hz, 1H), 5.28 (d, *J* = 2.0 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.0, 159.6, 155.3, 152.4, 144.7, 133.8, 129.9, 129.2, 128.6, 128.4, 128.1, 126.8, 126.3, 125.9, 125.1, 123.3, 120.9, 117.2, 112.7, 101.9, 55.2; MS (ESI): *m/z*: 355 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{23}H_{19}N_2O_2$: 355.14410 $[M+H]^+$; found: 355.14291.

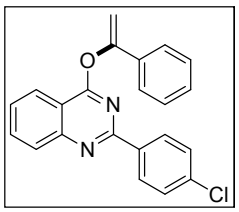
2-(4-Fluorophenyl)-4-((1-phenylvinyl)oxy)quinazoline (22).



Yield: 79% (135 mg); pale yellow solid; mp: 141–143 °C; IR (neat): ν_{max} = 2924, 2853, 1720, 1602, 1573, 1510, 1492, 1268, 1151, 1109, 909, 767, 696 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.38 (dd, *J* = 8.1, 0.6 Hz,

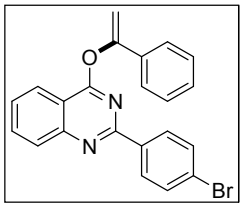
1H), 8.29 (dd, *J* = 8.8, 5.7 Hz, 2H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.90 – 7.85 (m, 1H), 7.62 – 7.58 (m, 3H), 7.34 – 7.28 (m, 2H), 7.18 (dd, *J* = 7.2, 4.7 Hz, 1H), 7.06 (t, *J* = 8.7 Hz, 2H), 5.61 (d, *J* = 2.0 Hz, 1H), 5.27 (d, *J* = 2.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.1, 163.3, 159.0, 155.3, 152.4, 135.0, 134.0, 130.5 (d, *J* = 8.6 Hz), 129.1, 128.7, 128.4, 128.0, 126.8, 126.2, 125.2, 123.4, 115.19 (d, *J* = 21.6 Hz), 101.9; MS (ESI): *m/z*: 343 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{16}FN_2O$: 343.12412 $[M+H]^+$; found: 343.12450.

2-(4-Chlorophenyl)-4-((1-phenylvinyl)oxy)quinazoline (23).



Yield: 77% (138 mg); pale yellow solid; mp: 135–136 °C; IR (neat): ν_{max} = 2923, 2852, 1621, 1574, 1555, 1494, 1453, 1261, 1091, 945, 770, 698 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.39 (d, *J* = 8.1 Hz, 1H), 8.23 (d, *J* = 8.5 Hz, 2H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.91 – 7.86 (m, 1H), 7.64 – 7.58 (m, 3H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.32 – 7.27 (m, 2H), 7.23 – 7.17 (m, 1H), 5.61 (d, *J* = 1.5 Hz, 1H), 5.27 (d, *J* = 1.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.1, 158.9, 155.2, 152.4, 136.6, 136.2, 134.0, 129.7, 129.1, 128.7, 128.4, 128.1, 126.9, 126.2, 125.2, 123.4, 114.8, 101.9; MS (ESI): *m/z*: 359 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{16}ClN_2O$: 359.09457 $[M+H]^+$; found: 359.09517.

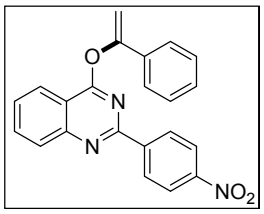
2-(4-Bromophenyl)-4-((1-phenylvinyl)oxy)quinazoline (24).



Yield: 74% (149 mg); yellow solid; mp: 125–127 °C; IR (neat): ν_{max} = 3058, 3028, 2923, 2853, 1620, 1574, 1554, 1491, 1451, 1260, 768, 698 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.38 (d, *J* = 8.1 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 2H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.90 – 7.85 (m, 1H), 7.63 – 7.55 (m, 3H), 7.51 (d, *J* = 8.6 Hz, 1H), 7.38 – 7.28 (m, 3H), 7.21 – 7.16 (m, 1H), 5.60 (d, *J* = 2.0 Hz, 1H), 5.27 (d, *J* = 2.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.1, 159.0, 155.2, 152.4, 136.6, 135.0, 134.0, 131.4, 130.0, 128.7, 128.4, 128.2, 128.1, 127.0, 125.2, 123.4, 114.9, 102.0; MS (ESI): *m/z*:

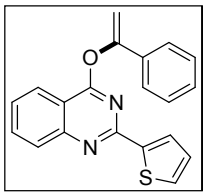
405 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{16}BrN_2O$: 403.04405 $[M+H]^+$; found: 403.04432.

2-(4-Nitrophenyl)-4-((1-phenylvinyl)oxy)quinazoline (25).



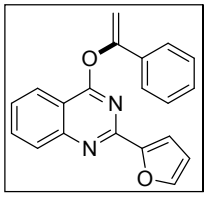
Yield: 77% (142 mg); white solid; mp: 179–180 °C; IR (neat): ν_{max} = 2921, 2852, 1727, 1593, 1517, 1343, 1219, 1109, 970, 854, 772, 687 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.44 (d, *J* = 8.9 Hz, 2H), 8.22 (d, *J* = 8.9 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.97 – 7.94 (m, 2H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.36 – 7.31 (m, 2H), 5.63 (d, *J* = 2.0 Hz, 1H), 5.29 (d, *J* = 2.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.3, 157.7, 155.2, 152.3, 149.0, 143.5, 134.3, 133.0, 129.1, 128.9, 128.5, 128.4, 128.2, 127.8, 125.2, 123.4, 115.1, 102.1; MS (ESI): *m/z*: 370 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{16}N_3O_3$: 370.11862 $[M+H]^+$; found: 370.11743.

4-((1-Phenylvinyl)oxy)-2-(thiophen-2-yl)quinazoline (26).



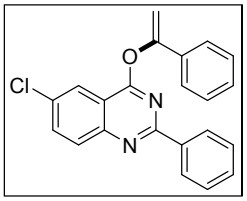
Yield: 67% (110 mg); light yellow solid; mp: 165–166 °C; IR (neat): ν_{max} = 3055, 3025, 2922, 2852, 1620, 1598, 1575, 1491, 1444, 1384, 1313, 1263, 1219, 1026, 896, 771, 698 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 7.94 (dd, *J* = 7.4, 1.0 Hz, 2H), 7.58 – 7.51 (m, 1H), 7.45 – 7.40 (m, 2H), 7.36 – 7.33 (m, 2H), 7.30 – 7.23 (m, 2H), 7.20 – 7.12 (m, 2H), 7.08 (dd, *J* = 5.9, 2.7 Hz, 1H), 5.57 (d, *J* = 2.0 Hz, 1H), 5.28 (d, *J* = 2.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 155.2, 152.3, 149.8, 146.3, 132.9, 129.3, 129.0, 128.4, 128.2, 127.7, 127.0, 126.1, 125.2, 123.3, 116.2, 114.1, 101.9; MS (ESI): *m/z*: 331 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{20}H_{15}N_2OS$: 331.08996 $[M+H]^+$; found: 331.08854.

2-(Furan-2-yl)-4-((1-phenylvinyl)oxy)quinazoline (27).



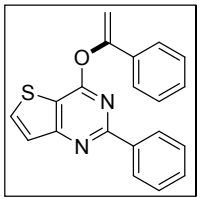
Yield: 71% (111 mg); white solid; mp: 153–155 °C; IR (neat): ν_{max} = 3055, 3024, 2921, 2852, 1730, 1598, 1574, 1491, 1443, 1312, 1263, 1219, 1025, 897, 772, 696 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 7.94 (dd, *J* = 5.1, 2.8 Hz, 2H), 7.55 – 7.51 (m, 1H), 7.45 – 7.40 (m, 2H), 7.36 – 7.27 (m, 4H), 7.20 – 7.17 (m, 2H), 7.08 – 7.06 (m, 1H), 5.54 (d, *J* = 3.4 Hz, 1H), 5.31 (d, *J* = 3.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 157.6, 149.8, 146.3, 143.9, 142.0, 132.9, 129.0, 128.4, 128.2, 128.0, 127.7, 127.0, 126.5, 126.1, 116.2, 114.1, 101.9; MS (ESI): *m/z*: 315 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{20}H_{15}N_2O_2$: 315.11280 $[M+H]^+$; found: 315.11146.

6-Chloro-2-phenyl-4-((1-phenylvinyl)oxy)quinazoline (28).



Yield: 72% (129 mg); yellow solid; mp: 151–152 °C; IR (neat): ν_{max} = 3059, 3026, 2921, 2851, 1571, 1555, 1260, 764, 700 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.37 (d, *J* = 2.3 Hz, 1H), 8.28 (dd, *J* = 7.7, 1.9 Hz, 2H), 7.97 (d, *J* = 9.0 Hz, 1H), 7.81 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.59 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.35 – 7.27 (m, 3H), 7.21 – 7.16 (m, 2H), 5.61 (d, *J* = 2.1 Hz, 1H), 5.28 (d, *J* = 2.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.3, 160.3, 155.1, 150.9, 134.7, 130.7, 129.8, 128.8, 128.5, 128.3, 128.1, 127.8, 126.2, 125.2, 122.5, 115.5, 114.2, 102.1; MS (ESI): *m/z*: 359 $[M+H]^+$; HRMS (ESI): *m/z*: calcd for $C_{22}H_{16}ClN_2O$: 359.09457 $[M+H]^+$; found: 359.09480.

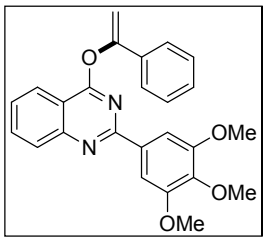
2-Phenyl-4-((1-phenylvinyl)oxy)thieno[3,2-*d*]pyrimidine (29).



Yield: 77% (127 mg); colorless solid; mp: 148–149 °C IR (neat): ν_{max} = 3057, 3027, 2923, 2853, 1722, 1599, 1565, 1526, 1260, 773, 696 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.26 (d, *J* = 2.0 Hz, 1H), 8.24 (dd, *J* = 2.7, 1.8 Hz, 1H), 7.94 (d, *J* = 5.4 Hz, 1H), 7.60 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.58 (d, *J* = 5.4 Hz, 1H), 7.41 (d, *J* = 8.3 Hz, 1H), 7.39 (dd, *J* = 5.2, 1.9 Hz, 1H), 7.33 – 7.28 (m, 2H), 7.25 – 7.23 (m, 1H), 7.18 (d, *J* = 8.0 Hz, 1H), 7.14 (d, *J* = 7.1 Hz, 1H), 5.60 (d, *J* = 2.2 Hz, 1H), 5.30 (d, *J* =

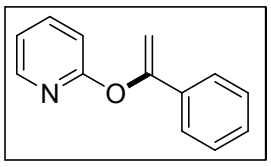
2.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1, 163.3, 161.2, 154.8, 144.4, 137.5, 134.7, 133.8, 130.2, 129.3, 129.1, 128.6, 128.3, 125.3, 115.4, 102.0; MS (ESI): *m/z*: 331 $[M+H]^+$.

4-((1-Phenylvinyl)oxy)-2-(3,4,5-trimethoxyphenyl)quinazoline (30).



Yield: 91% (188 mg); pale yellow solid; mp: 136–137 °C; IR (neat): ν_{max} = 3057, 2933, 2838, 1598, 1492, 1454, 1376, 770, 698 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.38 (d, *J* = 8.1 Hz, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.85 (t, *J* = 7.7 Hz, 1H), 7.59 – 7.57 (m, 2H), 7.44 – 7.40 (m, 1H), 7.37 – 7.33 (m, 1H), 7.29 – 7.23 (m, 2H), 7.18 – 7.17 (m, 1H), 5.58 (s, 1H), 5.27 (s, 1H), 3.87 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.8, 159.3, 155.3, 152.8, 152.3, 140.1, 133.8, 132.9, 128.6, 128.4, 127.9, 126.6, 126.1, 124.9, 123.3, 114.5, 105.3, 101.7, 60.7, 55.9; MS (ESI): *m/z*: 415 $[M+H]^+$; HRMS (ESI): *m/z* calcd for $C_{25}H_{23}N_2O_4$: 415.16523 $[M+H]^+$; found: 415.16502.

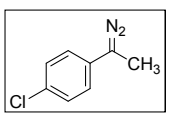
2-((1-Phenylvinyl)oxy)pyridine (31).[1]



Yield: 78% (76 mg); white solid; IR (neat): ν_{max} = 2922, 2852, 1728, 1643, 1592, 1492, 1466, 1429, 1266, 1243, 1075, 963, 772, 694 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (dd, *J* = 4.8, 1.3 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.59 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.34 – 7.28 (m, 3H), 6.96 – 6.92 (m, 2H), 5.42 (d, *J* = 2.0 Hz, 1H), 4.96 (d, *J* = 2.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.1, 156.1, 147.9, 139.3, 134.8, 128.6, 128.3, 125.4, 118.3, 111.4, 99.1; MS (ESI): *m/z*: 198 $[M+H]^+$.

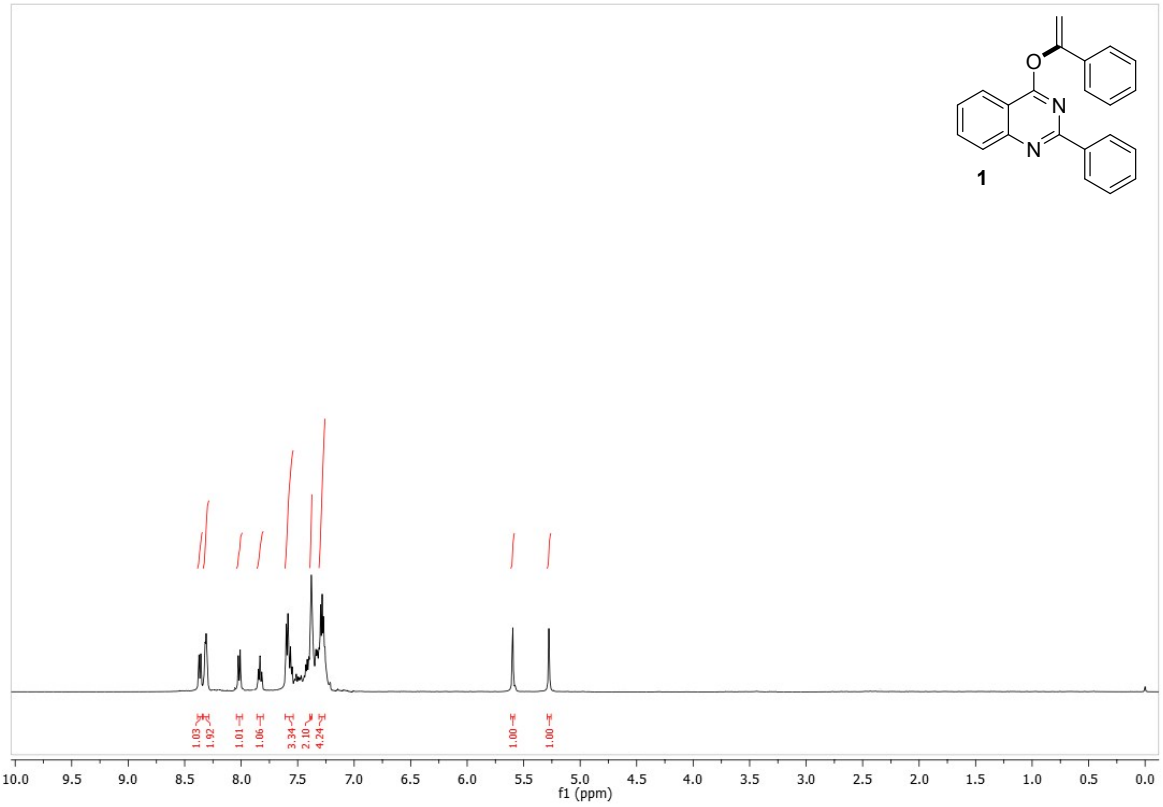
1. J. Yang and G. B. Dudley, *Adv. Synth. Catal.*, 2010, **352**, 3438.

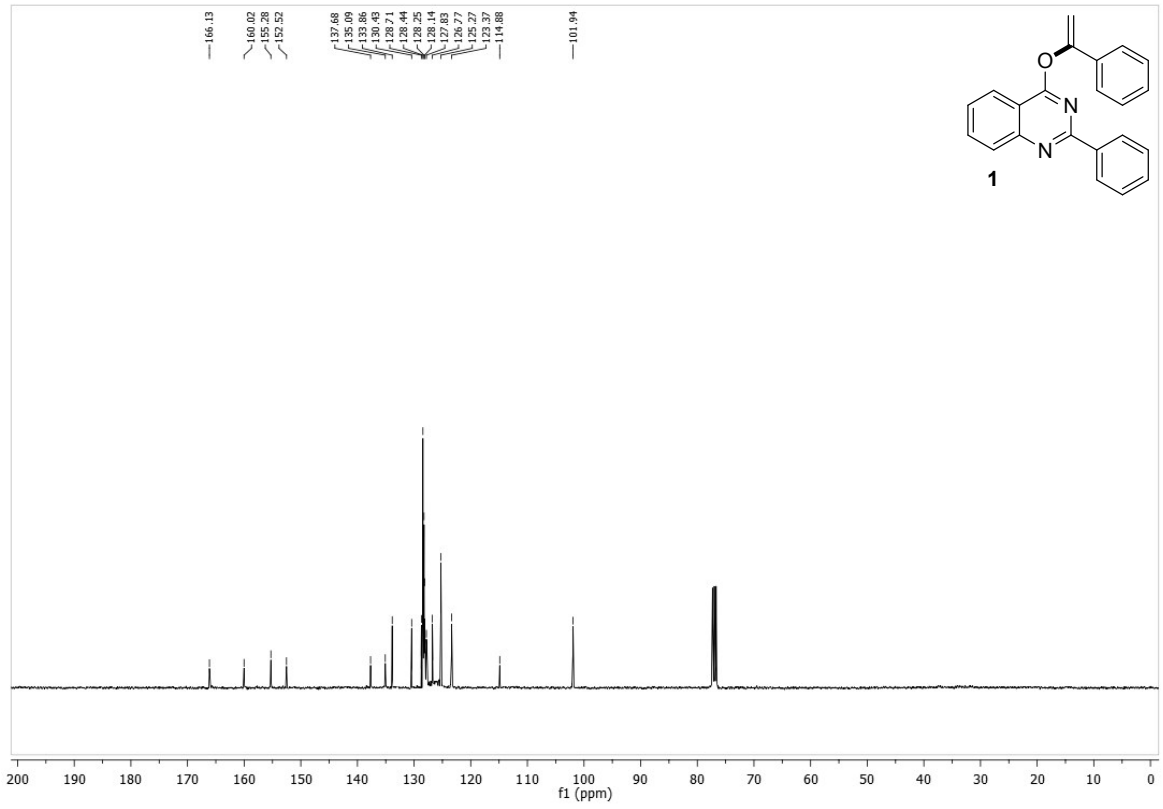
1-Chloro-4-(1-diazoethyl)benzene.

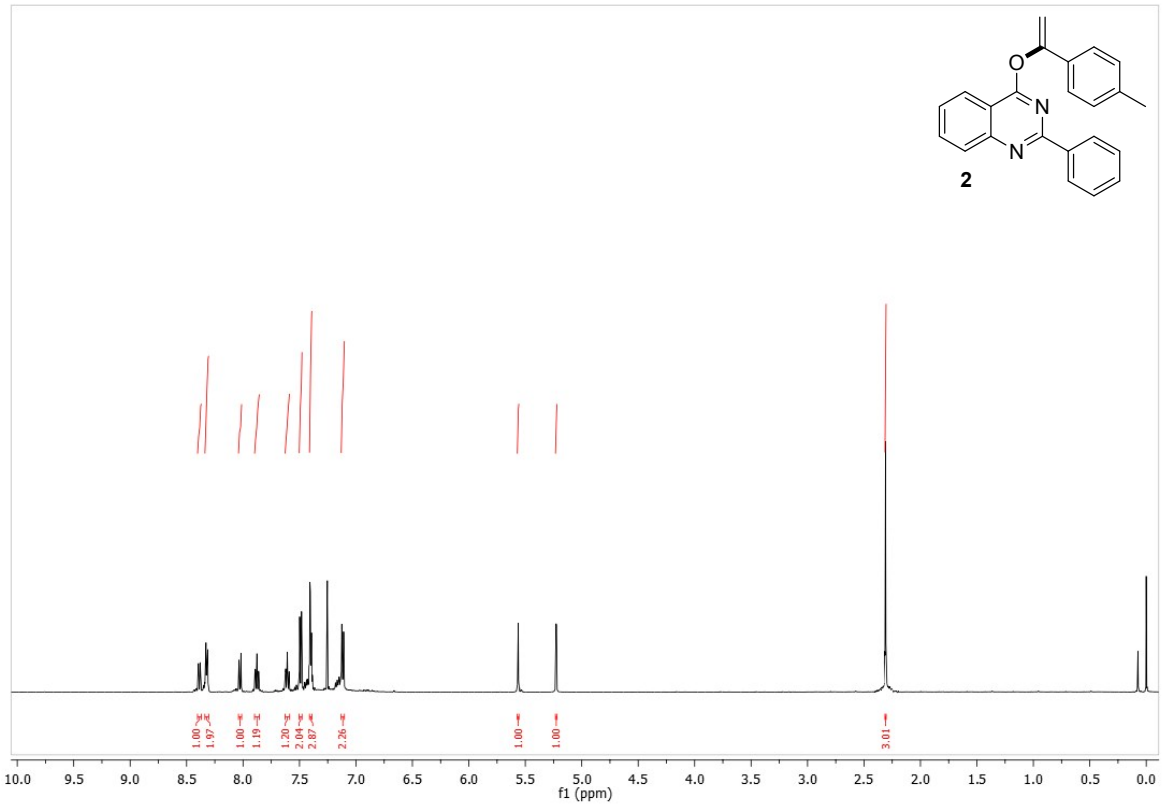


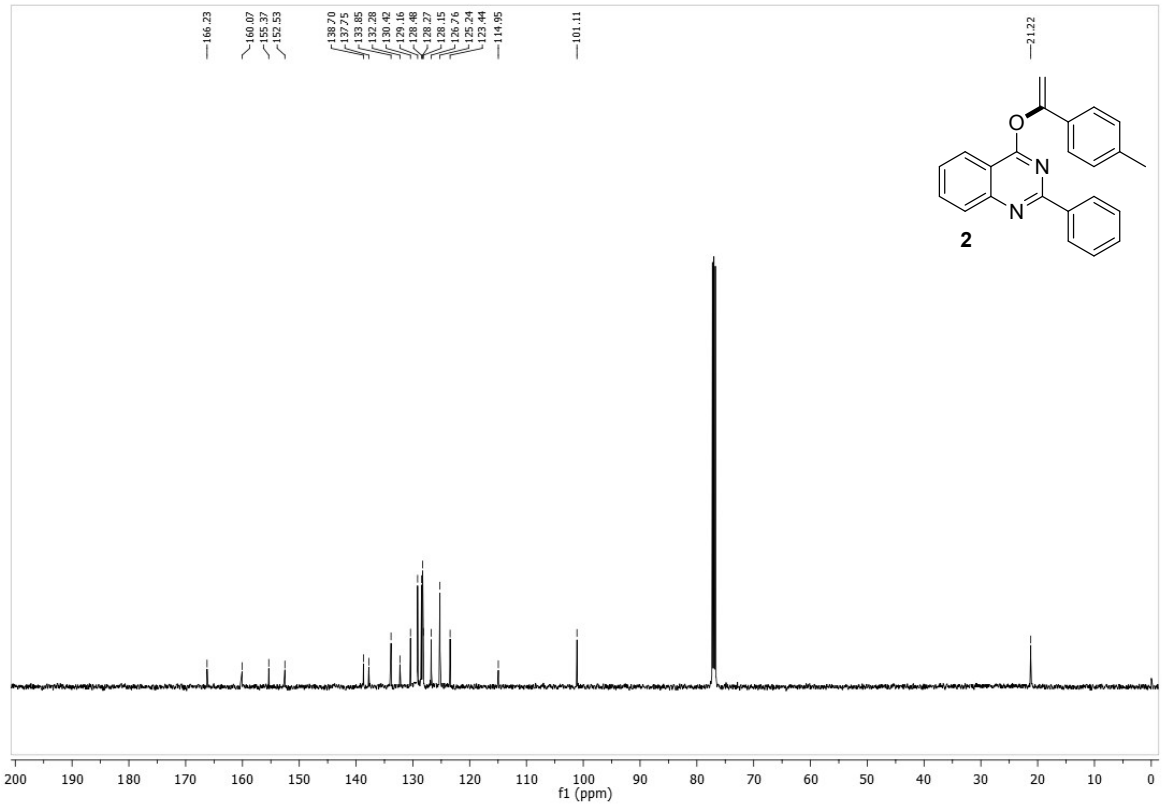
Yield: 94%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.89 (d, *J* = 8.6 Hz, 2H), 7.43 (d, *J* = 8.6 Hz, 2H), 2.59 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 196.7, 139.5, 135.3, 129.6, 128.8, 26.5; MS (ESI): *m/z*: 189 $[M+Na]^+$.

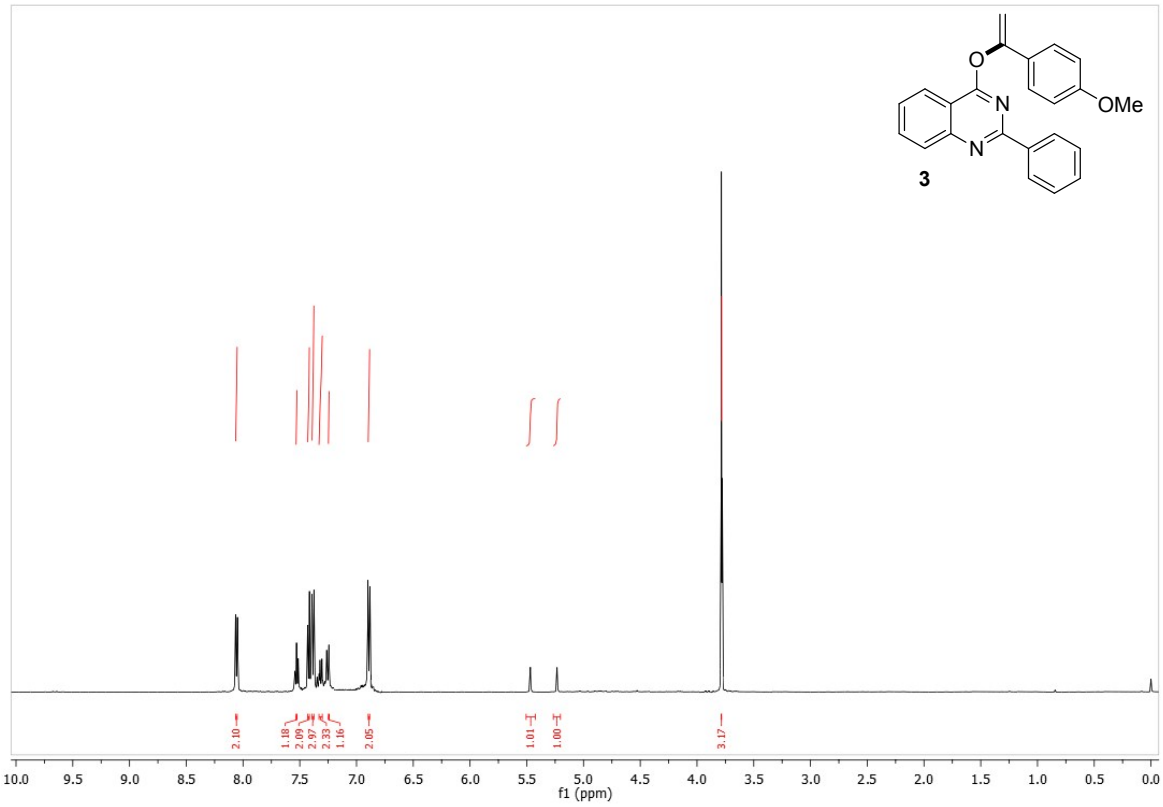
1.5 ^{1}H and ^{13}C NMR Spectra for compounds (1-30)

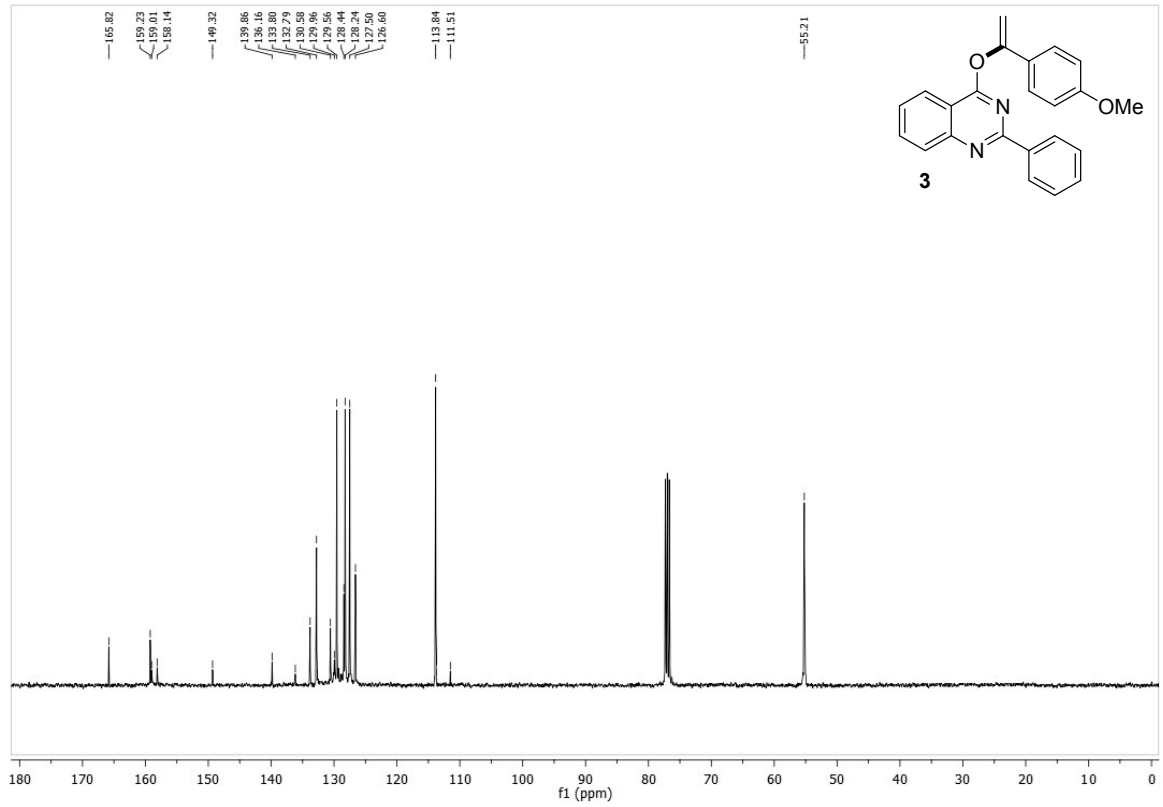


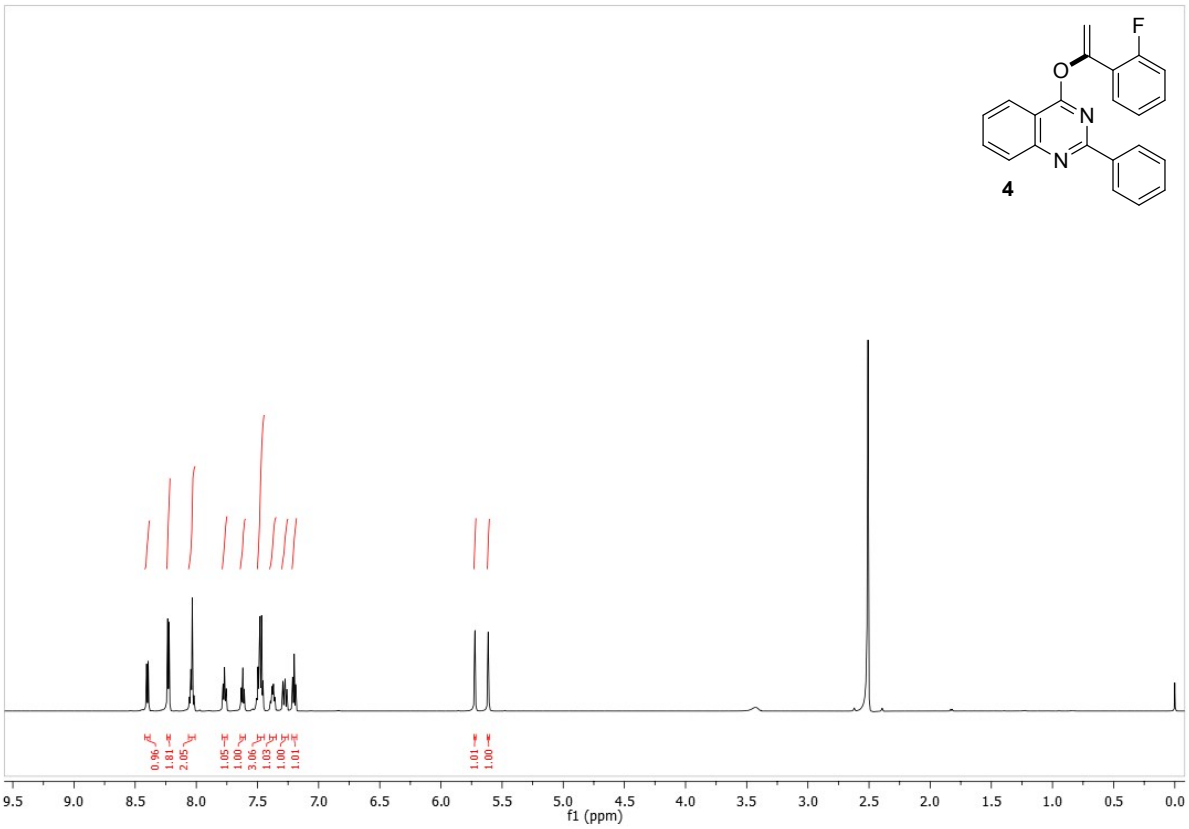


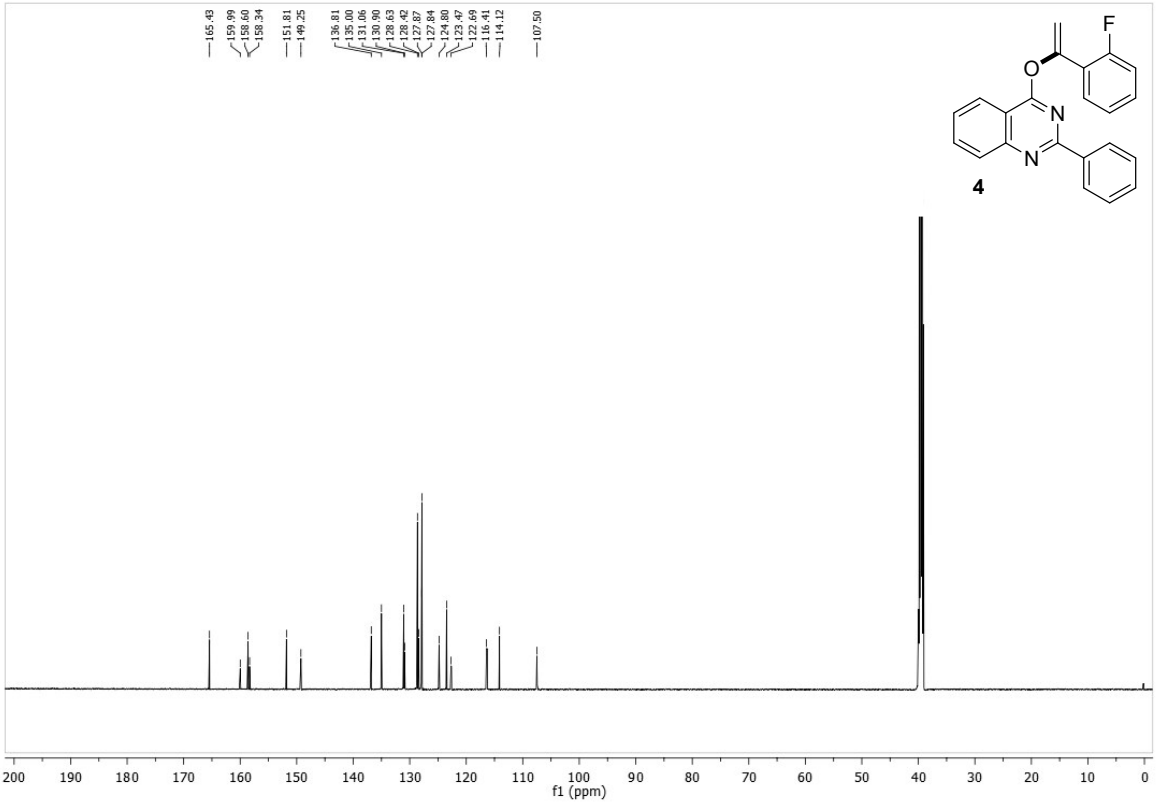

O
N
N
2
1.00
1.97
1.00
1.19
1.20
2.04
2.87
2.26
1.00
1.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

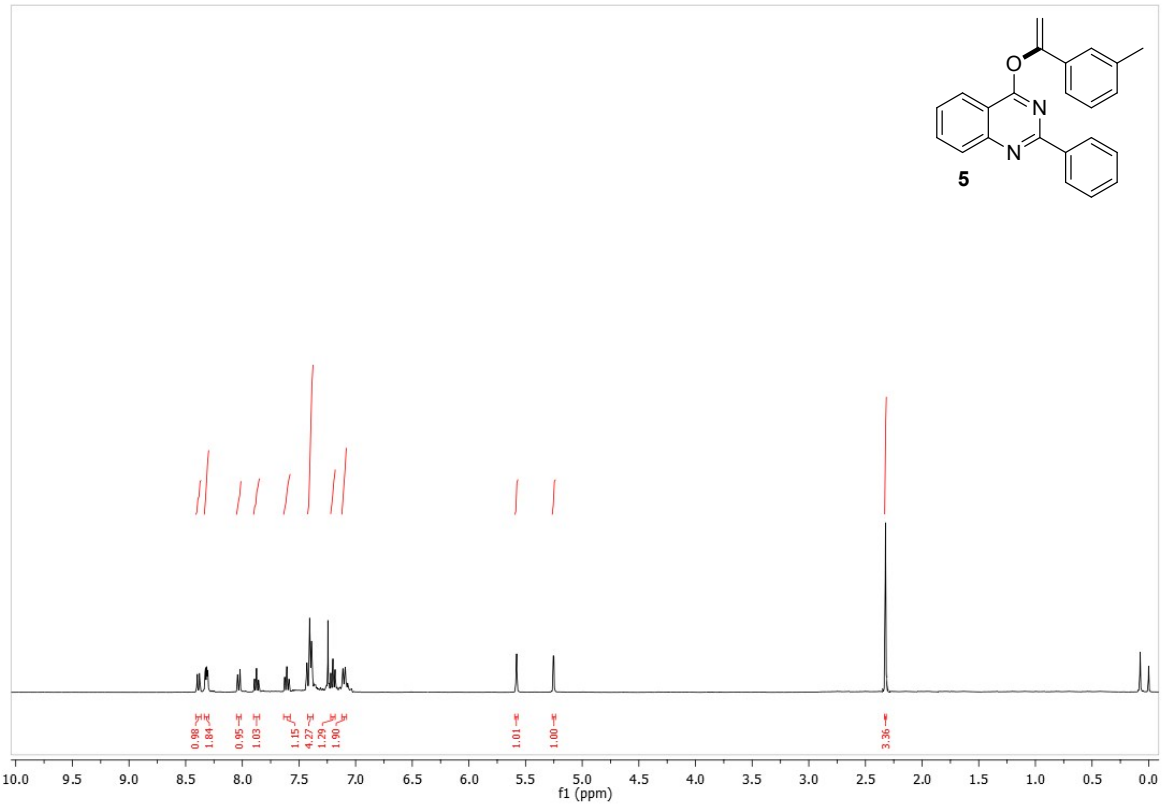

166.23
160.07
155.37
152.53
138.70
137.75
133.85
132.28
130.42
129.16
128.48
128.27
128.15
126.76
125.24
123.44
114.95
101.11
21.22
O
N
N
2
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

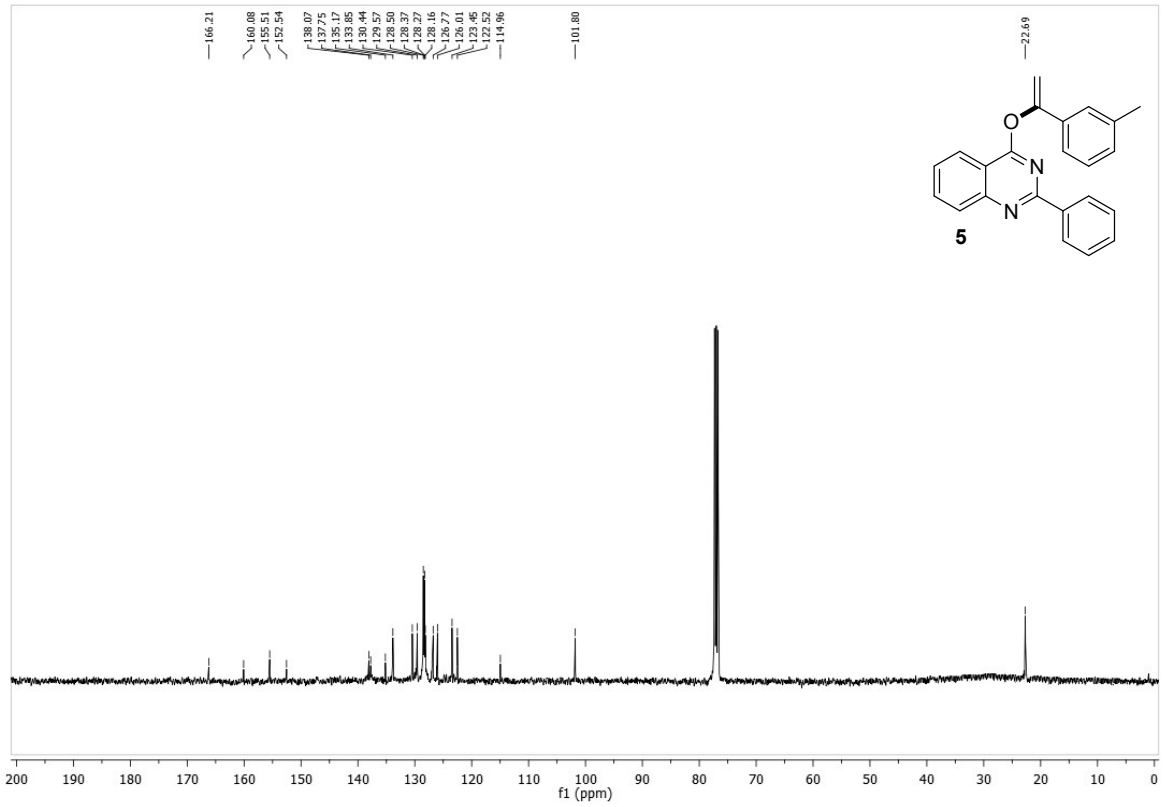

O
N
N
OMe
3
2.10
1.18
2.09
2.97
2.33
1.16
2.05
1.01
1.00
3.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

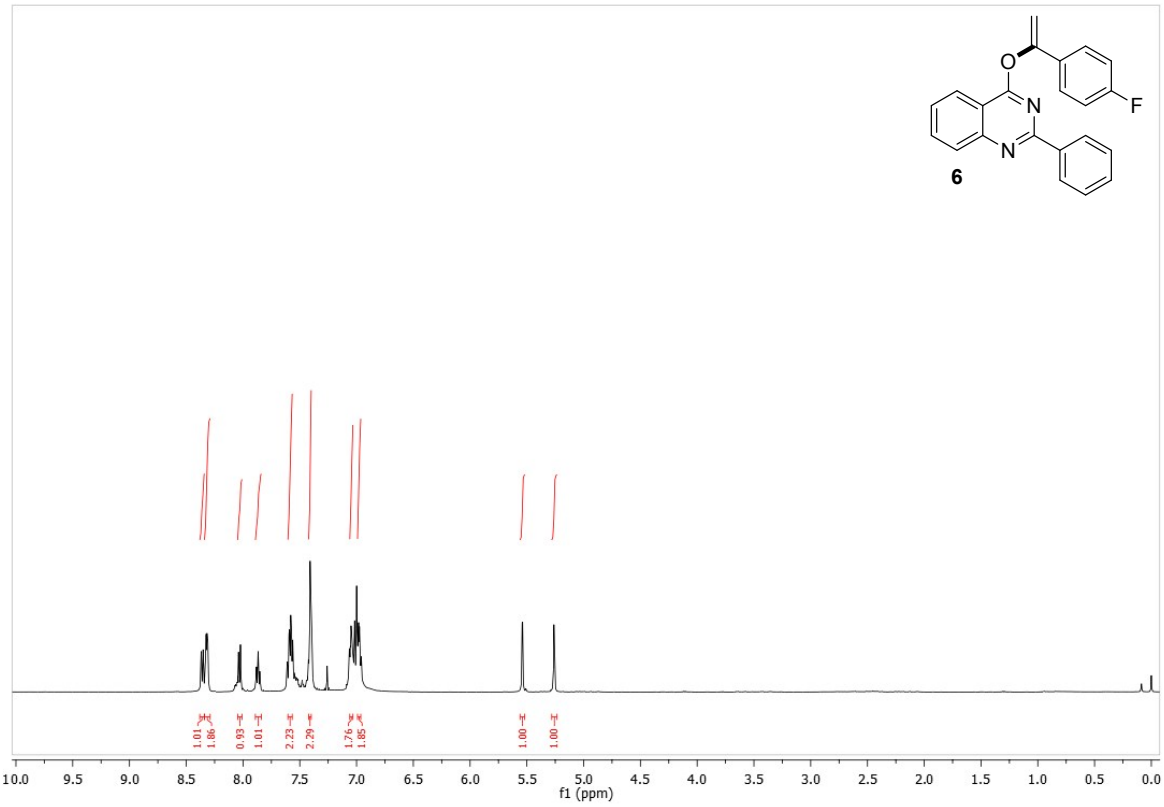

165.82
159.23
159.01
158.14
149.32
139.86
136.16
133.80
132.79
130.58
129.96
129.56
128.44
128.24
127.50
126.60
113.84
111.51
55.21
O
N
N
OMe
3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

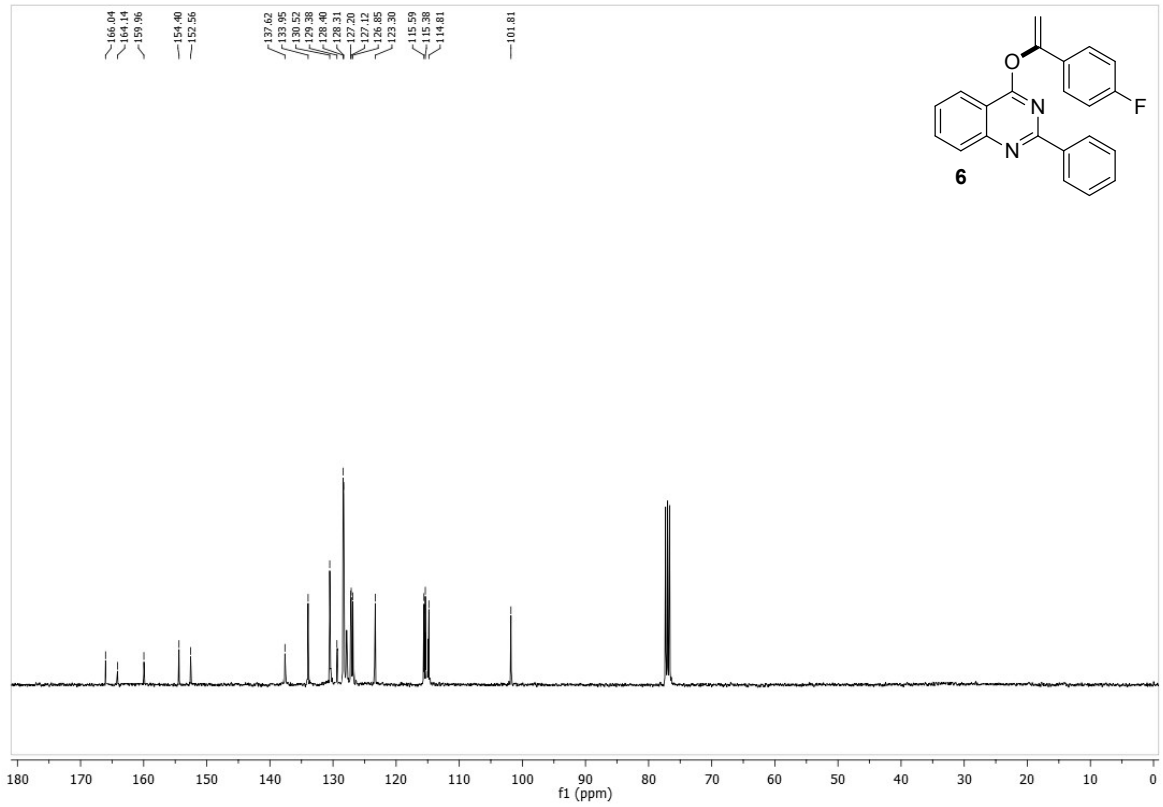

F
O
N
N
4
0.96
1.81
2.05
1.05
1.00
3.06
3.03
1.00
1.01
1.01
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

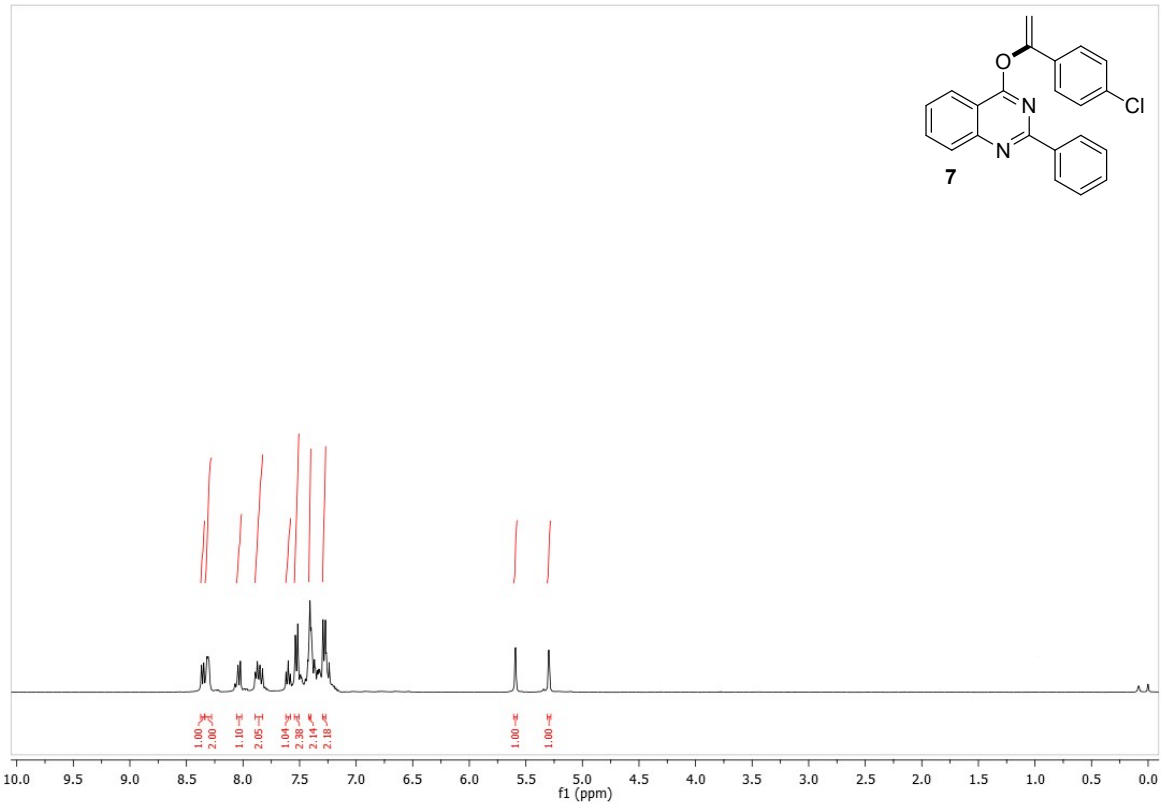

165.43
159.99
158.60
158.34
151.81
149.25
136.81
135.00
131.06
130.90
128.63
128.42
127.87
127.84
124.80
123.47
122.69
116.41
114.12
107.50
F
O
N
N
4
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

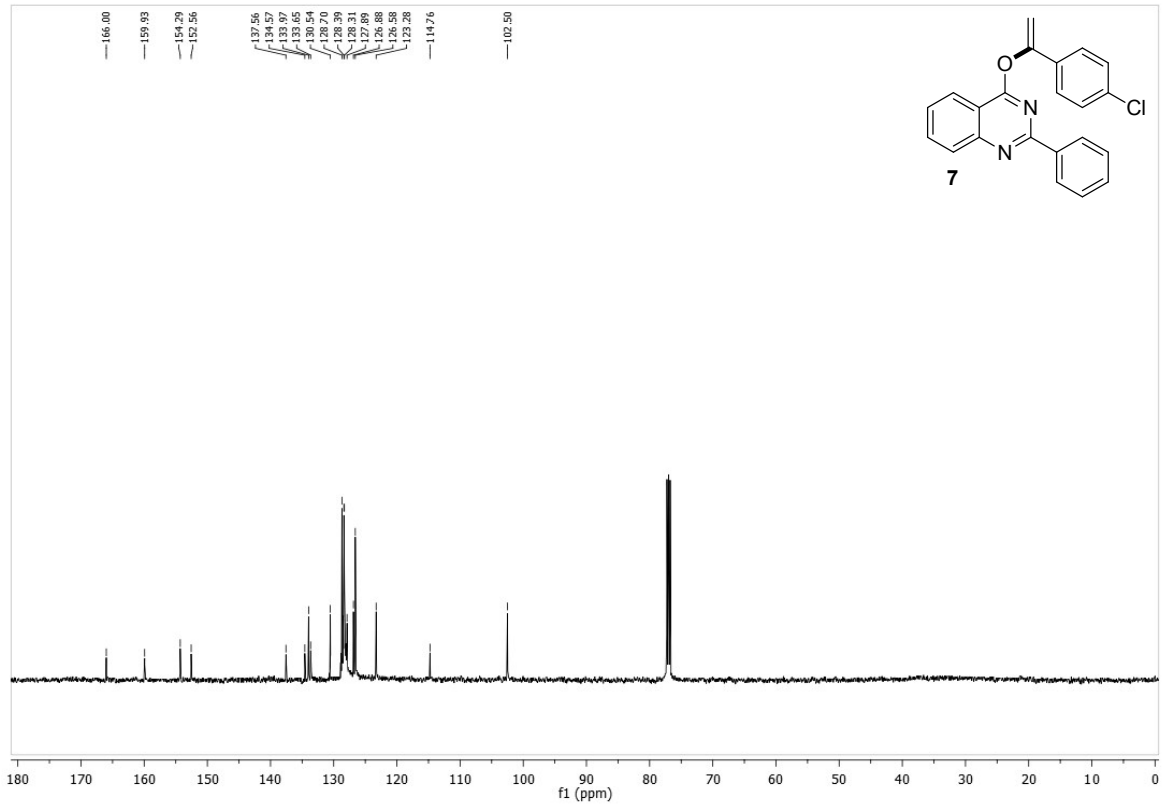

O
N
N
5
0.98
1.84
0.95
1.03
1.15
4.27
1.29
1.90
1.01
1.00
3.36
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

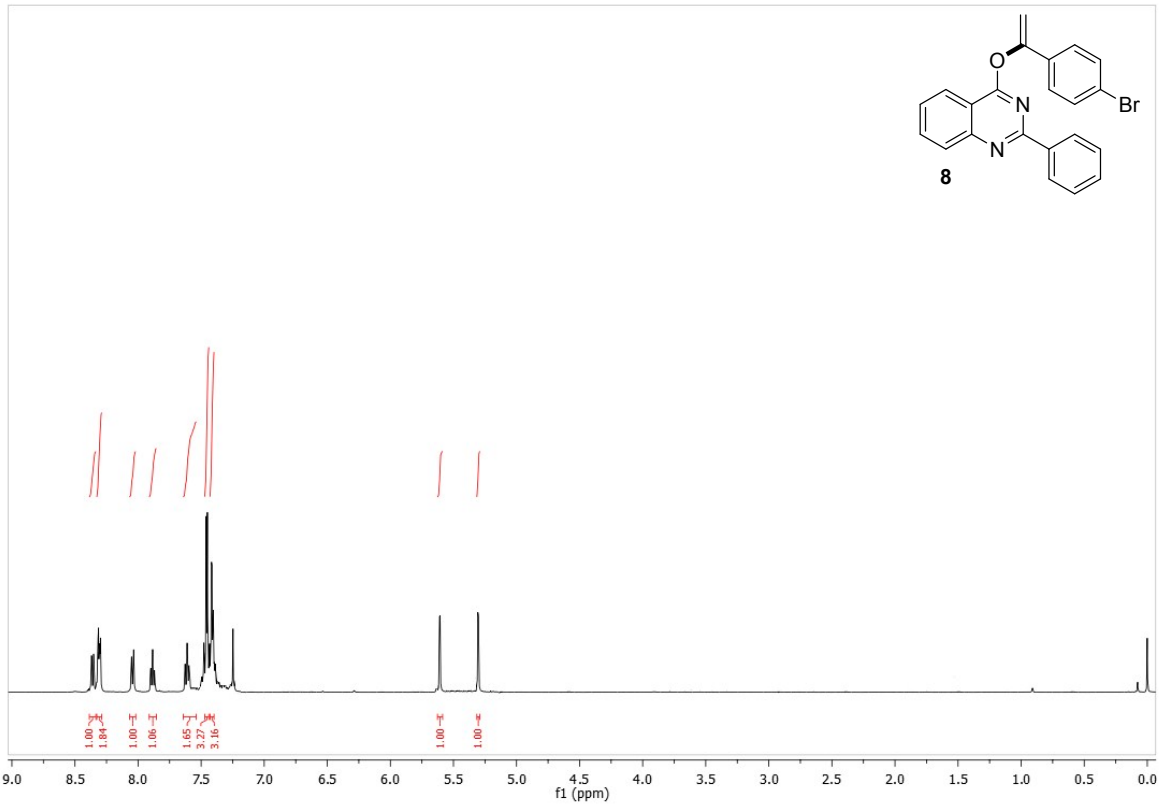

166.21
160.08
155.51
152.54
138.07
137.75
135.17
133.85
130.44
129.57
128.50
128.37
128.27
128.16
126.77
126.01
123.45
122.52
114.96
101.80
22.69
O
N
N
5
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

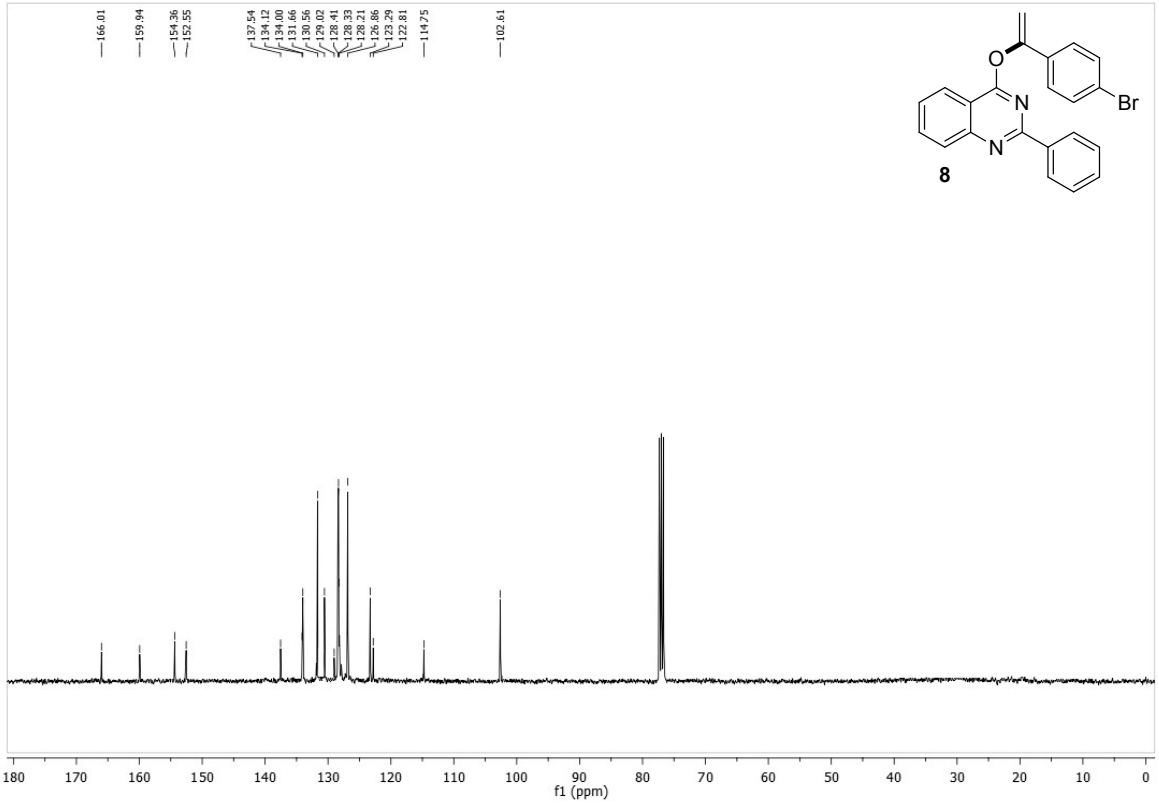

O
N
N
F
6
1.01
1.86
0.93
1.01
2.23
2.29
1.76
1.85
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

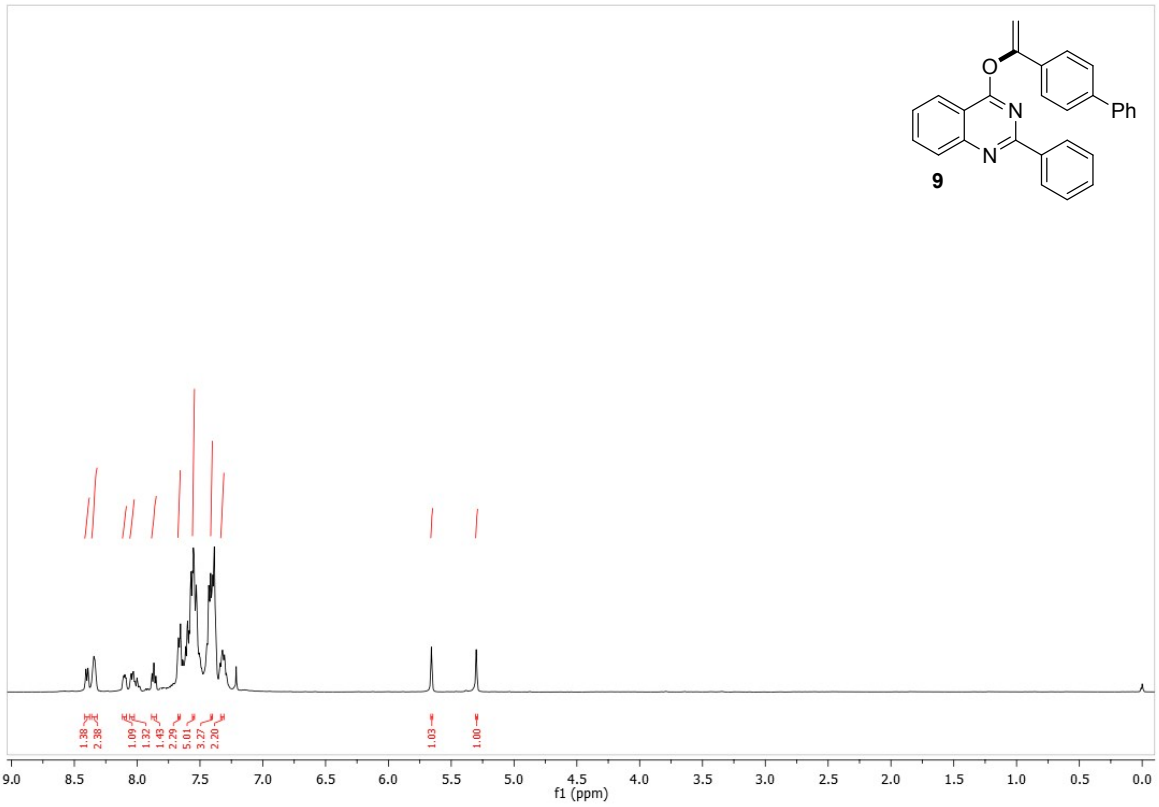

166.04
164.14
159.96
154.40
152.56
137.62
133.95
130.52
129.38
128.40
128.31
127.20
127.12
126.85
123.30
115.59
115.38
114.81
101.81
O
N
N
F
6
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

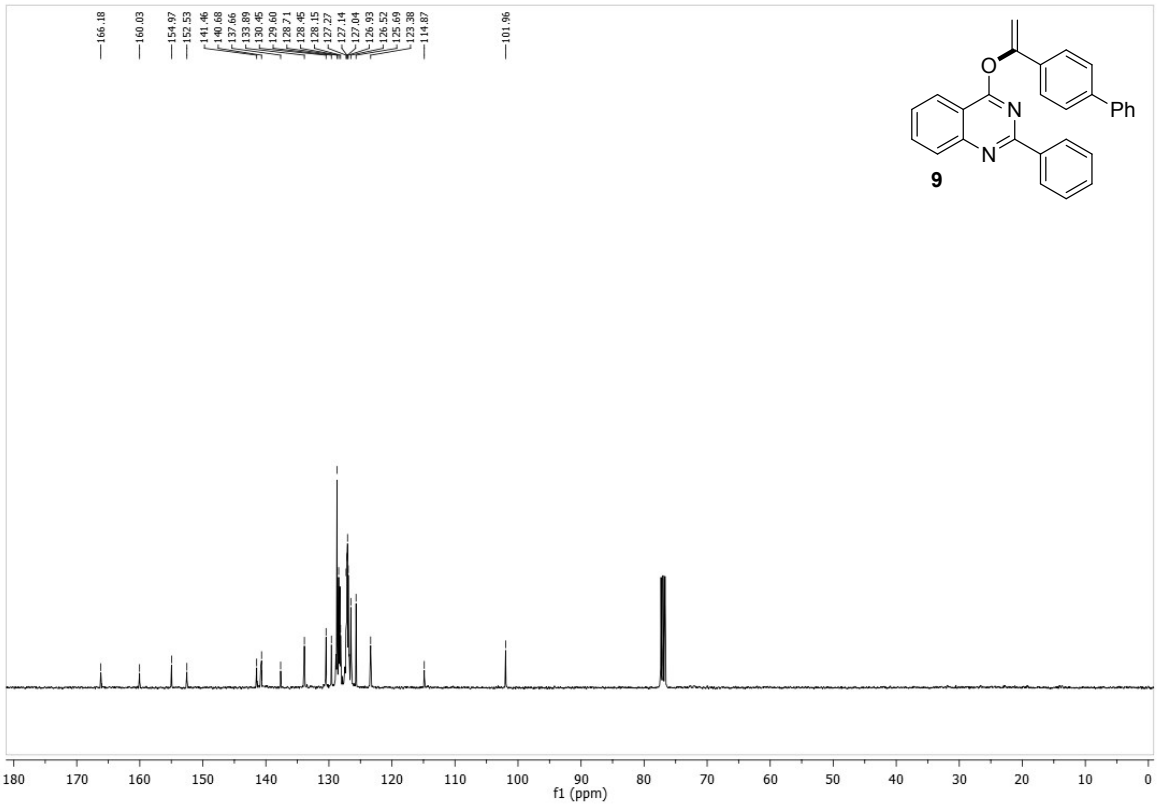

O
N
N
Cl
7
1.00
2.00
1.10
2.05
1.04
2.38
2.14
2.18
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

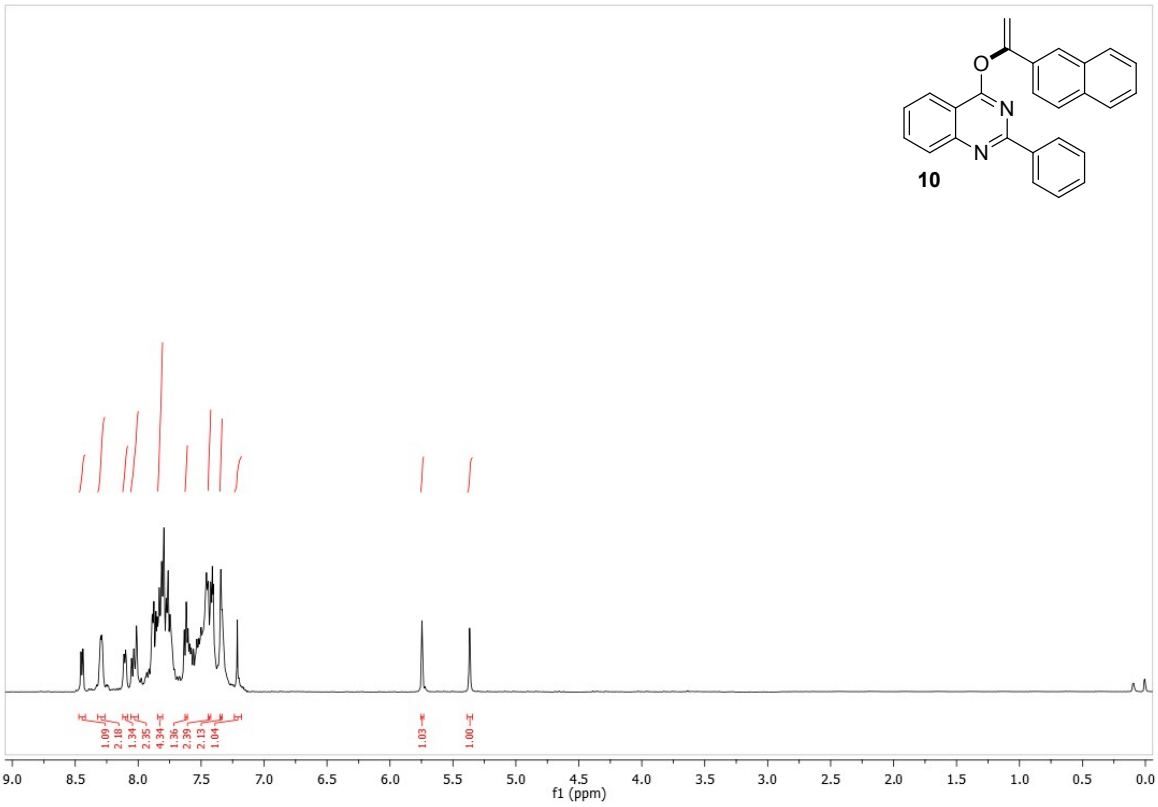

166.00
159.93
154.29
152.56
137.56
134.57
133.97
133.65
130.54
128.70
128.39
128.31
127.88
126.88
126.58
123.28
114.76
102.50
O
N
N
Cl
7
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

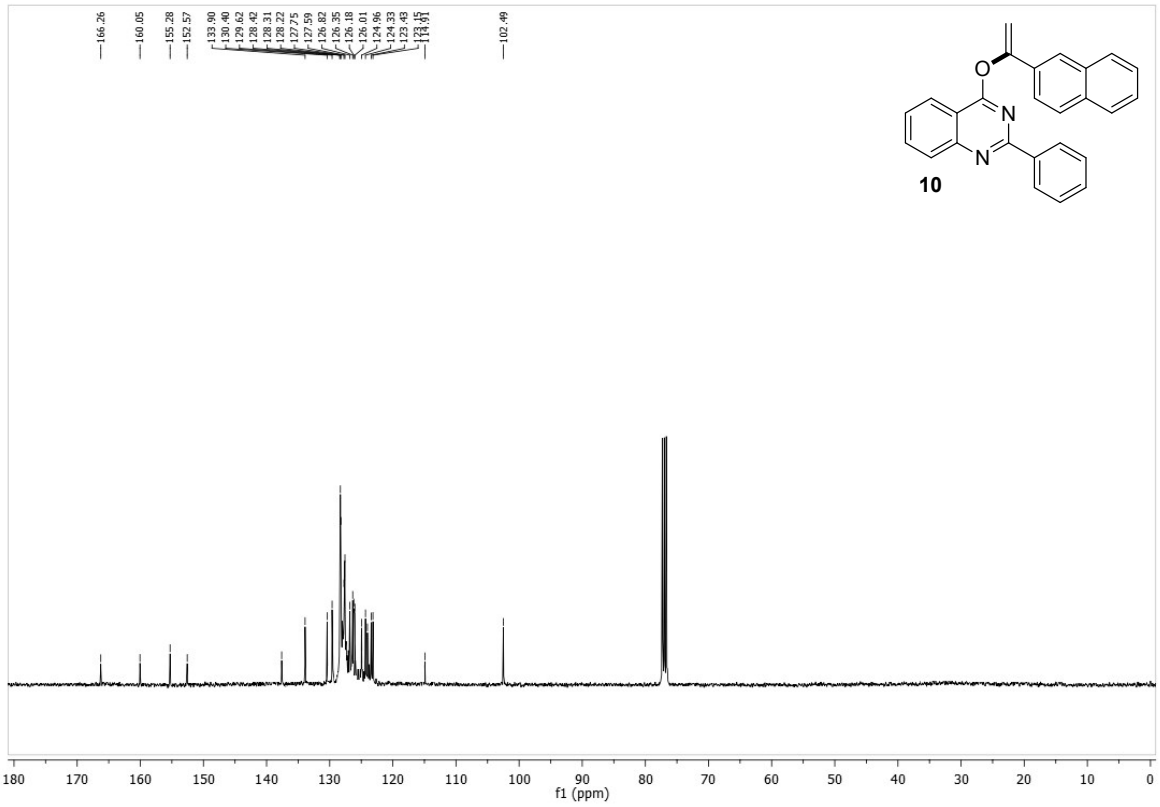

O
N
N
Br
8
1.00
1.84
1.00
1.06
1.65
3.27
3.16
1.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

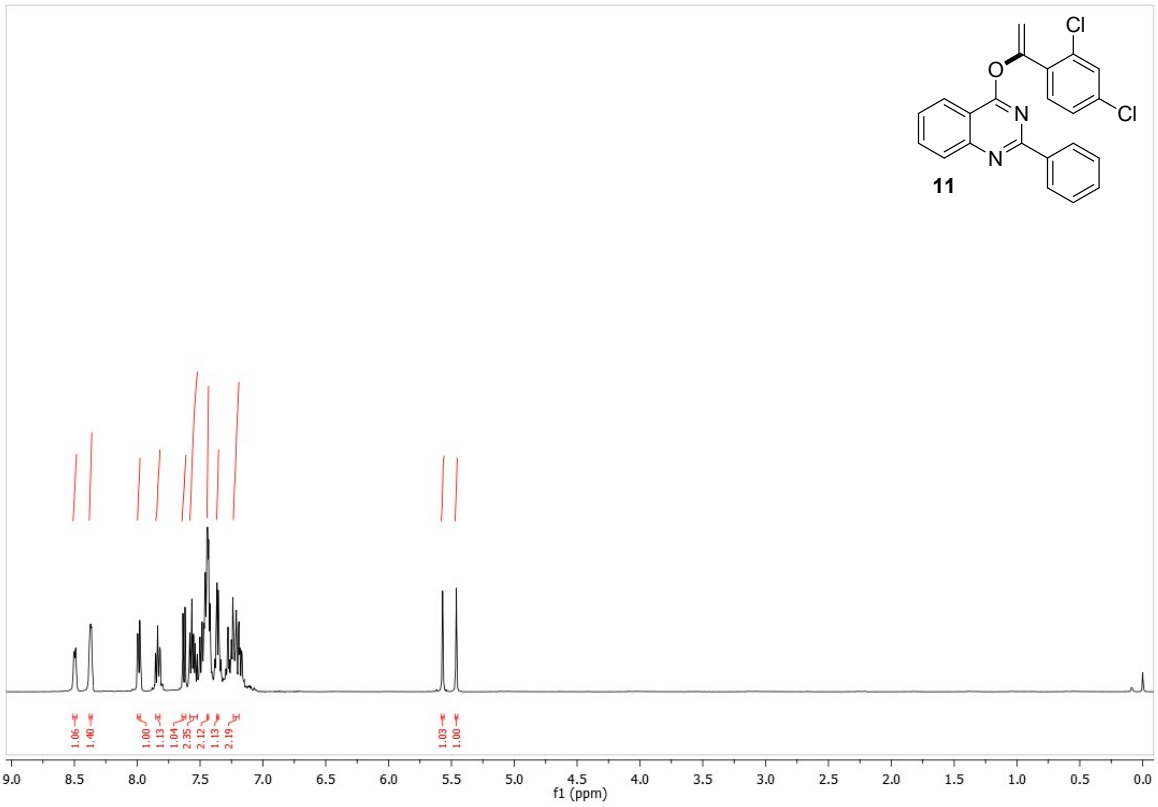

166.01
159.94
154.36
152.55
137.54
134.12
134.00
131.66
130.56
129.02
128.41
128.33
128.21
126.86
123.29
122.81
114.75
102.61
O
N
N
Br
8
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

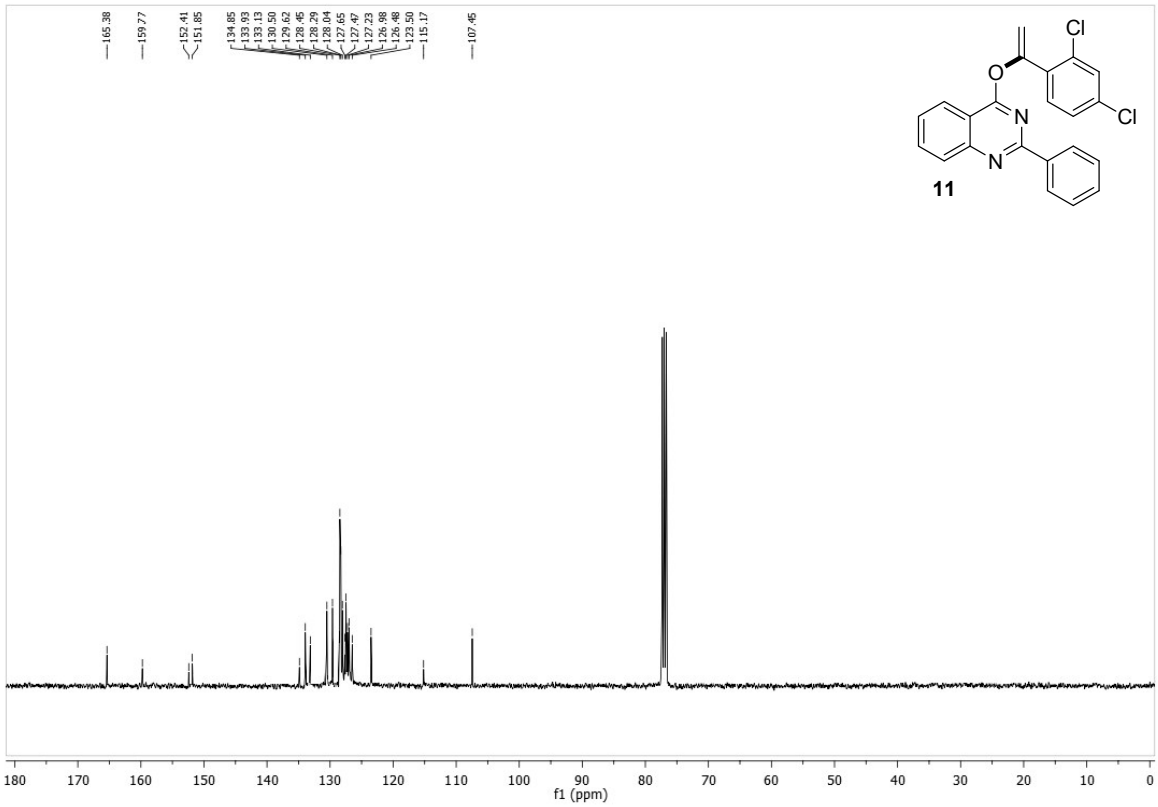

O
N
N
Ph
9
1.38
2.38
1.09
1.32
1.43
2.29
5.01
3.27
2.20
1.03
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

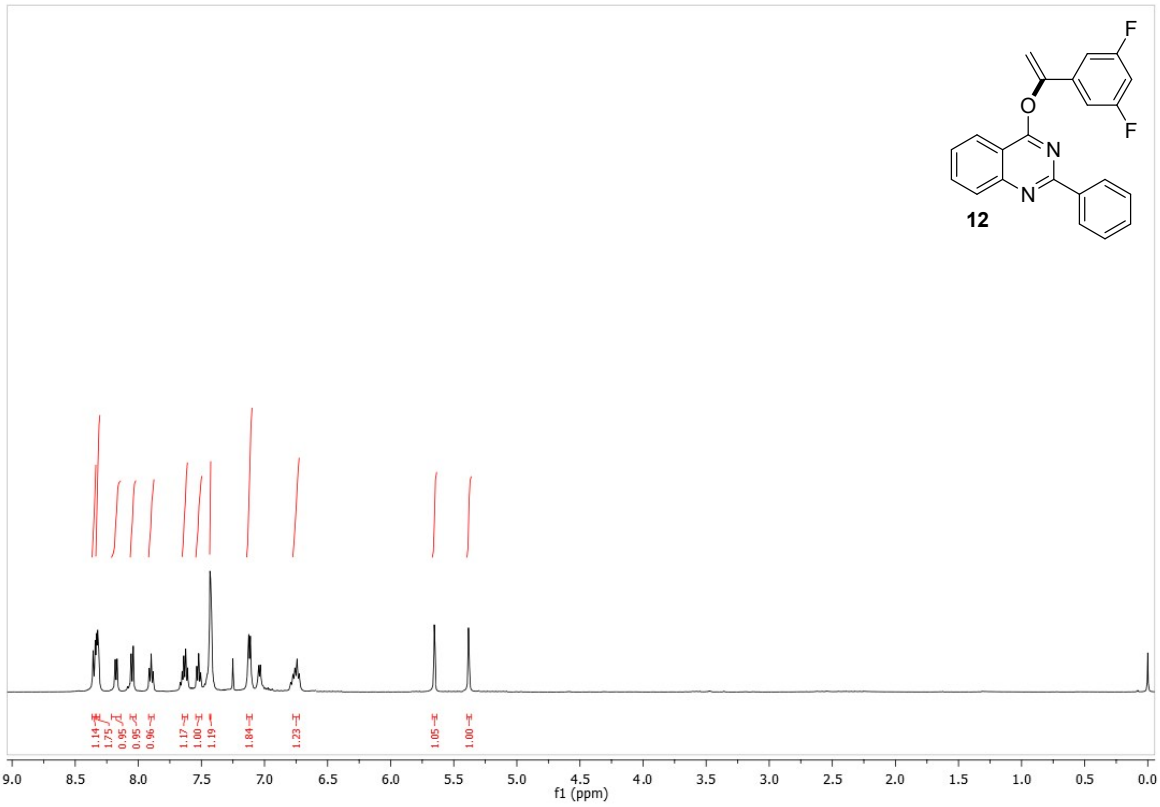

166.18
160.03
154.97
152.53
141.46
140.68
137.66
133.89
130.45
129.60
128.71
128.45
128.15
127.27
127.14
127.04
126.93
126.52
125.69
123.38
114.87
101.96
O
N
N
Ph
9
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

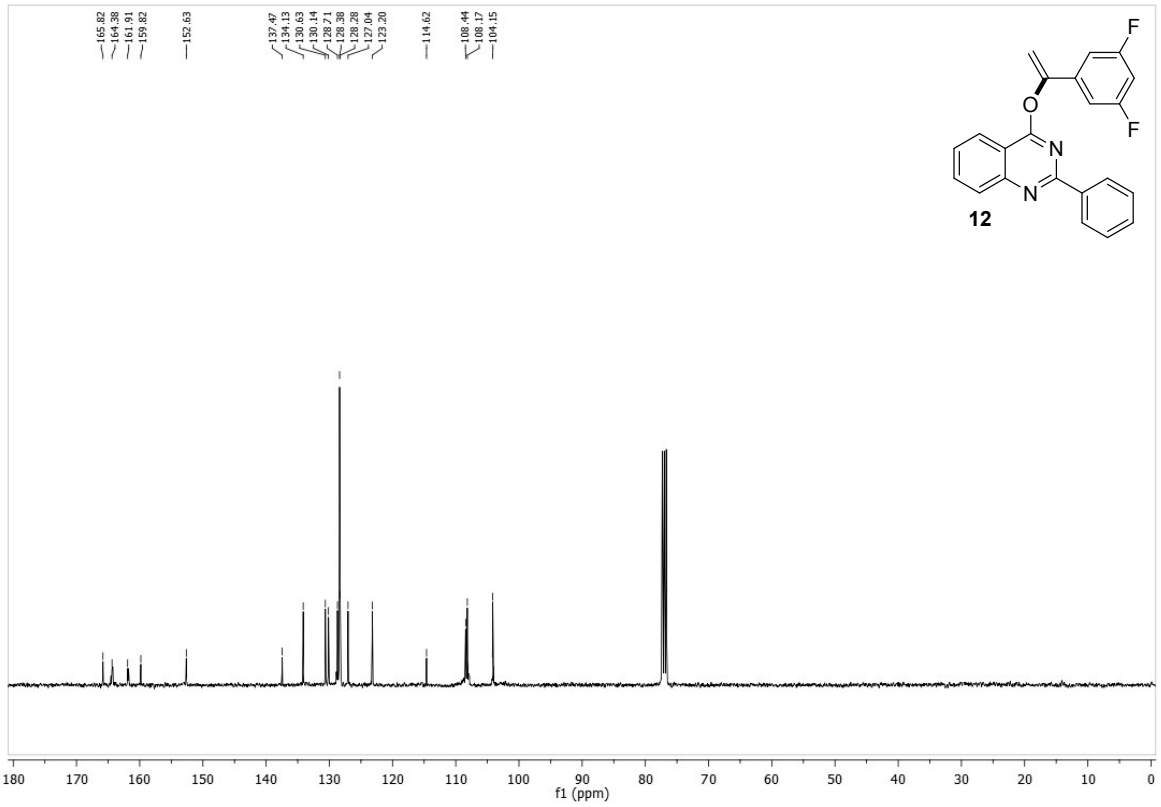

10
1.09
2.18
1.34
2.35
4.34
1.36
2.39
2.13
1.04
1.03
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

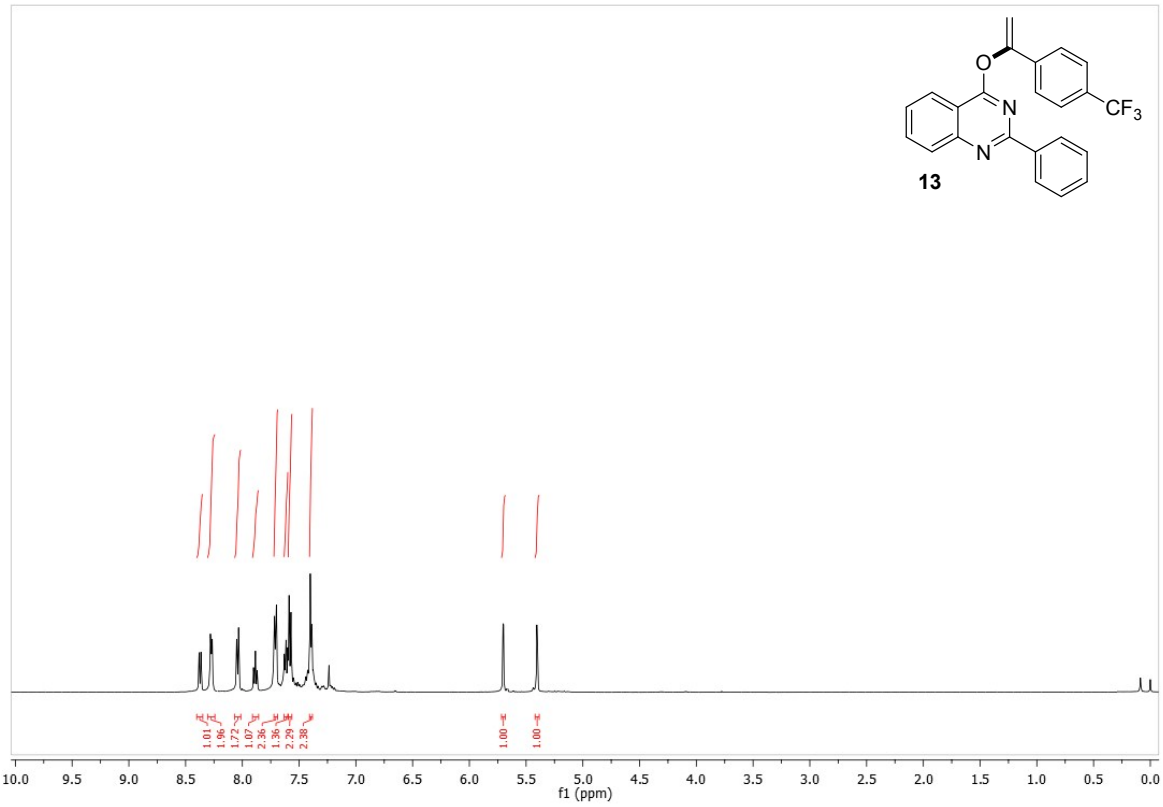

166.26
160.05
155.28
152.57
133.90
130.40
129.62
128.42
128.31
128.22
127.75
127.59
126.82
126.35
126.18
126.01
124.96
124.33
123.48
114.51
114.31
102.49
10
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

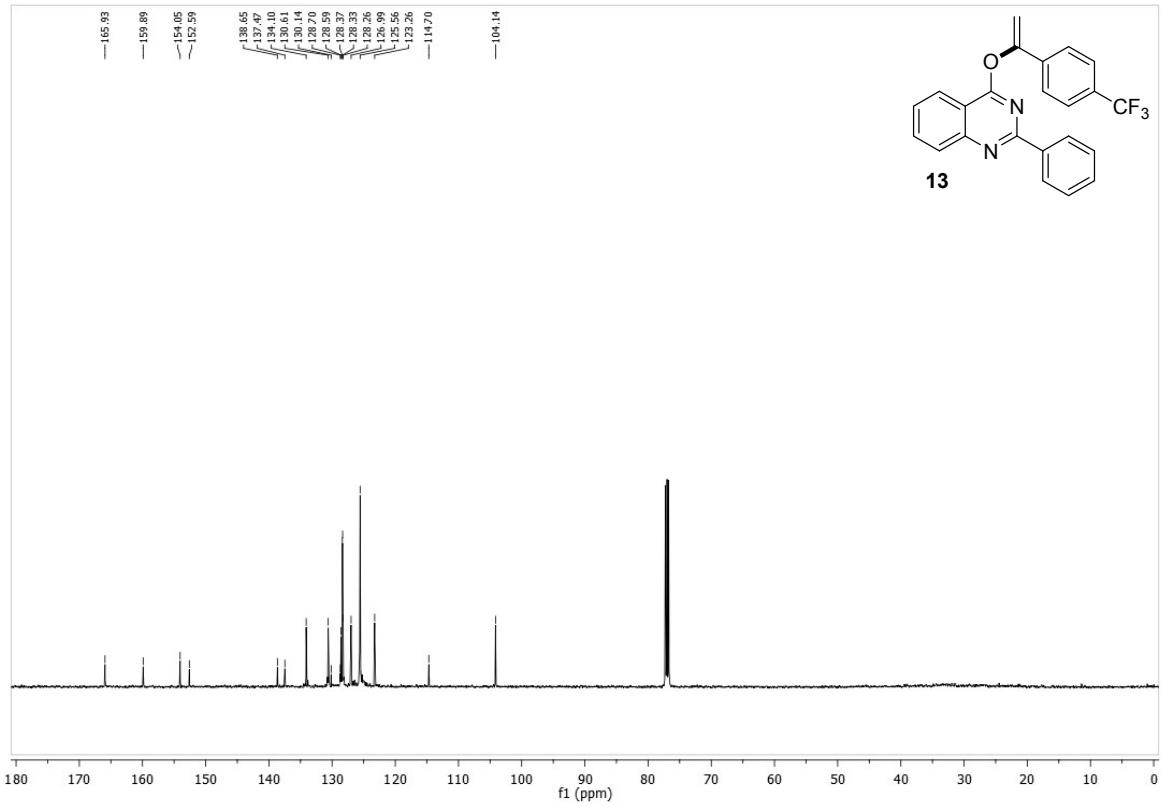

Cl
O
N
N
Cl
11
1.06
1.40
1.00
1.13
1.04
2.35
2.12
1.13
2.19
1.03
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

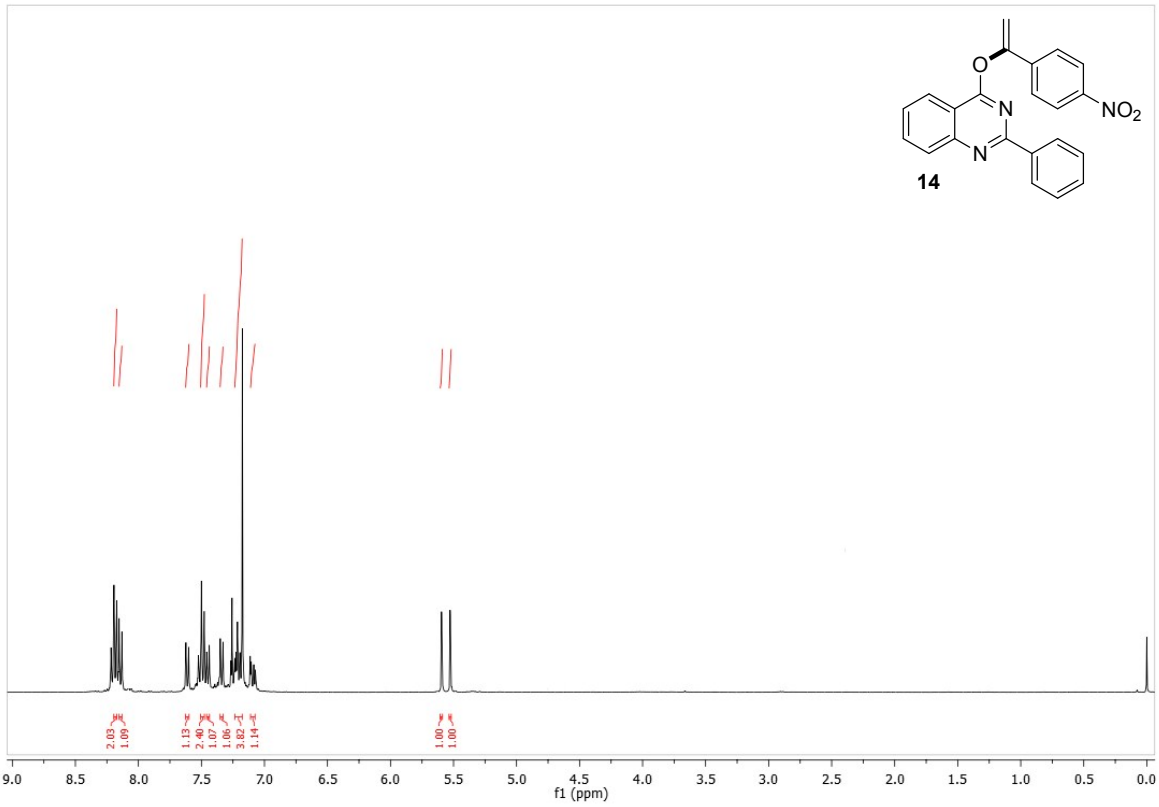

165.38
159.77
152.41
151.85
134.85
133.93
133.13
130.50
129.62
128.45
128.29
128.04
127.65
127.47
127.23
126.98
126.48
123.50
115.17
107.45
Cl
O
N
N
Cl
11
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

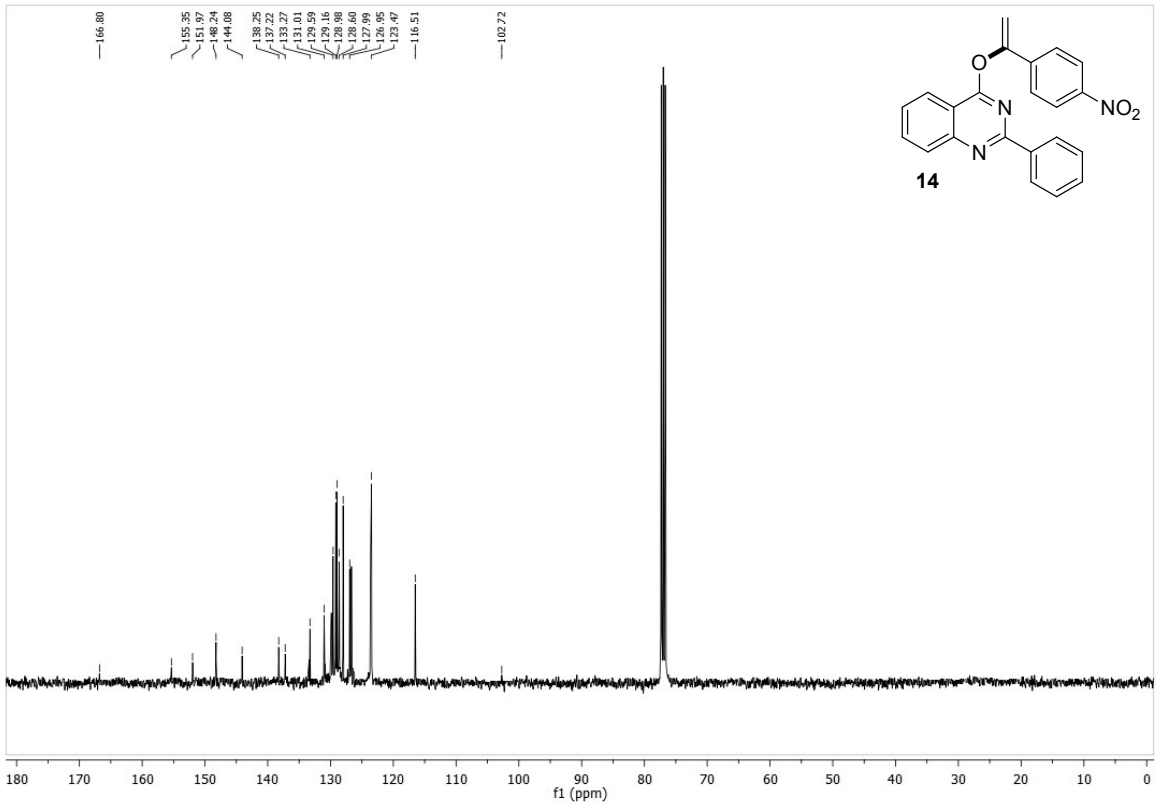

F
F
O
N
N
12
1.14
1.75
0.95
0.95
0.96
1.17
1.00
1.19
1.84
1.23
1.05
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

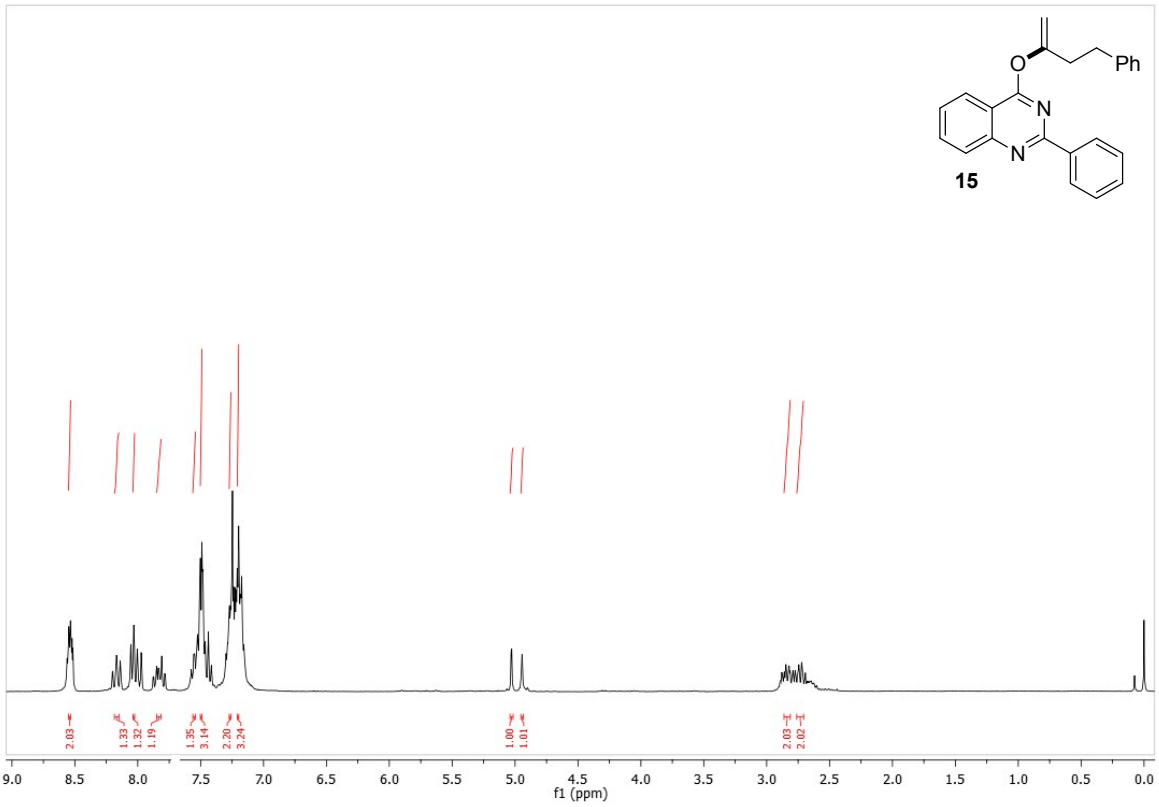

165.82
164.38
161.91
159.82
152.63
137.47
134.13
130.63
130.14
128.71
128.38
128.28
127.04
123.20
114.62
108.44
108.17
104.15
F
F
O
N
N
12
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

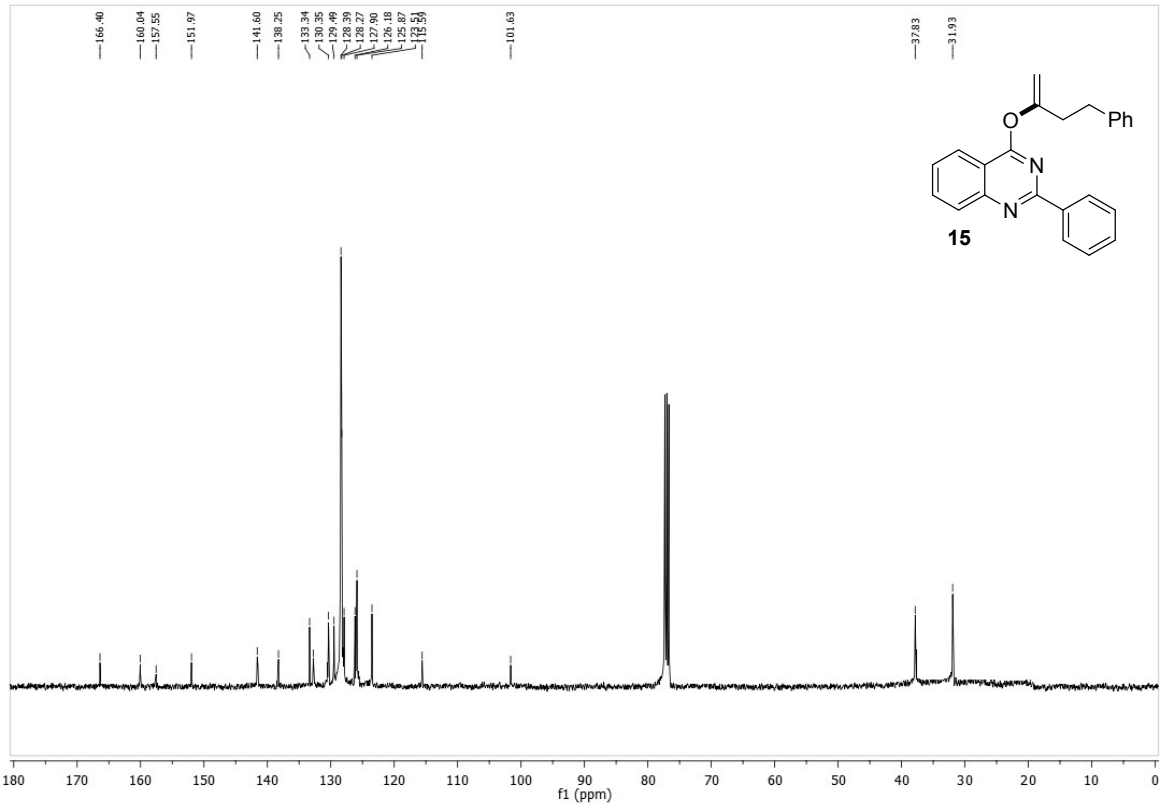

O
N
N
CF3
13
1.01
1.96
1.72
1.07
2.36
1.36
2.29
2.38
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

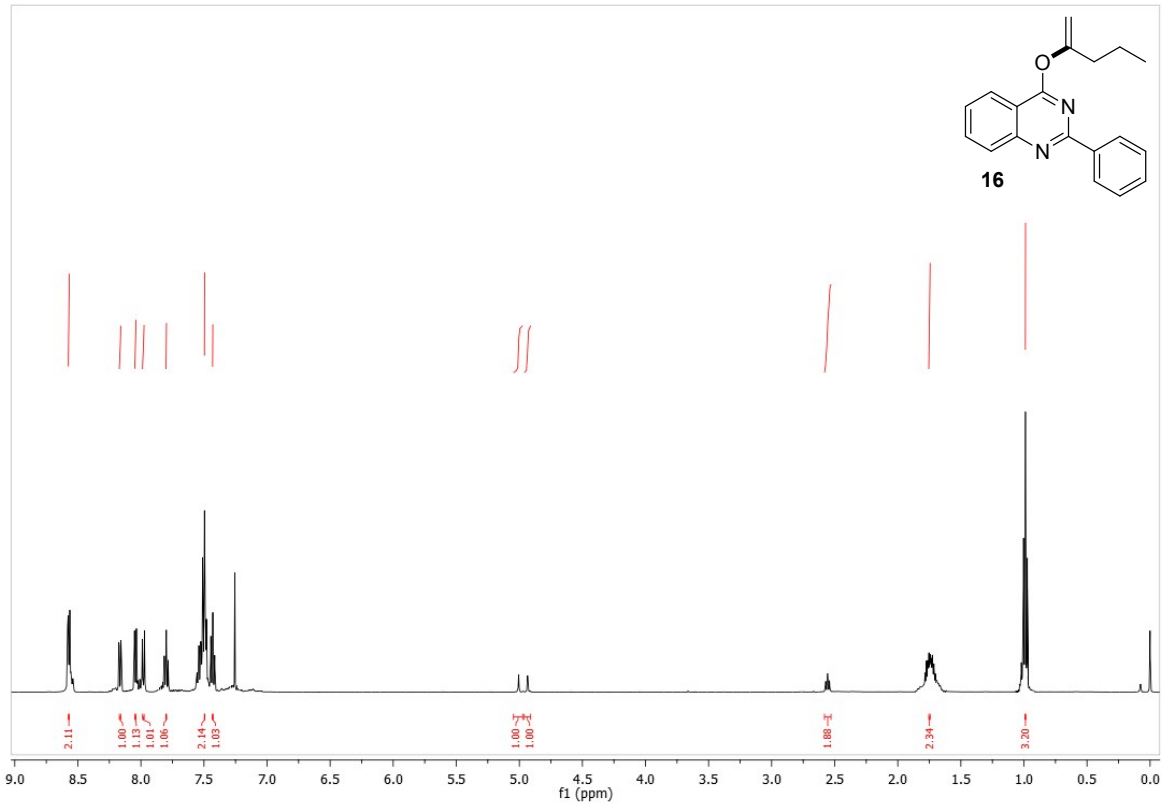

165.93
159.89
154.05
152.59
138.65
137.47
134.10
130.61
130.14
128.70
128.59
128.37
128.33
128.26
126.99
125.56
123.26
114.70
104.14
O
N
N
CF3
13
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

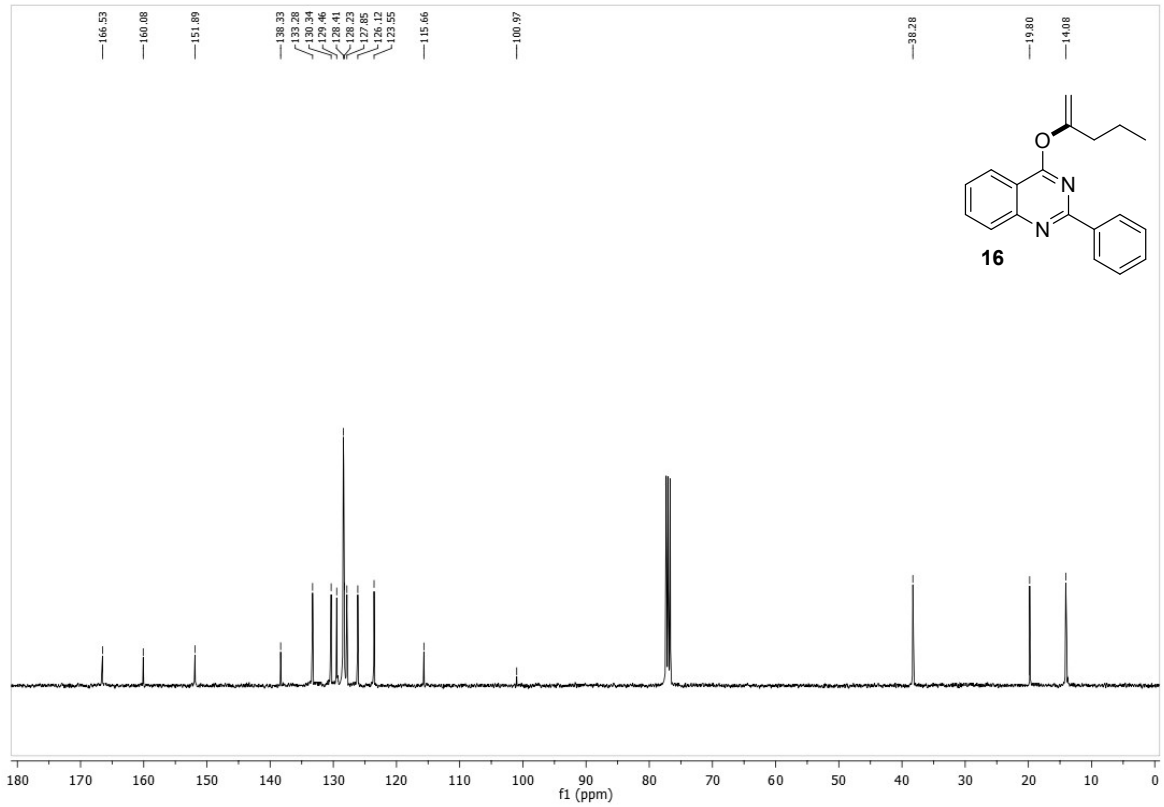

O
N
N
NO2
14
2.03
1.09
1.13
2.40
1.07
1.06
3.82
1.14
1.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

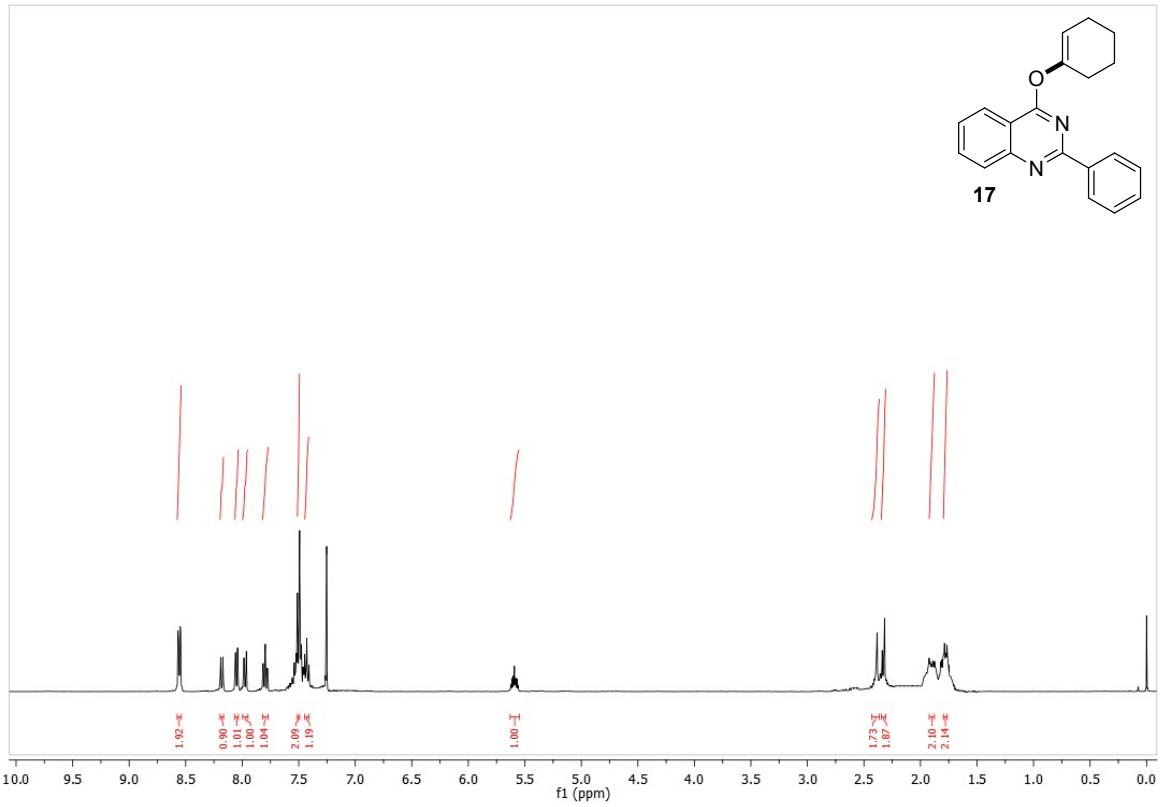

166.80
155.35
151.97
148.24
144.08
138.25
137.22
133.27
131.01
129.59
129.16
128.98
128.60
127.99
126.95
123.47
116.51
102.72
O
N
N
NO2
14
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

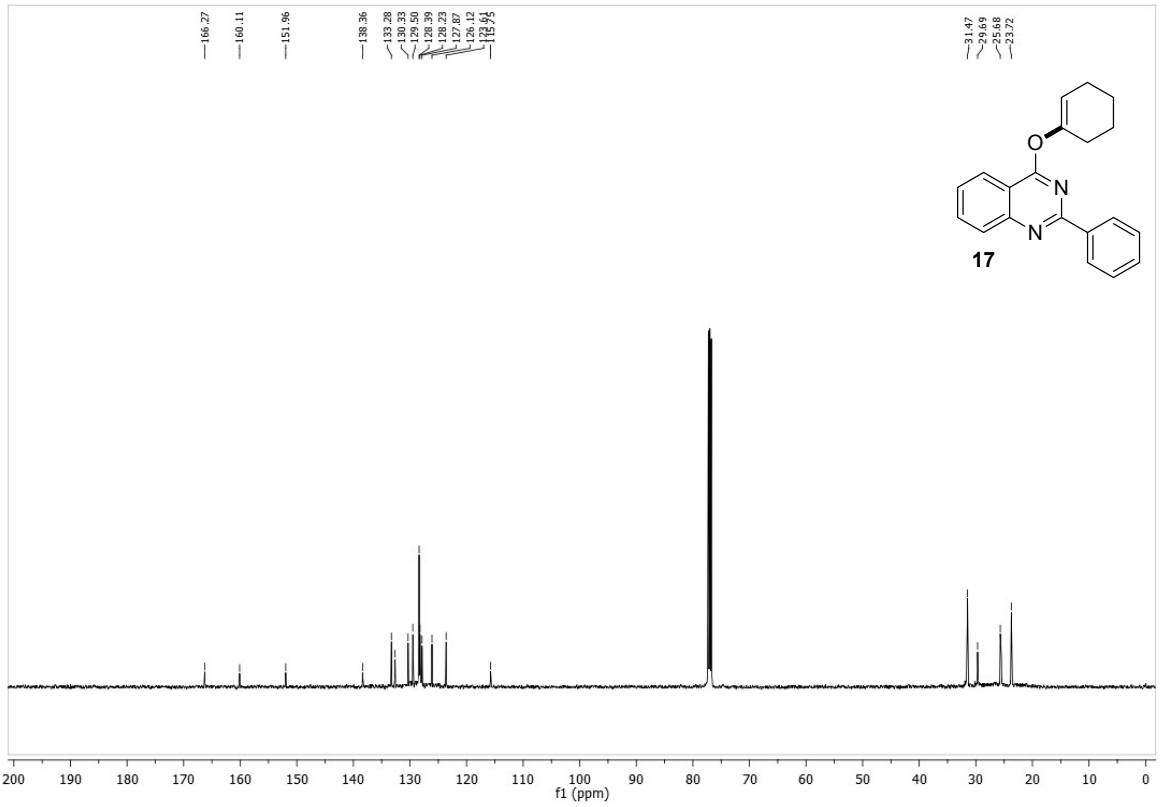

O
Ph
N
N
15
2.03
1.33
1.32
1.19
1.35
3.14
2.20
3.24
1.00
1.01
2.03
2.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

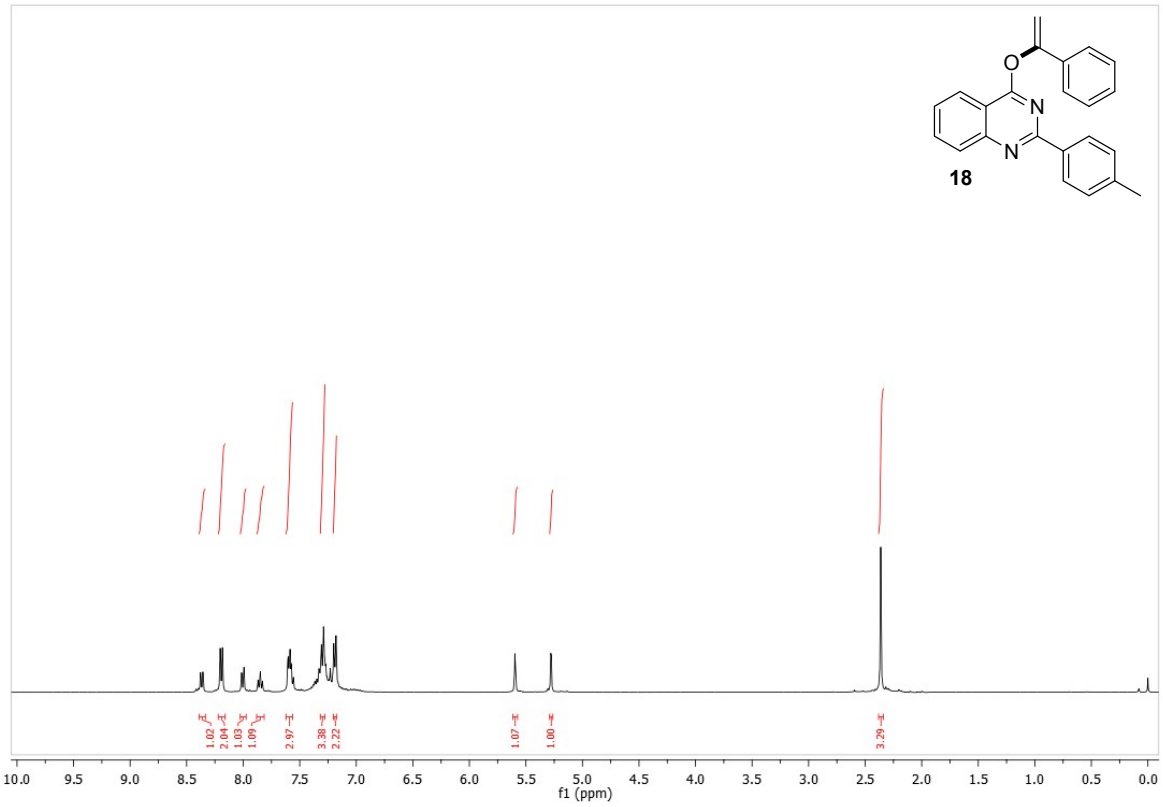

166.40
160.04
157.55
151.97
141.60
138.25
133.34
130.35
129.49
128.39
128.27
127.90
126.18
125.87
123.51
115.59
101.63
37.83
31.93
O
Ph
N
N
15
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

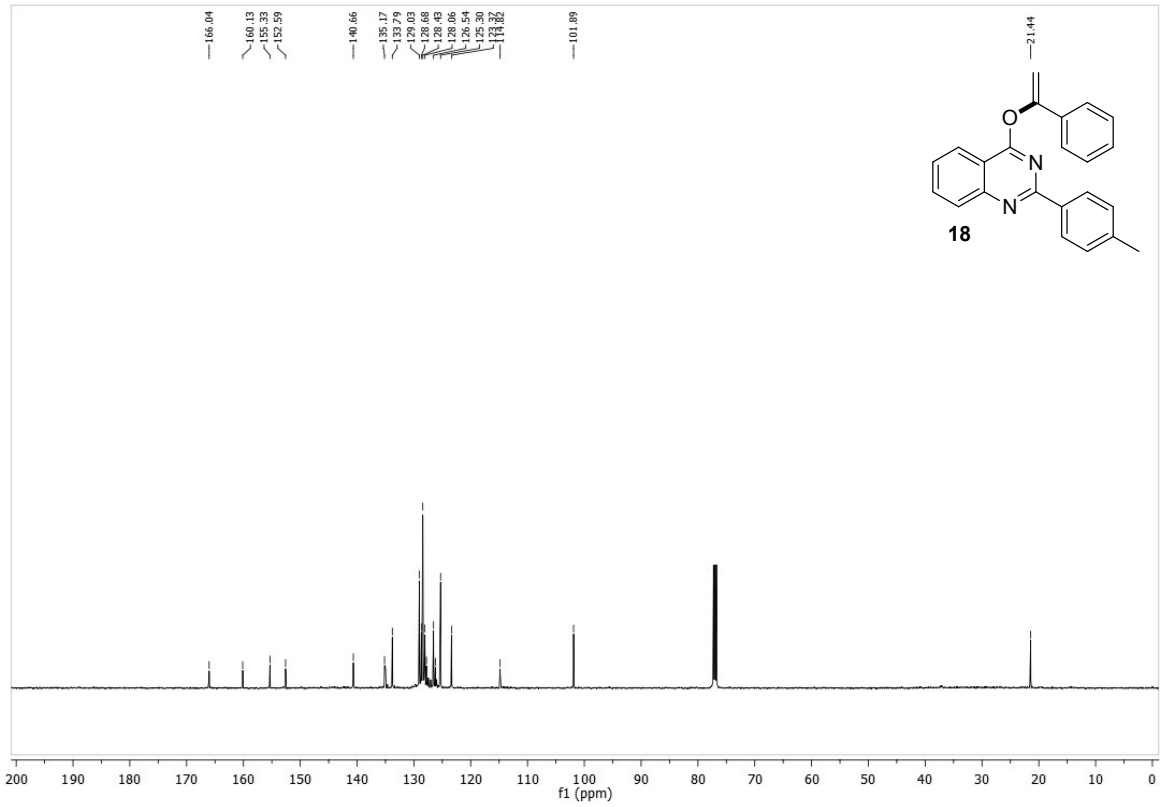

16
2.11
1.00
1.13
1.01
1.06
2.14
1.03
1.00
1.00
1.88
2.34
3.20
f1 (ppm)

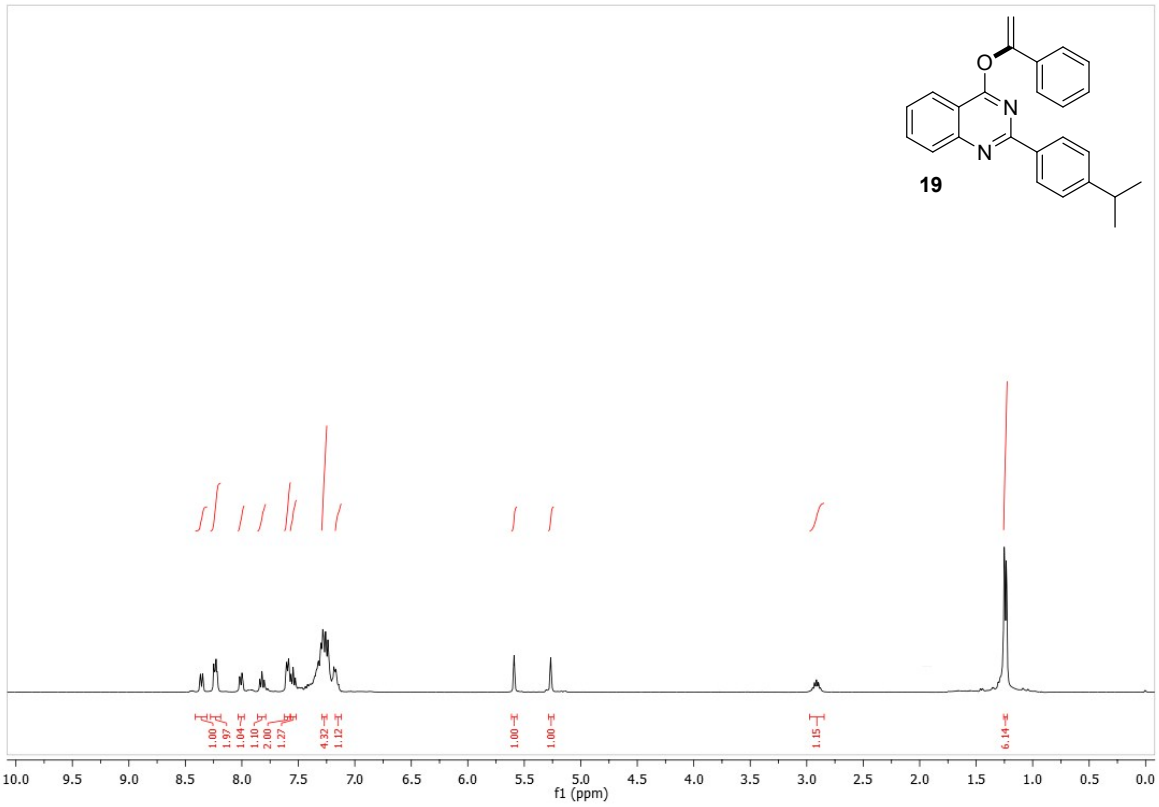

166.53
160.08
151.89
138.33
133.28
130.34
129.46
128.41
128.23
127.05
126.12
123.55
115.66
100.97
38.28
19.80
14.08
16
f1 (ppm)

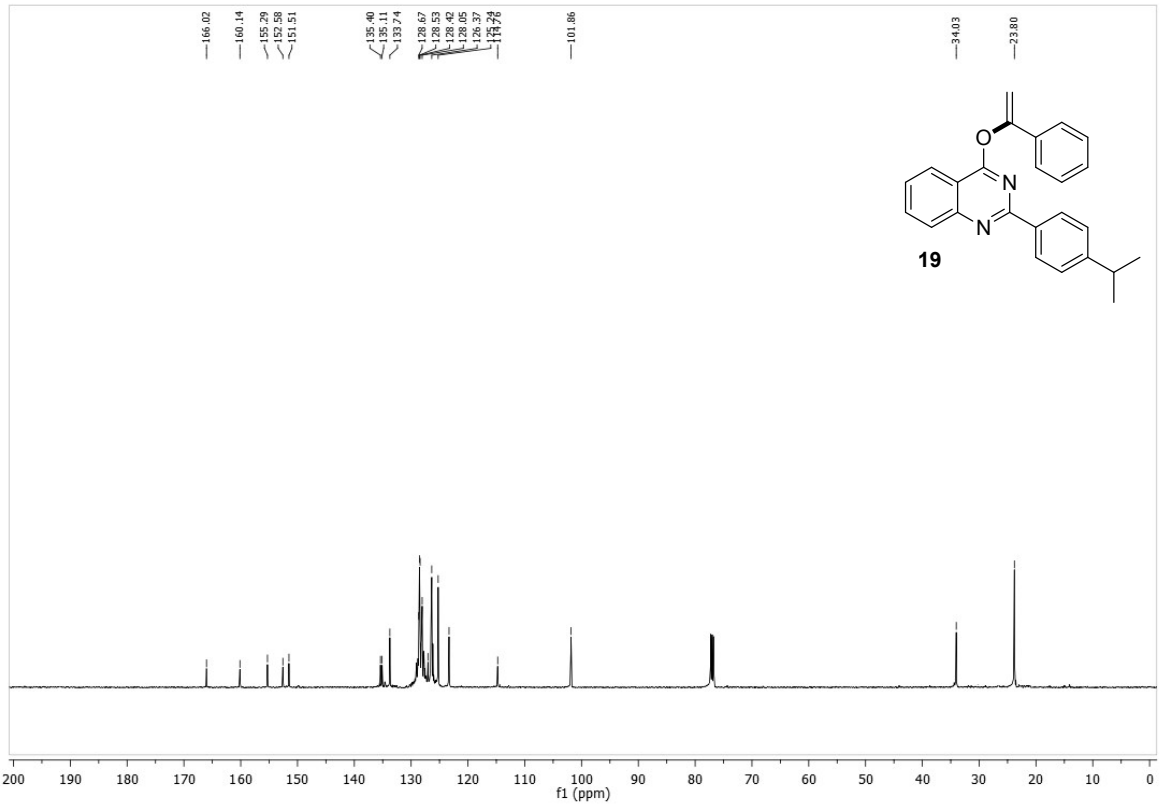

17
1.92
0.90
1.01
1.00
1.04
2.09
1.19
1.00
1.73
1.87
2.10
2.14
f1 (ppm)

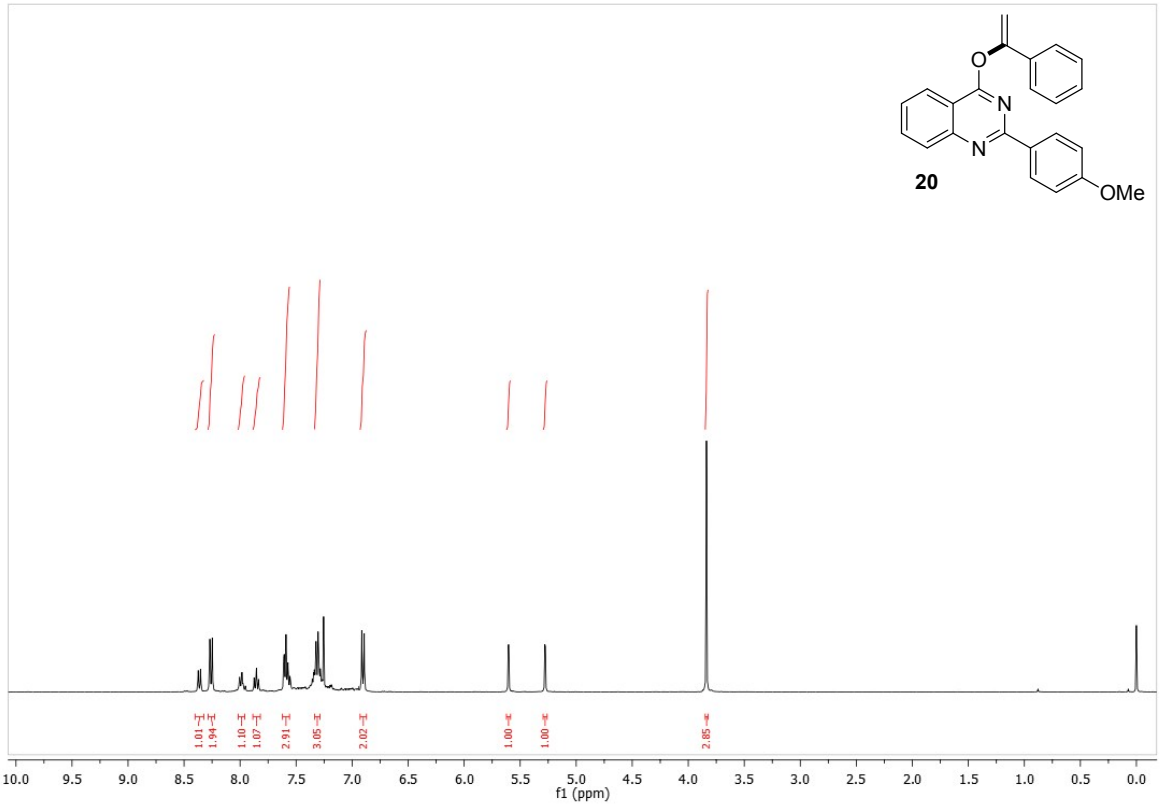

166.27
160.11
151.96
138.36
133.28
130.33
129.50
128.39
128.23
127.87
126.12
123.61
115.75
31.47
29.69
25.68
23.72
17
f1 (ppm)

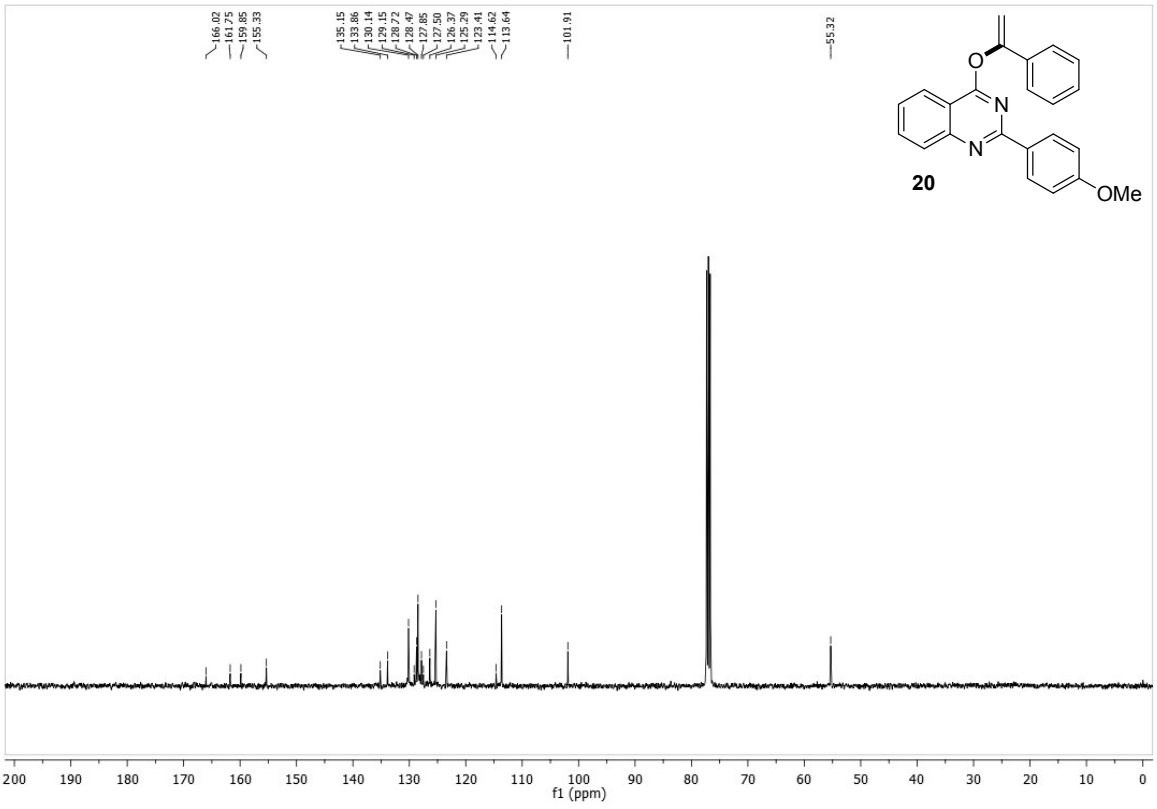

18
1.02
2.04
1.03
1.09
2.97
3.38
2.22
1.07
1.00
3.29
f1 (ppm)

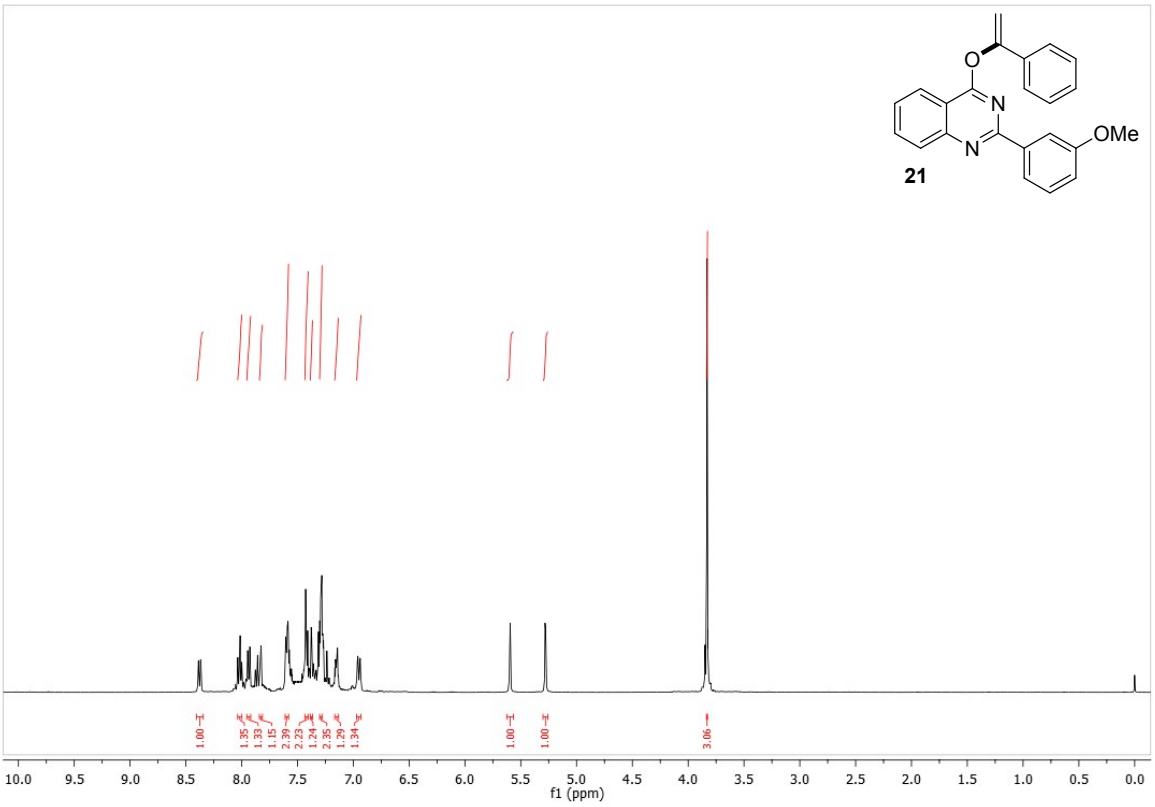

166.04
160.13
155.33
152.59
140.66
135.17
133.79
129.03
128.68
128.43
128.06
126.54
125.30
101.89
21.44
18
f1 (ppm)

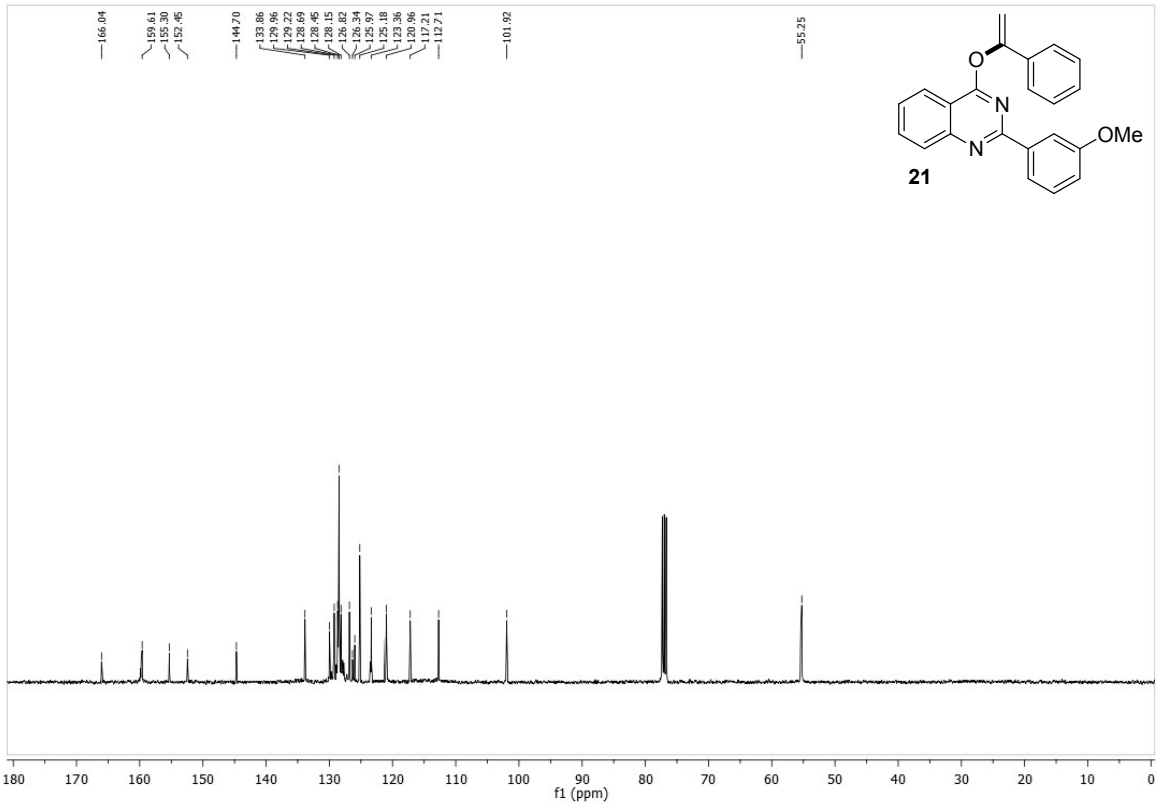

19
1.00
1.97
1.04
1.10
2.00
1.27
4.32
1.12
1.00
1.00
1.15
6.14
f1 (ppm)

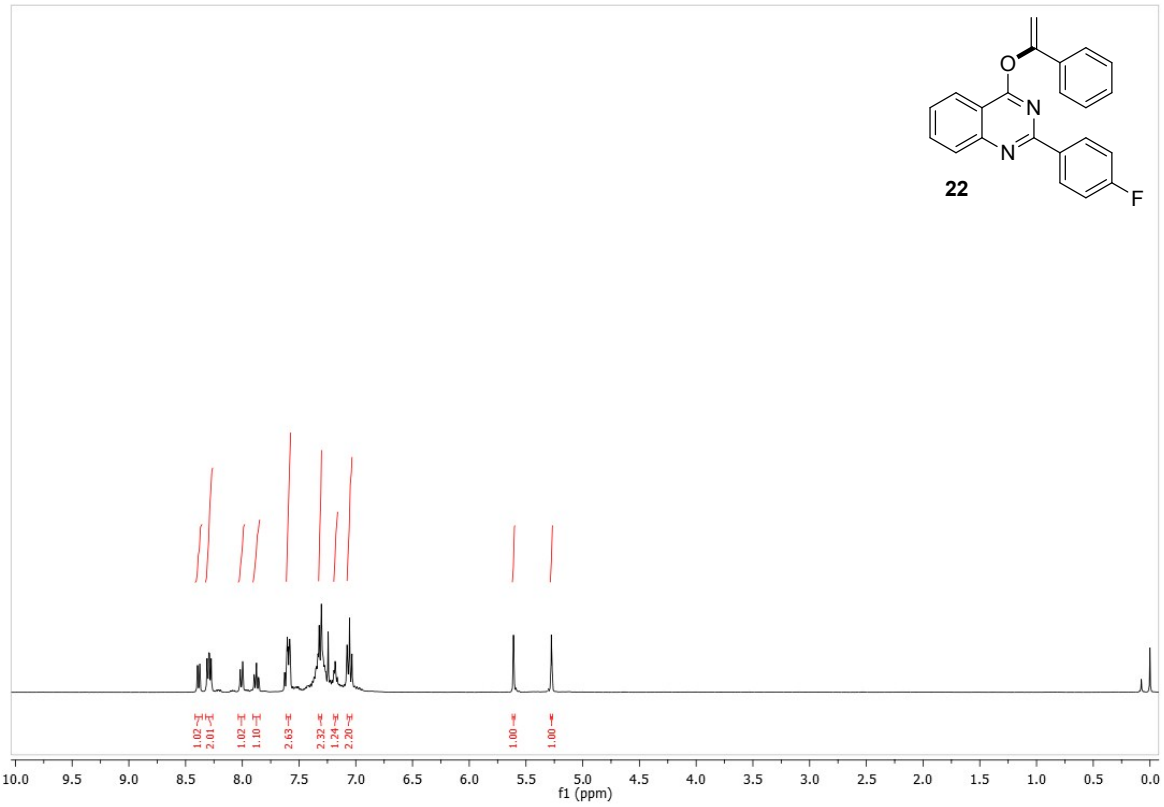

166.02
160.14
155.29
152.58
151.51
135.40
135.11
133.74
128.67
128.53
128.42
128.05
126.37
101.86
34.03
23.80
19
f1 (ppm)

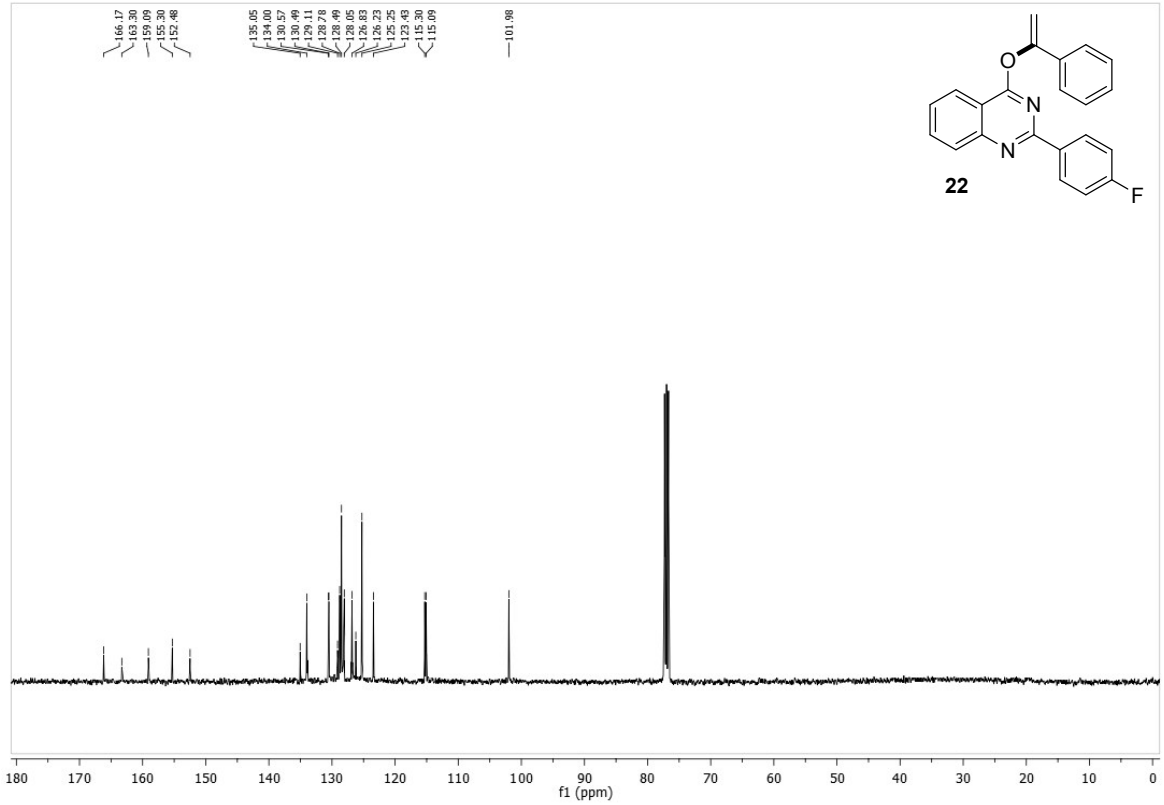

20
OMe
1.01
1.94
1.10
1.07
2.91
3.05
2.02
1.00
1.00
2.85
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.02
161.75
159.85
155.33
135.15
133.86
130.14
129.15
128.72
128.47
127.85
127.50
126.37
125.29
123.41
114.62
113.64
101.91
55.32
20
OMe
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N
N
OMe
21
1.00
1.35
1.33
1.15
2.39
2.23
1.24
2.35
1.29
1.34
1.00
1.00
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.04
159.61
155.30
152.45
144.70
133.86
129.96
129.22
128.69
128.45
128.15
126.82
126.34
125.97
125.18
123.36
120.96
117.21
112.71
101.92
55.25
O
N
N
OMe
21
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


22
1.02
2.01
1.02
1.10
2.63
2.32
1.24
2.20
1.00
1.00
f1 (ppm)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159.09
155.30
152.48
135.05
134.00
130.57
130.49
129.11
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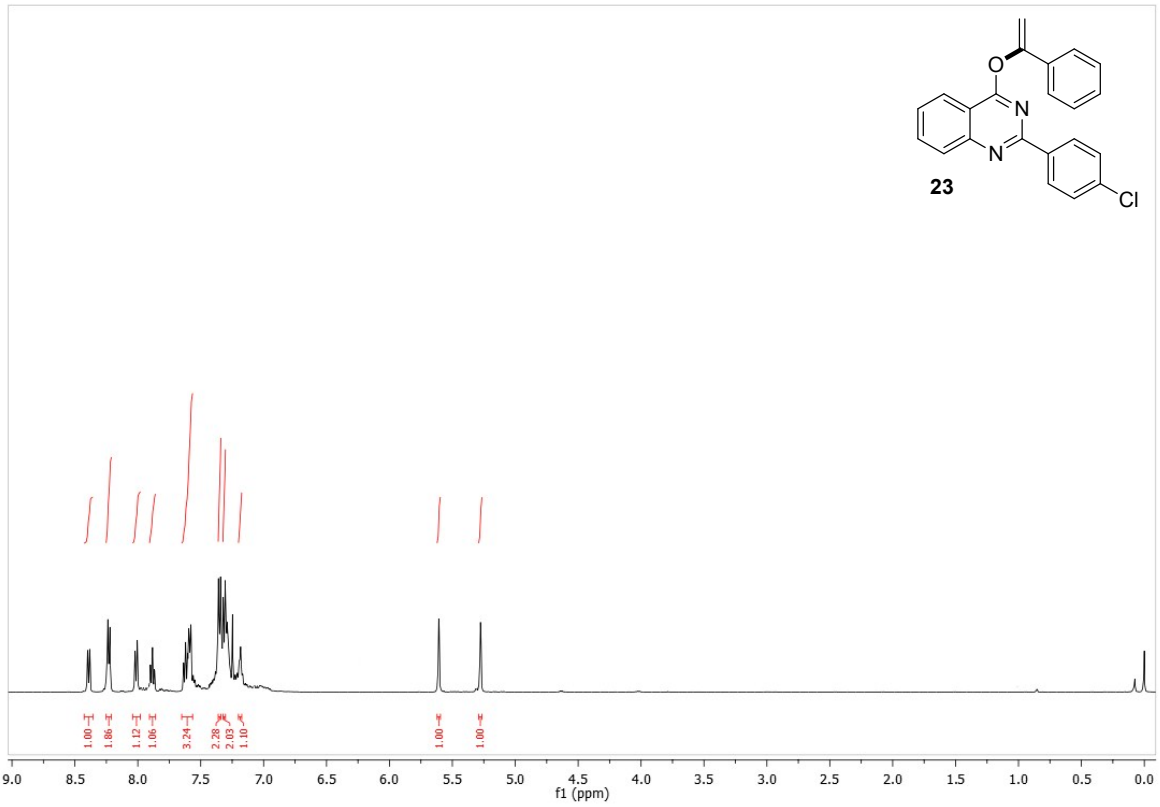
126.83
126.23
125.25
123.43
115.30
115.09
101.98
22
f1 (ppm)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N
Cl
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1.86
1.12
1.06
3.24
2.28
2.03
1.10
1.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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3.5
3.0
2.5
2.0
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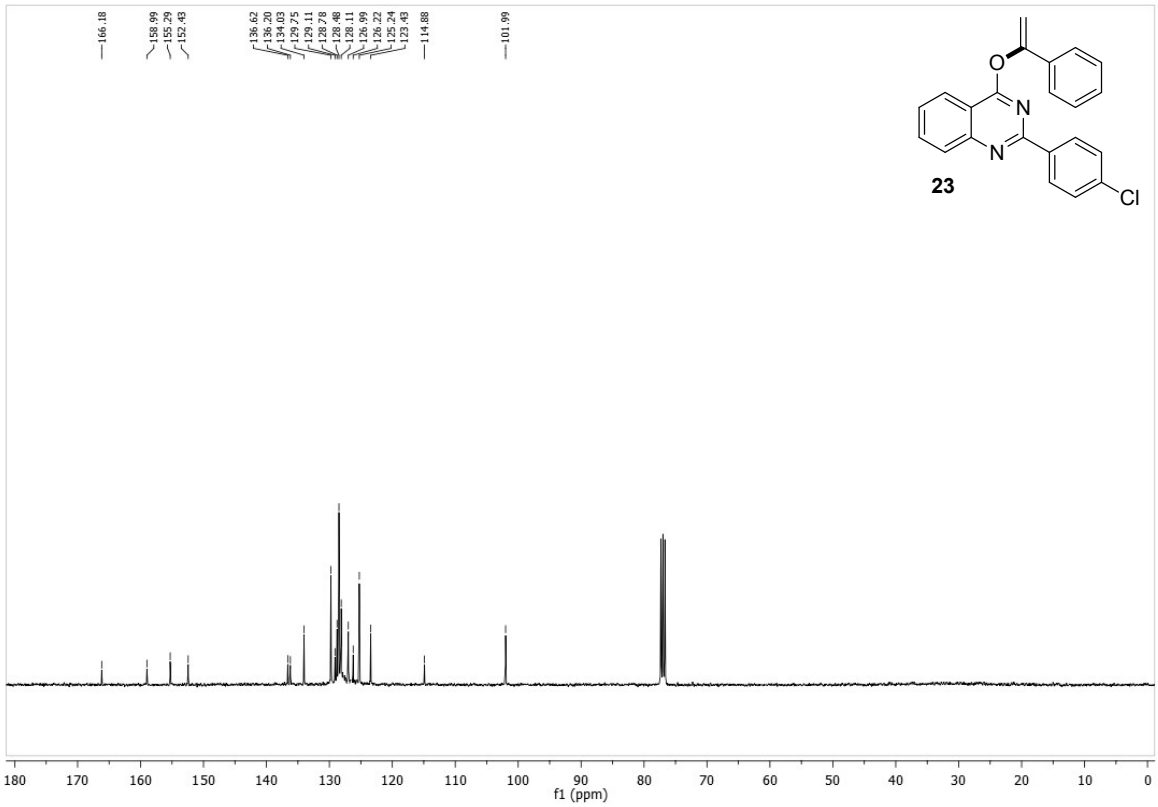
1.0
0.5
0.0
f1 (ppm)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136.20
134.03
129.75
129.11
128.78
128.48
128.11
126.99
126.22
125.24
123.43
114.88
101.99
O
N
N
Cl
23
180
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130
120
110
100
90
80
70
60
50
40
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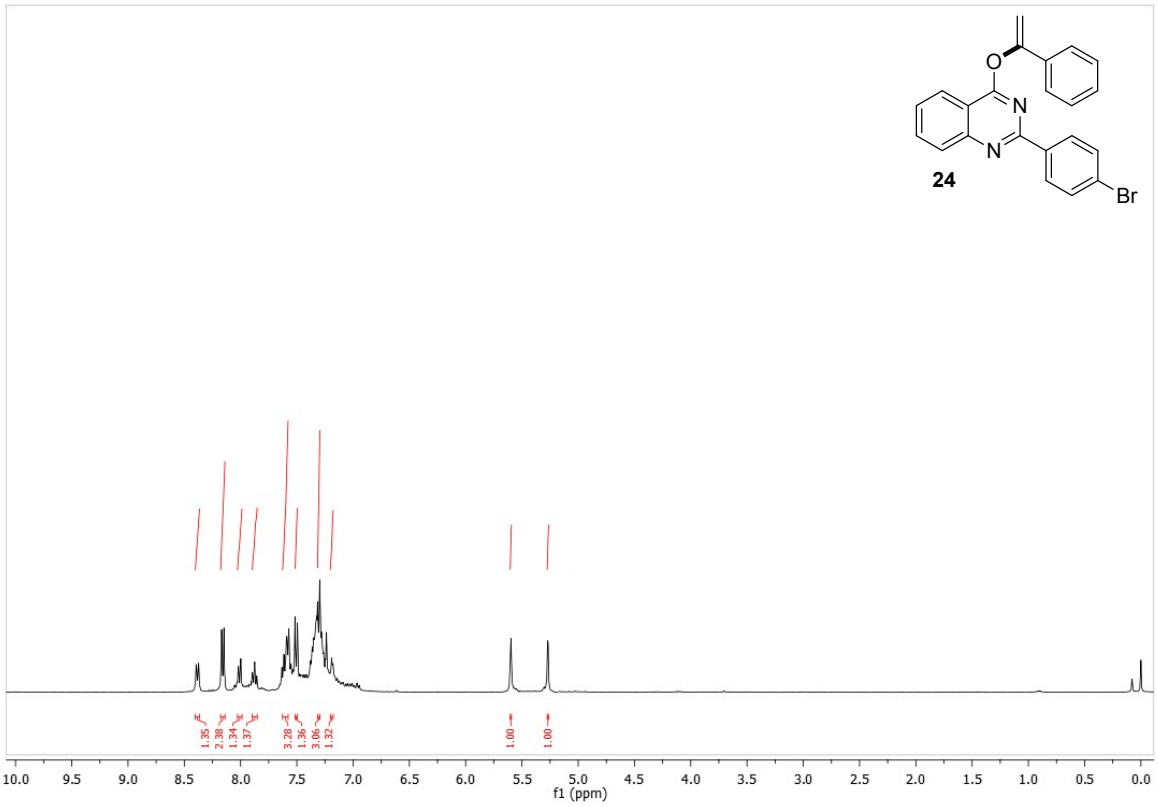
20
10
0
f1 (ppm)


24
Br
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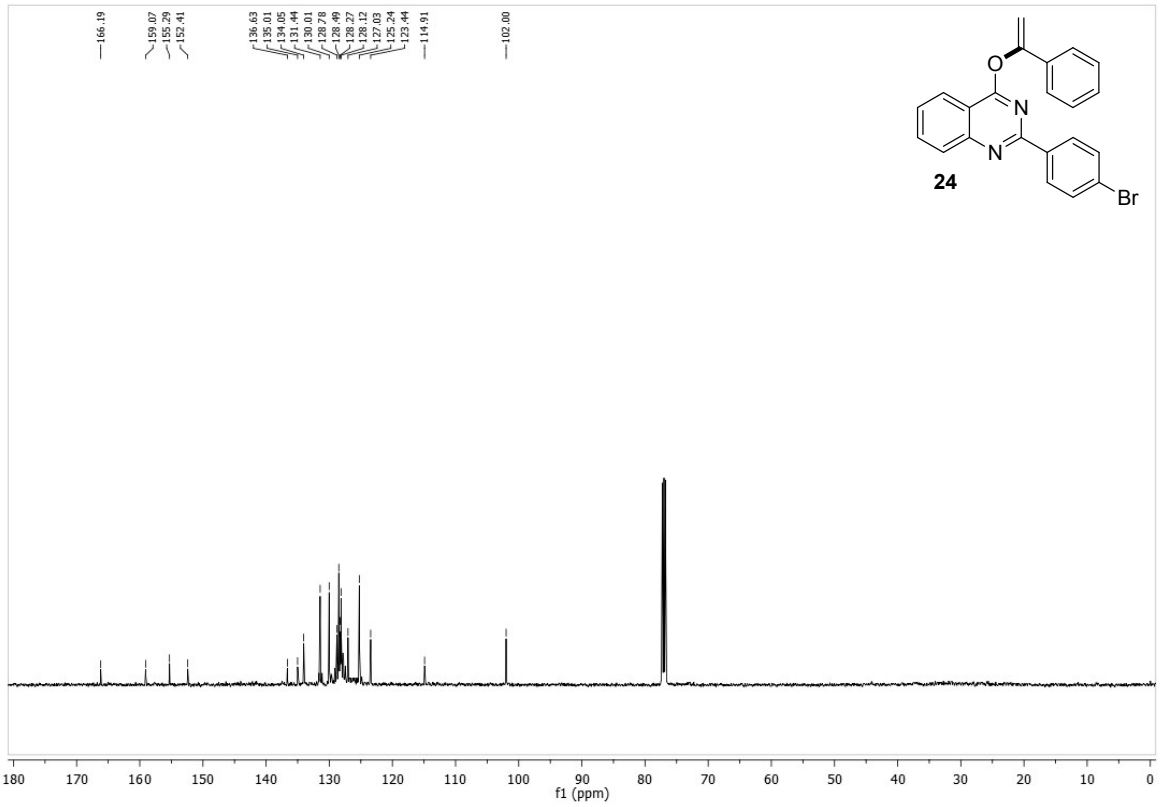
2.38
1.34
1.37
3.28
1.36
3.06
1.32
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.01
134.05
131.44
130.01
128.78
128.49
128.27
128.12
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123.44
114.91
102.00
24
Br
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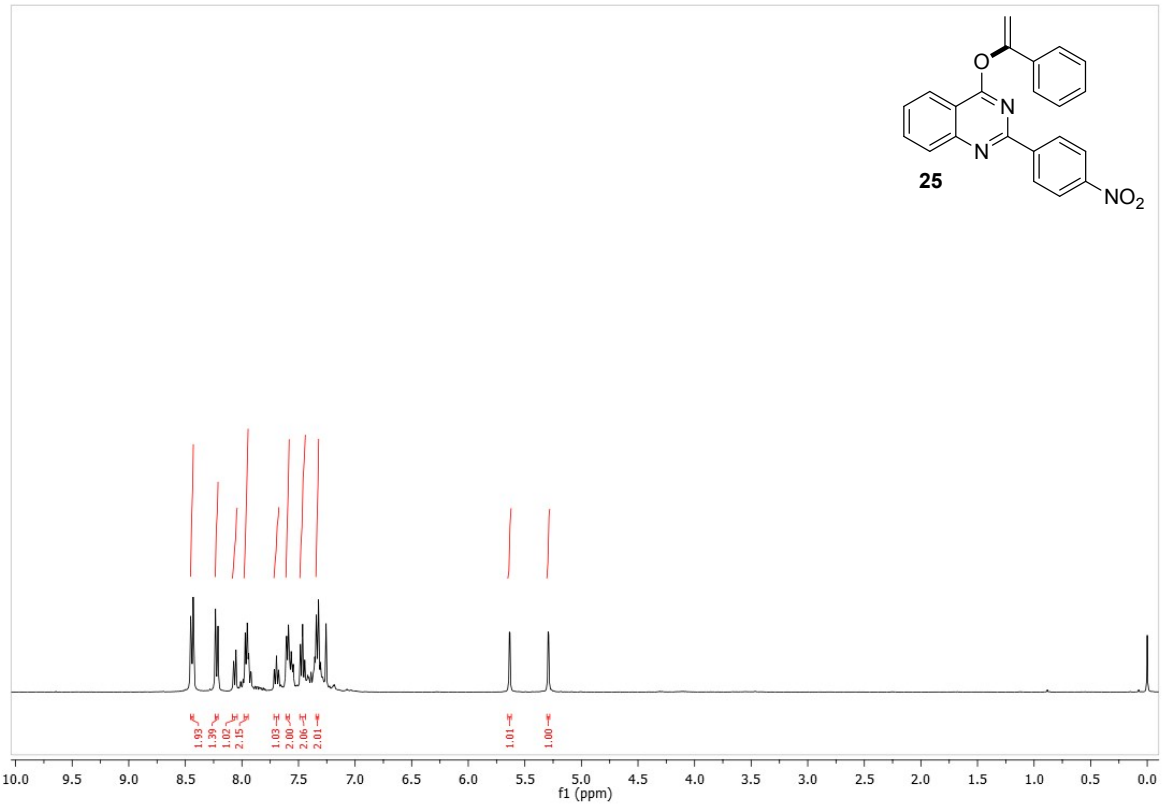
f1 (ppm)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N
N
NO2
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1.39
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2.15
1.03
2.00
2.06
2.01
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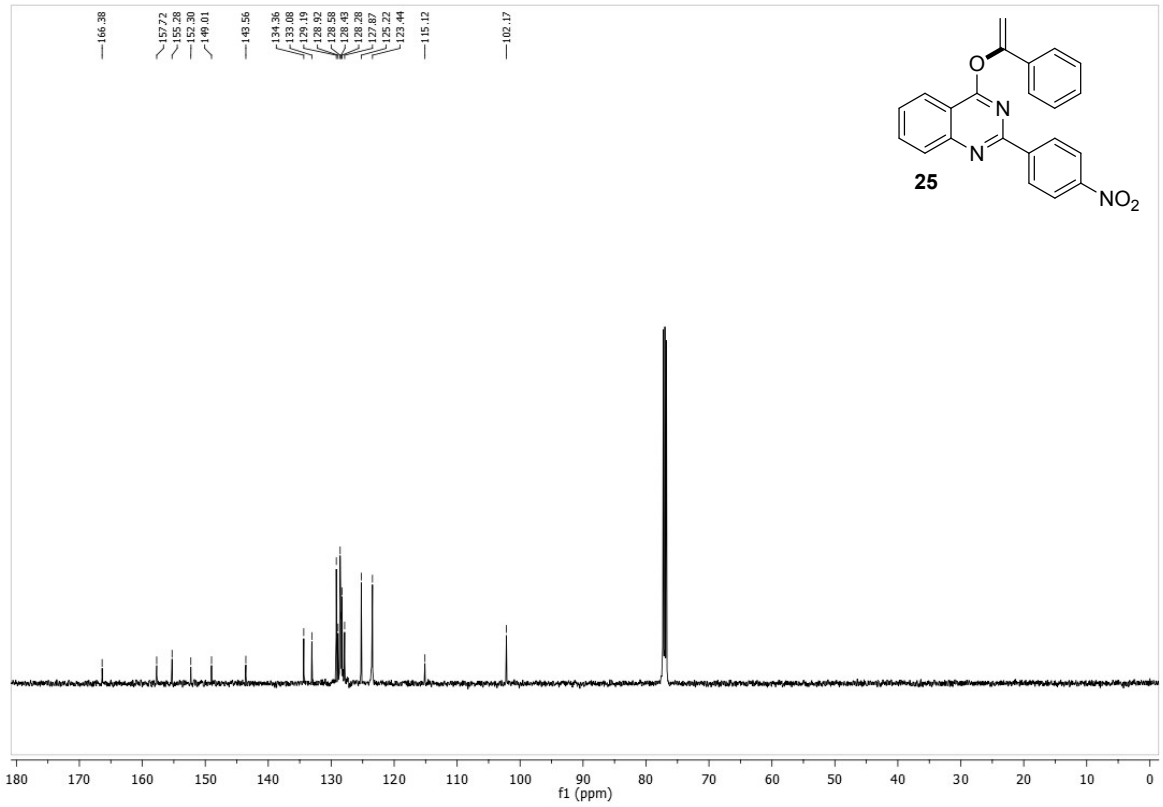
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.08
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128.58
128.43
128.28
127.87
125.22
123.44
115.12
102.17
O
N
N
NO2
25
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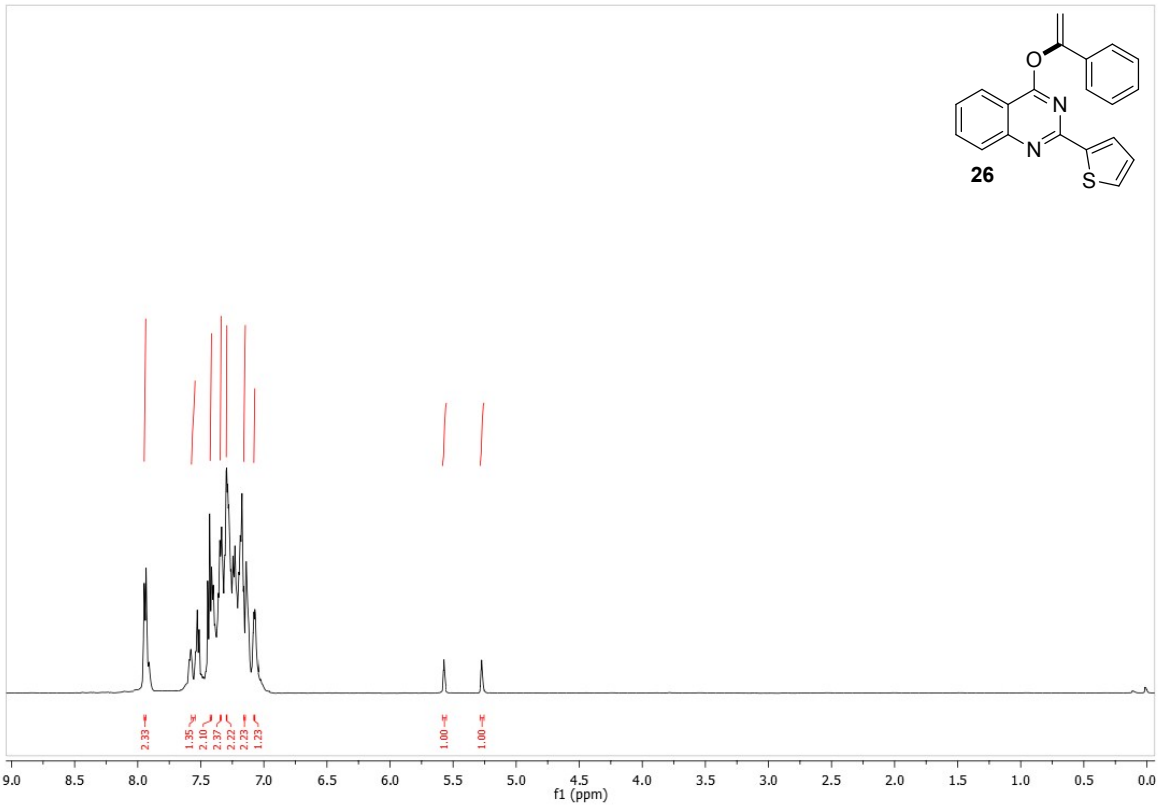
f1 (ppm)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N
N
S
26
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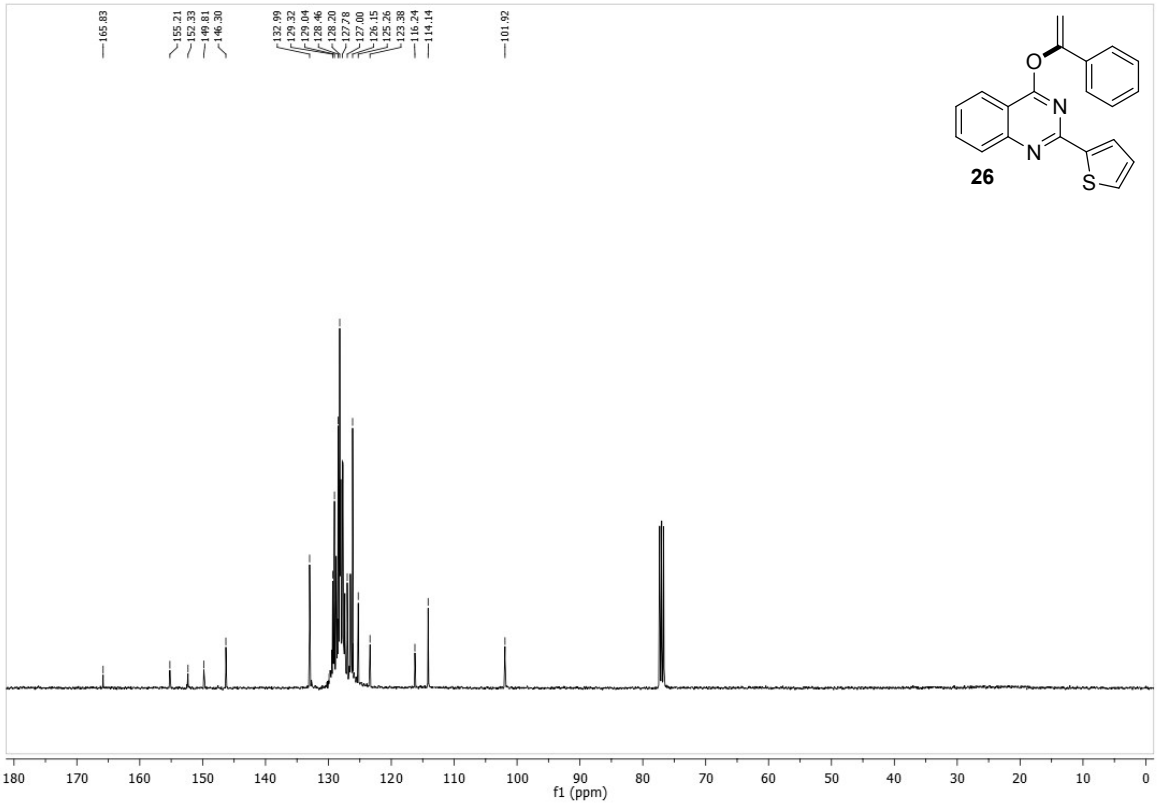
1.35
2.10
2.37
2.22
2.23
1.23
1.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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146.30
132.99
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129.04
128.46
128.20
127.78
127.08
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125.76
123.38
116.24
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101.92
O
N
N
S
26
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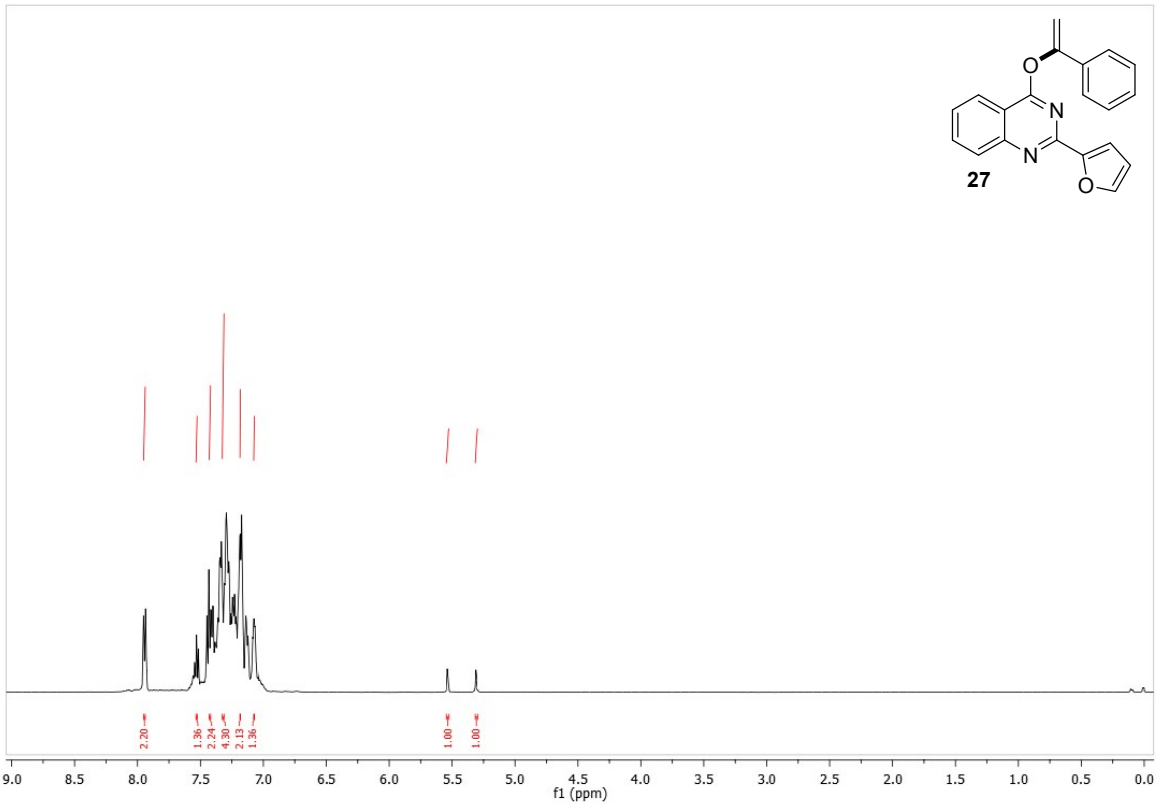
f1 (ppm)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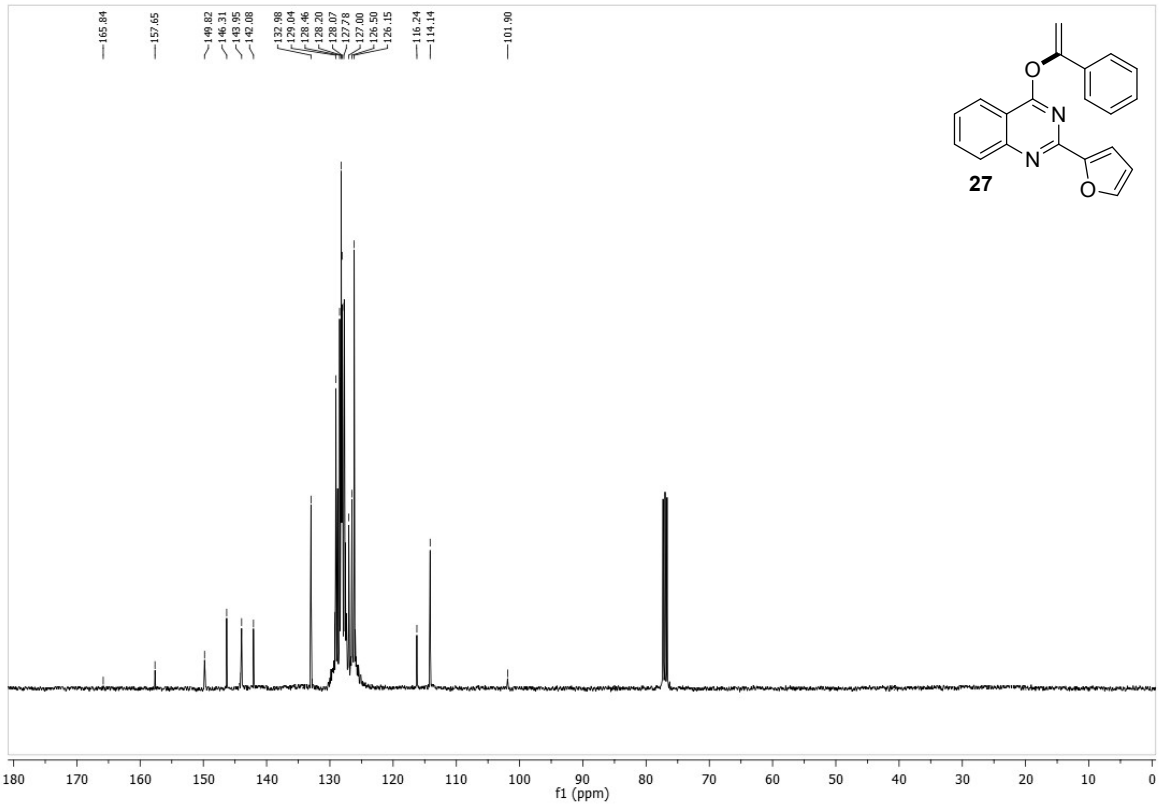
2.20
1.36
2.24
4.30
2.13
1.36
1.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.07
127.78
127.00
126.50
126.15
116.24
114.14
101.90
27
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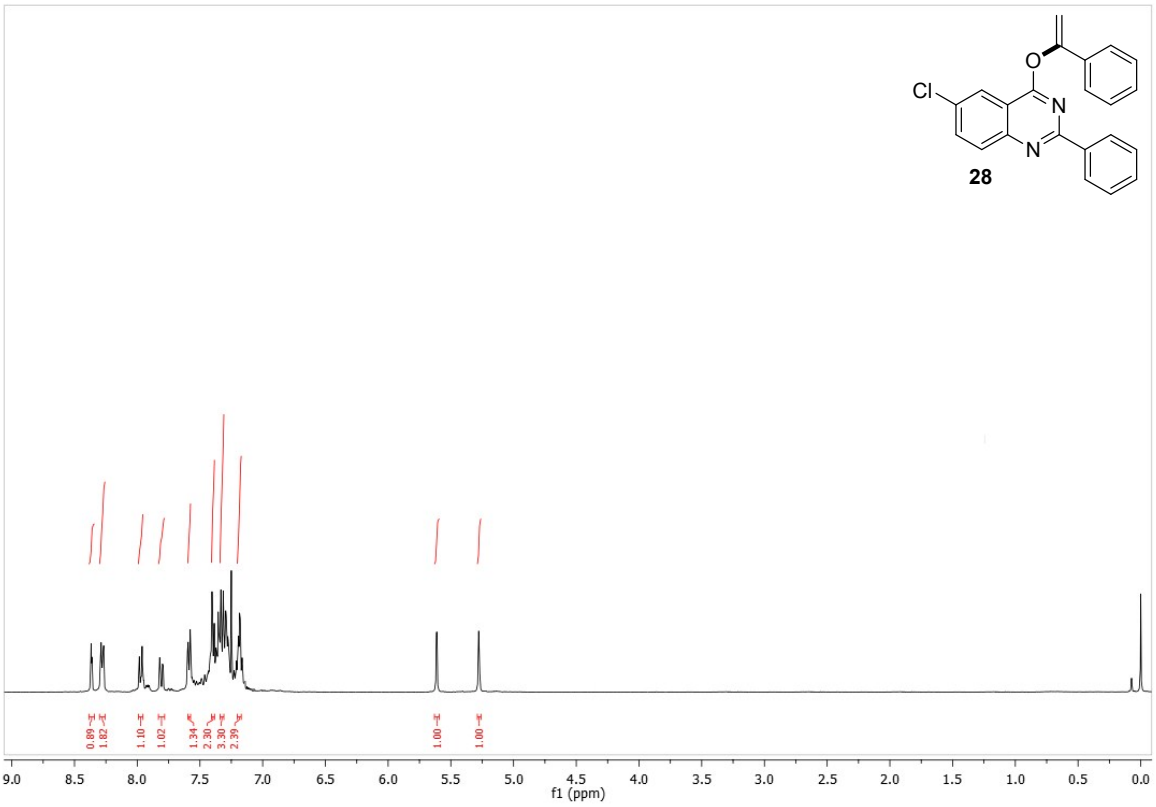
f1 (ppm)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O
N
N
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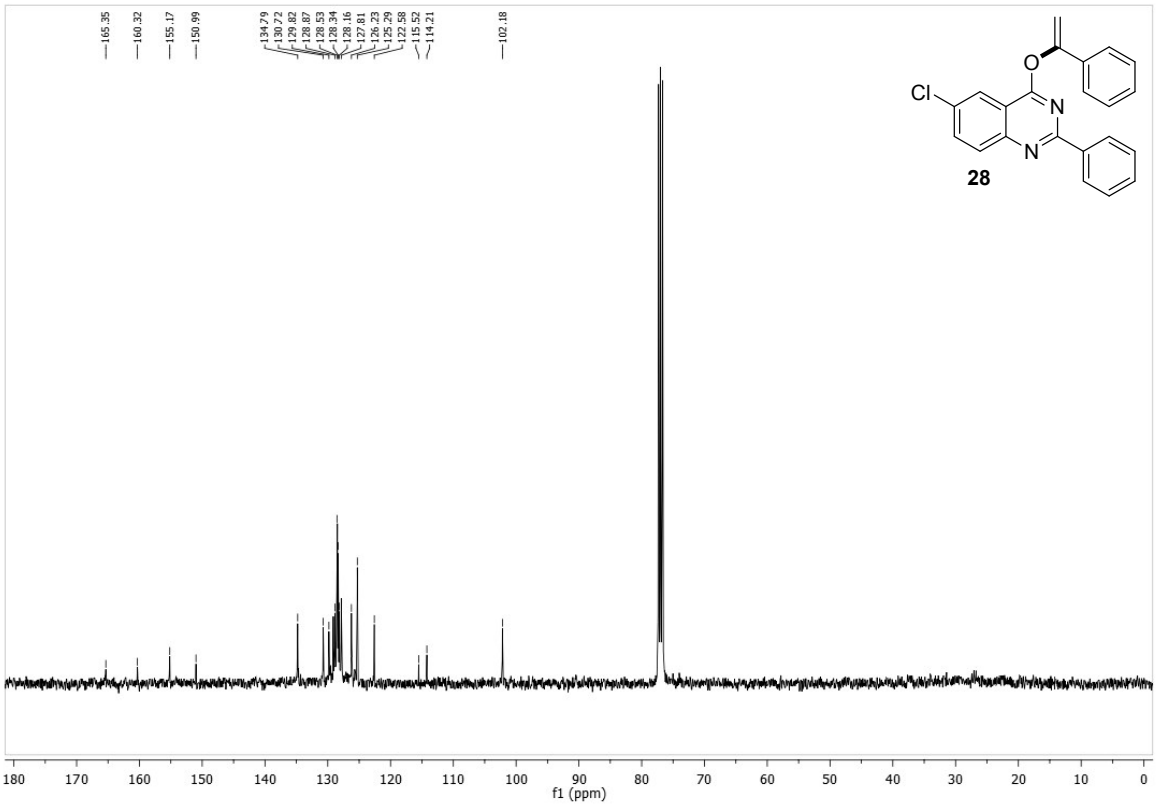
0.89
1.82
1.10
1.02
1.34
2.30
3.30
2.39
1.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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155.17
150.99
134.79
130.72
129.82
128.87
128.53
128.34
128.16
127.81
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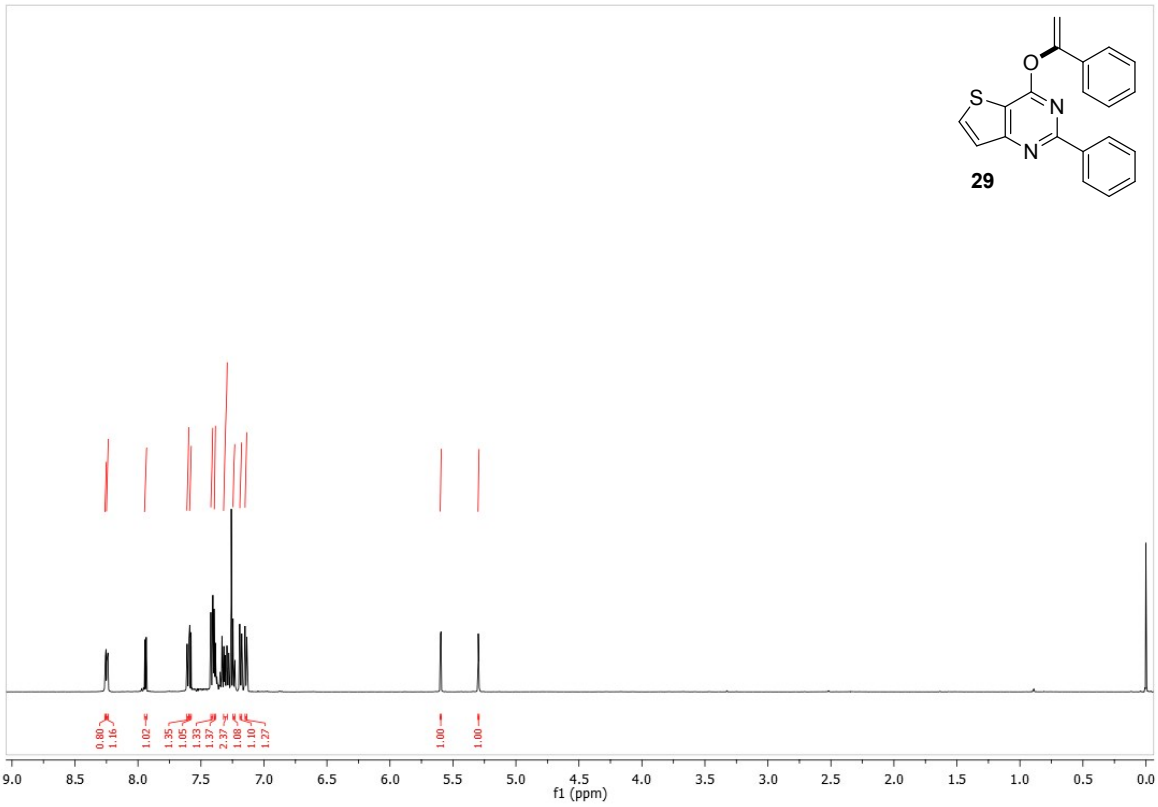
125.29
122.58
115.52
114.21
102.18
Cl
O
N
N
28
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
S
N
N
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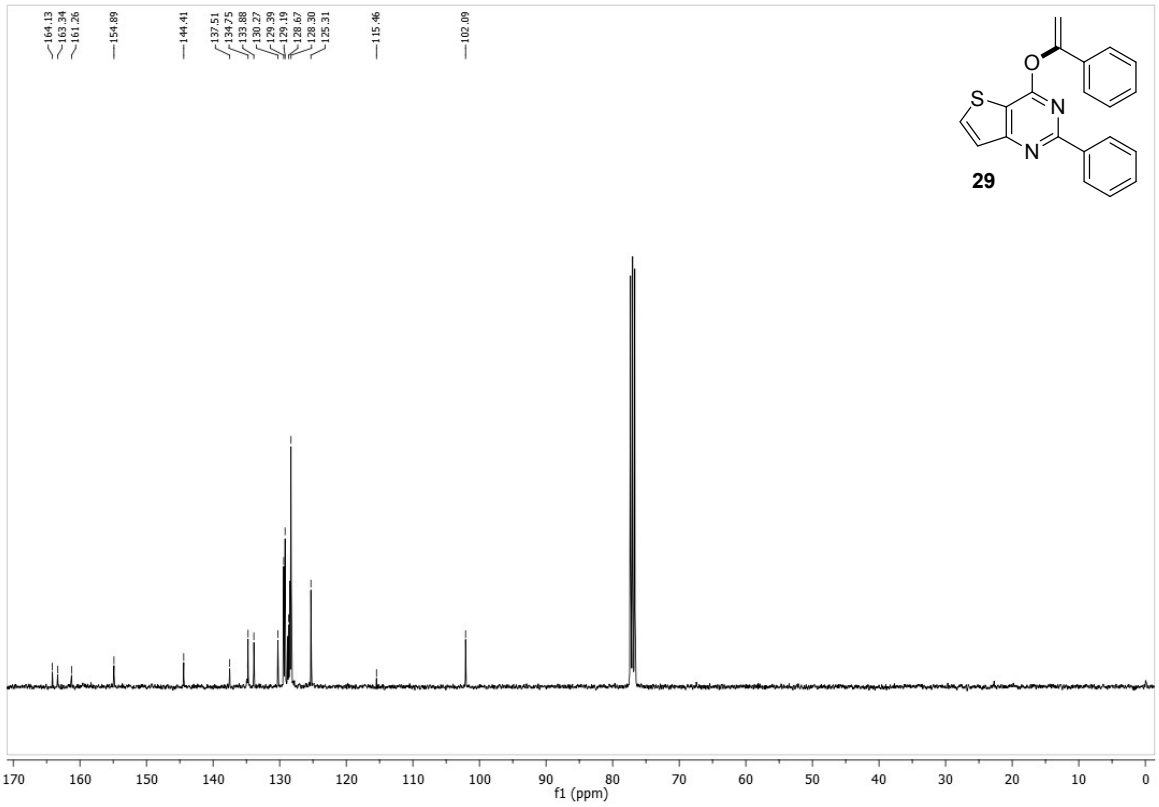
1.16
1.02
1.35
1.05
1.33
1.37
2.37
1.08
1.10
1.27
1.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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154.89
144.41
137.51
134.75
133.88
130.27
129.39
129.19
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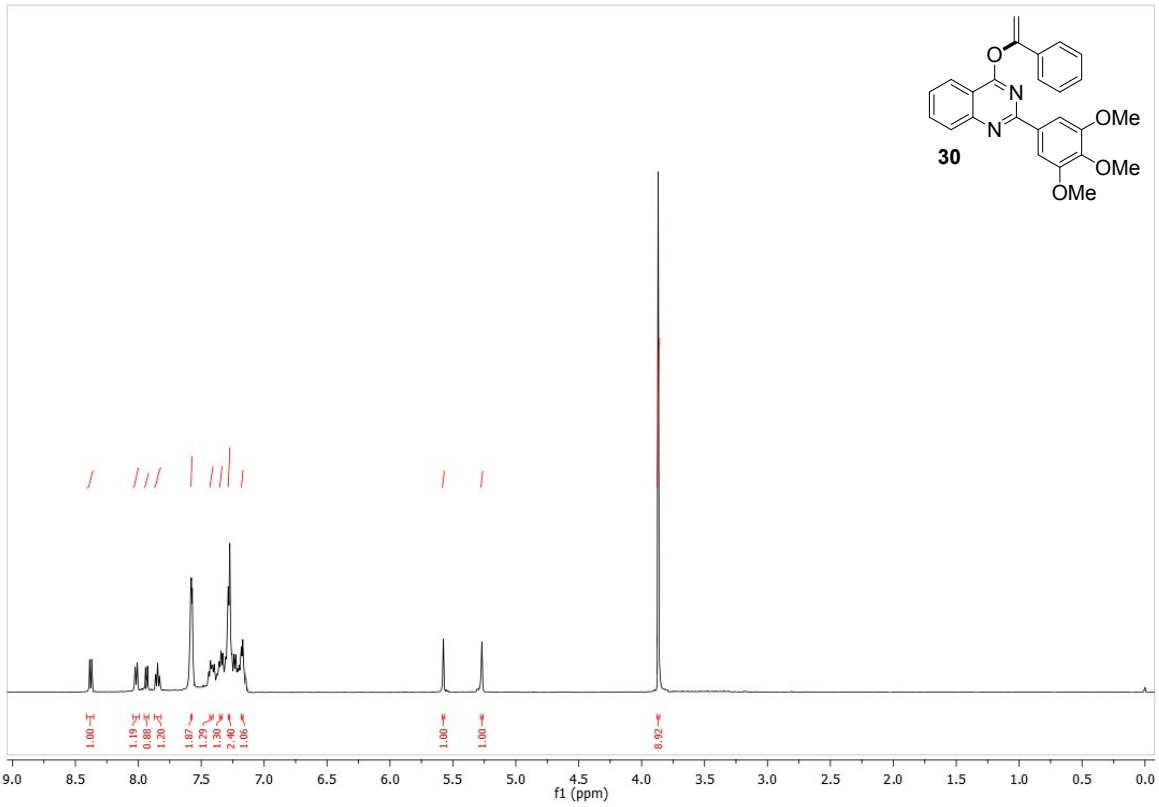
128.30
125.31
115.46
102.09
O
S
N
N
29
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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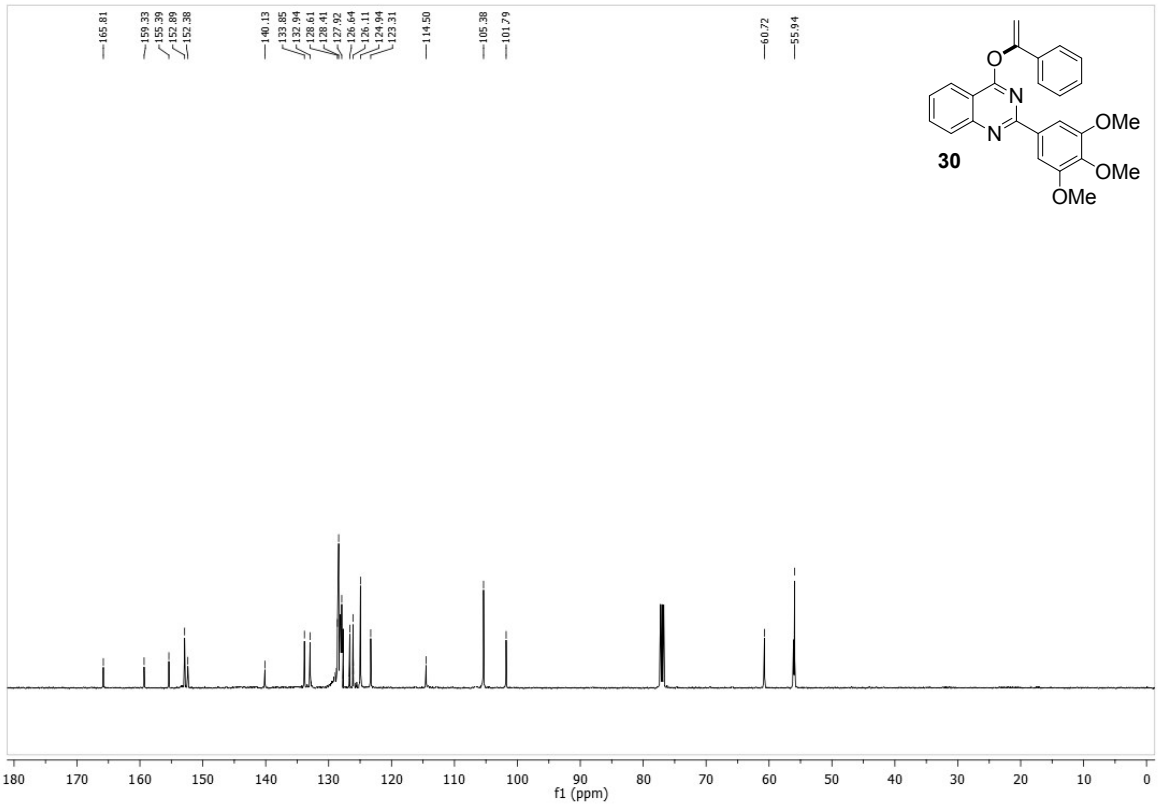
N
N
OMe
OMe
OMe
30
1.00
1.19
0.88
1.20
1.87
1.29
1.30
2.40
1.06
1.00
1.00
8.92
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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152.89
152.38
140.13
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132.94
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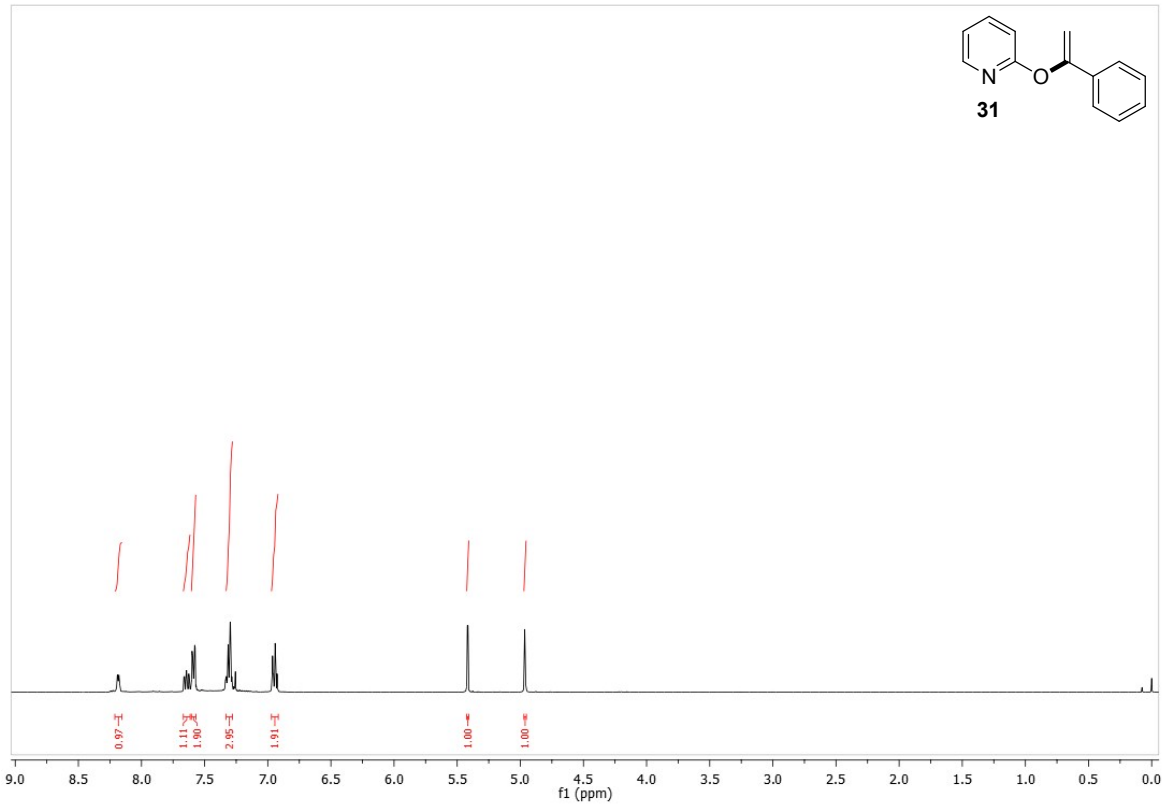
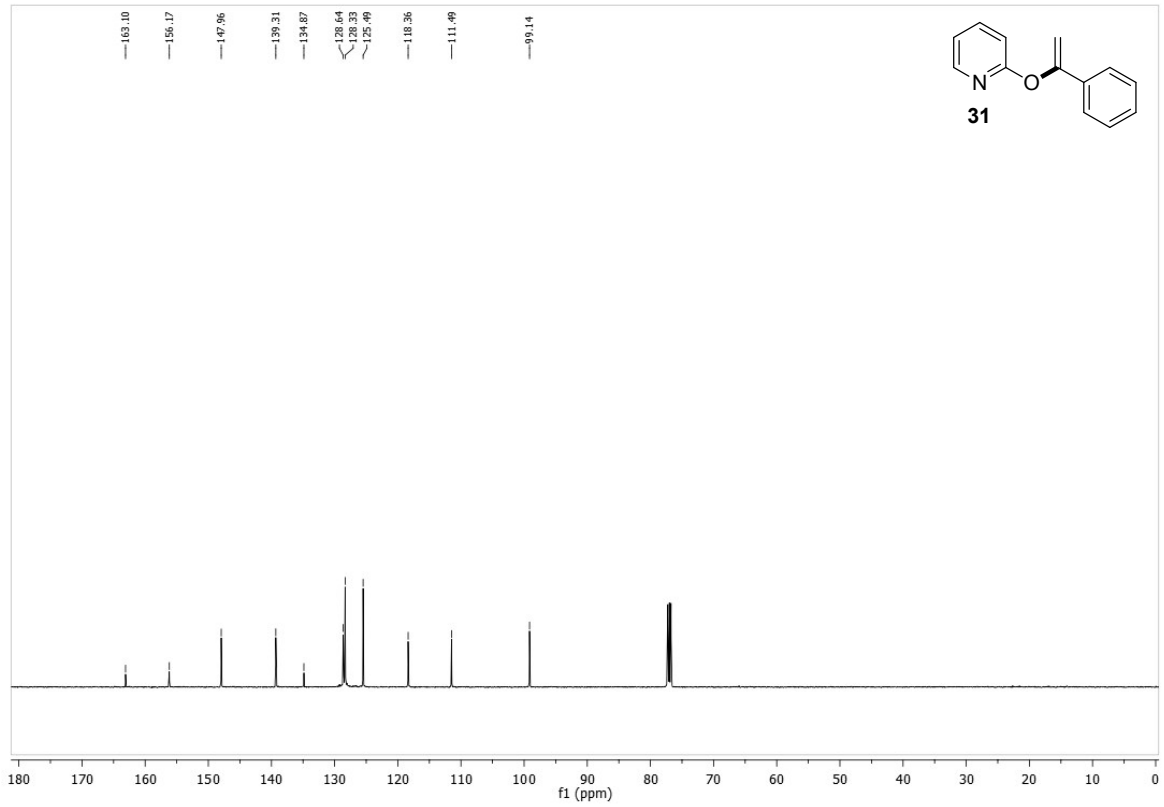
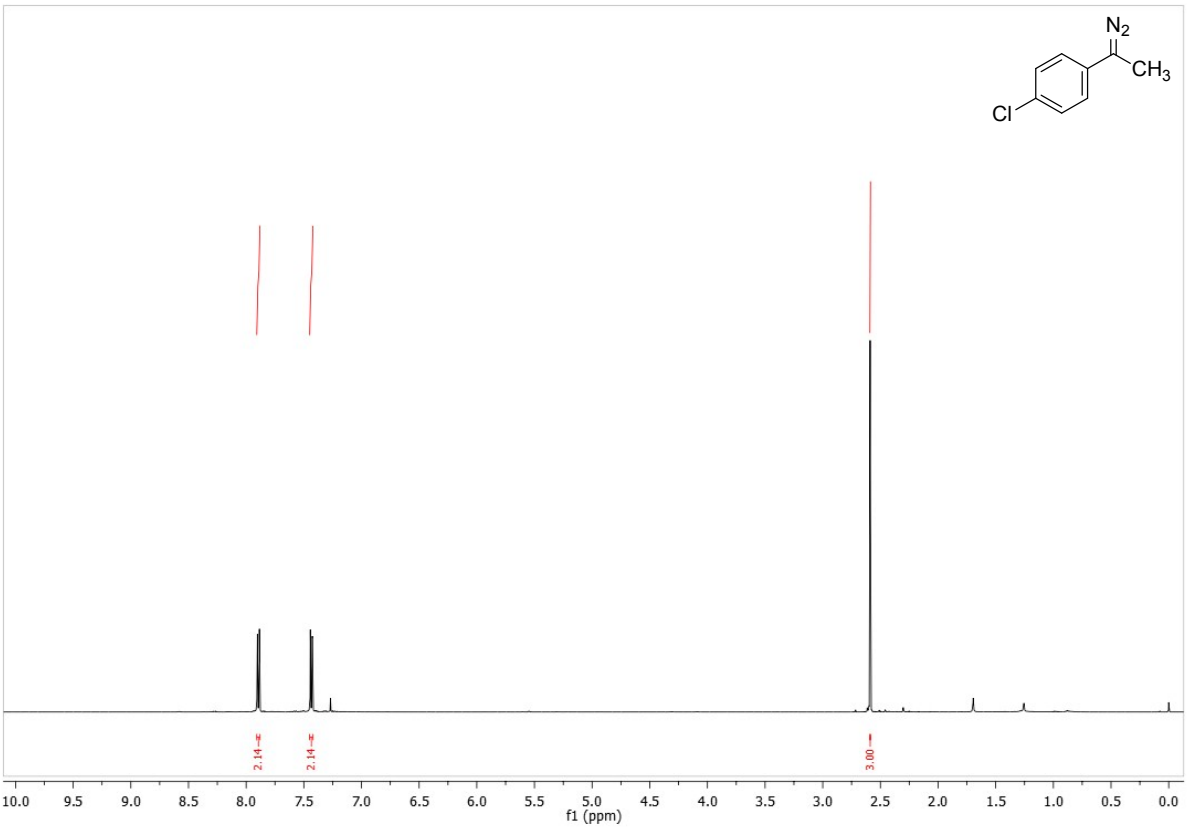
128.41
127.92
126.64
126.11
124.94
123.31
114.50
105.38
101.79
60.72
55.94
O
N
N
OMe
OMe
OMe
30
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


31
0.97
1.11
1.90
2.95
1.91
1.00
1.00
f1 (ppm)


163.10
156.17
147.96
139.31
134.87
128.64
128.33
125.49
118.36
111.49
99.14
31
f1 (ppm)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CH3
Cl
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2.14
3.00
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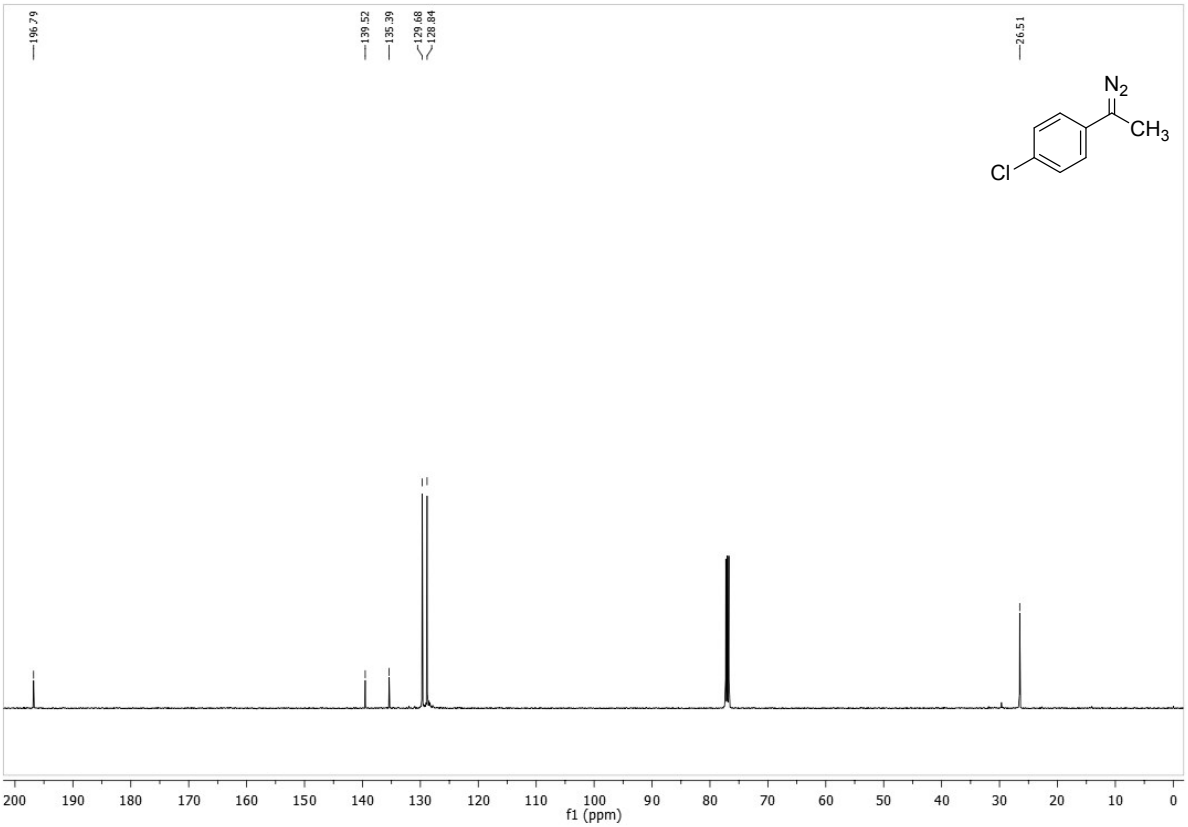
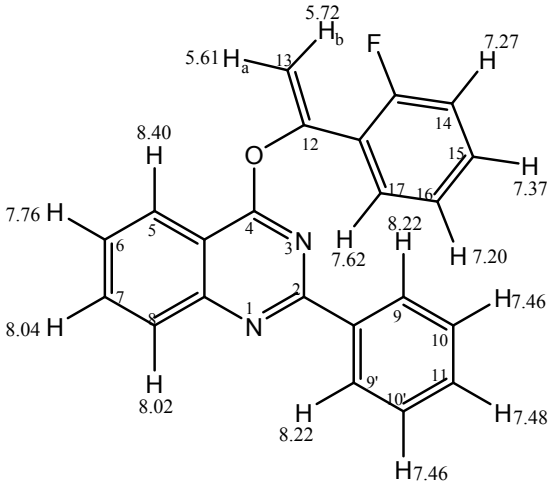
f1 (ppm)


196.79
139.52
135.39
129.68
128.84
26.51
N2
CH3
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

1.6 2D NMR Studies of **4**

Chemical shifts:

^{1}H: δ 8.40 (1H, H-5), 8.22 (2H, H-9, H-9'), 8.04 (1H, H-7), 8.02 (1H, H-8), 7.76 (1H, H-6) 7.62 (1H, H-17), 7.48 (1H, H-11), 7.46 (2H, H-10, H-10'), 7.37 (1H, H-15), 7.27 (1H, H-14), 7.20 (1H, H-16), 5.72 (1H, H_b-13), 5.61 (1H, H_a-13).



^{1}H-Chemical shifts

^{13}C: 165.41, 159.97, 158.58, 158.32, 151.79, 149.24, 136.79, 134.98, 131.04, 130.85, 128.61, 128.40, 127.85, 127.82, 124.77, 123.45, 122.63, 116.31, 114.10, 107.46, 39.50.

The structure of compound **4** was derived by extensive NMR experiments including 2-D Double Quantum Filtered Correlation Spectroscopy (DQF-COSY), Nuclear Overhauser Effect Spectroscopy (NOESY) and Heteronuclear-Single Quantum correlation (HSQC) and Heteronuclear-multiple Quantum correlation (HMBC) experiments. The resonance signal at 5.72 ppm is giving NOE with 7.62 and peak at 5.61 is interestingly showing weak intense NOE with 8.40 and 8.22 peaks. This NOE observation is initiating the resonance assignments of all the aromatic ring protons of substituted quinazoline ring system of compound **4**.

Herein the NOESY correlation structure and expanded NOESY Spectrum of compound **4** (Figure 1 and 2) have been illustrated.

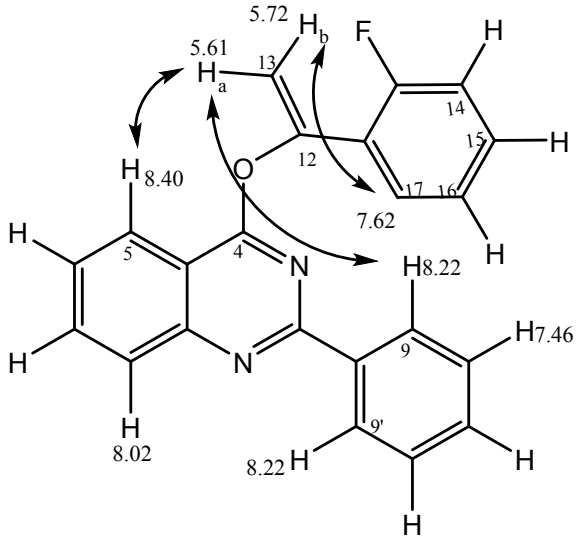


Figure 1. NOE correlations of H_b-13/ H-17, H_a-13/ H-5, H-9

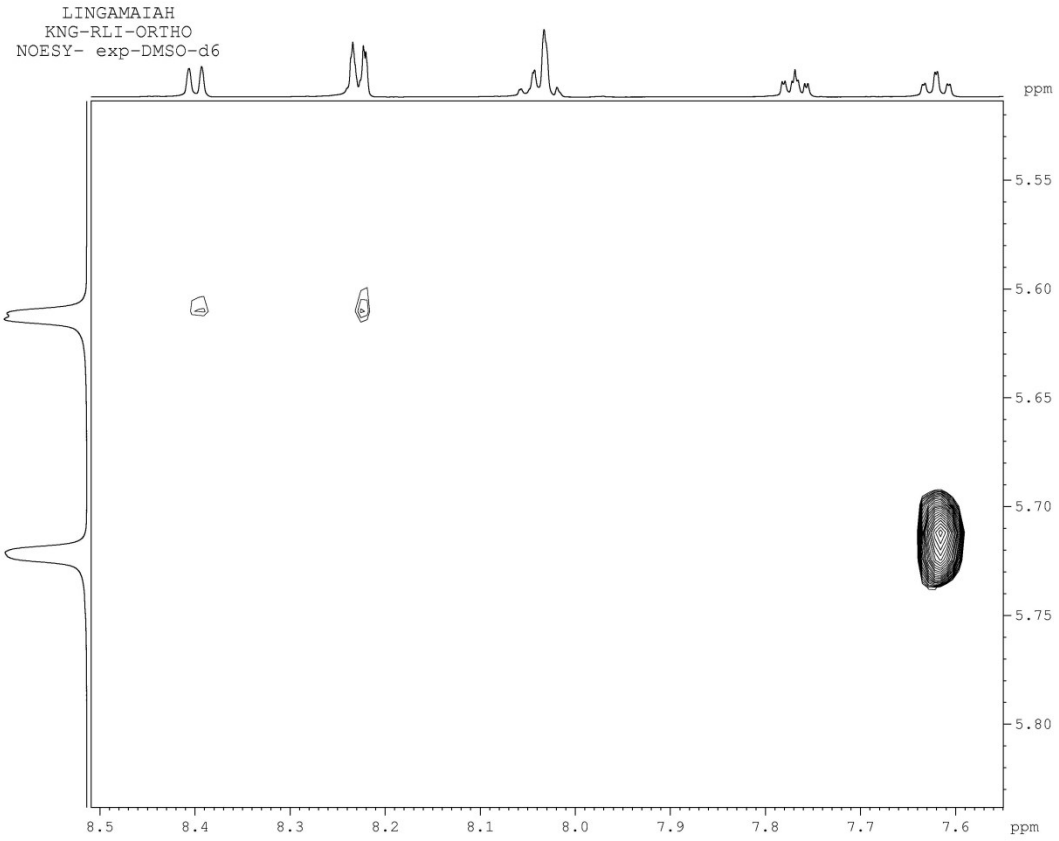
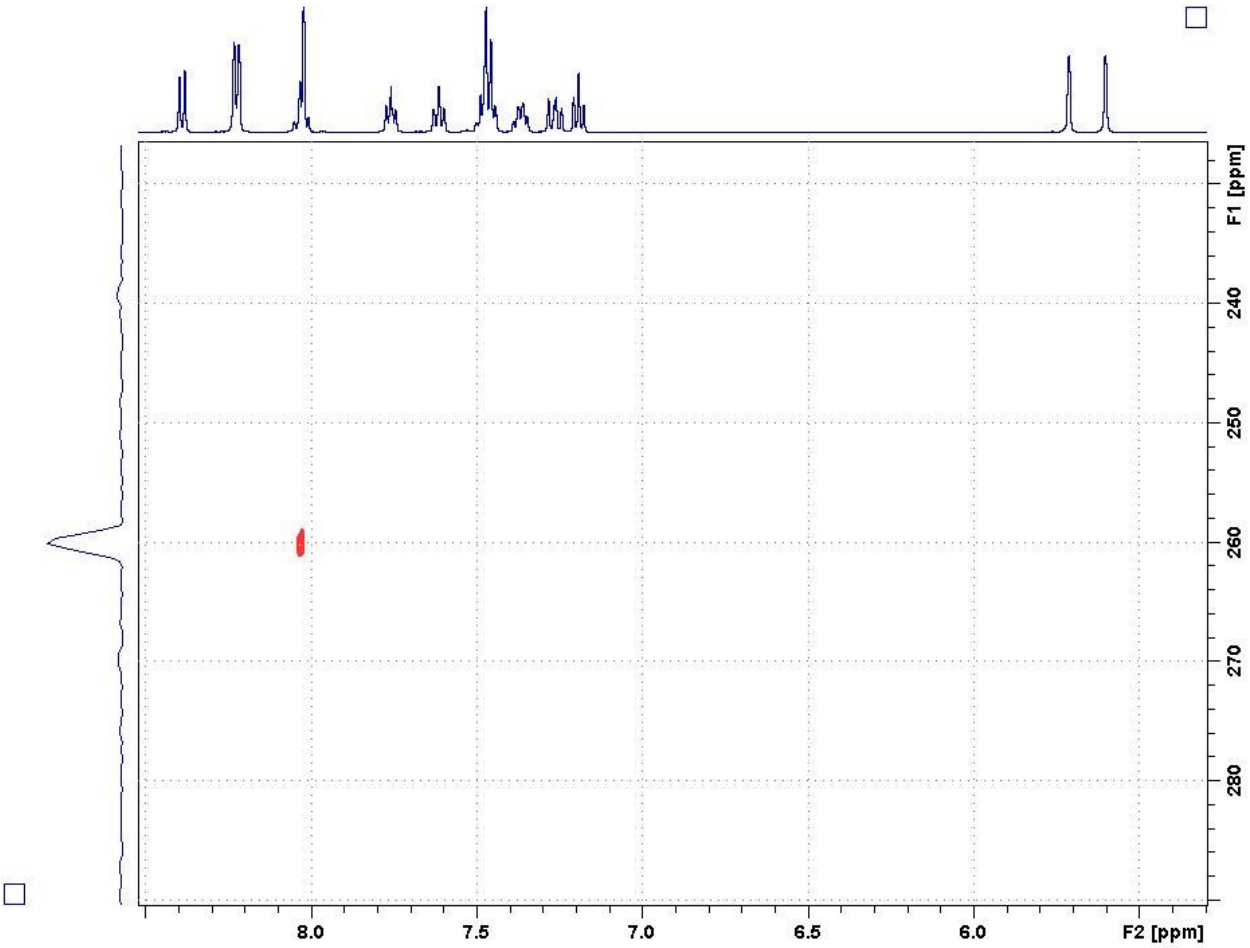


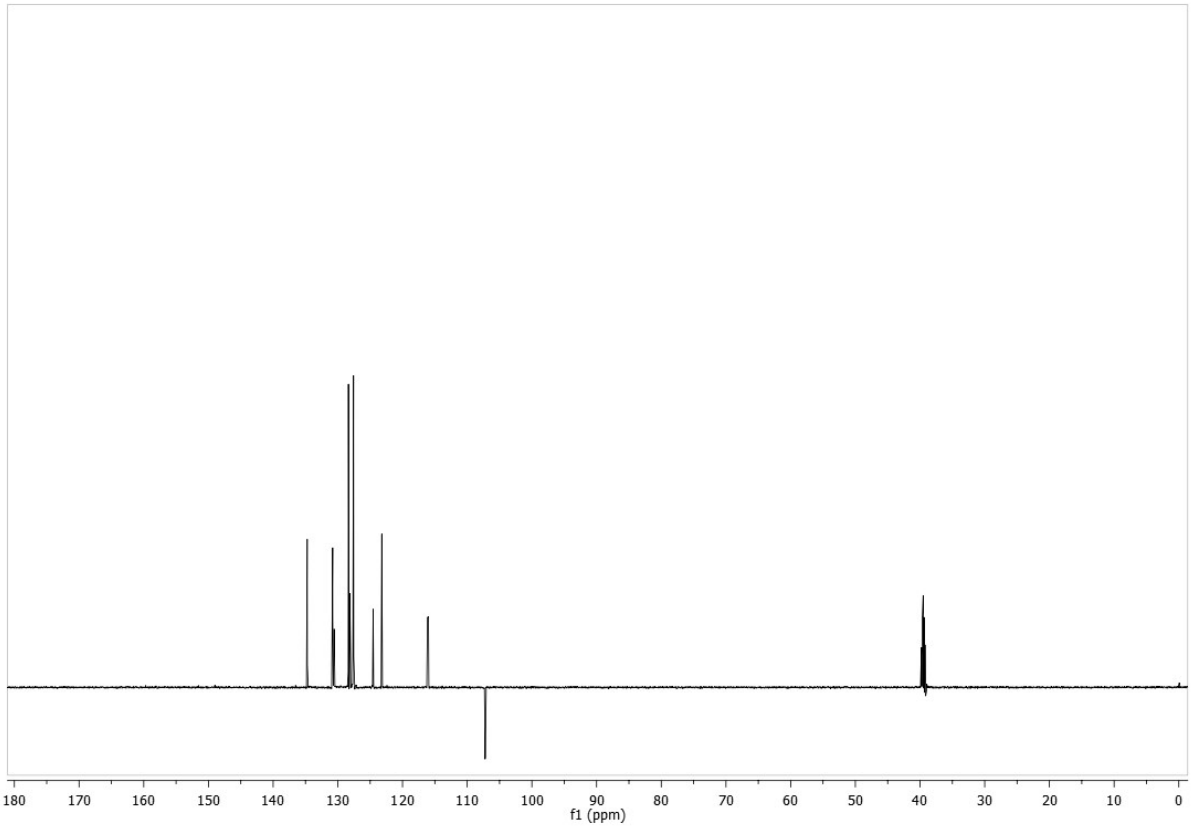
Figure 2. 2D-NOESY-Expansion



^{15}N-HMBC-Expansion

In Nitrogen Hetero nuclear multiple quantum correlation experiment (^{15}N-HMBC), H-13 protons be supposed to show 3 bond correlation with Nitrogen (N-2) if fluoro, vinyl substituted phenyl ring was present on (N-2) of the molecule. But observed significant 3-bond correlation between Nitrogen (N-1) and H-8 (δ 8.02) and observed not even 4 bond correlations between N-1 and H-9 (δ 8.22) of the molecule. Remaining spectral assignments were in agreement with assigned structure depicted in Figure 1.

DEPT-135 NMR spectrum of compound **4**



1.7 X-ray crystallography for 4

The CCDC deposition number for **4** is **1514723**; Crystal data: $C_{22}H_{15}N_2OF$, M = 342.36, 0.45 x 0.32 x 0.20 mm^3, monoclinic, space group C2/*c* (No. 15), a = 38.444(4), b = 6.2239(6), c = 14.5234(13) Å, β = 96.834(3)°, V = 3450.4(6) Å^3, Z = 8, D_c = 1.318 g/cm^3, F_{000} = 1424, CCD area detector, MoKα radiation, λ = 0.71073Å, T = 293(2)K, $2\theta_{max}$ = 56.6°, 19058 reflections collected, 4173 unique (R_{int} = 0.030), Final *GooF* = 1.03, $R1$ = 0.0443, $wR2$ = 0.1325, R indices based on 4173 reflections with I > 2σ(I) (refinement on F^2), 235 parameters, μ = 0.089 mm^{-1}, Min and Max Resd. Dens. = -0.17 and 0.26 e/Å^3. X-ray data for the compound were collected at room temperature using a Bruker Smart Apex CCD diffractometer. CCDC **1514723** contains the supplementary crystallographic data for this paper which can be obtained free of charge at https://summary.ccdc.cam.ac.uk/structure-summary-form or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk.

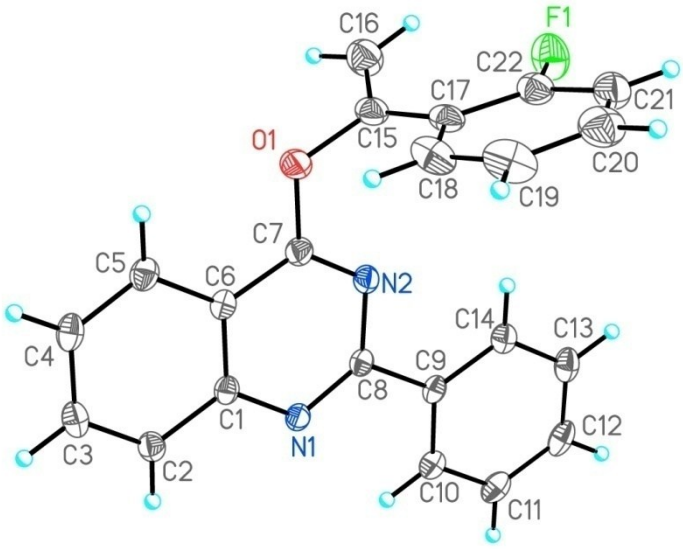


Figure 3. ORTEP diagram for compound **4**, with displacement ellipsoids drawn at the 20% probability level.