Electronic Supplementary Material (ESI) for Chemical Communications

Electronic Supplementary Information

UV Promoted Phenanthridine Syntheses from Oxime Carbonate Derived Iminyl Radicals

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General Experimental Section

All reagents and solvents were purchased from either Sigma Aldrich or Alfa Aesar and used without further purification. Toluene was distilled over sodium and dichloromethane distilled over calcium hydride. 4'-Methoxybiphenyl-2-carbaldehyde,[1] 2-acetyl-biphenyl oxime,[2] 2-acetyl-3-bromofuran[3] and 6-phenylbenzo[*d*][1,3]dioxole-5-carbaldehyde oxime[2] were prepared according to the literature procedures. Column chromatography was carried out using Silica 60A (particle size 40-63 µm, Silicycle, Canada) as the stationary phase, and TLC was performed on precoated silica gel plates (0.20 mm thick, Sil G UV_{254}, Macherey-Nagel, Germany) and observed under UV light. ^{1}H and ^{13}C NMR spectra were recorded on Bruker AV II 400 and Bruker AV 300 instruments. Chemical shifts are reported in parts per million (ppm) from low to high frequency and referenced to the residual solvent resonance. Coupling constants (*J*) are reported in hertz (Hz). Standard abbreviations indicating multiplicity were used as follows: s = singlet, d = doublet, t = triplet, dd = double doublet, q = quartet, m = multiplet, b = broad. Melting points (M.p.) were determined using a Sanyo Gallenkamp apparatus and are reported uncorrected. Mass spectrometry was carried out by the services at the University of St Andrews and the EPSRC National Mass Spectrometry Service Centre, Swansea, UK.

EPR Spectroscopy

EPR spectra were obtained with a Bruker EMX 10/12 spectrometer fitted with a rectangular ER4122 SP resonant cavity and operating at 9.5 GHz with 100 kHz modulation. Stock solutions of each oxime carbonate (2 to 15 mg) and MAP (1 equiv wt/wt) in *tert*-butylbenzene or benzene (0.5 mL) were prepared and sonicated if necessary. An aliquot (0.2 mL), to which any additional reactant had been added, was placed in a 4 mm o.d. quartz tube, de-aerated by bubbling nitrogen for 15 min, and photolysed in the resonant cavity by unfiltered light from a 500 W super pressure mercury arc lamp. The majority of EPR spectra

were recorded with 2.0 mW power, 0.8 G_{pp} modulation intensity and gain of *ca.* 10^6. In all cases where spectra were obtained, hfs were assigned with the aid of computer simulations using the Bruker SimFonia and NIEHS Winsim2002 software packages. EPR signals were digitally filtered and double integrated using the Bruker WinEPR software.

Suzuki Coupling General Procedure

To a stirred solution of aryl bromide (1.0 equiv.) and aryl boronic acid (1.2 equiv.) in a toluene/ethanol (4:1, 0.1 M) mixture was added potassium carbonate (3.0 equiv.) and tetrakis(triphenylphosphine) palladium(II) (0.1 equiv.). The resulting suspension was heated at reflux under an atmosphere of Ar for 18 h. The solvent was removed under reduced pressure and the crude residue was redissolved in H_2O (100 mL) and extracted with EtOAc (3 × 100 mL). The combined organic layers were washed with brine (100 mL) and dried over $MgSO_4$. The filtrate was concentrated under reduced pressure and purified by column chromatography (CH_2Cl_2 as eluent).

Oxime Formation General Procedure

To a stirred solution of carbonyl (1.0 equiv.) in EtOH (0.1 M) was added hydroxylamine hydrochloride (2.0 equiv.) and sodium acetate (2.0 equiv.). The resulting suspension was heated at reflux for 18 h. The solvent was removed under reduced pressure and the crude residue redissolved in H_2O (100 mL) and extracted with CH_2Cl_2 (3 × 100 mL). The combined organic layers were dried over $MgSO_4$, concentrated under reduced pressure and used without further purification.

Oxime Carbonate Formation General Procedure

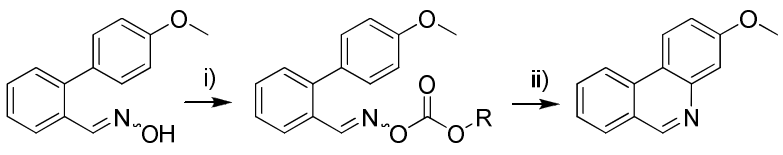
To a stirred solution of oxime (1.0 equiv.) in CH_2Cl_2 (0.1 M) was added ethyl chloroformate or phenyl chloroformate (1.0 equiv.) and pyridine (1.0 equiv.). The yellow solution was stirred at rt for 18 h. The reaction mixture was diluted with CH_2Cl_2 (100 mL) and washed

with 1 M HCl, saturated aqueous $NaHCO_3$ (100 mL) and brine (100 mL). The organic layer was dried over $MgSO_4$, concentrated under reduced pressure and purified by column chromatography (CH_2Cl_2 as eluent).

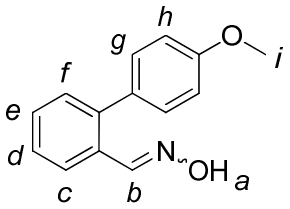
UV Cyclisation of Oxime Carbonate Derivatives General Procedure

A quartz tube was charged with oxime carbonate (1.0 equiv.), 4-methoxyacetophenone (MAP) (1 equiv. *wt/wt*) and benzotrifluoride (3 mL). The reaction mixture was degassed by bubbling Ar through the solution for 15 min. The solution was irradiated with UV light (400 W medium pressure Hg lamp) for 3 h. The solvent was removed under reduced pressure and the crude residue purified by column chromatography (CH_2Cl_2:EtOAc 9:1 as eluent).

Synthesis and Experimental Section



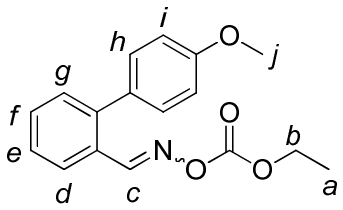
Scheme S1: Synthesis of 3-methoxyphenanthridine derivatives. Reagents and conditions: i) $NH_2OH.HCl$, NaOAc, EtOH, reflux, 18 h, 96%; ii) $EtOCO_2Cl$ or $PhOCO_2Cl$, pyridine, CH_2Cl_2, rt, 18 h; iv) MAP, UV irradiation, 3 h.



4'-Methoxybiphenyl-2-carbaldehyde oxime

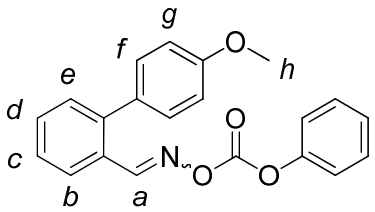
Prepared from 4'-methoxybiphenyl-2-carbaldehyde[1] (0.999 g, 4.71 mmol), hydroxylamine hydrochloride (0.655 g, 9.42 mmol) and sodium acetate (0.772 g, 9.47 mmol). Colourless oil (1.028 g, yield = 96%). ^{1}H NMR (400 MHz, $CDCl_3$, 294 K): δ = 3.86 (s, 3H, H_i), 6.98 (d, J =

8.8 Hz, 2H, H_h), 7.25 (d, *J* = 8.8 Hz, 2H, H_g), 7.32-7.38 (m, 2H, $H_{d,f}$), 7.43 (dd, *J* = 1.5 Hz, 7.5 Hz, 1H, H_e), 7.52 (br, 1H, H_a), 7.86 (d, *J* = 7.5 Hz, 1H, H_c), 8.12 (s, 1H, H_b); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 55.4, 113.8, 126.1, 127.3, 129.6, 129.7, 130.3, 130.9, 131.8, 141.9, 150.0, 159.2; LR-ESIMS: *m/z* = 250 $[MNa]^+$; HR-ESIMS: *m/z* = 250.0848 (calcd. for $C_{14}H_{13}NO_2Na$, 250.0828).



4'-Methoxybiphenyl-2-carbaldehyde *O*-ethoxycarbonyl oxime – 1a

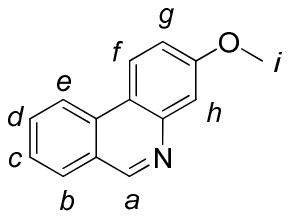
Prepared from 4'-methoxybiphenyl-2-carbaldehyde oxime (0.470 g, 2.07 mmol), ethyl chloroformate (0.22 mL, 2.36 mmol) and pyridine (0.19 mL, 2.36 mmol). Tan coloured solid (0.372 g, 53%). M.p. = 67-69 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$, 294 K): δ = 1.36 (t, *J* = 7.1 Hz, 3H, H_a), 3.86 (s, 3H, H_j), 4.34 (d, *J* = 7.1 Hz, 2H, H_b), 6.97 (d, *J* = 8.8 Hz, 2H, H_i), 7.22 (d, *J* = 8.8 Hz, 2H, H_h), 7.36-7.41 (m, 2H, $H_{e,g}$), 7.50 (dd, *J* = 1.4 Hz, 7.5 Hz, 1H, H_f), 8.10 (dd, *J* = 1.2 Hz, 7.8 Hz, 1H, H_d), 8.34 (s, 1H, H_c); ^{13}C NMR (100 MHz, $CDCl_3$, 294 K): δ = 14.3, 55.4, 64.8, 114.0, 127.4, 127.4, 127.5, 130.3, 130.9, 131.2, 131.3, 143.2, 153.8, 155.4, 159.5; LR-ESIMS: *m/z* = 322 $[MNa]^+$; HR-ESIMS: *m/z* = 322.1055 (calcd. for $C_{17}H_{17}NO_4Na$, 322.1055).



4'-Methoxybiphenyl-2-carbaldehyde *O*-phenoxycarbonyl oxime – 1b

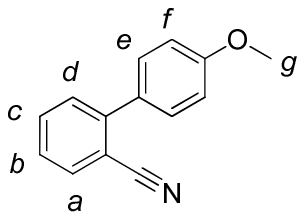
Prepared from 4'-methoxybiphenyl-2-carbaldehyde oxime (0.470 g, 2.07 mmol), phenyl chloroformate (0.26 mL, 2.07 mmol) and pyridine (0.17 mL, 2.07 mmol). Tan coloured solid

(0.598 g, 83%). M.p. = 105-107 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 3.88 (s, 3H, H_h), 7.01 (d, J = 8.8 Hz, 2H, H_g), 7.26 (m, 5H, $H_{f,ArH}$), 7.38-7.44 (m, 4H, $H_{c,e,ArH}$), 7.53 (dd, J = 1.4 Hz, 7.5 Hz, 1H, H_d), 8.13 (dd, J = 1.2 Hz, 8.8 Hz, 1H, H_b), 8.44 (s, 1H, H_a); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 55.4, 114.1, 120.9, 126.3, 127.3, 127.4, 127.5, 129.6, 130.3, 130.9, 131.1, 131.5, 143.4, 150.9, 152.2, 156.2, 159.5; LR-ESIMS: m/z = 365 [MNH_4]$^{+}$; HR-ESIMS: m/z = 365.1499 (calcd. for $C_{21}H_{21}O_4N_2$, 365.1496).



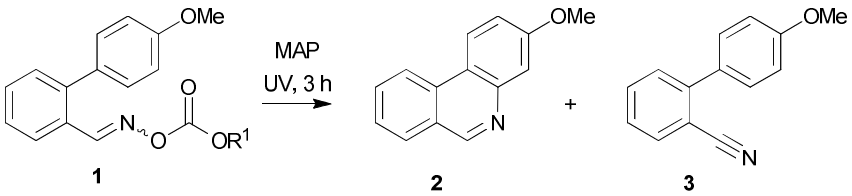
3-Methoxyphenanthridine - 2

^{1}H NMR spectrum was consistent with that reported in the literature.[1] ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 4.00 (s, 3H, H_i), 7.33 (dd, J = 2.7 Hz, 9.0 Hz, 1H, H_g), 7.61 (d, J = 2.7 Hz, 1H, H_h), 7.64 (d, J = 1.0 Hz, 7.1 Hz, 1H, H_d), 7.84 (dd, J = 1.3 Hz, 7.0 Hz, 1H, H_c), 8.03 (d, J = 8.0 Hz, 1H, H_e), 8.48 (d, J = 9.0 Hz, 1H, H_f), 8.52 (d, J = 8.1 Hz, 1H, H_b), 9.26 (s, 1H, H_a).



4'-Methoxybiphenyl-2-carbonitrile – 3

^{1}H NMR spectrum was consistent with that reported in the literature.[4] ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 3.87 (s, 3H, H_g), 7.02 (d, J = 8.9 Hz, 2H, H_f), 7.40 (dd, J = 1.4 Hz, 7.7 Hz, 1H, H_c), 7.51 (m, 3H, $H_{a,e}$), 7.62 (dd, J = 1.4 Hz, 7.7 Hz, 1H, H_b), 7.74 (ddd, J = 05 Hz, 1.4 Hz, 7.7 Hz, 1H, H_d).

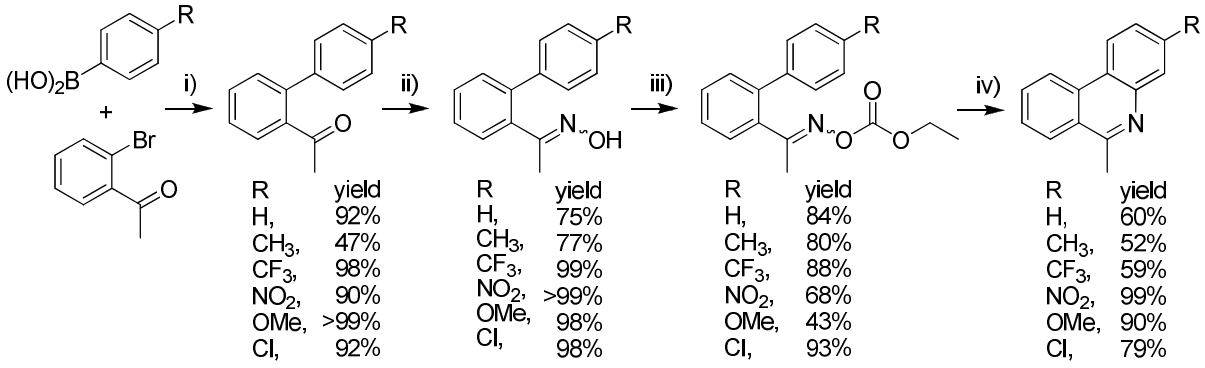


Scheme S2: Synthesis of 3-methoxyphenanthridine **2** and nitrile **3**, see table S1 for conditions and results.

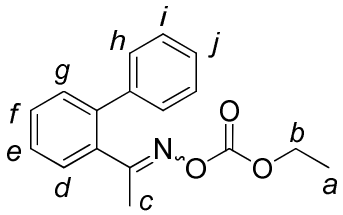
Table S1: Solvent screening results for the UV photolysis of **1**.

Entry	R^1	Solvent	Yield of **2** (%)	Yield of **3** (%)
1	Et	$PhCF_3$	30	27
2	Ph	$PhCF_3$	41	40
3	Ph	MeCN	40[a]	45[a]
4	Ph	DMF	41[a]	36[a]
5	Ph	*t*BuOH	75	20

[a] ^{1}H NMR estimated yields using CH_2Br_2 as an internal standard.



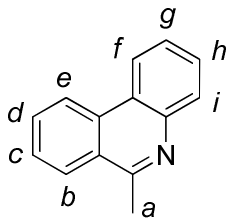
Scheme S3: Synthesis of substituted 6-methylphenanthridine derivatives. Reagents and conditions: i) $Pd(PPh_3)_4$, K_2CO_3, toluene, EtOH, reflux, 18 h, Ar; ii) $NH_2OH.HCl$, NaOAc, EtOH, reflux, 18 h; iii) $EtOCO_2Cl$, pyridine, CH_2Cl_2, rt, 18 h; iv) MAP, $PhCF_3$, UV irradiation, 3 h.



2-Acetyl-biphenyl *O*-ethoxycarbonyl oxime – 4a

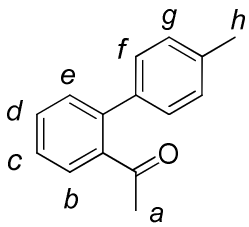
Prepared from 2-acetyl-biphenyl oxime[2] (0.600 g, 2.84 mmol), ethyl chloroformate (0.27 mL, 2.84 mmol) and pyridine (0.33 mL, 2.84 mmol). Yellow oil (0.683 g, yield = 84%). ^{1}H NMR

(400 MHz, $CDCl_3$, 295 K): δ = 1.38 (t, J = 7.1 Hz, 3H, H_a), 1.76 (s, 3H, H_c), 4.35 (q, J = 7.1 Hz, 2H, H_b), 7.33-7.42 (m, 7H, H_{ArH}), 7.45-7.54 (m, 2H, H_{ArH}); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 14.3, 18.0, 64.7, 127.4, 127.7, 128.6, 128.9, 129.7, 129.9, 130.3, 134.9, 140.4, 140.6, 153.9, 166.7; LR-ESIMS: m/z = 306 $[MNa]^+$; HR-ESIMS: m/z = 306.1109 (calcd. for $C_{17}H_{17}NO_3Na$, 306.1106).



6-Methylphenanthridine - 5a

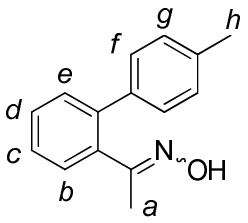
Prepared from 2-acetyl-biphenyl *O*-ethoxycarbonyl oxime (0.059 g, 0.021 mmol). Colourless solid (0.024 g, yield = 60%). ^{1}H and ^{13}C NMR spectrum were consistent with those reported in the literature.[2] M.p. = 65 °C; ^{1}H NMR (300 MHz, $CDCl_3$, 296 K): δ = 3.09 (s, 3H, H_a), 7.64-7.76 (m, 3H, $H_{d,g,h}$), 7.87 (dd, J = 1.3 Hz, 7.7 Hz, 1H, H_c), 8.18 (d, J = 8.0 Hz, 1H, H_i), 8.25 (d, J = 8.2 Hz, 1H, H_e), 8.55 (d, J = 8.1 Hz, 1H, H_f), 8.65 (d, J = 8.3 Hz, 1H, H_b); ^{13}C NMR (75 MHz, $CDCl_3$, 296 K): δ = 23.8, 122.4, 122.7, 124.2, 126.3, 126.7, 127.0, 127.7, 129.1, 129.8, 130.9, 133.0, 144.1, 159.3.



2-*p*-Tolylacetophenone

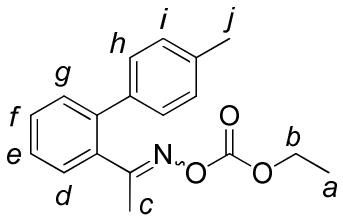
Prepared from *p*-tolylboronic acid (0.400 g, 3.00 mmol), 2'-bromoacetophenone (0.33 mL, 2.50 mmol), tetrakis(triphenylphosphine)palladium(II) (0.283 g, 0.25 mmol) and potassium carbonate (1.016 g, 7.40 mmol). Colourless oil (0.271 g, yield = 47%). ^{1}H and ^{13}C NMR

spectra were consistent with those reported in the literature.[5] ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 2.01 (s, 3H, H_a), 2.41 (s, 3H, H_h), 7.24 (s, 4H, $H_{f,g}$), 7.37-7.42 (m, 2H, $H_{c,d}$), 7.48-7.54 (m, 2H, $H_{b,e}$); ^{13}C NMR (75 MHz, $CDCl_3$, 296 K): δ = 21.6, 30.9, 127.6, 128.2, 129.2, 129.8, 130.6, 131.1, 138.2 (× 2), 140.9, 141.3, 205.6.



2-*p*-Tolylacetophenone oxime

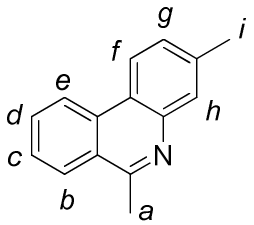
Prepared from 2-*p*-tolylacetophenone (0.246 g, 1.20 mmol), hydroxylamine hydrochloride (0.163 g, 2.30 mmol) and sodium acetate (0.192 g, 2.30 mmol). Colourless oil (0.209 g, yield = 77%). Two isomers (1:4). ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 1.70/1.76 (s, 3H, H_a), 2.39 (s, 3H, H_h), 7.19-7.22 (m, 2H, H_g), 7.28-7.30 (m, 2H, H_f), 7.32-7.45 (m, 4H, $H_{b,c,d,e}$); ^{13}C NMR (75 MHz, $CDCl_3$, 296 K): δ = 16.3, 21.6, 127.6, 129.2, 129.4, 129.5, 129.6, 130.7, 137.1, 137.5, 138.4, 141.0, 160.0; LR-ESIMS: *m/z* = 248 $[MNa]^+$; HR-ESIMS: *m/z* = 248.1048 (calcd. for $C_{15}H_{15}NONa$, 248.1051).



2-*p*-Tolylacetophenone *O*-ethoxycarbonyl oxime – 4b

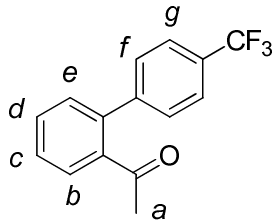
Prepared from 2-*p*-tolylacetophenone oxime (0.142 g, 0.63 mmol), ethyl chloroformate (0.06 mL, 0.63 mmol) and pyridine (0.05 mL, 0.63 mmol). Colourless oil (0.150 g, yield = 80%). Two isomers (1:3). ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 1.39 (t, J = 7.1 Hz, 3H, H_a), 1.77/2.05 (s, 3H, H_c), 2.39/2.40 (s, 3H, H_j), 4.36 (q, J = 7.1 Hz, 2H, H_b), 7.21 (d, J = 7.8 Hz,

2H, H_i), 7.29-7.52 (m, 5H, $H_{e,f,g,h}$), 7.75 (m, 1H, H_d); ^{13}C NMR (100 MHz, $CDCl_3$, 297 K): δ = 14.7, 18.4, 21.6, 65.1, 127.4, 127.6, 129.0, 129.2, 129.7, 130.1, 130.3, 130.6, 137.9, 141.0, 153.4, 167.3; LR-ESIMS: *m/z* = 320 $[MNa]^+$; HR-ESIMS: *m/z* = 320.1256 (calcd. for $C_{18}H_{19}NO_3Na$, 320.1263).



3,6-Dimethylphenanthridine – 5b

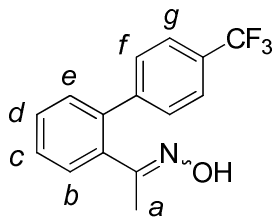
Prepared from 2-*p*-tolylacetophenone *O*-ethoxycarbonyl oxime (0.051 g, 0.172 mmol). Tan coloured solid (0.018 g, yield = 52%). M.p. = 89-91 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 2.59 (s, 3H, H_i), 3.04 (s, 3H, H_a), 7.45 (d, *J* = 8.3 Hz, 1H, H_g), 7.66 (m, 1H, H_d), 7.82 (m, 1H, H_c), 7.91 (s, 1H, H_h), 8.20 (dd, *J* = 0.4 Hz, 1H, H_e), 8.42 (d, *J* = 8.3 Hz, 1H, H_f), 8.59 (d, *J* = 8.3 Hz, 1H, H_b); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 21.6, 23.4, 121.4, 121.7, 122.1, 125.6, 126.5, 126.8, 128.0, 129.0, 130.4, 132.7, 138.8, 143.8, 158.9; LR-EIMS: *m/z* = 207 $[M]^+$; HR-ESIMS: *m/z* = 207.1042 (calcd. for $C_{15}H_{13}N$, 207.1043).



2-*p*-Trifluoromethylphenylacetophenone

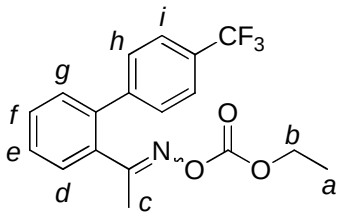
Prepared from 4-trifluromethylphenylboronic acid (0.407 g, 2.14 mmol), 2'-bromoacetophenone (0.356 g, 1.79 mmol), tetrakis(triphenylphosphine) palladium(II) (0.208 g, 0.18 mmol), and potassium carbonate (0.746 g, 5.40 mmol). Yellow oil (0.466 g, yield = 98%). ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 2.14 (s, 3H, H_a), 7.37 (dd, *J* = 1.0 Hz,

7.5 Hz, 1H, H_e), 7.44-7.60 (m, 3H, $H_{d,g}$), 7.55 (dd, J = 1.5 Hz, 7.5 Hz, 1H, H_c), 7.62 (dd, J = 1.2 Hz, 7.6 Hz, 1H, H_b), 7.69 (d, J = 8.0 Hz, 2H, H_g); ^{13}C NMR (100 MHZ, $CDCl_3$, 295 K): δ = 30.4, 125.5 (q, $^3J_{CF}$ = 3.6 Hz), 126.9 (q, $^1J_{CF}$ = 281.1 Hz), 128.2 (× 2), 129.1, 129.9 (q, $^2J_{CF}$ = 33.0 Hz), 130.5, 131.0, 139.2, 140.4, 144.6, 203.5; ^{19}F NMR (400 MHz, $CDCl_3$, 295 K): δ = -62.96 (CF_3); LR-EIMS: *m/z* = 264 $[M]^+$: HR-MS: *m/z* = 264.0756 (calcd. for $C_{15}H_{11}OF_3$, 264.0757).



2-*p*-Trifluoromethylphenylacetophenone oxime

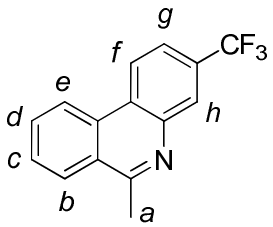
Prepared from 2-*p*-trifluoromethylphenylacetophenone (0.264 g, 3.4 mmol), hydroxylamine hydrochloride (0.473 g, 6.8 mmol) and sodium acetate (0.558 g, 6.8 mmol). Colourless oil (0.734 g, yield >99%). Two isomers 1:6.6. ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 1.94/2.07 (s, 3H, H_a), 7.30 (dd, J = 1.0 Hz, 7.2 Hz, 1H, H_b), 7.38 (d, J = 8.0 Hz, 2H, H_f), 7.42 (dd, J = 1.4 Hz, 7.5 Hz, 1H, H_e), 7.48 (m, 1H, H_c), 7.54 (m, 1H, H_d), 7.62 (d, J = 8.0 Hz, 2H, H_g); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 30.8, 126.0, 126.4, 128.6, 129.3, 129.5, 130.9, 131.4, 135.3, 138.9, 142.5, 145.0, 164.9;^{19}F NMR (400 MHz, $CDCl_3$, 296 K): δ = -63.0 (CF_3).



2-*p*-Trifluoromethylphenylacetophenone *O*-ethoxycarbonyl oxime – 4c

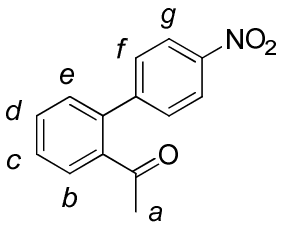
Prepared from 2-*p*-trifluoromethylphenylacetophenone oxime (0.466 g, 1.70 mmol), ethyl chloroformate (0.13 mL, 1.70 mmol) and pyridine (0.16 mL, 1.70 mmol). Colourless oil

(0.528 g, yield = 88%). Two isomers 1:2.5. ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 1.29/1.39 (t, J = 7.1 Hz, 3H, H_a), 1.79/2.01 (s, 3H, H_c), 4.23/4.35 (q, J = 7.1 Hz, 2H, H_b), 7.37-7.57 (m, 6H, H_{ArH}), 7.63-7.70 (m, 2H, H_{ArH}); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 14.3, 18.2, 64.8, 125.6 (q, $^{3}J_{CF}$ = 3.5 Hz), 126.8 (q, $^{1}J_{CF}$ = 269.0 Hz), 128.3, 129.3, 129.7 (q, $^{2}J_{CF}$ = 36.7 Hz), 129.8, 130.1, 130.2, 135.0, 139.0, 144.1, 153.8, 165.9; ^{19}F NMR (400 MHz, $CDCl_3$, 295 K): δ = -63.0 (CF_3); LR-ESIMS: *m/z* = 352 $[MH]^+$; HR-ESIMS: *m/z* = 352.1158 (calcd. for $C_{18}H_{17}O_3NF_3$, 352.1155).



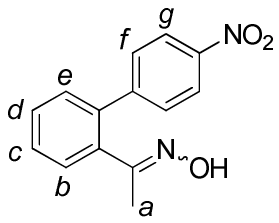
6-Methyl-3-(trifluoromethyl)phenanthridine – 5c

Prepared from 2-*p*-trifluoromethylphenylacetophenone *O*-ethoxycarbonyl oxime (0.059 g, 0.168 mmol). Colourless solid (0.026 g, yield = 59%). M.p. = 72 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$, 300 K): δ = 3.05 (s, 3H, H_a), 7.75-7.81 (m, 2H, $H_{d,g}$), 7.87-7.91 (m, 1H, H_c), 8.25 (dd, J = 0.7 Hz, 8.2 Hz, 1H, H_f), 8.38 (s, 1H, H_h), 8.59-8.63 (m 2H, $H_{b,e}$); ^{13}C NMR (100 MHz, $CDCl_3$, 297 K): δ = 23.4, 122.2 (q, $^{3}J_{CF}$ = 3.4 Hz), 122.7, 123.0, 124.2 (q, $^{1}J_{CF}$ = 272.2 Hz), 126.1, 126.5, 126.7, 126.9 (q, $^{3}J_{CF}$ = 4.0 Hz), 128.5, 130.4, (q, $^{2}J_{CF}$ = 32.6 Hz), 131.0, 131.7, 143.0, 160.5; ^{19}F NMR (400 MHz, $CDCl_3$, 296 K): δ = -62.75 (CF_3); LR-EIMS: *m/z* = 261 $[M]^+$; HR-ESIMS: *m/z* = 261.0762 (calcd. for $C_{15}H_{10}NF_3$, 261.0760).



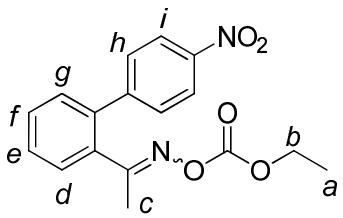
2-*p*-Nitrophenylacetophenone

Prepared from 4-nitrophenylboronic acid (0.235 g, 1.41 mmol), 2'-bromoacetophenone (0.16 mL, 1.17 mmol), tetrakis(triphenylphosphine) palladium(II) (0.139 g, 0.12 mmol), and potassium carbonate (0.487 g, 3.52 mmol). Colourless solid (0.308 g, yield = 90%). M.p. = 95 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 2.26 (s, 3H, H_a), 7.36 (d, J = 7.5 Hz, 1H, H_b),7.47 (d, J = 8.7 Hz, 2H, H_f), 7.52 (m, 1H, H_d), 7.58 (m, 1H, H_c), 7.69 (d, J = 7.5 Hz, 1H, H_e), 8.28 (d, J = 8.7 Hz, 2H, H_g); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 30.1, 123.7, 128.6, 128.7, 129.6, 130.5, 131.3, 133.1, 138.7, 139.7, 148.0, 202.4; LR-EIMS: *m/z* = 241 $[M]^+$; HR-ESIMS: *m/z* = 241.0732 (calcd. for $C_{14}H_{11}O_3N$, 241.0733).



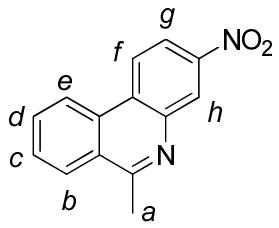
2-*p*-Nitrophenylacetophenone oxime

Prepared from 2-*p*-nitrophenylacetophenone (0.302 g, 1.25 mmol), hydroxylamine hydrochloride (0.174 g, 2.50 mmol) and sodium acetate (0.205 g, 2.50 mmol). Colourless oil (0.344 g, yield >99%). Two isomers 1:2.5. ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 1.72/1.76 (s, 3H, H_a), 7.29-7.33 (m, 2H, $H_{c,d}$), 7.37-7.42 (m, 2H, $H_{b,e}$), 7.47 (d, J = 8.9 Hz, 2H, H_g), 8.20 (d, J = 8.9 Hz, 2H, H_f); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 16.1, 123.6, 126.0, 127.8, 128.6, 129.0, 129.3, 129.4, 136.8, 147.1, 147.9, 158.0; LR-ESIMS: *m/z* = 256 $[M]^+$.



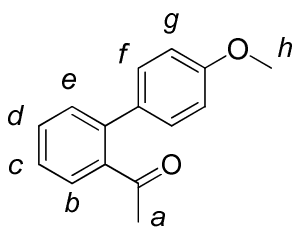
2-*p*-Nitrophenylacetophenone *O*-ethoxycarbonyl oxime – 4d RM1-11 RG13

Prepared from 2-*p*-nitrophenylacetophenone oxime (0.335 g, 1.31 mmol), ethyl chloroformate (0.12 mL, 1.31 mmol) and pyridine (0.10 mL, 1.31 mmol). Tan coloured solid (0.279 g, yield = 68%); M.p. = 91-92˚C; ^{1}H NMR (400 MHz, $CDCl_3$, 300 K): δ = 1.38 (t, J = 7.1 Hz, 3H, H_a), 1.84 (s, 3H, H_c), 4.34 (q, J = 7.1 Hz, 2H, H_b), 7.40 (dd, J = 0.6 Hz, 7.1 Hz, 1H, H_g), 7.47 (dd, J 1.4 Hz, 6.7 Hz, 1H, H_e), 7.51-7.55 (m, 2H, $H_{d,f}$), 7.59 (d, J = 8.58 Hz, 2H, H_g), 8.28 (d, J = 8.8 Hz, 2H, H_f); ^{13}C NMR (75 MHz, $CDCl_3$, 300 K): δ = 14.7, 18.7, 65.3, 124.2, 129.2, 130.3 (× 2), 130.6 (× 2), 135.5, 138.6, 147.6, 147.7, 154.1, 165.7; LR-ASAPMS: *m/z* = 329 $[MH]^+$; HR-ASAPMS: *m/z* = 329.1133 (calcd. for $C_{17}H_{17}O_5N_2$, 329.1132).



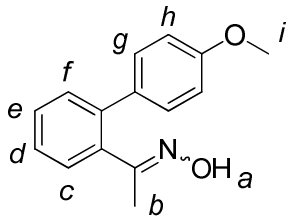
6-Methyl-3-nitrophenanthridine – 5d

Prepared from 2-*p*-nitrophenylacetophenone *O*-ethoxycarbonyl oxime (0.088 g, 0.27 mmol). Tan coloured solid (0.058 g, yield = 99%). M.p. = 167 ˚C (dec.); ^{1}H NMR (400 MHz, $CDCl_3$, 300 K): δ = 3.09 (s, 3H, H_a), 7.85 (m, 1H, H_d), 7.95 (m, 1H, H_c), 8.30 (dd, J = 0.7 Hz, 8.2 Hz, 1H, H_e), 8.40 (dd, J = 2.4 Hz, 9.0 Hz, 1H, H_g), 8.65 (d, J = 9.0 Hz, 1H, H_f), 8.66 (d, J = 8.1 Hz, 1H, H_b), 8.96 (d, J = 2.4 Hz, 1H, H_h); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K): δ = 25.5, 120.1, 123.2, 123.4, 125.2, 126.8, 126.9, 128.5, 129.4, 131.3, 131.4, 143.2, 147.5, 161.7; LR-EIMS: *m/z* = 238 $[M]^+$; HR-ESIMS: *m/z* = 238.0737 (calcd. for $C_{14}H_{10}O_2N_2$, 238.0737).



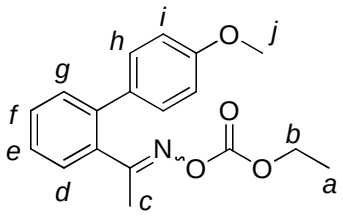
2-*p*-Methoxyphenylacetophenone

Prepared from 4-methoxyphenylboronic acid (0.396 g, 2.61 mmol), 2'-bromoacetophenone (0.3 mL, 2.17 mmol), tetrakis(triphenylphosphine) palladium(II) (0.254 g, 0.22 mmol), and potassium carbonate (0.899 g, 6.51 mmol). Colourless oil (0.573 g, yield >99%). ^{1}H NMR spectrum was consistent with that reported in the literature.[6] ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 2.01 (s, 3H, H_a), 3.86 (s, 3H, H_h), 6.67 (d, J = 8.8 Hz, 2H, H_g), 7.27 (d, J = 8.8 Hz, 2H, H_f), 7.36-7.40 (m, 2H, $H_{c,e}$), 7.47-7.53 (m, 2H, $H_{b,d,}$).



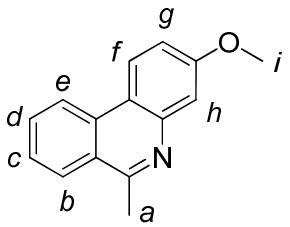
2-*p*-Methoxyphenylacetophenone oxime

Prepared from 2-*p*-methoxyphenylacetophenone (0.573 g, 2.53 mmol), hydroxylamine hydrochloride (0.352 g, 5.06 mmol) and sodium acetate (0.415 g, 5.06 mmol). Colourless solid (0.601 g, yield = 98%). M.p. = 108-112 ˚C; Two isomers 1:3.45. ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 1.70/1.76 (s, 3H, H_b), 3.85 (s, 3H, H_i), 6.94 (d, J = 8.8 Hz, 2H, H_h), 7.30-7.45 (m, 6H, H_{ArH}), 8.22-8.62 (br, 1H, H_a); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K): δ = 16.3, 55.7, 114.2, 114.3, 127.4, 129.4, 129.6, 130.5, 130.6, 133.8, 137.1, 140.6, 159.5; LR-ESIMS: *m/z* = 242 $[MH]^+$; HR-ESIMS: *m/z* = 242.1177 (calcd. for $C_{15}H_{16}NO_2$, 242.1176).



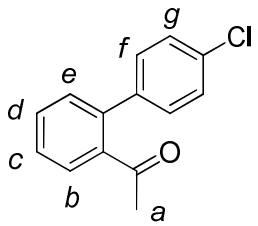
2-*p*-Methoxyphenylacetophenone *O*-ethoxycarbonyl oxime – 4e

Prepared from 2-*p*-methoxyphenylacetophenone oxime (0.393 g, 1.63 mmol), ethyl chloroformate (0.15 mL, 1.63 mmol) and pyridine (0.13 mL, 1.63 mmol). Colourless oil (0.220 g, yield = 43%). ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 1.39 (t, J = 7.1 Hz, 3H, H_a), 1.78 (s, 3H, H_c), 3.85 (s, 3H, H_j), 4.36 (q, J = 7.1 Hz, 2H, H_b), 6.94 (d, J = 8.8 Hz, 2H, H_i), 7.32-7.38 (m, 4H, H_{ArH}), 7.44-7.51 (m, 2H, H_{ArH}); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 14.3, 18.0, 55.3, 64.7, 114.1, 127.0, 129.7, 129.9, 130.1, 130.2, 132.8, 134.8, 140.2, 153.9, 159.3, 166.9; LR-ESIMS: *m/z* = 336 $[MNa]^+$; HR-ESIMS: *m/z* = 336.1209 (calcd. for $C_{18}H_{19}NO_4Na$, 336.1212).



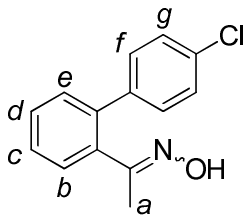
3-Methoxy-6-methylphenanthridine – 5e

Prepared from 2-*p*-methoxyphenylacetophenone *O*-ethoxycarbonyl oxime (0.050 g, 0.16 mmol). Yellow oil (0.032 g, yield = 90%). ^{1}H NMR (300 MHz, $CDCl_3$, 300 K): δ = 3.02 (s, 3H, H_a), 3.97 (s, 3H, H_i), 7.24 (dd, J = 2.6 Hz, 9.0 Hz, 1H, H_g), 7.51 (d, J = 2.6 Hz, 1H, H_h), 7.60 (m, 1H, H_c), 7.78 (m, 1H, H_d), 8.17 (d, J = 8.2 Hz, 1H, H_b), 8.40 (d, J = 9.0 Hz, 1H, H_f), 8.49 (d, J = 8.3 Hz, 1H, H_e); ^{13}C NMR (75 MHz, $CDCl_3$, 300 K): δ = 23.8, 56.0, 109.7, 117.7, 118.2, 122.2, 123.6, 125.4, 126.6, 127.0, 131.0, 133.2, 145.7, 159.8, 160.5; LR-ESIMS: *m/z* = 224 $[MH]^+$; HR-ESIMS: *m/z* = 224.1069 (calcd. for $C_{15}H_{14}NO$, 224.1075).



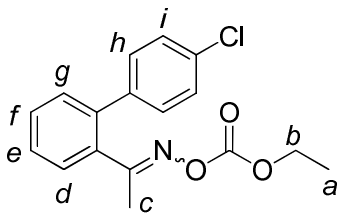
2-*p*-Chlorophenylacetophenone

Prepared from 2'-bromoacetophenone (0.920 g, 4.60 mmol), 4-chlorophenylboronic acid (1.080 g, 6.89 mmol), tetrakis(triphenylphosphine) palladium(II) (0.797 g, 0.69 mmol), and potassium carbonate (2.861 g, 20.7 mmol). Yellow oil (0.980 g, yield = 92%). ^{1}H NMR (400 MHz, $CDCl_3$, 297 K): δ = 2.12 (s, 3H, H_a), 7.30 (d, J = 8.6 Hz, 2H, H_g), 7.38 (dd, J = 1.2 Hz, 7.6 Hz, 1H, H_e), 7.42-7.48 (m, 3H, $H_{c,f}$), 7.52-7.61 (m, 2H, $H_{b,d}$); ^{13}C NMR (100 MHz, $CDCl_3$, 297 K): δ = 30.5, 98.7, 127.8, 128.1, 128.9, 130.1, 130.3, 130.9, 134.1, 139.3, 140.6, 204.2; LR-EIMS: m/z = 230 $[M]^+$; HR-ESIMS: m/z = 230.0495 (calcd. for $C_{11}H_{14}O^{35}Cl$, 230.0493).



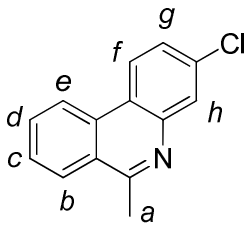
2-*p*-Chlorophenylacetophenone oxime

Prepared from 2-*p*-chlorophenylacetophenone (0.900 g, 3.90 mmol), hydroxylamine hydrochloride (0.540 g, 7.80 mmol) and sodium acetate (0.538 g, 7.80 mmol). White solid (0.950 g, yield = 98%). M.p. = 110-114 ˚C; Two isomers 1:3.25. ^{1}H NMR (400 MHz, $CDCl_3$, 297 K): δ = 1.74/1.79 (s, 3H, H_a), 7.31-7.47 (m, 8H, H_{ArH}), 8.20-10.00 (br, 1H, H_a); ^{13}C NMR (100 MHz, $CDCl_3$, 297 K): (major isomer) δ = 16.2, 127.8, 128.7, 129.2, 129.3, 130.2, 130.3, 133.6, 136.7, 139.3, 139.4, 158.8; LR-EIMS: m/z = 246 $[MH]^+$; HR-MS: m/z = 246.0683 (calcd. for $C_{14}H_{13}ON^{35}Cl$, 246.0680).



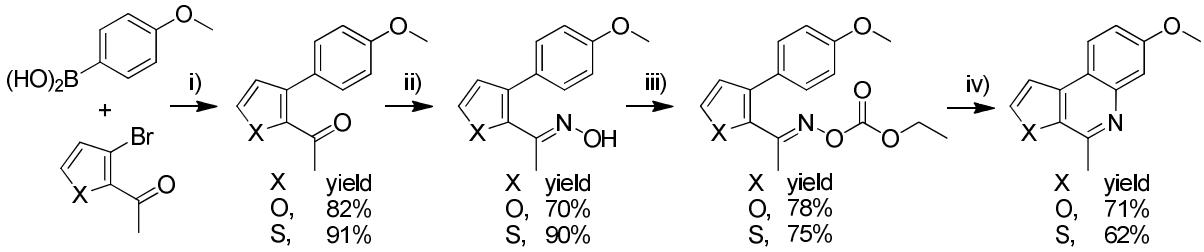
2-*p*-Chlorophenylacetophenone *O*-ethoxycarbonyl oxime - 4f

Prepared from 2-*p*-chlorophenylacetophenone oxime (0.800 g, 3.26 mmol), ethyl chloroformate (0.31 mL, 3.26 mmol) and pyridine (0.26 mL, 3.26 mmol). Yellow oil (0.970 g, yield = 93%). Two isomers 1:2.4. ^{1}H NMR (400 MHz, $CDCl_3$, 297 K): δ = 1.29/1.38 (t, J = 7.1 Hz, 3H, H_a), 1.79/1.98 (s, 3H, H_c), 4.23/4.35 (q, J = 7.1 Hz, 2H, H_b), 7.21-7.28 (m, 1H, H_{ArH}), 7.33-7.51 (m, 7H, H_{ArH}); ^{13}C NMR (100 MHz, $CDCl_3$, 297 K): (major isomer) δ = 14.3, 18.1, 64.7, 127.8, 128.8, 129.7, 130.0, 130.1, 130.2, 133.9, 134.9, 138.9, 139.3, 153.8, 166.2; LR-ESIMS: *m/z* = 340 $[MNa]^+$; HR-ESIMS: *m/z* = 340.0713 (calcd. for $C_{17}H_{16}NO_3Na^{35}Cl$, 340.0716).

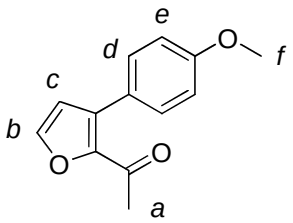


3-Chloro-6-methylphenanthridine – 5f

Prepared from 2-*p*-chlorophenylacetophenone *O*-ethoxycarbonyl oxime (0.053 g, 0.17 mmol). Colourless solid (0.030 g, yield = 79%). M.p. = 120-122 ˚C; ^{1}H NMR (300 MHz, $CDCl_3$, 297 K): δ = 3.02 (s, 3H, H_a), 7.55 (dd, J = 2.2 Hz, 8.8 Hz, 1H, H_g), 7.70 (m, 1H, H_c), 7.84 (m, 1H, H_d), 8.08 (d, J = 2.2 Hz, 1H, H_h), 8.20 (d, J = 7.6 Hz, 1H, H_b), 8.41 (d, J = 8.8 Hz, 1H, H_f), 8.53 (d, J = 8.2 Hz, 1H, H_e); ^{13}C NMR (75 MHz, $CDCl_3$, 298 K): δ = 23.8, 122.6, 123.7, 126.2, 127.1, 127.3, 128.0, 129.0, 131.3, 132.5, 134.6, 144.7, 160.7 (× 2); LR-EIMS: *m/z* = 227 $[M]^+$; HR-ESIMS: *m/z* = 227.0499 (calcd. for $C_{14}H_{10}N^{35}Cl$, 227.0496).

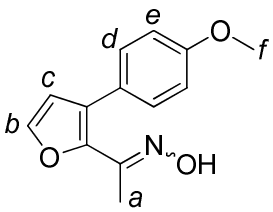


Scheme S4: Synthesis of quinoline derivatives. Reagents and conditions: i) $Pd(PPh_3)_4$, K_2CO_3, toluene, EtOH, reflux, 18 h, Ar; ii) $NH_2OH.HCl$, NaOAc, EtOH, reflux, 18 h; iii) $EtOCO_2Cl$, pyridine, CH_2Cl_2, rt, 18 h; iv) MAP, $PhCF_3$, UV irradiation, 3 h.



2-Acetyl-3-*p*-methoxyphenylfuran

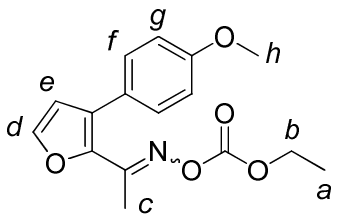
Prepared from 4-methoxyphenylboronic acid (0.202 g, 1.33 mmol), 2-acetyl-3-bromofuran[3] (0.209 g, 1.11 mmol), tetrakis(triphenylphosphine) palladium(II) (0.127 g, 0.11 mmol) and potassium carbonate (0.460 g, 3.33 mmol). Yellow oil (0.233 g, yield = 91%). ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 2.47 (s, 3H, H_a), 3.85 (s, 3H, H_f), 6.64 (d, J = 1.7 Hz, 1H, H_c), 6.94 (d, J = 8.9 Hz, 2H, H_e), 7.53 (d, J = 1.7 Hz, 1H, H_b), 7.63 (d, J = 8.9 Hz, 2H, H_d); %). ^{1}H NMR (100 MHz, $CDCl_3$, 296 K): δ = 27.7, 55.3, 113.6, 114.8, 124.1, 130.6, 133.3, 144.5, 147.0, 159.9, 188.0; LR-ESIMS: *m/z* = 239 $[MNa]^+$; HR-ESIMS: *m/z* = 239.0692 (calcd. for $C_{13}H_{12}O_3Na$, 239.0684).



2-Acetyl-3-*p*-methoxyphenylfuran oxime

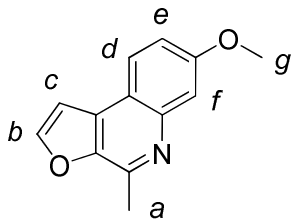
Prepared from 2-acetyl-3-*p*-methoxyphenylfuran (0.193 g, 0.89 mmol), hydroxylamine hydrochloride (0.124 g, 1.80 mmol) and sodium acetate (0.148 g, 1.80 mmol). Off-white

solid (0.186 g, yield = 90%). M.p. = 130-132 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 2.08 (s, 3H, H_a), 3.83 (s, 3H, H_f), 6.50 (d, J = 1.8 Hz, 1H, H_c), 6.91 (d, J = 8.8 Hz, 2H, H_e), 7.37 (d, J = 8.8 Hz, 2H, H_d), 7.44 (d, J = 1.8 Hz, 1H, H_b); ^{13}C NMR (75 MHz, $CDCl_3$, 296 K): δ = 12.8, 55.7, 114.1, 114.5, 120.9, 126.0, 126.2, 129.8, 130.5, 142.7, 150.3; LR-ESIMS: *m/z* = 254 $[MNa]^+$; HR-ESIMS: *m/z* = 254.0787 (calcd. for $C_{13}H_{13}NO_3Na$, 254.0793).



2-Acetyl-3-*p*-methoxyphenylfuran *O*-ethoxycarbonyl oxime – 6a

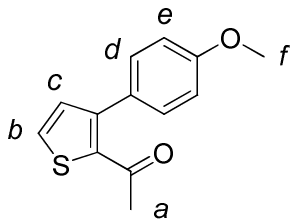
Prepared from 2-acetyl-3-*p*-methoxyphenylfuran oxime (0.179 g, 4.30 mmol), ethyl chloroformate (0.41 mL, 4.30 mmol) and pyridine (0.35 mL, 4.30 mmol). Colourless oil (0.178 g, yield = 75%). ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 1.37 (t, J = 7.1 Hz, 3H, H_a), 2.19 (s, 3H, H_c), 3.84 (s, 3H, H_h), 4.34 (q, J = 7.1 Hz, 2H, H_b), 6.56 (d, J = 1.8 Hz, 1H, H_e), 6.93 (d, J = 8.8 Hz, 2H, H_g), 7.48-7.52 (m, 3H, $H_{d,f}$); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 14.3, 14.3, 55.3, 64.8, 113.7, 114.5, 124.8, 129.1, 130.7, 142.3, 143.5, 153.6, 155.5, 159.5; LR-ESIMS: *m/z* = 326 $[M]^+$; HR-ESIMS: *m/z* = 326.1016 (calcd. for $C_{16}H_{17}NO_5Na$, 326.1004).



7-Methoxy-4-methylfuro[2,3-c]quinoline – 7a

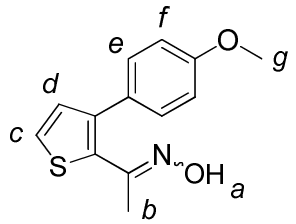
Prepared from 2-acetyl-3-*p*-methoxyphenylfuran *O*-ethoxycarbonyl oxime (0.052 g, 0.17 mmol). Colourless oil (0.026 g, yield = 71%). ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 2.90

(s, 3H, H_a), 3.95 (s, 3H, H_g), 7.19 (d, J = 2.0 Hz, 1H, H_c), 7.23 (dd, J = 2.5 Hz, 8.9 Hz, 1H, H_e), 7.53 (d, J = 2.5 Hz, 1H, H_f), 7.83 (d, J = 2.0 Hz, 1H, H_b), 7.95 (d, J = 8.9 Hz, 1H, H_d); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 19.8, 55.9, 105.8, 108.5, 117.6, 118.6, 124.7, 129.8, 145.9, 146.2, 147.4 (× 2), 159.6; LR-ESIMS: *m/z* = 214 $[MH]^+$; HR-ESIMS: *m/z* = 214.0862 (calcd. for $C_{13}H_{12}NO_2$, 214.0868).



2-Acetyl-3-*p*-methoxyphenylthiophene

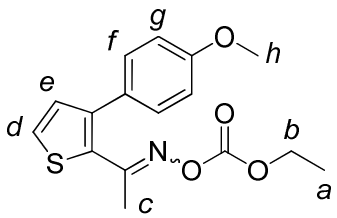
Prepared from 4-methoxyphenylboronic acid (0.180 g, 1.18 mmol), 2-acetyl-3-bromothiophene (0.202 g, 1.00 mmol), tetrakis(triphenylphosphine) palladium(II) (0.116 g, 0.01 mmol) and potassium carbonate (0.415 g, 3.00 mmol). Yellow oil (0.192 g, yield = 82%). ^{1}H NMR (300 MHz, $CDCl_3$, 295 K): δ = 2.15 (s, 3H, H_a), 3.84 (s, 3H, H_f), 6.94 (d, J = 8.8 Hz, 2H, H_e), 7.02 (d, J = 5.0 Hz, 1H, H_c), 7.29 (d, J = 8.8 Hz, 2H, H_d), 7.52 (d, J = 5.0 Hz, 1H, H_b); ^{13}C NMR (75 MHz, CDCl3, 295 K): δ = 29.3, 55.3, 113.8, 128.6, 130.4, 130.9, 132.1, 139.5, 146.7, 159.7, 192.3; LR-ESIMS: *m/z* =233 $[M]^+$; HR-ESIMS: *m/z* = 233.0639 (calcd. for $C_{13}H_{13}O_2S$, 233.0636).



2-Acetyl-3-*p*-methoxyphenylthiophene oxime

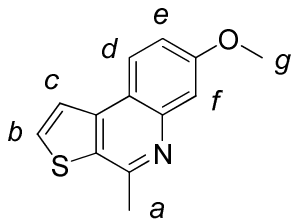
Prepared from 2-acetyl-3-*p*-methoxyphenylthiophene (0.186 g, 0.80 mmol), hydroxylamine hydrochloride (0.111 g, 1.60 mmol) and sodium acetate (0.131 g, 1.60 mmol). Colourless oil

(0.138 g, yield = 70%). ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 1.83 (s, 3H, H_a), 3.76 (s, 3H, H_g), 6.85 (d, J = 8.2 Hz, 2H, H_f), 6.98 (d, J = 5.1 Hz, 1H, H_d), 7.17 (d, J = 5.1 Hz, 1H, H_c), 7.23 (d, J = 8.2 Hz, 2H, H_e), 8.70-9.70 (br, 1H, H_a); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 15.1, 55.3, 113.9, 114.0, 125.1, 128.8, 130.0, 130.5, 133.0, 153.4, 159.2; LR-ESIMS: m/z = 270 $[MNa]^+$; HR-ESIMS: m/z = 270.0569 (calcd. for $C_{13}H_{13}NO_2NaS$, 270.0565).



2-Acetyl-3-*p*-methoxyphenylthiophene *O*-ethoxycarbonyl oxime – 6b

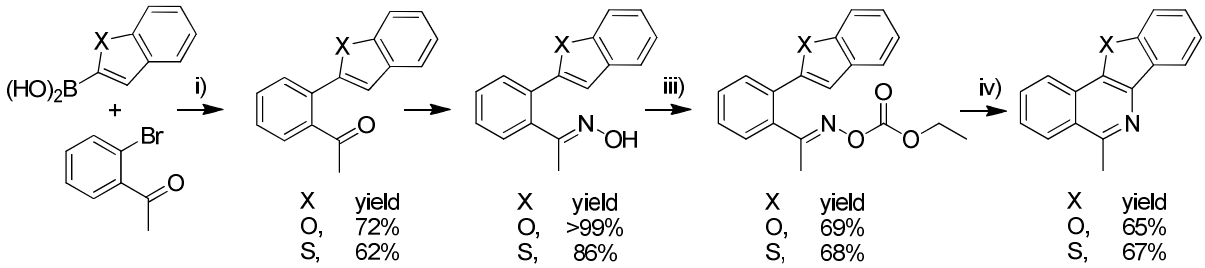
Prepared from 2-acetyl-3-*p*-methoxyphenylthiophene oxime (0.138 g, 0.56 mmol), ethyl chloroformate (0.05 mL, 0.56 mmol) and pyridine (0.05 mL, 0.56 mmol). Colourless oil (0.140 g, yield = 78%). ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 1.36 (t, J = 7.1 Hz, 3H, H_a), 1.97 (s, 3H, H_c), 3.83 (s, 3H, H_h), 4.34 (q, J = 7.1 Hz, 2H, H_b), 6.91 (d, J = 8.7 Hz, 2H, H_g), 7.07 (d, J = 5.1 Hz, 1H, H_e), 7.28 (d, J = 8.7 Hz, 2H, H_f), 7.34 (d, J = 5.1 Hz, 1H, H_d); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 14.3, 17.0, 55.3, 64.8, 114.0, 126.8, 128.4, 130.0, 130.4, 130.5, 143.2, 153.6, 159.5, 160.4; LR-ESIMS: m/z = 230 $[M]^+$; HR-ESIMS: m/z = 342.0770 (calcd. for $C_{16}H_{17}NO_4Na$, 342.0776).



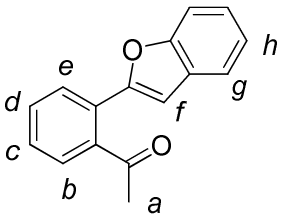
7-Methoxy-4-methylthieno[2,3-c]quinoline – 7b

Prepared from 2-acetyl-3-*p*-methoxyphenylthiophene *O*-ethoxycarbonyl oxime (0.056 g, 0.17 mmol). Colourless solid (0.025 g, yield = 62%). M.p. = 112 ˚C (dec.); ^{1}H NMR (300 MHz,

$CDCl_3$, 296 K): δ = 2.92 (s, 3H, H_a), 3.97 (s, 3H, H_g), 7.24 (dd, J = 2.6 Hz, 8.9 Hz, 1H, H_e), 7.54 (d, J = 2.6 Hz, 1H, H_f), 7.78 (d, J = 5.3 Hz, 1H, H_c), 7.89 (d, J = 5.3 Hz, 1H, H_b), 8.11 (d, J = 8.9 Hz, 1H, H_d); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 30.9, 127.0, 127.2, 128.6, 128.8, 129.3, 129.9, 130.0, 130.2, 134.9, 137.5, 140.6, 166.9; LR-EIMS: m/z = 229 $[M]^+$; HR-ESIMS: m/z = 229.0554 (calcd. for $C_{13}H_{11}ONS$, 229.0556).

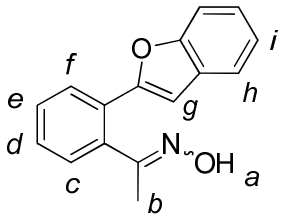


Scheme S5: Synthesis of isoquinoline derivatives. Reagents and conditions: i) $Pd(PPh_3)_4$, K_2CO_3, toluene, EtOH, reflux, 18 h, Ar; ii) $NH_2OH.HCl$, NaOAc, EtOH, reflux, 18 h; iii) $EtOCO_2Cl$, pyridine, CH_2Cl_2, rt, 18 h; iv) MAP, $PhCF_3$, UV irradiation, 3 h.



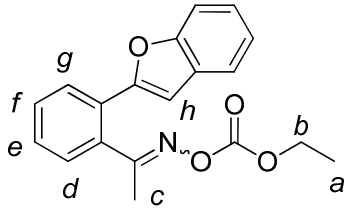
2-(Benzofuran-2-yl)acetophenone

Prepared from 2-benzofuranylboronic acid (0.406 g, 2.51 mmol), 2'-acetophenone (0.28 mL, 2.10 mmol), tetrakis(triphenylphosphine) palladium(II) (0.243 g, 0.21 mmol), and potassium carbonate (0.869 g, 6.30 mmol). Colourless oil (0.352 g, yield = 72%). ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 2.34 (s, 3H, H_a), 6.95 (d, J = 0.9 Hz, 1H, H_f), 7.25-7.34 (m, 2H, $H_{d,j}$), 7.44-7.55 (m, 4H, $H_{c,g,h,i}$), 7.61-7.63 (m, 1H, H_e), 7.74-7.77 (m, 1H, H_b); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 30.1, 105.0, 111.4, 121.3, 123.3, 124.8, 127.3, 128.0, 128.5, 128.9, 129.0, 130.4, 140.4, 154.3, 155.2, 204.4; LR-EIMS: m/z = 236 $[M]^+$; HR-ESIMS: m/z = 236.0834 (calcd. for $C_{16}H_{12}O_2$, 236.0832).



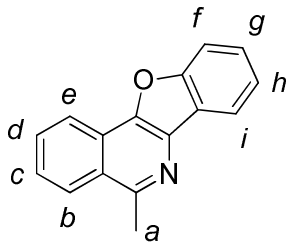
2-(Benzofuran-2-yl)acetophenone oxime

Prepared from 2-(benzofuran-2-yl)acetophenone (0.351 g, 1.50 mmol), hydroxylamine hydrochloride (0.207 g, 3.00 mmol) and sodium acetate (0.366 g, 3.00 mmol). Yellow oil (0.389 g, yield >99%). ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 2.08 (s, 3H, H_b), 6.87 (d, J = 0.9 Hz, 1H, H_g), 7.22-7.27 (m, 2H, $H_{i,j}$), 7.37-7.42 (m, 2H, $H_{e,h}$), 7.45-7.54 (m, 2H, $H_{k,d}$), 7.60 (m, 1H, H_f), 7.87 (d, J =7.6 Hz, 1H, H_c); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 15.8, 105.4, 111.3, 121.2, 123.0, 124.6, 126.1, 128.3, 128.5, 128.7, 129.0, 129.0, 129.5, 136.0, 154.3, 154.8; LR-ESIMS: *m/z* = 274 $[MNa]^+$; HR-ESIMS: *m/z* = 274.0848 (calcd. for $C_{16}H_{13}NO_2Na$, 274.0844).



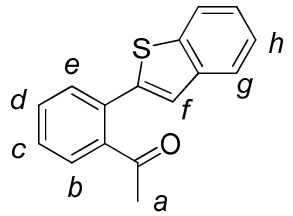
2-(Benzofuran-2-yl)acetophenone *O*-ethylcarbonyl oxime – 8a

Prepared from 2-(benzofuran-2-yl)acetophenone oxime (0.374 g, 1.50 mmol), ethyl chloroformate (0.12 mL, 1.50 mmol) and pyridine (0.14 mL, 1.50 mmol). Colourless oil (0.333 g, yield = 69%). ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 1.42 (t, J = 7.1 Hz, 3H, H_a), 2.18 (s, 3H, H_c), 4.39 (q, J = 7.1 Hz, 2H, H_b), 6.92 (s, 1H, H_h), 7.24-7.28 (m, 1H, H_f), 7.32 (dd, J 1.3 Hz, 7.3 Hz, 1H, H_e), 7.40-7.55 (m, 4H, H_{ArH}), 7.61 (dd, J = 1.1 Hz, 7.7 Hz, 1H, H_g), 7.86 (dd, J = 1.0 Hz, 7.7 Hz, 1H, H_d); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 14.8, 18.4, 65.2, 106.1, 111.7, 121.7, 123.5, 125.2, 127.4, 128.7, 129.0, 129.2, 129.3, 130.2, 130.3, 134.4, 154.2, 155.3, 166.6; LR-EIMS: *m/z* = 278 $[M]^+$.



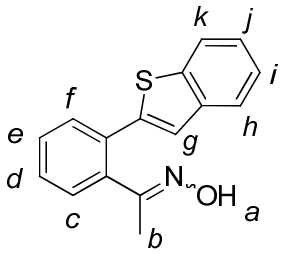
5-Methylbenzofuro[3,2-c]isoquinoline – 9a

Prepared from 2-(benzofuran-2-yl)acetophenone *O*-ethoxycarbonyl oxime (0.028 g, 0.087 mmol). Colourless oil (0.013 g, yield = 65%). ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 3.12 (s, 3H, H_a), 7.46 (m, 1H, H_c), 7.53 (m, 1H, H_d), 7.66-7.72 (m, 2H, $H_{e,g}$), 7.85 (m, 1H, H_h), 8.26-8.29 (m, 2H, $H_{b,f}$), 8.40 (d, J = 8.0 Hz, 1H, H_i); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 22.8, 112.0, 120.3, 120.6, 123.4, 123.5, 124.2, 126.7, 126.9, 127.1, 129.8, 130.5, 155.1, 156.2, 169.6, 190.3; LR-EIMS: *m/z* = 233 $[M]^+$; HR-ESIMS: *m/z* = 233.0836 (calcd. for $C_{16}H_{11}ON$, 233.0835).



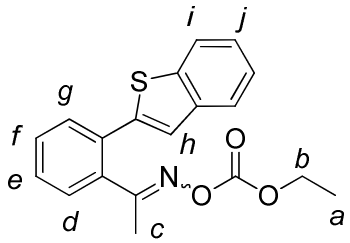
2-(Benzothiophen-2-yl)acetophenone

Prepared from benzo[b]thiophene-2-boronic acid (0.400 g, 2.25 mmol), 2'-bromoacetophenone (0.25 mL, 1.87 mmol), tetrakis(triphenylphosphine) palladium(II) (0.216 g, 0.19 mmol) and potassium carbonate (0.776 g, 5.61 mmol). Colourless oil (0.293 g, yield = 62%). ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 2.22 (s, 3H, H_a), 7.22 (d, J = 0.6 Hz, 1H, H_f), 7.34-7.42 (m, 2H, $H_{c,d}$), 7.43-7.59 (m, 4H, $H_{g,h,i,j}$), 7.77-7.80 (m, 1H, H_e), 7.85-7.87 (m, 1H, H_b); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 30.4, 122.2, 123.9, 124.4, 124.8, 127.6, 128.3, 128.6, 130.6, 130.8, 132.3, 133.1, 140.2, 140.5, 141.7, 204.8; LR-EIMS: *m/z* = 252 $[M]^+$; HR-ESIMS: *m/z* = 252.0605 (calcd. for $C_{16}H_{12}OS$, 252.0603).



2-(Benzothiophen-2-yl)acetophenone oxime

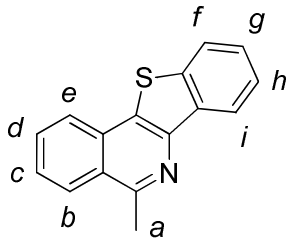
Prepared from 2-(benzothiophen-2-yl)acetophenone (0.283 g, 1.10 mmol), hydroxylamine hydrochloride (0.156 g, 2.20 mmol) and sodium acetate (0.184 g, 2.20 mmol). Colourless oil (0.325 g, yield = 86%). Two isomers 1:3.25. ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 1.94/1.98 (s, 3H, H_b), 7.31 (d, J = 05 Hz, 1H, H_g), 7.32-7.48 (m, 4H, $H_{d,e,i,j}$), 7.59 (d, J = 7.4 Hz, 1H, H_f), 7.64 (m, 1H, H_c), 7.79 (dd, J = 1.7 Hz, 6.9 Hz, 1H, H_k), 7.84 (dd, 1.4 Hz, 7.9 Hz, 1H, H_h), 7.94-8.19 (br, 1H, H_a); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 15.9, 122.2, 124.4, 124.5, 126.0, 128.4, 128.5, 129.1, 129.5, 130.8, 133.1, 137.2, 140.2, 140.4, 142.3, 159.2; LR-ESIMS: *m/z* = 290.3 $[MNa]^+$; HR-ESIMS: *m/z* = 290.0608 (calcd. for $C_{16}H_{13}NONaS$, 290.0616).



2-(Benzothiophen-2-yl)acetophenone *O*-ethoxycarbonyl oxime – 8b

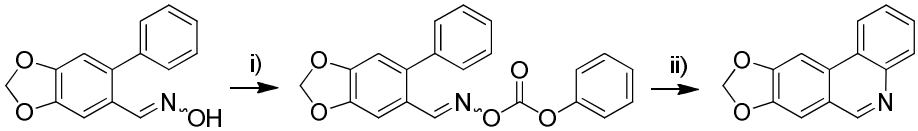
Prepared from 2-(benzothiophen-2-yl)acetophenone oxime (0.306 g, 1.15 mmol), ethyl chloroformate (0.11 mL, 1.15 mmol) and pyridine (0.09 mL, 1.15 mmol). Colourless oil (0.267 g, yield = 68%). Two isomers 1:1.3. ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 1.39/1.40 (t, J = 7.1 Hz, 3H, H_a), 2.01/2.40 (s, 3H, H_c), 4.36/4.38 (q, J = 7.1 Hz, 2H, H_b), 7.32 (d, J = 0.5 Hz, 1H, H_h), 7.34-7.44 (m, 3H, $H_{e,j,k}$), 7.47-7.52 (m, 1H, H_f), 7.59 (dd, J = 1.2 Hz, 7.7 Hz, 1H, H_g), 7.74 (dd, J = 1.4 Hz, 8.0 Hz, 1H, H_d), 7.79 (d, J = 6.6 Hz, 1H, H_l), 7.84

(dd, J = 0.5 Hz, 7.1 Hz, 1H, H_i); ^{13}C NMR (100 MHz, $CDCl_3$, 296 K): δ = 14.3, 17.9, 64.8, 122.2, 123.9, 124.3, 124.6, 124.6, 127.0, 128.6, 129.9, 130.8, 133.2, 135.4, 140.2, 140.4, 141.6, 153.9, 166.3; LR-ESIMS: *m/z* = 362 $[MNa]^+$; HR-ESIMS: *m/z* = 362.0838 (calcd. for $C_{19}H_{17}NO_3NaS$, 362.0827).

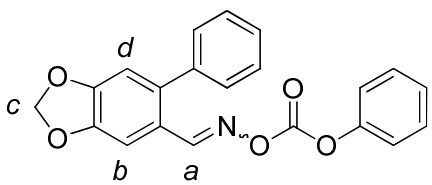


5-Methylbenzo[4,5]thieno[3,2-c]isoquinoline – 9b

Prepared from 2-(benzothiophen-2-yl)acetophenone *O*-ethoxycarbonyl oxime (0.051 g, 0.15 mmol). Colourless oil (0.025 g, yield = 67%). ^{1}H NMR (400 MHz, $CDCl_3$, 296 K): δ = 3.13(s, 3H, H_a), 7.51-7.58 (m, 2H, $H_{c,d}$), 7.65-7.70 (m, 1H, H_h), 7.79-7.83 (m, 1H, H_g), 7.94 (d, J = 7.1 Hz, 1H, H_e), 8.09 (d, J = 8.2 Hz, 1H, H_f), 8.27 (d, J = 8.4 Hz, 1H, H_i), 8.54 (d, J = 7.1 Hz, 1H, H_b); ^{13}C NMR (125 MHz, $CDCl_3$, 294 K): δ = 22.7, 122.7, 122.8, 124.2, 124.9, 126.0 (×2), 127.0, 127.1 (× 2), 128.1, 130.5, 130.6, 131.7, 156.5 (× 2).

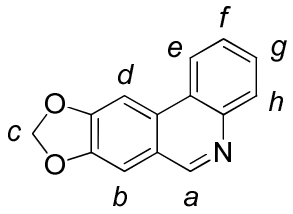


Scheme S6: Synthesis of trispheridine from 6-phenylbenzo[*d*][1,3]dioxole-5-carbaldehyde oxime.[2] Reagents and conditions: i) $PhOCO_2Cl$, pyridine, CH_2Cl_2, rt, 18 h, 66%; ii) MAP, *t*-BuOH, UV irradiation, 3 h, 49%.



6-Phenylbenzo[*d*][1,3]dioxole-5-carbaldehyde *O*-phenoxycarbonyl oxime – 10

Prepared from 6-phenylbenzo[*d*][1,3]dioxole-5-carbaldehyde oxime[2] (0.257 g, 1.07 mmol), phenyl chloroformate (0.13 mL, 1.07 mmol) and pyridine (0.08 mL, 1.07 mmol). Colourless solid (0.254 g, yield = 66%). M.p. = 115-117 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 6.07 (s, 2H, H_c), 6.83 (s, 1H, H_d), 7.22-7.29 (m, 5H, H_{ArH}), 7.37-7.47 (m, 5H, H_{ArH}), 7.62 (s, 1H, H_b), 8.29 (s, 1H, H_a); ^{13}C NMR (100 MHz, $CDCl_3$, 295 K): δ = 53.9, 102.4, 106.5, 110.5, 121.4, 126.7, 128.4, 129.0, 130.0, 130.2, 139.0, 140.4, 148.0, 151.0, 151.3, 152.6, 155.9; LR-ESIMS: *m/z* = 384 $[MNa]^+$; HR-ESIMS: *m/z* = 384.0859 (calcd. for $C_{21}H_{15}NO_5Na$, 384.0848).



Trispheridine - 11

Prepared from 6-phenylbenzo[*d*][1,3]dioxole-5-carbaldehyde *O*-phenoxycarbonyl oxime (0.049 mg, 0.136 mmol). Colourless solid (0.015 g, yield = 49%). ^{1}H and ^{13}C NMR spectra were consistent with those reported in the literature.[2] M.p. = 130-132 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$, 295 K): δ = 6.17 (s, 2H, H_c), 7.34 (s, 1H, H_d), 7.61-7.71 (m, 2H, $H_{f,g}$), 7.92 (s, 1H, H_b), 8.14 (dd, *J* = 1.1 Hz, 8.2 Hz, 1H, H_e), 8.38 (dd, *J* = 1.2 Hz, 8.1 Hz, 1H, H_h), 9.09 (s, 1H, H_a); ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 100.0, 101.9, 105.5, 122.0, 123.1, 124.3, 126.7, 128.0, 130.1, 130.3, 144.1, 148.2, 151.5, 151.8.

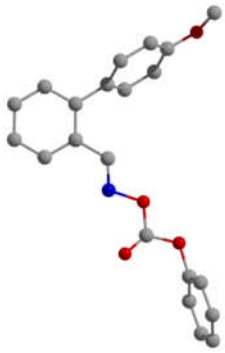


Figure S1: The X-ray crystal structure of **1b**.

Table S2: Crystal data and structure refinement for **1b**.

Identification code	**1b**	
Empirical formula	$C_{21}H_{17}NO_4$	
Formula weight	347.36	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.5885(19) Å	α = 90°.
	b = 13.388(3) Å	β = 90°.
	c = 15.162(4) Å	γ = 90°.
Volume	1743.4(7) $Å^3$	
Z	4	
Density (calculated)	1.323 Mg/m^3	
Absorption coefficient	0.092 mm^{-1}	
F(000)	728	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.03 to 25.33°.	
Index ranges	$-8 \le h \le 10$, $-16 \le k \le 13$, $-17 \le l \le 18$	
Reflections collected	11104	
Independent reflections	3181 [R(int) = 0.0433]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.000 and 0.851	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3181 / 0 / 236	
Goodness-of-fit on F^2	0.987	
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0751	
R indices (all data)	R1 = 0.0441, wR2 = 0.0795	
Absolute structure parameter	0.0(9)	
Largest diff. peak and hole	0.147 and -0.182 e.$Å^{-3}$	

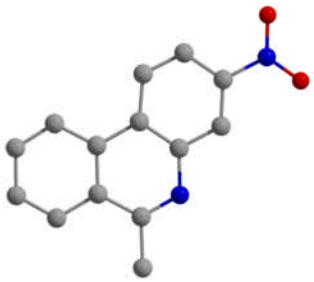


Figure S2: The X-ray crystal structure of **5d**.

Table S3: Crystal data and structure refinement for **5d**.

Identification code	**5d**	
Empirical formula	$C_{14}H_{10}N_2O_2$	
Formula weight	238.24	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 4.469(3) Å	α = 90°.
	b = 13.268(10) Å	β = 96.36(2)°.
	c = 18.459(16) Å	γ = 90°.
Volume	1087.8(15) $Å^3$	
Z	4	
Density (calculated)	1.455 Mg/m^3	
Absorption coefficient	0.816 mm^{-1}	
F(000)	496	
Crystal size	0.10 x 0.03 x 0.03 mm^3	
Theta range for data collection	4.11 to 68.25°.	
Index ranges	$-5 \le h \le 5$, $-15 \le k \le 15$, $-22 \le l \le 22$	
Reflections collected	13762	
Independent reflections	1978 [R(int) = 0.1630]	
Completeness to theta = 67.00°	99.7 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.000 and 0.516	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1978 / 0 / 165	
Goodness-of-fit on F^2	1.244	
Final R indices [I>2sigma(I)]	R1 = 0.1223, wR2 = 0.3345	
R indices (all data)	R1 = 0.1570, wR2 = 0.3712	
Extinction coefficient	0.028(9)	
Largest diff. peak and hole	0.382 and -0.384 $e.Å^{-3}$	

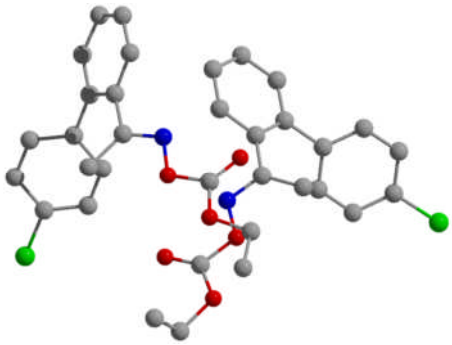


Figure S3: The X-ray crystal structure of **4f**.

Table S4: Crystal data and structure refinement for **4f**.

Identification code	**4f**	
Empirical formula	$C_{17}H_{16}ClNO_3$	
Formula weight	317.76	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 24.039(14) Å	α = 90°.
	b = 7.017(5) Å	β = 95.759(14)°.
	c = 19.280(12) Å	γ = 90°.
Volume	3236(4) $Å^3$	
Z	8	
Density (calculated)	1.305 Mg/m^3	
Absorption coefficient	2.191 mm^{-1}	
F(000)	1328	
Crystal size	0.12 x 0.02 x 0.02 mm^3	
Theta range for data collection	2.30 to 68.08°.	
Index ranges	$-28 \le h \le 28$, $-8 \le k \le 8$, $-22 \le l \le 22$	
Reflections collected	20550	
Independent reflections	5616 [R(int) = 0.2075]	
Completeness to theta = 67.00°	99.6 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.000 and 0.756	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5616 / 1 / 400	
Goodness-of-fit on F^2	1.203	
Final R indices [I>2sigma(I)]	R1 = 0.1423, wR2 = 0.3619	
R indices (all data)	R1 = 0.1656, wR2 = 0.3976	
Absolute structure parameter	0.09(5)	
Extinction coefficient	0.0053(8)	
Largest diff. peak and hole	0.723 and -0.600 $e.Å^{-3}$	

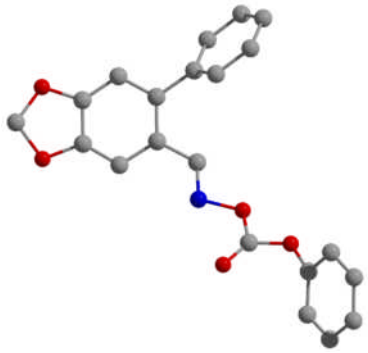


Figure S4: The X-ray crystal structure of **10**.

Table S5: Crystal data and structure refinement for **10**.

Identification code	**10**	
Empirical formula	$C_{21}H_{15}NO_5$	
Formula weight	361.34	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.119(8) Å	α = 97.856(18)°.
	b = 9.581(7) Å	β = 96.761(13)°.
	c = 10.232(8) Å	γ = 104.70(2)°.
Volume	845.7(12) $Å^3$	
Z	2	
Density (calculated)	1.419 Mg/m^3	
Absorption coefficient	0.102 mm^{-1}	
F(000)	376	
Crystal size	0.10 x 0.10 x 0.10 mm^3	
Theta range for data collection	2.23 to 25.32°.	
Index ranges	$-10 \le h \le 10$, $-9 \le k \le 11$, $-12 \le l \le 10$	
Reflections collected	5292	
Independent reflections	2969 [R(int) = 0.0681]	
Completeness to theta = 25.00°	96.8 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.000 and 0.8540	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2969 / 0 / 244	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0783, wR2 = 0.1996	
R indices (all data)	R1 = 0.0858, wR2 = 0.2115	
Largest diff. peak and hole	0.633 and -0.543 $e.Å^{-3}$	

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1. F. Portela-Cubillo, J. S. Scott and J. C. Walton, *J. Org Chem.* 2008, **73**, 5558.

2. F. Portela-Cubillo, J. Lymer, E. M. Scanlan, J. S. Scott and J. C. Walton, *Tetrahedron*, 2008, **64**, 11908.

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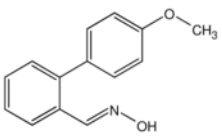
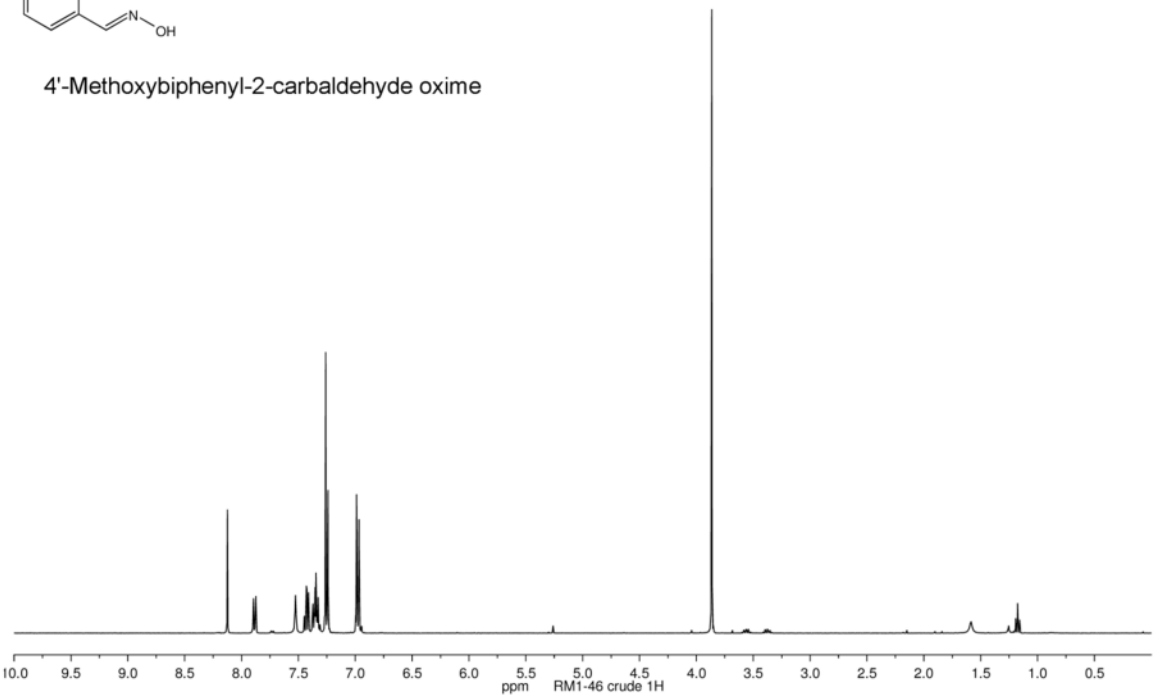
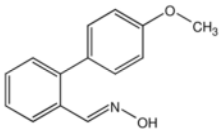
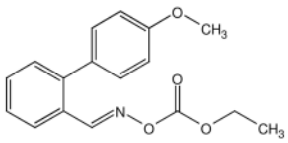
^{1}H and ^{13}C NMR spectra of novel compounds



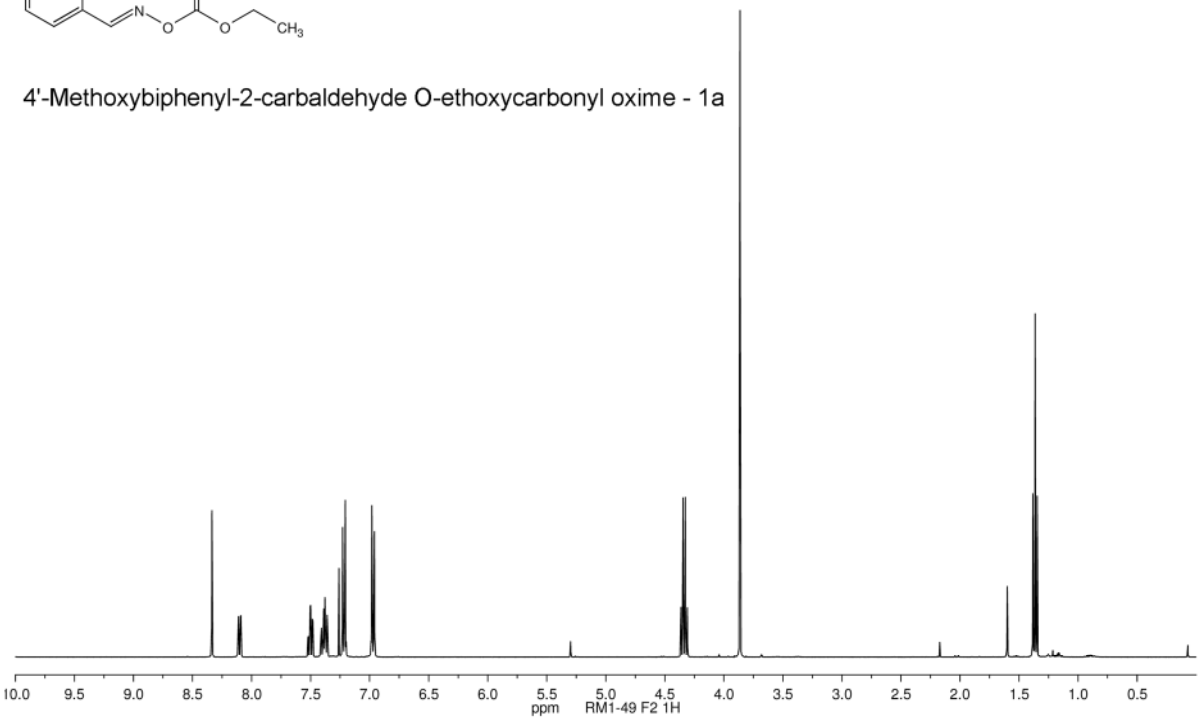
4'-Methoxybiphenyl-2-carbaldehyde oxime

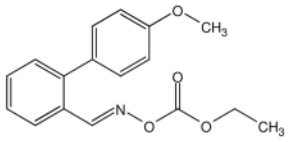


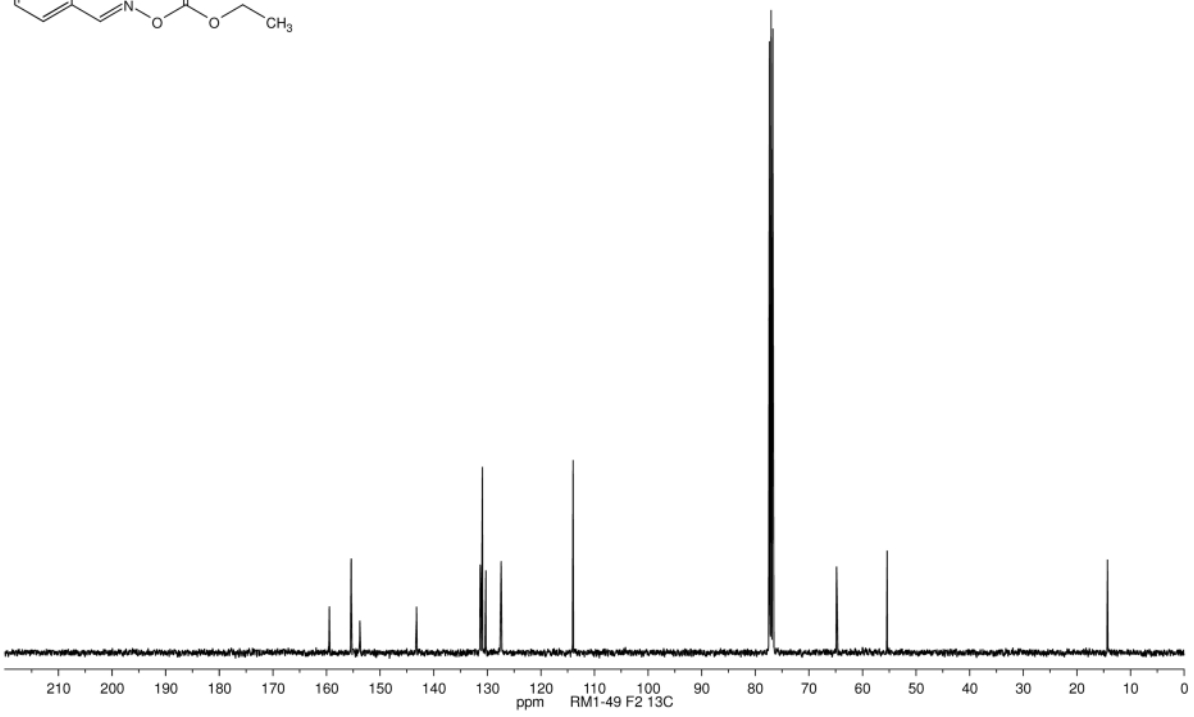


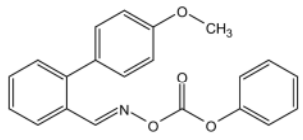


4'-Methoxybiphenyl-2-carbaldehyde O-ethoxycarbonyl oxime - 1a

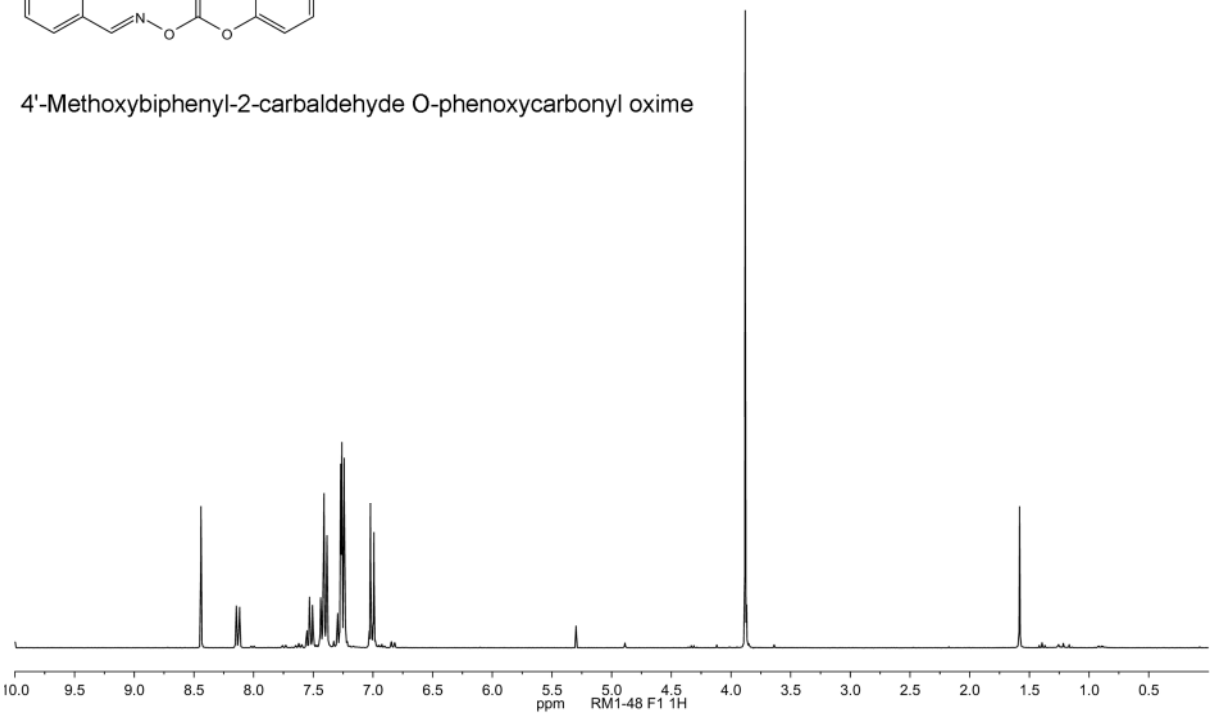


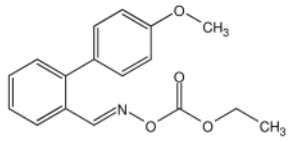


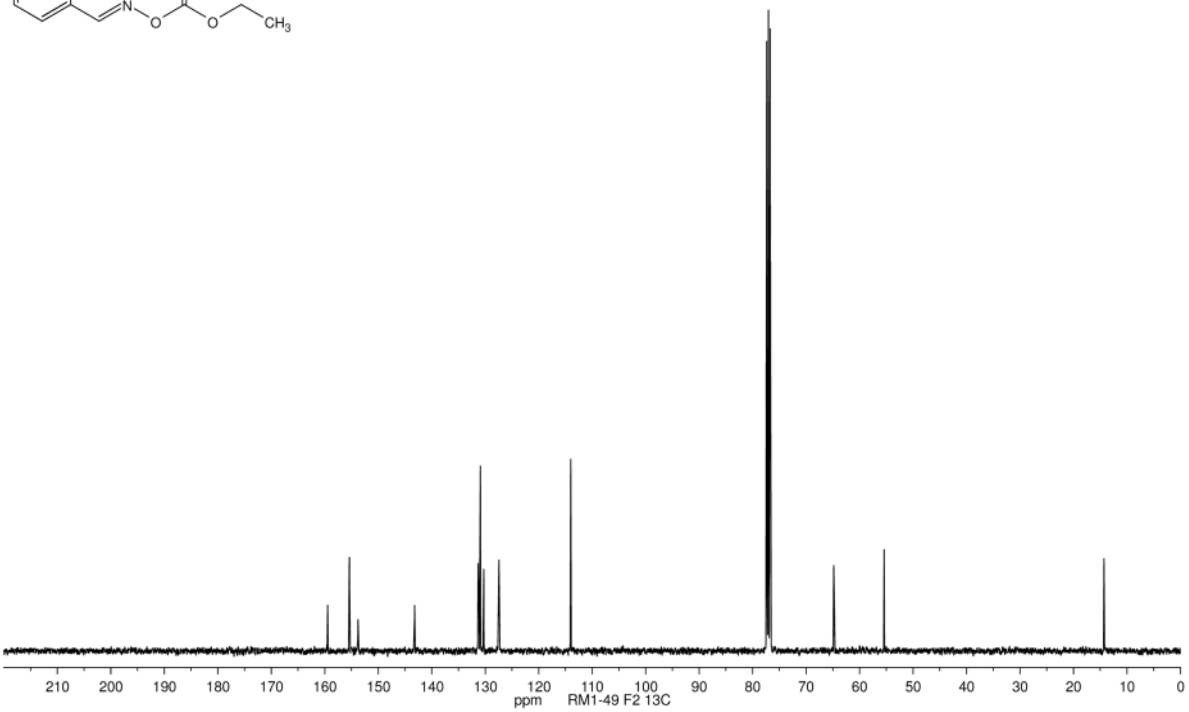


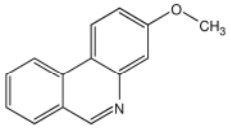


4'-Methoxybiphenyl-2-carbaldehyde O-phenoxycarbonyl oxime

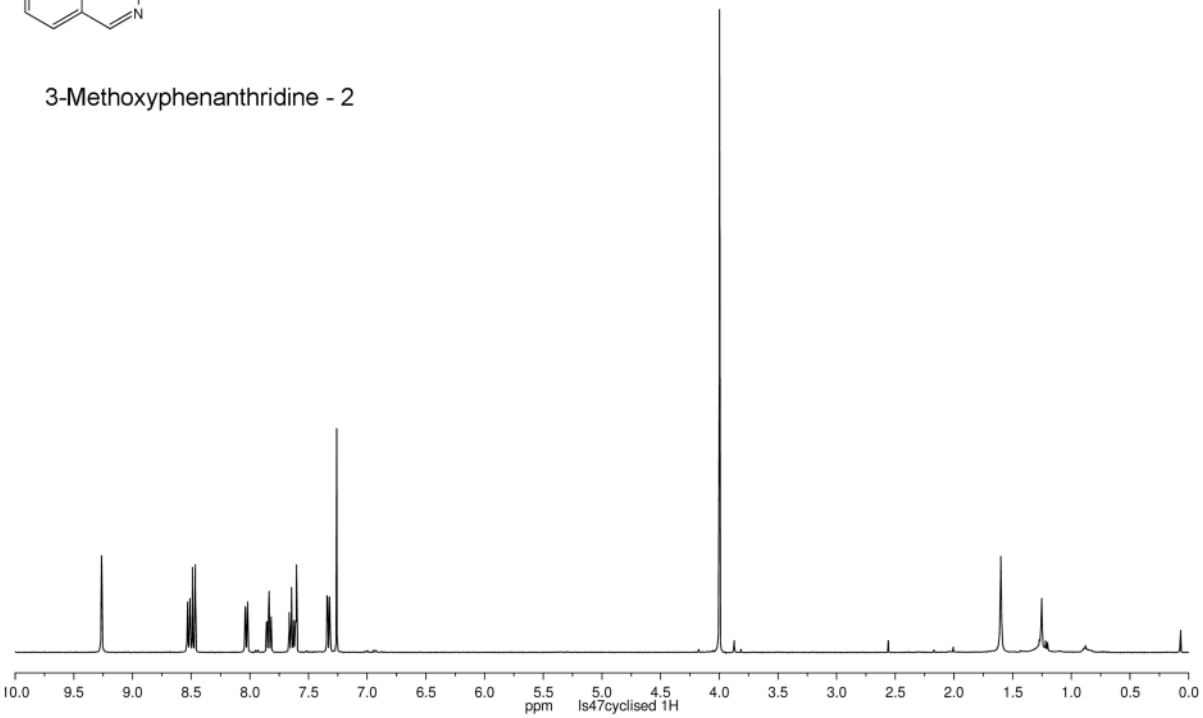


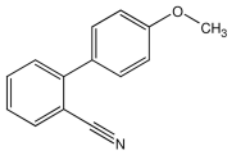




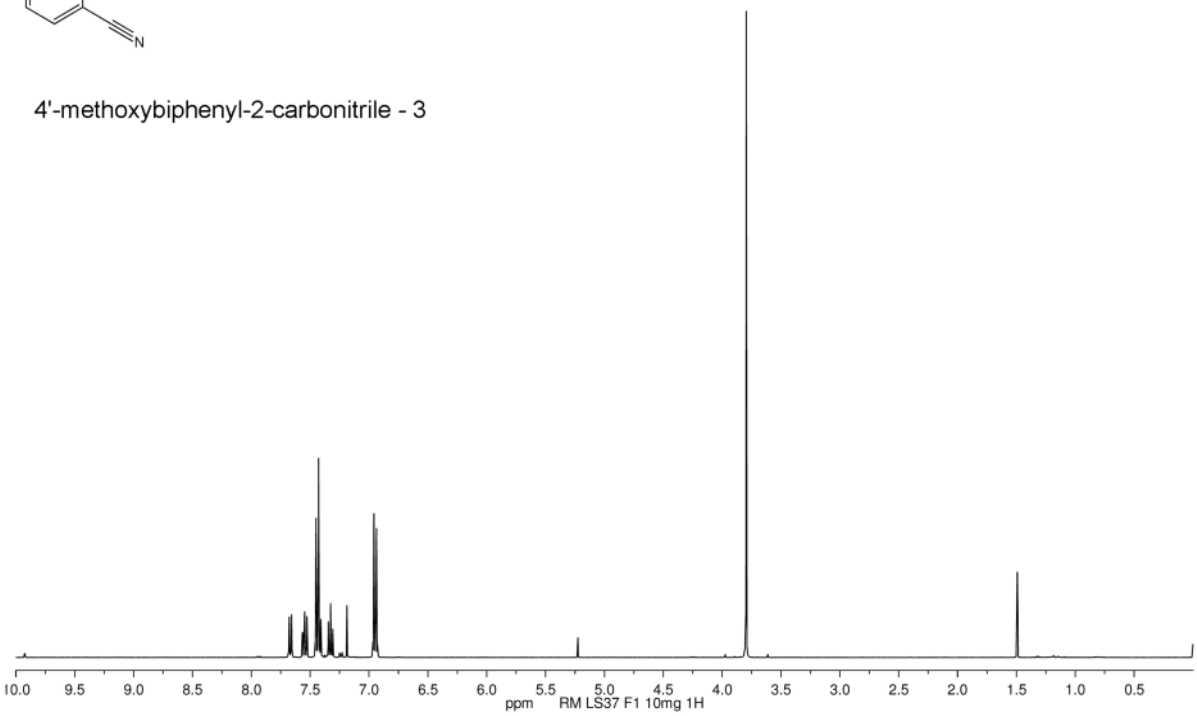


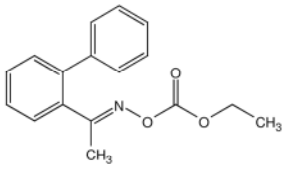
3-Methoxyphenanthridine - 2



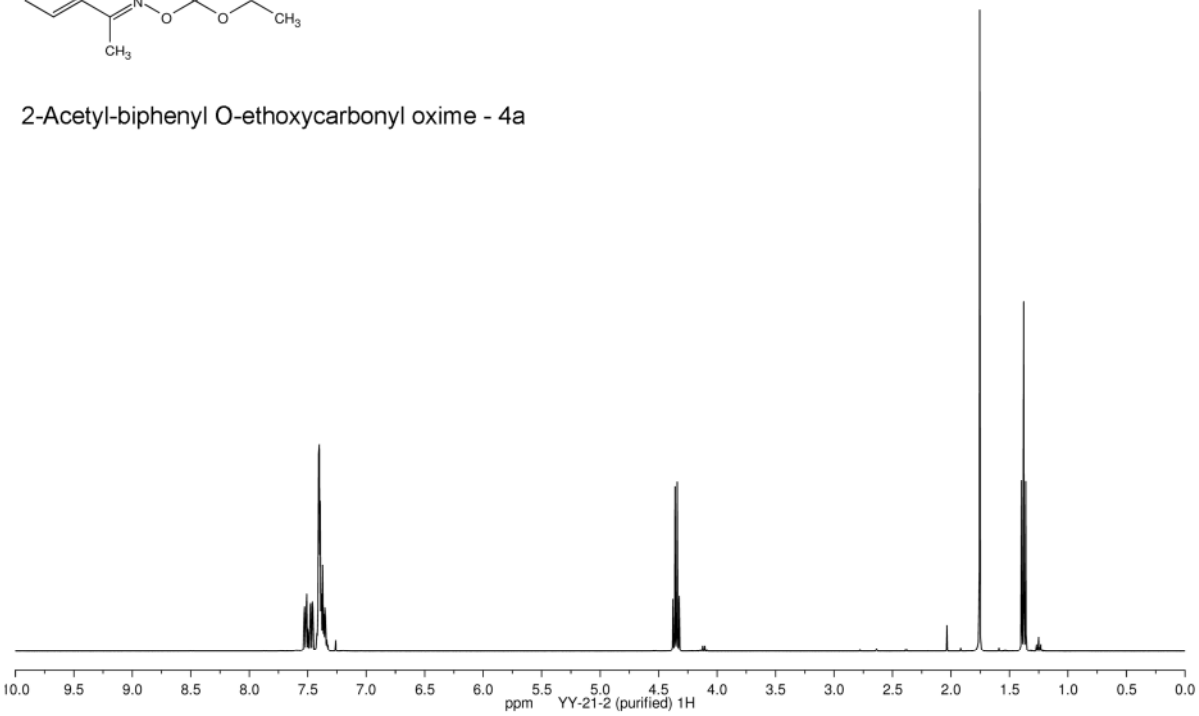


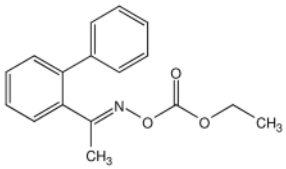
4'-methoxybiphenyl-2-carbonitrile - 3

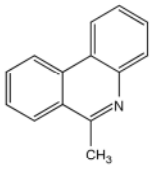




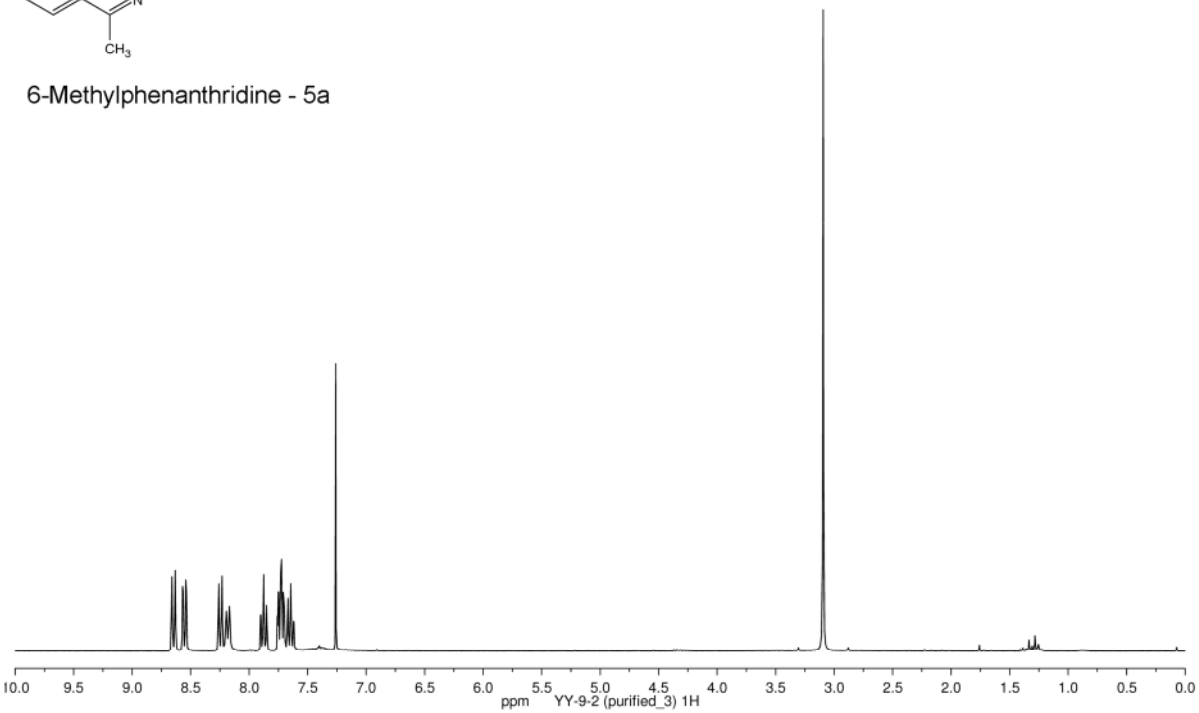
2-Acetyl-biphenyl O-ethoxycarbonyl oxime - 4a

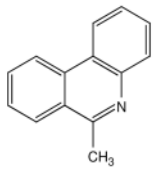


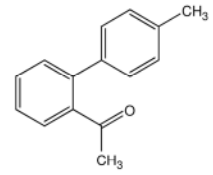




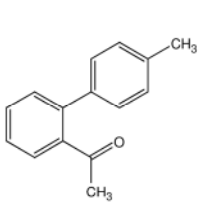
6-Methylphenanthridine - 5a

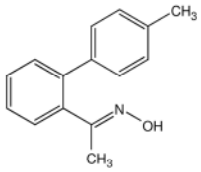




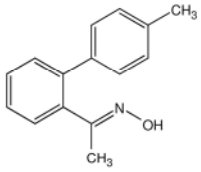


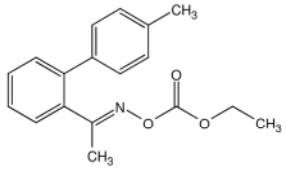
2-p-Tolylacetophenone



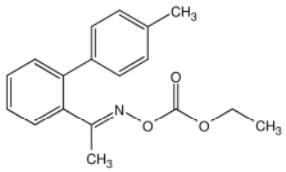


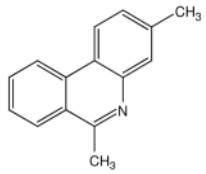
2-p-Tolylacetophenone oxime



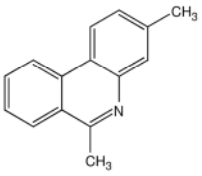


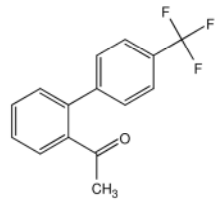
2-p-Tolylacetophenone O-ethoxycarbonyl oxime - 4b



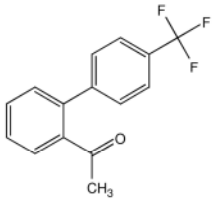


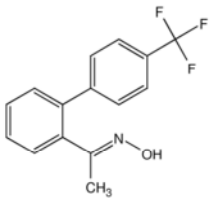
3,6-Dimethylphenanthridine - 5b



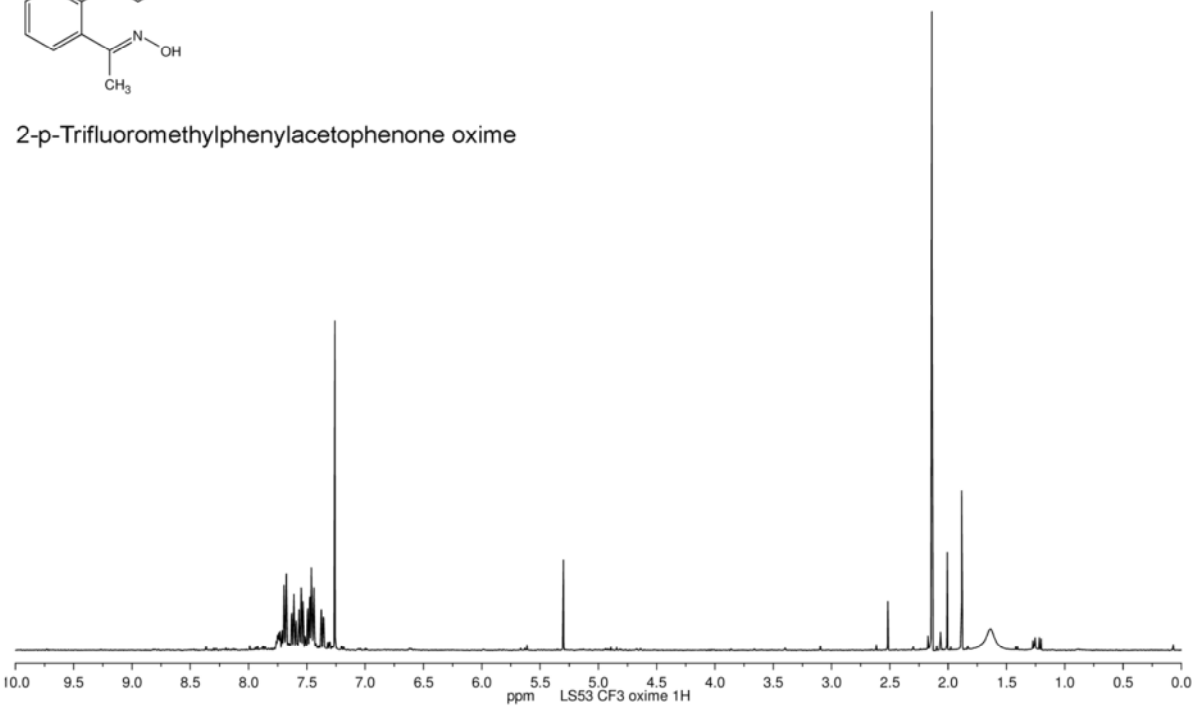


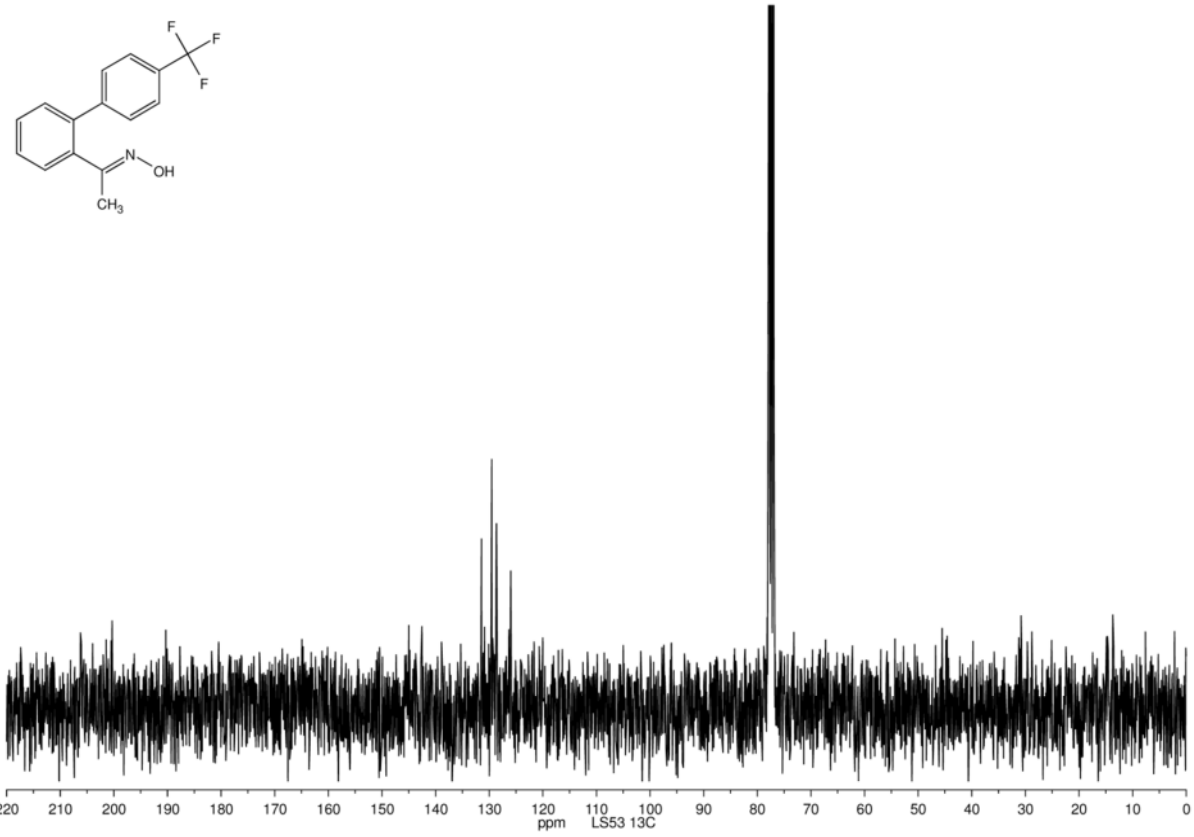
2-p-Trifluoromethylphenylacetophenone

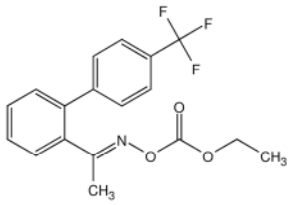




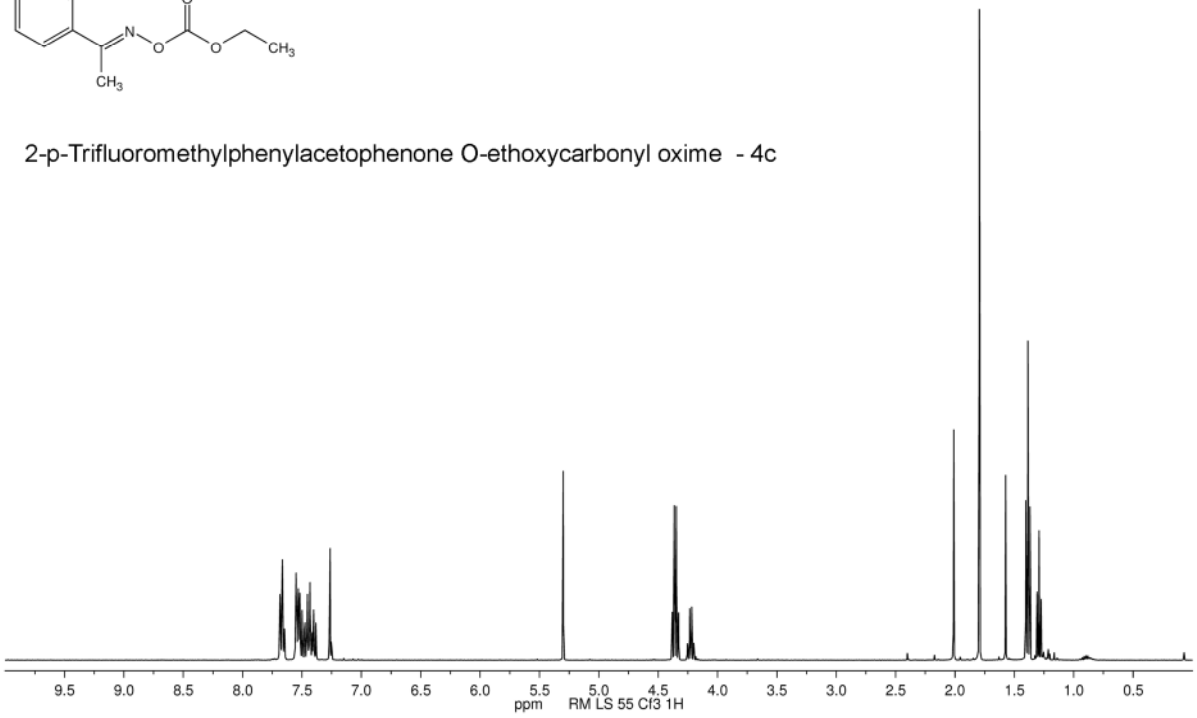
2-p-Trifluoromethylphenylacetophenone oxime

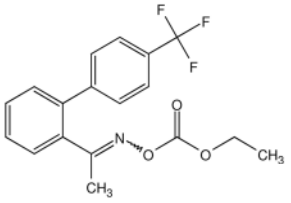


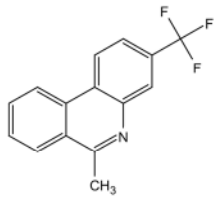




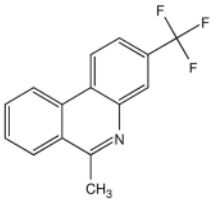
2-p-Trifluoromethylphenylacetophenone O-ethoxycarbonyl oxime - 4c

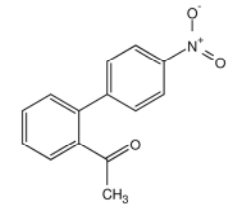




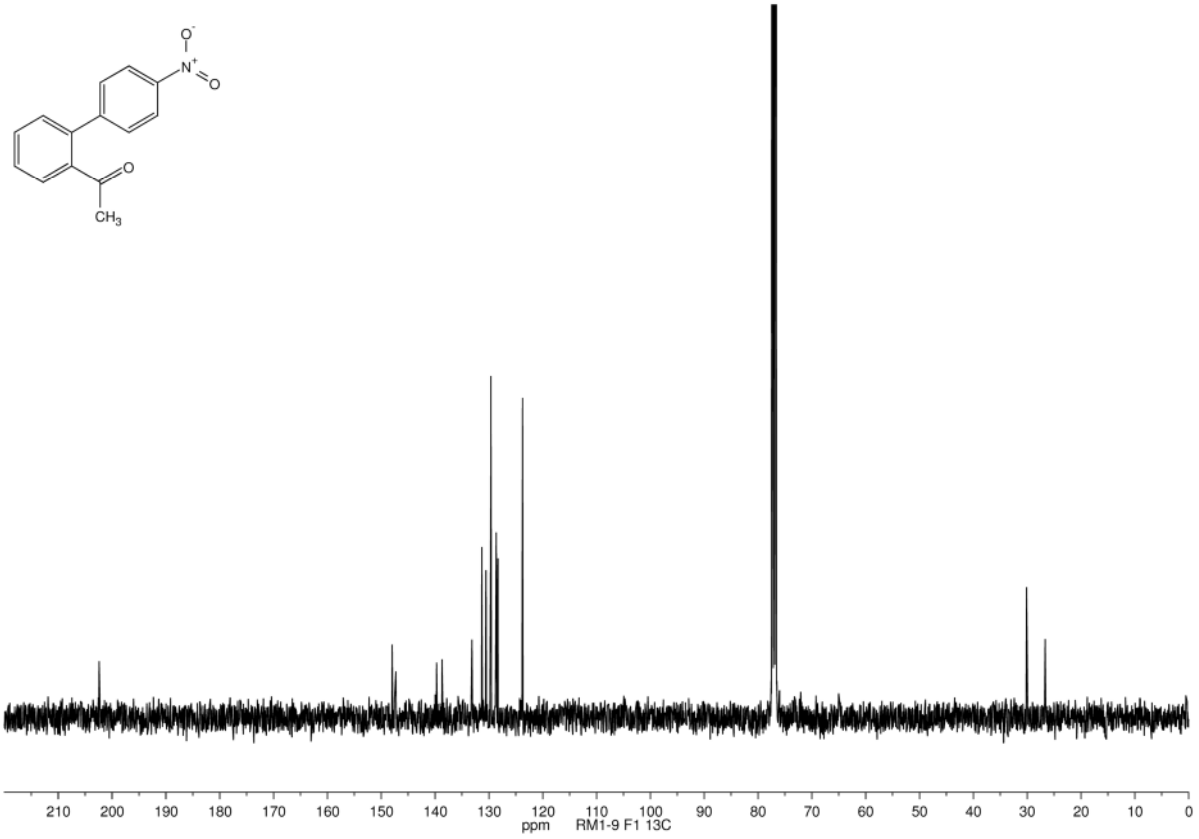


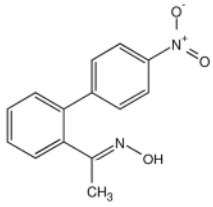
6-methyl-3-(trifluoromethyl)phenanthridine - 5c



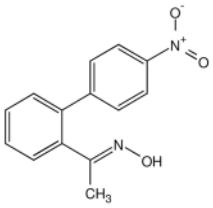


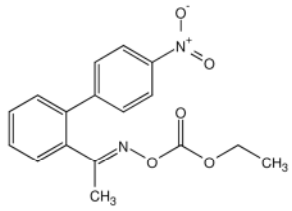
2-p-Nitrophenylacetophenone



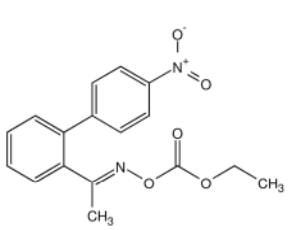


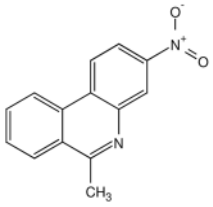
2-p-Nitrophenylacetophenone oxime



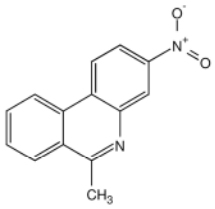


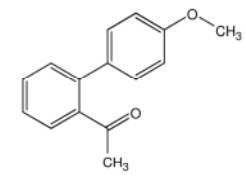
2-p-Nitrophenylacetophenone O-ethoxycarbonyl oxime - 4d



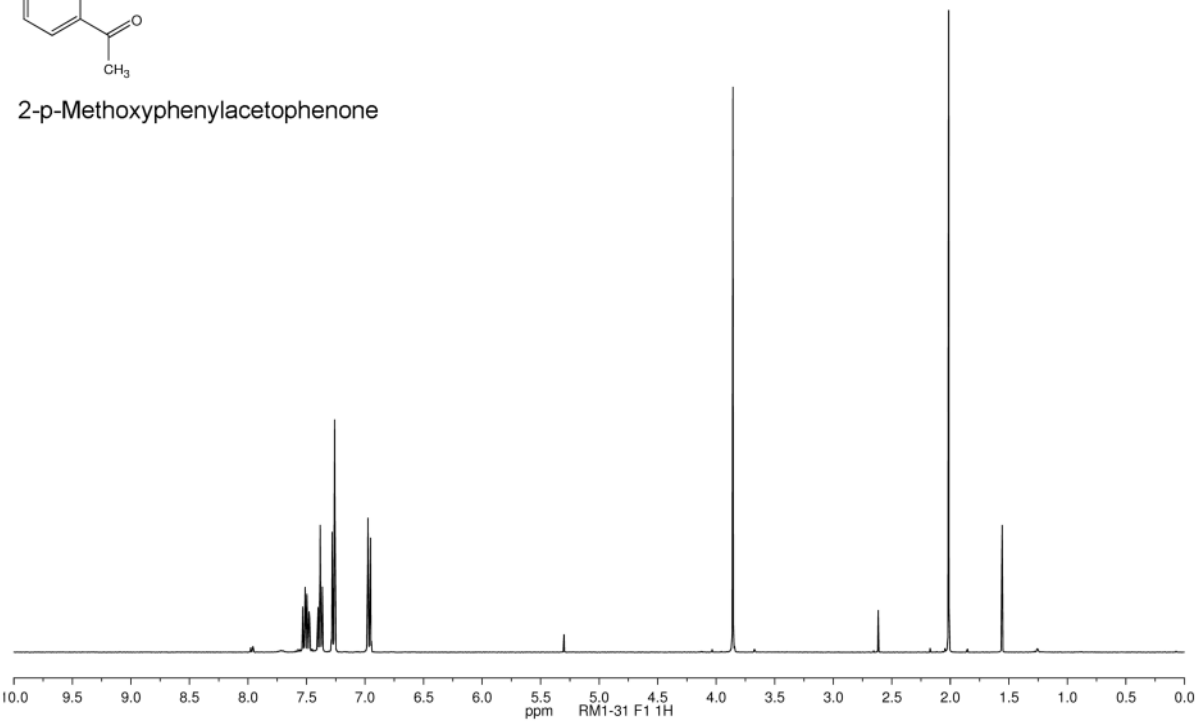


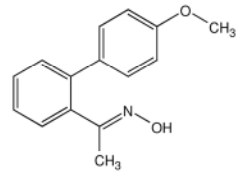
6-Methyl-3-nitrophenanthridine - 5d



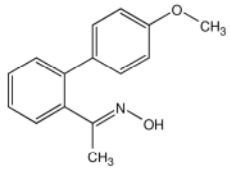


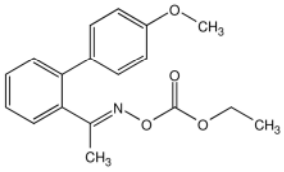
2-p-Methoxyphenylacetophenone



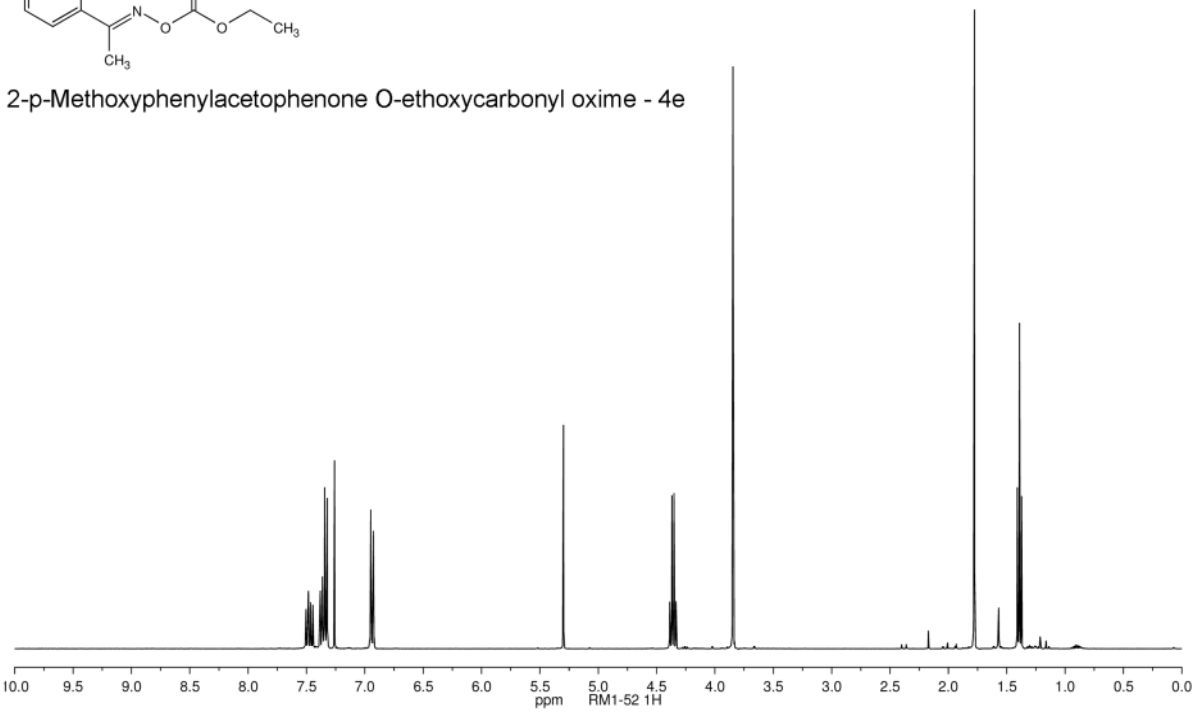


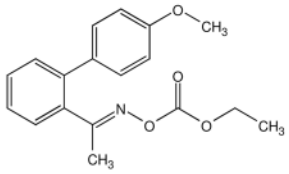
2-p-Methoxyphenylacetophenone oxime

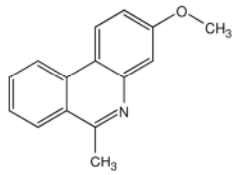




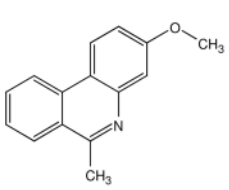
2-p-Methoxyphenylacetophenone O-ethoxycarbonyl oxime - 4e

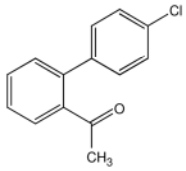




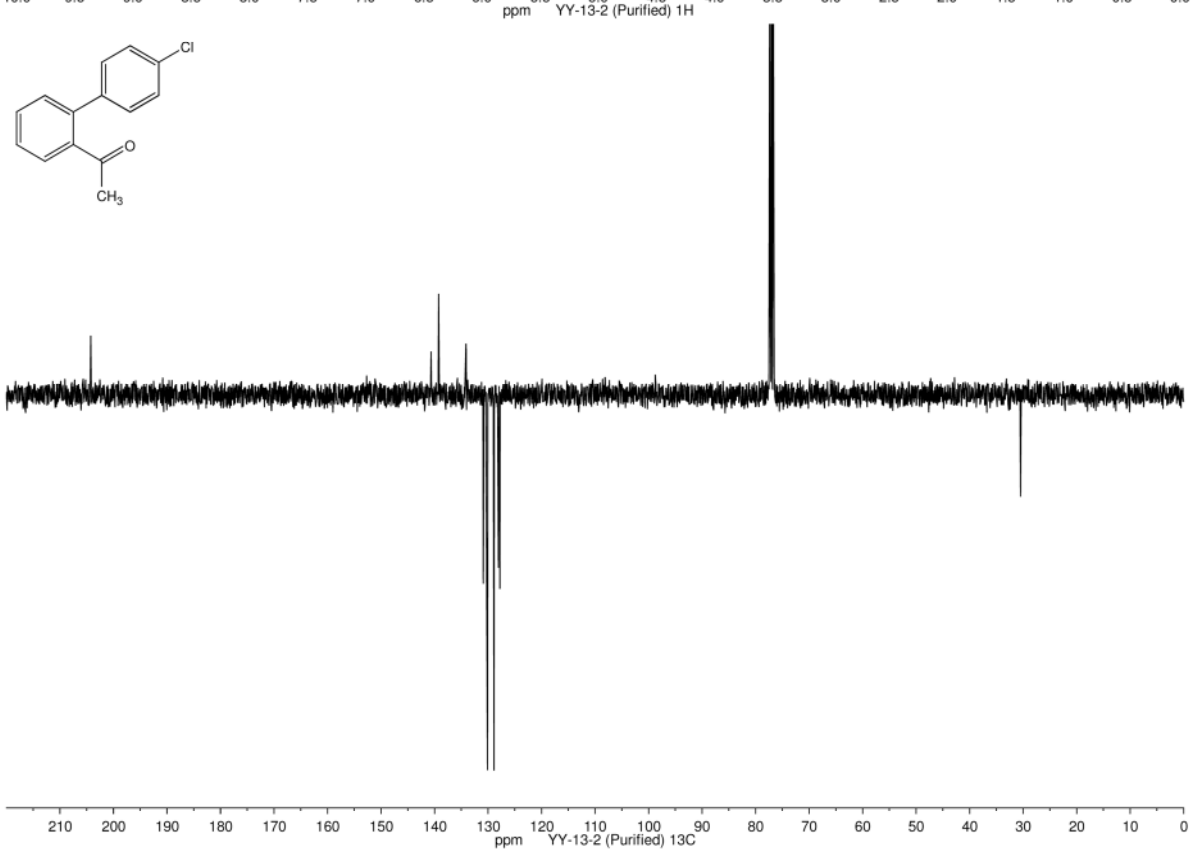


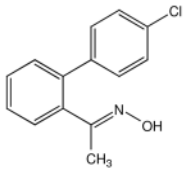
3-Methoxy-6-methylphenanthridine - 5e



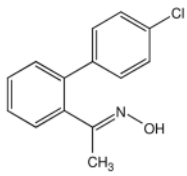


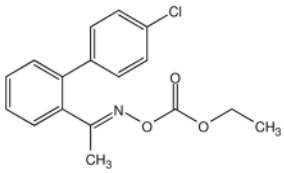
2-p-Chlorophenylacetophenone



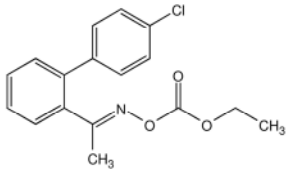


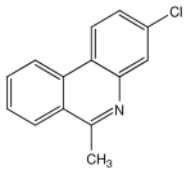
2-p-Chlorophenylacetophenone oxime



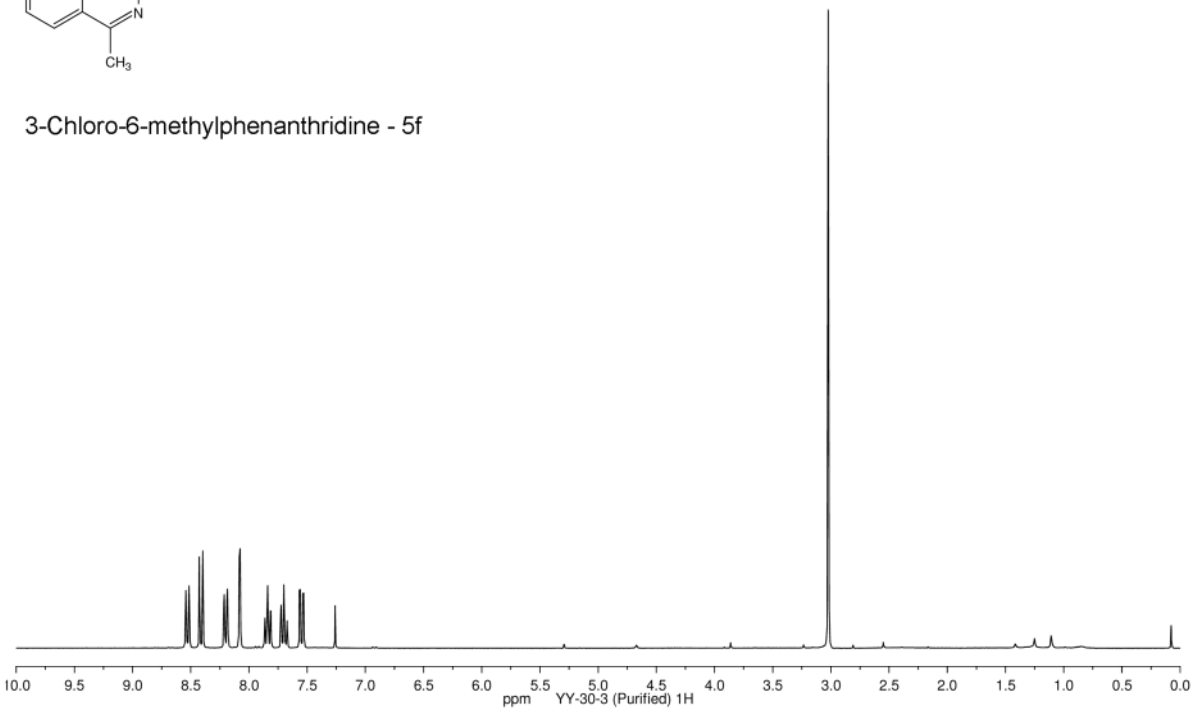


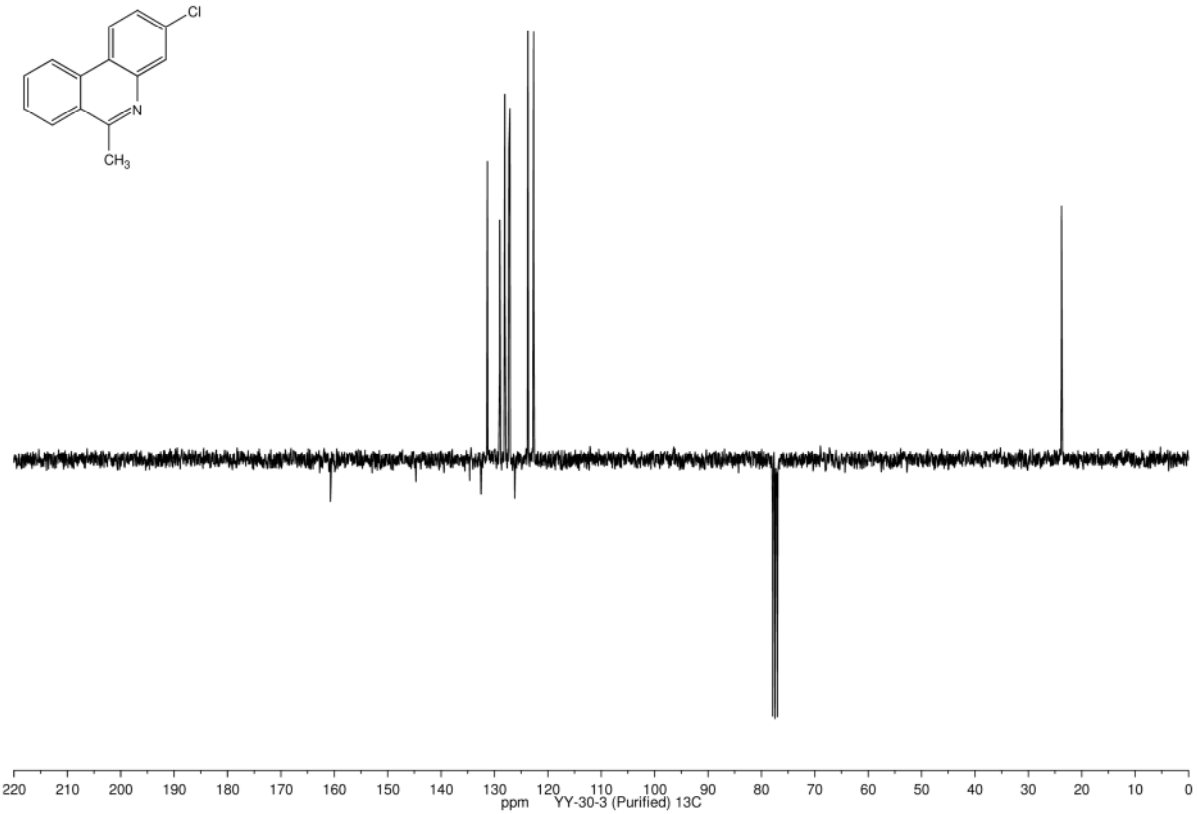
2-p-Chlorophenylacetophenone O-ethoxycarbonyl oxime - 4f

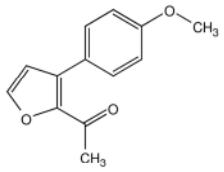




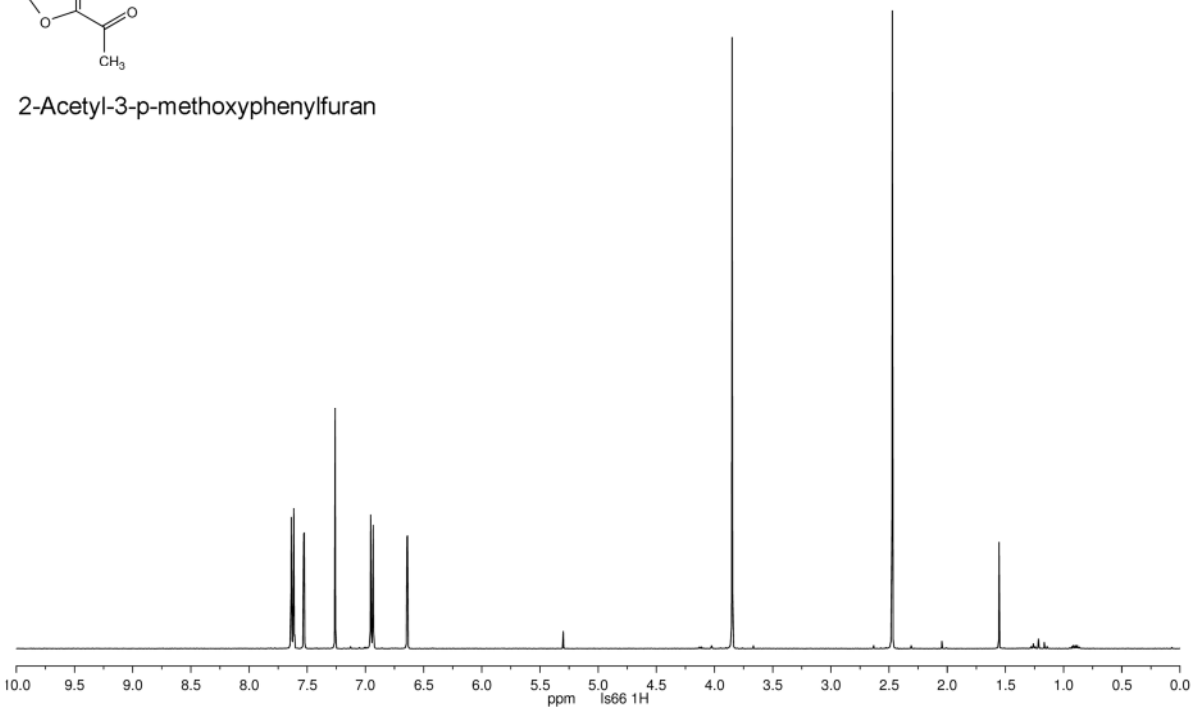
3-Chloro-6-methylphenanthridine - 5f

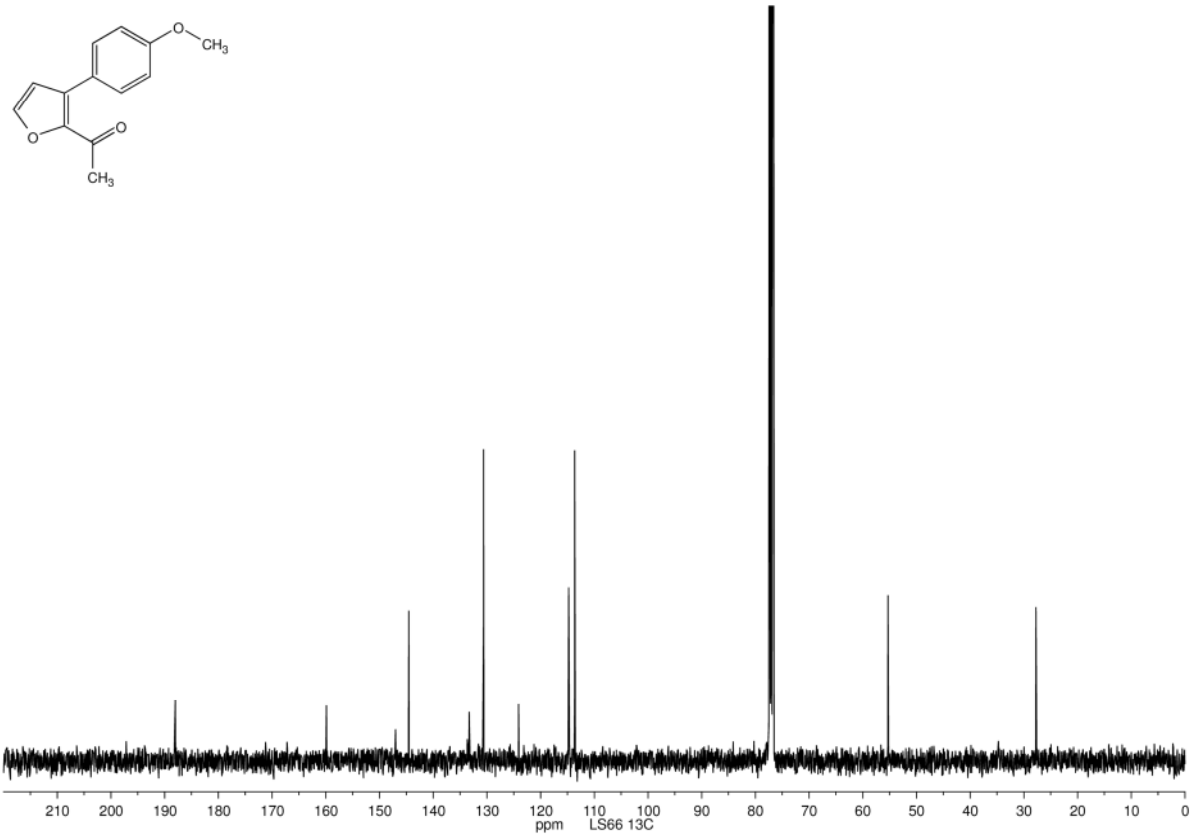


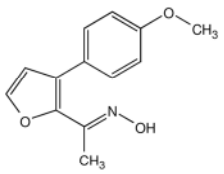




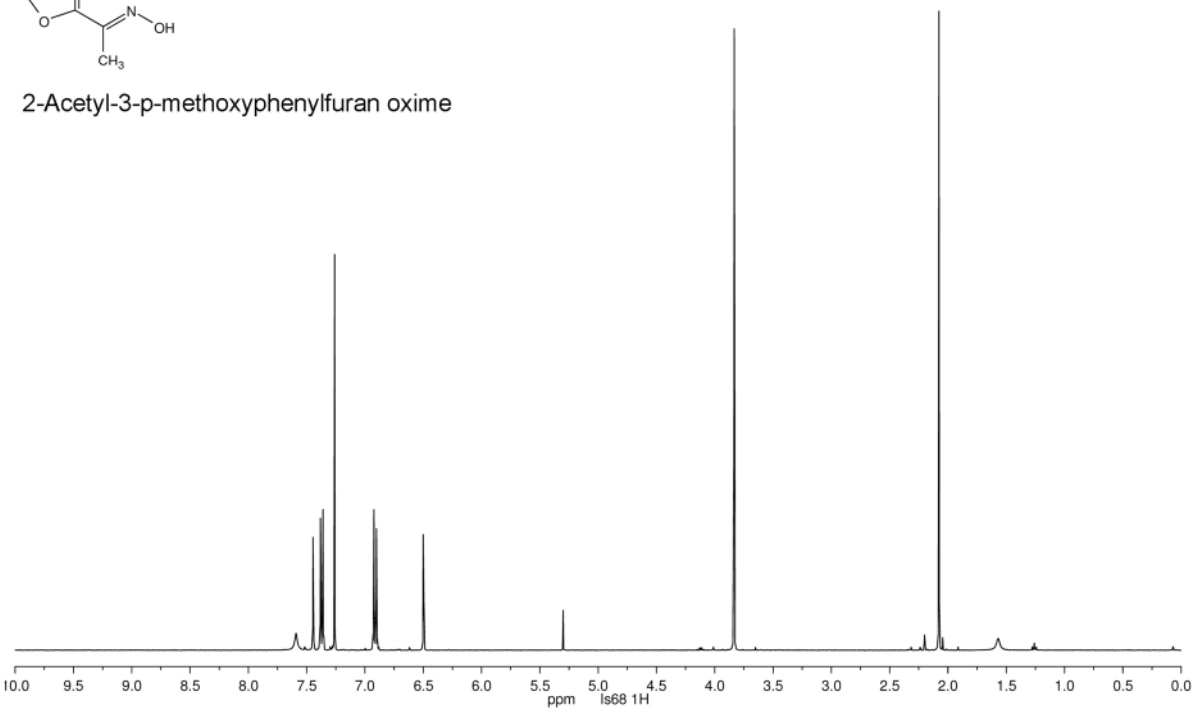
2-Acetyl-3-p-methoxyphenylfuran

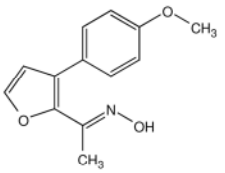


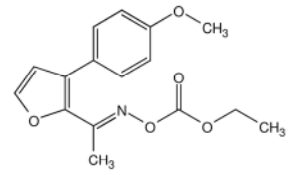




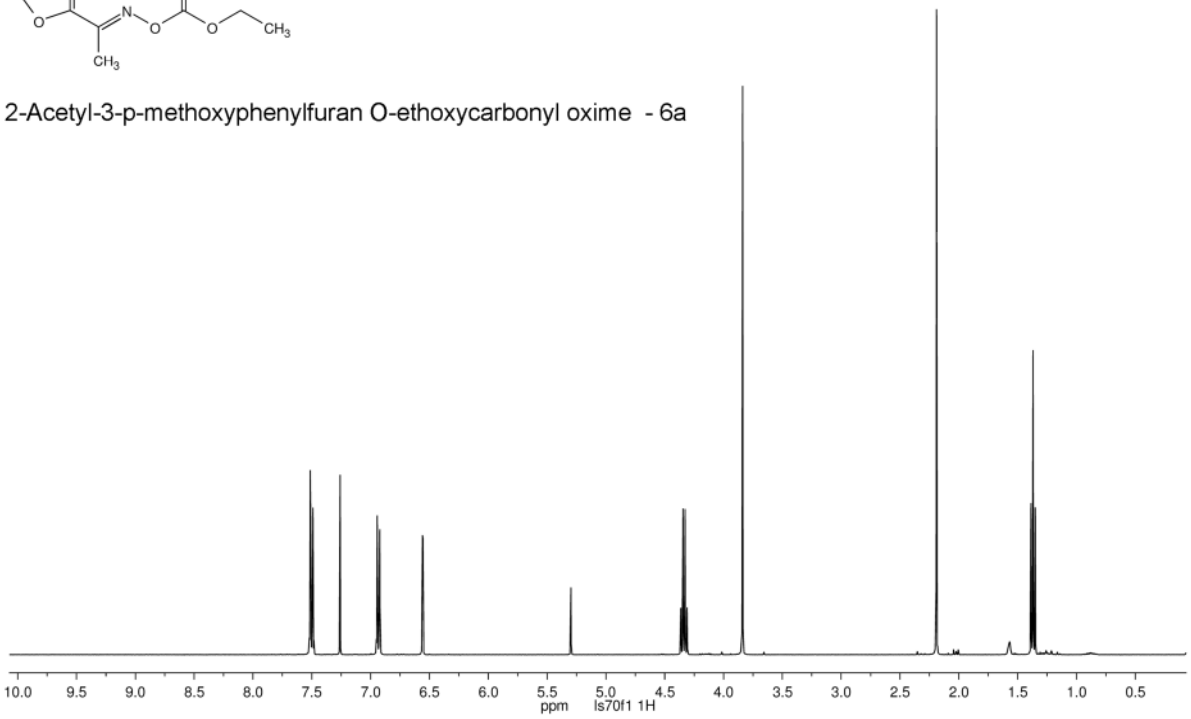
2-Acetyl-3-p-methoxyphenylfuran oxime

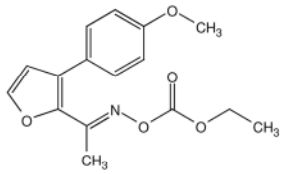


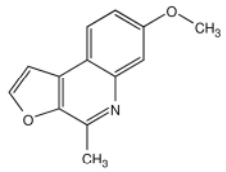




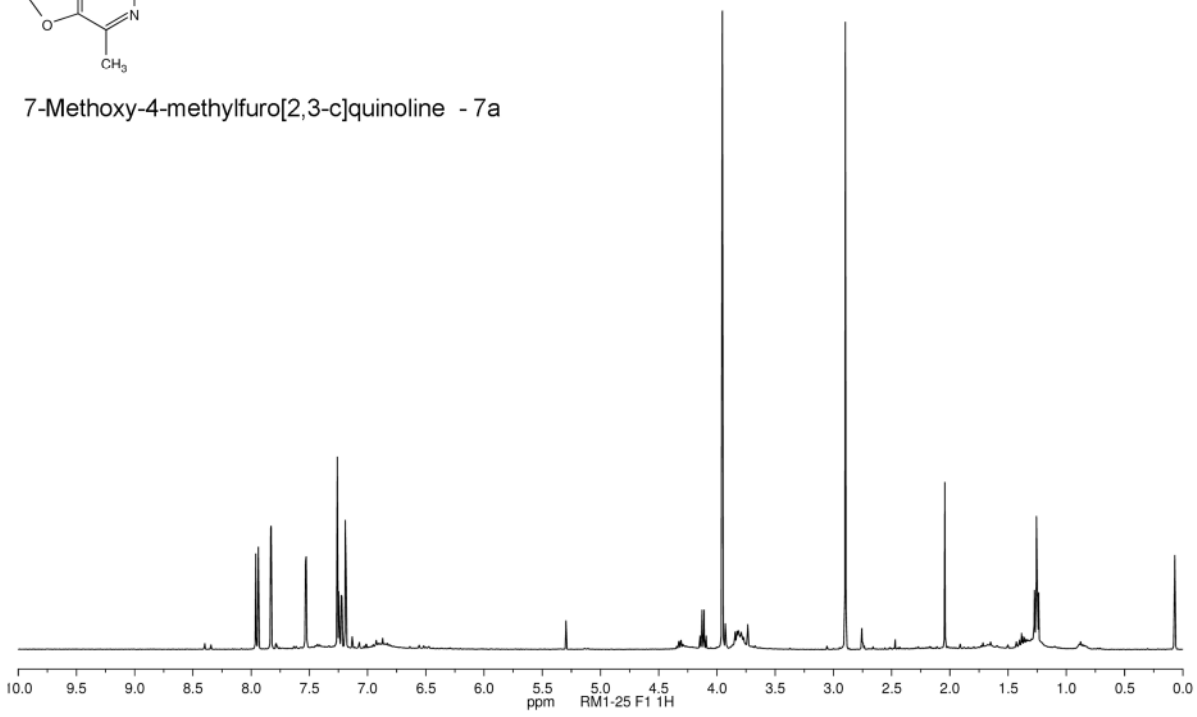
2-Acetyl-3-p-methoxyphenylfuran O-ethoxycarbonyl oxime - 6a

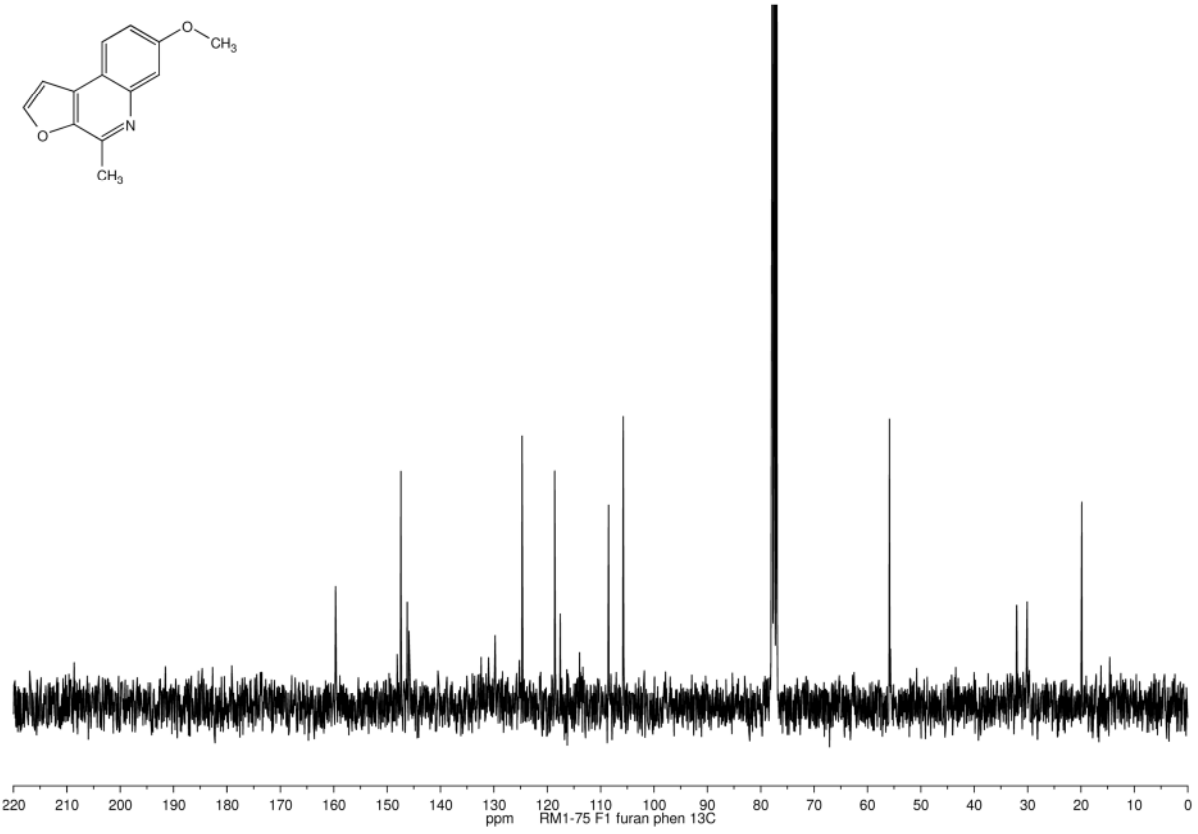


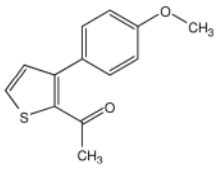




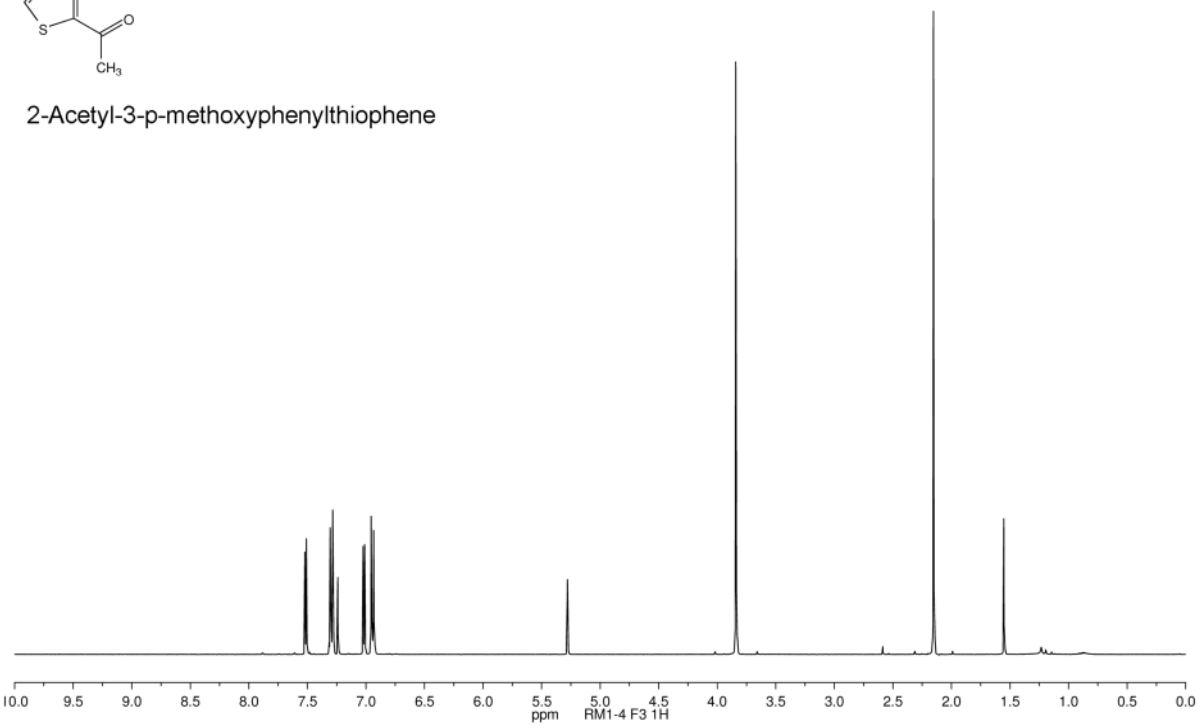
7-Methoxy-4-methylfuro[2,3-c]quinoline - 7a

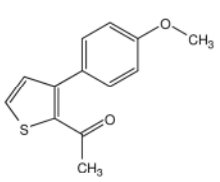


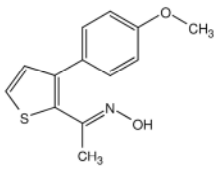




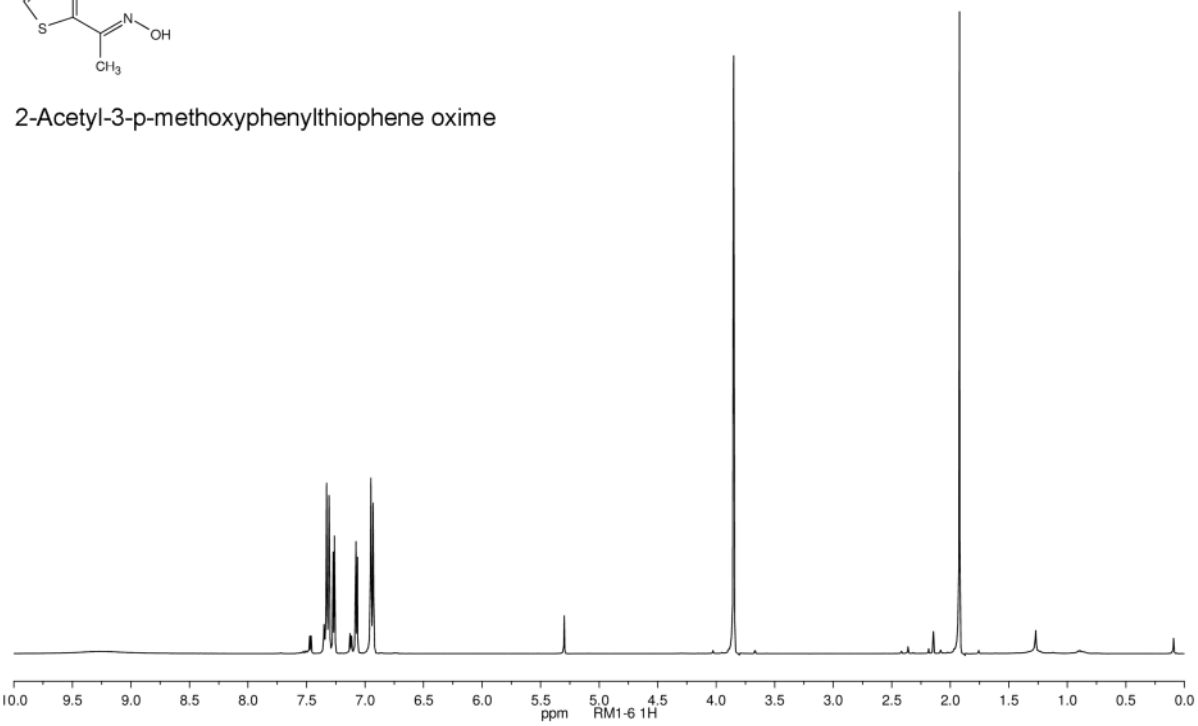
2-Acetyl-3-p-methoxyphenylthiophene

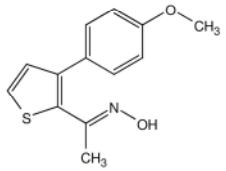


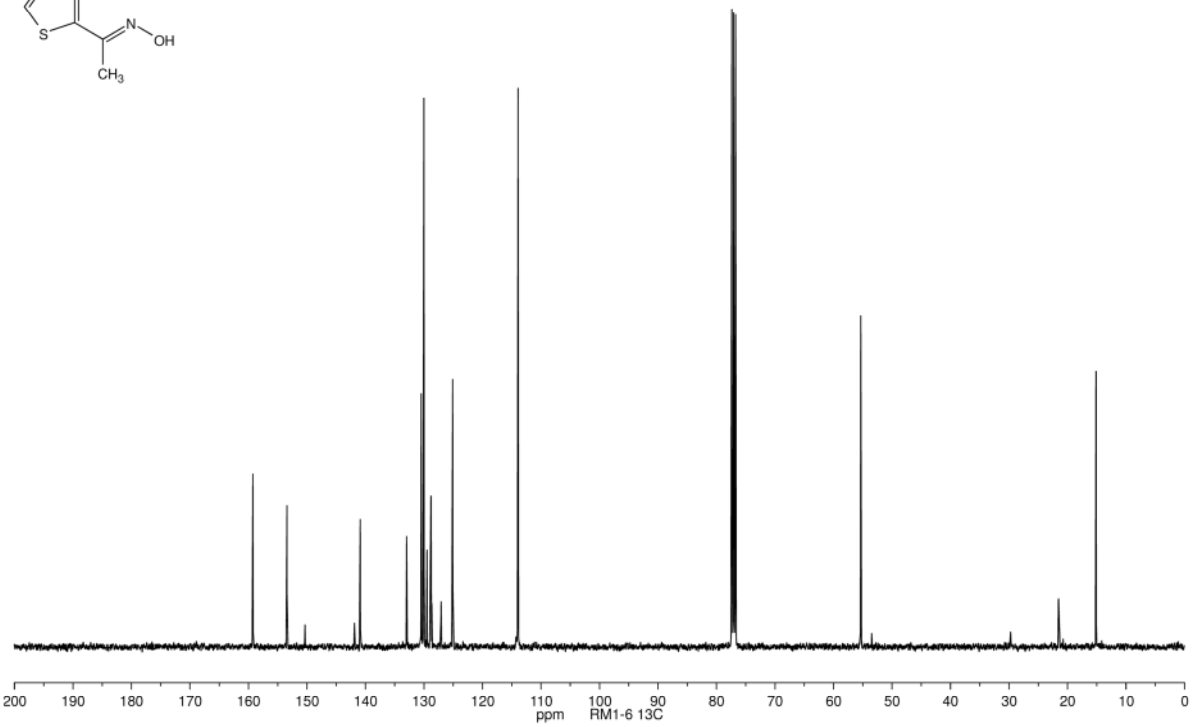


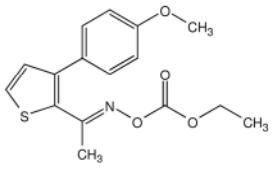


2-Acetyl-3-p-methoxyphenylthiophene oxime

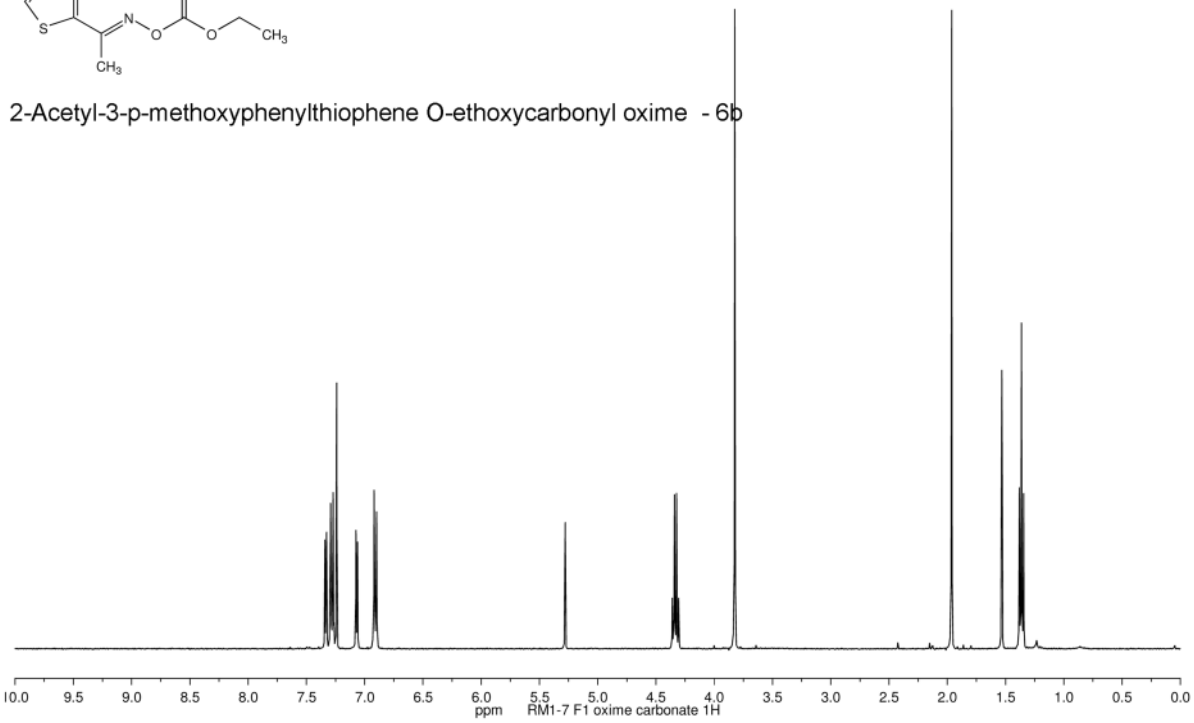


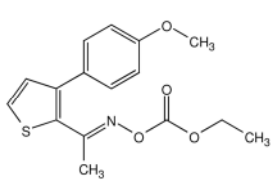


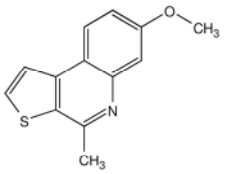




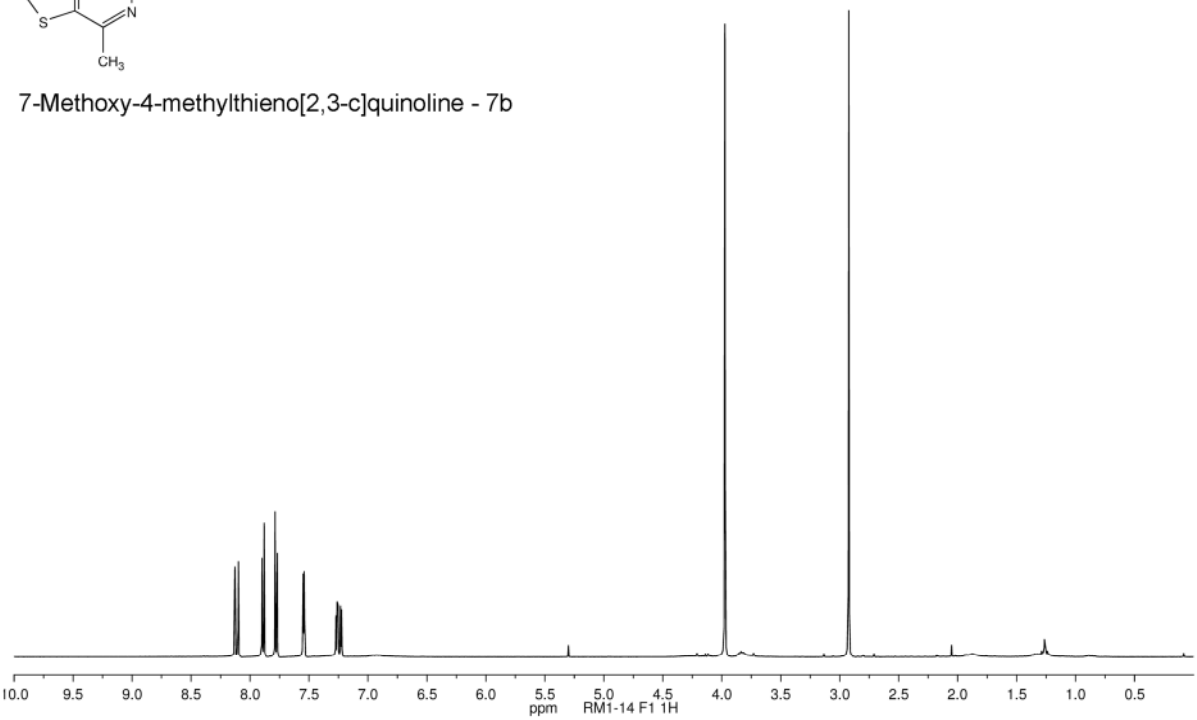
2-Acetyl-3-p-methoxyphenylthiophene O-ethoxycarbonyl oxime - 6b

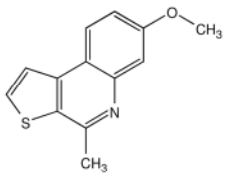


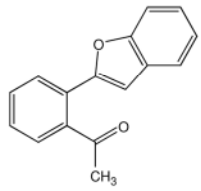




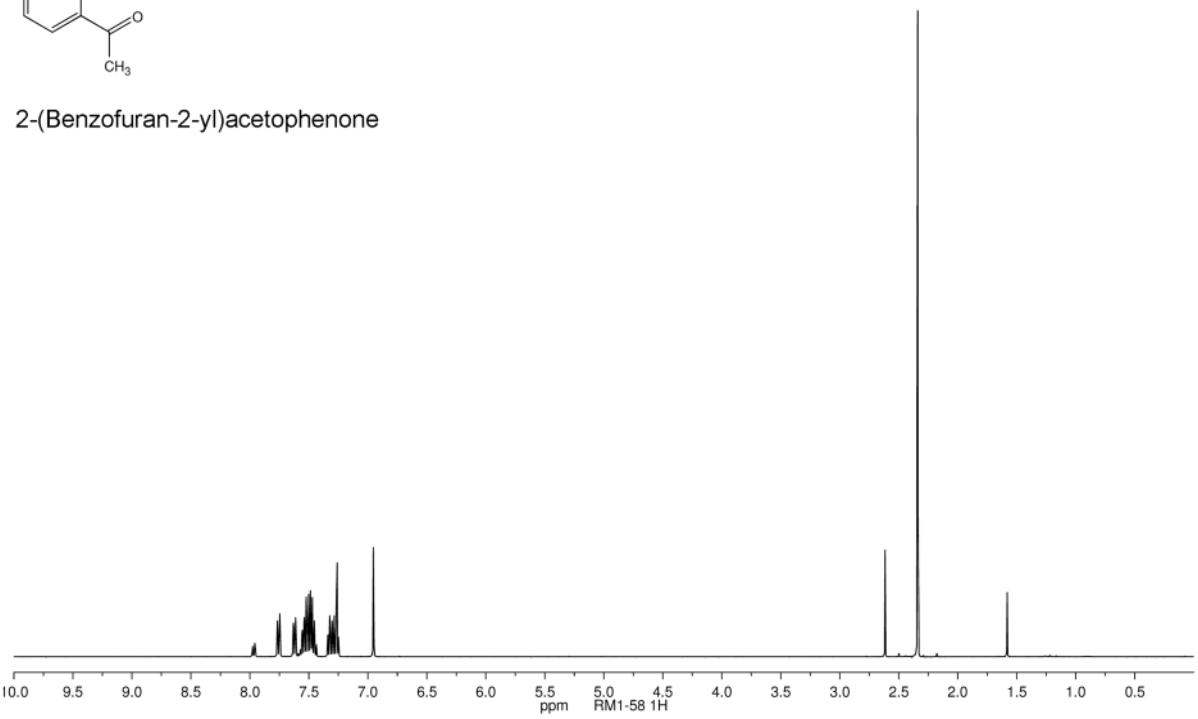
7-Methoxy-4-methylthieno[2,3-c]quinoline - 7b

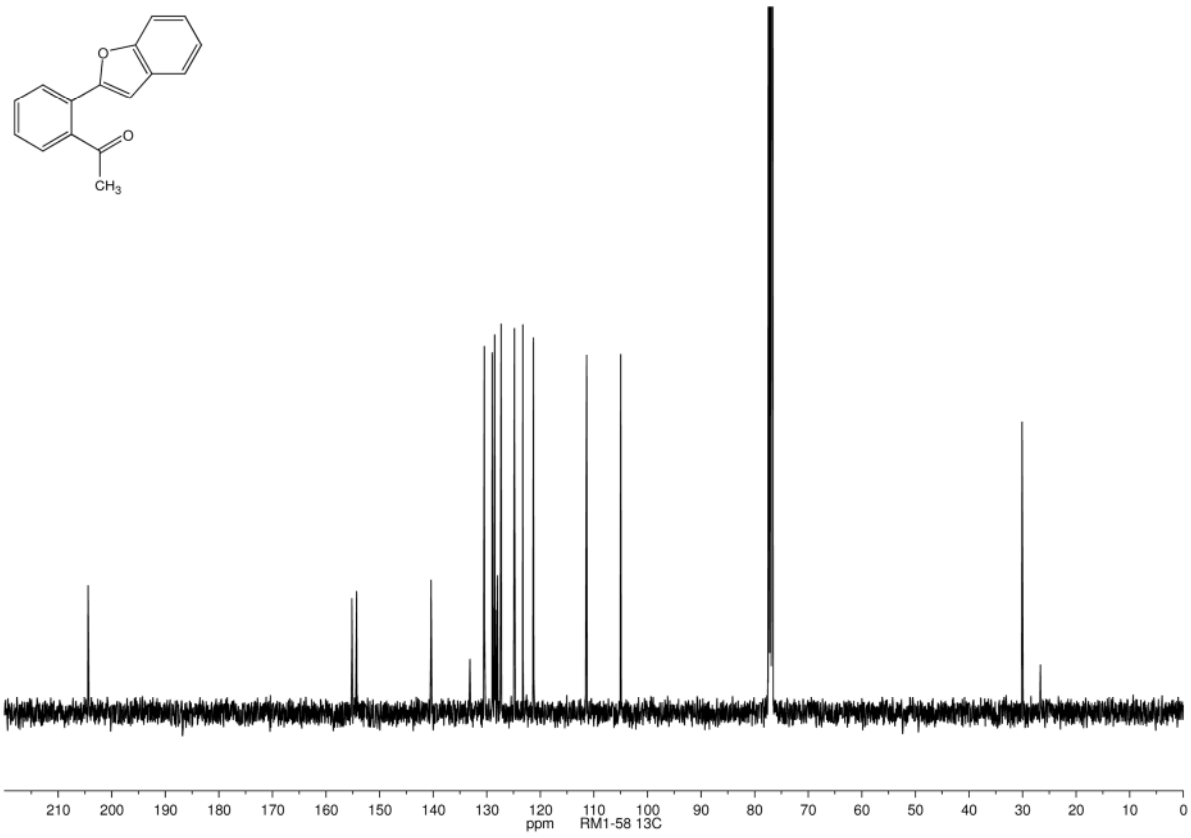


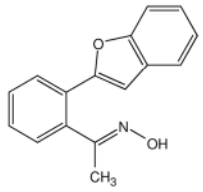




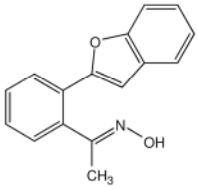
2-(Benzofuran-2-yl)acetophenone

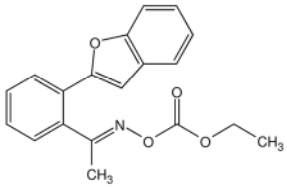




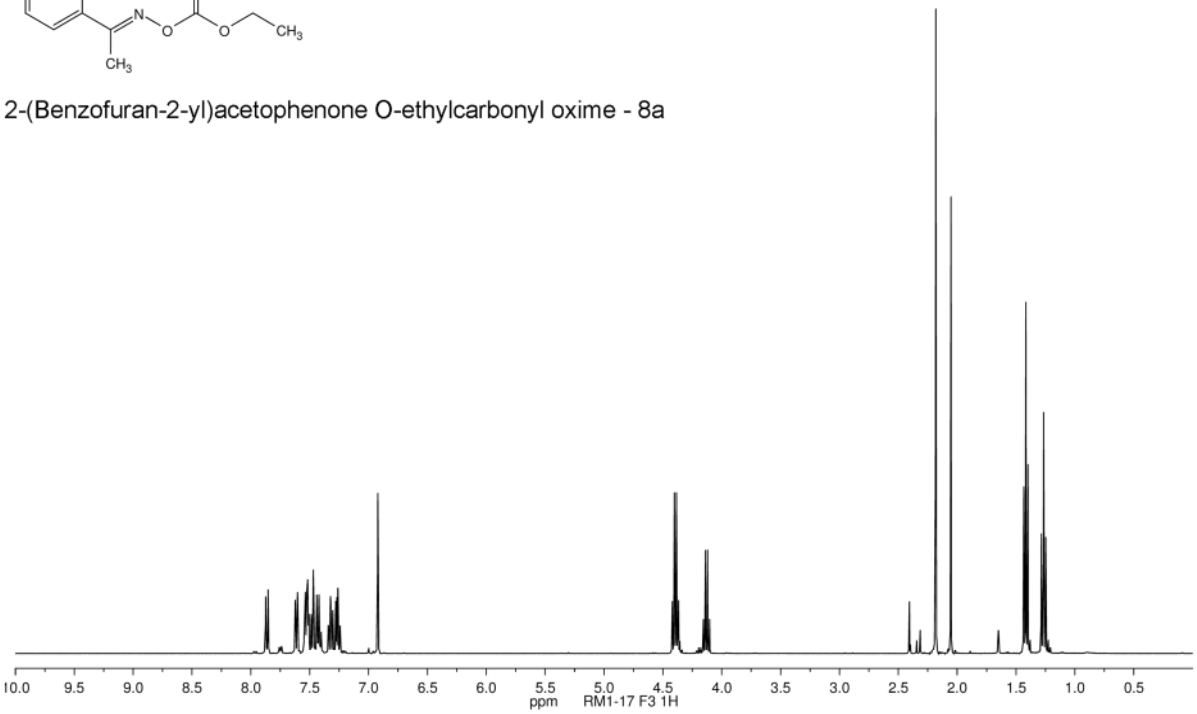


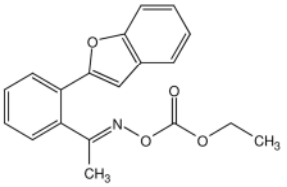
2-(Benzofuran-2-yl)acetophenone oxime

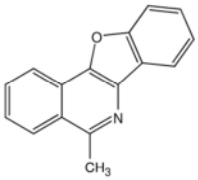




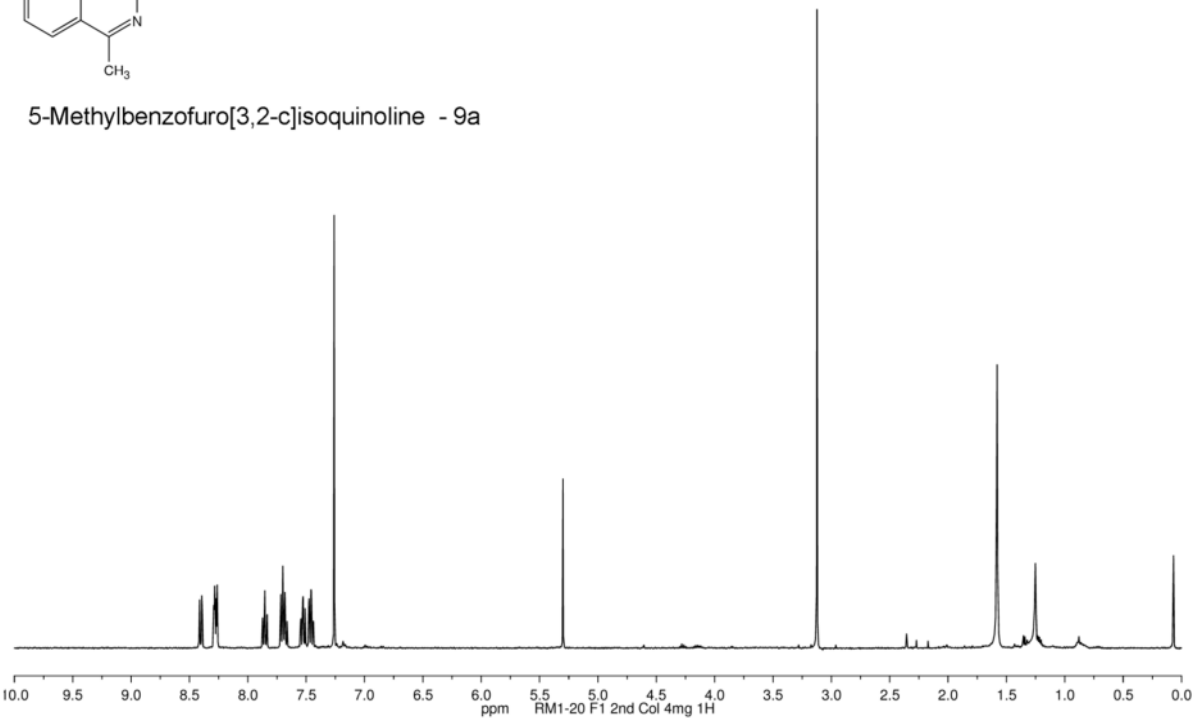
2-(Benzofuran-2-yl)acetophenone O-ethylcarbonyl oxime - 8a

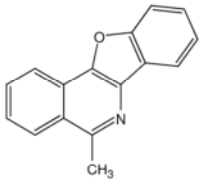


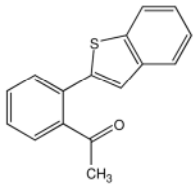




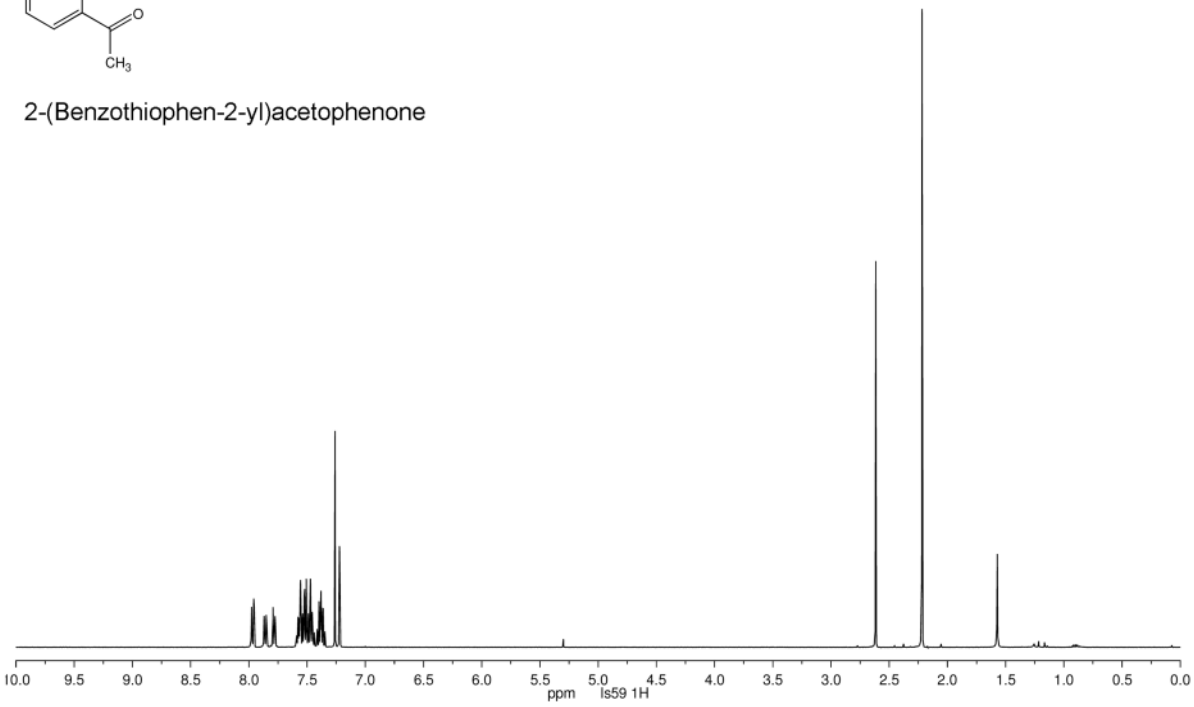
5-Methylbenzofuro[3,2-c]isoquinoline - 9a

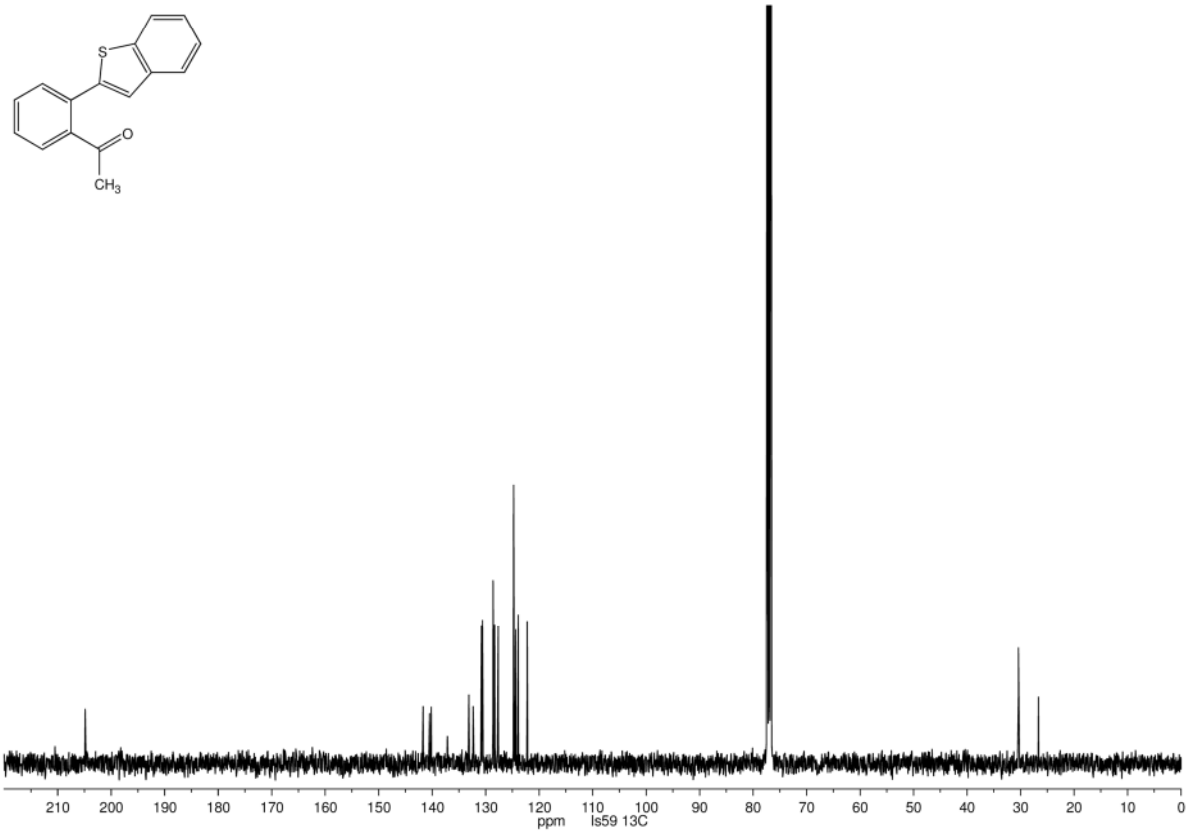


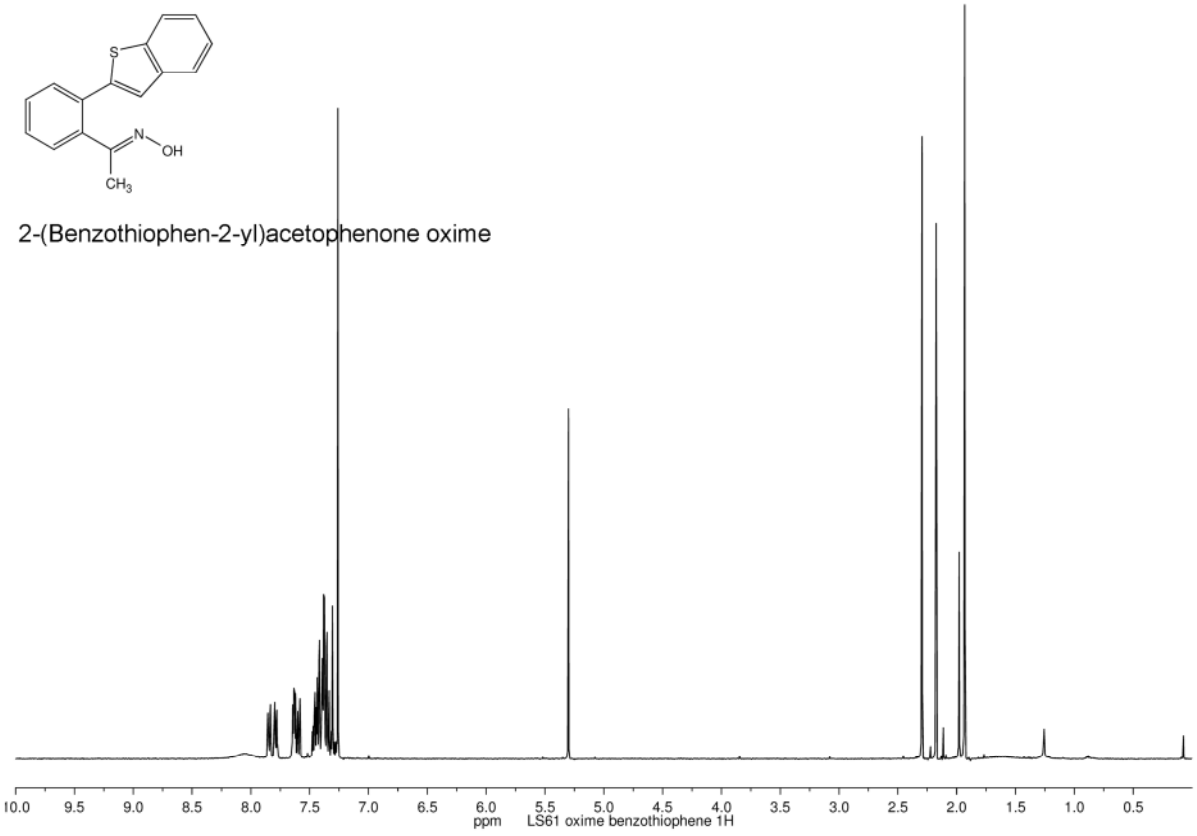


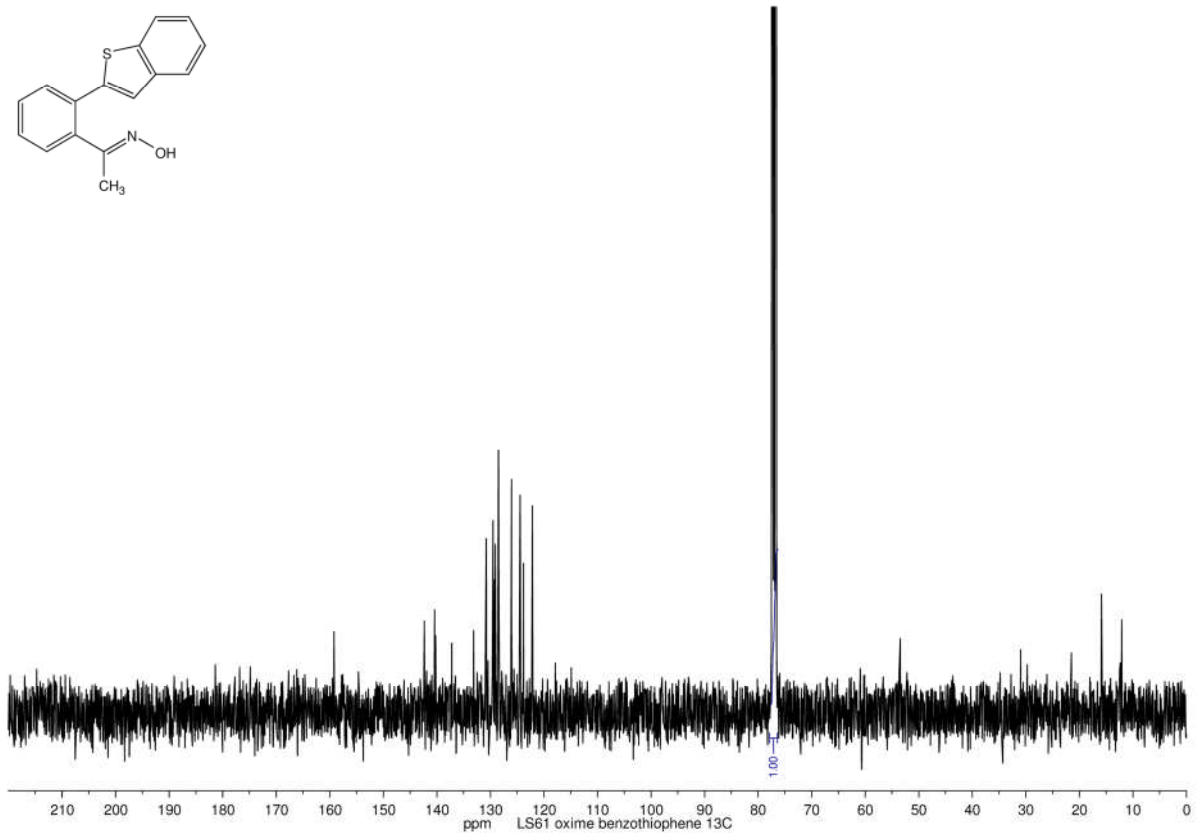


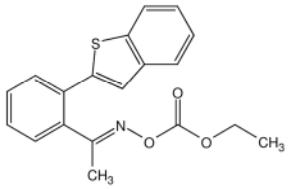
2-(Benzothiophen-2-yl)acetophenone



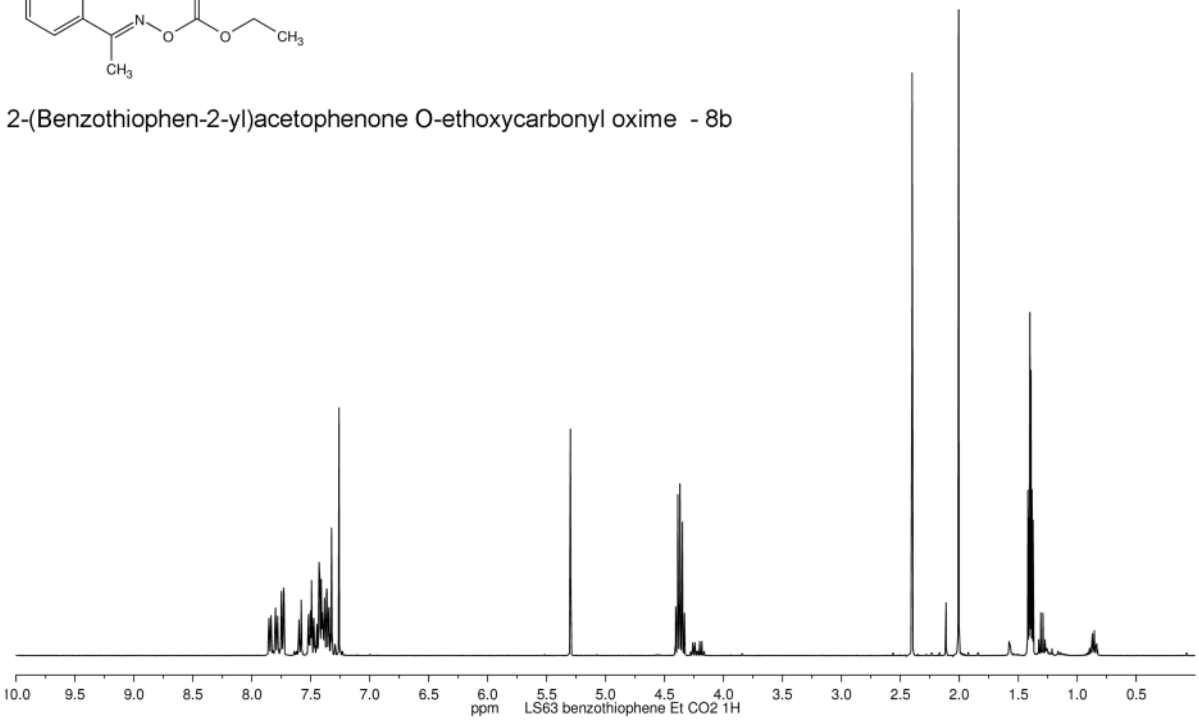


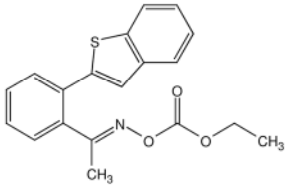

S
N
OH
CH3
2-(Benzothiophen-2-yl)acetophenone oxime
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm
LS61 oxime benzothiophene 1H

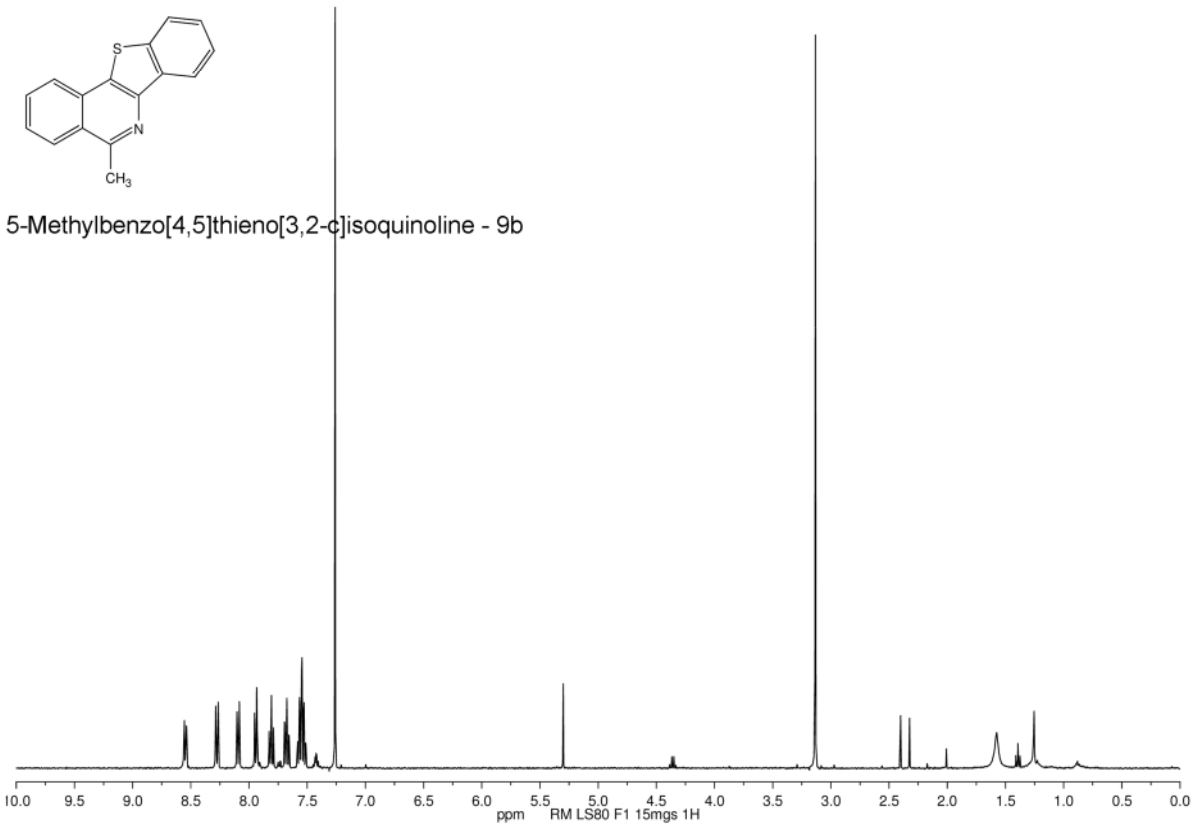

S
N
OH
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm
LS61 oxime benzothiophene 13C

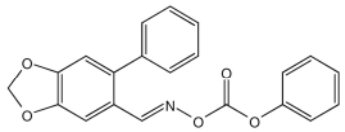


2-(Benzothiophen-2-yl)acetophenone O-ethoxycarbonyl oxime - 8b









6-Phenylbenzo[d][1,3]dioxole-5-carbaldehyde *O*-phenoxy oxime - 10