Facile Synthesis of 2-Alkynyloxazoles *via* $Ce(OTf)_3$-Catalyzed Cascade Reaction of Alkynyl Carboxylic Acids with *tert*-Butyl Isocyanide

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Experimental

General methods and materials. Proton nuclear magnetic resonance spectra (^{1}H NMR) and carbon nuclear magnetic resonance spectra (^{13}C NMR) were recorded at 400 MHz and 100 MHz or 500 MHz and 125 MHz, respectively, using $CDCl_3$ as reference standard (δ 7.26 ppm) for ^{1}H NMR and (δ 77.04 ppm) for ^{13}C NMR. HRMS were recorded using ESI. Melting points were uncorrected. Precoated silica gel plates F-254 were used for analytical thin-layer chromatography. Column chromatography was performed on silica gel (300-400 mesh). Starting material alkynyl carboxylic acids were readily prepared according to literature procedures. Unless otherwise noted, all reagents were obtained commercially and used without further purification.

General procedure for the synthesis of 2-alkynyloxazole 2a.

1a **2a**, 82%

A mixture of phenylpropiolic acid **1a** (1.0 equiv, 0.5 mmol), *tert*-butyl isocyanide (3.0 equiv, 1.5 mmol), $Ce(OTf)_3$ (10 mol%, 0.05 mmol) and 2 mL of toluene was stirred at 60 °C for 1 h. The progress of the reaction was monitored by thin-layer chromatography. After the reaction was complete, the reaction mixture was subjected to column chromatographic separation (petroleum ether/ethyl acetate) to afford 2-alkynyloxazole **2a**.

Procedure of anticancer activity assay.

The MGC-803, T-24, Hep-G2 and A549 cell lines used in this study were all obtained from the Institute of Biochemistry and Cell Biology, China Academy of Sciences. Cells were cultured in Dulbecco's modified Eagle's medium (DMEM) or RPMI-1640, which supplemented with 10% fetal bovine serum in a humidified atmosphere of 5% CO_2/95% air at 37 ℃. The 180 μL cell suspensions (4500-5000 cells/mL) was seeded

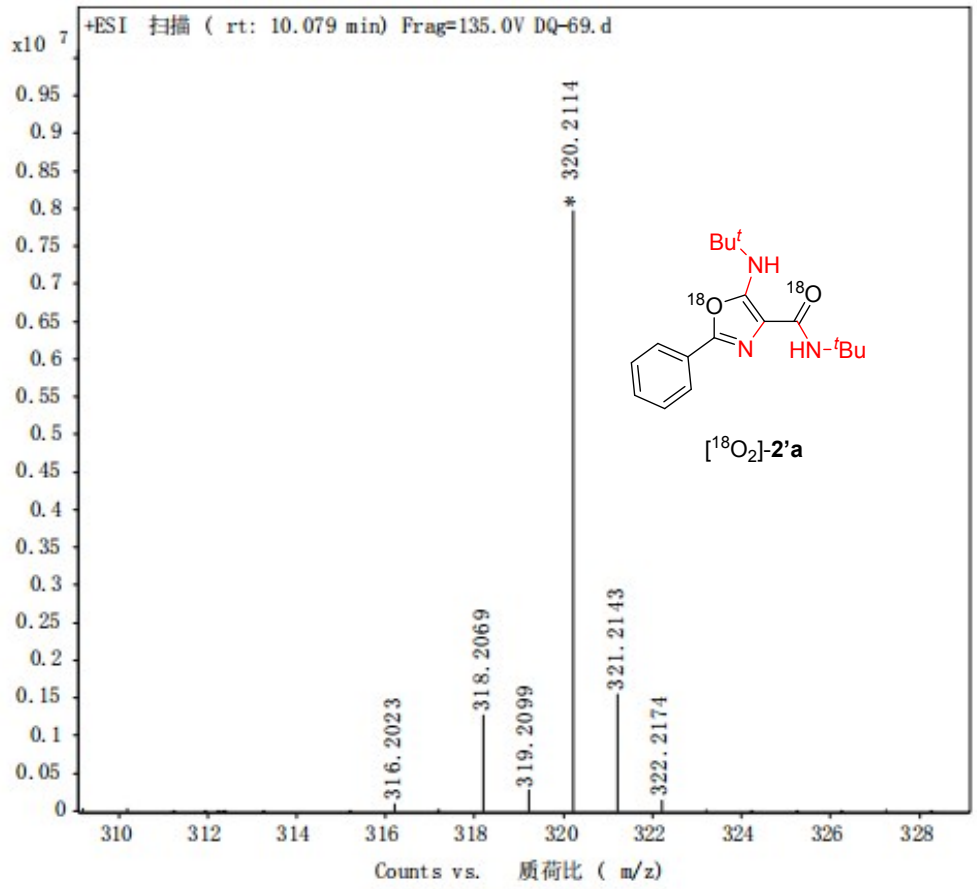
in 96-well plates and incubated for 24 h. All compounds and 5-FU were dissolved in the Phosphate Buffered Saline (PBS) with 1% DMSO to give various concentrations (2.5, 5, 10, 20, 40 μM, respectively) to 96-well plates and control wells contained supplemented media with 1% DMSO. Continue incubating for 48 h at 37 ℃ and in 5% CO_2 atmosphere and then the MTT solution (10 μL, 5 mg/mL) was added into each well and the cultures were incubated further for 4~6 h. After removal of the supernatant, DMSO (100 uL) was added to dissolve the formazan crystals. The absorbance was read by enzyme labeling instrument with 570/630 nm double wavelength measurement. The cytotoxicity was estimated based on the percentage cell survival in a dose dependent manner relative to the negative control. The final IC_{50} (a drug concentration killing 50% cells) values were calculated by the Bliss method (n ¼ 5). All the tests were repeated in at least three independent experiments.

Table S1 Effect of compounds 2a-v against cell viability of different cell lines[a]

Compound	IC_{50} ± SD (μM)[a]			
	MGC803	T24	HepG2	A549
2a	35.49±1.14	26.33±0.46	28.44±0.31	57.23±0.73
2b	17.88±1.7	11.56±0.09	27.34±0.37	24.01±1.22
2c	77.46±0.68	27.52±2.93	89.93±2.31	44.52±4.02
2d	28.96±1.28	29.17±2.43	31.05±0.75	28.36±0.81
2e	27.22±2.69	34.69±2.54	35.79±0.59	54.79±1.61
2f	49.43±3.02	21.44±0.86	59.20±0.4	50.17±0.9
2g	84.64±2.21	32.61±1.45	21.93±0.61	39.40±0.37
2h	16.86±1.37	32.94±1.03	29.32±0.55	28.69±0.91
2i	100.98±1.56	50.50±2.32	45.87±0.93	25.53±1.24
2j	40.78±2.16	80.51±0.71	25.84±1.92	44.50±1.16
2k	15.61±1.96	29.54±0.97	24.80±2.61	42.53±1.22
2m	48.10±2.12	62.12±0.77	41.15±0.36	59.10±2.14
2n	15.92±1.24	50.86±2.62	59.95±0.39	45.36±0.67
2o	20.26±1.54	73.22±2.43	28.00±1.17	80.70±0.46
2p	19.69±1.09	62.12±3.04	50.38±1.27	58.79±0.27
2q	55.50±2.03	65.76±1.72	27.73±1.35	53.62±0.94
2s	57.13±2.11	56.76±0.78	30.06±1.45	43.72±0.79
2t	18.67±1 .15	34.84±1.11	39.33±1.96	43.83±0.93
2v	45.49±2.03	40.48±1.74	20.10±0.82	23.82±1.03
5-FU	45.76±1.97	40.14±2.14	23.60±2.11	34.32±2.19

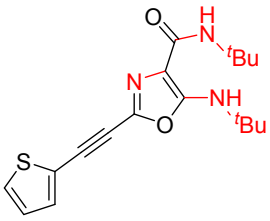
[a] IC_{50} (μmol L^{-1}) values are presented as the mean ± SD (standard error of the mean) from the three separate experiments; 5-FU: 5-fluorouracil.

HRMS analysis of [$^{18}O_2$]-2'a



[$^{18}O_2$]-**2'a**

X-ray data for compound 2s



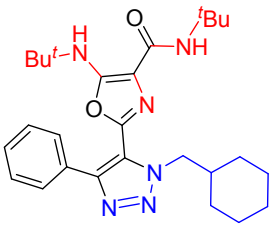
2s

Table S2 Crystal data and structure refinement for 2s

Compound	**2s**
Empirical formula	$C_{18}H_{23}N_3O_2S$
Formula weight	345.45
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.6688(3)

b/Å	10.6008(3)
c/Å	31.1741(9)
α/°	90
β/°	100.107(3)
γ/°	90
Volume/Å^3	3796.35(19)
Z	8
ρ_{calc}g/cm^3	1.209
μ/mm^{-1}	1.629
F(000)	1472.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.76 to 147.504
Index ranges	-14 ≤ h ≤ 10, -7 ≤ k ≤ 13, -38 ≤ l ≤ 38
Reflections collected	14668
Independent reflections	7409 [R_{int} = 0.0356, R_{sigma} = 0.0445]
Data/restraints/parameters	7409/8/471
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0564, wR_2 = 0.1439
Final R indexes [all data]	R_1 = 0.0638, wR_2 = 0.1515
Largest diff. peak/hole / e Å^{-3}	0.52/-0.40

X-ray data for compound 3a



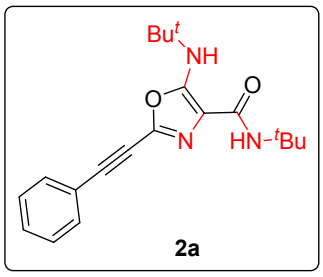
3a

Table S3 Crystal data and structure refinement for 3a

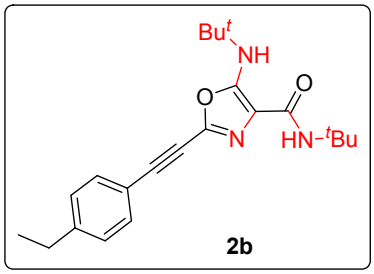
Compound	**3a**
Empirical formula	$C_{27}H_{38}N_6O_2$
Formula weight	478.63
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	Pbca

a/Å	19.2320(3)
b/Å	11.92476(17)
c/Å	23.5435(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	5399.40(15)
Z	8
ρ_{calc}g/cm^3	1.178
μ/mm^{-1}	0.607
F(000)	2064.0
Crystal size/mm^3	0.12 × 0.11 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.51 to 147.242
Index ranges	-22 ≤ h ≤ 23, -11 ≤ k ≤ 14, -29 ≤ l ≤ 27
Reflections collected	14096
Independent reflections	5342 [R_{int} = 0.0358, R_{sigma} = 0.0400]
Data/restraints/parameters	5342/0/322
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0435, wR_2 = 0.1067
Final R indexes [all data]	R_1 = 0.0540, wR_2 = 0.1146
Largest diff. peak/hole / e Å^{-3}	0.47/-0.44

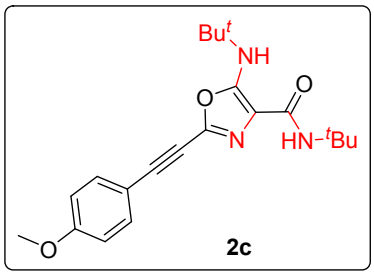
Spectral data of all compounds



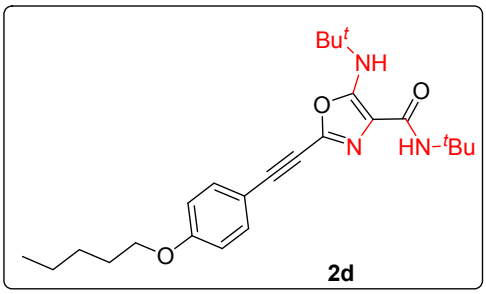
***N*-*tert*-butyl-5-(*tert*-butylamino)-2-(2-phenylethynyl)oxazole-4-carboxamide (2a):** light yellow solid, m.p. 44.2–46.5 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.58 (dd, *J* = 7.4, 1.6 Hz, 2H), 7.41–7.34 (m, 3H), 6.80 (s, 1H), 6.30 (s, 1H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.2, 157.1, 134.0, 131.9, 129.5, 128.5, 121.0, 107.7, 91.1, 77.2, 52.9, 51.0, 29.9, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{20}H_{26}O_2N_3$ 340.2025 $[M+H]^+$; found 340.2012.



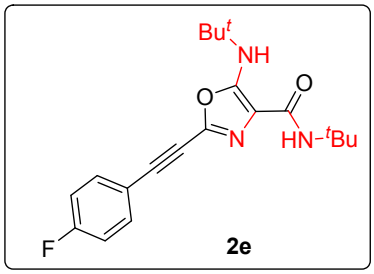
***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(4-ethylphenyl)ethynyl)oxazole-4-carboxamide (2b):** yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55–7.45 (m, 2H), 7.20 (d, *J* = 8.3 Hz, 2H), 6.78 (s, 1H), 6.30 (s, 1H), 2.67 (q, *J* = 7.6 Hz, 2H), 1.44 (s, 9H), 1.43 (s, 9H), 1.24 (t, *J* = 7.6 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.2, 157.1, 146.2, 134.2, 131.9, 128.1, 118.1, 107.6, 91.4, 52.9, 51.0, 29.9, 29.3, 28.9, 15.2 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{22}H_{30}O_2N_3$ 368.2338 $[M+H]^+$; found 368.2328.



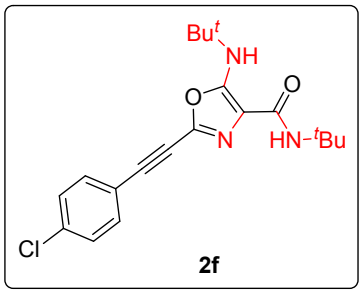
***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(4-methoxyphenyl)ethynyl)oxazole-4-carboxamide (2c):** yellow solid, m.p. 47.1–48.8 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55–7.46 (m, 2H), 6.91–6.86 (m, 2H), 6.76 (s, 1H), 6.29 (s, 1H), 3.83 (s, 3H), 1.44 (s, 9H), 1.42 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.2, 160.6, 157.0, 134.4, 133.6, 114.2, 113.0, 107.6, 91.3, 76.2, 55.4, 52.8, 51.0, 29.9, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{21}H_{28}O_3N_3$ 370.2131 $[M+H]^+$; found 370.2119.



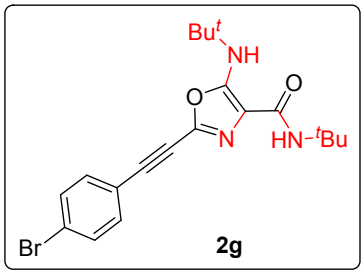
***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(4-(pentyloxy)phenyl)ethynyl)oxazole-4-carboxamide (2d):** yellow solid, m.p. 43.1–45.5 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.56–7.43 (m, 2H), 6.91–6.81 (m, 2H), 6.76 (s, 1H), 6.29 (s, 1H), 3.97 (t, *J* = 6.6 Hz, 2H), 1.85–1.73 (m, 2H), 1.50–1.34 (m, 22H), 0.93 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.2, 160.2, 157.0, 134.4, 133.6, 114.7, 112.6, 107.6, 91.4, 76.1, 68.16, 52.8, 51.0, 29.9, 29.3, 28.8, 28.2, 22.4, 14.0 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{25}H_{36}O_3N_3$ 426.2757 $[M+H]^+$; found 426.2742.



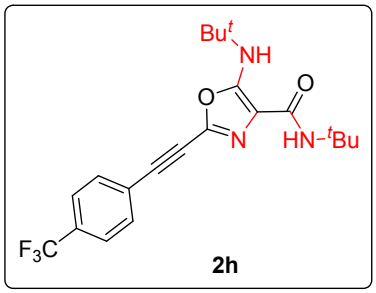
***N*-(*tert*-butyl)-5-(*tert*-butylamino)-2-((4-fluorophenyl)ethynyl)oxazole-4-carboxamide (2e):** yellow solid, m.p. 47.2–50.1 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.60–7.52 (m, 2H), 7.10–7.03 (m, 2H), 6.81 (s, 1H), 6.29 (s, 1H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.1, 162.2 (d, $^1J_{CF}$ = 250 Hz), 157.13, 134.0 (d, $^3J_{CF}$ = 8.0 Hz), 133.8, 117.2 (d, $^4J_{CF}$ = 4.0 Hz), 116.0 (d, $^2J_{CF}$ = 22.0 Hz), 107.7, 90.0, 77.2, 52.9, 51.0, 29.8, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{20}H_{25}O_2N_3F$ 358.1931 $[M+H]^+$; found 358.1921.



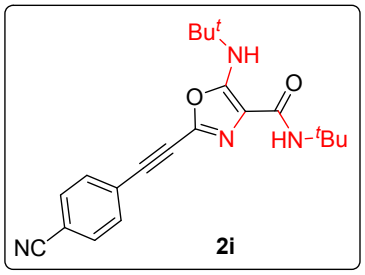
1-*tert*-butyl-5-(*tert*-butylamino)-4-(4-chlorophenyl)pyridin-2(1*H*)-one (2f): light yellow solid, m.p. 50.1–53.2 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.54–7.47 (m, 2H), 7.39–7.32 (m, 2H), 6.83 (s, 1H), 6.29 (s, 1H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.1, 157.2, 135.7, 133.7, 133.0, 129.0, 119.5, 107.8, 90.0, 78.3, 52.9, 51.0, 29.8, 30.0 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{20}H_{25}O_2N_3Cl$ 374.1635 $[M+H]^+$; found 374.1625.



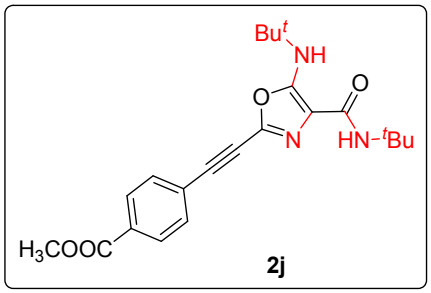
2-(2-(4-bromophenyl)ethynyl)-*N*-*tert*-butyl-5-(*tert*-butylamino)oxazole-4-carboxamide (2g): yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.59–7.49 (m, 2H), 7.42–7.35 (m, 2H), 6.80 (s, 1H), 6.30 (s, 1H), 1.44 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.2, 157.2, 133.2, 131.9, 129.5, 128.5, 121.0, 107.7, 91.1, 78.4, 52.9, 51.0, 29.9, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{16}H_{25}O_4N_2$ 309.1814 $[M+H]^+$; found 309.1791.



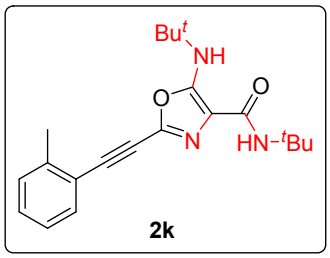
***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(4-(trifluoromethyl)phenyl)ethynyl)oxazole-4-carboxamide (2h): yellow oil; ^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.69–7.62 (m, 4H), 6.88 (s, 1H), 6.29 (s, 1H), 1.46 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.0, 157.3, 133.4, 132.0, 131.2, 126.5 (q, J = 272.6 Hz), 125.5 (q, J = 4.4 Hz), 124.9 (q, J = 1.7 Hz), 108.0, 89.6, 79.5, 53.0, 51.1, 29.8, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{21}H_{25}O_2N_3F_3$ 408.1899 $[M+H]^+$; found 408.1886.



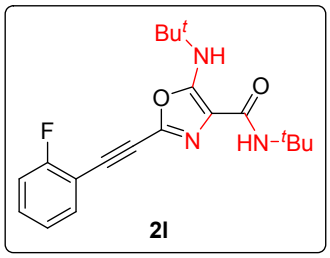
***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(4-cyanophenyl)ethynyl)oxazole-4-carboxamide (2i):** yellow solid, m.p. 51.2–53.9 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.66 (s, 4H), 6.92 (s, 1H), 6.29 (s, 1H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 162.9, 157.4, 133.1, 132.2, 132.1, 126.0, 118.2, 112.6, 108.2, 89.4, 81.4, 53.00, 51.1, 29.8, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{21}H_{25}N_4O_2$ 365.1978 $[M+H]^+$; found 365.1967.



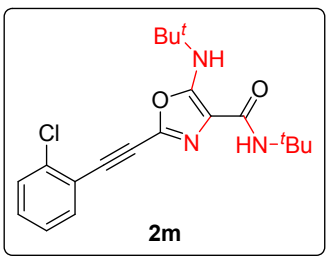
***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(4-(trifluoromethyl)phenyl)ethynyl)oxazole-4-carboxamide (2j):** yellow solid, m.p. 44.2–46.5 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.06–8.00 (m, 2H), 7.66–7.58 (m, 2H), 6.86 (s, 1H), 6.29 (s, 1H), 3.93 (s, 3H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.3, 163.0, 157.3, 133.5, 131.7, 130.5, 129.6, 125.6, 108.0, 90.3, 80.0, 53.0, 52.3, 51.1, 29.8, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{22}H_{28}N_3O_4$ 398.2080 $[M+H]^+$; found 398.2071.



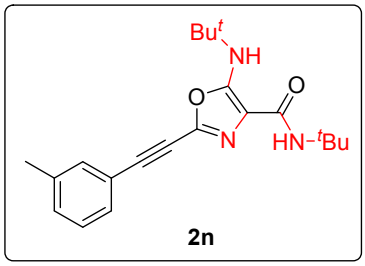
***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-o-tolylethynyl)oxazole-4-carboxamide (2k):** light yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.54 (d, J = 7.6 Hz, 1H), 7.32–7.16 (m, 3H), 6.79 (s, 1H), 6.31 (s, 1H), 2.52 (s, 3H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.2, 157.1, 141.0, 134.1, 132.3, 129.7, 129.5, 125.7, 120.8, 107.7, 90.1, 80.92, 52.87, 50.99, 29.85, 29.31, 20.65 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{21}H_{28}O_2N_3$ 354.2182 $[M+H]^+$; found 354.2171.



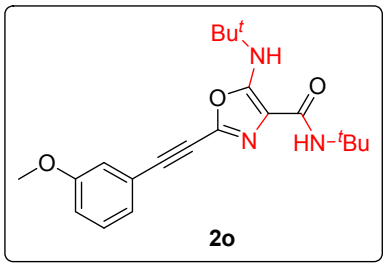
***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(2-fluorophenyl)ethynyl)oxazole-4-carboxamide (2l):**light yellow solid**,** m.p. 51.1–53.5 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.38–7.32 (m, 2H), 7.29–7.25 (m, 1H), 7.14–7.06 (m, 1H), 6.84 (s, 1H), 6.29 (s, 1H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.13, 162.9 (d, $^1J_{CF}$ = 253 Hz), 157.2, 133.6, 131.3 (d, $^3J_{CF}$ = 8.0 Hz), 124.1 (d, $^4J_{CF}$ = 4.0 Hz), 115.8 (d, $^2J_{CF}$ = 20.0 Hz), 109.9, 107.8, 84.6, 82.0, 78.1, 52.9, 51.0, 29.8, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{20}H_{25}O_2N_3F$ 358.1931 $[M+H]^+$; found 358.1921.



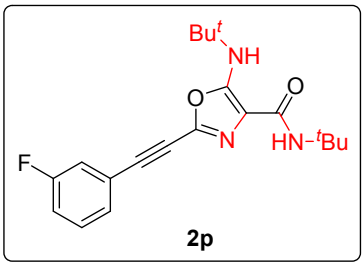
***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(2-chlorophenyl)ethynyl)oxazole-4-carboxamide (2m):** light yellow solid, m.p. 53.2–55.7 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.60 (dd, J = 7.6, 1.7 Hz, 1H), 7.44 (dd, J = 8.0, 1.1 Hz, 1H), 7.35–7.26 (m, 2H), 6.83 (s, 1H), 6.32 (s, 1H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.1, 157.3, 136.3, 133.6, 130.4, 129.5, 126.6, 121.3, 107.9, 87.7, 82.0, 52.9, 51.0, 29.8, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{20}H_{25}O_2N_3Cl$ 374.1635 $[M+H]^+$; found 374.1625.



***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-m-tolylethynyl)oxazole-4-carboxamide (2n):** light yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.42–7.36 (m, 2H), 7.27–7.19 (m, 2H), 6.79 (s, 1H), 6.30 (s, 1H), 2.36 (s, 3H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.2, 157.1, 138.3, 134.1, 132.4, 130.4, 129.0, 128.4, 120.8, 107.7, 91.3, 52.9, 51.0, 29.9, 29.3, 21.2 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{21}H_{28}O_2N_3$ 354.2182 $[M+H]^+$; found 354.2169.

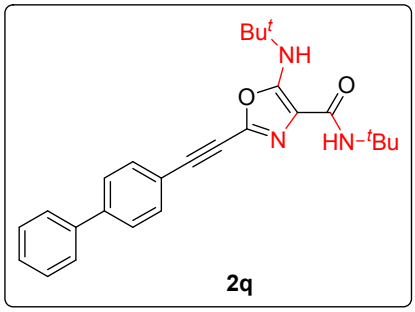


***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(3-methoxyphenyl)ethynyl)oxazole-4-carboxamide (2o):** light yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.29–7.25 (m, 1H), 7.18 (dt, *J* = 7.6, 1.1 Hz, 1H), 7.10–7.09 (m, 1H), 6.95 (ddd, *J* = 8.3, 2.6, 0.9 Hz, 1H), 6.81 (s, 1H), 6.30 (s, 1H), 3.82 (s, 3H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.2, 159.4, 157.1, 134.0, 129.6, 124.4, 122.0, 116.5, 116.3, 107.7, 91.0, 77.1, 55.4, 52.9, 51.0, 29.9, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{21}H_{28}O_3N_3$ 370.2131 $[M+H]^+$; found 370.2119.



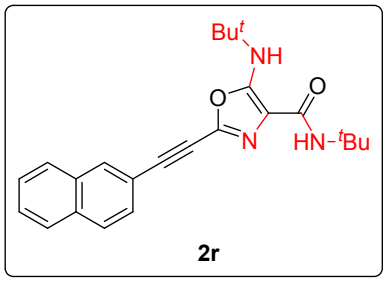
***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(3-fluorophenyl)ethynyl)oxazole-4-carboxamide (2p):** yellow solid, m.p. 53.4–56.5 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.38–7.30 (m, 2H), 7.28–7.25 (m, 1H), 7.13–7.06 (m, 1H), 6.84 (s, 1H), 6.29 (s, 1H), 1.45 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.1, 162.3 (d, $^1J_{CF}$ = 246.0 Hz), 157.2, 133.6, 130.2 (d, $^3J_{CF}$ = 9.0 Hz), 127.7 (d, $^4J_{CF}$ = 4.0 Hz), 122.9 (d, $^3J_{CF}$ = 10.0 Hz), 118.6 (d, $^2J_{CF}$ = 23.0 Hz), 117.9 (d, $^2J_{CF}$ = 21.0 Hz), 107.8, 89.7, 78.1, 52.9,

51.0, 29.8, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{20}H_{25}O_2N_3F$ 358.1931 $[M+H]^+$; found 358.1921.



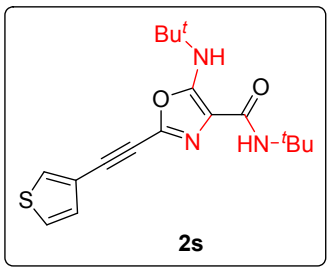
2q

2-([1,1'-biphenyl]-4-ylethynyl)-*N*-(*tert*-butyl)-5-(*tert*-butylamino)oxazole-4-carboxamide (2q): yellow solid, m.p. 47.5–49.8 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.64–7.59 (m, 5H), 7.49–7.35 (m, 4H), 6.82 (s, 1H), 6.31 (s, 1H), 1.46 (s, 9H), 1.44 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.2, 157.2, 142.2, 140.0, 134.1, 132.3, 128.9, 128.0, 127.2, 127.2, 119.8, 107.7, 91.1, 78.0, 52.9, 51.0, 29.9, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{26}H_{30}O_2N_3$ 416.2338 $[M+H]^+$; found 416.2328.



2r

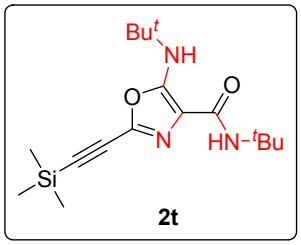
***N*-*tert*-butyl-5-(*tert*-butylamino)-2-(2-(naphthalen-2-yl)ethynyl)oxazole-4-carboxamide (2r):** yellow solid, m.p. 42.3–45.1 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.12 (s, 1H), 7.83 (dd, J = 9.2, 3.4 Hz, 3H), 7.59 (dd, J = 8.5, 1.5 Hz, 1H), 7.55–7.50 (m, 2H), 6.83 (s, 1H), 6.32 (s, 1H), 1.46 (s, 9H), 1.44 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.2, 157.2, 134.1, 133.3, 132.8, 132.4, 128.3, 128.0, 127.9, 127.9, 127.4, 126.9, 118.3, 107.8, 91.6, 77.6, 52.9, 51.0, 29.9, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{21}H_{28}O_3N_3$ 370.2131 $[M+H]^+$; found 370.2119.



2s

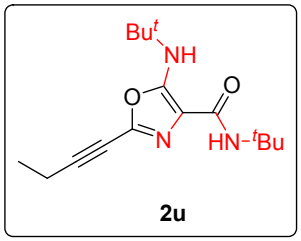
***N*-*tert*-butyl-5-(*tert*-butylamino)-2-(2-(thiophen-3-yl)ethynyl)oxazole-4-carboxamide (2s): light yellow solid,** m.p. 45.3–48.2 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.65 (dd, J = 3.0, 1.2 Hz, 1H), 7.32 (dd, J = 5.0, 3.0 Hz, 1H), 7.23 (dd, J = 5.0, 1.2 Hz, 1H), 6.79 (s, 1H), 6.29 (s, 1H), 1.44 (s, 9H), 1.43 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.2, 157.1,

134.0, 130.9, 129.7, 125.8, 120.1, 107.6, 86.4, 77.0, 52.9, 51.0, 29.8, 29.3 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{18}H_{24}O_2N_3S$ 346.1589 $[M+H]^+$; found 346.1578.



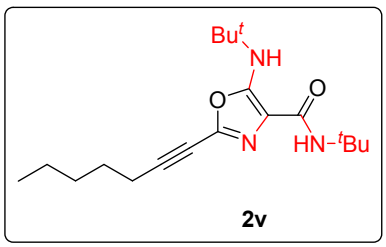
2t

***N-tert*-butyl-5-(*tert*-butylamino)-2-(2-(trimethylsilyl)ethynyl)oxazole-4-carboxamide (2t):** light yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 6.77 (s, 1H), 6.26 (s, 1H), 1.42 (s, 9H), 1.40 (s, 9H), 0.27 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.6, 157.4, 134.2, 107.8, 98.9, 92.0, 53.4, 51.5, 30.3, 29.8, 0.00 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{17}H_{30}O_2N_3$ Si 366.2107 $[M+H]^+$; found 366.2097.



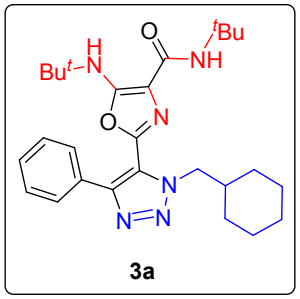
2u

2-(but-1-ynyl)-*N-tert*-butyl-5-(*tert*-butylamino)oxazole-4-carboxamide (2u): white solid, m.p. 52.6–54.3 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 6.66 (s, 1H), 6.25 (s, 1H), 2.45 (q, *J* = 7.5 Hz, 2H), 1.41 (s, 18H), 1.25 (t, *J* = 7.5 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.3, 156.7, 134.2, 107.0, 94.3, 68.4, 52.7, 50.9, 29.9, 29.3, 13.1, 13.0 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{16}H_{26}N_3O_2$ 292.2025 $[M+H]^+$; found 292.2014.

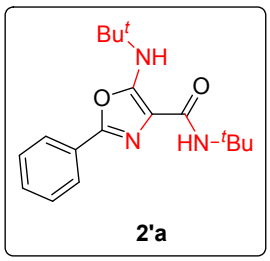


2v

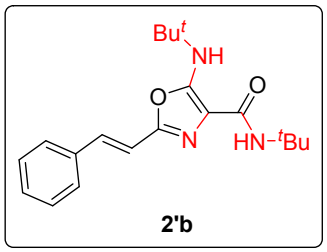
***tert*-butyl-5-(*tert*-butylamino)-2-(hept-1-ynyl)oxazole-4-carboxamide (2v):** yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 6.66 (s, 1H), 6.25 (s, 1H), 2.43 (t, *J* = 7.2 Hz, 2H), 1.67–1.59 (m, 2H), 1.47–1.43 (m, 2H), 1.41 (s, 18H), 1.37–1.32 (m, 2H), 0.92 (t, *J* = 7.2 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.3, 156.7, 134.3, 106.9, 93.3, 70.0, 52.7, 50.9, 31.1, 29.9, 29.3, 27.7, 22.1, 19.3, 13.9 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{19}H_{32}O_2N_3$ 334.2494 $[M+H]^+$; found 334.2484.



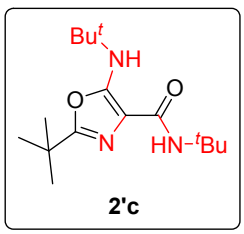
***N*-(*tert*-butyl)-5-(*tert*-butylamino)-2-(1-(cyclohexylmethyl)-4-phenyl-1*H*-1,2,3-triazol-5-yl)oxazole-4-carboxamide (3a)**: yellow solid, m.p. 85.1–87.2 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.62 (dd, *J* = 7.5, 1.5 Hz, 2H), 7.42–7.35 (m, 3H), 6.61 (s, 1H), 6.25 (s, 1H), 4.49 (d, *J* = 7.1 Hz, 2H), 1.76–1.67 (m, 6H), 1.45 (s, 9H), 1.29–1.19 (m, 5H), 1.15 (s, 9H) ppm; **^{13}C NMR** (100MHz, $CDCl_3$): δ 163.3, 156.9, 146.7, 138.7, 130.5, 128.6, 128.6, 128.5, 122.0, 108.0, 55.9, 52.7, 51.0, 38.4, 30.5, 29.5, 29.3, 26.2, 25.6 ppm; **HRMS** (m/z) (ESI): calcd for $C_{27}H_{39}O_2N_6$ 479.3134 $[M+H]^+$; found 479.3107.



***N-tert*-butyl-5-(*tert*-butylamino)-2-phenyloxazole-4-carboxamide (2'a):** light yellow solid, m.p. 91.3–93.8 °C (lit.[1] 92–94 °C); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.6 Hz, 2H), 7.39 (dt, *J* = 27.5, 6.8 Hz, 3H), 6.55 (s, 1H), 6.38 (s, 1H), 1.47 (s, 18H) ppm; **^{13}C NMR** (125 MHz, $CDCl_3$): δ 164.0, 157.1, 149.2, 129.2, 128.8, 127.3, 125.1, 108.2, 52.8, 50.9, 30.0, 29.4 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{18}H_{26}O_2N_3$ 316.2020 $[M+H]^+$; found 316.2029.



(*E*)-*N-tert*-butyl-5-(*tert*-butylamino)-2-styryloxazole-4-carboxamide (2'b): yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.48 (d, *J* = 7.4 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 2H), 7.32–7.25 (m, 1H), 7.16 (d, *J* = 16.3 Hz, 1H), 6.74 (d, *J* = 16.3 Hz, 1H), 6.66 (s, 1H), 6.28 (s, 1H), 1.47 (s, 9H), 1.45 (s, 9H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 163.8, 156.9, 149.4, 135.9, 132.5, 128.9, 128.6, 126.8, 113.4, 108.4, 52.7, 50.9, 29.9, 29.4 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{20}H_{28}O_2N_3$ 342.2176 $[M+H]^+$; found 342.2186.

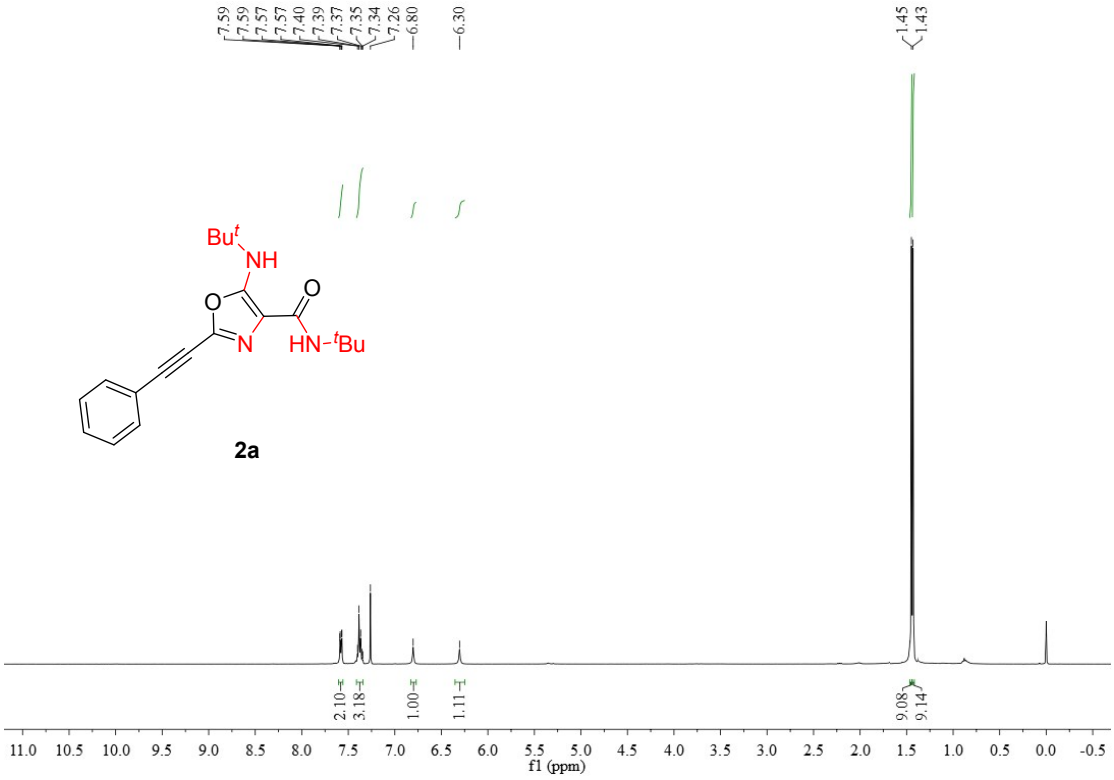


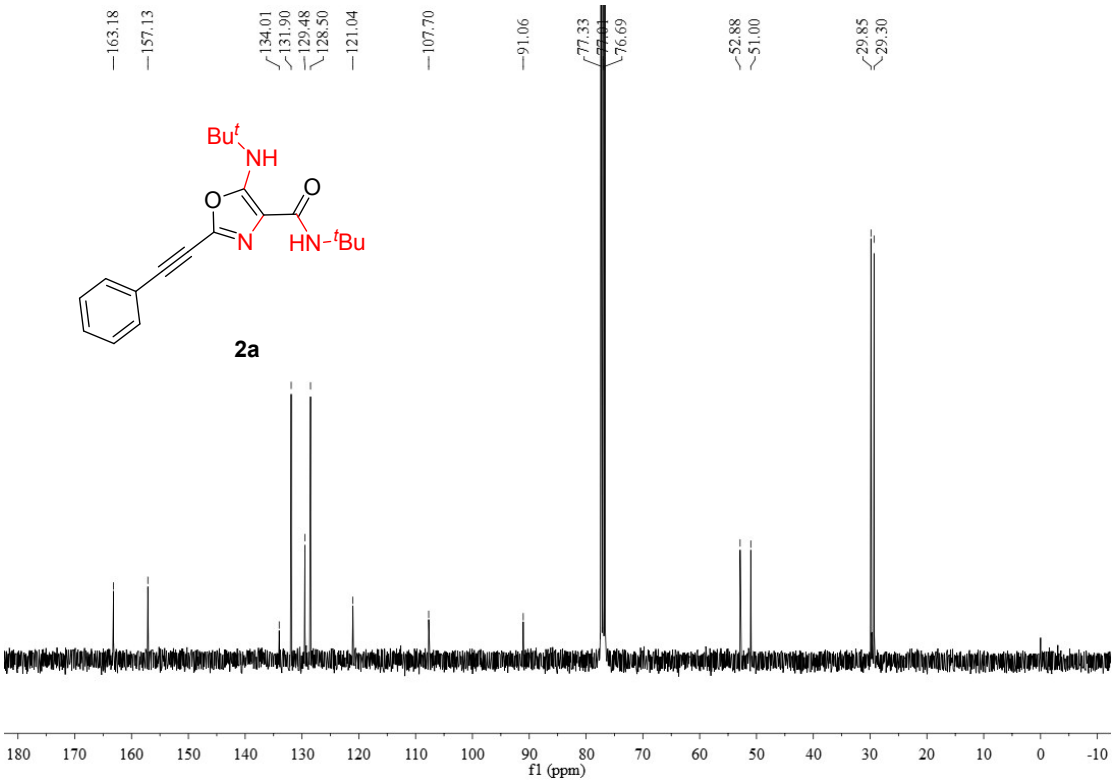
***N*,2-di-*tert*-butyl-5-(*tert*-butylamino)oxazole-4-carboxamide (2'c):** colorless solid, m.p. 67.2–69.7 °C (lit.[1] 68–70 °C); **^{1}H NMR** (500 MHz, $CDCl_3$): δ 6.28 (s, 1H), 6.25 (s, 1H), 1.46 (s, 9H), 1.40 (s, 9H), 1.35 (s, 9H) ppm; **^{13}C NMR** (125 MHz, $CDCl_3$): δ 164.2, 158.6, 156.9, 106.3, 52.5, 50.7, 33.3, 30.0,

29.4, 28.4 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{16}H_{30}O_2N_3$ 296.2333 $[M+H]^+$; found 296.2344.

1. Y. Odabachian, S. Tong, Q. Wang, M.-X. Wang and J.-P. Zhu, *Angew. Chem. Int. Ed.,* 2013, **52**, 10878–10882.

Copies of ^{1}H NMR and ^{13}C NMR spectra of all compounds

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128.50
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91.06
77.33
77.01
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51.00
29.85
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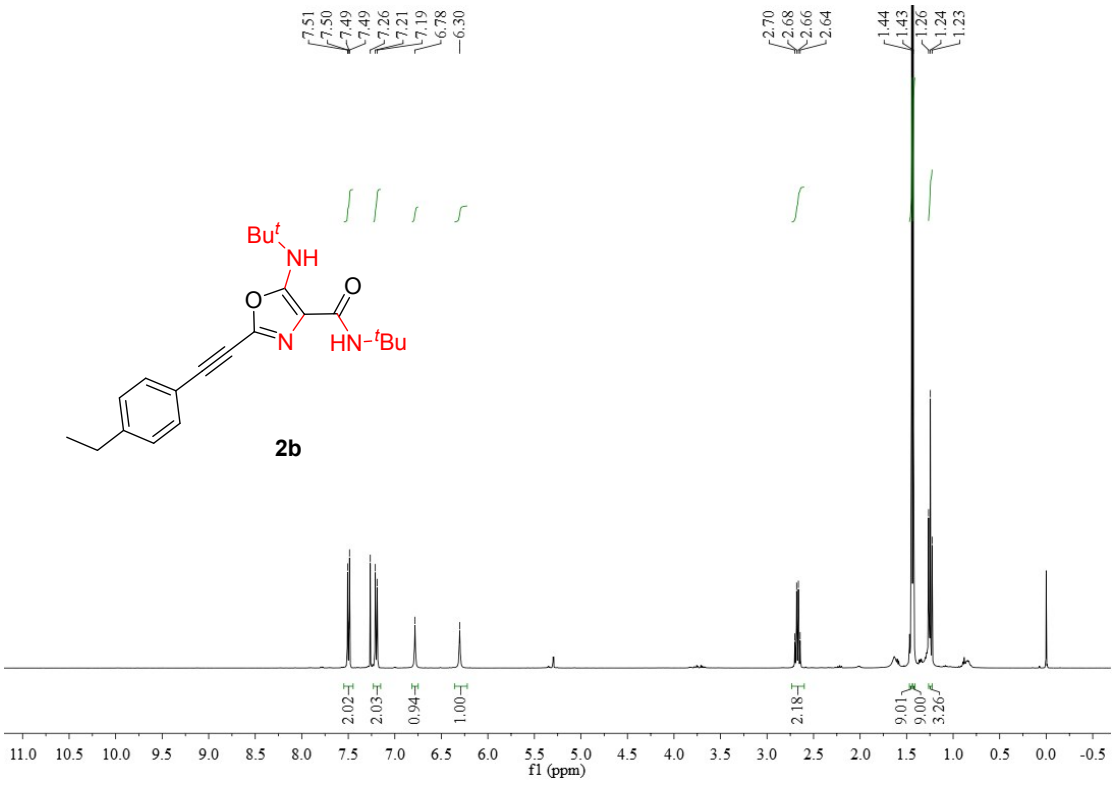
Bu^t
NH
O
O
N
HN-^tBu
2a
f1 (ppm)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1.43
1.26
1.24
1.23
Bu^t
NH
O
O
N
HN-^tBu
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0.94
1.00
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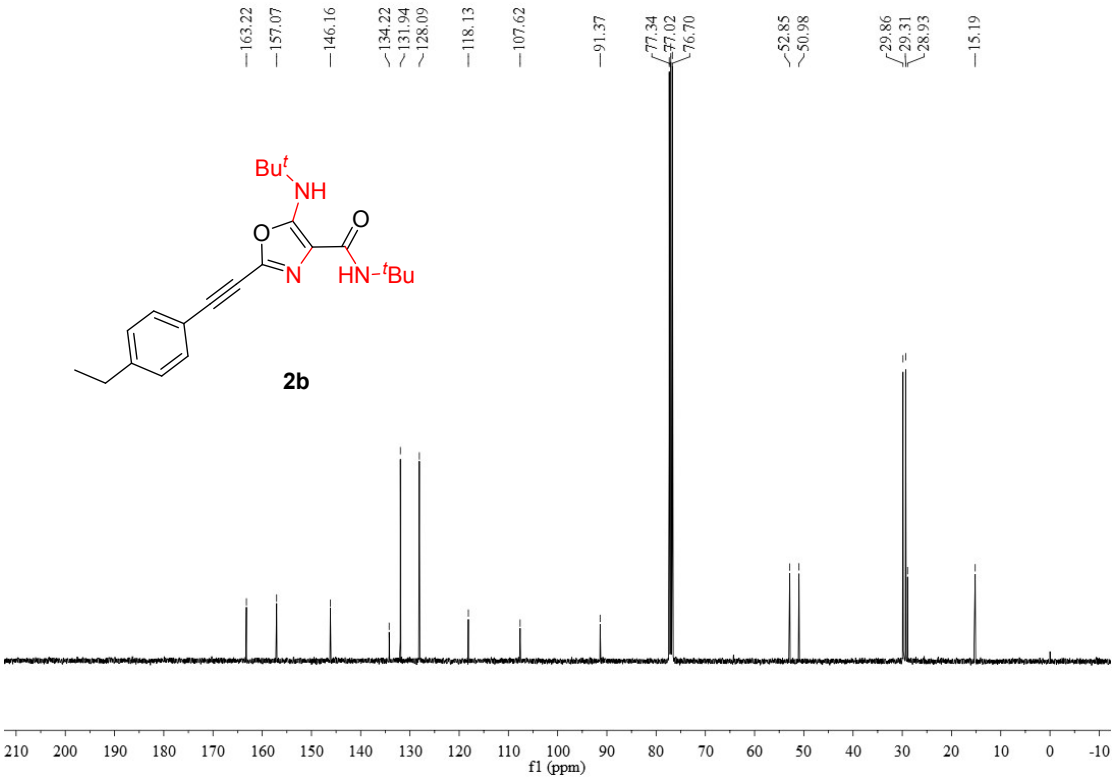
9.01
9.00
3.26
f1 (ppm)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50.98
29.86
29.31
28.93
15.19
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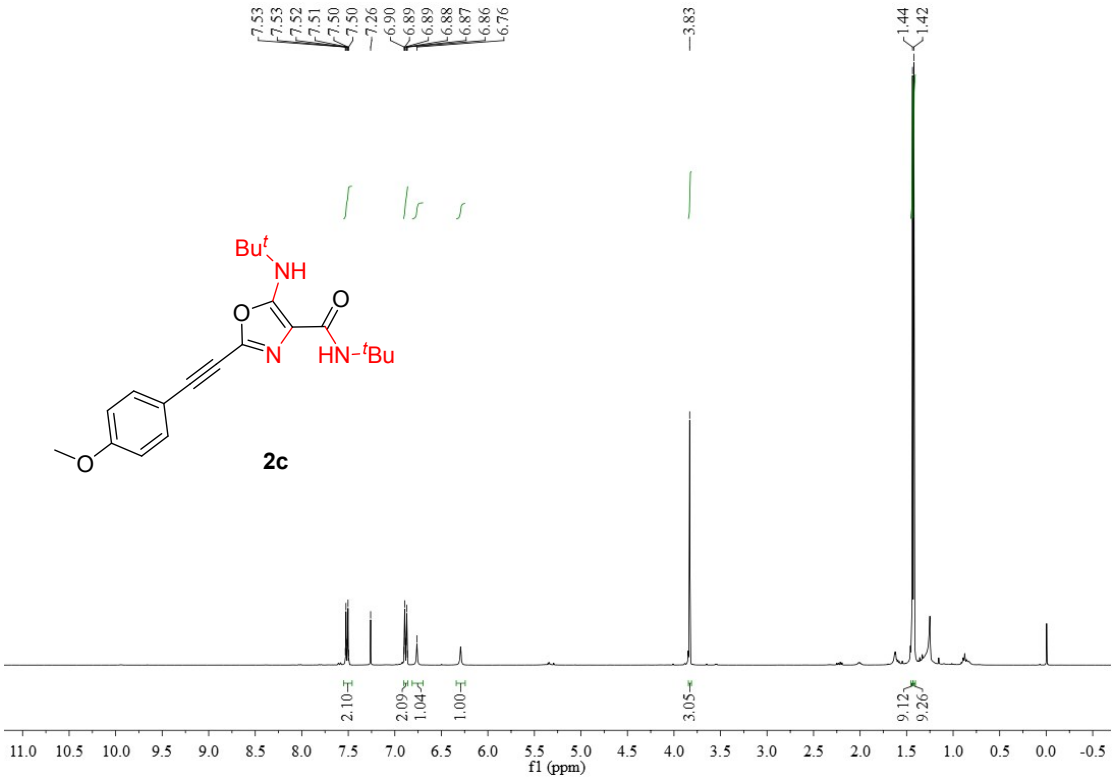
N
HN-^{t}Bu
2b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.89
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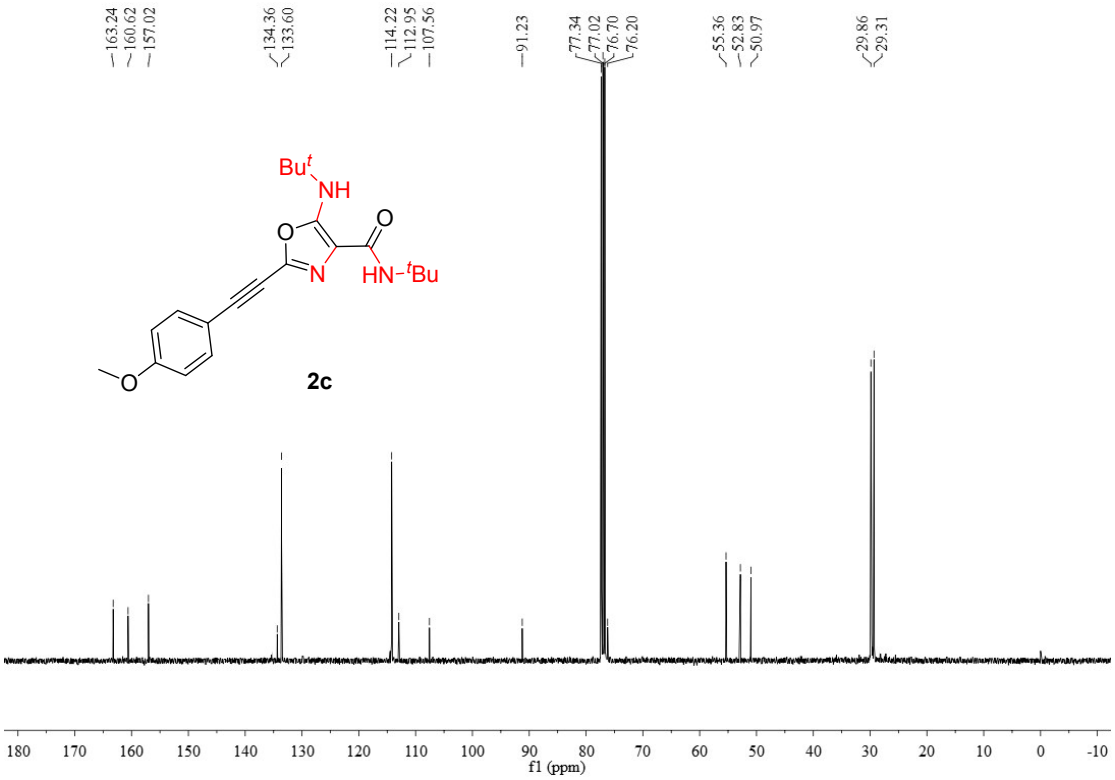
6.76
3.83
1.44
1.42
Bu^t
NH
O
O
N
HN-^{t}Bu
O
2c
2.10
2.09
1.04
1.00
3.05
9.12
9.26
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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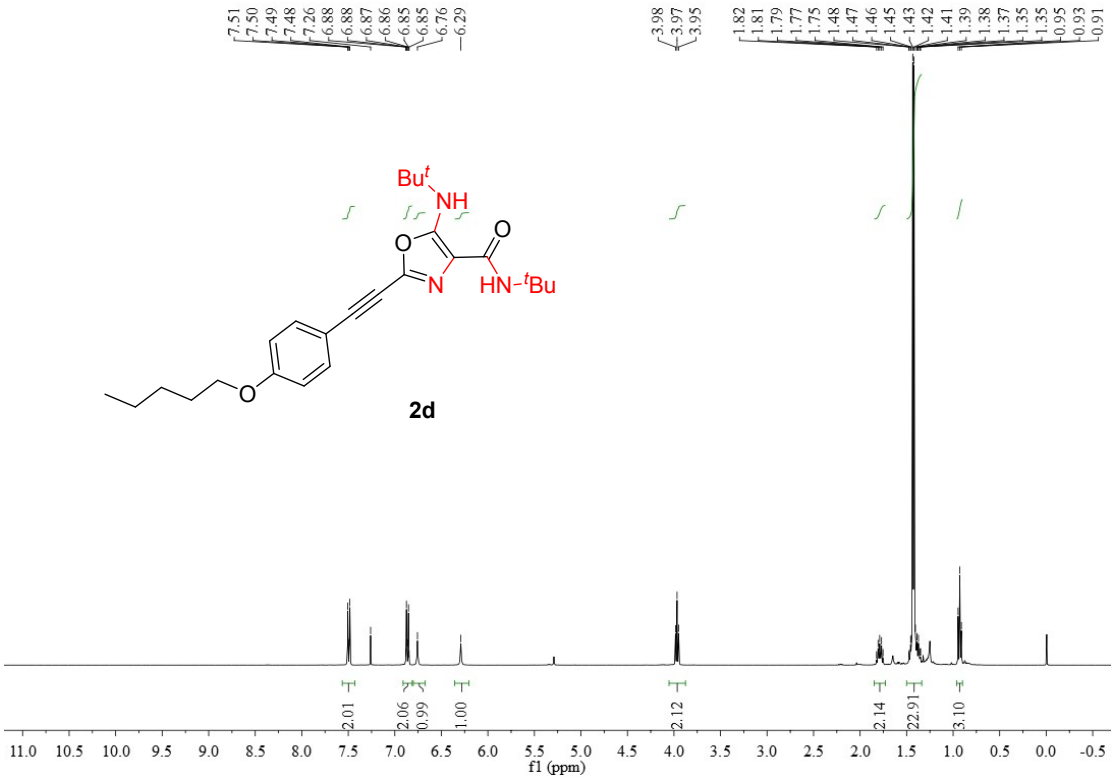
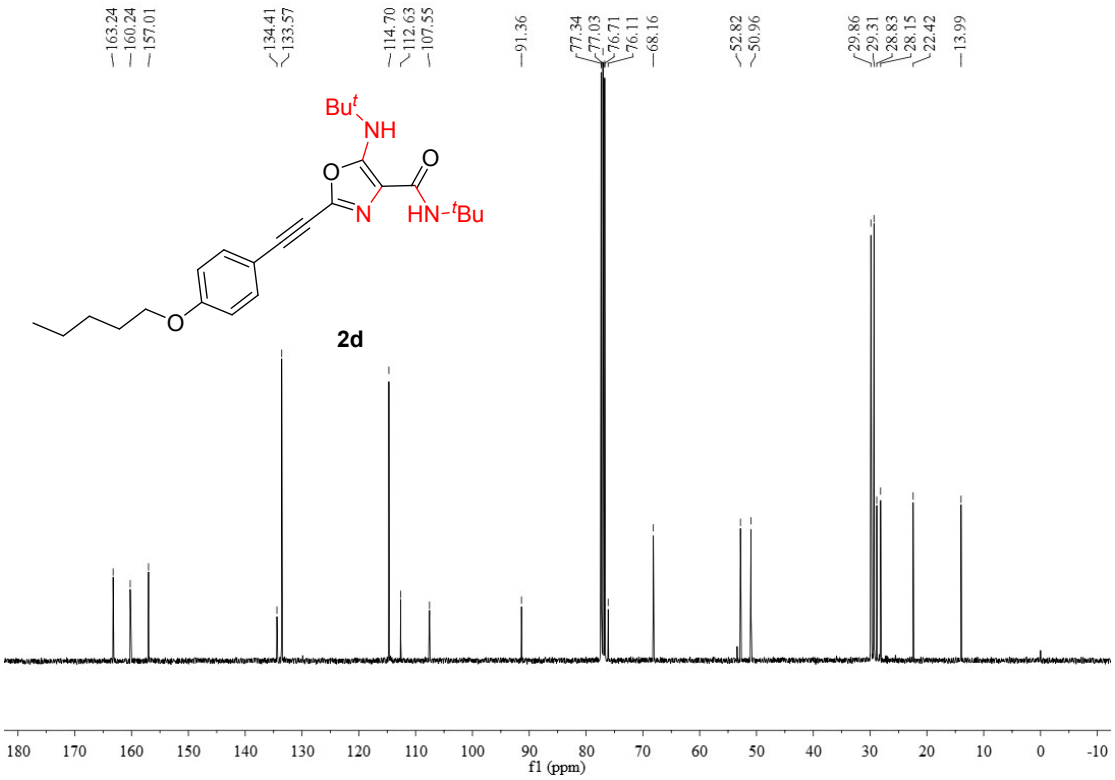
134.36
133.60
114.22
112.95
107.56
91.23
77.34
77.02
76.70
76.20
55.36
52.83
50.97
29.86
29.31
Bu^t
NH
O
N
HN-^{t}Bu
O
2c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.51
7.50
7.49
7.48
7.26
6.88
6.88
6.87
6.86
6.85
6.85
6.76
6.29
3.98
3.97
3.95
1.82
1.81
1.79
1.77
1.75
1.48
1.47
1.46
1.45
1.43
1.42
1.41
1.39
1.38
1.37
1.35
1.35
0.95
0.93
0.91
Bu^t
NH
O
N
HN-^{t}Bu
O
2d
2.01
2.06
0.99
1.00
2.12
2.14
22.91
3.10
11.0 10.5 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 -0.5
f1 (ppm)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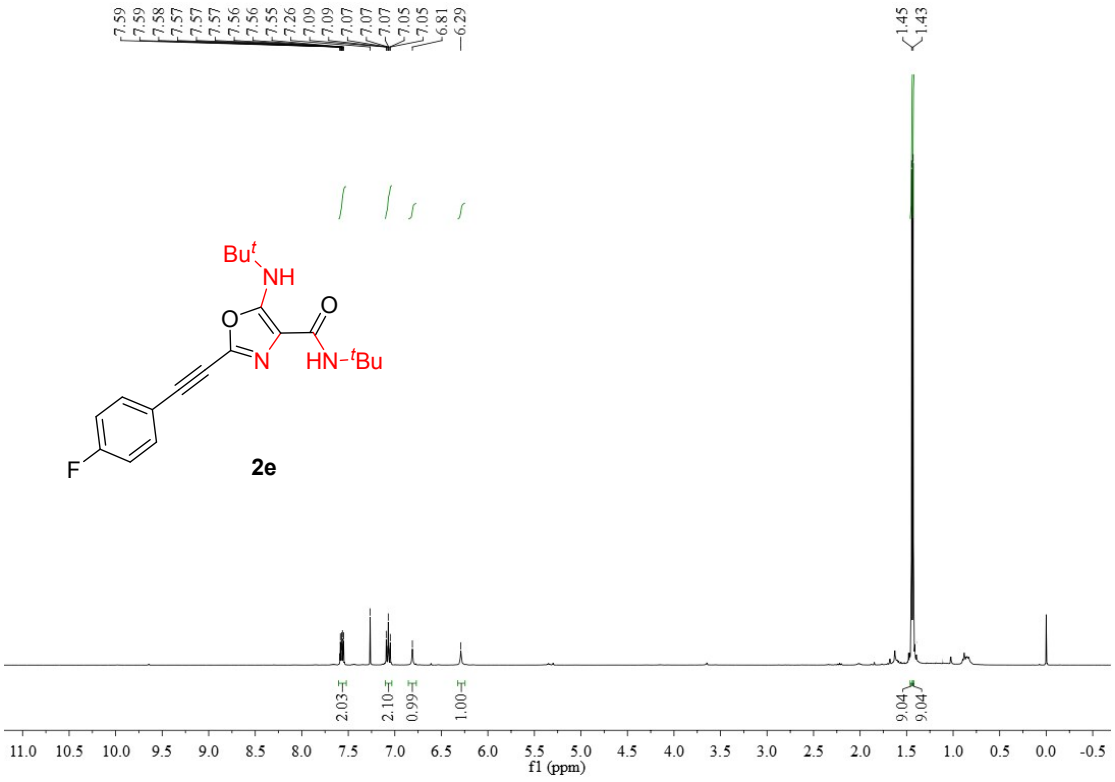
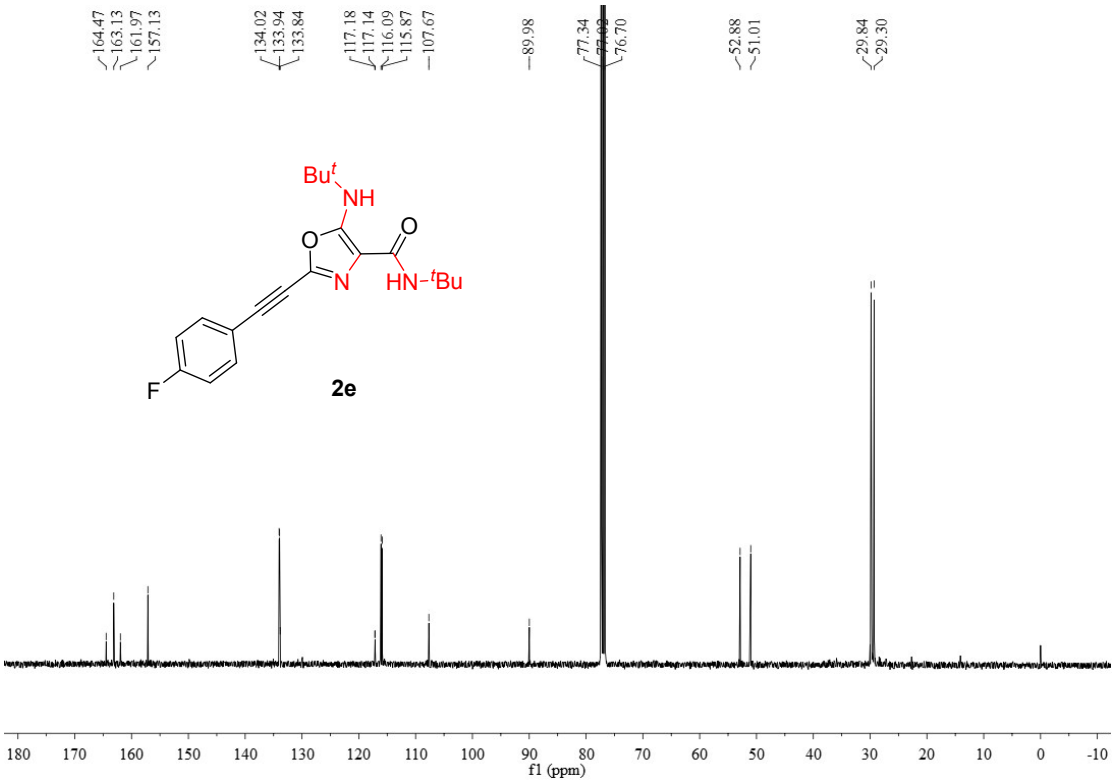
160.24
157.01
134.41
133.57
114.70
112.63
107.55
91.36
77.34
77.03
76.71
76.11
68.16
52.82
50.96
29.86
29.31
28.83
28.15
22.42
13.99
Bu^t
NH
O
O
N
HN-^{t}Bu
O
2d
f1 (ppm)


7.59
7.59
7.58
7.57
7.57
7.57
7.56
7.56
7.55
7.26
7.09
7.09
7.07
7.07
7.07
7.05
7.05
6.81
6.29
1.45
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
F
2e
2.03
2.10
0.99
1.00
9.04
9.04
f1 (ppm)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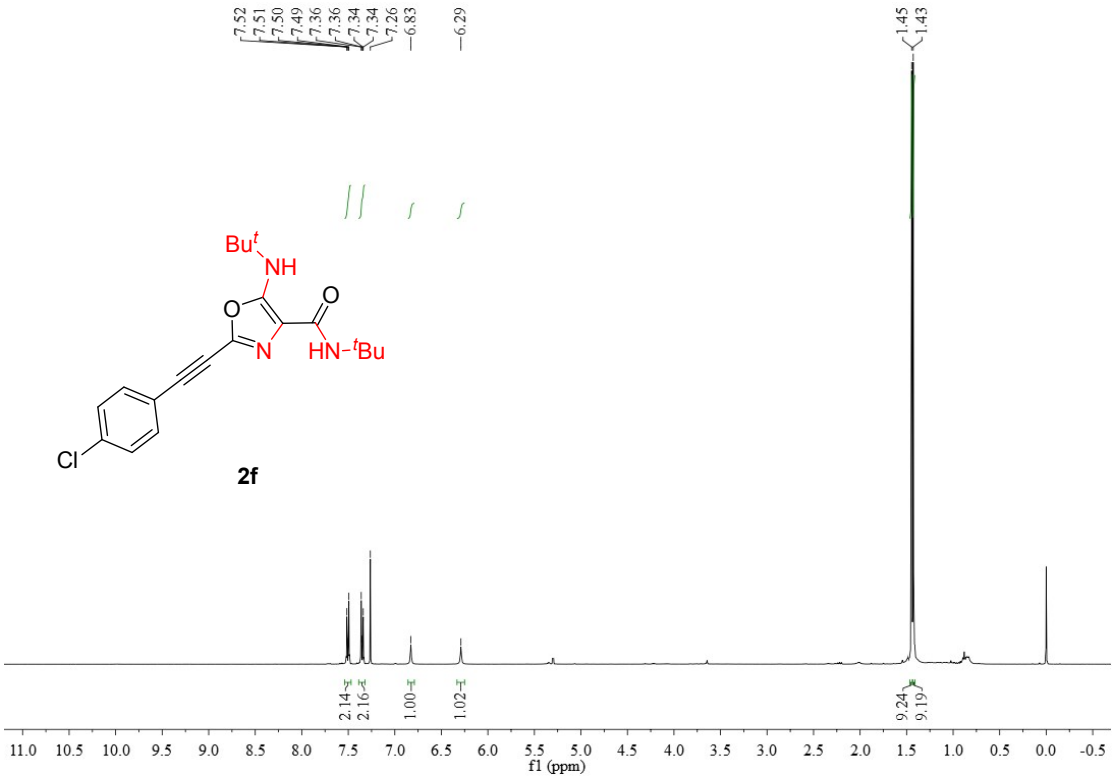
133.94
133.84
117.18
117.14
116.09
115.87
107.67
89.98
77.34
76.70
52.88
51.01
29.84
29.30
Bu^t
NH
O
O
N
HN-^{t}Bu
F
2e
f1 (ppm)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7.51
7.50
7.49
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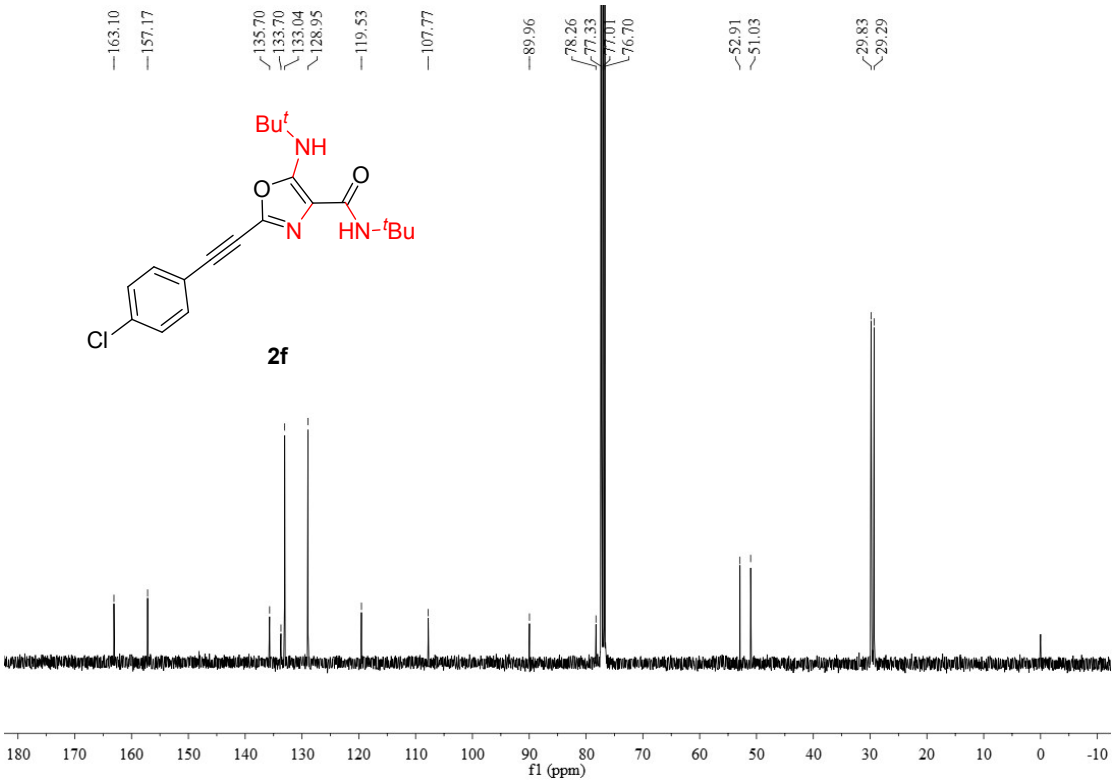
7.36
7.34
7.34
7.26
6.83
6.29
1.45
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
Cl
2f
2.14
2.16
1.00
1.02
9.24
9.19
f1 (ppm)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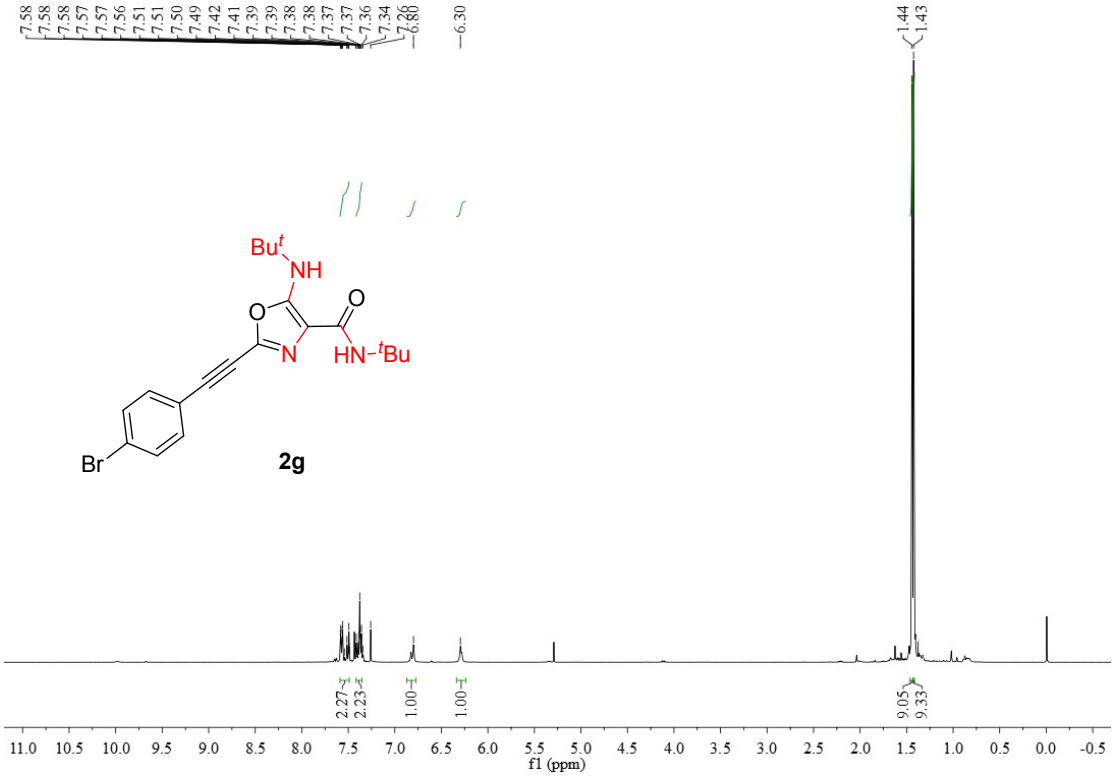
128.95
119.53
107.77
89.96
78.26
77.33
77.01
76.70
52.91
51.03
29.83
29.29
Bu^t
NH
O
O
N
HN-^{t}Bu
Cl
2f
f1 (ppm)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7.58
7.57
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7.51
7.50
7.49
7.42
7.41
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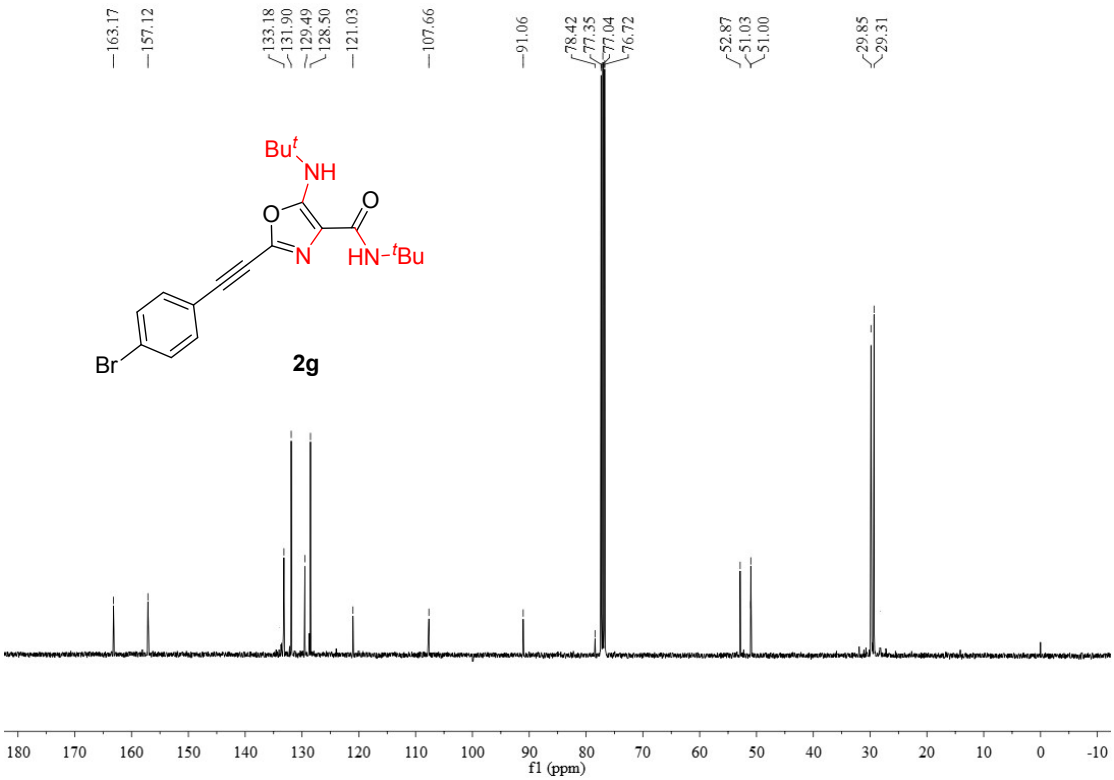
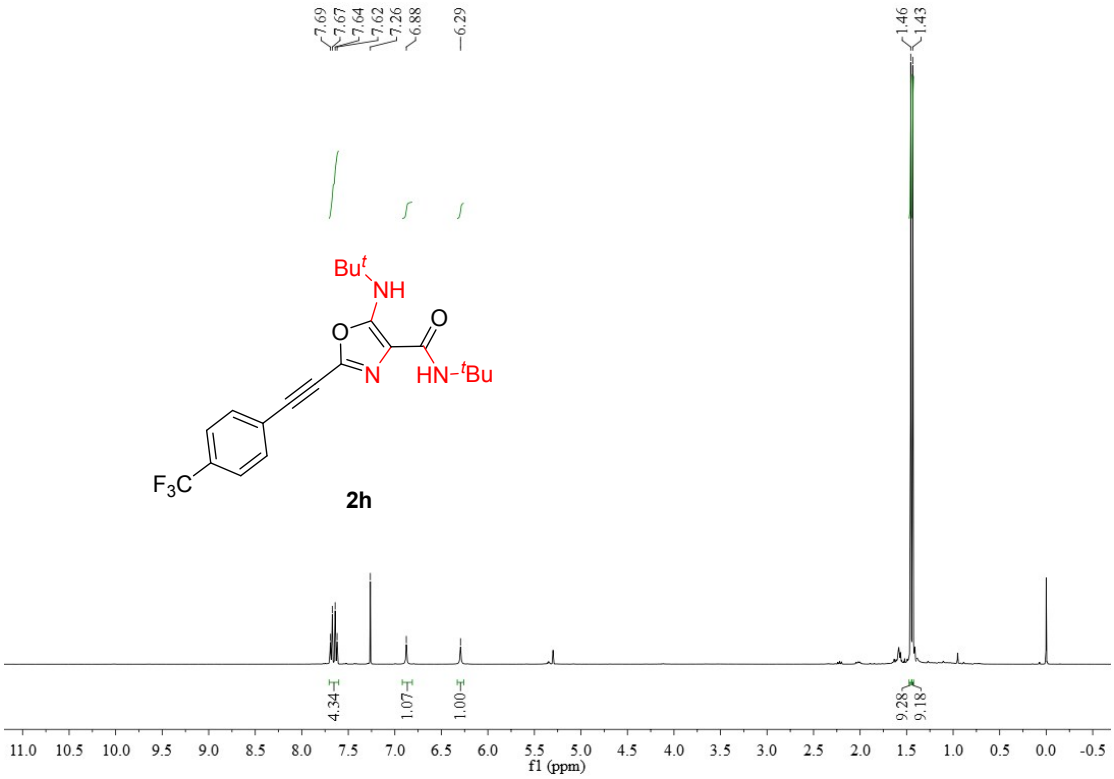
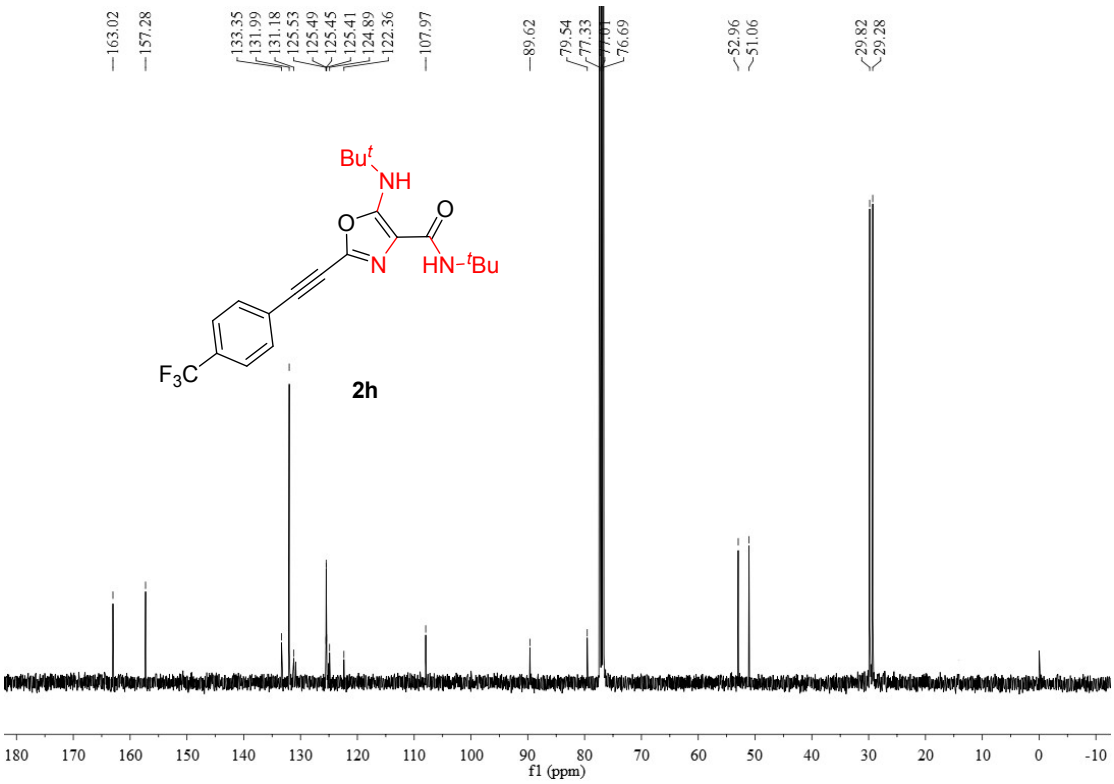
7.39
7.38
7.38
7.37
7.37
7.36
7.34
7.26
6.80
6.30
1.44
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
Br
2g
2.27
2.23
1.00
1.00
9.05
9.33
f1 (ppm)


163.17
157.12
133.18
131.90
129.49
128.50
121.03
107.66
91.06
78.42
77.35
77.04
76.72
52.87
51.03
51.00
29.85
29.31
Bu^t
NH
O
O
N
HN-^{t}Bu
Br
2g
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.69
7.67
7.64
7.62
7.26
6.88
6.29
1.46
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
F$_3$C
2h
4.34
1.07
1.00
9.28
9.18
11.0 10.5 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 -0.5
f1 (ppm)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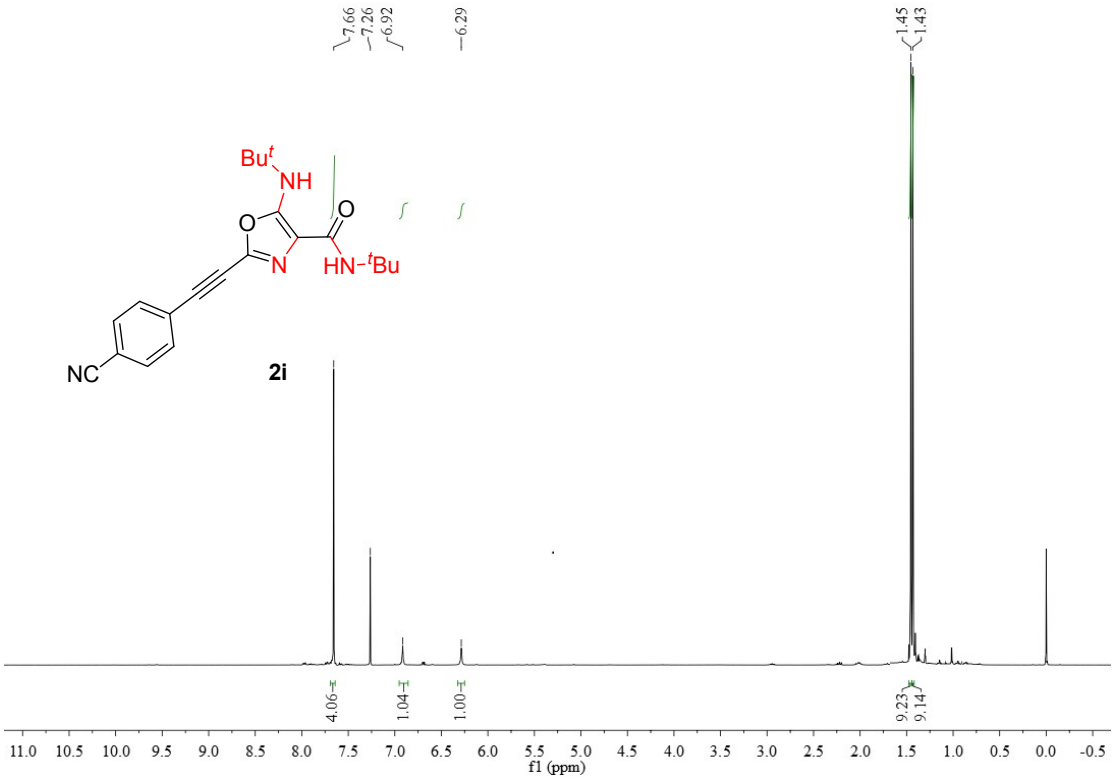
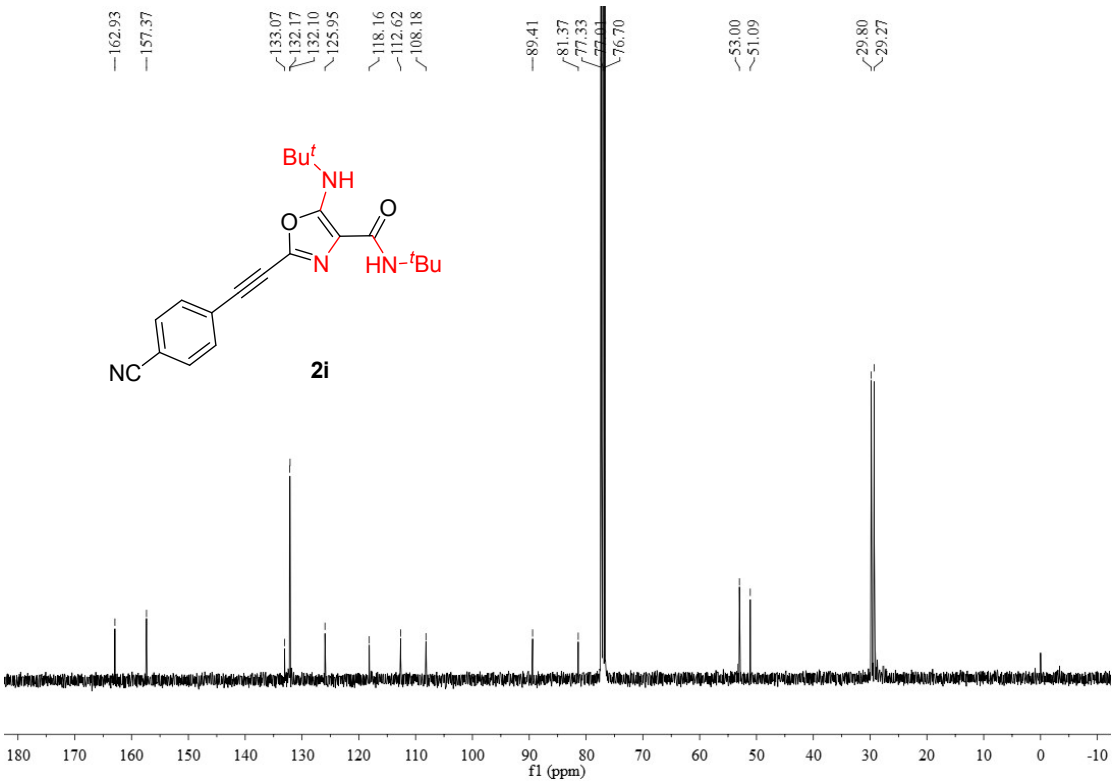
125.53
125.49
125.45
125.41
124.89
122.36
107.97
89.62
79.54
77.33
76.69
52.96
51.06
29.82
29.28
Bu^t
NH
O
O
N
HN-^{t}Bu
F$_3$C
2h
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.66
7.26
6.92
6.29
1.45
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
NC
2i
4.06
1.04
1.00
9.23
9.14
11.0 10.5 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 -0.5
f1 (ppm)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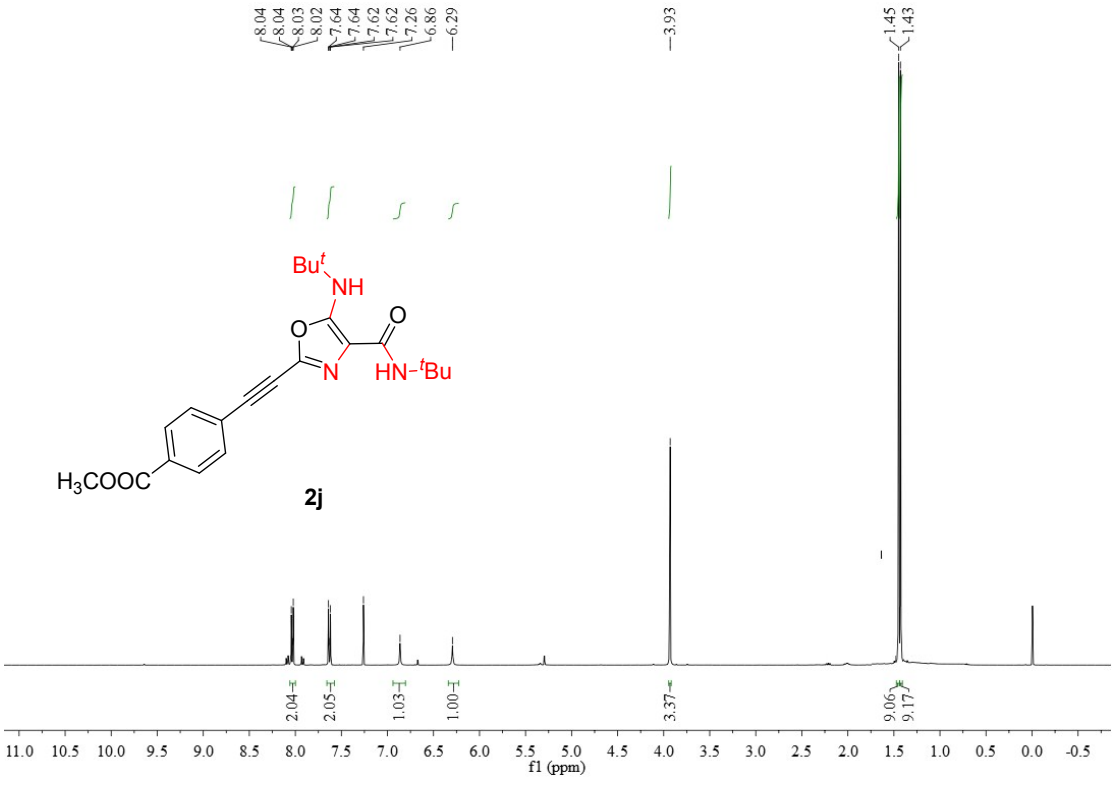
118.16
112.62
108.18
89.41
81.37
77.33
77.01
76.70
53.00
51.09
29.80
29.27
Bu^t
NH
O
O
N
HN-^tBu
NC
2i
f1 (ppm)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8.04
8.03
8.02
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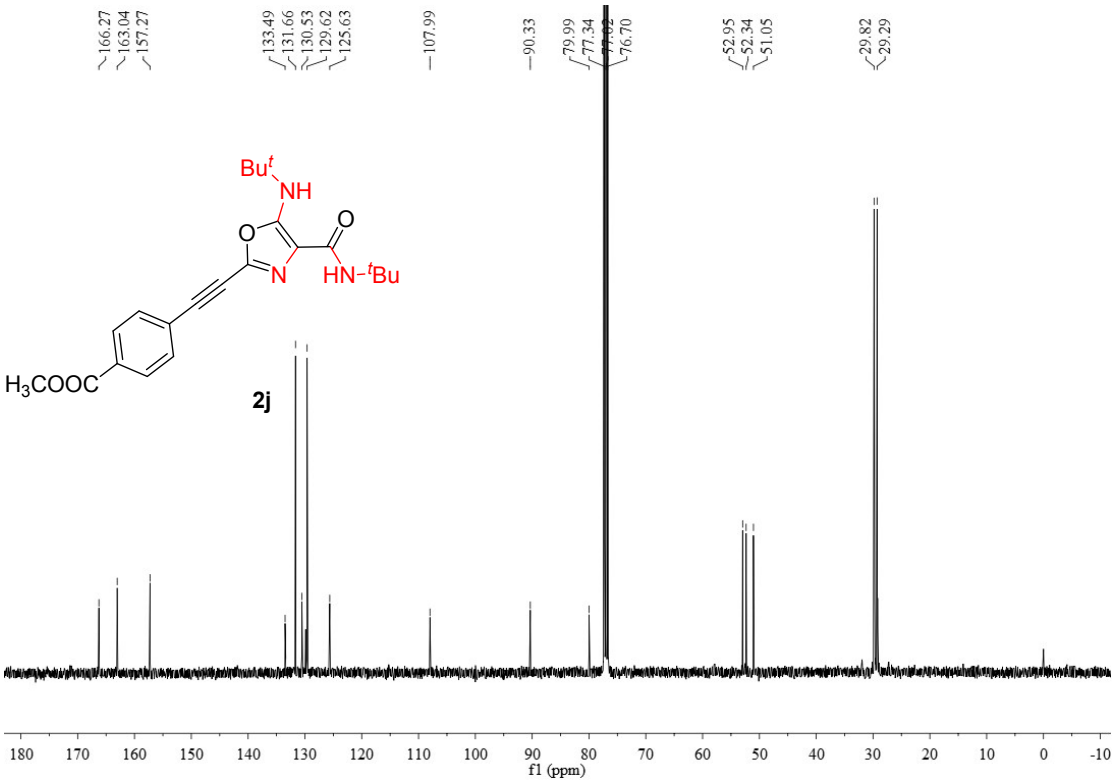
7.64
7.62
7.62
7.26
6.86
6.29
3.93
1.45
1.43
Bu^t
NH
O
O
N
HN-^tBu
H3COOC
2j
2.04
2.05
1.03
1.00
3.37
9.06
9.17
f1 (ppm)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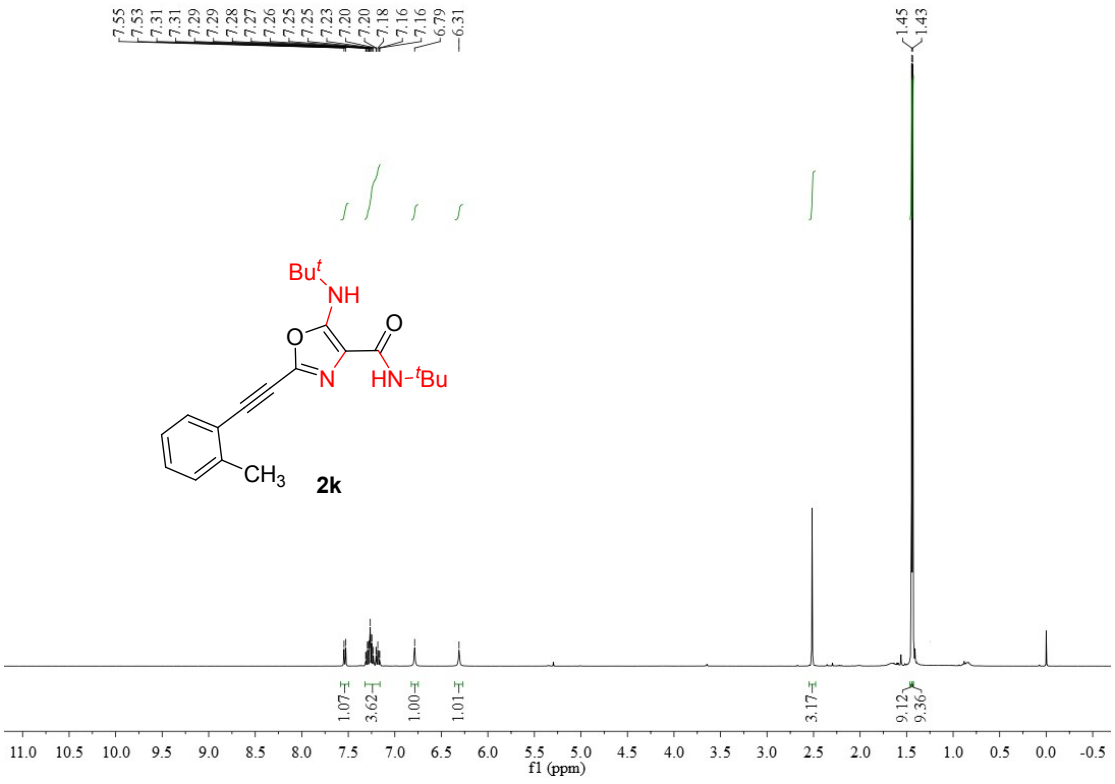
130.53
129.62
125.63
107.99
90.33
79.99
77.34
76.70
52.95
52.34
51.05
29.82
29.29
Bu^t
NH
O
O
N
HN-^tBu
H3COOC
2j
f1 (ppm)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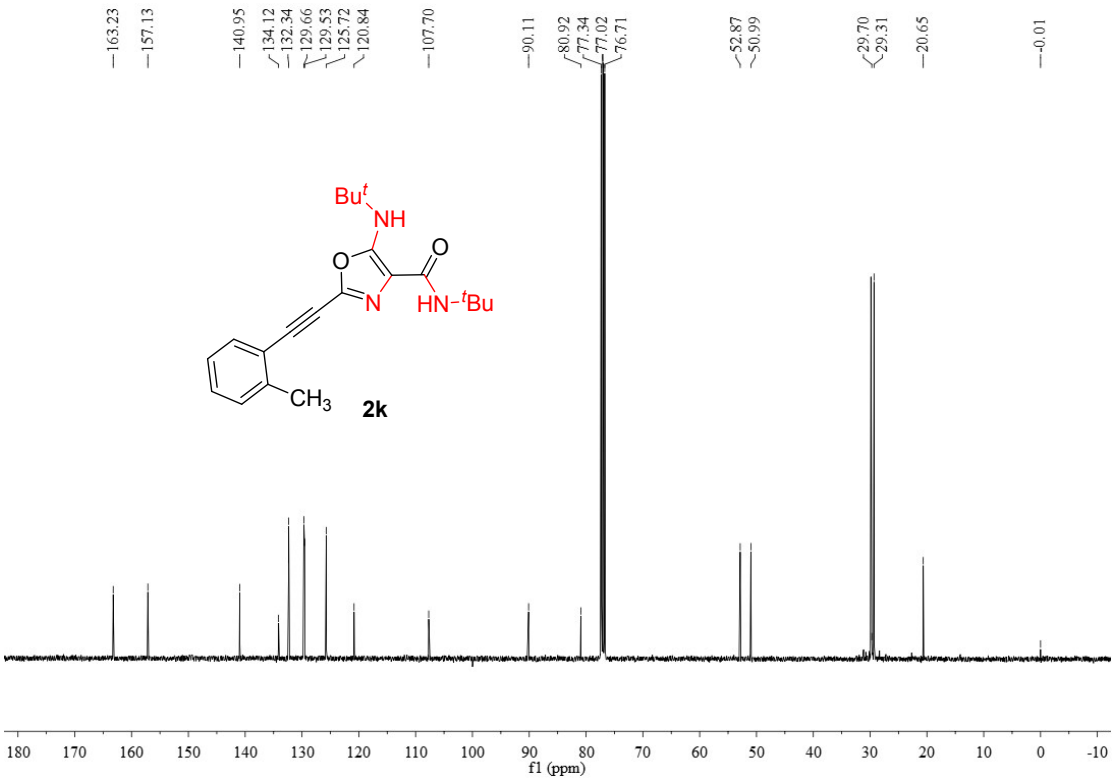
7.25
7.25
7.23
7.20
7.20
7.18
7.16
7.16
6.79
6.31
1.45
1.43
Bu^t
NH
O
O
N
HN-^tBu
CH3
2k
1.07
3.62
1.00
1.01
3.17
9.12
9.36
f1 (ppm)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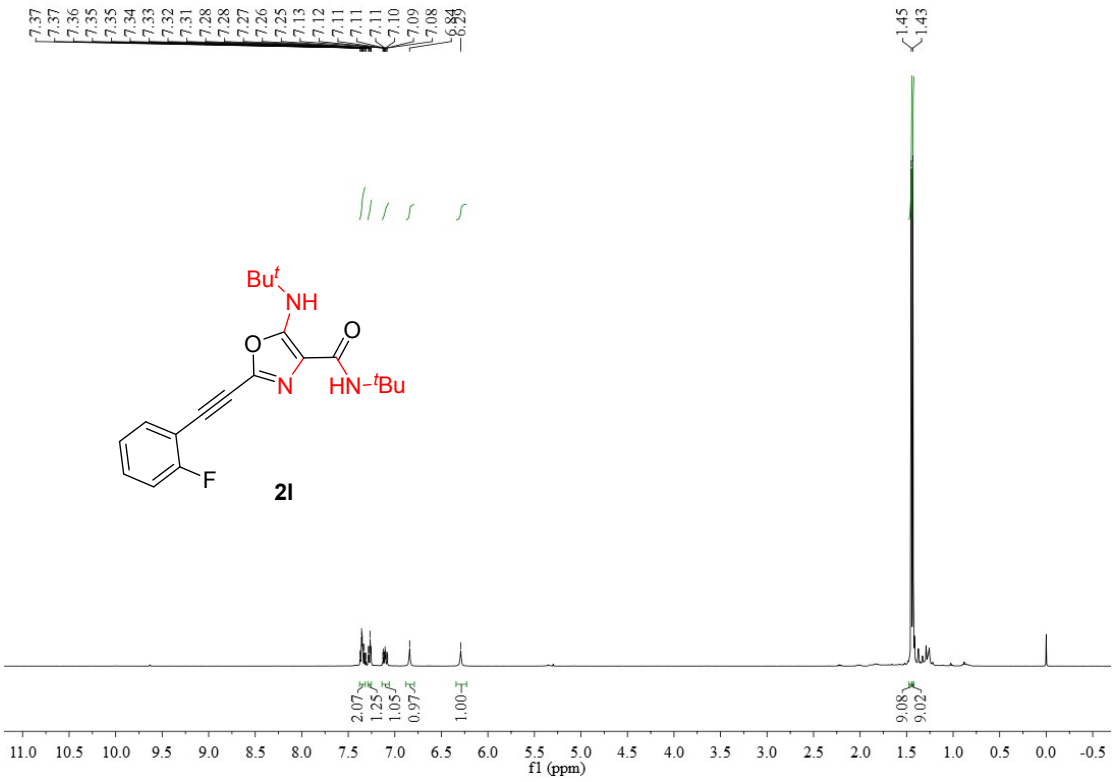
132.34
129.66
129.53
125.72
120.84
107.70
90.11
80.92
77.34
77.02
76.71
52.87
50.99
29.70
29.31
20.65
-0.01
Bu^t
NH
O
O
N
HN-^{t}Bu
CH$_3$
2k
f1 (ppm)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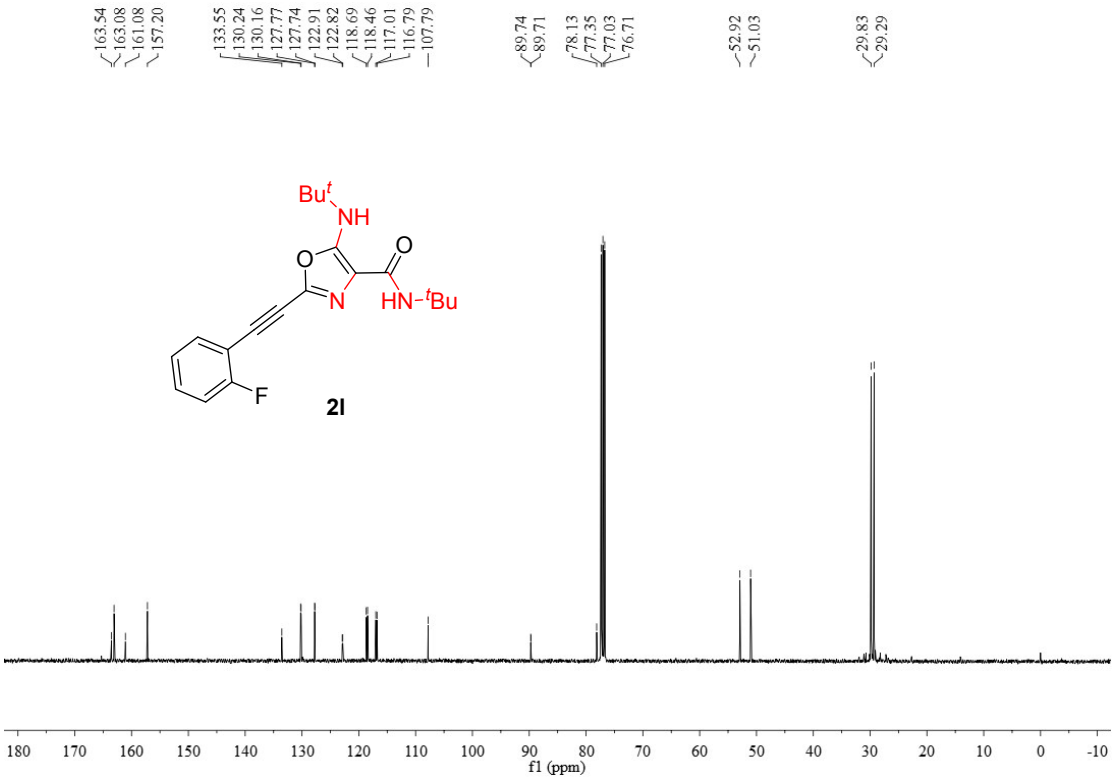
7.26
7.25
7.13
7.12
7.11
7.11
7.11
7.10
7.09
7.08
6.84
6.83
1.45
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
F
2l
2.07
1.25
1.05
0.97
1.00
9.08
9.02
f1 (ppm)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122.82
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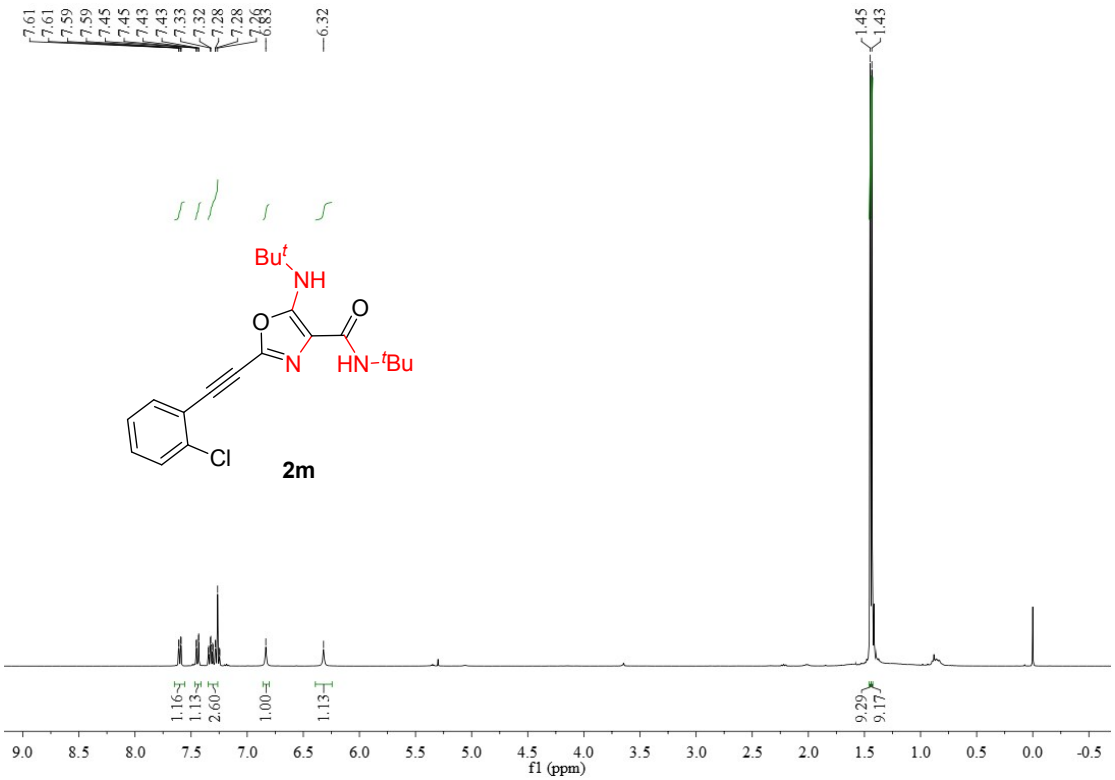
117.01
116.79
107.79
89.74
89.71
78.13
77.35
77.03
76.71
52.92
51.03
29.83
29.29
Bu^t
NH
O
O
N
HN-^{t}Bu
F
2l
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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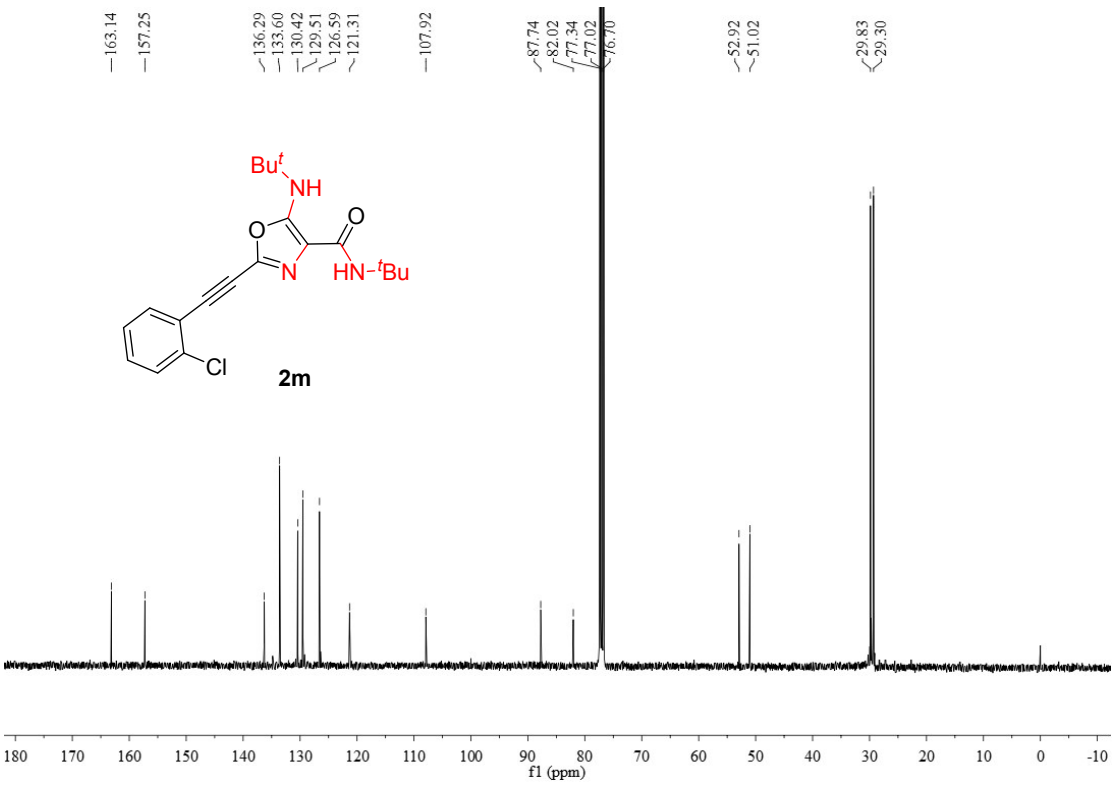
7.43
7.43
7.33
7.32
7.28
7.26
6.83
6.32
1.45
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
Cl
2m
1.16
1.13
2.60
1.00
1.13
9.29
9.17
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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121.31
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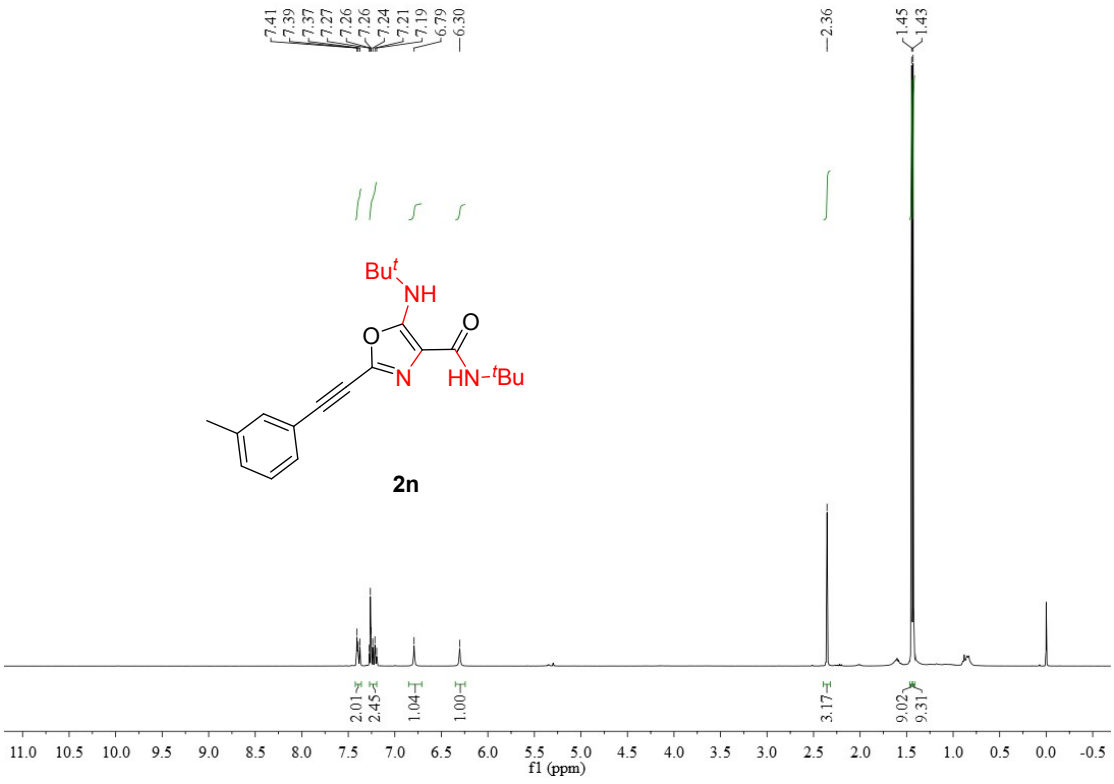
87.74
82.02
77.34
77.02
76.70
52.92
51.02
29.83
29.30
Bu^t
NH
O
O
N
HN-^{t}Bu
Cl
2m
f1 (ppm)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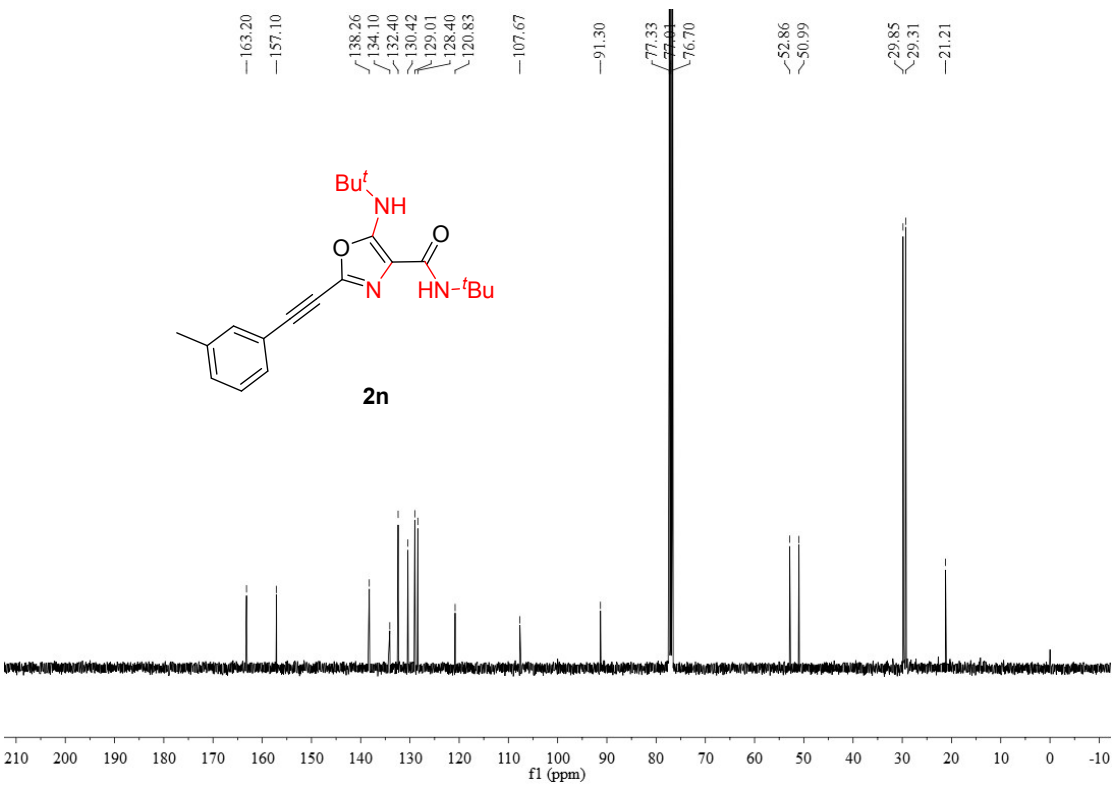
7.26
7.24
7.21
7.19
6.79
6.30
2.36
1.45
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
2n
2.01
2.45
1.04
1.00
3.17
9.02
9.31
f1 (ppm)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128.40
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91.30
77.33
77.01
76.70
52.86
50.99
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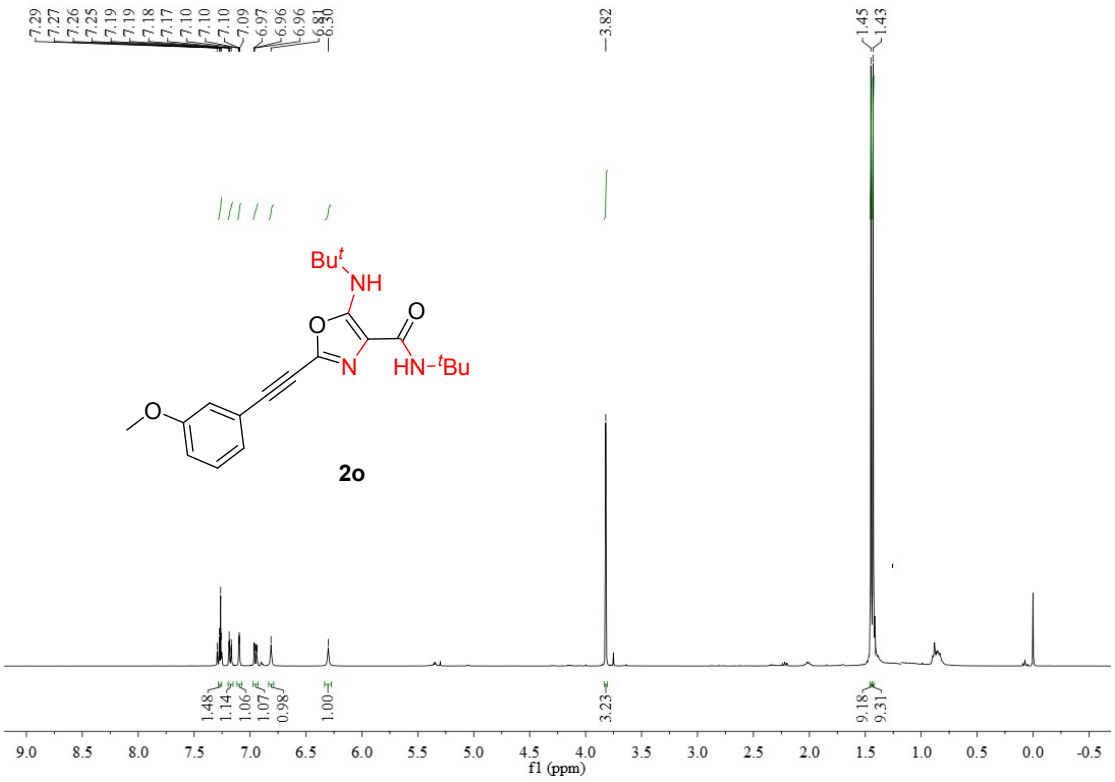
29.31
21.21
Bu^t
NH
O
O
N
HN-^{t}Bu
2n
f1 (ppm)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7.17
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7.10
7.09
6.97
6.96
6.96
6.81
6.80
3.82
1.45
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
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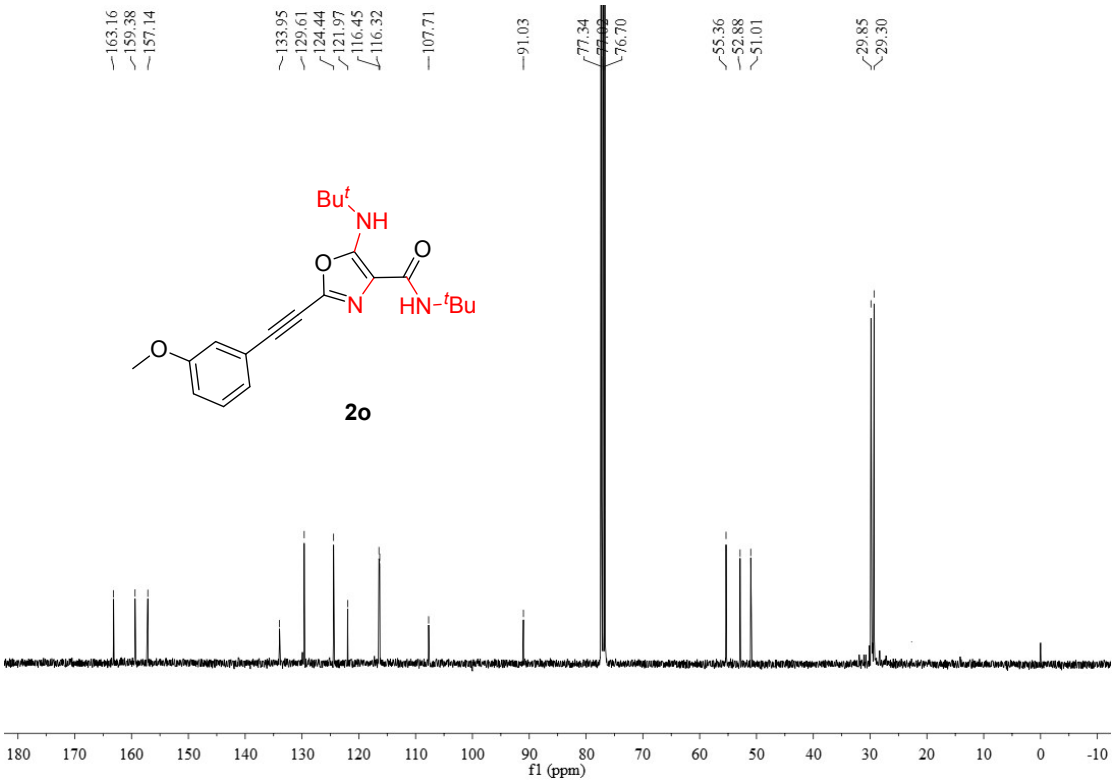
1.14
1.06
1.07
0.98
1.00
3.23
9.18
9.31
f1 (ppm)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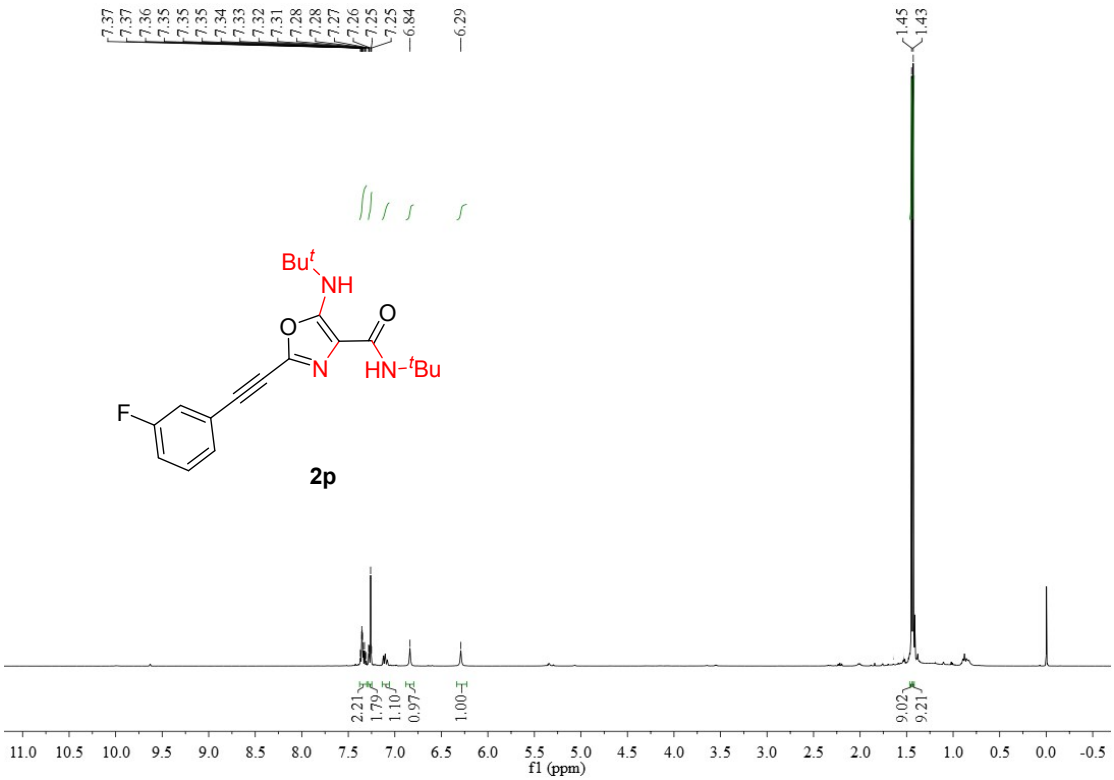
124.44
121.97
116.45
116.32
107.71
91.03
77.34
77.03
76.70
55.36
52.88
51.01
29.85
29.30
Bu^t
NH
O
O
N
HN-^{t}Bu
O
2o
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.28
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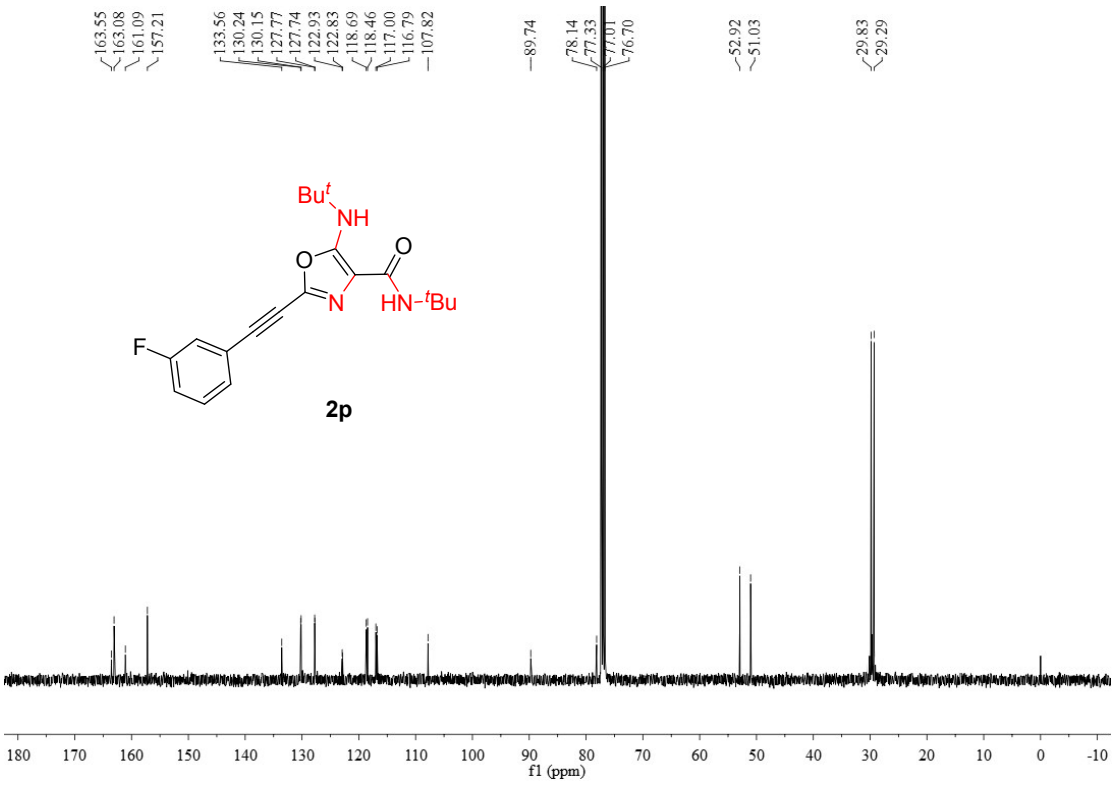
7.27
7.26
7.25
7.25
6.84
6.29
1.45
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
F
2p
2.21
1.79
1.10
0.97
1.00
9.02
9.21
f1 (ppm)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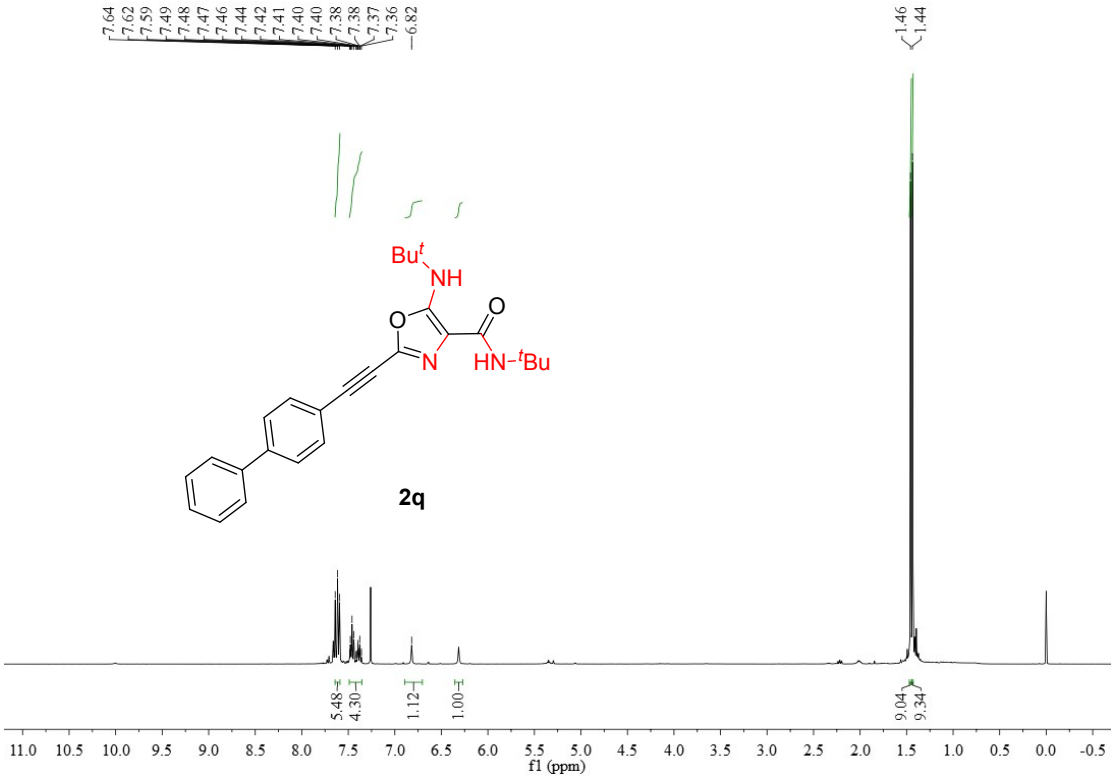
122.93
122.83
118.69
118.46
117.00
116.79
107.82
89.74
78.14
77.33
77.01
76.70
52.92
51.03
29.83
29.29
Bu^t
NH
O
O
N
HN-^{t}Bu
F
2p
f1 (ppm)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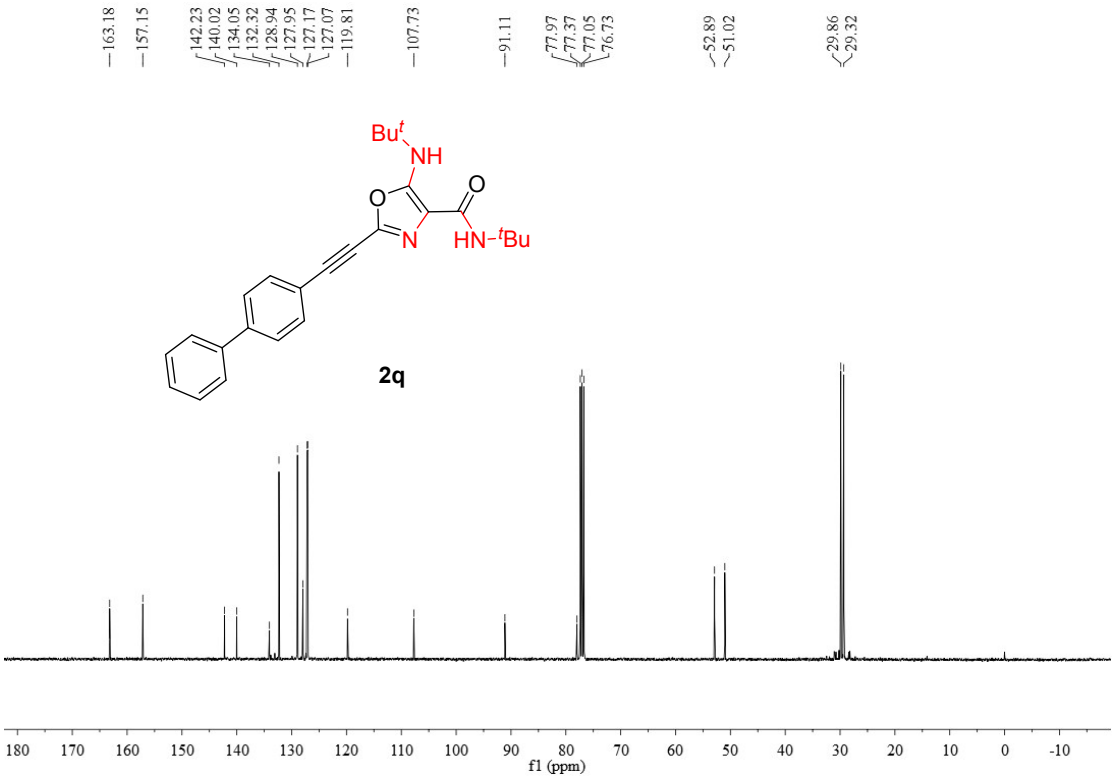
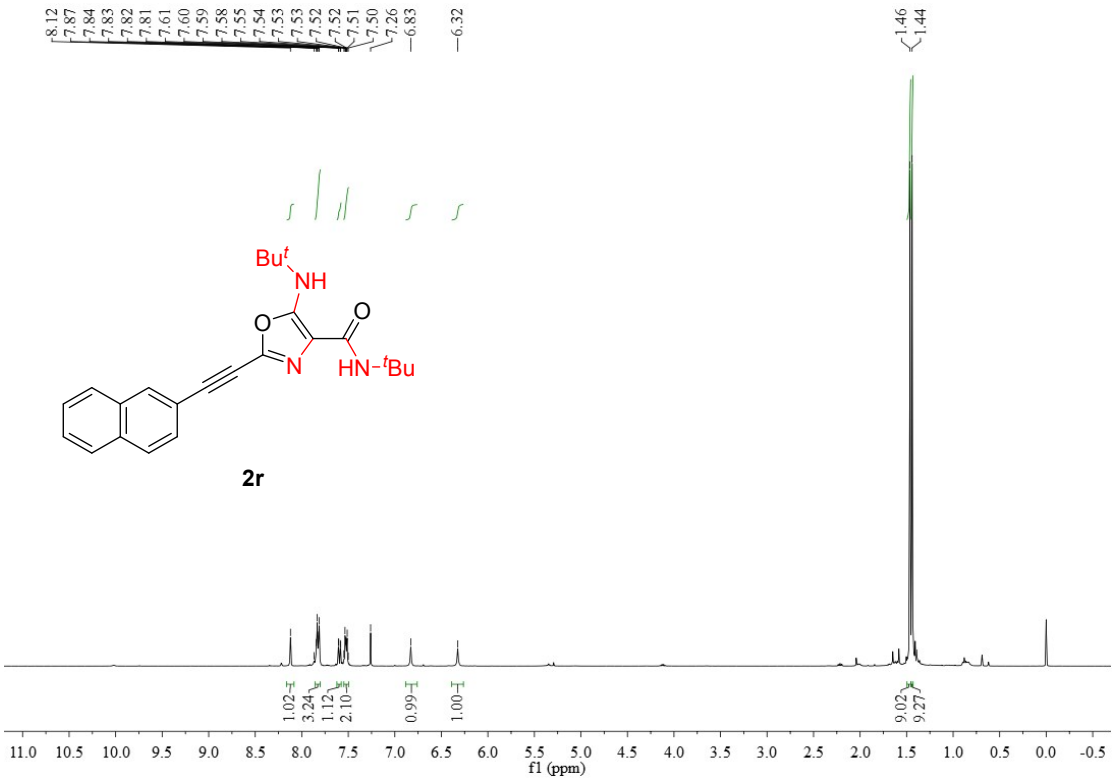
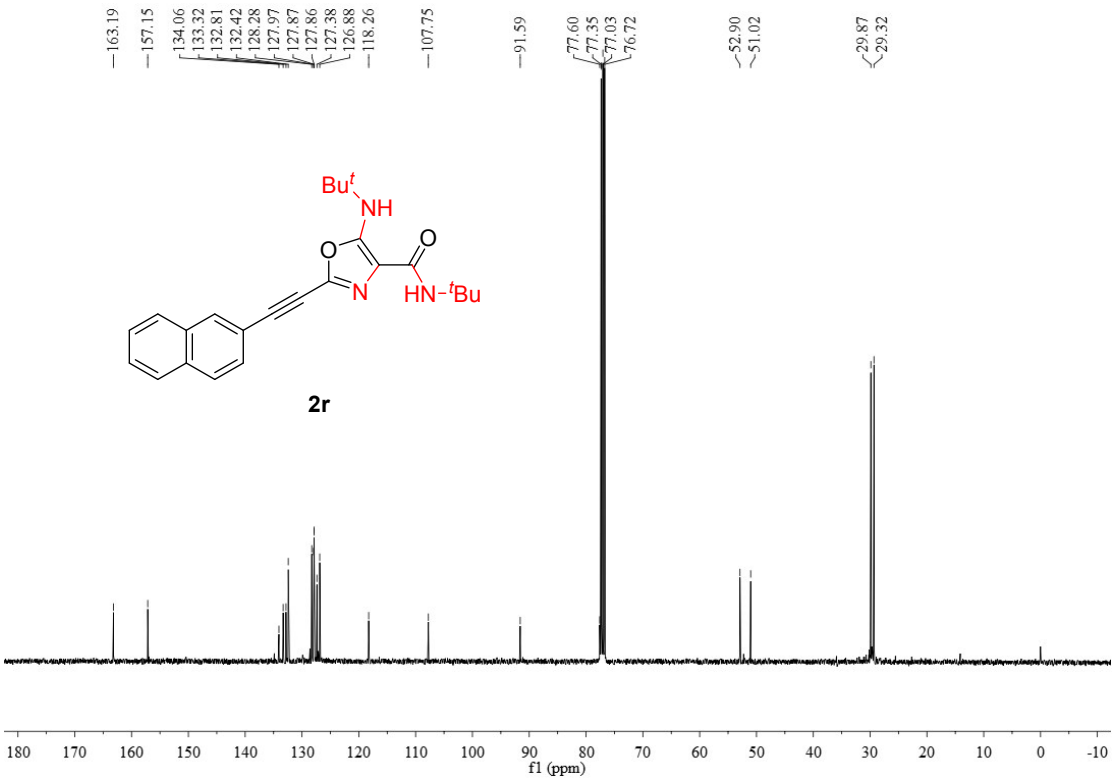
7.38
7.37
7.36
6.82
1.46
1.44
Bu^t
NH
O
O
N
HN-^tBu
2q
5.48
4.30
1.12
1.00
9.04
9.34
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

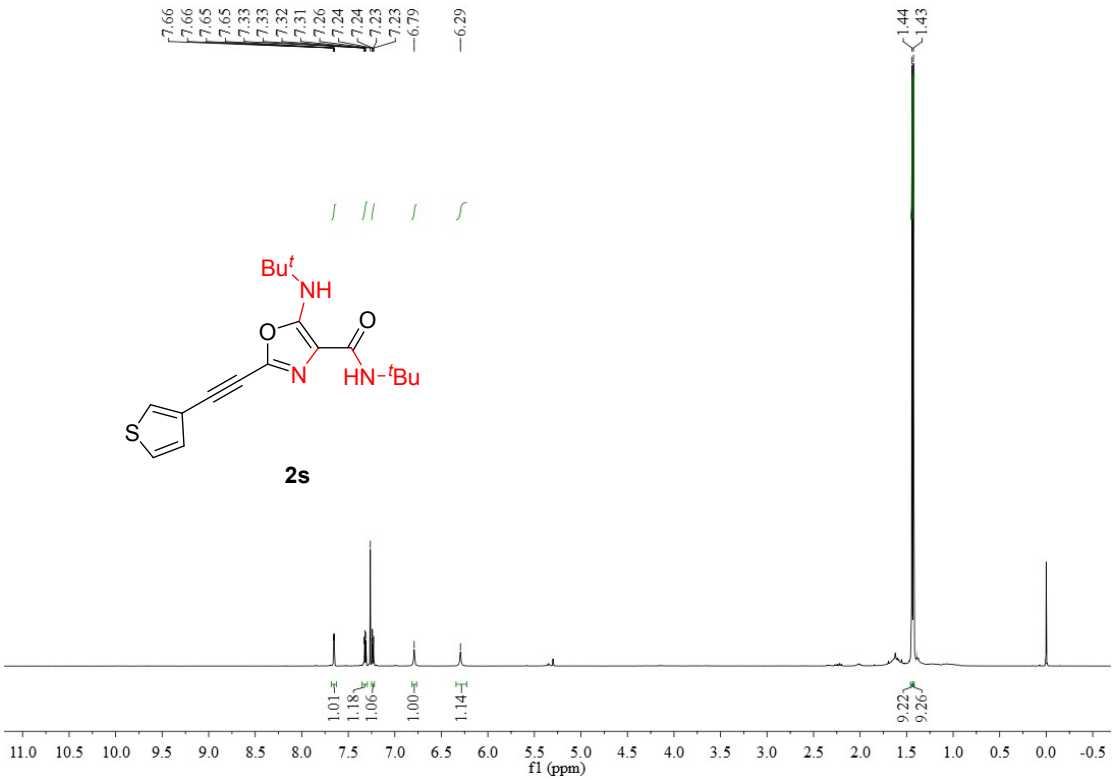

163.18
157.15
142.23
140.02
134.05
132.32
128.94
127.95
127.17
127.07
119.81
107.73
91.11
77.97
77.37
77.05
76.73
52.89
51.02
29.86
29.32
Bu^t
NH
O
O
N
HN-^tBu
2q
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

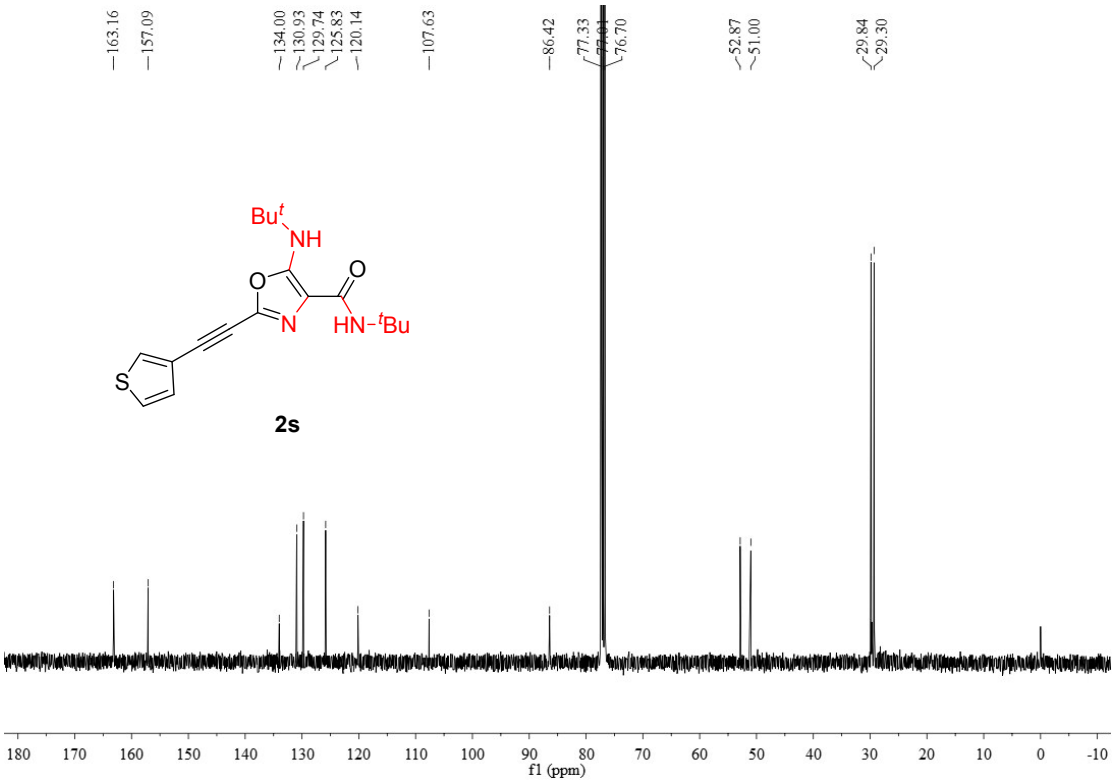

8.12
7.87
7.84
7.83
7.82
7.81
7.61
7.60
7.59
7.58
7.55
7.54
7.53
7.53
7.52
7.52
7.51
7.50
7.26
6.83
6.32
1.46
1.44
Bu^t
NH
O
O
N
HN-^{t}Bu
1.02
3.24
1.12
2.10
0.99
1.00
9.02
9.27
f1 (ppm)

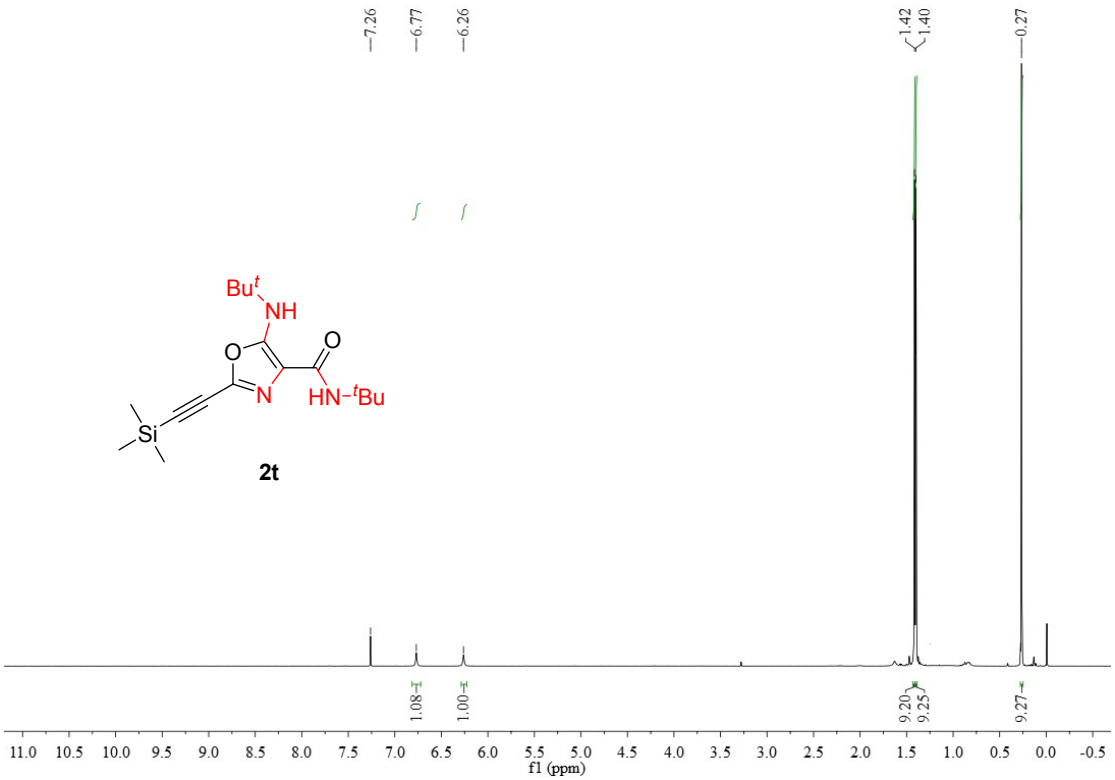
2r

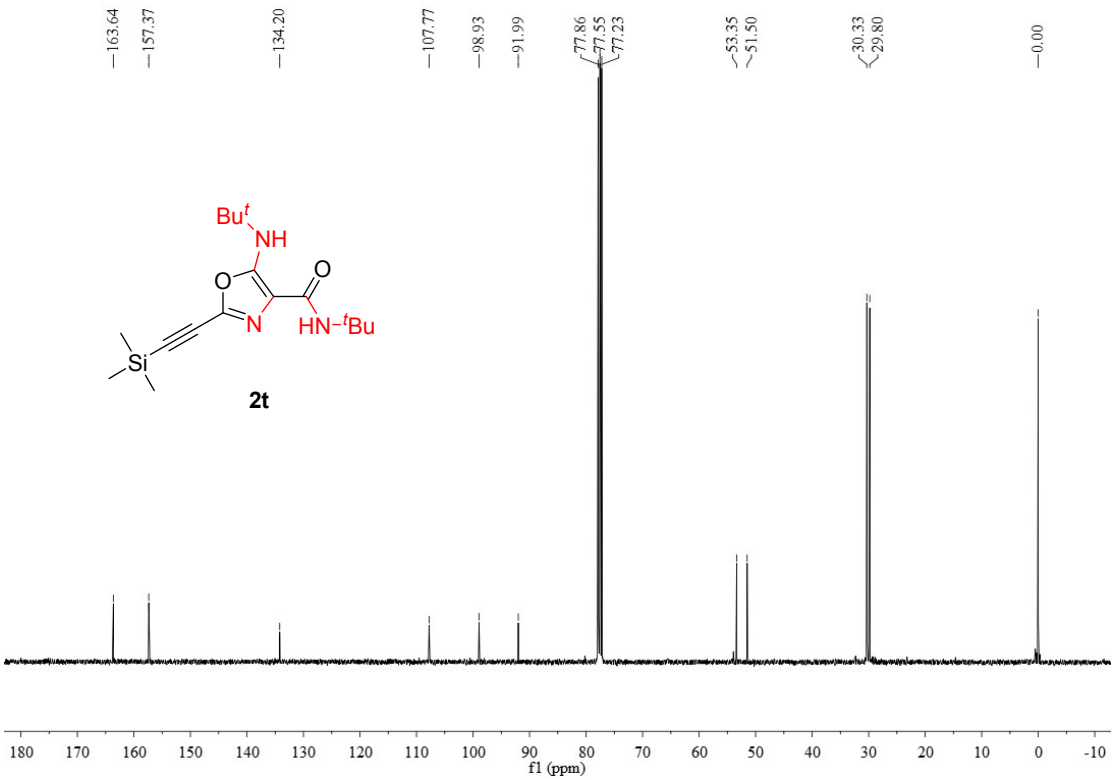

163.19
157.15
134.06
133.32
132.81
132.42
128.28
127.97
127.87
127.86
127.38
126.88
118.26
107.75
91.59
77.60
77.35
77.03
76.72
52.90
51.02
29.87
29.32
Bu^t
NH
O
O
N
HN-^{t}Bu
f1 (ppm)

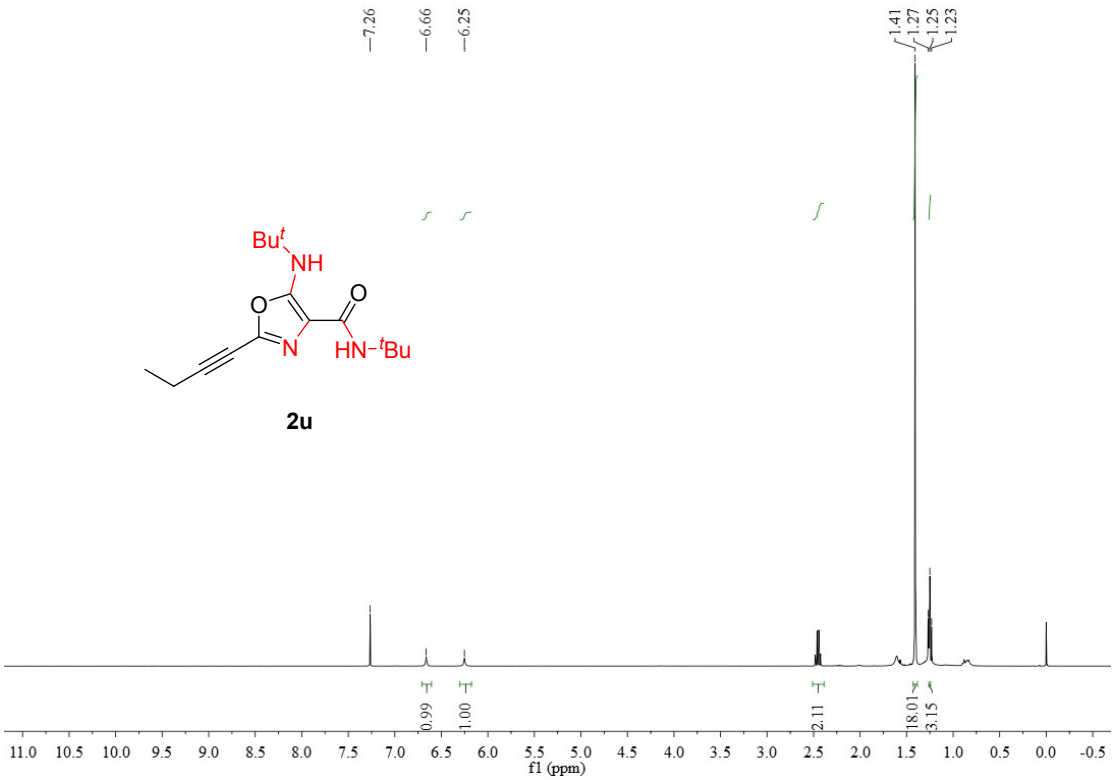
2r


7.66
7.66
7.65
7.65
7.33
7.33
7.32
7.31
7.26
7.24
7.24
7.23
7.23
6.79
6.29
1.44
1.43
Bu^t
NH
O
O
N
HN-^{t}Bu
S
2s
1.01
1.18
1.06
1.00
1.14
9.22
9.26
f1 (ppm)

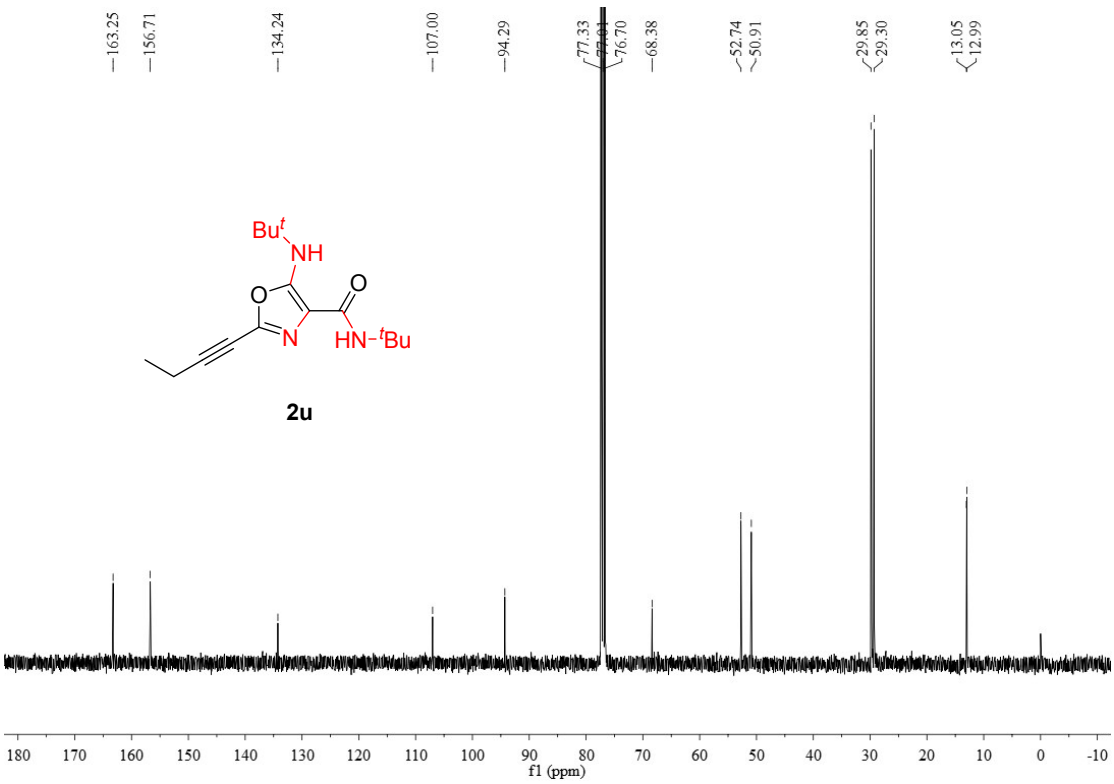

163.16
157.09
134.00
130.93
129.74
125.83
120.14
107.63
86.42
77.33
77.01
76.70
52.87
51.00
29.84
29.30
Bu^t
NH
O
O
N
HN-^{t}Bu
S
2s
f1 (ppm)


7.26
6.77
6.26
1.42
1.40
0.27
Bu^t
NH
O
O
N
HN-^{t}Bu
Si
2t
1.08
1.00
9.20
9.25
9.27
11.0 10.5 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 -0.5
f1 (ppm)

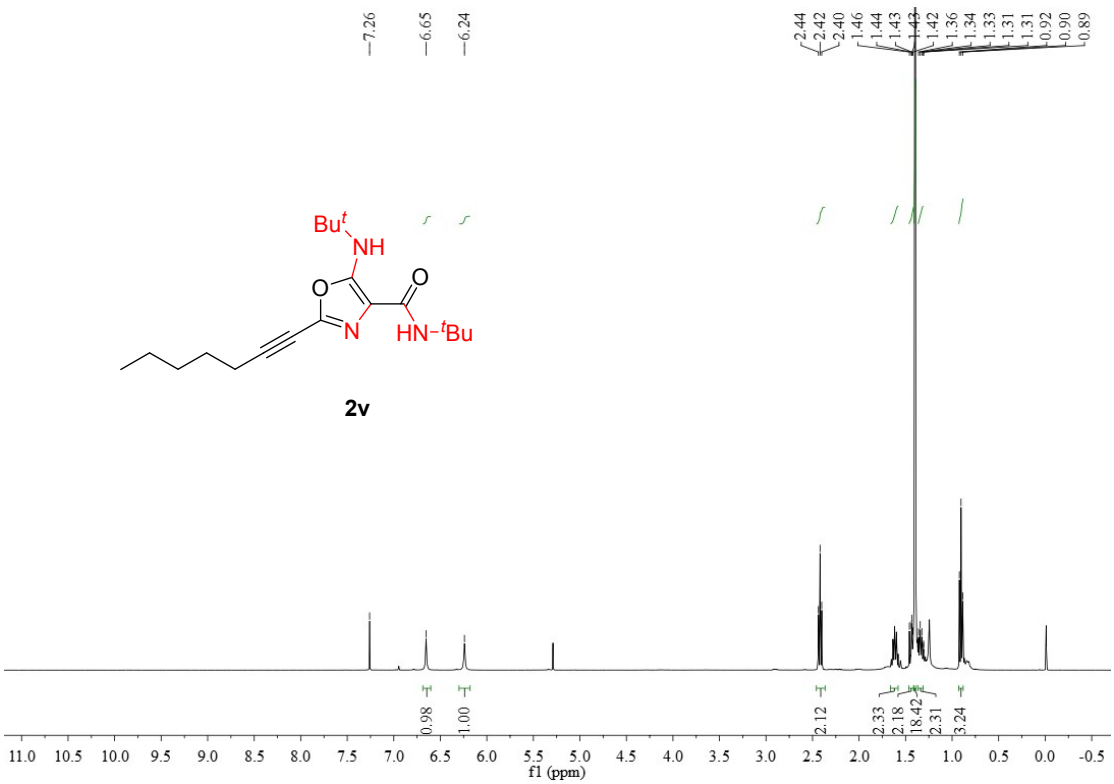

163.64
157.37
134.20
107.77
98.93
91.99
77.86
77.55
77.23
53.35
51.50
30.33
29.80
0.00
Bu^t
NH
O
O
N
HN-^{t}Bu
Si
2t
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.26
6.66
6.25
1.41
1.27
1.25
1.23
Bu^t
NH
O
O
N
HN-^tBu
0.99
1.00
2.11
18.01
3.15
f1 (ppm)

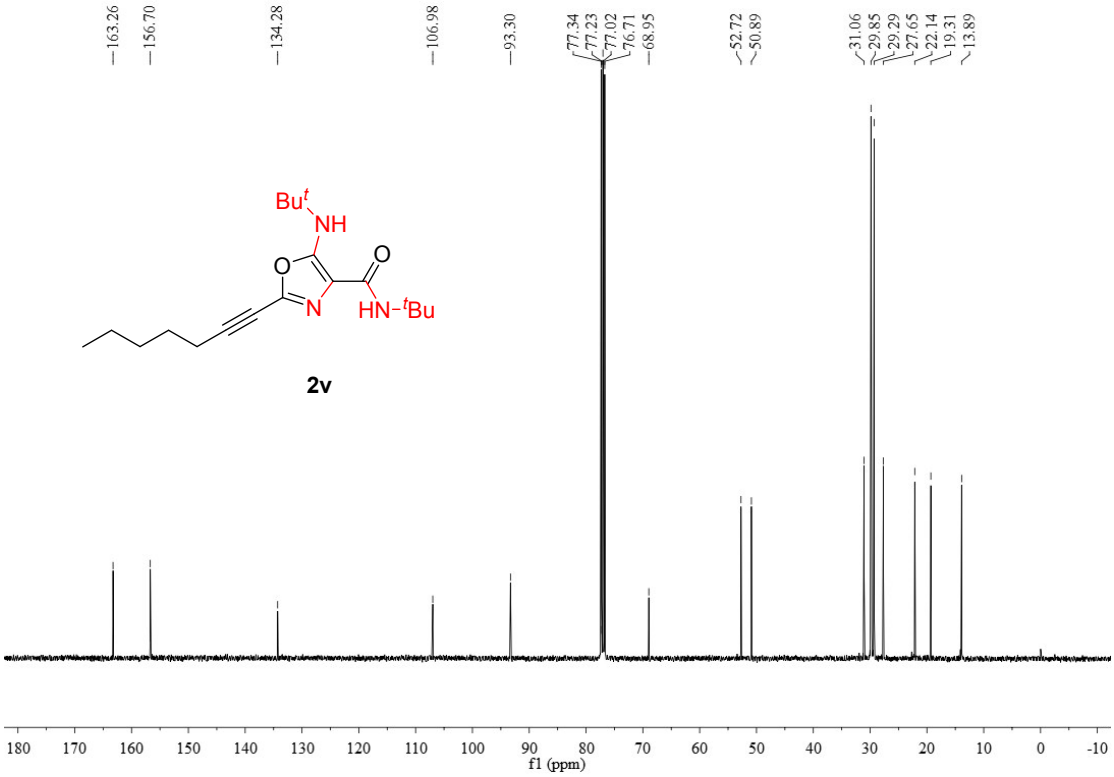
2u


163.25
156.71
134.24
107.00
94.29
77.33
77.01
76.70
68.38
52.74
50.91
29.85
29.30
13.05
12.99
Bu^t
NH
O
O
N
HN-^tBu
f1 (ppm)

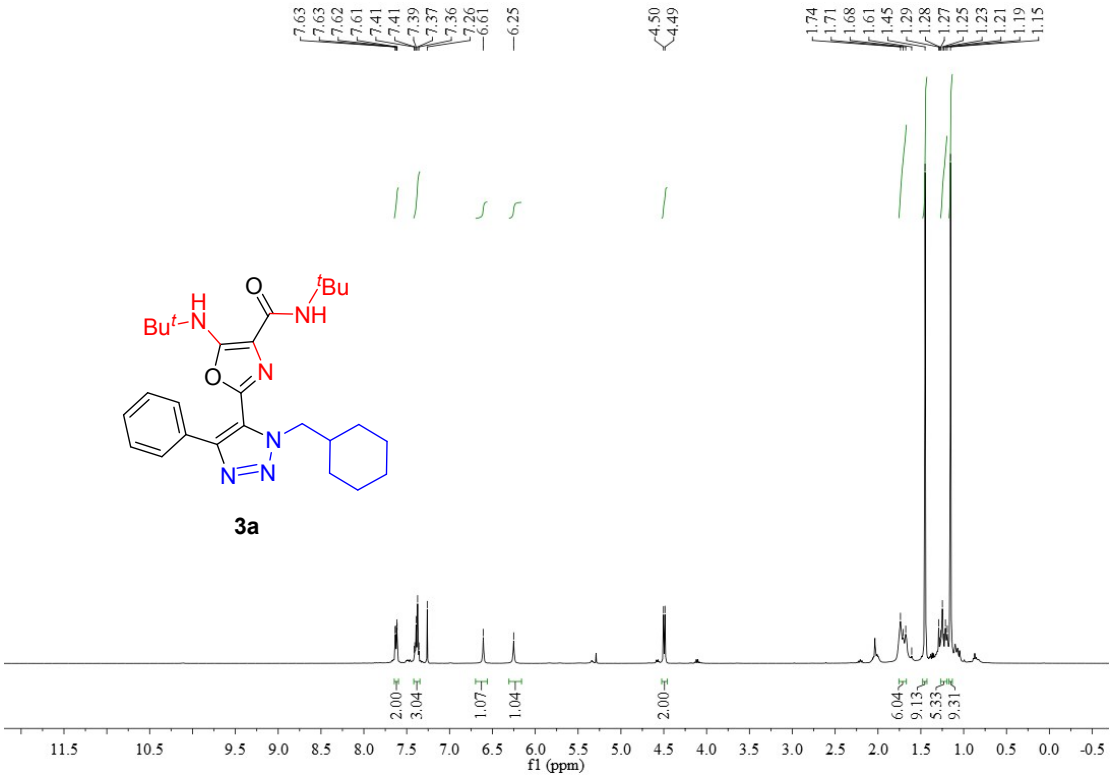
2u


7.26
6.65
6.24
2.44
2.42
2.40
1.46
1.44
1.43
1.42
1.36
1.34
1.33
1.31
0.92
0.90
0.89
Bu^t
NH
O
O
N
HN-^{t}Bu
0.98
1.00
2.12
2.33
2.18
18.42
2.31
3.24
f1 (ppm)

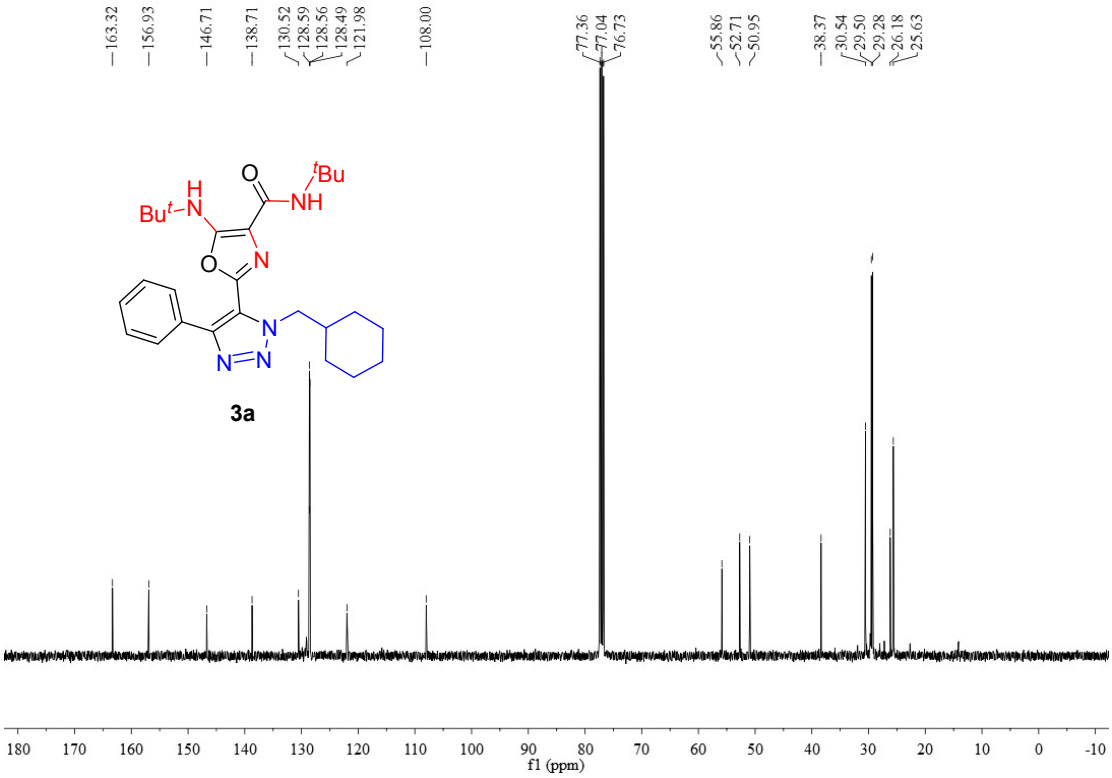
2v


163.26
156.70
134.28
106.98
93.30
77.34
77.23
77.02
76.71
68.95
52.72
50.89
31.06
29.85
29.29
27.65
22.14
19.31
13.89
Bu^t
NH
O
O
N
HN-^{t}Bu
f1 (ppm)

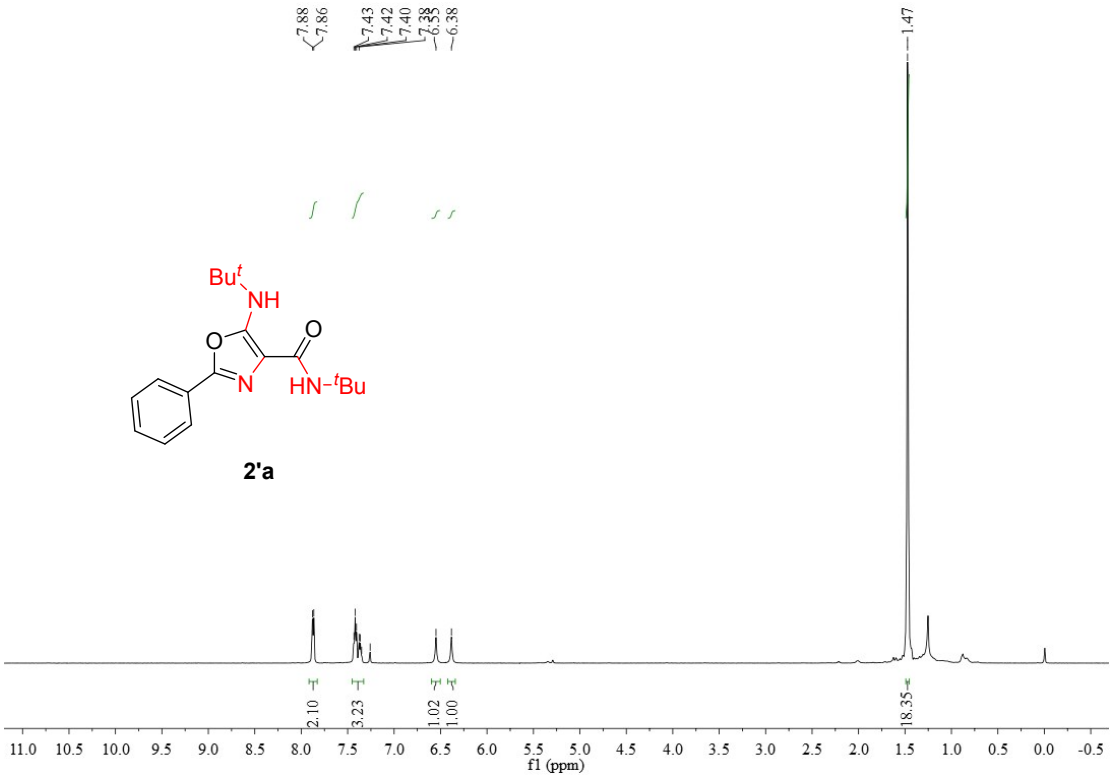
2v


7.63
7.63
7.62
7.61
7.41
7.41
7.39
7.37
7.36
7.26
6.61
6.25
4.50
4.49
1.74
1.71
1.68
1.61
1.45
1.29
1.28
1.27
1.25
1.23
1.21
1.19
1.15
2.00
3.04
1.07
1.04
2.00
6.04
9.13
5.33
9.31
f1 (ppm)

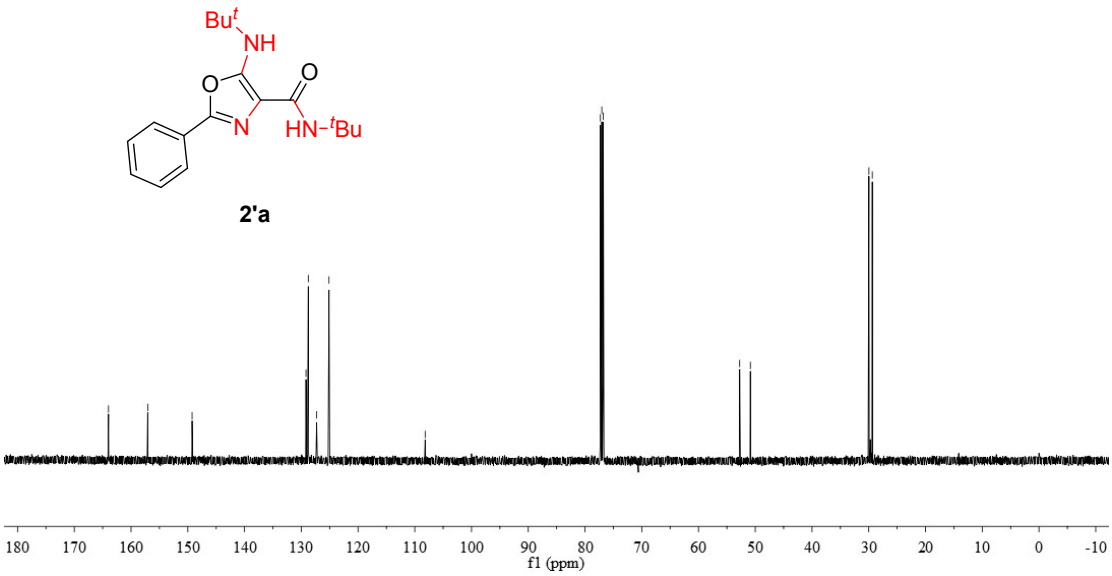
3a


163.32
156.93
146.71
138.71
130.52
128.59
128.56
128.49
121.98
108.00
77.36
77.04
76.73
55.86
52.71
50.95
38.37
30.54
29.50
29.28
26.18
25.63
f1 (ppm)

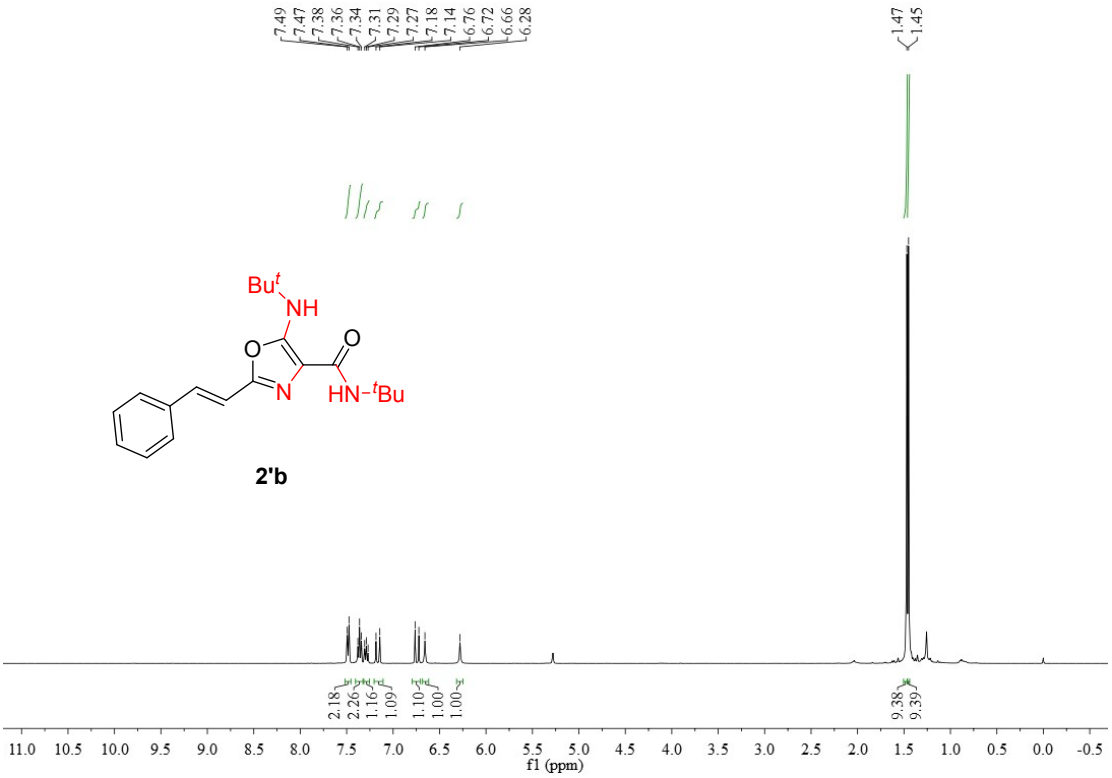
3a


7.88
7.86
7.43
7.42
7.40
7.38
7.35
6.38
1.47
Bu^t
NH
O
O
N
HN-^{t}Bu
2.10
3.23
1.02
1.00
18.35
11.0 10.5 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 -0.5
f1 (ppm)

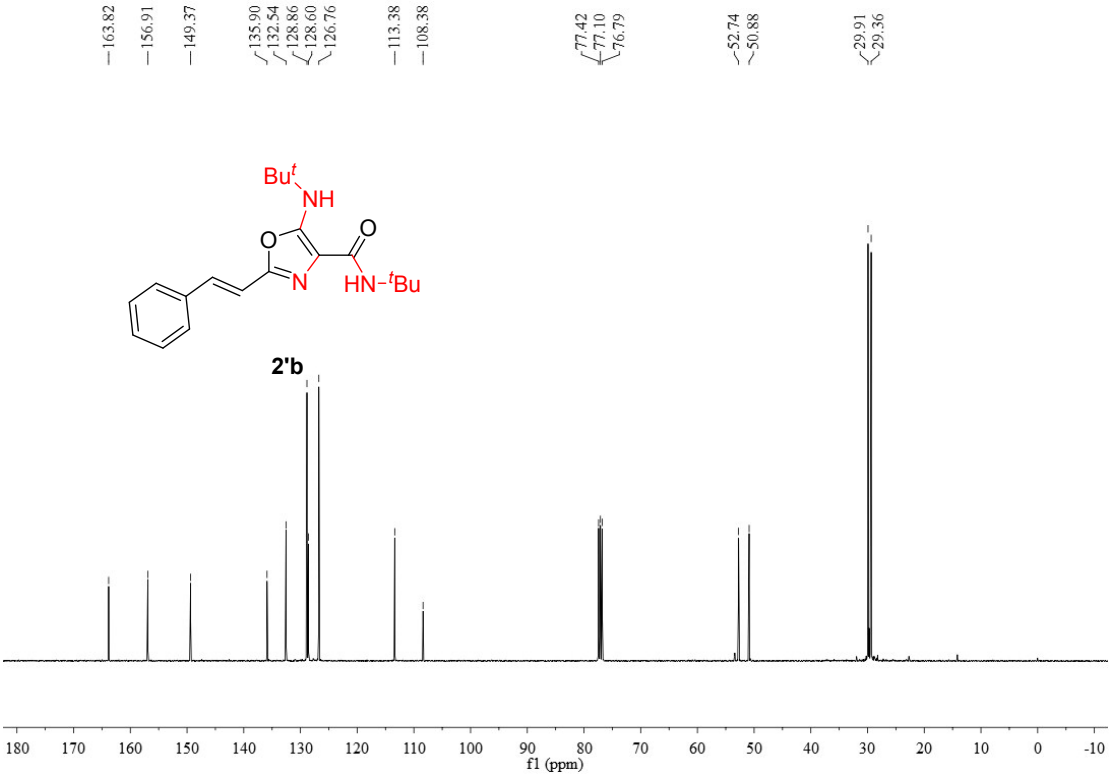
2'a


163.97
157.07
149.24
129.17
128.77
127.29
125.12
108.17
77.29
77.04
76.79
52.75
50.86
29.97
29.38
Bu^t
NH
O
O
N
HN-^{t}Bu
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

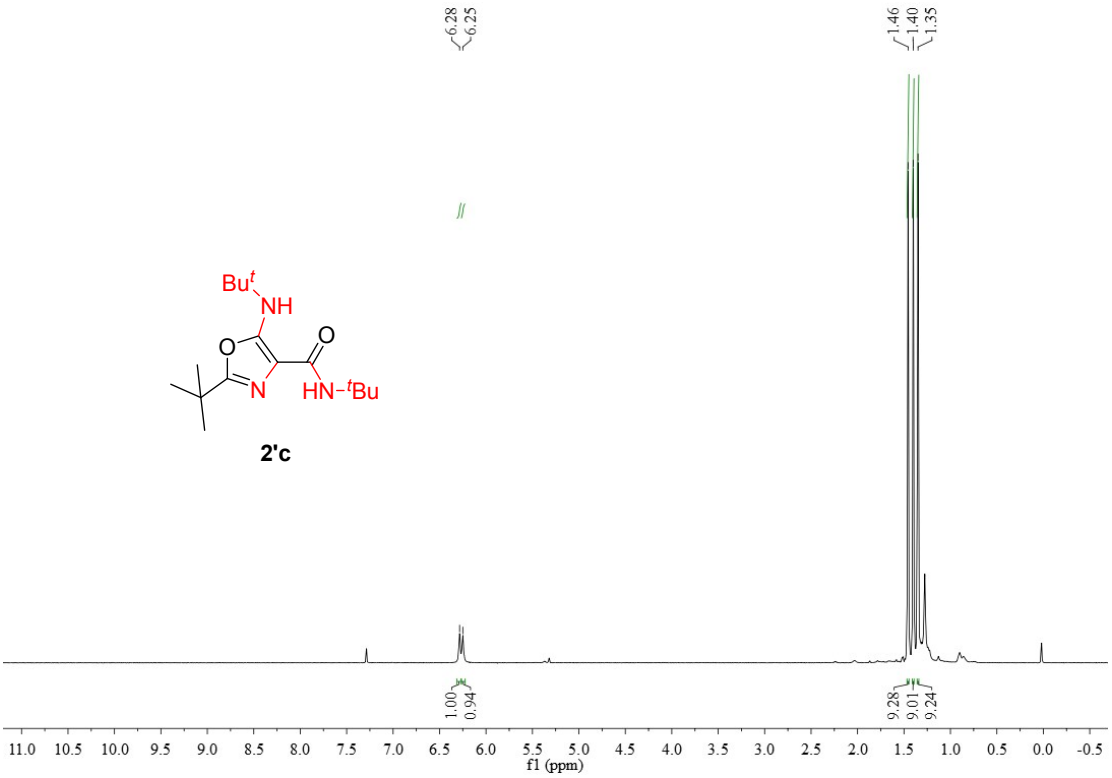
2'a


7.49
7.47
7.38
7.36
7.34
7.31
7.29
7.27
7.18
7.14
6.76
6.72
6.66
6.28
1.47
1.45
Bu^t
NH
O
O
N
HN-^{t}Bu
2.18
2.26
1.16
1.09
1.10
1.00
1.00
9.38
9.39
11.0 10.5 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 -0.5
f1 (ppm)

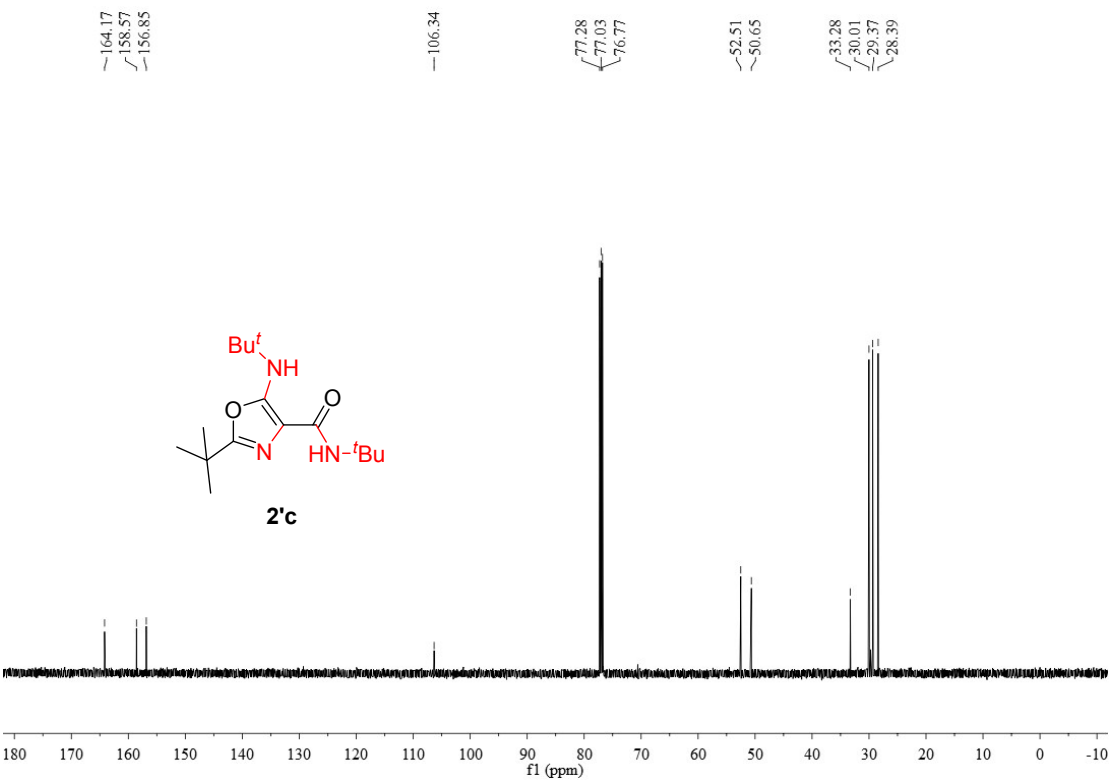
2'b


163.82
156.91
149.37
135.90
132.54
128.86
128.60
126.76
113.38
108.38
77.42
77.10
76.79
52.74
50.88
29.91
29.36
Bu^t
NH
O
O
N
HN-^{t}Bu
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2'b


6.28
6.25
1.46
1.40
1.35
Bu^t
NH
O
O
N
HN-^{t}Bu
1.00
0.94
9.28
9.01
9.24
f1 (ppm)

2'c


164.17
158.57
156.85
106.34
77.28
77.03
76.77
52.51
50.65
33.28
30.01
29.37
28.39
Bu^t
NH
O
O
N
HN-^{t}Bu
f1 (ppm)

2'c