



Supporting Information

for

Primary amine-catalyzed enantioselective 1,4-Michael addition reaction of pyrazolin-5-ones to α,β -unsaturated ketones

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Additional optimization studies, characterization data of compounds 3aa–na and *ent*-3aa–*ent*-3na, ^1H , ^{13}C NMR spectra of 3aa–na, ^1H NMR of *ent*-3aa–*ent*-3na and their HPLC traces and single crystal data of *ent*-3ba

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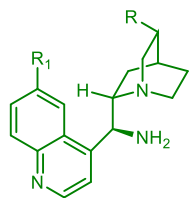
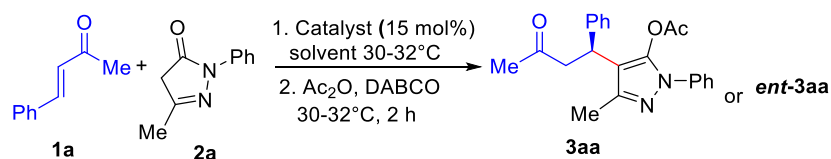
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1. General experimental

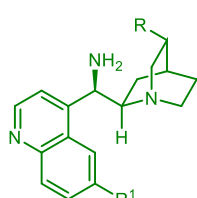
Solvent removal was performed with a rotary evaporator that was connected to a dry ice condenser. TLC (0.5 mm) was carried out using Merck TLC plate. Column chromatography was performed on SRL make silica gel (230–400 mesh). The ^1H and ^{13}C NMR spectroscopic data were recorded with a 500 MHz (^1H NMR: 500 MHz, ^{13}C NMR: 125 MHz) Varian spectrometer, ^{19}F spectroscopic data were recorded with 300 MHz (^{19}F NMR: 282 MHz). The ^1H and ^{13}C chemical shifts are given in ppm (δ scale) and are measured relative to CHCl_3 (7.27 ppm) and CDCl_3 (77.0 ppm), respectively, as internal standards. High resolution mass spectra were recorded at 60–70 eV with a Micromass Q-TOF spectrometer (ESI, Ar) or on an XEVO G2-XS QTOF. Enantiomeric excess (ee) values were determined by HPLC analysis with a Waters instrument fitted with a Daicel Chiralpak AD-H column, Daicel Chiralcel OD-H column and Daicel Chiralpak OJ-H with UV detector (λ fixed at 220 nm). Melting points (mp) were measured on a Büchi B-540 apparatus. The single-crystal X-ray diffraction data of *ent*-**3ba** was collected from were collected using a XtaLAB Synergy, Dualflex, HyPix diffractometer, operating at $T = 298(2)$ K, equipped with a micro-focus sealed X-ray Cu $K\alpha$ radiation ($\lambda = 1.54184$ Å). All the solvents were distilled out prior to use.

2. Reaction optimizations

Table S1: Catalyst and solvent screening^a



I, R = CH=CH₂, R¹ = H,
III, R = CH=CH₂, R¹ = OMe,
IV, R = CH₂CH₃, R¹ = OMe,



II R = CH=CH₂, R¹ = H,
V, R = CH=CH₂, R¹ = OMe,
VI, R = CH₂CH₃, R¹ = OMe,

Entry	Cat.	Solvent	Yield[%] of 3aa ^[b]	[%]ee ^[c] of 3aa
1	I	Toluene	58-62	74
2	II	Toluene	62	-66
3	III	Toluene	75	64
4	IV	Toluene	76	58
5	V	Toluene	69	-63
6	VI	Toluene	66	-59
7	I	C ₆ H ₅ CF ₃	ND	69
8	I	DCE	70	64
9	I	DCM	69	69
10	I	CH ₃ CN	58	42
11	I	EtOAc	70	60
12	I	CHCl ₃	77	74

^a Reaction conditions: **1a** (0.3 mmol), **2a** (0.2 mmol), 15 mol% of catalyst **I-VI** in 0.5 mL solvent for 12h-14h. Next, Ac₂O (0.52 mmol, 50 μ L) and DABCO (0.1mmol, 11 mg) were added and stirred for 2h at 30-32°C.

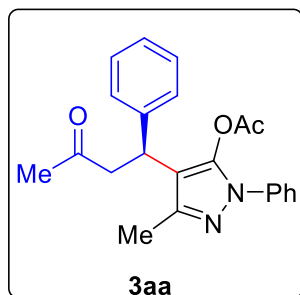
3. General procedure for the synthesis of *rac*-3

An oven-dried 4 mL glass vial equipped with a magnetic stirring bar was charged with catalyst ($\pm$)-*trans*-1,2-diaminocyclohexane (20 mol %, $\approx$ 4.6 mg). Next, CHCl_3 (1.0 mL) was added to the mixture and stirred for 5 min at room temperature (30–32 °C). The α,β -unsaturated ketone **1** (0.3 mmol, 1.5 equiv) and pyrazolone **2** were added sequentially, and the reaction mixture was stirred for 12 h. Ac_2O (50 μL , 0.52 mmol, 2.6 equiv) followed by DABCO (12 mg, 50 mol %) were added. The resulting reaction mixture was further stirred for 2 h at room temperature. The crude reaction mixture was directly loaded on the column and purified by column chromatography on silica gel (petroleum ether/EtOAc as the eluent) to give *rac*-3.

4. General procedure for the synthesis of **3** and *ent*-3

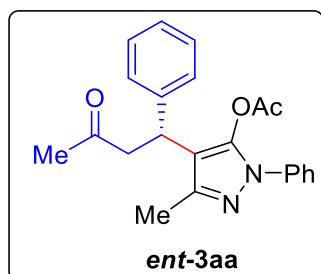
An oven-dried 4 mL glass vial equipped with a magnetic stirring bar was charged with catalyst **I** (15 mol %, $\approx$ 9.0 mg) and ($\pm$)-mandelic acid (30 mol %, 9.0 mg) or catalyst **II** (15 mol %, $\approx$ 9.0 mg) and ($\pm$)-mandelic acid (30 mol %). Next, CHCl_3 (1.0 mL) was added to the mixture and stirred for 5 min at room temperature (30–32 °C). The α,β -unsaturated ketone (0.3 mmol, 1.5 equiv) was added in one portion and the reaction mixture was further stirred for 5 min. Pyrazolin-5-one **2** (0.2 mmol, 1.0 equiv) was added to the reaction mixture and stirred for 4–14 h. Once the pyrazolone **2** was consumed (monitored by TLC), Ac_2O (50 μL , $\approx$ 0.52 mmol, 2.6 equiv) and DABCO (11 mg, 50 mol %) were sequentially added. The resulting reaction mixture was further stirred for 2 h at room temperature. The crude reaction mixture was directly loaded on the column and purified by column chromatography on silica gel (petroleum ether/EtOAc as the eluent) to give the product **3** or *ent*-3.

5. Characterization data



(S)-3-Methyl-4-(3-oxo-1-phenylbutyl)-1-phenyl-1H-pyrazol-5-yl acetate (3aa)

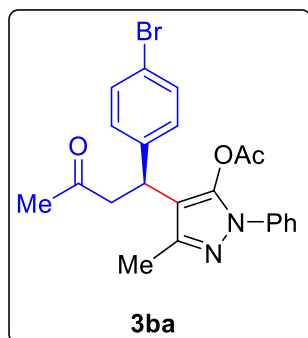
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/ petroleum ether-20% EtOAc/ petroleum ether. The above titled compound was isolated as yellow liquid (59 mg, 81%). **¹H NMR (500 MHz, CDCl₃):** δ 7.46-7.44 (m, 2 H), 7.39 (t, J = 7.7 Hz, 2 H), 7.28 (t, J = 7.2 Hz, 3 H), 7.23-7.22 (m, 2 H), 7.19 (t, J = 7.0, 1 H), 4.51 (t, J = 7.4 Hz, 1 H), 3.19 (dd, J = 17.0, 7.7 Hz, 1 H), 3.06 (dd, J = 17.0, 7.0 Hz, 1 H), 2.17 (s, 3 H), 2.14 (s, 3 H), 2.10 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 206.4, 167.4, 147.5, 141.8, 141.3, 137.8, 129.1 (2 C), 128.4 (2 C), 127.4, 127.2 (2 C), 126.4, 122.8 (2 C), 110.8, 47.3, 34.8, 30.4, 20.3, 13.5; **IR (ATR):** 2968, 1788, 1713, 1594, 1501, 1368, 1164, 754, 698 cm⁻¹; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 1.0 mL/min; λ = 220 nm; τ_{minor} = 7.77 min, τ_{major} = 9.0 min, $[\alpha]_{\text{D}}^{22}$ = -7.5 (*c* 3.0, CHCl₃, 94% ee); **HRMS (ESI)** calcd for C₂₂H₂₂N₂NaO₃ [M + Na]⁺: 385.1528, found: 385.1541.



(R)-3-Methyl-4-(3-oxo-1-phenylbutyl)-1-phenyl-1H-pyrazol-5-yl acetate (ent-3aa)

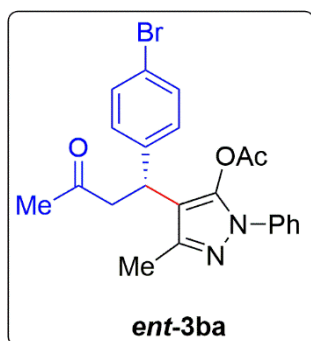
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/ petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as yellow

liquid (55 mg, 77%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 1.0 mL/min; $\lambda = 220$ nm; $\tau_{\text{major}} = 7.49$ min, $\tau_{\text{minor}} = 8.96$ min, $[\alpha]_{\text{D}}^{23} = +5.0$ (*c* 2.1, 87.5% ee CHCl₃).



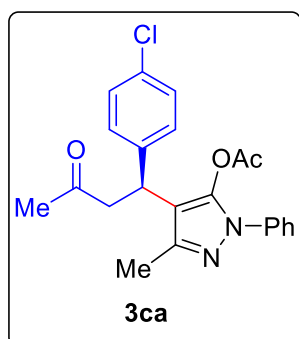
(S)-4-(1-(4-Bromophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (3ba)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as colourless liquid (75 mg, ~85%) which solidify on standing in refrigerator. M.p.: 105.5-106.5 °C (n-hexane/EtOAc : 99/1); ¹H NMR (500 MHz, CDCl₃): δ 7.44-7.43 (m, 2 H), 7.40-7.39 (m, 4 H), 7.29 (t, *J* = 7.3 Hz, 1 H), 7.10 (d, *J* = 8.2 Hz, 2 H), 4.45 (t, *J* = 7.3 Hz, 1 H), 3.14 (dd, *J* = 17.2, 7.9 Hz, 1 H), 3.04 (dd, *J* = 17.2, 6.8 Hz, 1 H), 2.14 (s, 6 H), 2.13 (s, 3 H); ¹³C NMR (125 MHz, CDCl₃): δ 206.0, 167.4, 147.3, 141.2, 141.0, 137.7, 131.4 (2 C), 129.2 (2 C), 129.1 (2 C), 127.3, 122.8 (2 C), 120.2, 110.2, 47.2, 34.2, 30.3, 20.3, 13.5; IR (ATR): 2926, 1790, 1719, 1590, 1502, 1370, 1161, 754, 694 cm⁻¹; HPLC: 92% ee, the ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; $\lambda = 220$ nm; $\tau_{\text{minor}} = 14.87$ min, $\tau_{\text{major}} = 17.41$ min, $[\alpha]_{\text{D}}^{23} = -5.7$ (*c* 1.0, CHCl₃, >99% ee); HRMS (ESI) calcd for C₂₂H₂₂BrN₂O₃ [M + H]⁺: 441.0813, found: 441.0817.



(R)-4-(1-(4-Bromophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (*ent*-3ba)

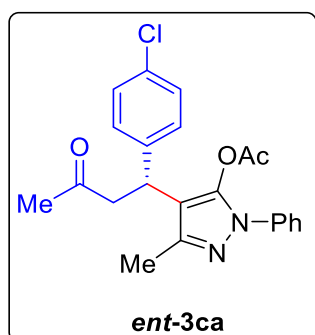
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as colourless liquid (75 mg, ~85%) which solidify in on standing in refrigerator. Mp. 106-108 °C (n-hexane/EtOAc : 99/1); The ee was determined by HPLC using a Daicel CHIRALCEL® OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; $\lambda = 220$ nm; $\tau_{\text{minor}} = 15.12$ min, $\tau_{\text{major}} = 18.12$ min, $[\alpha]_{\text{D}}^{25} = +2.3$ (c 1.0, CHCl₃, 98% ee). [CCDC: 2234286](#)



(S)-4-(1-(4-Chlorophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (3ca)

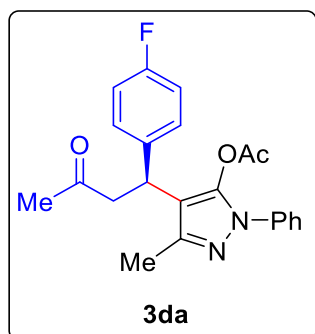
Purified by column chromatography on silica gel (230-400 mesh) using 15% EtOAc/petroleum ether-20%EtOAc/petroleum ether. The above titled compound was isolated as colourless liquid (77 mg, 97%) which solidify on standing. M.p.: 101-102 °C (n-hexane/ EtOAc : 99/1); **¹H NMR (500 MHz, CDCl₃):** δ 7.45-7.43 (m, 2 H), 7.40 (t, $J = 7.5$ Hz, 2 H), 7.30 (t, $J = 7.1$ Hz, 1 H), 7.25 (d, $J = 7.1$ Hz, 2 H), 7.16 (d, $J = 8.1$ Hz, 2 H), 4.47 (t, $J = 7.2$ Hz, 1 H), 3.15 (dd, $J = 17.2, 7.9$ Hz, 1 H), 3.04 (dd, J

= 17.1, 6.8 Hz, 1 H), 2.15 (s, 3 H), 2.14 (s, 3 H), 2.13 (s, 3 H); ^{13}C NMR (125 MHz, CDCl_3): δ 206.1, 167.5, 147.4, 141.3, 140.5, 137.8, 132.2, 129.1 (2 C), 128.8 (2 C), 128.5 (2 C), 127.3, 122.8 (2 C), 110.4, 47.3, 34.2, 30.4, 20.3, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 14.31 min, τ_{major} = 17.10 min, $[\alpha]_{\text{D}}^{25}$ = -6.6 (*c* 1.2, CHCl_3 , 97% ee); HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{22}\text{ClN}_2\text{O}_3$ $[\text{M} + \text{H}]^+$: 397.1319, found: 397.1324.



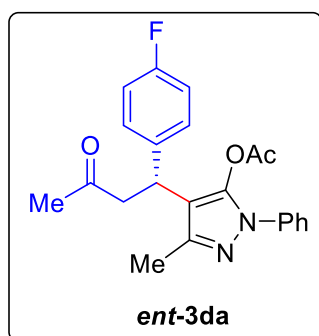
(R)-4-(1-(4-Chlorophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (ent-3ca)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15%EtOAc/petroleum ether-20%EtOAc/petroleum ether. The above titled compound was isolated as colourless liquid (77 mg, 97%) which solidify in on standing. M.p.: 99.5-100.5 °C (n-hexane/ IPA: 95/5); The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{major} = 14.26 min, τ_{minor} = 17.49 min, $[\alpha]_{\text{D}}^{23}$ = +6.7 (*c* 1.2, CHCl_3 , 97.5% ee)



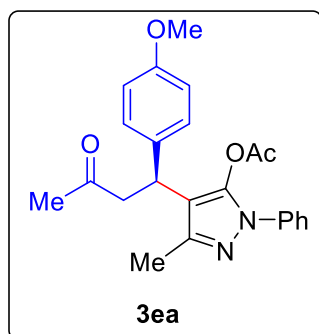
(S)-4-(1-(4-Fluorophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (3da)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as light-yellow liquid (55 mg, 72%). **¹H NMR (500 MHz, CDCl₃):** δ 7.46-7.44 (m, 2 H), 7.40 (t, J = 7.6 Hz, 2 H), 7.29 (t, J = 7.3 Hz, 1 H), 7.21-7.18 (m, 2 H), 6.97 (t, J = 8.6 Hz, 2 H), 4.48 (t, J = 7.4 Hz, 1 H), 3.14 (dd, J = 17.1, 7.9 Hz, 1 H), 3.05 (dd, J = 17.1, 6.9 Hz, 1 H), 2.14 (s, 3 H), 2.139 (s, 3 H), 2.132 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 206.2, 167.6, 161.4 (J_{C-F} = 243.6 Hz), 147.4, 141.2, 137.8, 137.7, 137.6, 129.2 (2 C), 129.0, 128.9, 127.3, 122.8 (2 C), 115.2 (J_{C-F} = 21.2 Hz), 110.7, 47.5, 34.1, 30.4, 20.3, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 13.50 min, τ_{major} = 16.34 min, $[\alpha]_{\text{D}}^{21}$ = -8.6 (c 2.4, CHCl₃, 95%ee); **HRMS (ESI)** calcd for C₂₂H₂₂FN₂O₃ [M + H]⁺: 381.1614, found: 381.1613.



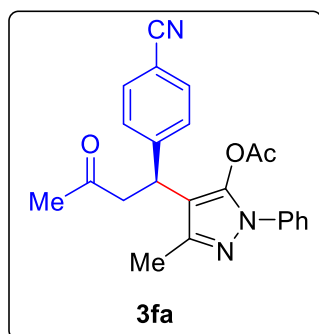
(R)-4-(1-(4-Fluorophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (*ent*-3da)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as light yellow liquid (59 mg, 77.5%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{major} = 13.55 min, τ_{minor} = 16.73 min, $[\alpha]_{\text{D}}^{22}$ = +6.9 (c 1.6, CHCl₃, >93% ee).



(S)-4-(1-(4-Methoxyphenyl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (3ea)

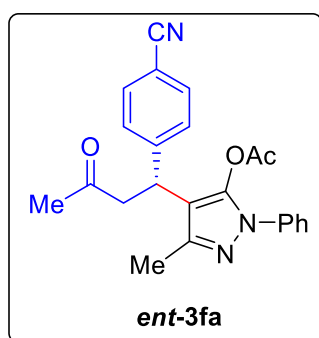
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-25% EtOAc/petroleum ether. The above titled compound was isolated as light yellow liquid (68 mg, 86%). **¹H NMR (500 MHz, CDCl₃):** δ 7.46-7.44 (m, 2 H), 7.39 (t, J = 7.9 Hz, 2 H), 7.28 (t, J = 7.1 Hz, 1 H), 7.14 (d, J = 8.4 Hz, 2 H), 6.81 (d, J = 8.6 Hz, 2 H), 4.44 (t, J = 7.4 Hz, 1 H), 3.77 (s, 3 H), 3.14 (dd, J = 16.8, 7.8 Hz, 1 H), 3.02 (dd, J = 16.8, 6.9 Hz, 1 H), 2.15 (s, 3 H), 2.13 (s, 3 H), 2.12 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 206.5, 167.5, 158.0, 147.5, 141.2, 137.9, 133.9, 129.1 (2 C), 128.4 (2 C), 127.2, 122.8 (2 C), 113.8 (2 C), 111.0, 55.2, 47.6, 34.1, 30.4, 20.3, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 17.64 min, τ_{major} = 19.79 min, $[\alpha]_{\text{D}}^{25}$ = -3.7 (*c* 2.1, CHCl₃, 90% ee); **HRMS (ESI)** calcd for C₂₃H₂₅N₂O₄ [M + H]⁺: 393.1814, found: 393.1825.



(S)-4-(1-(4-Cyanophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (3fa)

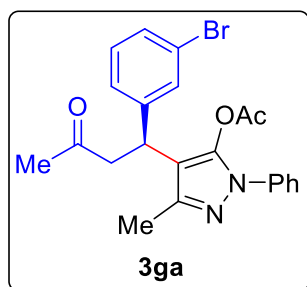
Purified by column chromatography on silica gel (230-400 mesh) using eluent 20% EtOAc/petroleum ether-35% EtOAc/petroleum ether. The above titled compound was isolated as white solid

(69 mg, 89%). **¹H NMR (500 MHz, CDCl₃):** δ 7.57 (d, J = 8.2 Hz, 2 H), 7.44-7.38 (m, 4 H), 7.34 (d, J = 8.1 Hz, 2 H), 7.30 (t, J = 7.0 Hz, 1 H), 4.54 (t, J = 7.1 Hz, 1 H), 3.17 (dd, J = 17.6, 7.8 Hz, 1 H), 3.08 (dd, J = 17.6, 6.6 Hz, 1 H), 2.16 (s, 3 H), 2.14 (s, 3 H), 2.10 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 205.6, 167.4, 147.6, 147.2, 141.3, 137.6, 132.2 (2 C), 129.2 (2 C), 128.3 (2 C), 127.4, 122.8 (2 C), 118.7, 110.3, 109.7, 46.8, 34.6, 30.3, 20.3, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 27.65 min, τ_{major} = 30.29 min; $[\alpha]_{\text{D}}^{26}$ = -9.9 (*c* 1.8, CHCl₃, 92% ee); **HRMS (ESI)** calcd for C₂₃H₂₂N₃O₃ [M + H]⁺: 388.1661, found: 388.1662.



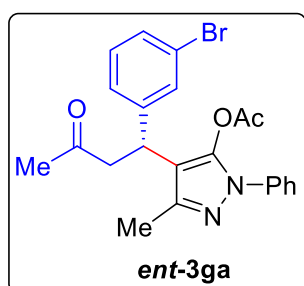
(*R*)-4-(1-(4-Cyanophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1*H*-pyrazol-5-yl acetate (*ent*-3fa)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 20% EtOAc/petroleum ether-35% EtOAc/petroleum ether. The above titled compound was isolated as white solid (64 mg, 82.5%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{major} = 27.02 min, τ_{minor} = 30.84 min. ; $[\alpha]_{\text{D}}^{26}$ = +10.8 (*c* 3.6, CHCl₃, 91.5% ee);



(S)-4-(1-(3-Bromophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (3ga)

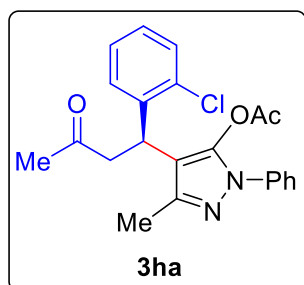
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as yellow liquid (73 mg, 82%). **¹H NMR (500 MHz, CDCl₃):** δ 7.44-7.43 (m, 2 H), 7.41-7.37 (m, 3 H), 7.33-7.32 (m, 1 H), 7.29 (t, J = 7.3 Hz, 1 H), 7.16-7.14 (m, 2 H), 4.48 (t, J = 7.3 Hz, 1 H), 3.15 (dd, J = 17.3, 7.7 Hz, 1 H), 3.05 (dd J = 17.3, 7.0 Hz, 1 H), 2.18 (s, 3 H), 2.15 (s, 3 H), 2.13 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 205.8, 167.4, 147.3, 144.3, 141.3, 137.8, 130.3, 130.0, 129.6, 129.1 (2 C), 127.3, 126.4, 123.8 (2 C), 122.5, 110.2, 47.1, 34.4, 30.4, 20.3, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OJ-H [hexane/*i*-PrOH (70/30)]; flow rate 1.0 mL/min; λ = 220 nm; τ_{major} = 34.14 min, τ_{minor} = 55.56 min, $[\alpha]_{\text{D}}^{25}$ = -26.3 (c 2.0, CHCl₃, 94.5% ee); **HRMS (ESI)** calcd for C₂₂H₂₂BrN₂O₃ [M + H]⁺: 441.0814, found: 441.0813.



(R)-4-(1-(3-Bromophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (ent-3ga)

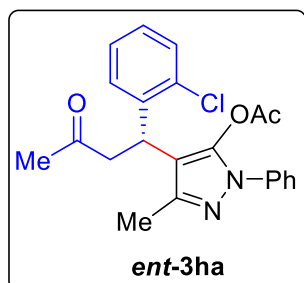
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as yellow liquid (70 mg, 79%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OJ-H

[hexane/*i*-PrOH (70/30)]; flow rate 1.0 mL/min; $\lambda = 220$ nm; $\tau_{\text{minor}} = 41.63$ min, $\tau_{\text{major}} = 51.72$ min, $[\alpha]_{\text{D}}^{25} = +23.26$ (*c* 2.8, CHCl₃, 94% ee);



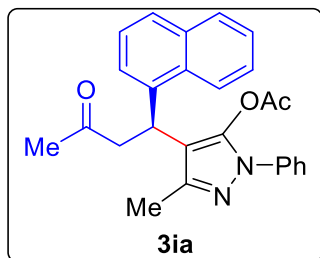
(*R*)-4-(1-(2-Chlorophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1*H*-pyrazol-5-yl acetate (3ha)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20%EtOAc/petroleum ether. The above titled compound was isolated as yellow liquid (61 mg, >76.5%). **¹H NMR (500 MHz, CDCl₃):** δ 7.44-7.42 (m, 2 H), 7.40-7.35 (m, 3 H), 7.29-7.26 (m, 2 H), 7.21 (t, *J* = 7.4 Hz, 1 H), 7.16 (t, *J* = 7.5 Hz, 1 H), 4.86 (t, *J* = 7.6 Hz, 1 H), 3.11 (dd *J* = 17.1, 7.3 Hz, 1 H), 3.06 (dd *J* = 17.4, 8.1 Hz, 1 H), 2.23 (s, 3 H), 2.17 (s, 3 H), 2.06 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 205.8, 167.3, 147.8, 141.5, 139.1, 137.8, 133.9, 130.0, 129.1 (2 C), 128.1, 127.9, 127.3, 126.7, 122.9 (2 C), 108.7, 46.8, 32.6, 29.9, 20.3, 13.4; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OJ-H [hexane/*i*-PrOH (70/30)]; flow rate 1.0 mL/min; $\lambda = 220$ nm; $\tau_{\text{minor}} = 34.77$ $\tau_{\text{major}} = 50.3$ min, $[\alpha]_{\text{D}}^{24} = +18.3$ (*c* 1.1, CHCl₃, >98.5% ee); **HRMS (ESI)** calcd for C₂₂H₂₂ClN₂O₃ [*M* + *H*]⁺: 397.1319, found: 397.1331.



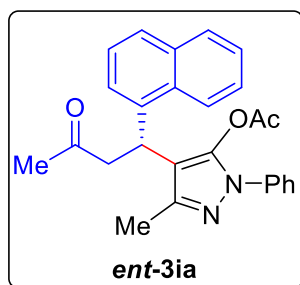
(*S*)-4-(1-(2-Chlorophenyl)-3-oxobutyl)-3-methyl-1-phenyl-1*H*-pyrazol-5-yl acetate (*ent*-3ha)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20%EtOAc/petroleum ether. The above titled compound was isolated as yellow liquid (58 mg, 73%). The ee was determined by HPLC using a Daicel CHIRALCEL® OJ-H [hexane/*i*-PrOH (70/30)]; flow rate 1.0 mL/min; $\lambda = 220$ nm; $\tau_{\text{major}} = 31.61$ $\tau_{\text{minor}} = 58.62$ min, $[\alpha]_{\text{D}}^{24} = -15.0$ (*c* 1.5, CHCl₃, 98% ee).



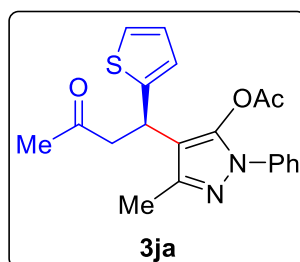
(S)-3-Methyl-4-(1-(naphthalen-1-yl)-3-oxobutyl)-1-phenyl-1H-pyrazol-5-yl acetate (3ia)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as white solid (64 mg, >77.5%). M.p.: 130°C –131.0°C; **¹H NMR (500 MHz, CDCl₃):** δ 8.03 (d, *J* = 8.3 Hz, 1 H), 7.85 (d, *J* = 7.6 Hz, 1 H), 7.75 (d, *J* = 8.0 Hz, 1 H), 7.52-7.46 (m, 2 H), 7.43-7.35 (m, 6 H), 7.28-7.25 (m, 1 H), 5.27 (t, *J* = 7.4 Hz, 1 H), 3.33 (dd, *J* = 17.4, 7.5 Hz, 1 H), 3.19 (dd, *J* = 17.4, 7.5 Hz, 1 H), 2.24 (s, 3 H), 2.20 (s, 3 H), 1.98 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 206.4, 167.5, 147.4, 141.4, 137.8, 137.0, 134.0, 131.3, 129.1 (2 C), 128.9, 127.6, 127.2, 126.3, 125.6, 124.9, 123.7, 123.3, 122.8 (2 C), 110.1, 47.4, 31.3, 30.4, 20.2, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL® OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; $\lambda = 220$ nm; $\tau_{\text{minor}} = 21.02$ min, $\tau_{\text{major}} = 27.22$ min, $[\alpha]_{\text{D}}^{26} = -17.2$ (*c* 1.2, CHCl₃, 98% ee); **HRMS (ESI)** calcd for C₂₆H₂₄N₂O₃K [M + K]⁺: 451.1424, found: 441.1436.



(R)-3-Methyl-4-(1-(naphthalen-1-yl)-3-oxobutyl)-1-phenyl-1H-pyrazol-5-yl acetate (*ent*-3ia)

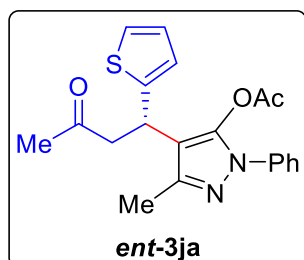
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as white solid (59 mg, >71.5%). M.p.: 129.0°C –130°C; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; $\lambda = 220$ nm; $\tau_{\text{major}} = 20.12$ min, $\tau_{\text{minor}} = 28.35$ min, $[\alpha]_{\text{D}}^{26} = +15.8$ (c 1.2, CHCl₃, 98% ee).



(R)-3-Methyl-4-(3-oxo-1-(thiophen-2-yl)butyl)-1-phenyl-1H-pyrazol-5-yl acetate (3ja)

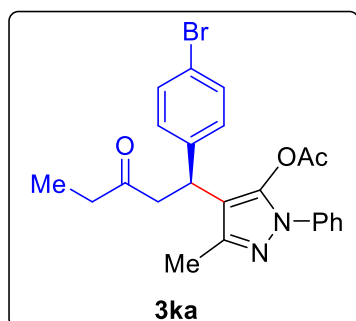
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as light-yellow liquid (59 mg, 80%). ¹H NMR (500 MHz, CDCl₃): δ 7.47-7.46 (m, 2 H), 7.40 (t, $J = 8.1$ Hz, 2 H), 7.29 (t, $J = 7.3$ Hz, 1 H), 7.14 (d, $J = 5.1$ Hz, 1 H), 6.90 (dd, $J = 5.0, 3.6$ Hz, 1 H), 6.80-6.79 (m, 1 H), 4.72 (t, $J = 7.2$ Hz, 1 H), 3.25 (dd, $J = 17.2, 7.5$ Hz, 1 H), 3.08 (dd, $J = 17.2, 6.9$ Hz, 1 H), 2.22 (s, 3 H), 2.17 (s, 3 H), 2.15 (s, 3 H); ¹³C NMR (125 MHz, CDCl₃): δ 205.8, 167.3, 147.3, 146.3, 141.2, 137.9, 129.1 (2 C), 127.3, 126.6, 124.1, 123.8, 122.8 (2 C), 110.7, 48.7, 30.4, 30.3, 20.3, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)];

flow rate 0.5 mL/min; $\lambda = 220$ nm; $\tau_{\text{minor}} = 15.36$ min, $\tau_{\text{major}} = 17.71$ min, $[\alpha]_{\text{D}}^{25} = -22.7$ (*c* 2.7, CHCl₃, 90% ee); **HRMS (ESI)** calcd for C₂₀H₂₀N₂O₃SNa [M + Na]⁺: 391.1092, found: 391.1102.



(S)-3-Methyl-4-(3-oxo-1-(thiophen-2-yl)butyl)-1-phenyl-1H-pyrazol-5-yl acetate (*ent*-3ja)

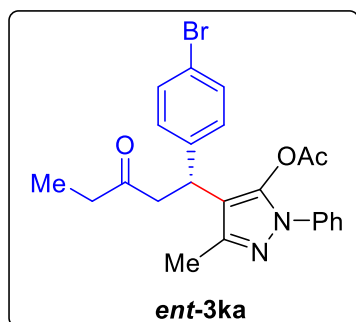
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as light-yellow liquid (54 mg, 73%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; $\lambda = 220$ nm; $\tau_{\text{major}} = 15.60$ min, $\tau_{\text{minor}} = 18.2$ min, $[\alpha]_{\text{D}}^{25} = +16.2$ (*c* 1.0, CHCl₃, 83.5% ee).



(S)-4-(1-(4-Bromophenyl)-3-oxopentyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (3ka)

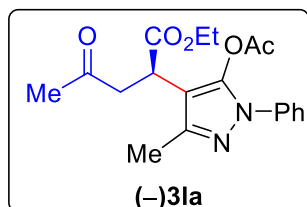
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20%EtOAc/petroleum ether. The above titled compound was isolated as colourless liquid (83 mg, 91%) which solidify in refrigerator on standing. M.p.: 100°C–101°C (hexane/*i*-PrOH :95/5); **¹H NMR (500 MHz, CDCl₃)**: δ 7.45-7.43 (m, 2 H), 7.42-7.39 (m, 4 H), 7.30 (d, *J* = 7.2 Hz, 1 H), 7.10 (d, *J* = 9.2 Hz, 2 H), 4.48 (t, *J* = 7.4 Hz, 1 H), 3.11 (dd, *J* = 16.9, 7.9 Hz, 1 H), 3.01 (dd, *J* = 16.9, 6.7 Hz, 1 H), 2.40 (q, *J* = 7.1 Hz, 2 H), 2.14 (s, 3 H), 2.13 (s, 3 H), 1.02 (t, *J* = 7.3 Hz, 3 H);

¹³C NMR (125 MHz, CDCl₃): δ 208.8, 167.5, 147.4, 141.3, 141.1, 137.7, 131.5 (2 C), 129.2 (2 C), 129.2 (2 C), 127.4, 122.8 (2 C), 120.3, 110.4, 46.0, 36.5, 34.3, 20.3, 13.5, 7.6; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 11.55 min, τ_{major} = 12.73 min, $[\alpha]_{\text{D}}^{24}$ = -9.4 (*c* 1.0, CHCl₃, >99.5% ee); **HRMS (ESI)** calcd for C₂₃H₂₄BrN₂O₃ [M + H]⁺: 455.0971, found: 455.0977.



(R)-4-(1-(4-Bromophenyl)-3-oxopentyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (ent-3ka)

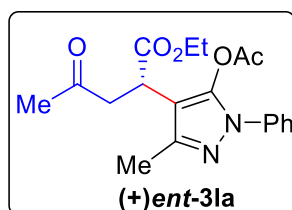
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as colourless liquid (83 mg, 91%) which solidify in refrigerator on standing. M.p.: 100°C–101°C (hexane/*i*-PrOH :95/5); The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{major} = 11.46 min, τ_{minor} = 12.77 min, $[\alpha]_{\text{D}}^{25}$ = +6.6 (*c* 1.0, CHCl₃, 96% ee);



Ethyl (R)-2-(5-acetoxy-3-methyl-1-phenyl-1H-pyrazol-4-yl)-4-oxopentanoate (-)3la

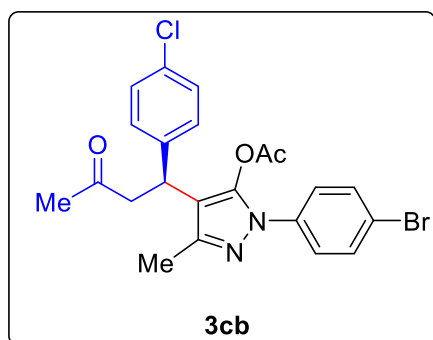
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-25% EtOAc/petroleum ether. The above titled compound was isolated as light-

yellow liquid (49 mg, >68%). **¹H NMR (500 MHz, CDCl₃):** δ 7.46-7.44 (m, 2 H), 7.39 (t, J = 7.8 Hz, 2 H), 7.29 (t, J = 7.3 Hz, 1 H), 4.15 (dq, J = 14.3, 7.2 Hz, 1 H), 4.06 (dq, J = 14.3, 7.1 Hz, 1 H), 3.98 (dd, J = 10.2, 4.0 Hz, 1 H), 3.35 (dd, J = 18.1, 10.2, Hz, 1 H), 2.59 (dd, J = 18.1, 4.0, Hz, 1 H), 2.28 (s, 3 H), 2.20 (s, 3 H), 2.18 (s, 3 H), 1.22 (t, J = 7.2 Hz, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 206.3, 172.1, 167.4, 147.3, 141.6, 137.6, 129.1 (2 C), 127.4, 122.7 (2 C), 105.8, 61.2, 44.2, 35.1, 29.9, 20.2, 14.0, 13.0; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 12.27 min, τ_{major} = 14.08 min, $[\alpha]_{\text{D}}^{23}$ = -58.1 (*c* 3.2, CH₂Cl₂, 95% ee); **HRMS (ESI)** calcd for C₁₉H₂₂NaN₂O₅ [M + Na]⁺: 381.1426, found: 381.1442.



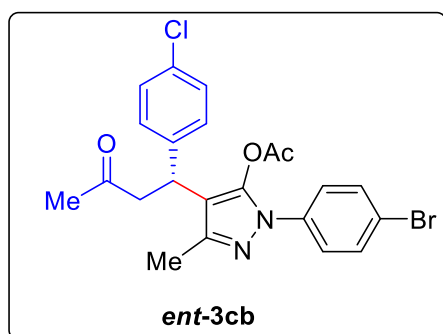
Ethyl (S)-2-(5-acetoxy-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)-4-oxopentanoate (+)3la

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as light-yellow liquid (51 mg, 71%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{major} = 12.21 min, τ_{minor} = 14.32 min, $[\alpha]_{\text{D}}^{22}$ = +59.1 (*c* 4.1, CH₂Cl₂, 90% ee);



(S)-1-(4-Bromophenyl)-4-(1-(4-chlorophenyl)-3-oxobutyl)-3-methyl-1H-pyrazol-5-yl acetate (3cb)

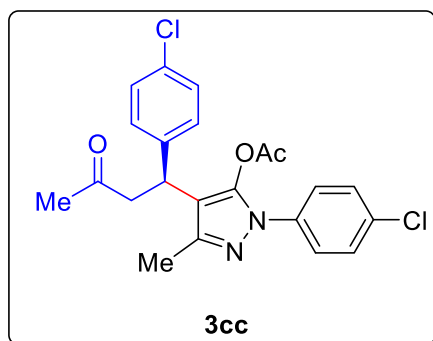
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as white solid (74 mg, 77.5 %). M.p.: 130.0°C –131.0°C ([n-hexane/*i*-PrOH (95/5)]; **¹H NMR (500 MHz, CDCl₃)**: δ 7.52 (d, *J* = 8.6 Hz, 2 H), 7.34 (d, *J* = 8.5 Hz, 2 H), 7.24 (d, *J* = 8.5 Hz, 2 H), 7.14 (d, *J* = 8.3 Hz, 2 H), 4.46 (t, *J* = 7.2 Hz, 1 H), 3.14 (dd, *J* = 17.3, 7.8 Hz, 1 H), 3.02 (dd, *J* = 17.2, 7.0 Hz, 1 H), 2.16 (s, 3 H), 2.14 (s, 3 H), 2.12 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃)**: δ 205.9, 167.3, 147.9, 141.2, 140.3, 136.9, 132.3 (2 C), 132.26, 128.8 (2 C), 128.6 (2 C), 124.1 (2 C), 120.8, 110.8, 47.2, 34.1, 30.4, 20.4, 13.6; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 12.77 min, τ_{major} = 13.78 min, [α]_D²⁵ = -6.5 (c 1.0, CHCl₃, 95% ee); **HRMS (ESI)** calcd for C₂₂H₂₁BrClN₂O₃ [M + H]⁺: 475.0424, found: 475.0432.



(S)-1-(4-Bromophenyl)-4-(1-(4-chlorophenyl)-3-oxobutyl)-3-methyl-1H-pyrazol-5-yl acetate (*ent*-3cb)

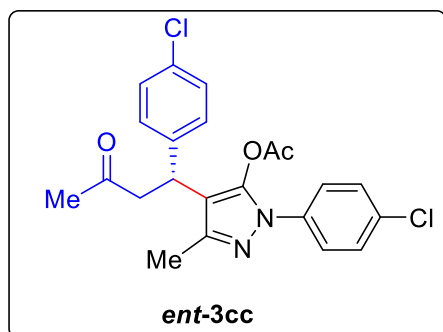
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as white solid (76 mg, >79.5%). M.p.: 130.0°C –131.0°C ([hexane/*i*-PrOH (95/5)]; The ee was determined by

HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; $\lambda = 220$ nm; $\tau_{\text{minor}} = 12.76$ min, $\tau_{\text{major}} = 13.87$ min, $[\alpha]_{\text{D}}^{25} = +6.0$ (c 1.0, CHCl₃, >95.5% ee);



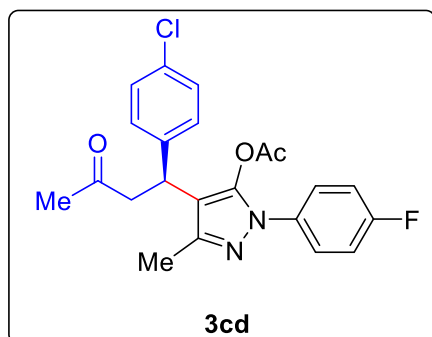
(S)-1-(4-Chlorophenyl)-4-(1-(4-chlorophenyl)-3-oxobutyl)-3-methyl-1*H*-pyrazol-5-yl acetate (3cc)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as white solid (74 mg, >85.5 %). M.p.: 129.0°C –130.0°C ([hexane/*i*-PrOH (95/5)]; **¹H NMR (500 MHz, CDCl₃):** δ 7.40-7.36 (m, 4 H), 7.24 (d, $J = 8.5$ Hz, 2 H), 7.14 (d, $J = 8.4$ Hz, 2 H), 4.46 (t, $J = 7.3$ Hz, 1 H), 3.13 (dd, $J = 17.3, 7.8$ Hz, 1 H), 3.02 (dd, $J = 17.3, 7.0$ Hz, 1 H), 2.15 (s, 3 H), 2.14 (s, 3 H), 2.12 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 205.8, 167.3, 147.8, 141.3, 140.3, 136.4, 132.8, 132.3, 129.3 (2 C), 128.8 (2 C), 128.5 (2 C), 123.9 (2 C), 110.7, 47.2, 34.1, 30.3, 20.3, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; $\lambda = 220$ nm; $\tau_{\text{minor}} = 12.51$ min, $\tau_{\text{major}} = 13.47$ min, $[\alpha]_{\text{D}}^{25} = -15$ (c 1.0, CHCl₃, 98% ee); **HRMS (ESI)** calcd for C₂₂H₂₁Cl₂N₂O₃ [M + H]⁺: 431.0925, found: 431.0914.



**(R)-1-(4-Chlorophenyl)-4-(1-(4-chlorophenyl)-3-oxobutyl)-3-methyl-1H-pyrazol-5-yl acetate
(ent-3cc)**

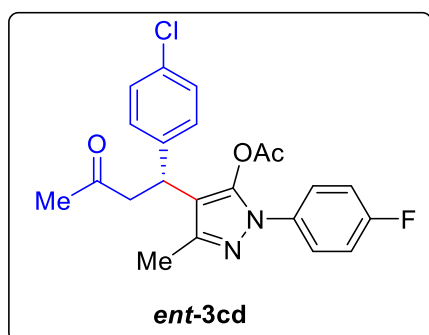
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as white solid (70 mg, 81%). M.p.: 129.5°C –130.0°C ([hexane/*i*-PrOH (95/5)]; The ee was determined by HPLC using a Daicel CHIRALCEL® OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; $\lambda = 220$ nm; $\tau_{\text{major}} = 12.53$ min, $\tau_{\text{minor}} = 13.59$ min, $[\alpha]_{\text{D}}^{25} = +13.1$ (*c* 1.0, CHCl₃, 95% ee).



**(S)-4-(1-(4-Chlorophenyl)-3-oxobutyl)-1-(4-fluorophenyl)-3-methyl-1H-pyrazol-5-yl acetate
(3cd)**

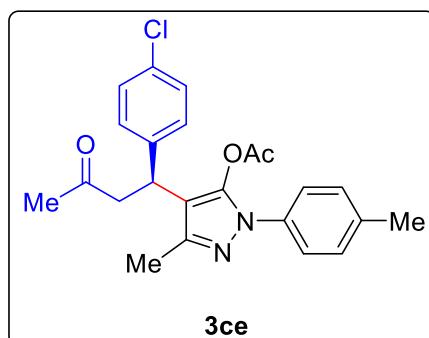
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-25% EtOAc/petroleum ether. The above titled compound was isolated as yellow thick liquid (67 mg, 80.5%). ¹H NMR (500 MHz, CDCl₃): δ 7.42-7.39 (m, 2 H), 7.24 (d, *J* = 8.5 Hz, 2 H), 7.15 (d, *J* = 8.4 Hz, 2 H), 7.08 (t, *J* = 8.6 Hz, 2 H), 4.46 (t, *J* = 7.3 Hz, 1 H), 3.13 (dd, *J* = 17.2, 7.8 Hz, 1 H), 3.03 (dd, *J* = 17.2, 6.9 Hz, 1 H), 2.14 (s, 3 H), 2.12 (s, 6 H); ¹³C NMR (125 MHz,

CDCl₃): δ 205.9, 167.4, 161.5 (d, J_{C-F} = 246.2 Hz), 147.5, 141.3, 140.4, 133.9 (d, J_{C-F} = 12.1 Hz), 132.2, 128.8 (2 C), 128.5 (2 C), 124.9 (d, J_{C-F} = 34.2 Hz, 2 C), 116.0 (d, J_{C-F} = 22.8 Hz, 2 C), 110.3, 42.2, 34.1, 30.4, 20.3, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 12.49 min, τ_{major} = 13.68 min, $[\alpha]_{\text{D}}^{22}$ = -4.8 (*c* 2.0, CHCl₃, 93% ee); **HRMS (ESI)** calcd for C₂₂H₂₁ClFN₂O₃ [M + H]⁺: 415.1224, found: 415.1229.



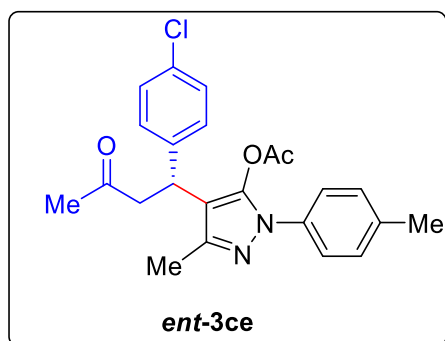
(R)-4-(1-(4-Chlorophenyl)-3-oxobutyl)-1-(4-fluorophenyl)-3-methyl-1H-pyrazol-5-yl acetate (ent-3cd)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-25% EtOAc/petroleum ether. The above titled compound was isolated as yellow thick liquid (65 mg, 78%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{major} = 12.52 min, τ_{minor} = 13.86 min, $[\alpha]_{\text{D}}^{21}$ = +4.6 (*c* 2.3, CHCl₃, 89% ee);



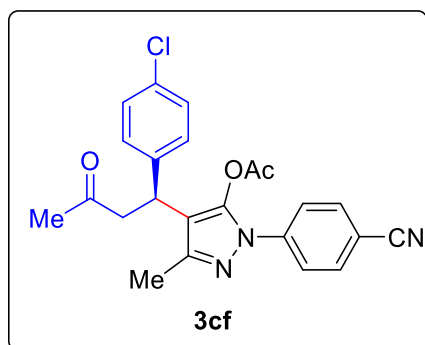
(S)-4-(1-(4-Chlorophenyl)-3-oxobutyl)-3-methyl-1-(p-tolyl)-1H-pyrazol-5-yl acetate (3ce)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as yellow thick liquid (64 mg, 78%). **¹H NMR (500 MHz, CDCl₃):** δ 7.30 (d, J = 8.4 Hz, 2 H), 7.24 (d, J = 8.5 Hz, 2 H), 7.19 (d, J = 8.2 Hz, 2 H), 7.15 (d, J = 8.4 Hz, 2 H), 4.46 (t, J = 7.3 Hz, 1 H), 3.14 (dd, J = 17.2, 8.0 Hz, 1 H), 3.03 (dd, J = 17.2, 6.8 Hz, 1 H), 2.35 (s, 3 H), 2.14 (s, 3 H), 2.13 (s, 3 H), 2.12 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 206.1, 167.5, 147.1, 141.2, 140.5, 137.2, 135.3, 132.1, 129.7 (2 C), 128.8 (2 C), 128.5 (2 C), 122.7 (2 C), 110.0, 47.3, 34.1, 30.4, 21.0, 20.3, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 13.37 min, τ_{major} = 16.02 min, $[\alpha]_{\text{D}}^{24}$ = -1.8 (*c* 1.4, CHCl₃, 89.5% ee); **HRMS (ESI)** calcd for C₂₃H₂₄ClN₂O₃ [M + H]⁺: 411.1475, found: 411.1478.



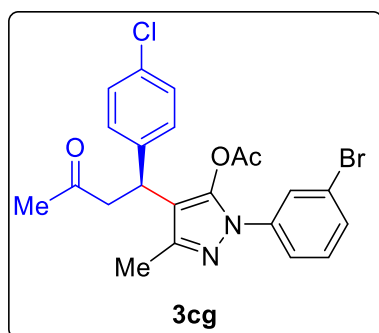
(R)-4-(1-(4-Chlorophenyl)-3-oxobutyl)-3-methyl-1-(p-tolyl)-1H-pyrazol-5-yl acetate (ent-3ce)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20%EtOAc/petroleum ether. The above titled compound was isolated as yellow thick liquid (69 mg, 84%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{major} = 13.25 min, τ_{minor} = 16.15 min, $[\alpha]_{\text{D}}^{24}$ = +1.8 (*c* 1.4, CHCl₃, 84.5% ee).



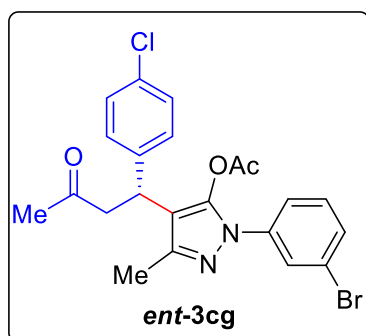
**(S)-4-(1-(4-Chlorophenyl)-3-oxobutyl)-1-(4-cyanophenyl)-3-methyl-1H-pyrazol-5-yl acetate
(3cf)**

Purified by column chromatography on silica gel (230-400 mesh) using eluent 25% EtOAc/petroleum ether-35% EtOAc/petroleum ether. The above titled compound was isolated as off-white amorphous solid (52 mg, 61.5%). **¹H NMR (500 MHz, CDCl₃):** δ 7.69 (d, J = 8.2 Hz, 2 H), 7.63 (d, J = 8.7 Hz, 2 H), 7.25 (d, J = 8.4 Hz, 2 H), 7.13 (d, J = 8.5 Hz, 2 H), 4.46 (t, J = 7.3 Hz, 1 H), 3.15 (dd, J = 17.4, 7.5 Hz, 1H), 3.03 (dd, J = 17.4, 7.1 Hz, 1 H), 2.21 (s, 3 H), 2.15 (s, 3 H), 2.13 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 205.7, 167.1, 149.1, 141.5, 141.3, 139.9, 133.2 (2 C), 132.4, 128.7 (2 C), 128.6 (2 C), 121.9 (2 C), 118.2, 111.9, 110.1, 46.9, 33.8, 30.4, 20.4, 13.6; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 22.61 min, τ_{major} = 24.17 min, $[\alpha]_{\text{D}}^{23}$ = -11.0 (c 2.8, CHCl₃, 95% ee); **HRMS (ESI)** calcd for C₂₃H₂₁ClN₃O₃ [M + H]⁺: 422.1271, found: 422.1268.



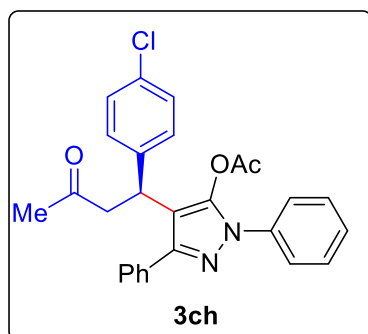
**(S)-1-(3-Bromophenyl)-4-(1-(4-chlorophenyl)-3-oxobutyl)-3-methyl-1H-pyrazol-5-yl acetate
(3cg)**

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20%EtOAc/petroleum ether. The above titled compound was isolated as off-white amorphous solid (83 mg, 87%). **¹H NMR (500 MHz, CDCl₃):** δ 7.66 (t, J = 1.8 Hz, 1H), 7.42-7.40 (m, 2 H), 7.26-7.24 (m, 3 H), 7.14 (d, J = 8.4 Hz, 2 H), 4.46 (t, J = 7.3 Hz, 1H), 3.14 (dd, J = 17.3, 7.7 Hz, 1H), 3.03 (dd, J = 17.2, 7.0 Hz, 1H), 2.18 (s, 3 H), 2.14 (s, 3 H), 2.12 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 205.8, 167.3, 148.0, 141.3, 140.2, 138.9, 132.2, 130.4, 130.0, 128.8 (2 C), 128.5 (2 C), 125.4, 122.6, 120.7, 111.0, 47.1, 34.0, 30.3, 20.3, 13.5; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 12.95 min, τ_{major} = 13.99 min, $[\alpha]_{\text{D}}^{21}$ = -4.2 (*c* 2.0, CHCl₃, 95.5% ee); **HRMS (ESI)** calcd for C₂₂H₂₁BrClN₂O₃ [M + H]⁺: 475.0424, found: 475.0432.



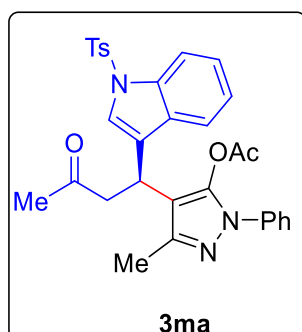
(R)-1-(3-Bromophenyl)-4-(1-(4-chlorophenyl)-3-oxobutyl)-3-methyl-1H-pyrazol-5-yl acetate (ent-3cg)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-20% EtOAc/petroleum ether. The above titled compound was isolated as off-white amorphous solid (83 mg, 87%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{major} = 12.91 min, τ_{minor} = 14.00 min, $[\alpha]_{\text{D}}^{24}$ = +2.5 (*c* 1.7, CHCl₃, 85% ee);



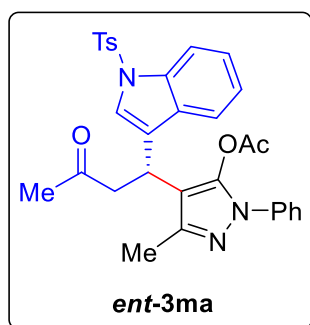
(S)-4-(1-(4-Chlorophenyl)-3-oxobutyl)-1,3-diphenyl-1H-pyrazol-5-yl acetate (3ch)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 10% EtOAc/petroleum ether-20%EtOAc/petroleum ether. The above titled compound was isolated as off-white amorphous solid (80 mg, 87%). **¹H NMR (500 MHz, CDCl₃):** δ 7.55 (d, J = 8.0 Hz, 2 H), 7.50 (dd, J = 7.7, 1.8 Hz, 2 H), 7.44 (t, J = 8.0 Hz, 2 H), 7.41-7.37 (m, 3 H), 7.33 (t, J = 7.4 Hz, 1 H), 7.24 (d, J = 8.5 Hz, 2 H), 7.14 (d, J = 8.4 Hz, 2 H), 4.73 (t, J = 7.3 Hz, 1H), 3.10 (dd, J = 17.4, 8.2 Hz, 1H), 3.02 (dd, J = 17.3, 6.6 Hz, 1H), 2.09 (s, 3 H), 2.05 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 205.8, 167.1, 150.5, 141.9, 140.9, 137.7, 133.2, 132.1, 129.2 (2 C), 128.9 (2 C), 128.5 (2 C), 128.48 (2 C), 128.4 (2 C), 128.2, 127.7, 123.03 (2 C), 110.1, 47.9, 34.3, 30.0, 20.2; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 12.05 min, τ_{major} = 13.44 min, $[\alpha]_{\text{D}}^{20}$ = -8.4 (*c* 1.0, CHCl₃, 90% ee); **HRMS (ESI)** calcd for C₂₇H₂₄ClN₂O₃ [M + H]⁺: 459.1475, found: 459.1487.



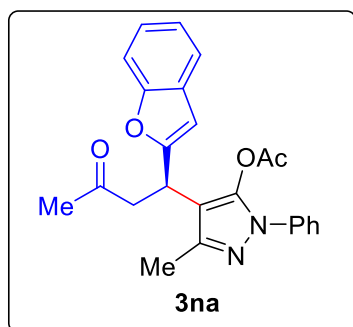
(S)-3-Methyl-4-(3-oxo-1-(1-tosyl-1H-indol-3-yl)butyl)-1-phenyl-1H-pyrazol-5-yl acetate (3ma)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 25% EtOAc/petroleum ether-35% EtOAc/petroleum ether. The above titled compound was isolated as colourless amorphous solid (107 mg, 96%). **¹H NMR (500 MHz, CDCl₃):** δ 7.95 (d, J = 8.3 Hz, 1 H), 7.70 (d, J = 8.3 Hz, 2 H), 7.42-7.37 (m, 4 H), 7.33-7.27 (m, 4 H), 7.20 (d, J = 8.2 Hz, 2 H), 7.17 (t, J = 7.8 Hz, 1 H), 4.59 (t, J = 7.1 Hz, 1 H), 3.20 (dd, J = 17.1, 6.9 Hz, 1 H), 3.09 (dd, J = 17.0, 6.9 Hz, 1 H), 2.33 (s, 3 H), 2.18 (s, 3 H), 2.13 (s, 3 H), 2.07 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 205.9, 167.4, 147.1, 144.9, 141.3, 137.7, 135.4, 134.9, 129.9, 129.7 (2 C), 129.1 (2 C), 127.2, 126.6 (2 C), 124.9, 123.7, 123.3, 122.7 (2 C), 122.4, 119.9, 113.6, 108.6, 46.7, 30.4, 26.4, 21.4, 20.1, 13.3; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{major} = 29.30 min, τ_{minor} = 33.60 min, $[\alpha]_{\text{D}}^{23}$ = -67.3 (c 1.7, CHCl₃, 90% ee); **HRMS (ESI)** calcd for C₃₁H₃₀N₃O₅S [M + H]⁺: 556.1906, found: 556.1908.



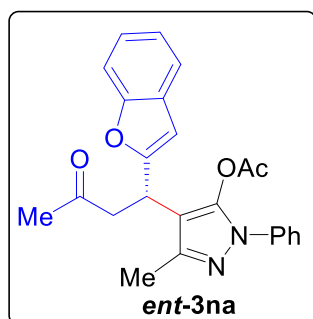
(R)-3-Methyl-4-(3-oxo-1-(1-tosyl-1H-indol-3-yl)butyl)-1-phenyl-1H-pyrazol-5-yl acetate (ent-3ma)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 25% EtOAc/petroleum ether-35% EtOAc/petroleum ether. The above titled compound was isolated as colourless amorphous solid (102 mg, 91.5%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{major} = 30.79 min, τ_{minor} = 34.58 min, $[\alpha]_{\text{D}}^{25}$ = +72.1 (c 1.7, CHCl₃, 84% ee);



(R)-4-(1-(Benzofuran-2-yl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (3na)

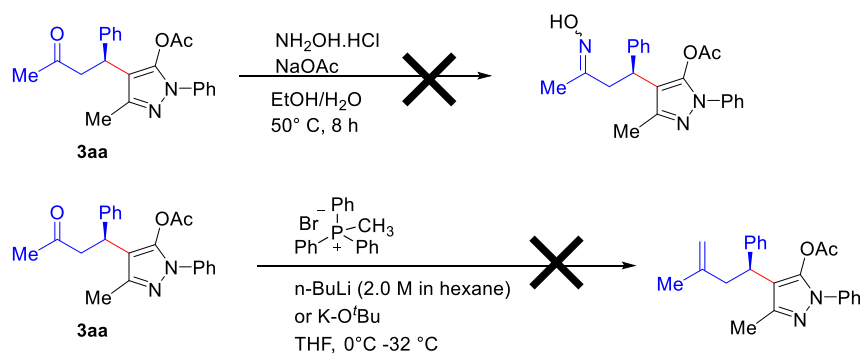
Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-25% EtOAc/petroleum ether. The above titled compound was isolated as yellowish thick liquid (69 mg, 85.5%). **¹H NMR (500 MHz, CDCl₃):** δ 7.47-7.46 (m, 3 H), 7.40 (t, J = 7.8 Hz, 3 H), 7.30 (t, J = 7.5 Hz, 1 H), 7.22 (td, J = 7.6, 1.1 Hz, 1 H), 7.18 (t, J = 7.3 Hz, 1 H), 6.42 (s, 1 H), 4.69 (t, J = 7.0 Hz, 1 H), 3.37 (dd, J = 17.5, 7.5 Hz, 1 H), 3.04 (dd, J = 17.5, 6.7 Hz, 1 H), 2.31 (s, 3 H), 2.21 (s, 3 H), 2.08 (s, 3 H); **¹³C NMR (125 MHz, CDCl₃):** δ 205.6, 167.4, 157.8, 154.7, 147.4, 141.7, 137.8, 129.2 (2 C), 128.4, 127.4, 123.7, 122.8 (2 C), 122.7, 120.6, 110.9, 108.1, 102.9, 45.9, 30.3, 29.4, 20.3, 13.4; The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; λ = 220 nm; τ_{minor} = 16.24 min, τ_{major} = 17.41 min, $[\alpha]_{\text{D}}^{24}$ = -40.3 (c 1.3, CHCl₃, 95.5% ee); **HRMS (ESI)** calcd for C₂₄H₂₃N₂O₄ [M + H]⁺: 403.1657, found: 403.1657.



(S)-4-(1-(Benzofuran-2-yl)-3-oxobutyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl acetate (ent-3na)

Purified by column chromatography on silica gel (230-400 mesh) using eluent 15% EtOAc/petroleum ether-25% EtOAc/petroleum ether. The above titled compound was isolated as yellowish thick liquid (69 mg, 85.5%). The ee was determined by HPLC using a Daicel CHIRALCEL[®] OD-H [hexane/*i*-PrOH (80/20)]; flow rate 0.5 mL/min; $\lambda = 220$ nm; $\tau_{\text{major}} = 16.56$ min, $\tau_{\text{minor}} = 18.11$ min, $[\alpha]_{\text{D}}^{22} = +36.5$ (*c* 2.0 CHCl₃, 91.5% ee).

Unsuccessful synthetic transformation



6. Single crystal X-ray diffraction analysis of *ent*-3ba

X-ray structure of *ent*-3ba ([CCDC 2234286](#))

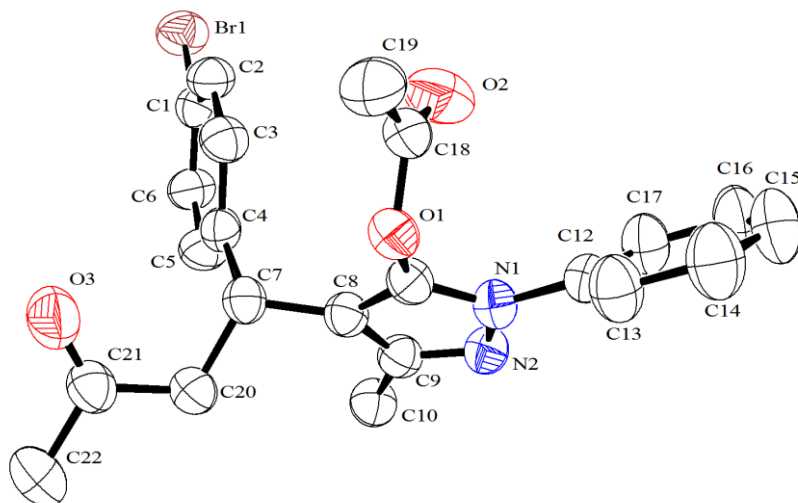


Table 1. Crystal data and structure refinement for BOD-PG-45-new

CCDC number	
Empirical formula	C ₂₂ H ₂₁ BrN ₂ O ₃
Formula weight	441.32
Temperature [K]	298(2)
Crystal system	monoclinic
Space group (number)	C2 (5)
<i>a</i> [Å]	27.4766(3)
<i>b</i> [Å]	6.15110(10)
<i>c</i> [Å]	12.3067(2)
α [°]	90
β [°]	100.7590(10)
γ [°]	90
Volume [Å ³]	2043.41(5)
<i>Z</i>	4
ρ_{calc} [g/cm ³]	1.435
μ [mm ⁻¹]	2.946

$F(000)$	904
Crystal size [mm ³]	0.100×0.050×0.050
Crystal colour	colourless
Crystal shape	needle
Radiation	Cu K_{α} ($\lambda=1.54184$ Å)
2 θ range [°]	6.55 to 154.68 (0.79 Å)
Index ranges	$-34 \leq h \leq 34$ $-7 \leq k \leq 7$ $-15 \leq l \leq 15$
Reflections collected	40865
Independent reflections	4274 $R_{\text{int}} = 0.0848$ $R_{\text{sigma}} = 0.0282$
Completeness to $\theta = 67.684^{\circ}$	100.0 %
Data / Restraints / Parameters	4274/1/256
Goodness-of-fit on F^2	1.195
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0343$ $wR_2 = 0.0993$
Final R indexes [all data]	$R_1 = 0.0706$ $wR_2 = 0.1550$
Largest peak/hole [eÅ ³]	0.64/-0.58
Flack X parameter	-0.031(7)

Table 2. Bond lengths and angles for BOD-PG-45-new.

Atom– AtomAtom– Atom–Atom	Length [Å]Angle [°]
C1–C6	1.376(8)
C1–C2	1.382(8)
C1–Br1	1.905(5)
C2–C3	1.380(8)
C3–C4	1.396(7)
C4–C5	1.394(7)
C4–C7	1.521(7)
C5–C6	1.388(8)
C7–C8	1.511(6)
C7–C20	1.539(7)
C8–C11	1.371(7)
C8–C9	1.417(8)
C9–N2	1.333(7)
C9–C10	1.489(7)
C11–N1	1.349(7)
C11–O1	1.369(6)
C12–C17	1.373(8)
C12–C13	1.380(8)
C12–N1	1.428(6)
C13–C14	1.388(9)
C14–C15	1.368(11)
C15–C16	1.380(11)
C16–C17	1.380(9)
C18–O2	1.181(9)
C18–O1	1.385(7)
C18–C19	1.488(10)
C20–C21	1.512(8)
C21–O3	1.191(9)
C21–C22	1.507(9)
N1–N2	1.367(7)
C6–C1–C2	121.4(5)
C6–C1–Br1	118.5(4)
C2–C1–Br1	120.0(4)
C3–C2–C1	118.3(5)
C2–C3–C4	122.6(5)
C5–C4–C3	116.8(5)
C5–C4–C7	123.3(5)
C3–C4–C7	119.7(5)
C6–C5–C4	121.8(5)
C1–C6–C5	119.0(5)
C8–C7–C4	109.9(4)
C8–C7–C20	111.3(4)

C4–C7–C20	115.6(4)
C11–C8–C9	103.0(4)
C11–C8–C7	125.1(5)
C9–C8–C7	131.8(5)
N2–C9–C8	112.1(4)
N2–C9–C10	118.3(5)
C8–C9–C10	129.5(5)
N1–C11–O1	122.8(5)
N1–C11–C8	109.4(5)
O1–C11–C8	127.6(5)
C17–C12–C13	121.0(5)
C17–C12–N1	118.5(5)
C13–C12–N1	120.6(5)
C12–C13–C14	118.4(6)
C15–C14–C13	121.3(7)
C14–C15–C16	119.4(6)
C17–C16–C15	120.2(6)
C12–C17–C16	119.7(6)
O2–C18–O1	121.8(6)
O2–C18–C19	129.3(6)
O1–C18–C19	108.9(6)
C21–C20–C7	113.5(4)
O3–C21–C22	121.6(6)
O3–C21–C20	122.9(5)
C22–C21–C20	115.5(6)
C11–N1–N2	110.4(4)
C11–N1–C12	129.1(5)
N2–N1–C12	120.2(4)
C9–N2–N1	105.0(4)
C11–O1–C18	118.2(4)

A colourless block-shaped crystal with dimensions $0.05 \times 0.05 \times 0.10 \text{ mm}^3$ was mounted. Data were collected using a XtaLAB Synergy, Dualflex, HyPix diffractometer, operating at $T = 298(2) \text{ K}$, equipped with a micro-focus sealed X-ray Cu $K\alpha$ radiation ($\lambda = 1.54184 \text{ \AA}$). All data were integrated with CrysAlisPro 1.171.40.57a (Rigaku OD, 2019) and a multi-scan absorption correction using SCALE3 ABSPACK was applied.^[1] The structure were solved by iterative methods using SHELXT and refined by full-matrix least-squares methods against F^2 by SHELXL-2017/1.^[2,3] All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom

positions were calculated geometrically and refined using the riding model. ORTEP diagrams were prepared with 50% probability using ORTEP 3 for windows.^[4]

Crystallographic data (including structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre (CCDC No. 2234286).

[1] CrysAlisPro (Rigaku, V1.171.40.57a, 2019), Rigaku Oxford Diffraction, Poland.

[2] G. M. Sheldrick, *Acta Cryst.***2015**, *A71*, 3–8, doi:10.1107/S2053273314026370.

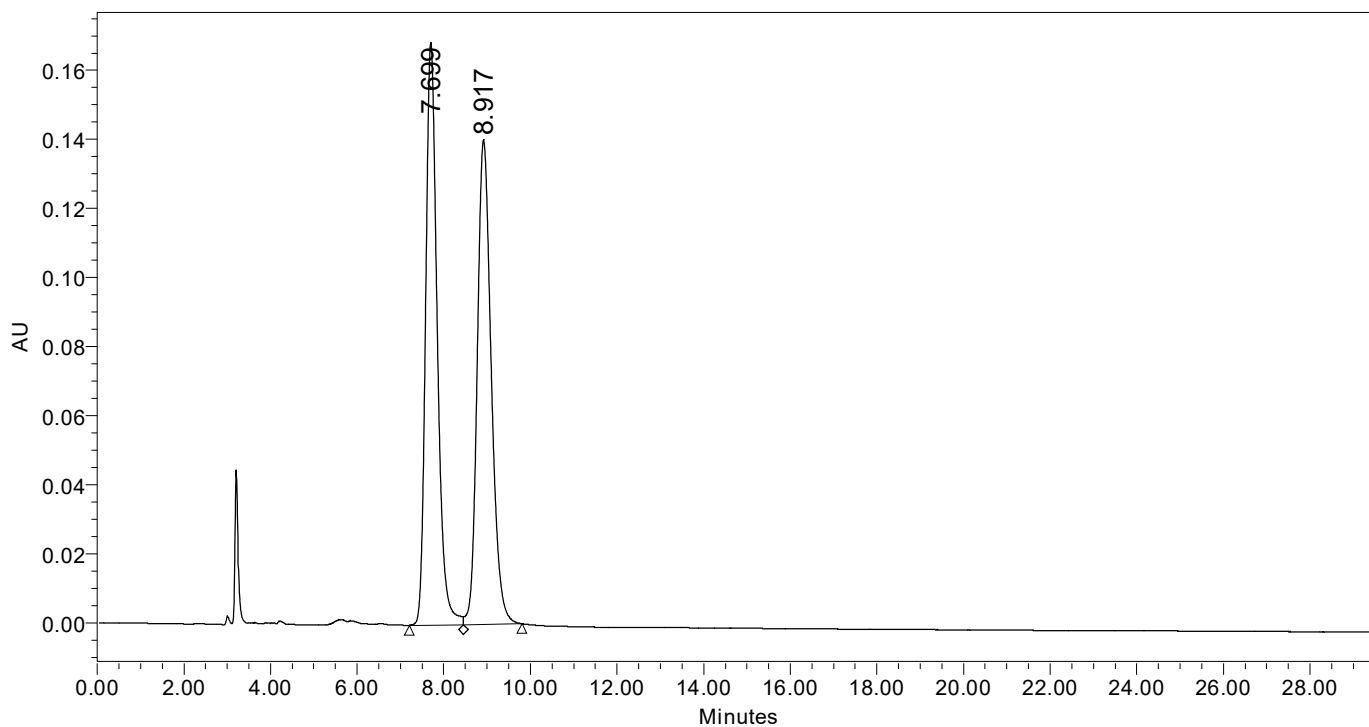
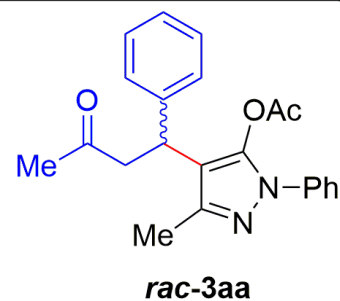
[3] G. M. Sheldrick, *Acta Cryst.***2015**, *C71*, 3–8, doi:10.1107/S2053229614024218.

[4] L. J. Farrugia, *J. Appl. Crystallogr.*, 1997, 30, 565.

SAMPLE INFORMATION

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Sample Type: Unknown
Vial: 1
Injection #: 14
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

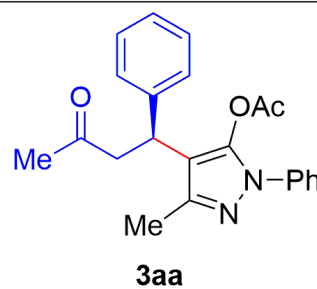


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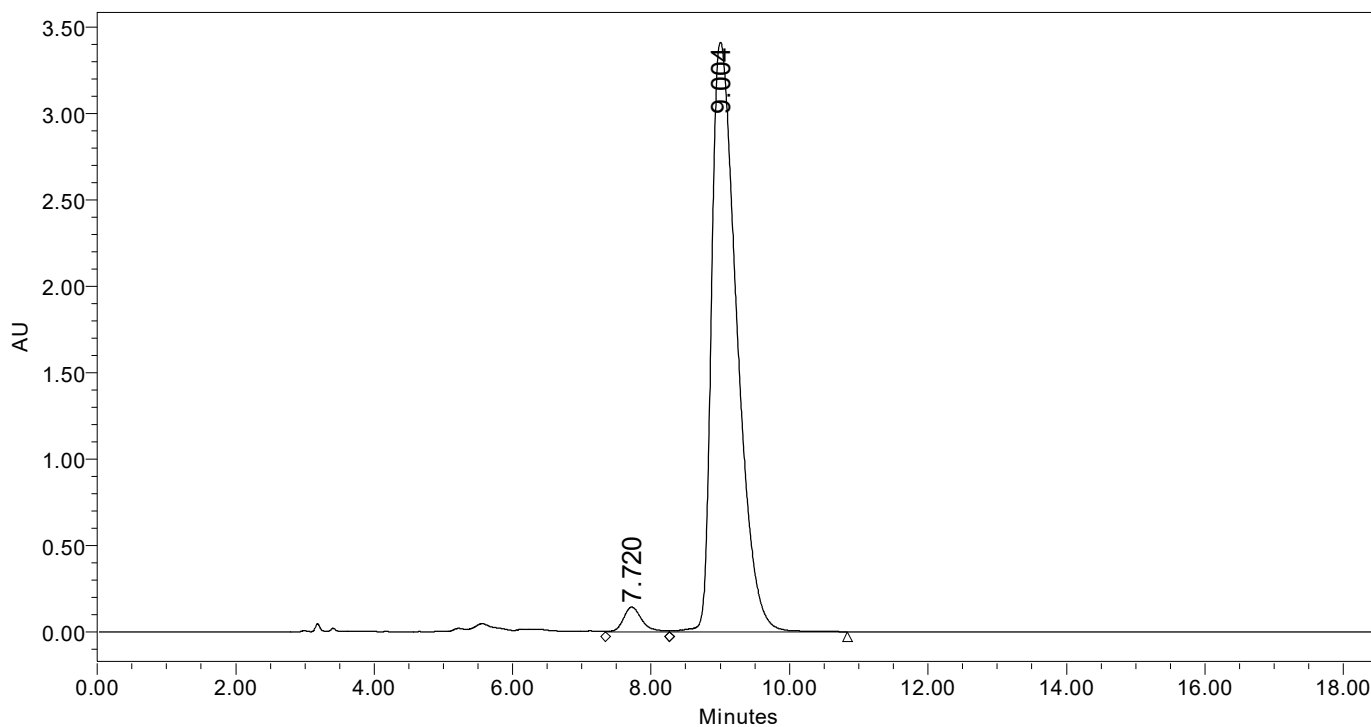
SAMPLE INFORMATION

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Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 21-10-2022 19:14:13 IST
Date Processed: 28-10-2022 14:12:04 IST

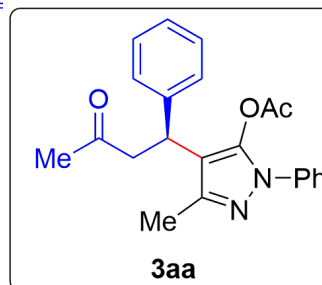


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2	9.004	86150145	97.04	3412864

SAMPLE INFORMATION

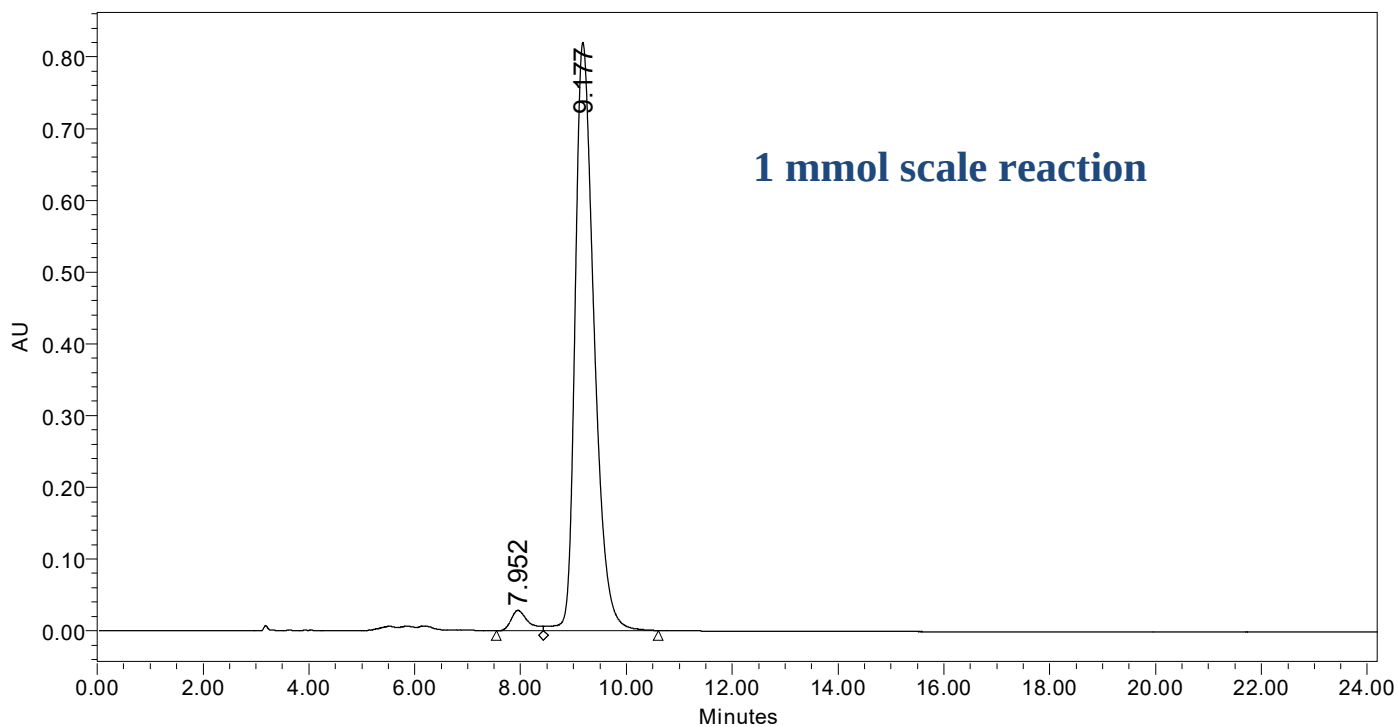
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Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 05-01-2023 14:58:10 IST
Date Processed: 21-03-2023 19:23:12 IST

1 mmol scale reaction

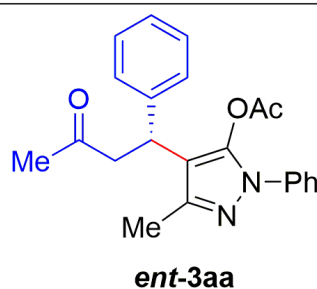


	RT	Area	% Area	Height
1	7.952	631769	3.00	28313
2	9.177	20441814	97.00	820052

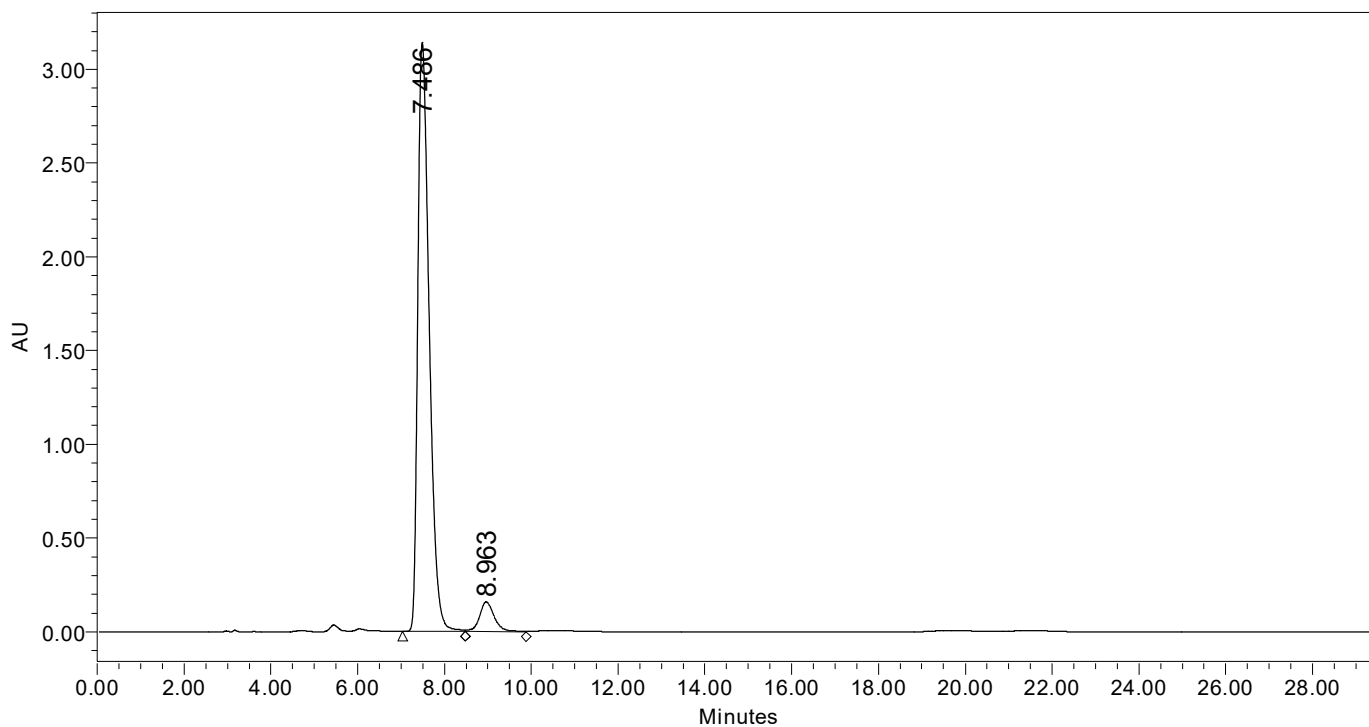
SAMPLE INFORMATION

Sample Name: PG43-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 7
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 27-10-2022 13:36:52 IST
Date Processed: 30-11-2022 13:36:32 IST

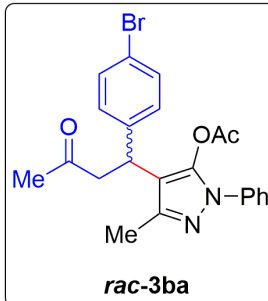


	RT	Area	% Area	Height
1	7.486	57369937	93.83	3143419
2	8.963	3774962	6.17	159145

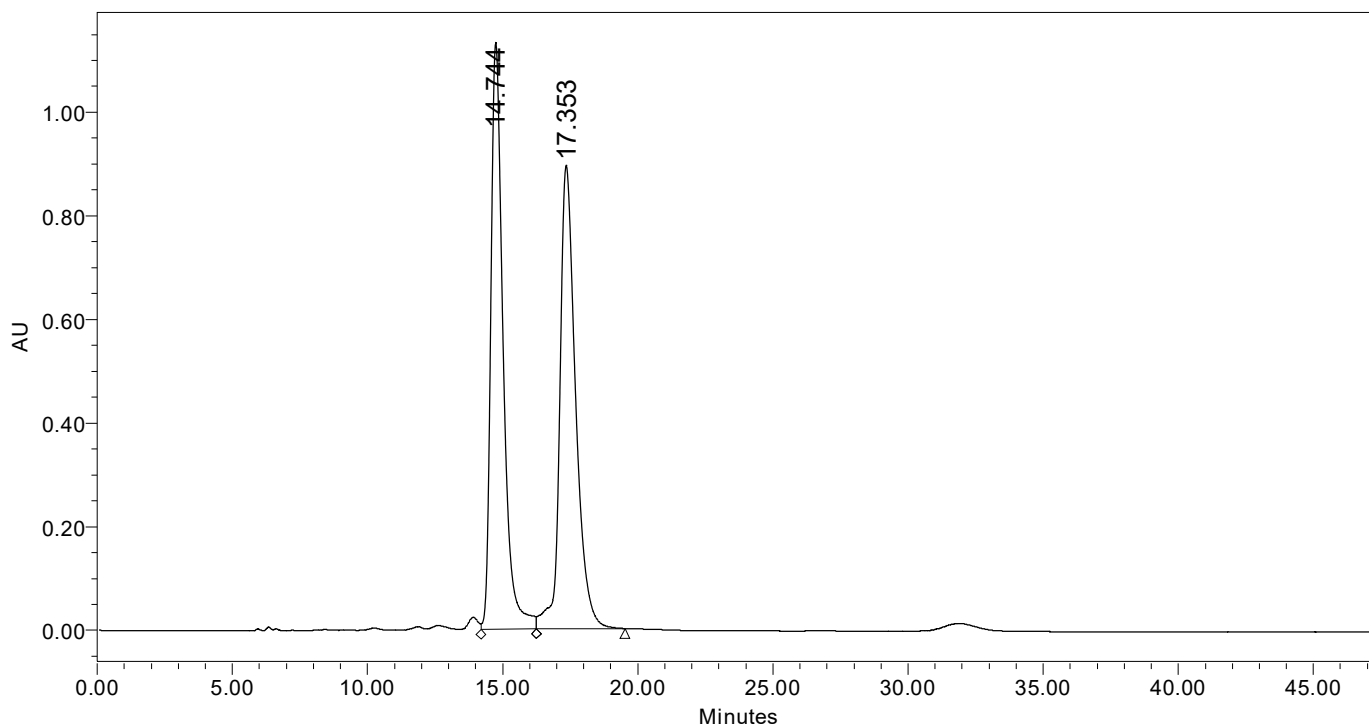
SAMPLE INFORMATION

Sample Name: PG93-ODH
Sample Type: Unknown
Vial: 1
Injection #: 5
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 01-12-2022 12:43:10 IST
Date Processed: 05-01-2023 18:00:58 IST



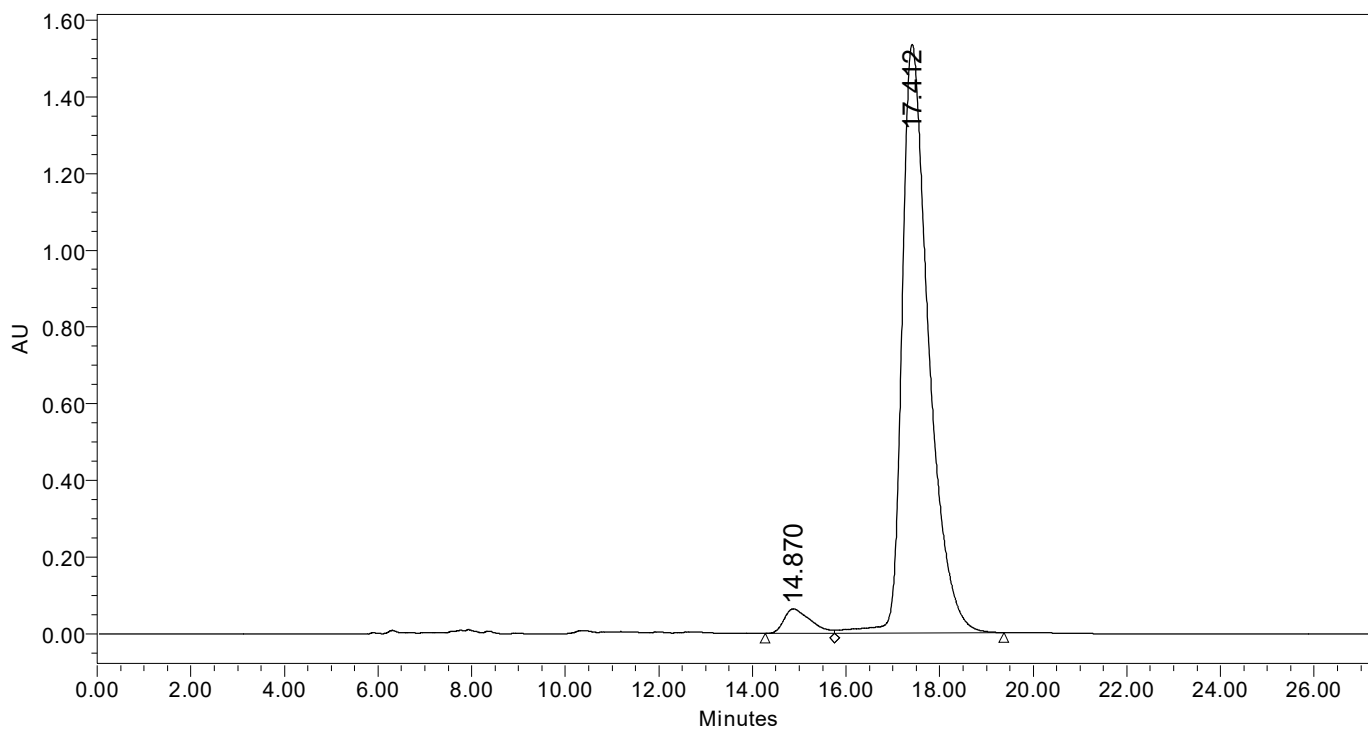
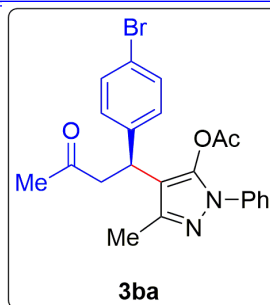
	RT	Area	% Area	Height
1	14.744	36044872	49.66	1133263
2	17.353	36536584	50.34	894938

SAMPLE INFORMATION

Sample Name: PG44-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Date Acquired: 28-10-2022 13:49:39 IST
Date Processed: 28-10-2022 14:17:35 IST

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

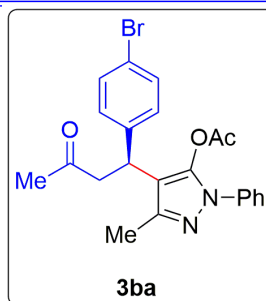


	RT	Area	% Area	Height
1	14.870	2490680	3.96	63884
2	17.412	60478795	96.04	1534578

SAMPLE INFORMATION

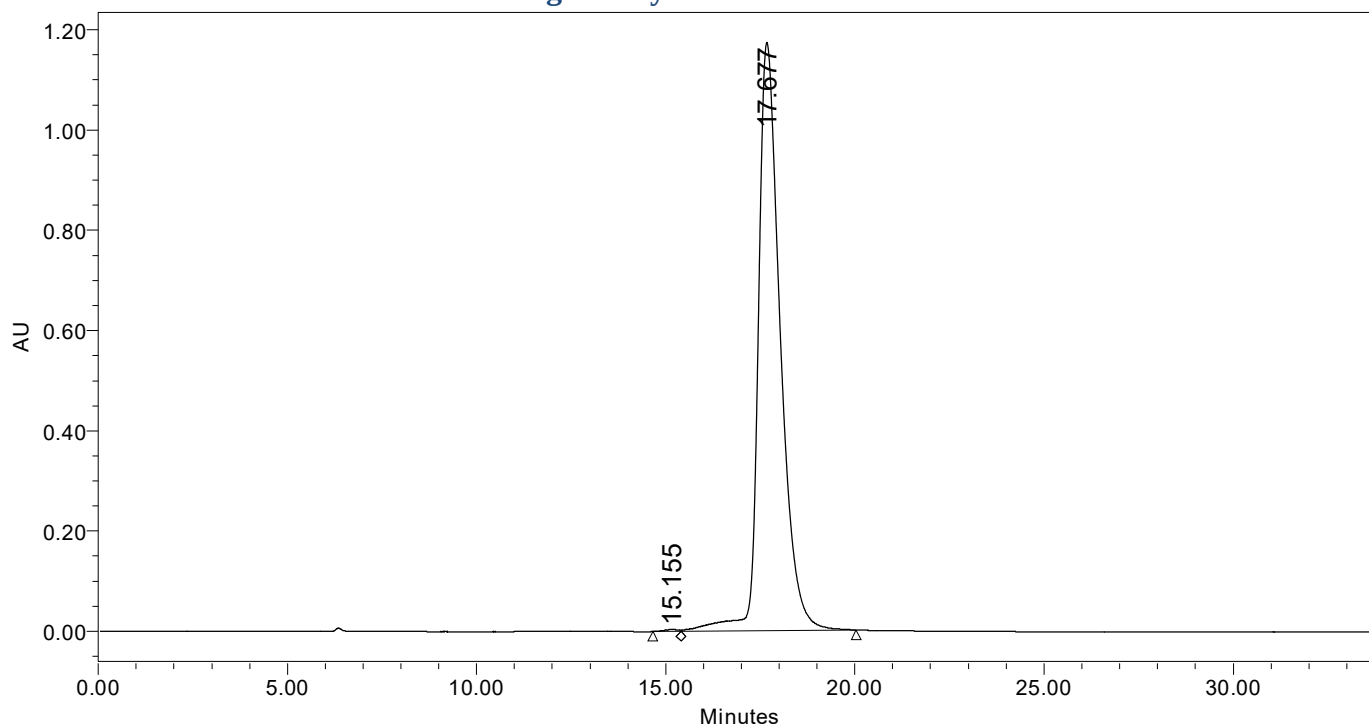
Sample Name: PG44-CRYSTAL
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 11-01-2023 13:15:15 IST
Date Processed: 13-01-2023 11:30:28 IST

After single recrystallization



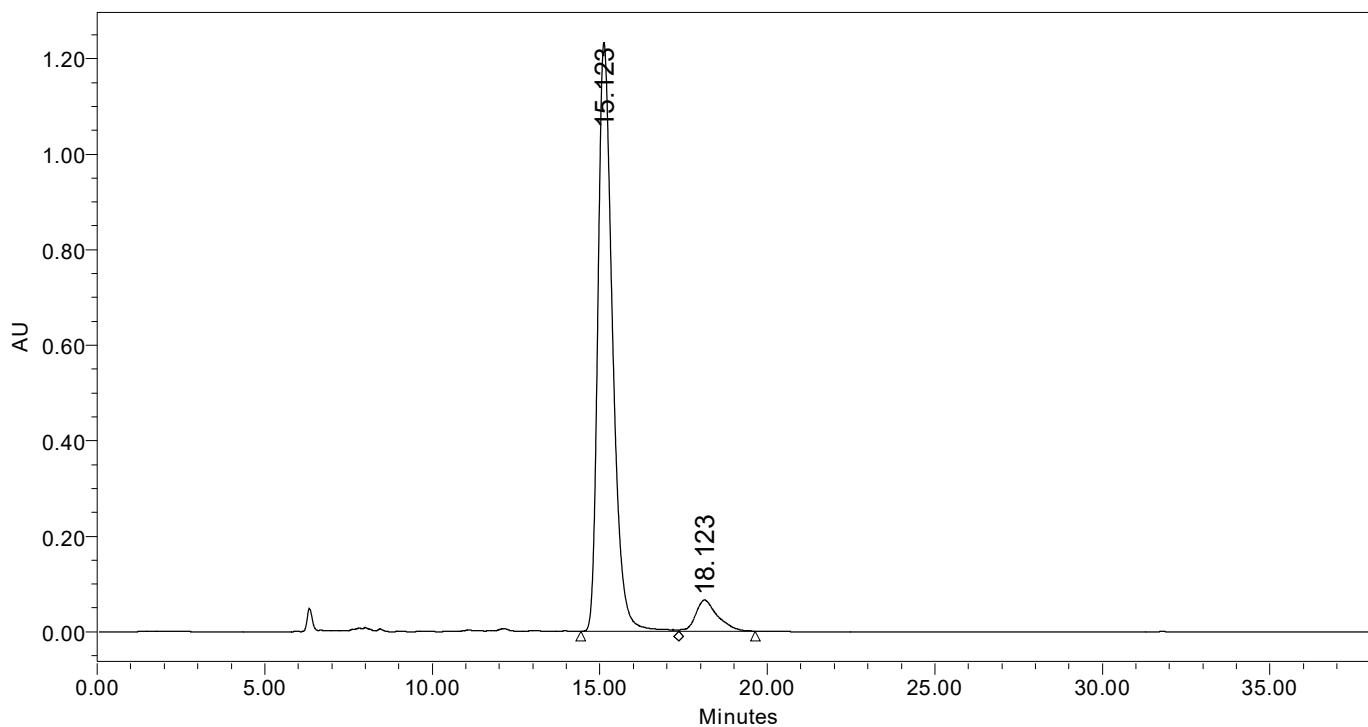
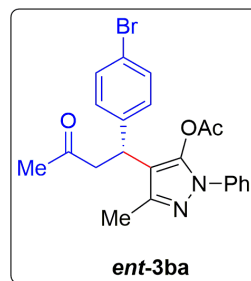
	RT	Area	% Area	Height
1	15.155	101420	0.21	3728
2	17.677	47603373	99.79	1173813

SAMPLE INFORMATION

Sample Name: PG45-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 6
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Date Acquired: 28-10-2022 14:46:48 IST
Date Processed: 28-10-2022 15:24:33 IST

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

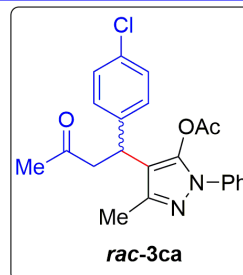


	RT	Area	% Area	Height
1	15.123	37490359	92.65	1233815
2	18.123	2975849	7.35	65127

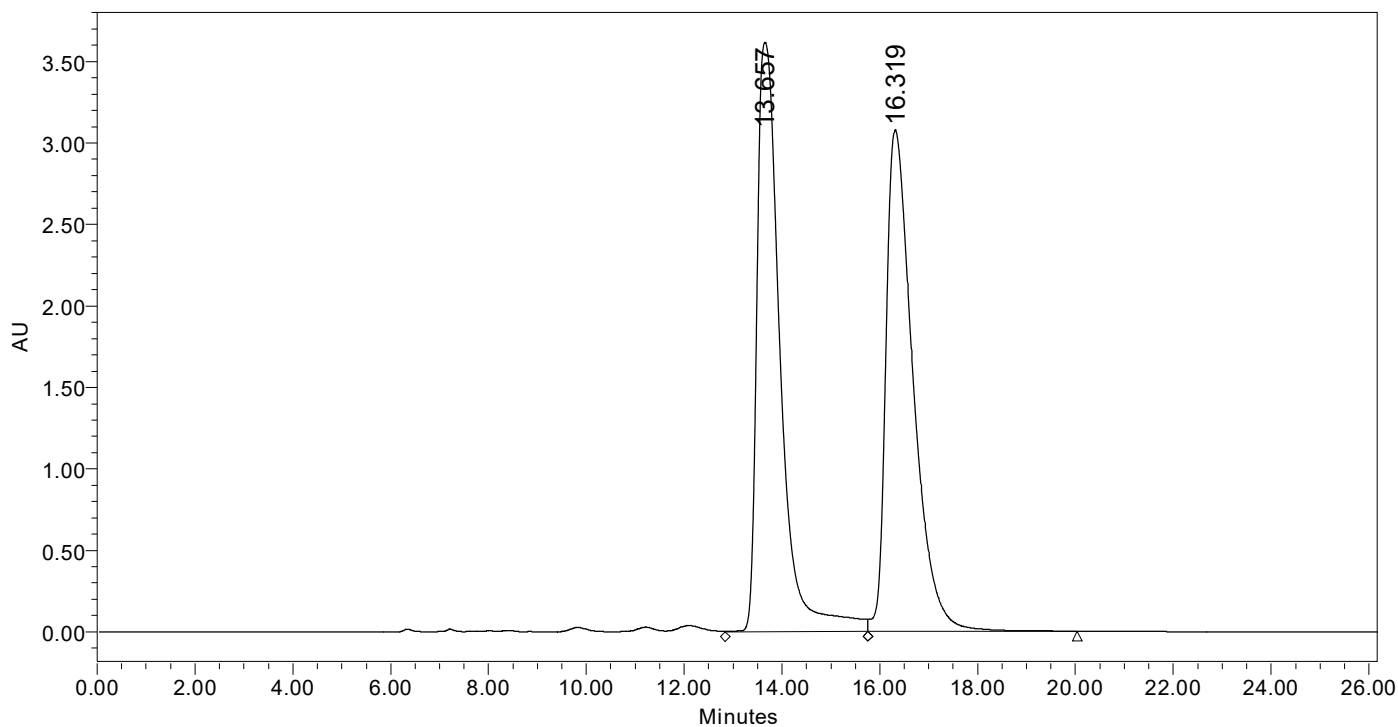
SAMPLE INFORMATION

Sample Name: PG92-ODH
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 01-12-2022 11:52:30 IST
Date Processed: 01-12-2022 18:05:32 IST

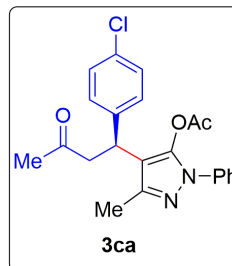


	RT	Area	% Area	Height
1	13.657	120011936	50.29	3616219
2	16.319	118644424	49.71	3078780

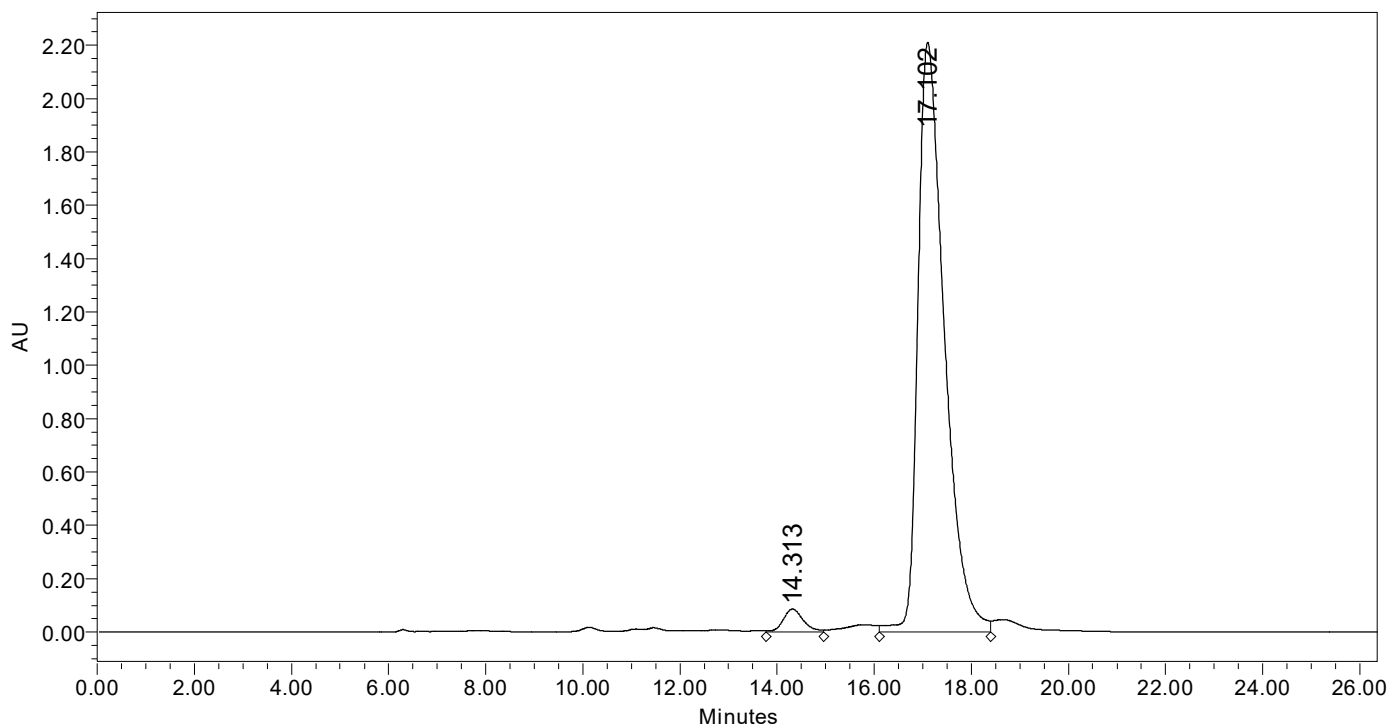
SAMPLE INFORMATION

Sample Name: PG55-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 03-11-2022 14:39:20 IST
Date Processed: 04-11-2022 15:06:54 IST

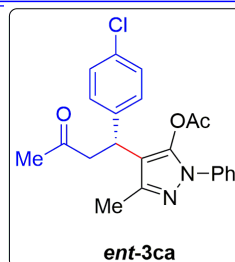


	RT	Area	% Area	Height
1	14.313	2432605	2.83	85500
2	17.102	83518750	97.17	2209887

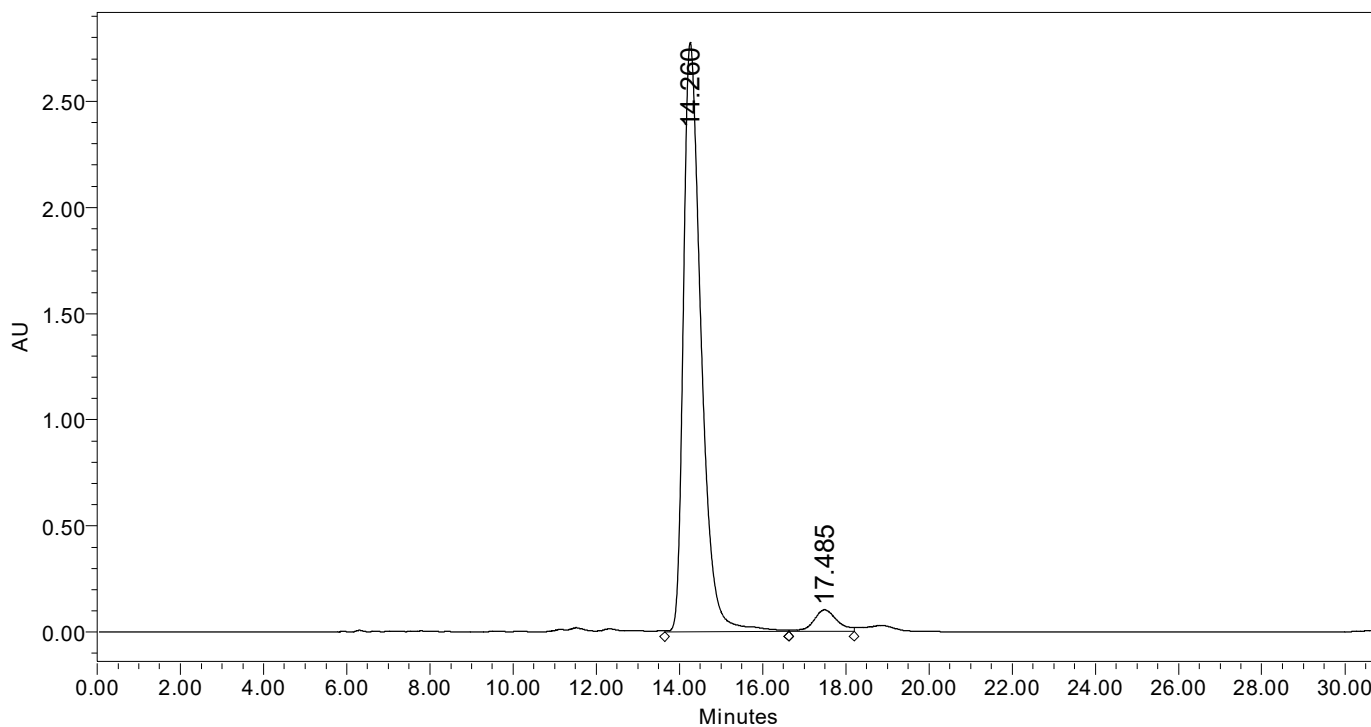
SAMPLE INFORMATION

Sample Name: PG56-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 03-11-2022 15:27:23 IST
Date Processed: 11-11-2022 14:41:53 IST

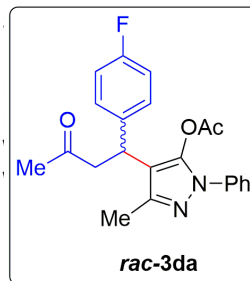


	RT	Area	% Area	Height
1	14.260	82147153	95.26	2776418
2	17.485	4088503	4.74	102285

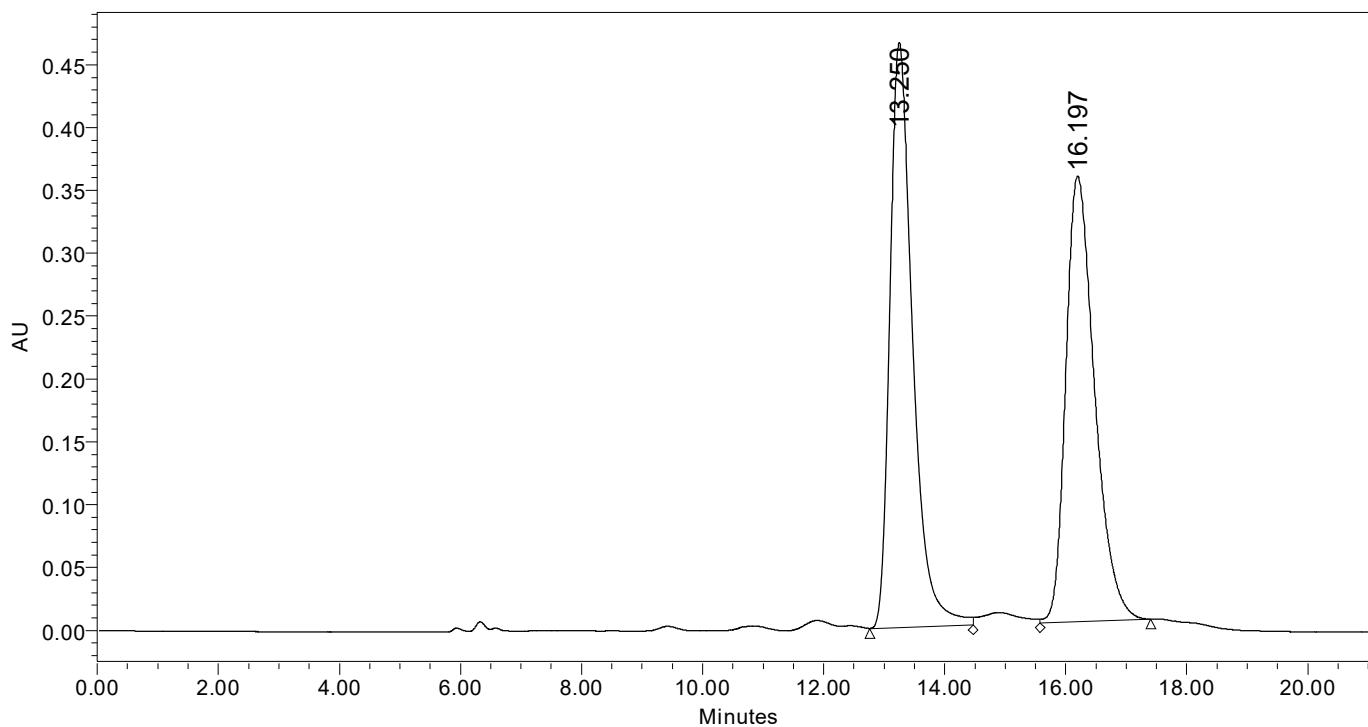
SAMPLE INFORMATION

Sample Name: PG100-ODH
Sample Type: Unknown
Vial: 1
Injection #: 5
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 28-12-2022 12:39:48 IST
Date Processed: 28-12-2022 17:30:07 IST



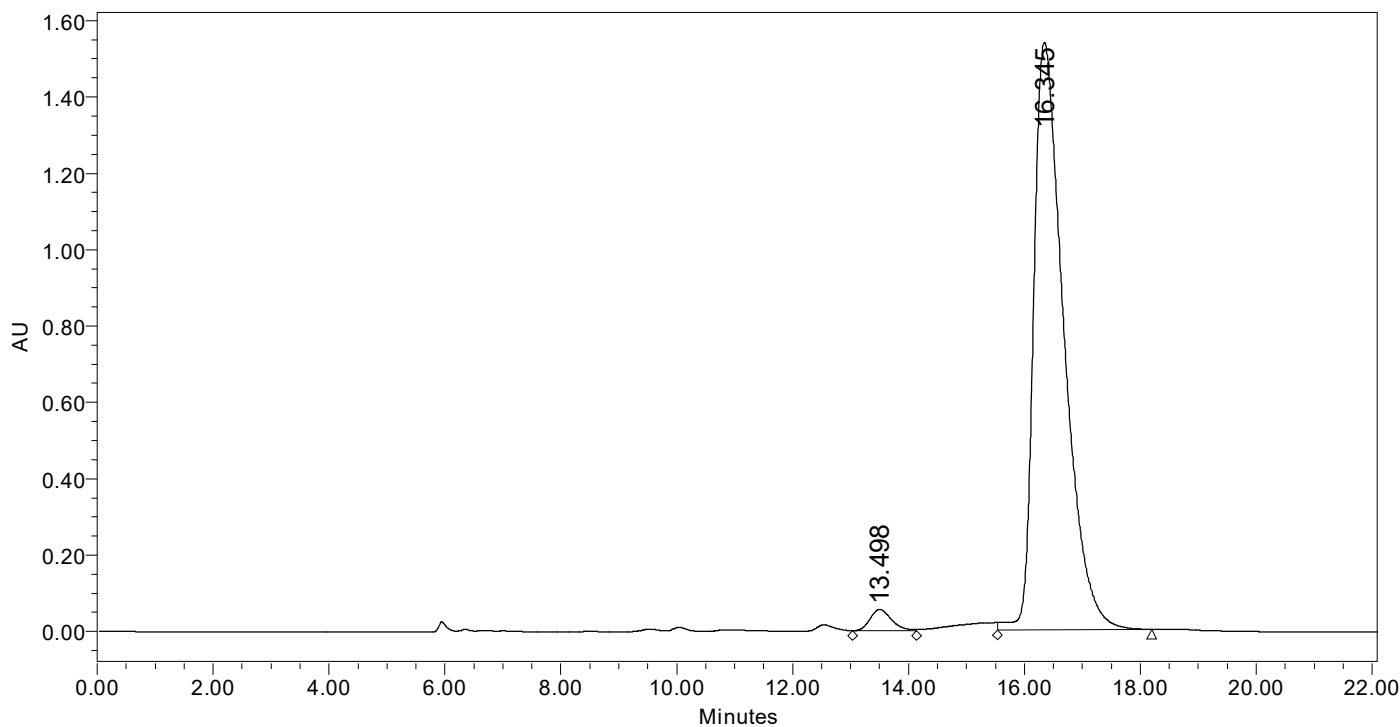
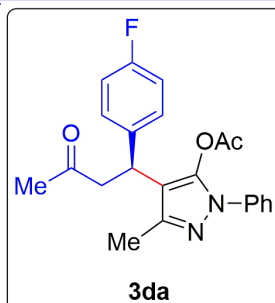
	RT	Area	% Area	Height
1	13.250	12177405	51.01	465531
2	16.197	11696466	48.99	354300

SAMPLE INFORMATION

Sample Name: PG155
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Date Acquired: 08-02-2023 14:49:25 IST
Date Processed: 21-03-2023 19:38:44 IST

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

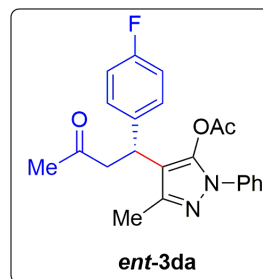


	RT	Area	% Area	Height
1	13.498	1459269	2.56	55988
2	16.345	55510958	97.44	1539264

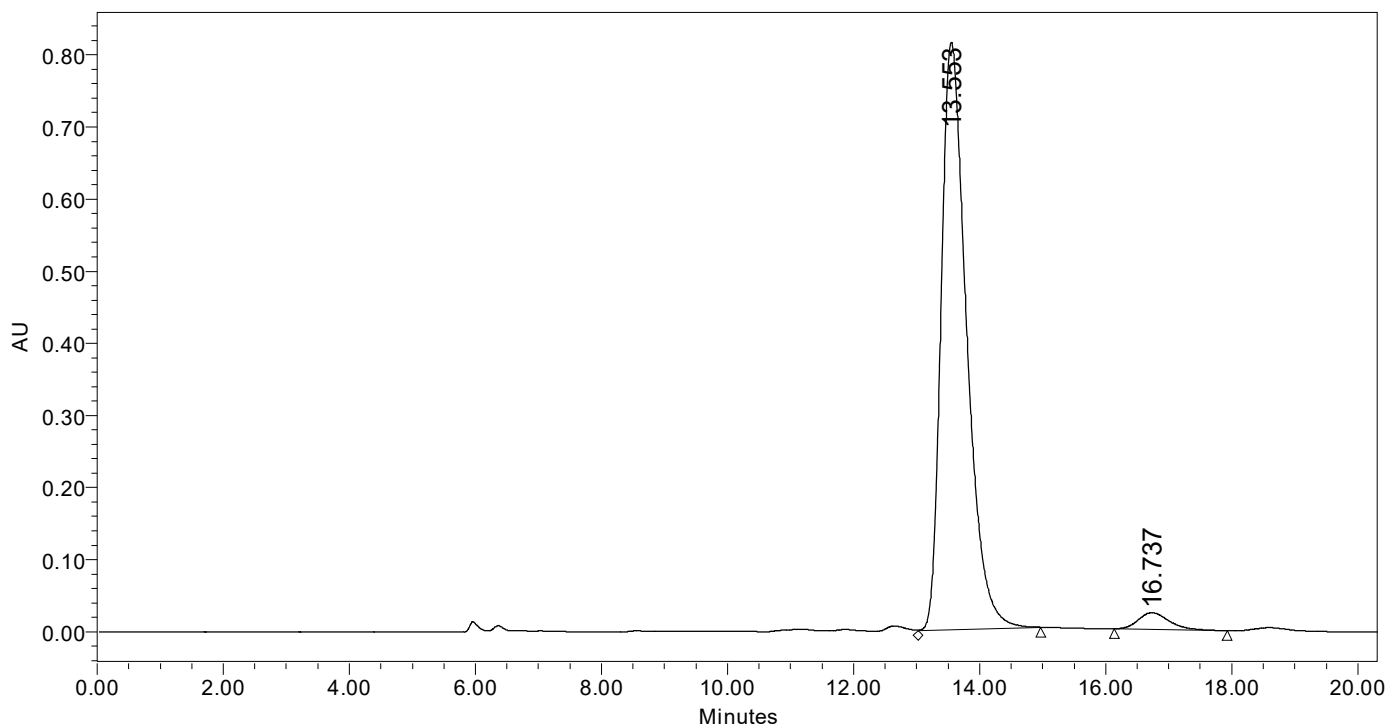
SAMPLE INFORMATION

Sample Name: PG156
Sample Type: Unknown
Vial: 1
Injection #: 6
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 08-02-2023 15:54:27 IST
Date Processed: 16-03-2023 18:56:50 IST

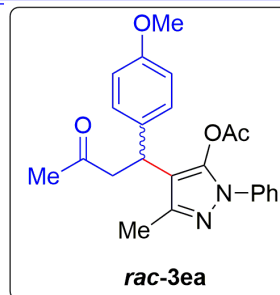


	RT	Area	% Area	Height
1	13.553	22763661	96.71	814289
2	16.737	775139	3.29	23020

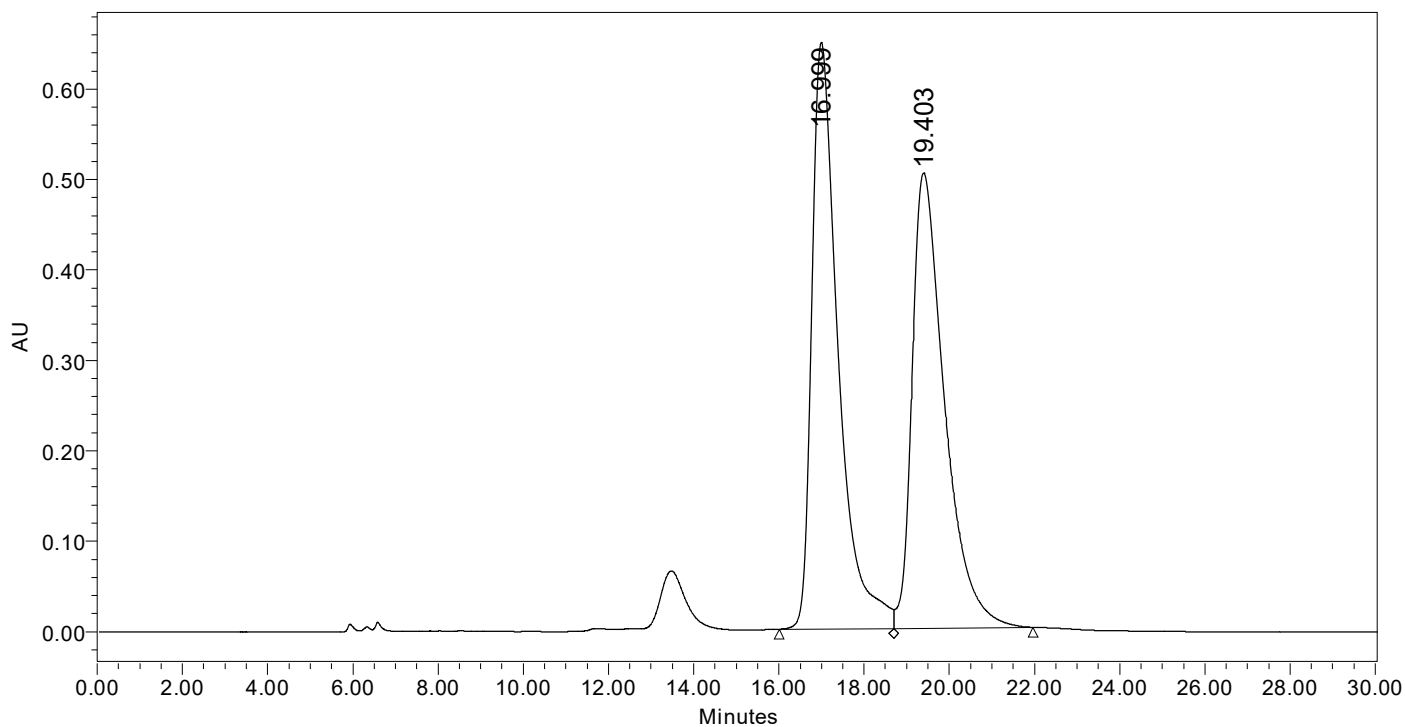
SAMPLE INFORMATION

Sample Name: PG99-ODH
Sample Type: Unknown
Vial: 1
Injection #: 7
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 28-12-2022 13:46:33 IST
Date Processed: 28-12-2022 17:29:14 IST

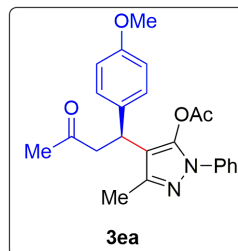


	RT	Area	% Area	Height
1	16.999	27917751	51.15	648798
2	19.403	26664037	48.85	503707

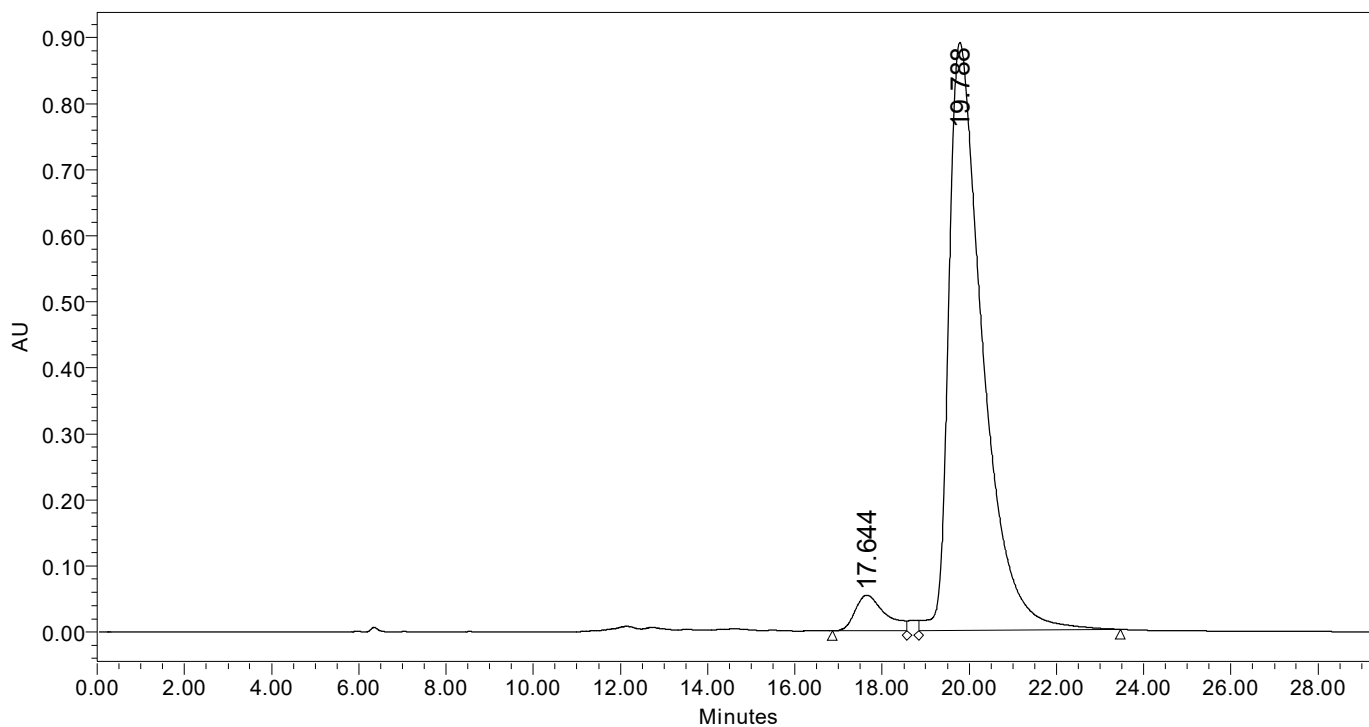
SAMPLE INFORMATION

Sample Name: PG157
Sample Type: Unknown
Vial: 1
Injection #: 7
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 09-02-2023 15:44:12 IST
Date Processed: 09-02-2023 17:17:54 IST

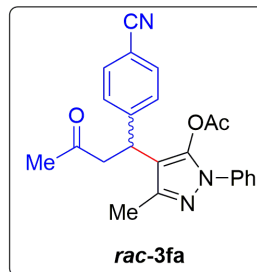


	RT	Area	% Area	Height
1	17.644	2542718	5.04	53729
2	19.788	47892578	94.96	890381

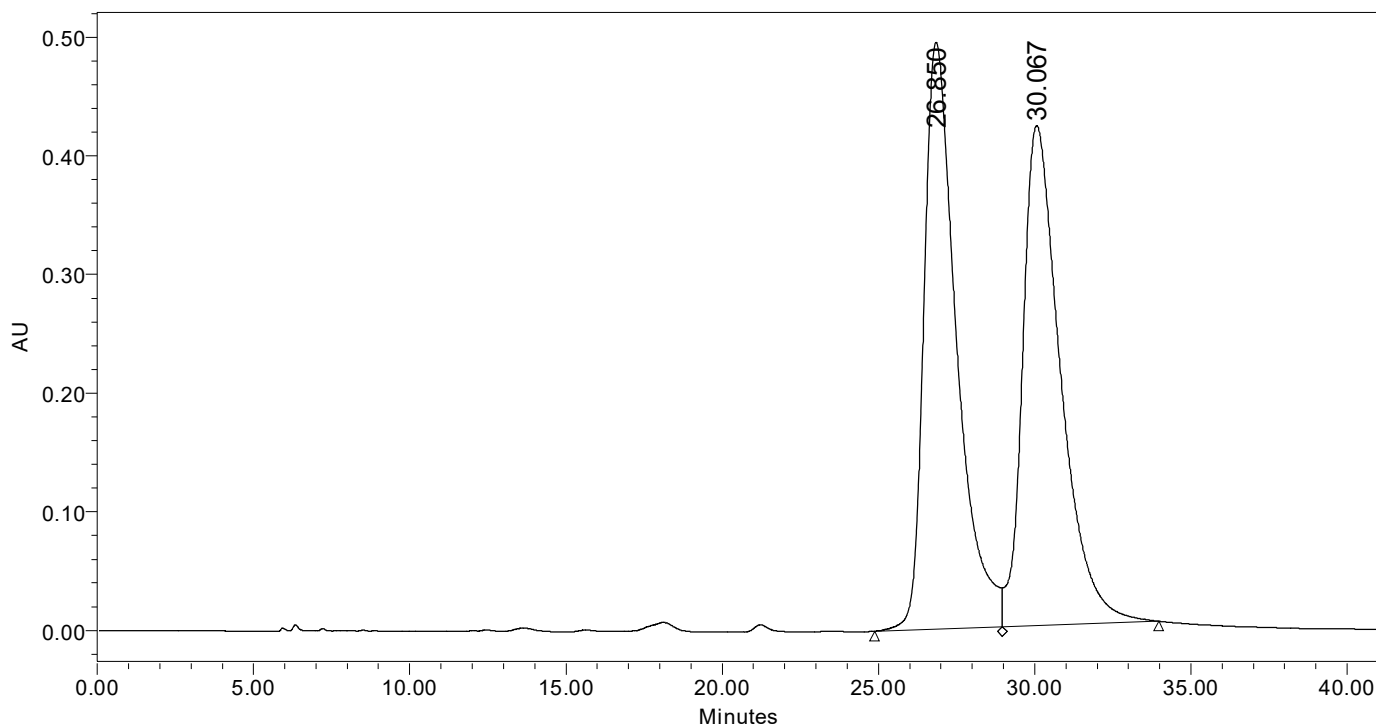
SAMPLE INFORMATION

Sample Name: PG89-ODH
Sample Type: Unknown
Vial: 1
Injection #: 8
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 30-11-2022 13:22:55 IST
Date Processed: 30-11-2022 14:04:46 IST

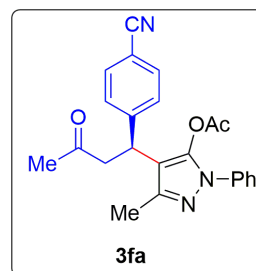


	RT	Area	% Area	Height
1	26.850	35950030	50.24	494515
2	30.067	35599754	49.76	421418

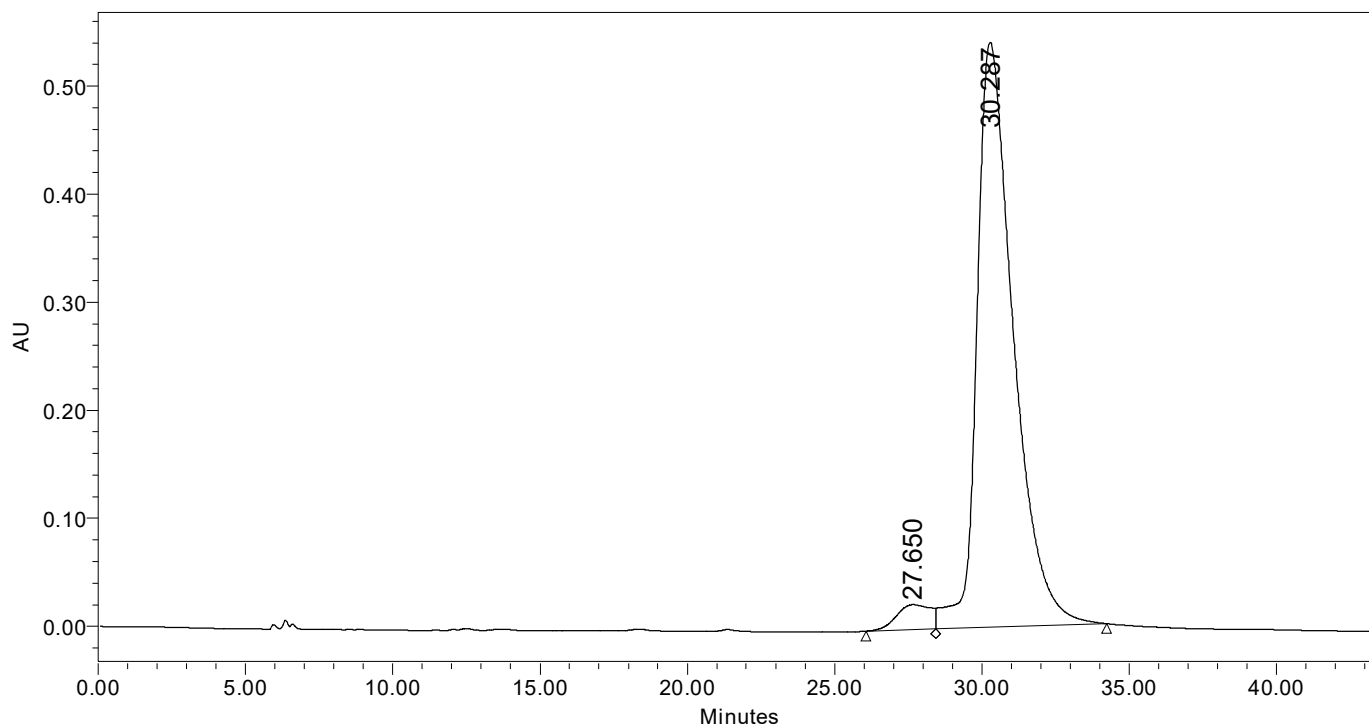
SAMPLE INFORMATION

Sample Name: PG85-ODH
Sample Type: Unknown
Vial: 1
Injection #: 6
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 30-11-2022 11:50:54 IST
Date Processed: 30-11-2022 13:31:53 IST

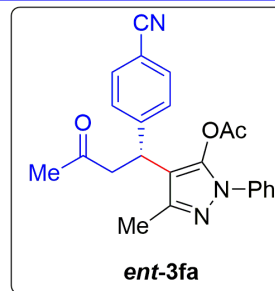


	RT	Area	% Area	Height
1	27.650	1887183	3.89	23163
2	30.287	46649969	96.11	541444

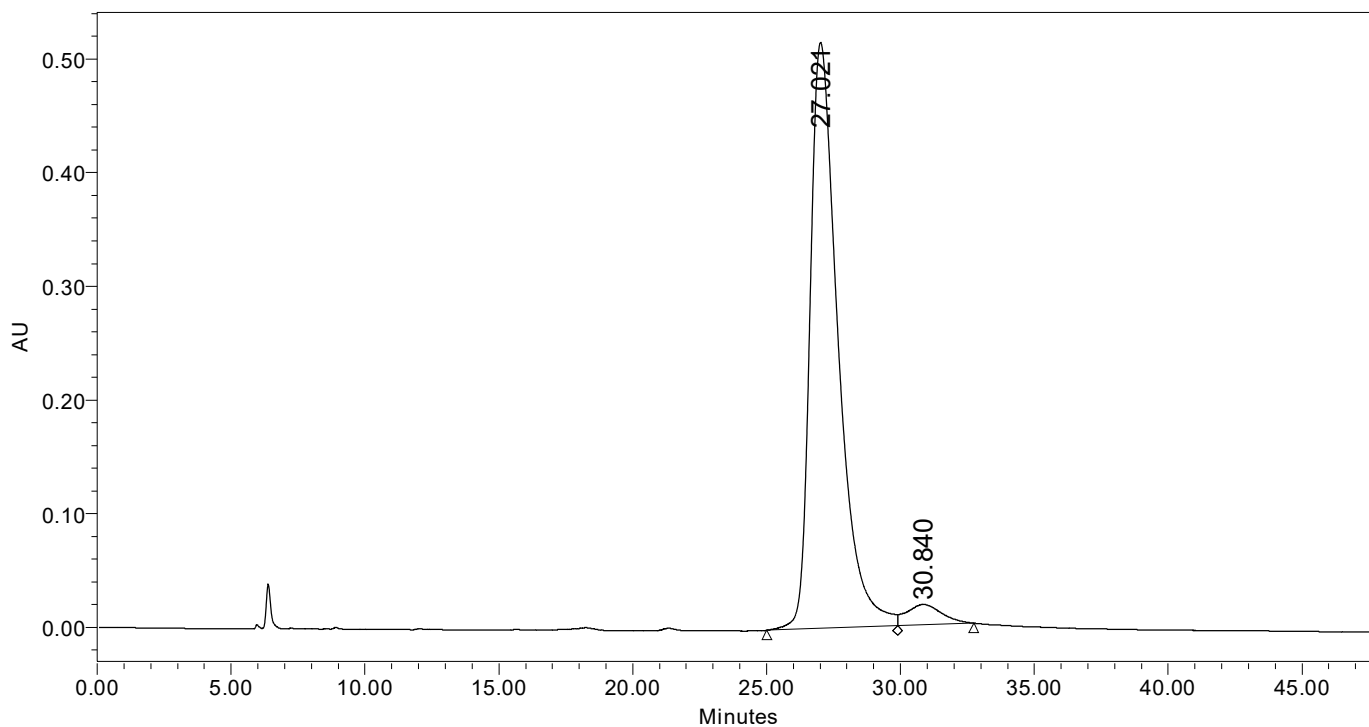
SAMPLE INFORMATION

Sample Name: PG86-ODH
Sample Type: Unknown
Vial: 1
Injection #: 7
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 30-11-2022 12:34:42 IST
Date Processed: 30-11-2022 13:33:17 IST

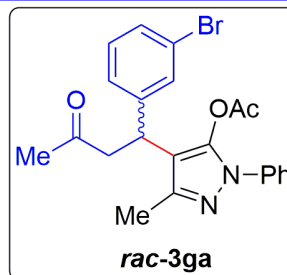


	RT	Area	% Area	Height
1	27.021	37463824	95.76	515567
2	30.840	1657709	4.24	17925

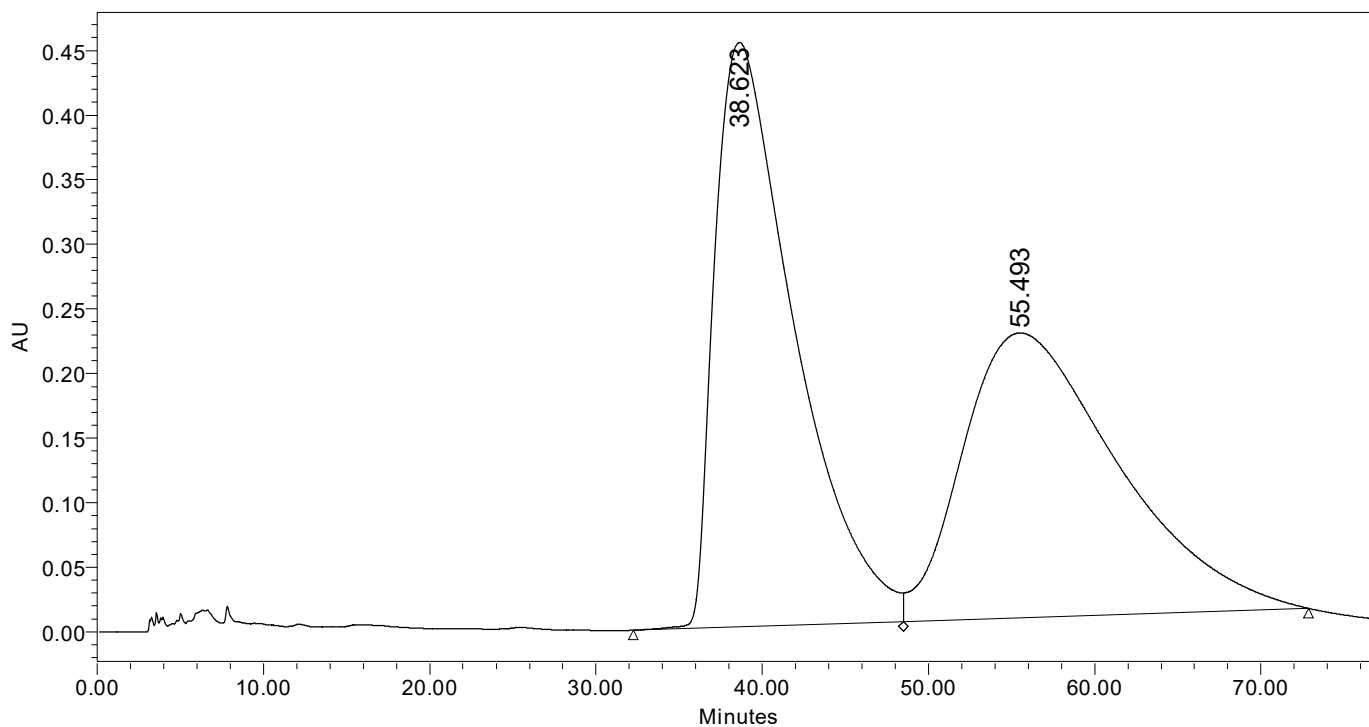
SAMPLE INFORMATION

Sample Name: PG67-68-OJH
Sample Type: Unknown
Vial: 1
Injection #: 6
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 17-11-2022 18:05:22 IST
Date Processed: 21-11-2022 15:47:30 IST



	RT	Area	% Area	Height
1	38.623	151231394	51.37	452384
2	55.493	143190385	48.63	220389

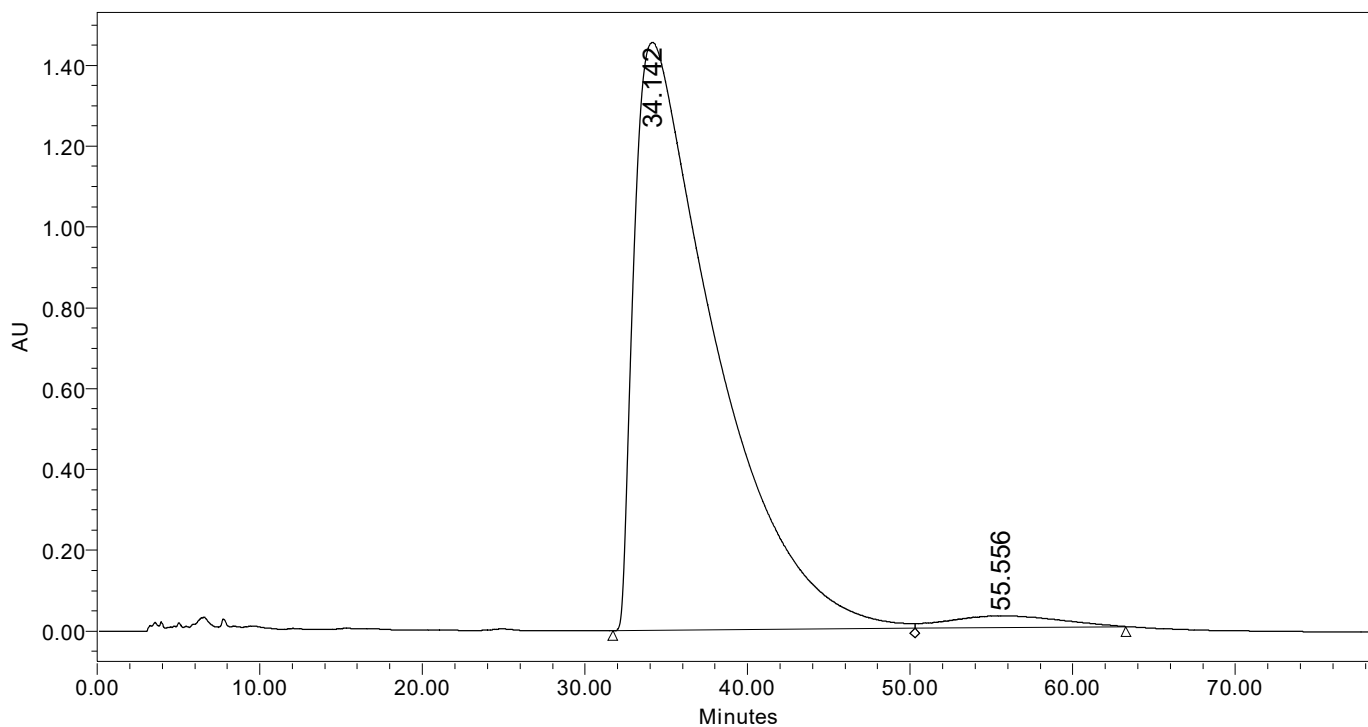
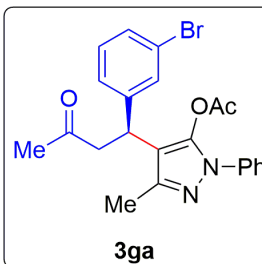
SAMPLE INFORMATION

Sample Name: PG67-OJH
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Date Acquired: 18-11-2022 14:06:59 IST
Date Processed: 21-11-2022 15:51:08 IST

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

System



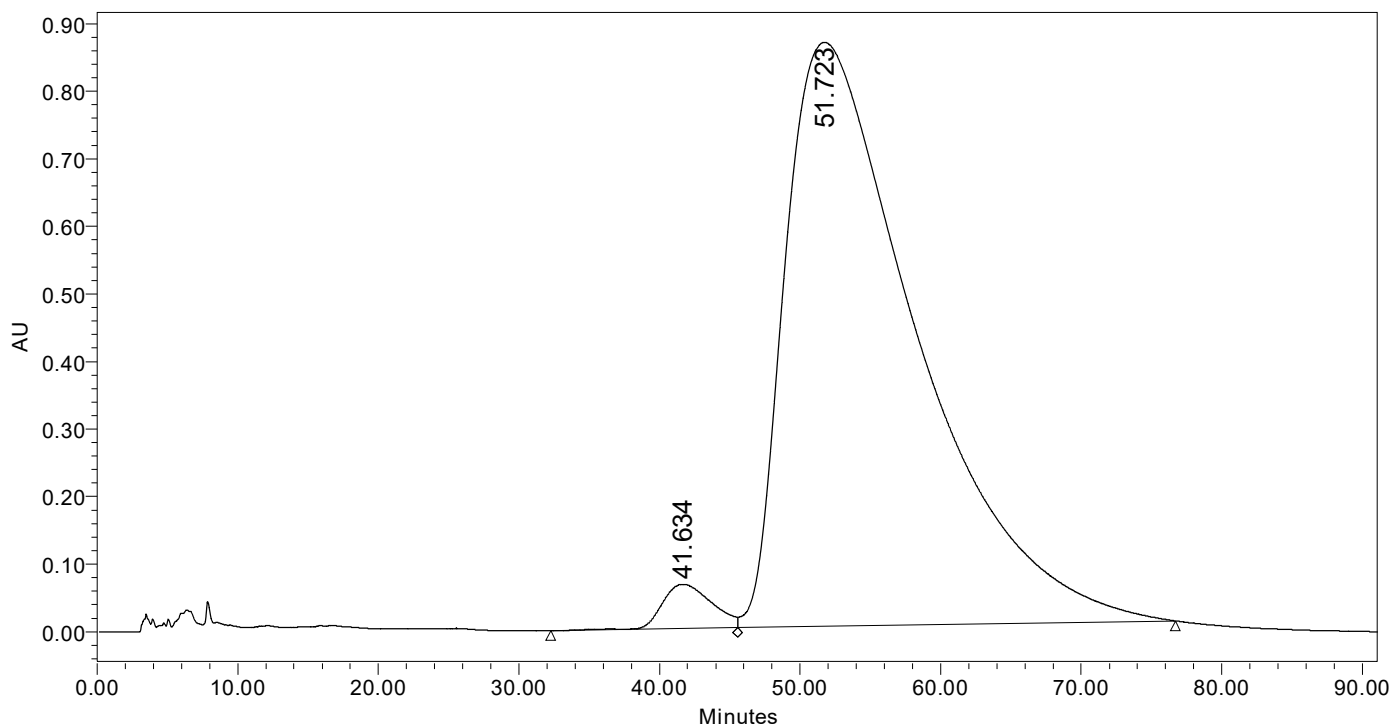
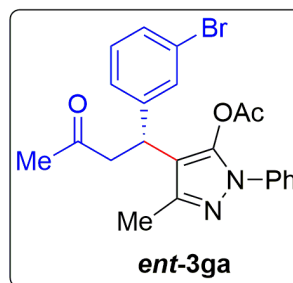
	RT	Area	% Area	Height
1	34.142	507143983	97.34	1455265
2	55.556	13840728	2.66	28942

SAMPLE INFORMATION

Sample Name: PG68-OJH
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Date Acquired: 18-11-2022 12:35:39 IST
Date Processed: 21-11-2022 15:52:14 IST

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

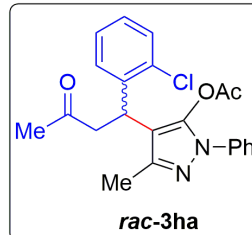


	RT	Area	% Area	Height
1	41.634	16058557	2.77	65761
2	51.723	563389567	97.23	864614

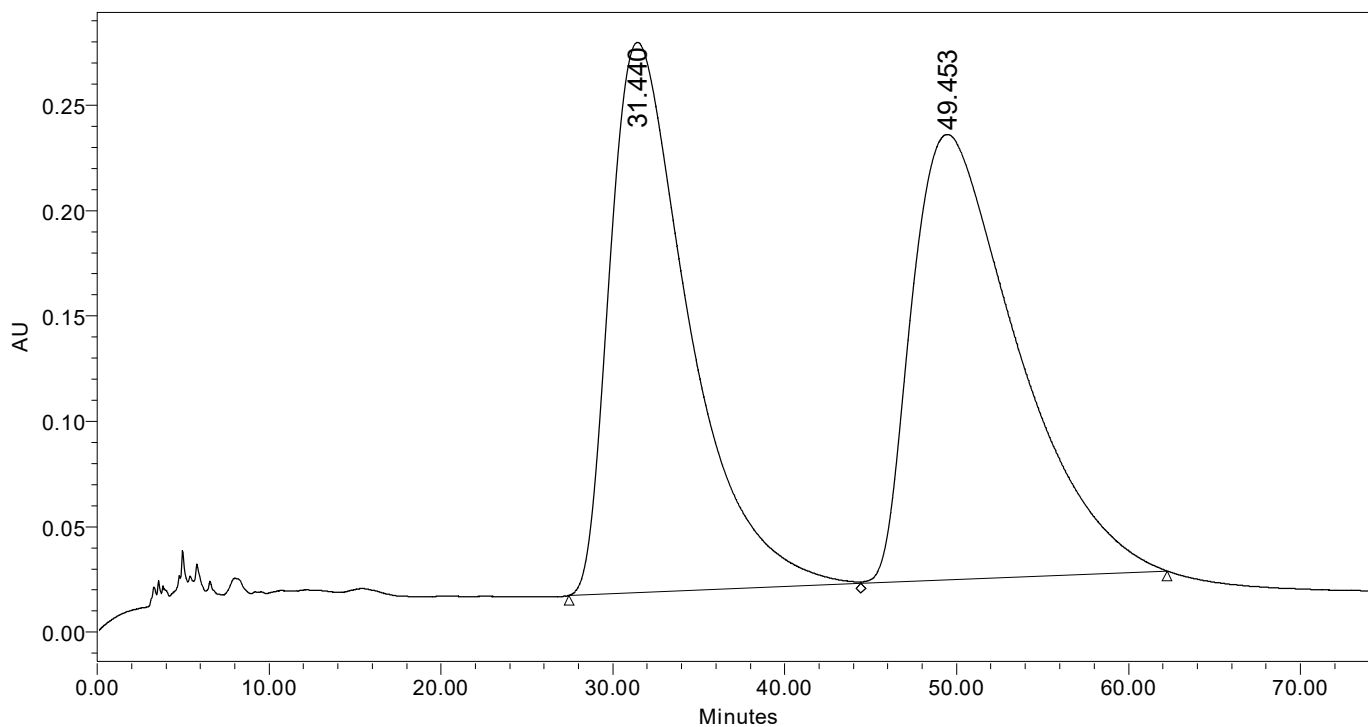
SAMPLE INFORMATION

Sample Name: PG69-70-OJH
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 17-11-2022 14:02:02 IST
Date Processed: 21-11-2022 15:53:54 IST

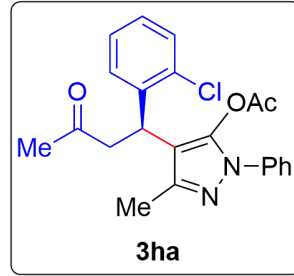


	RT	Area	% Area	Height
1	31.440	83613550	48.08	261211
2	49.453	90276211	51.92	211459

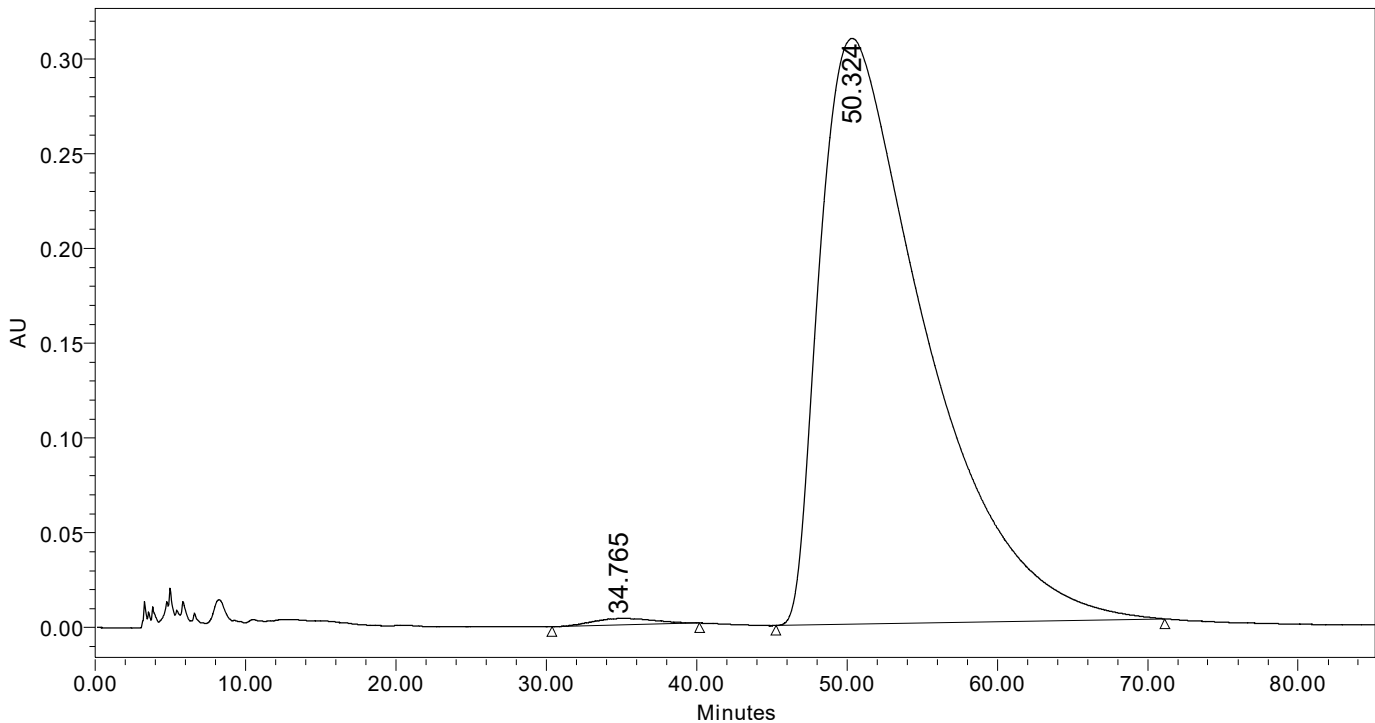
SAMPLE INFORMATION

Sample Name: PG69-OJH
Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 17-11-2022 15:16:54 IST
Date Processed: 17-11-2022 17:58:24 IST

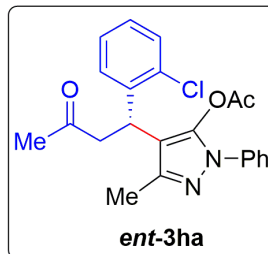


	RT	Area	% Area	Height
1	34.765	996392	0.65	3484
2	50.324	151760560	99.35	309184

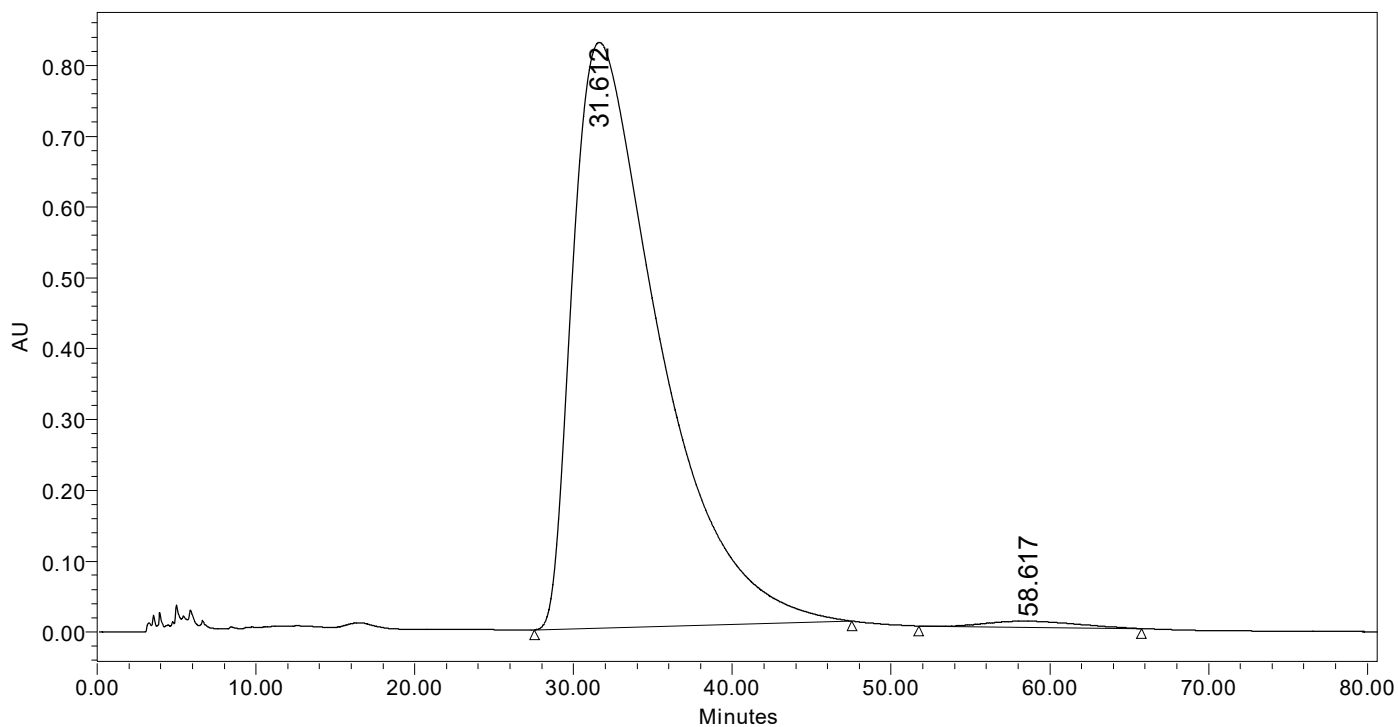
SAMPLE INFORMATION

Sample Name: PG70-OJH
Sample Type: Unknown
Vial: 1
Injection #: 5
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 17-11-2022 16:43:43 IST
Date Processed: 05-01-2023 18:07:35 IST

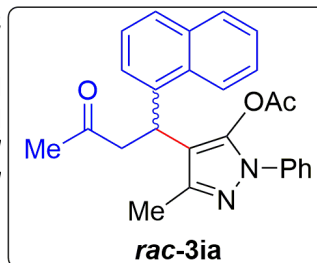


	RT	Area	% Area	Height
1	31.612	313265985	98.93	827224
2	58.617	3376038	1.07	8527

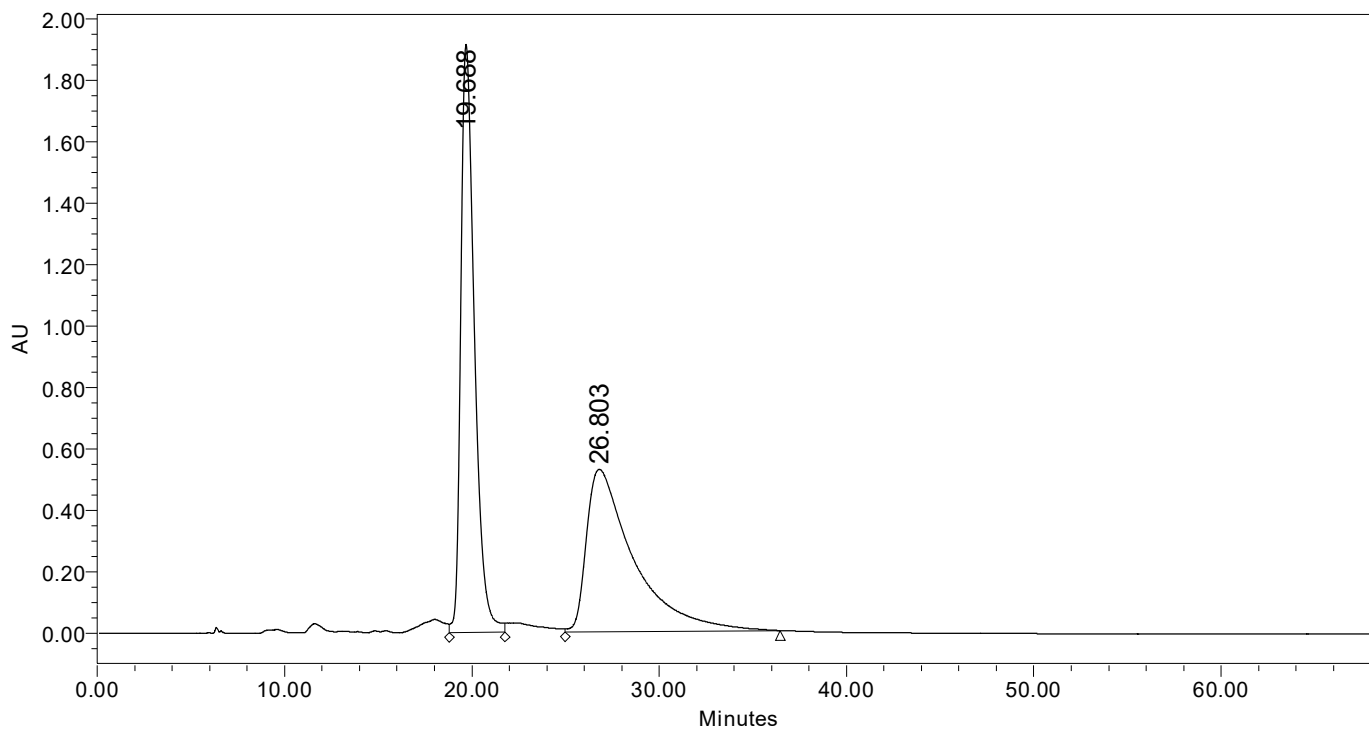
SAMPLE INFORMATION

Sample Name: PG94-ODH
Sample Type: Unknown
Vial: 1
Injection #: 6
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 01-12-2022 13:30:50 IST
Date Processed: 05-01-2023 18:11:25 IST

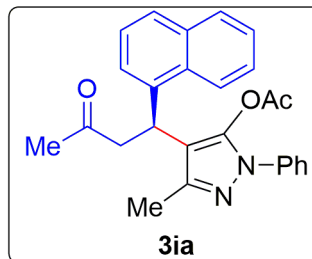


	RT	Area	% Area	Height
1	19.688	97264760	51.30	1914310
2	26.803	92347787	48.70	528374

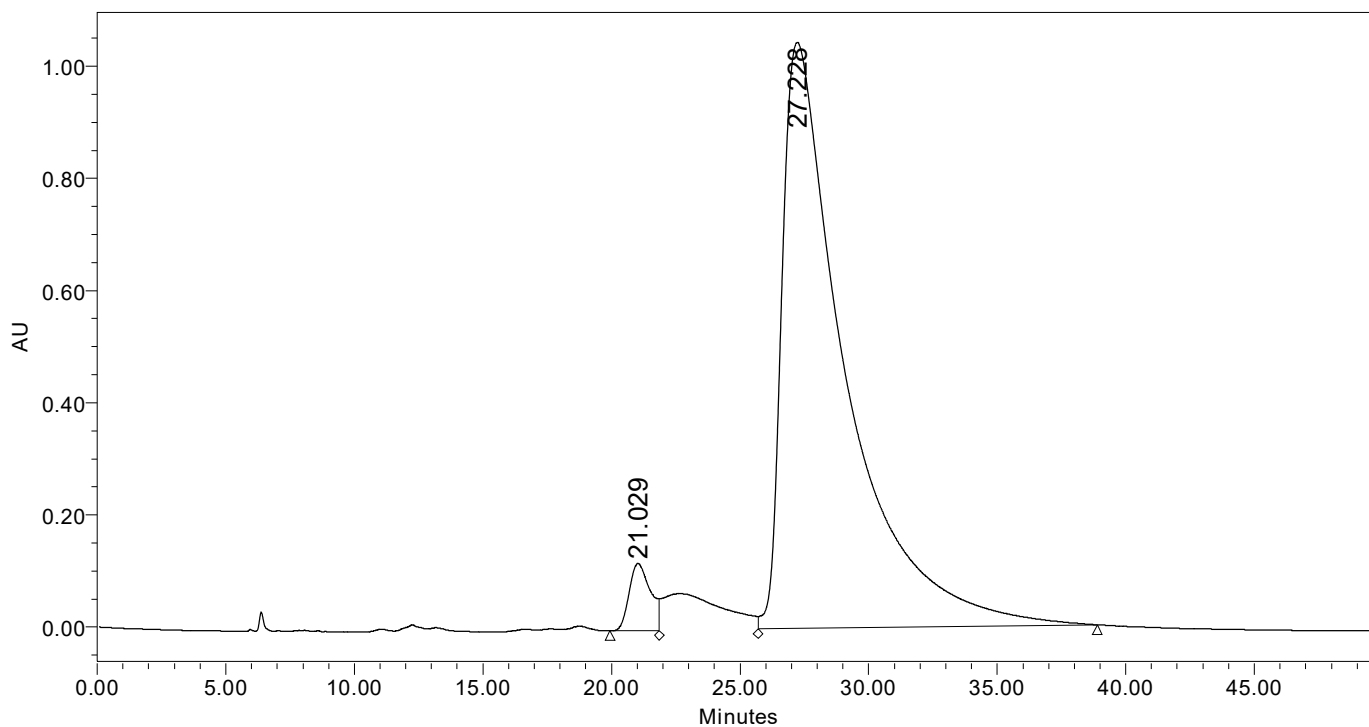
SAMPLE INFORMATION

Sample Name: PG71-ODH
Sample Type: Unknown
Vial: 1
Injection #: 8
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 18-11-2022 18:33:41 IST
Date Processed: 05-01-2023 18:13:29 IST

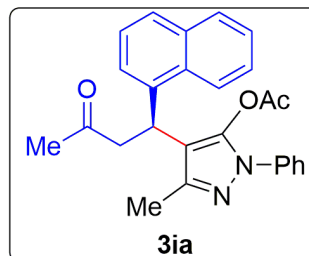


	RT	Area	% Area	Height
1	21.029	6931970	3.72	119451
2	27.228	179338232	96.28	1045594

SAMPLE INFORMATION

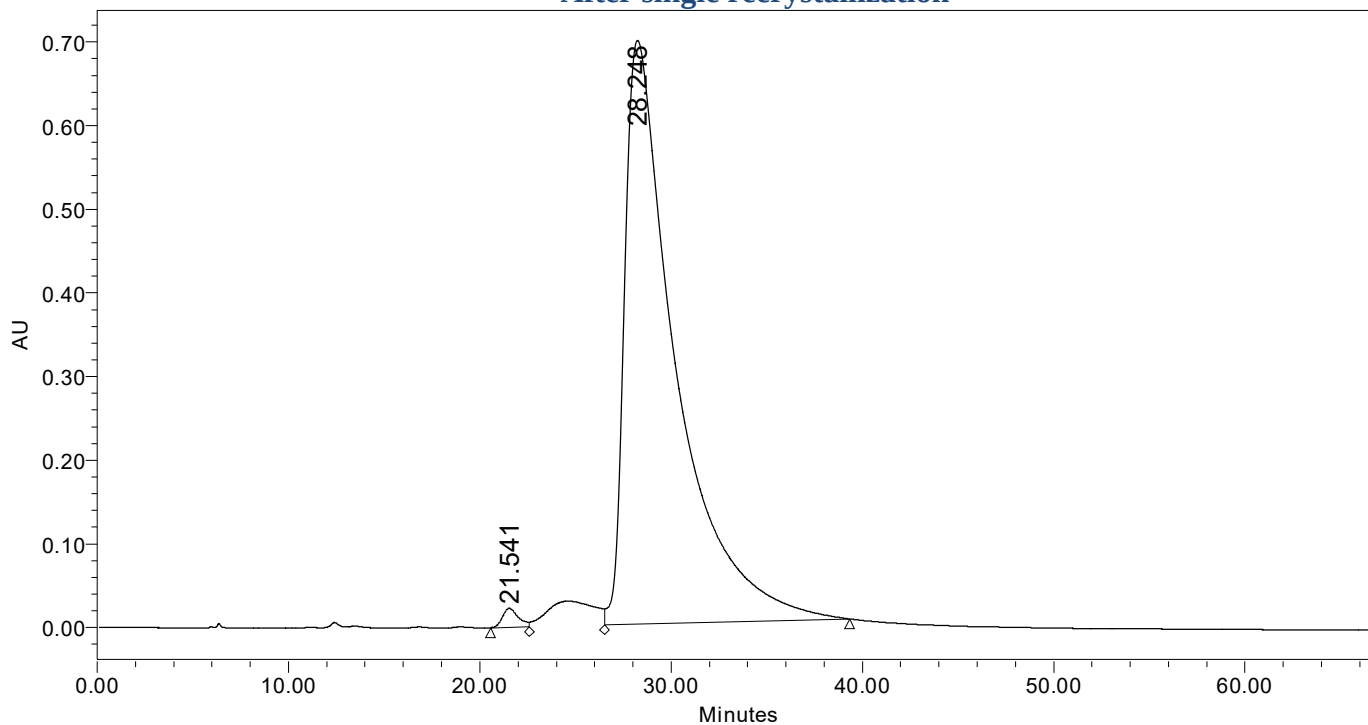
Sample Name: PG71-CRYSTAL
Sample Type: Unknown
Vial: 1
Injection #: 5
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 10-01-2023 12:52:40 IST
Date Processed: 10-01-2023 16:47:34 IST

After single recrystallization

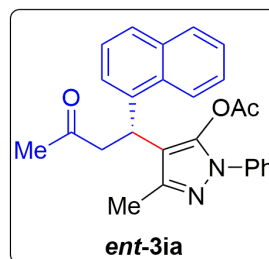


	RT	Area	% Area	Height
1	21.541	1321728	1.01	22629
2	28.248	129626219	98.99	698126

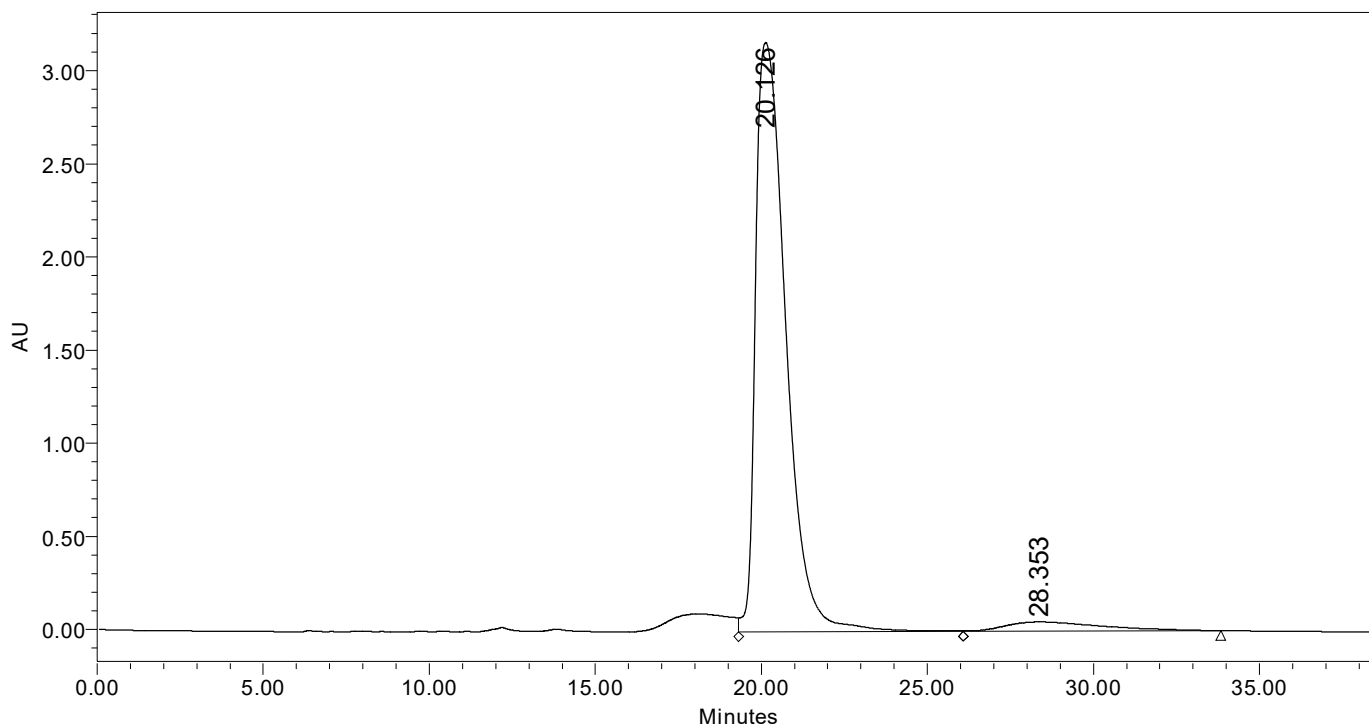
SAMPLE INFORMATION

Sample Name: PG72-ODH
Sample Type: Unknown
Vial: 1
Injection #: 6
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 18-11-2022 17:16:34 IST
Date Processed: 05-01-2023 18:14:30 IST

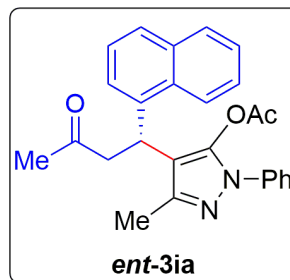


	RT	Area	% Area	Height
1	20.126	200627154	95.30	3163869
2	28.353	9884915	4.70	49079

SAMPLE INFORMATION

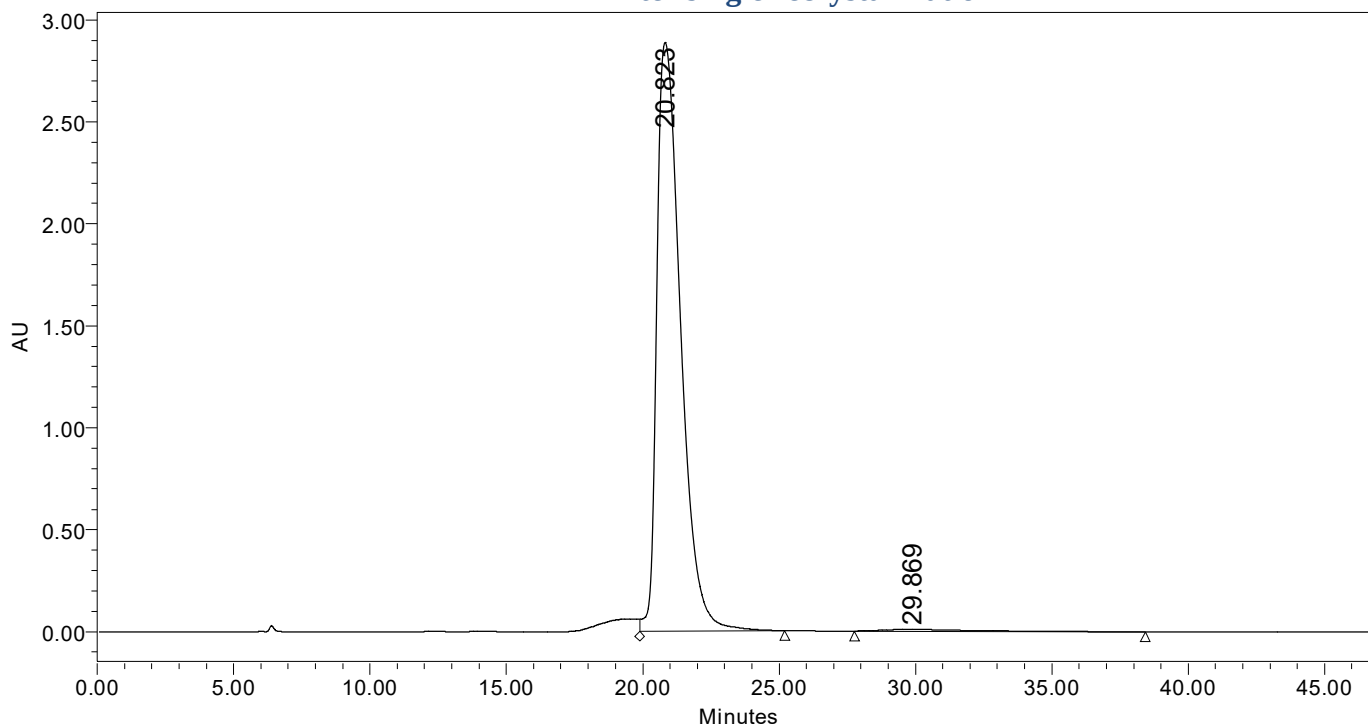
Sample Name: PG72-CRYSTAL
Sample Type: Unknown
Vial: 1
Injection #: 6
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 10-01-2023 14:04:25 IST
Date Processed: 10-01-2023 16:48:15 IST

After single recrystallization

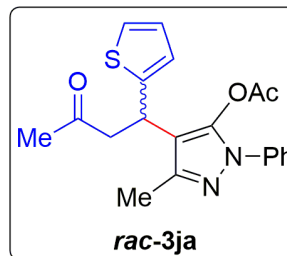


	RT	Area	% Area	Height
1	20.823	175328032	98.88	2887774
2	29.869	1979149	1.12	8729

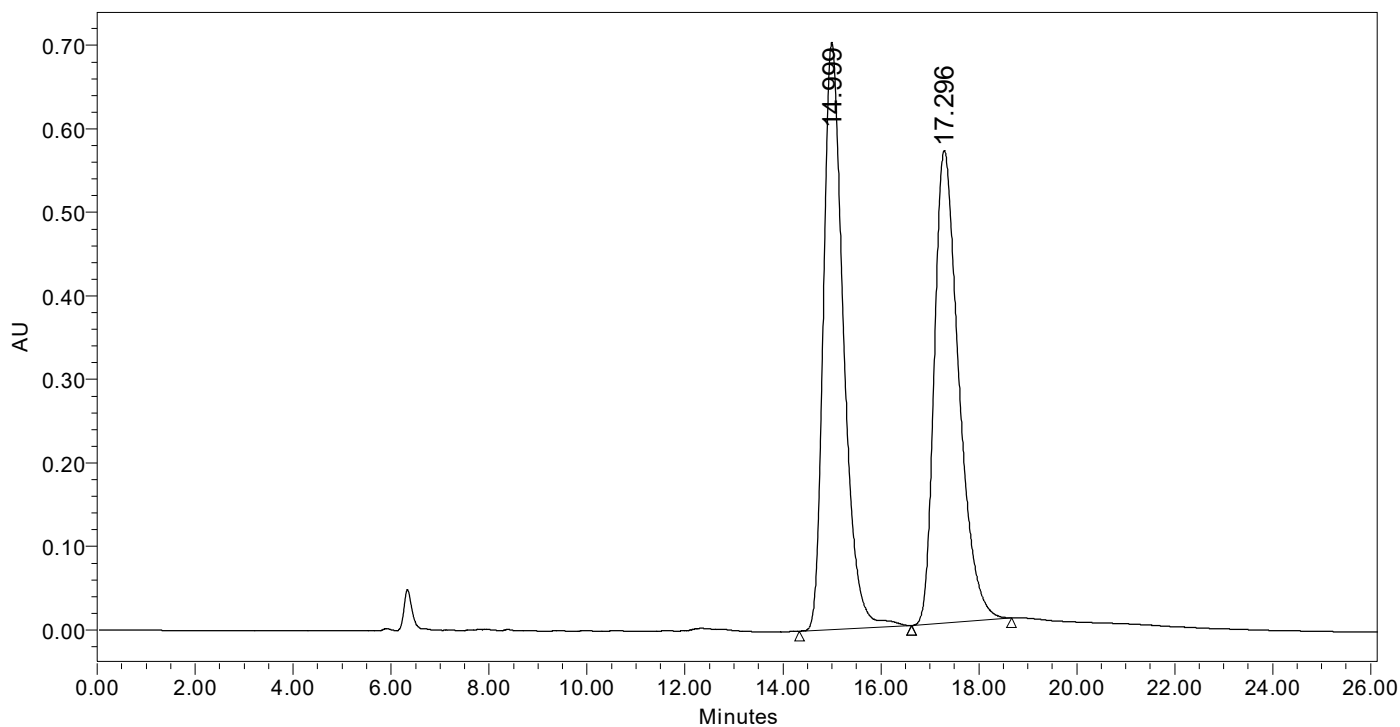
SAMPLE INFORMATION

Sample Name: PG90-ODH
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 29-11-2022 18:18:57 IST
Date Processed: 29-11-2022 18:45:29 IST

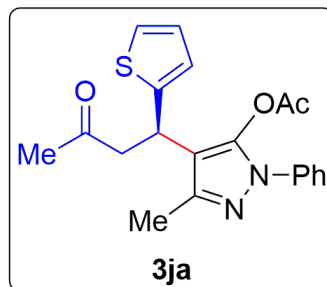


	RT	Area	% Area	Height
1	14.999	20014798	50.51	703234
2	17.296	19614171	49.49	566125

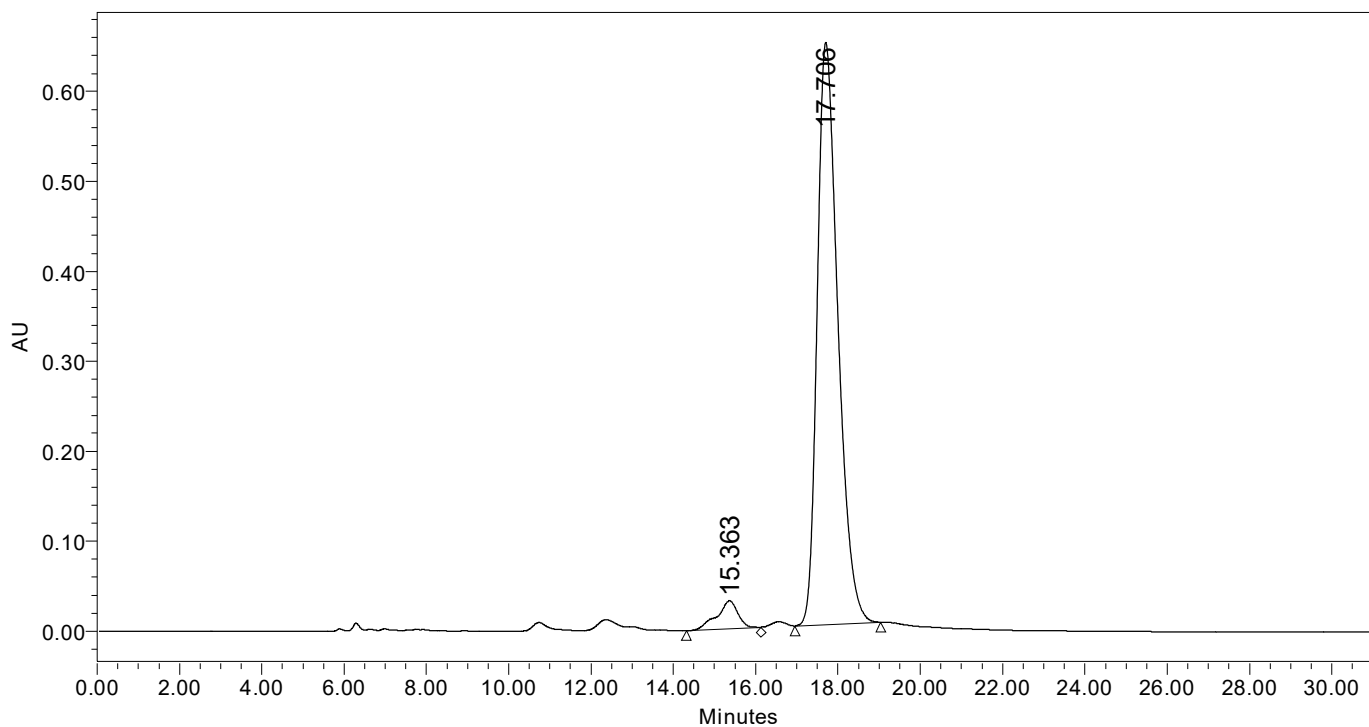
SAMPLE INFORMATION

Sample Name: PG61-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 11-11-2022 11:23:34 IST
Date Processed: 29-11-2022 18:44:27 IST

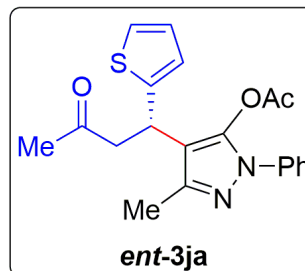


	RT	Area	% Area	Height
1	15.363	1115204	4.70	31144
2	17.706	22595514	95.30	647379

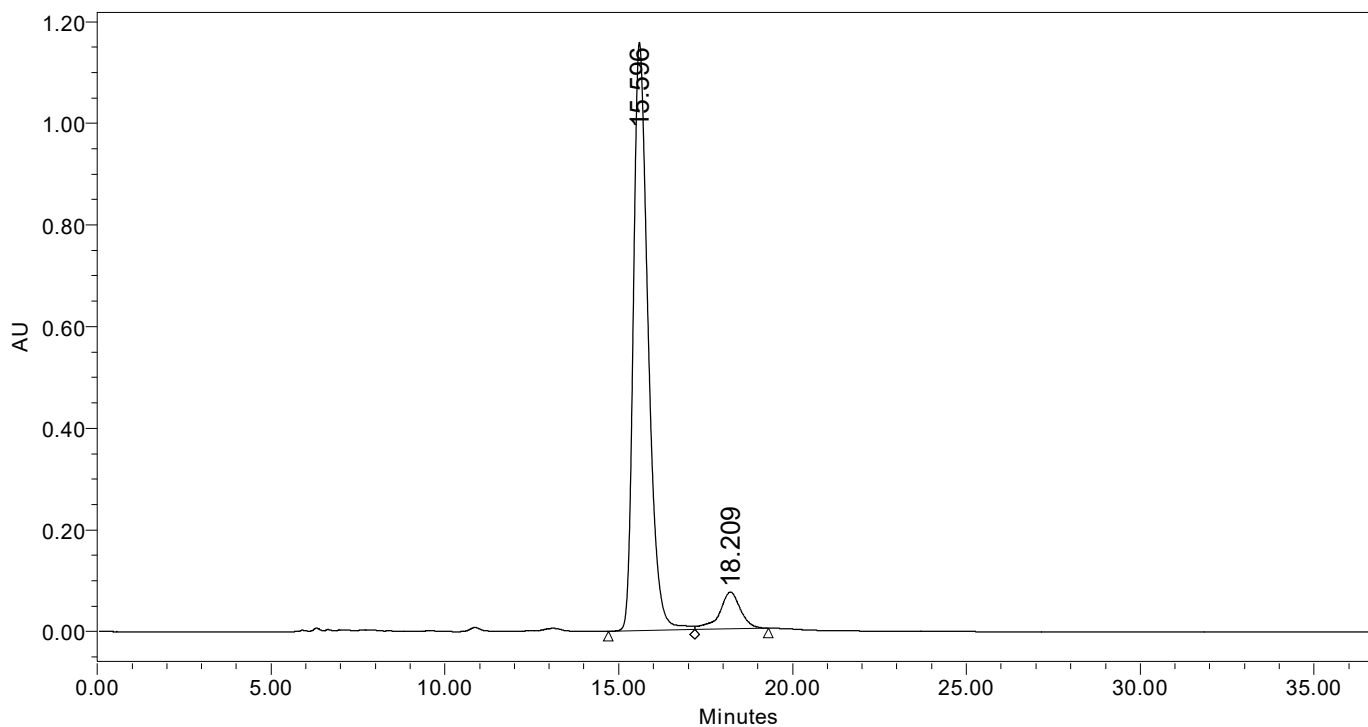
SAMPLE INFORMATION

Sample Name: PG62-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 11-11-2022 11:55:00 IST
Date Processed: 29-11-2022 18:43:23 IST

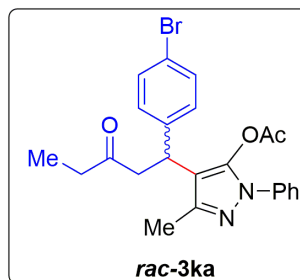


	RT	Area	% Area	Height
1	15.596	34189213	91.75	1157872
2	18.209	3072533	8.25	72535

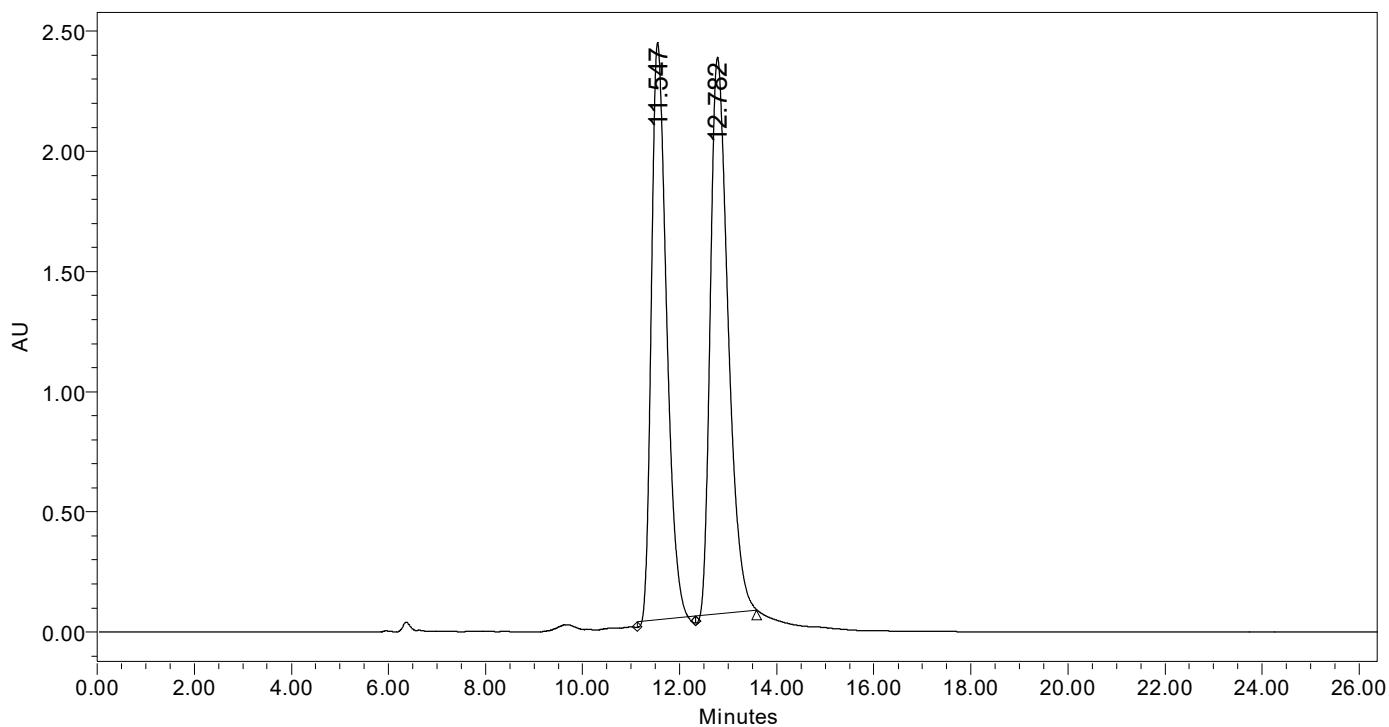
SAMPLE INFORMATION

Sample Name: PG73-74-ODH
Sample Type: Unknown
Vial: 1
Injection #: 5
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 21-11-2022 17:52:34 IST
Date Processed: 21-11-2022 18:19:56 IST

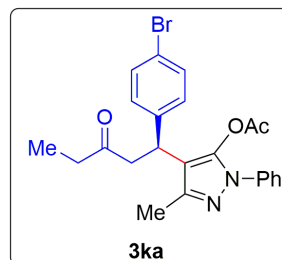


	RT	Area	% Area	Height
1	11.547	52298184	47.06	2402773
2	12.782	58838386	52.94	2314849

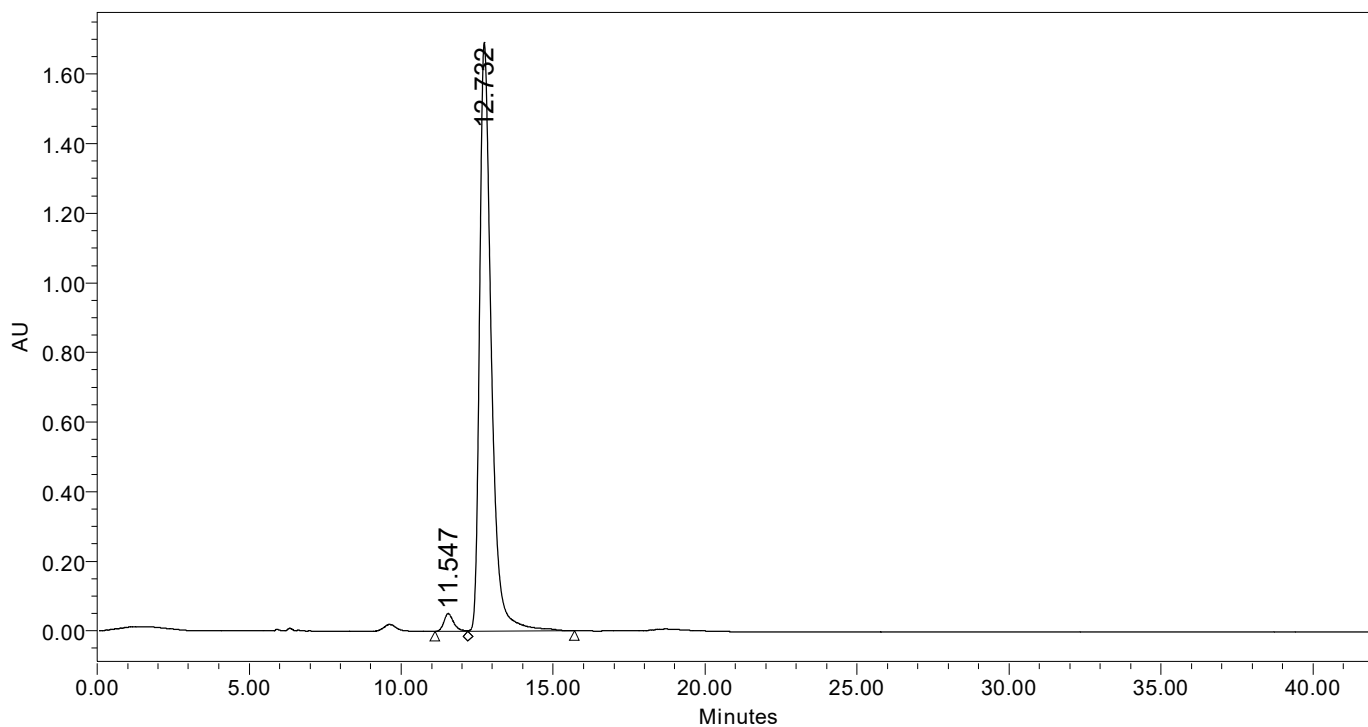
SAMPLE INFORMATION

Sample Name: PG73-ODH
Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 21-11-2022 17:09:04 IST
Date Processed: 21-11-2022 18:20:51 IST

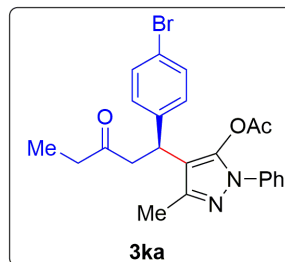


	RT	Area	% Area	Height
1	11.547	1137990	2.44	50589
2	12.732	45443346	97.56	1692533

SAMPLE INFORMATION

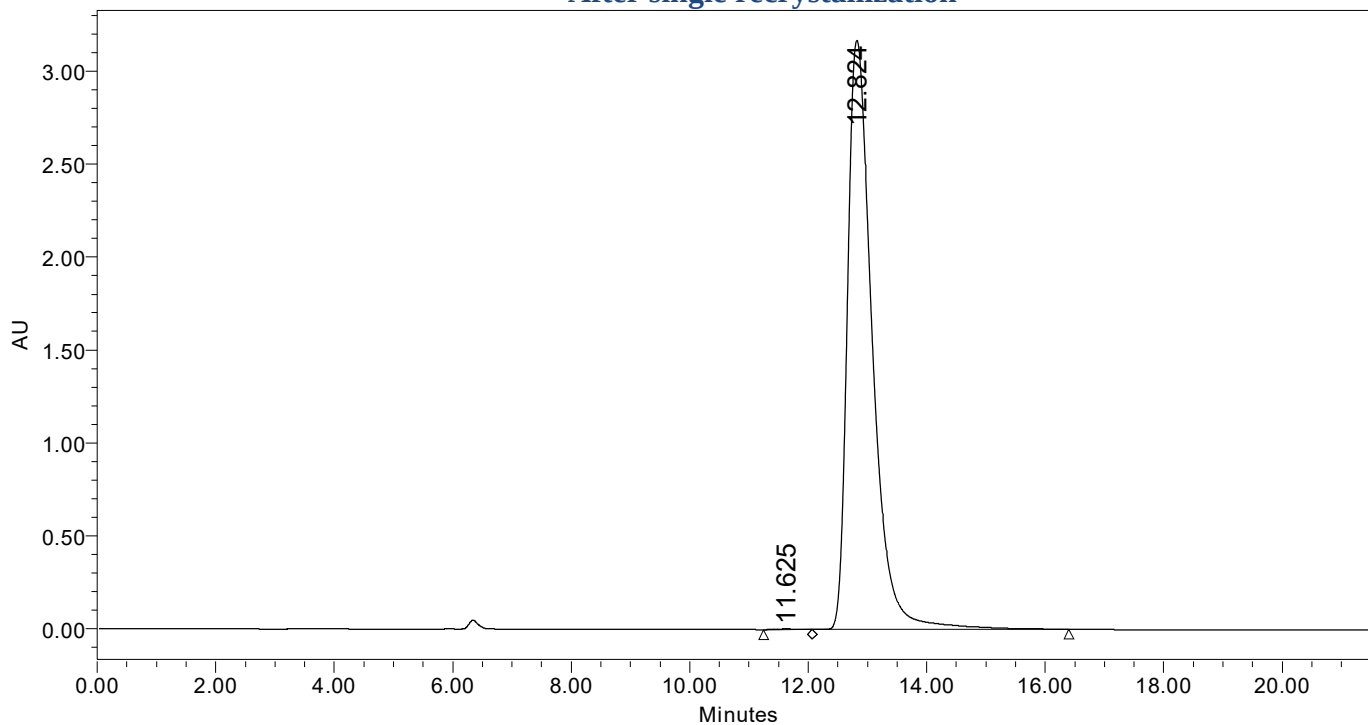
Sample Name: PG73-CRYSTAL
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 10-01-2023 11:23:27 IST
Date Processed: 10-01-2023 16:45:48 IST

After single recrystallization

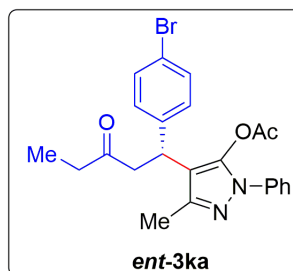


	RT	Area	% Area	Height
1	11.625	70652	0.08	3386
2	12.824	92497025	99.92	3170912

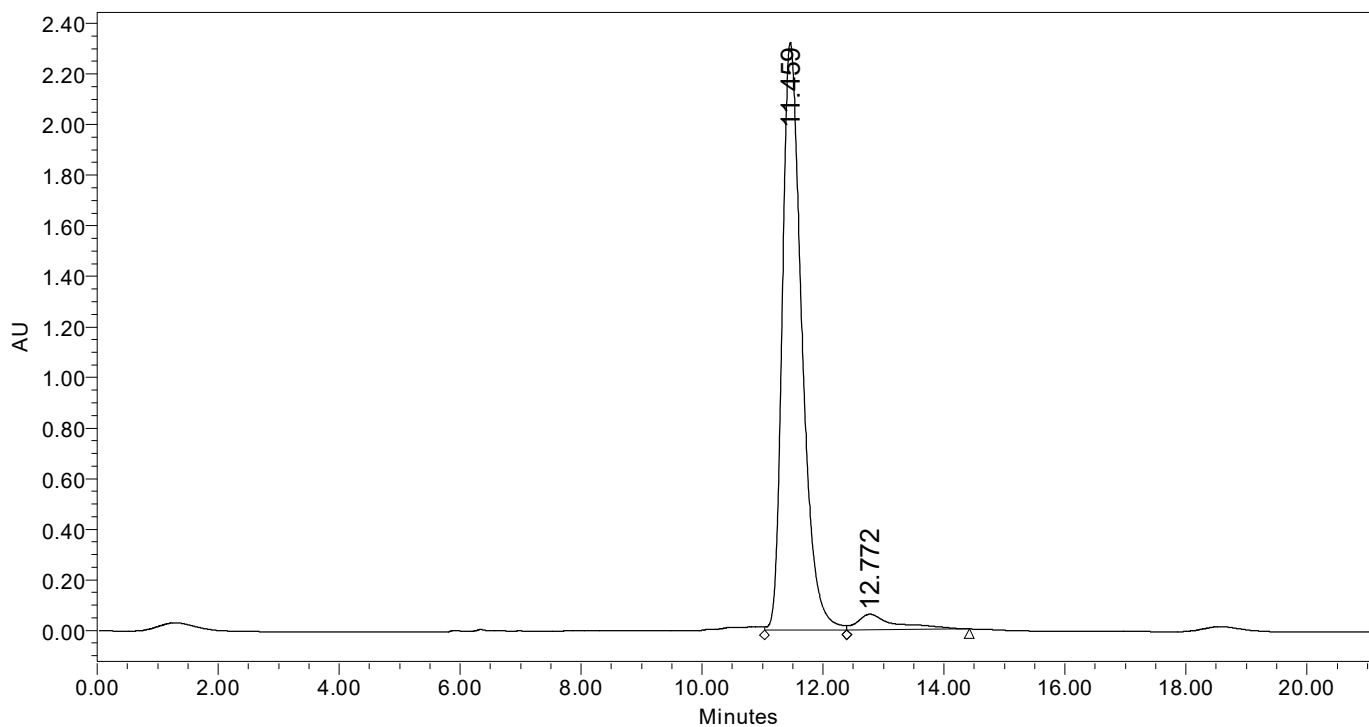
SAMPLE INFORMATION

Sample Name: PG74-ODH
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 21-11-2022 16:47:28 IST
Date Processed: 21-11-2022 18:21:58 IST

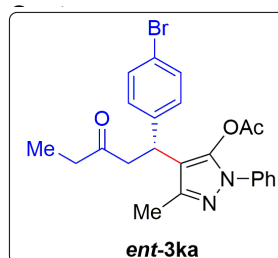


	RT	Area	% Area	Height
1	11.459	52228139	95.15	2323576
2	12.772	2659323	4.85	61064

SAMPLE INFORMATION

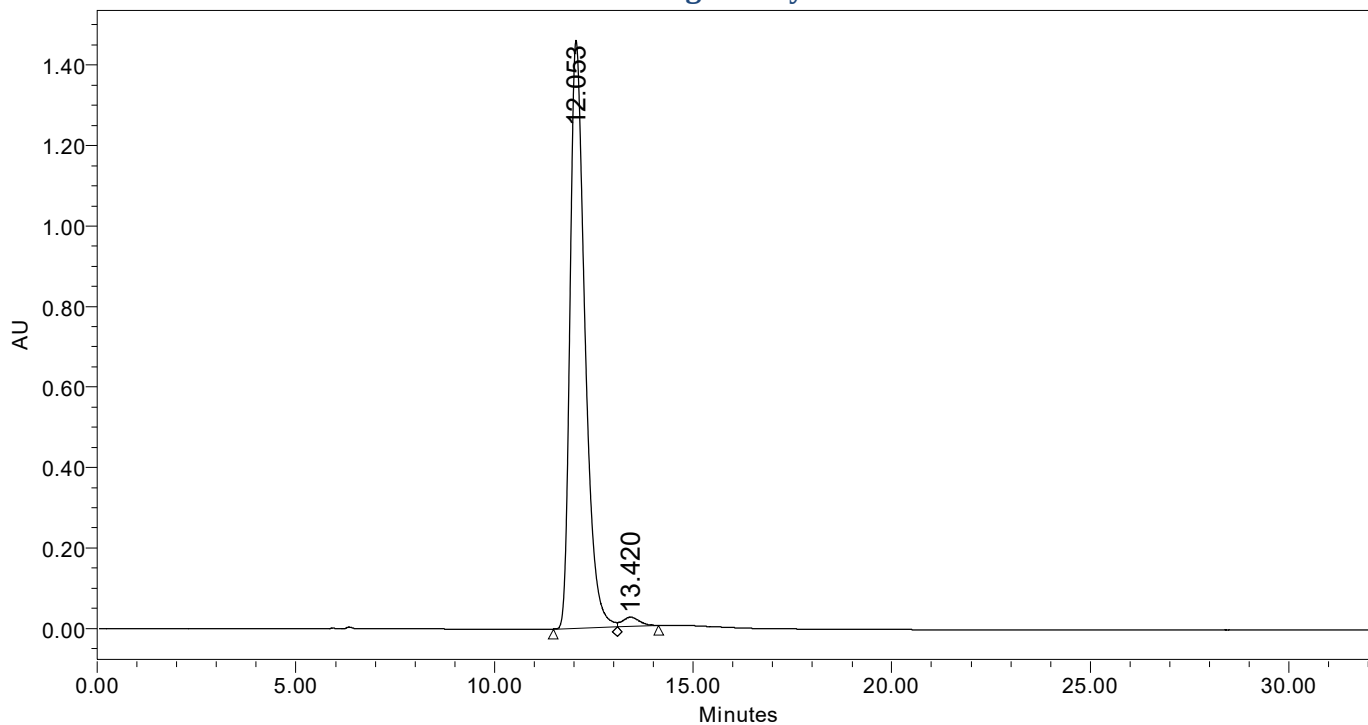
Sample Name: PG74-CRYSTAL
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 10-01-2023 11:45:31 IST
Date Processed: 10-01-2023 16:46:40 IST

After single recrystallization

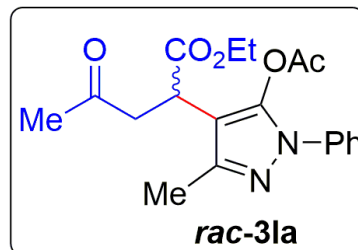


	RT	Area	% Area	Height
1	12.053	38089922	98.23	1461076
2	13.420	685749	1.77	22829

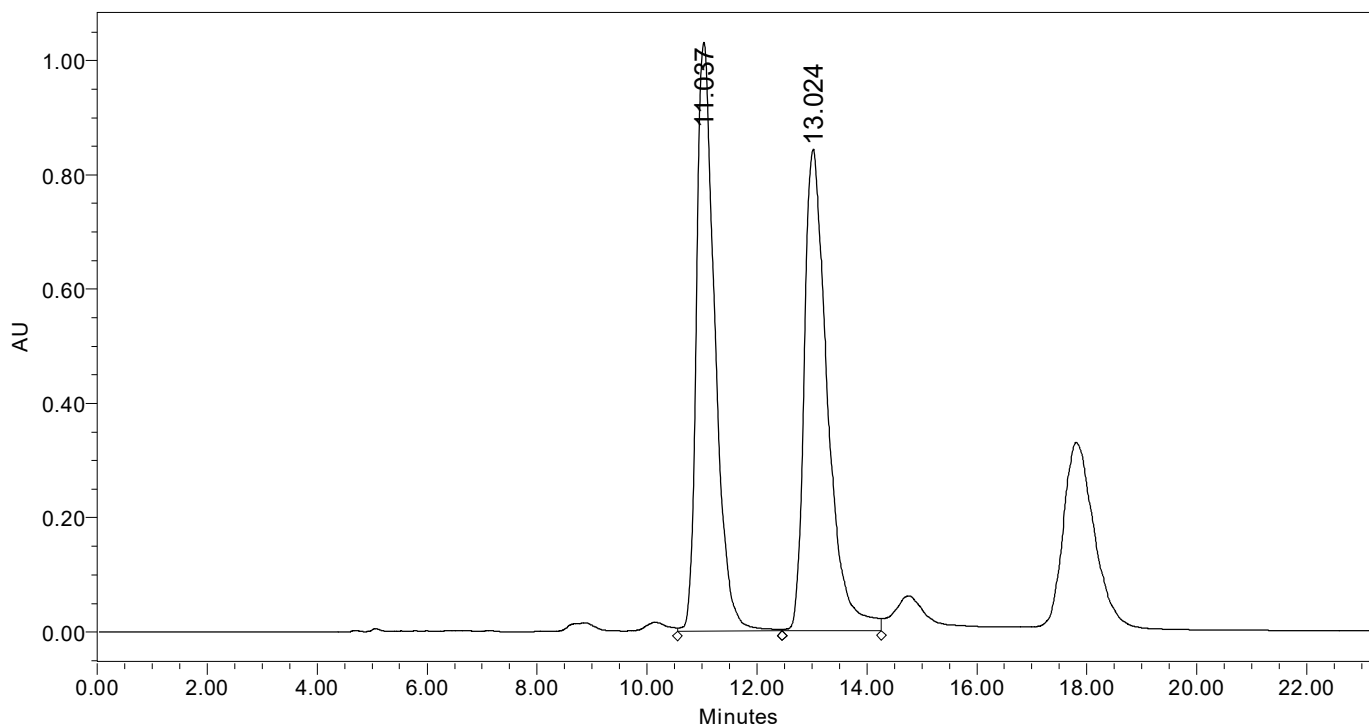
SAMPLE INFORMATION

Sample Name: PD16-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 5
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 19-10-2022 17:16:14 IST
Date Processed: 05-01-2023 18:03:44 IST

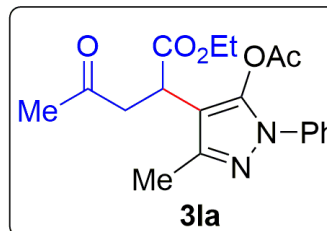


	RT	Area	% Area	Height
1	11.037	23992096	49.30	1030252
2	13.024	24677237	50.70	842260

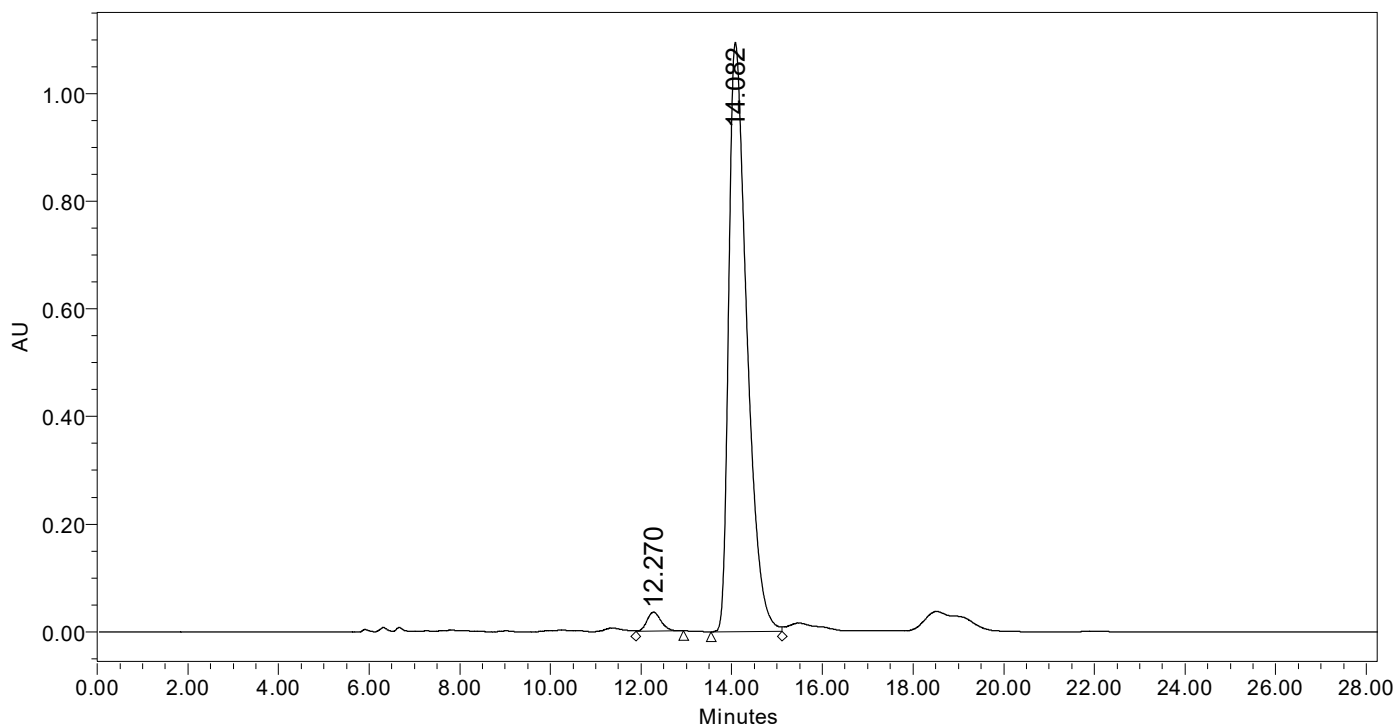
SAMPLE INFORMATION

Sample Name: PG46-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 8
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 28-10-2022 15:55:34 IST
Date Processed: 28-10-2022 16:23:08 IST

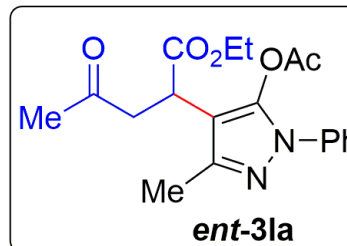


	RT	Area	% Area	Height
1	12.270	767204	2.46	35629
2	14.082	30453488	97.54	1095596

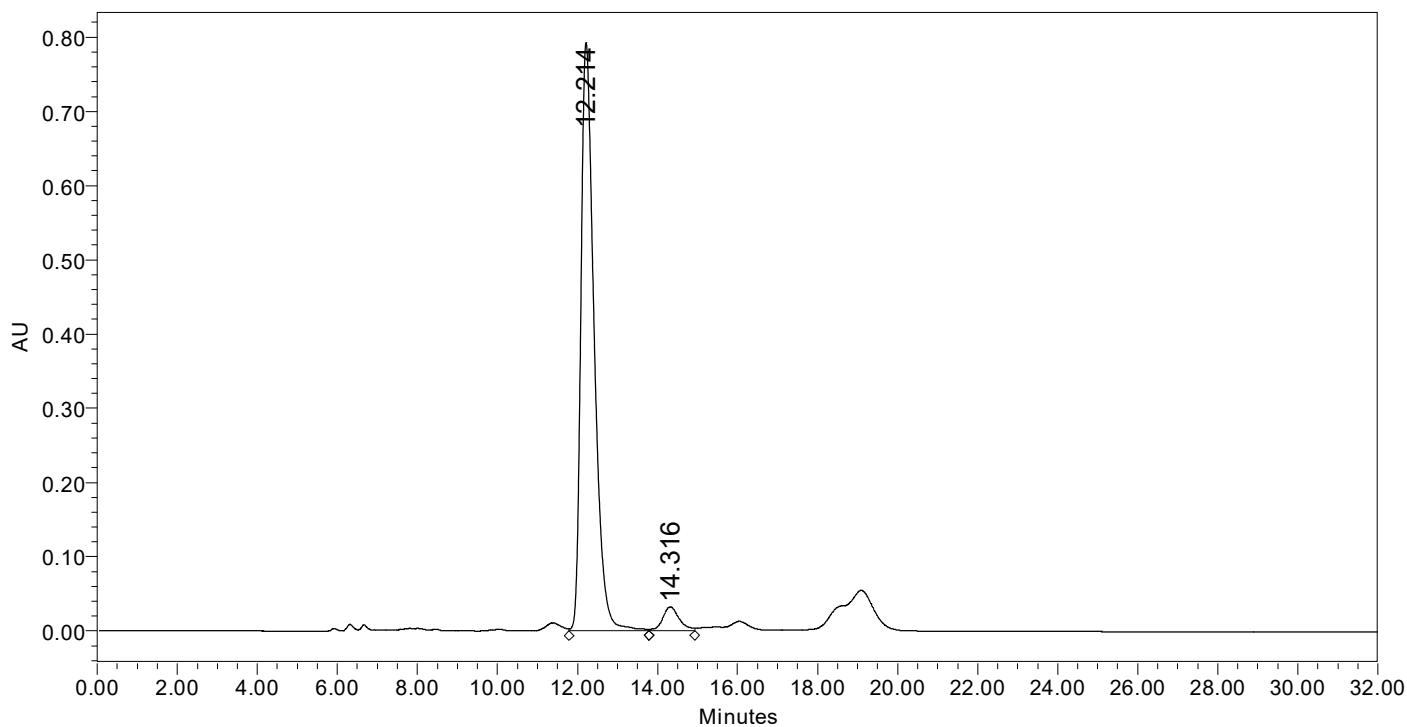
SAMPLE INFORMATION

Sample Name: PG47-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 10
Injection Volume: 5.00 ul
Run Time: 120.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 28-10-2022 16:51:04 IST
Date Processed: 28-10-2022 17:24:05 IST

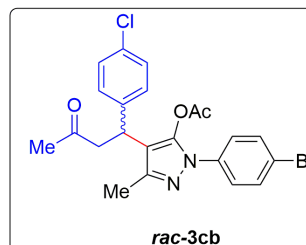


	RT	Area	% Area	Height
1	12.214	18248661	95.32	792879
2	14.316	896587	4.68	31713

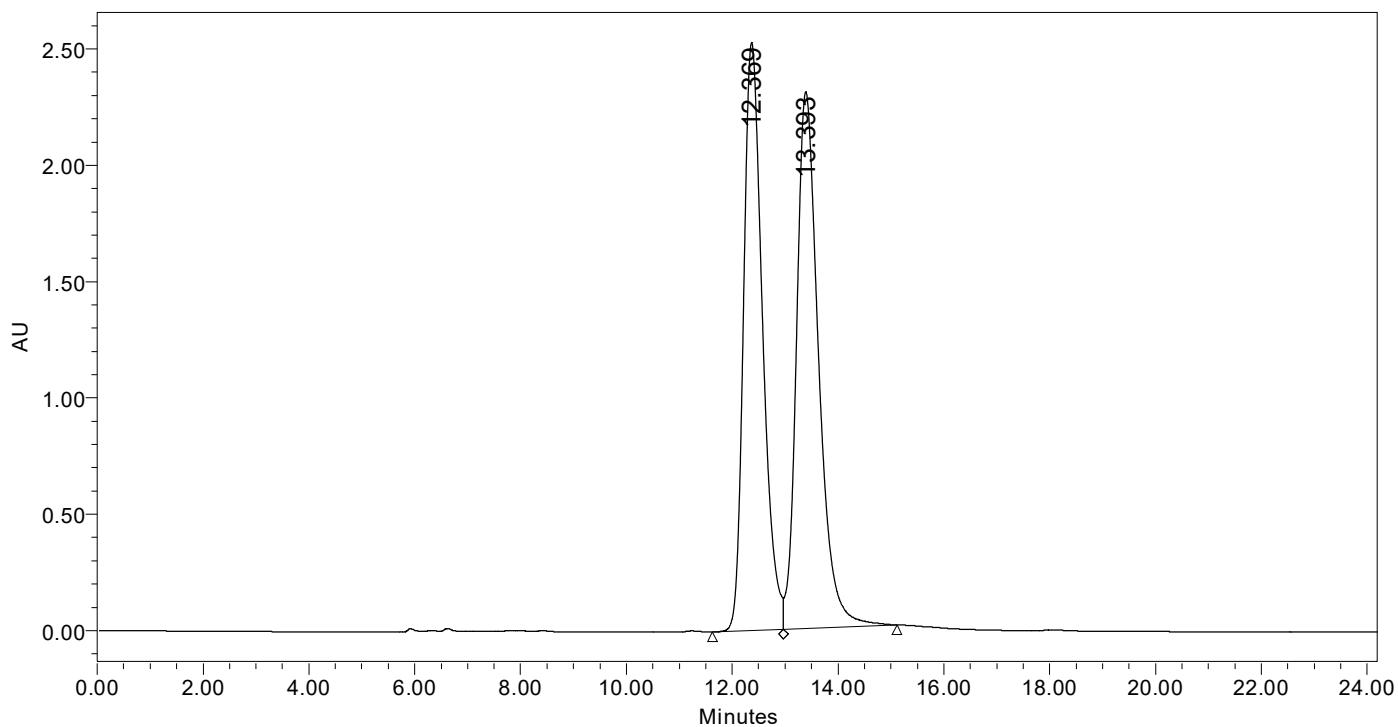
SAMPLE INFORMATION

Sample Name: AKD-640-ODH
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 02-12-2022 16:31:34 IST
Date Processed: 02-12-2022 18:04:00 IST

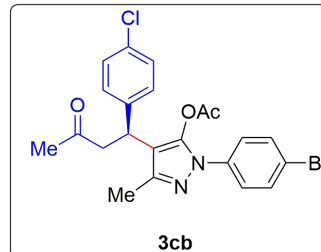


	RT	Area	% Area	Height
1	12.369	62972586	48.48	2528478
2	13.393	66918108	51.52	2306666

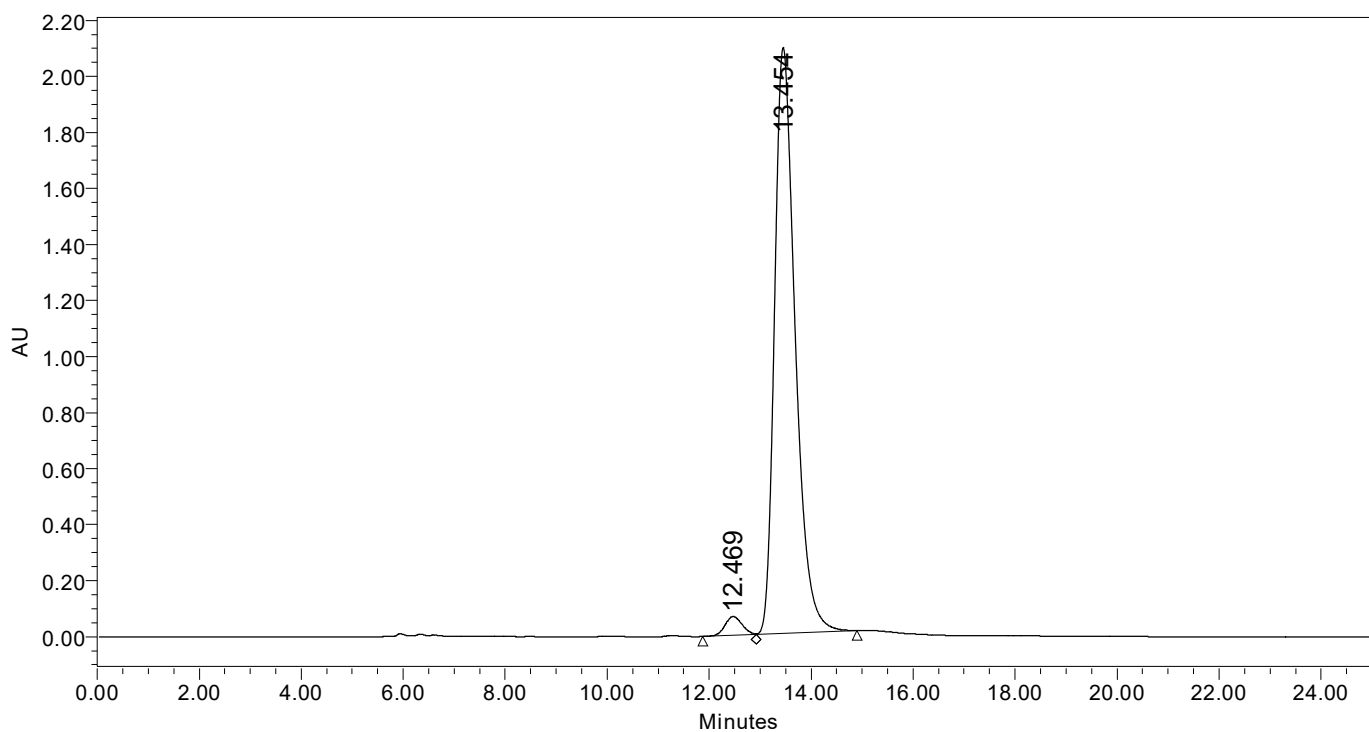
SAMPLE INFORMATION

Sample Name: PG97-ODH
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 02-12-2022 16:56:12 IST
Date Processed: 02-12-2022 18:04:47 IST

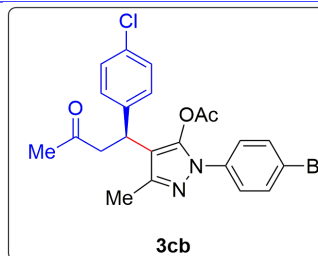


	RT	Area	% Area	Height
1	12.469	1563532	2.60	66887
2	13.454	58606545	97.40	2091950

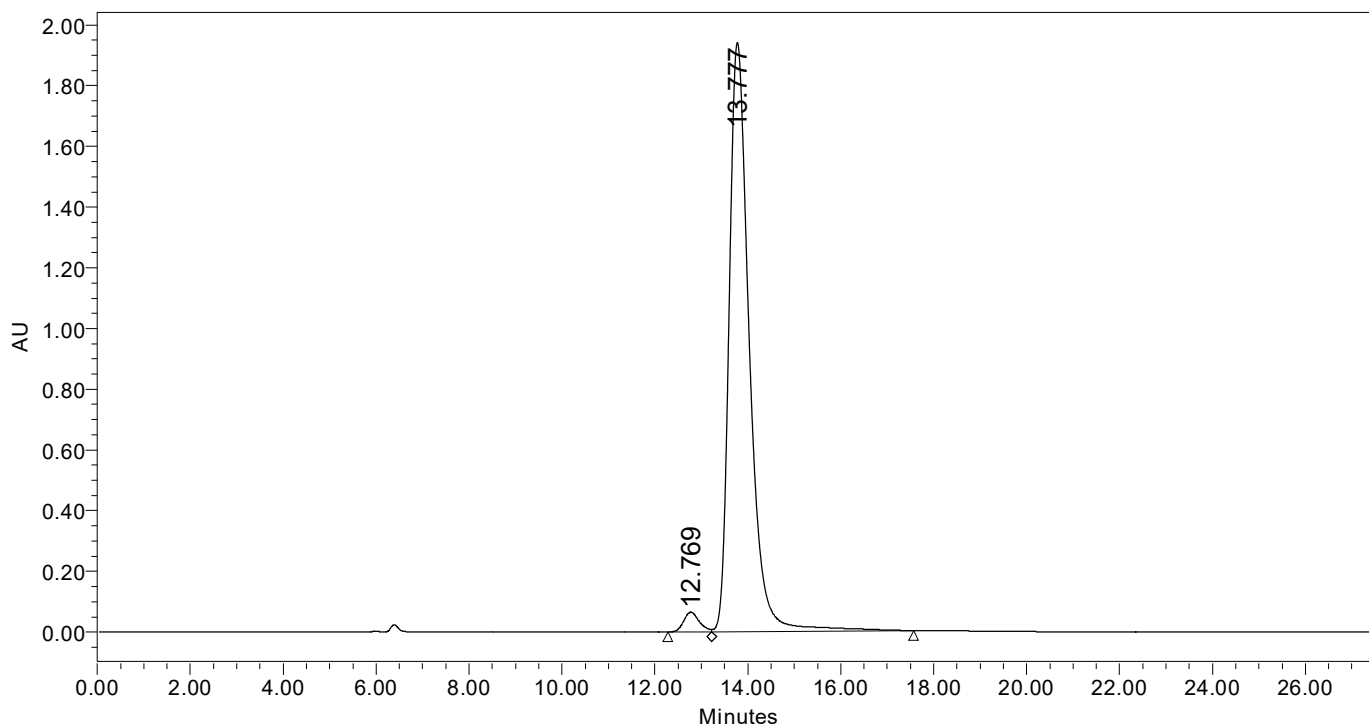
SAMPLE INFORMATION

Sample Name: PG97-CRYSTAL
Sample Type: Unknown
Vial: 1
Injection #: 10
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 10-01-2023 18:12:09 IST
Date Processed: 13-01-2023 11:32:37 IST

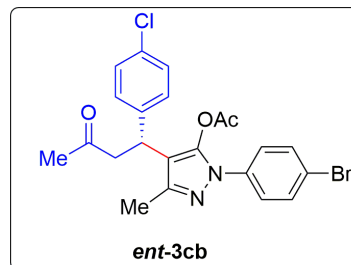


	RT	Area	% Area	Height
1	12.769	1512814	2.52	64702
2	13.777	58514028	97.48	1941482

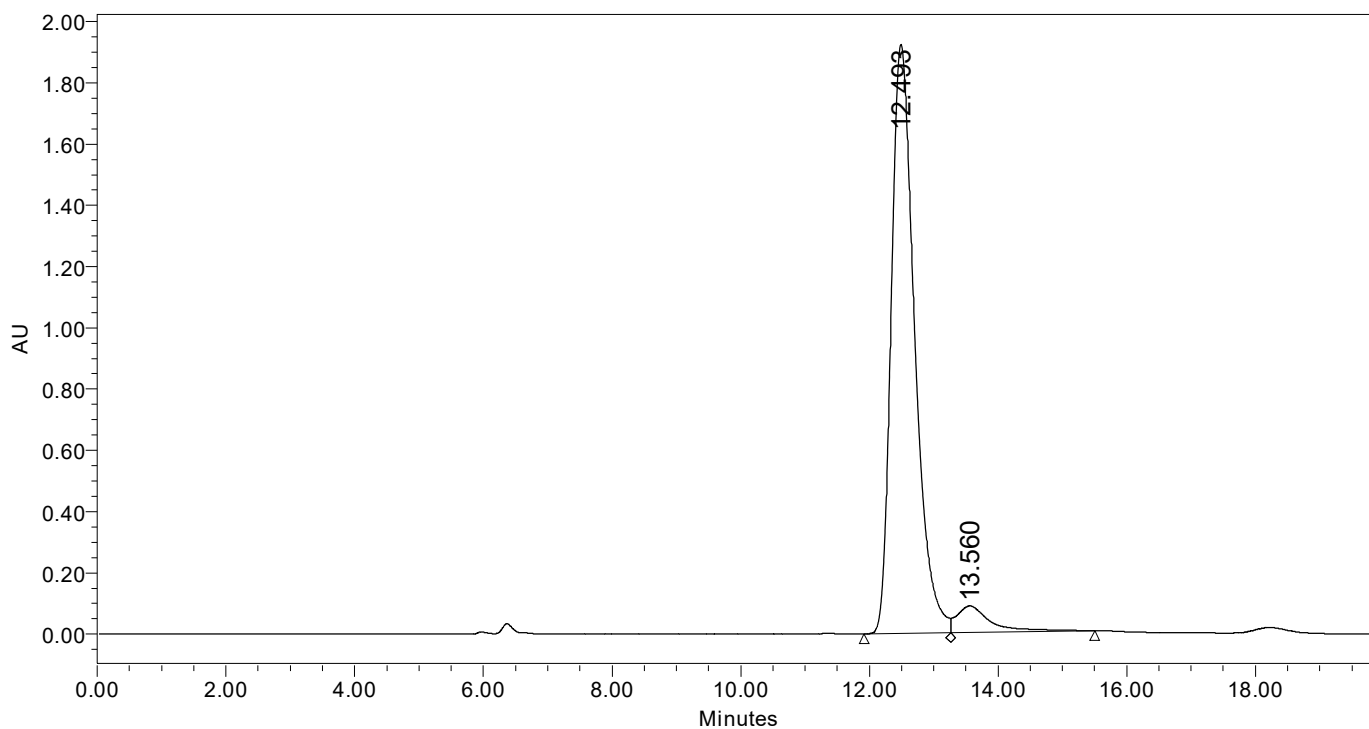
SAMPLE INFORMATION

Sample Name: PG98-ODH
Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 02-12-2022 17:48:27 IST
Date Processed: 02-12-2022 18:06:02 IST

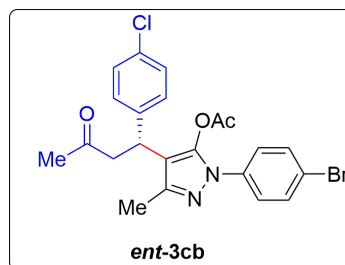


	RT	Area	% Area	Height
1	12.493	48515680	93.82	1923904
2	13.560	3196385	6.18	86538

SAMPLE INFORMATION

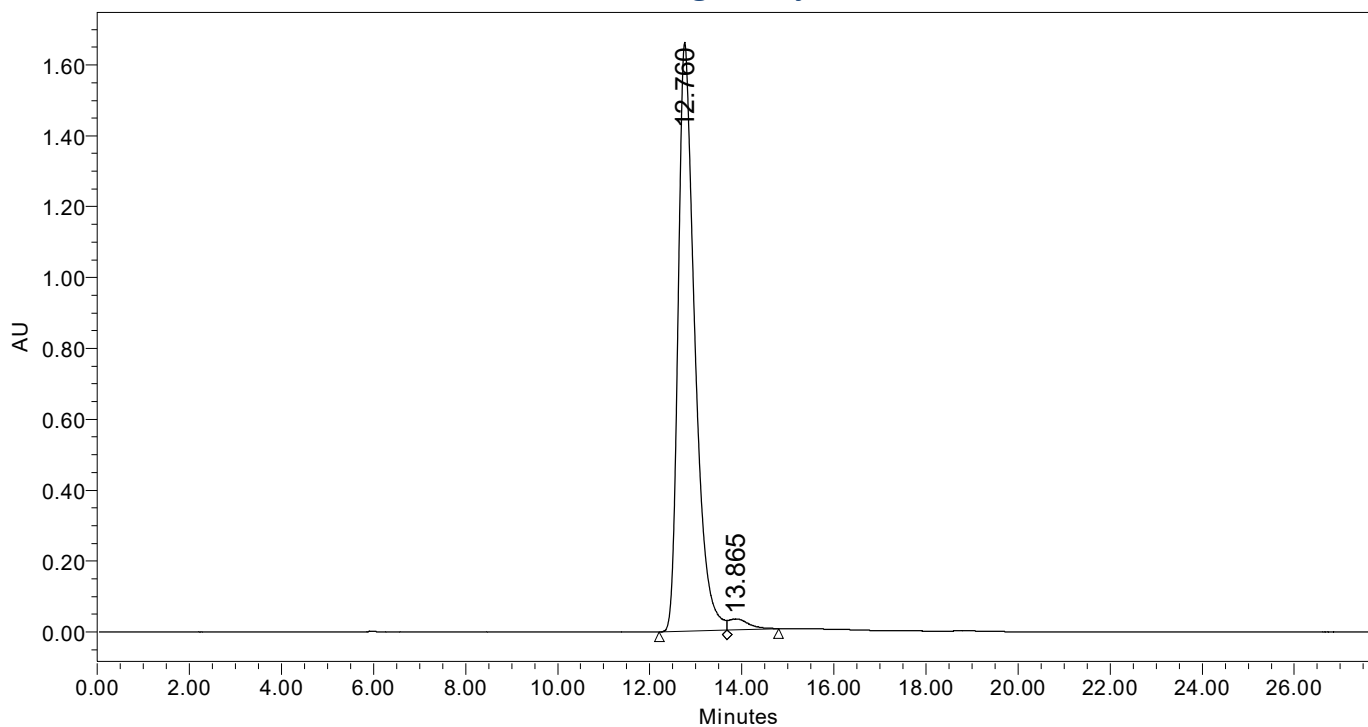
Sample Name: PG98-CRYSTAL
Sample Type: Unknown
Vial: 1
Injection #: 11
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 10-01-2023 18:40:02 IST
Date Processed: 13-01-2023 11:31:49 IST

After single recrystallization

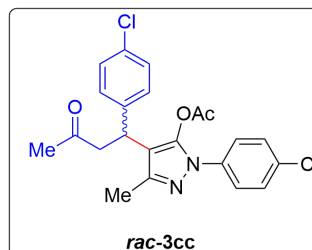


	RT	Area	% Area	Height
1	12.760	41757493	97.85	1661616
2	13.865	915439	2.15	30407

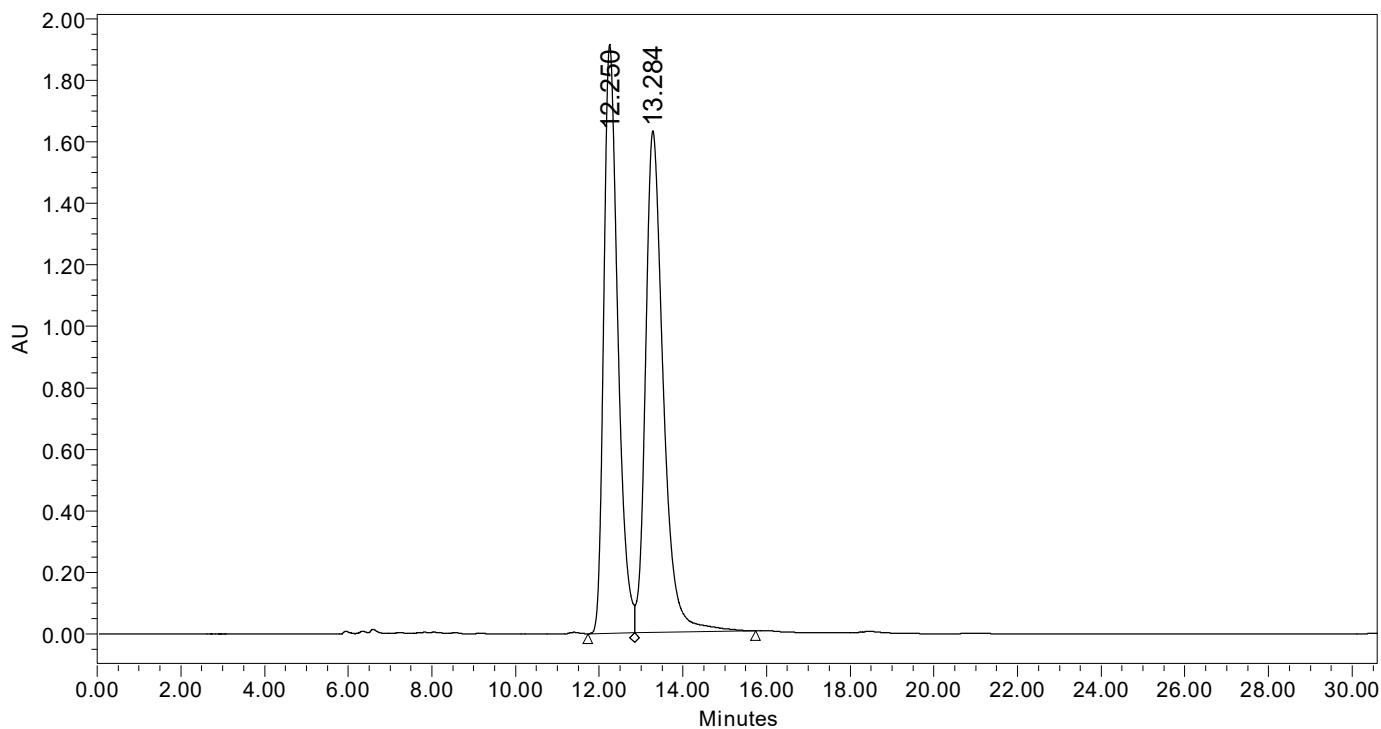
SAMPLE INFORMATION

Sample Name: AKD-641-ODH
Sample Type: Unknown
Vial: 1
Injection #: 10
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 01-12-2022 18:22:08 IST
Date Processed: 05-01-2023 18:16:12 IST

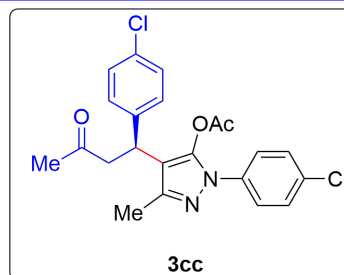


	RT	Area	% Area	Height
1	12.250	44809995	48.17	1914279
2	13.284	48223287	51.83	1630586

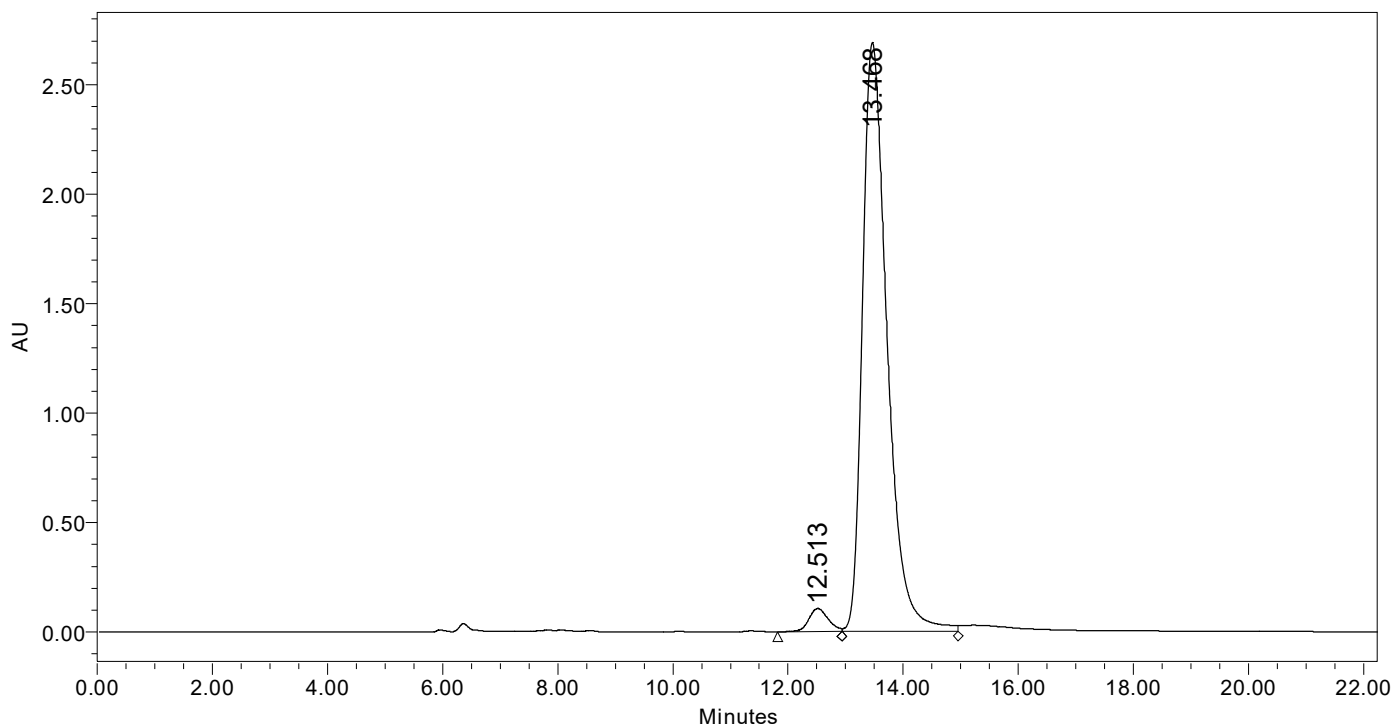
SAMPLE INFORMATION

Sample Name: PG95-ODH
Sample Type: Unknown
Vial: 1
Injection #: 8
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 01-12-2022 17:33:13 IST
Date Processed: 02-12-2022 18:01:35 IST

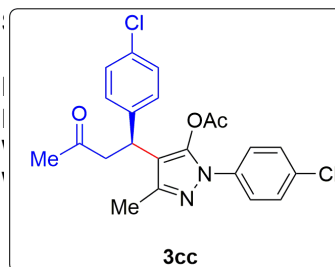


	RT	Area	% Area	Height
1	12.513	2499088	3.04	105584
2	13.468	79695968	96.96	2691451

SAMPLE INFORMATION

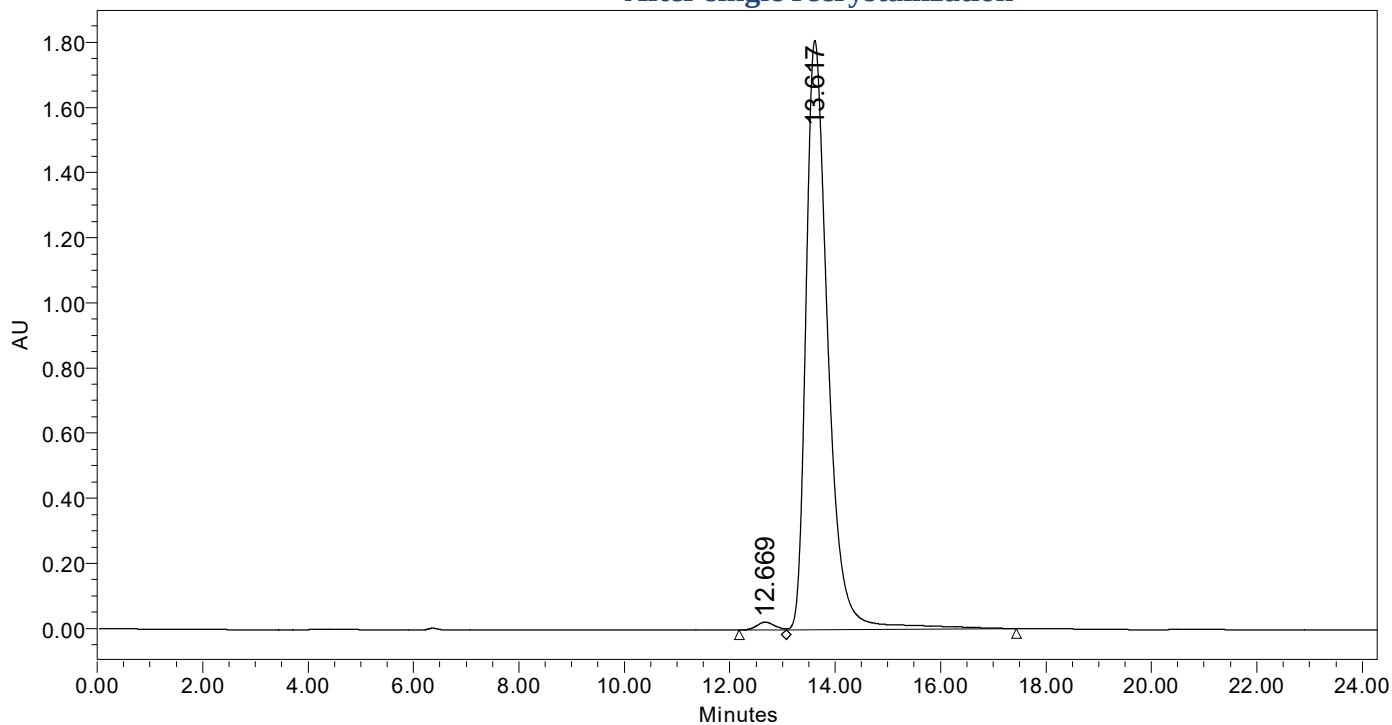
Sample Name: PG95-CRYSTAL
Sample Type: Unknown
Vial: 1
Injection #: 8
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 10-01-2023 17:06:05 IST
Date Processed: 10-01-2023 18:07:35 IST

After single recrystallization

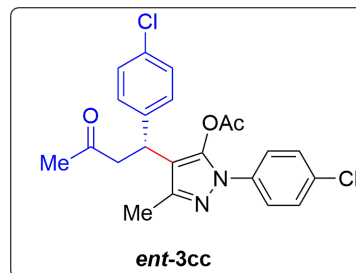


	RT	Area	% Area	Height
1	12.669	553428	1.04	23763
2	13.617	52426960	98.96	1809397

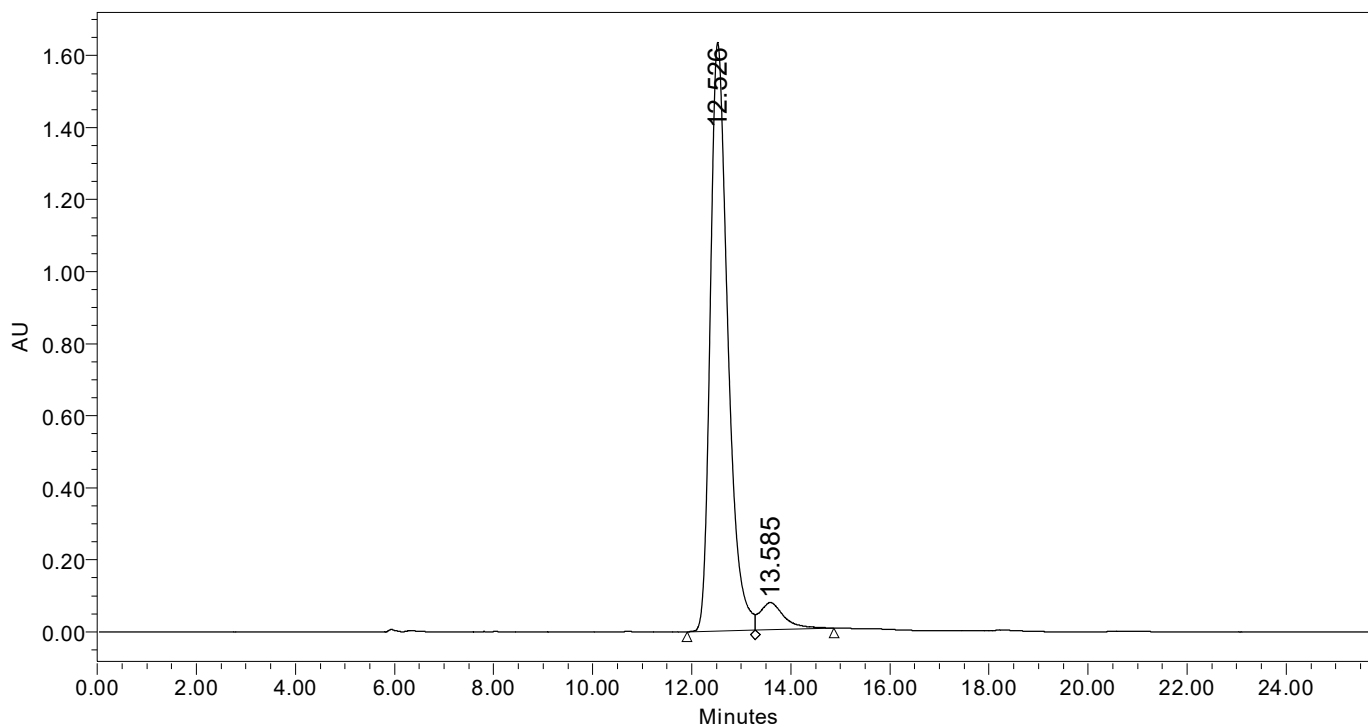
SAMPLE INFORMATION

Sample Name: PG96-ODH
Sample Type: Unknown
Vial: 1
Injection #: 9
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 01-12-2022 17:55:46 IST
Date Processed: 02-12-2022 18:02:41 IST

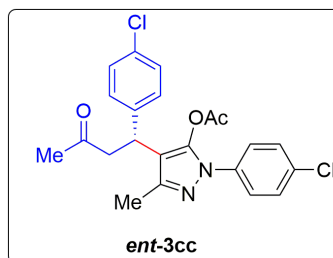


	RT	Area	% Area	Height
1	12.526	40190837	94.04	1634201
2	13.585	2548071	5.96	74790

SAMPLE INFORMATION

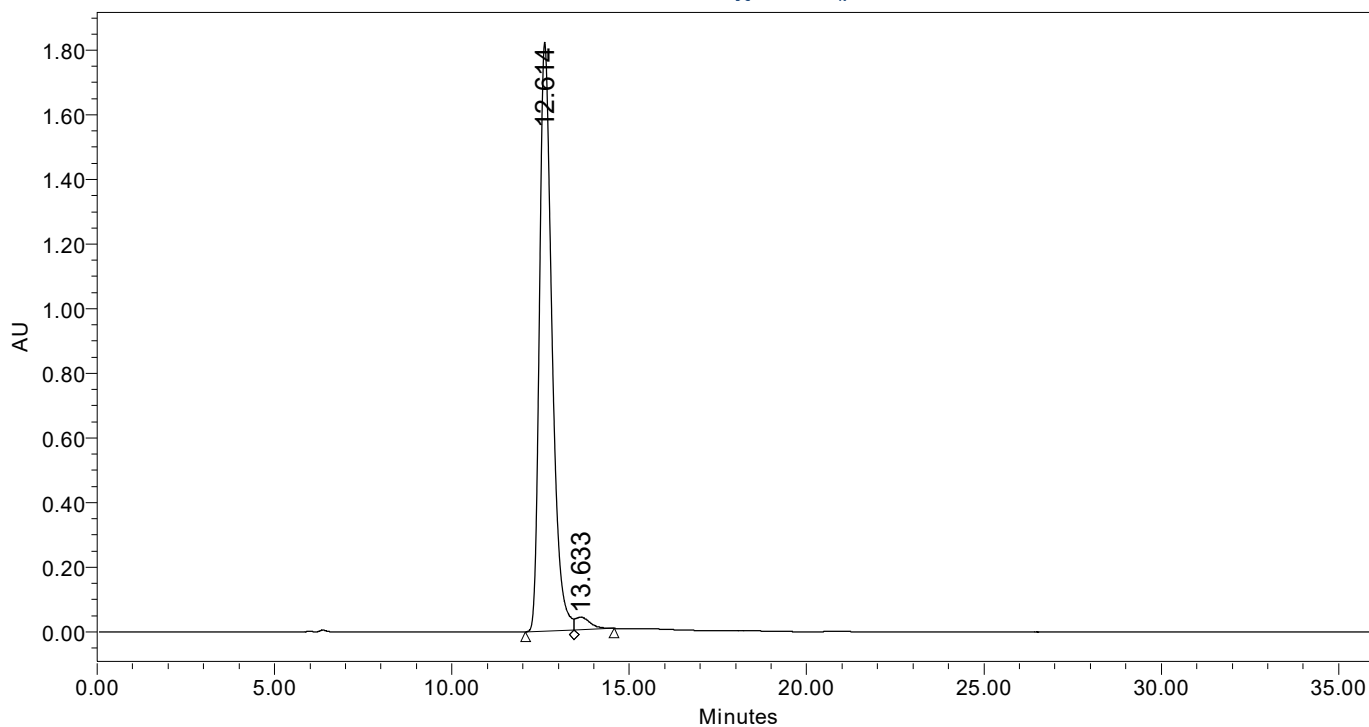
Sample Name: PG96-CRYSTAL
Sample Type: Unknown
Vial: 1
Injection #: 9
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 10-01-2023 17:30:43 IST
Date Processed: 10-01-2023 18:08:55 IST

After single recrystallization

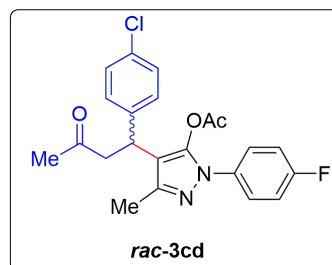


	RT	Area	% Area	Height
1	12.614	44685057	97.54	1822013
2	13.633	1128881	2.46	38441

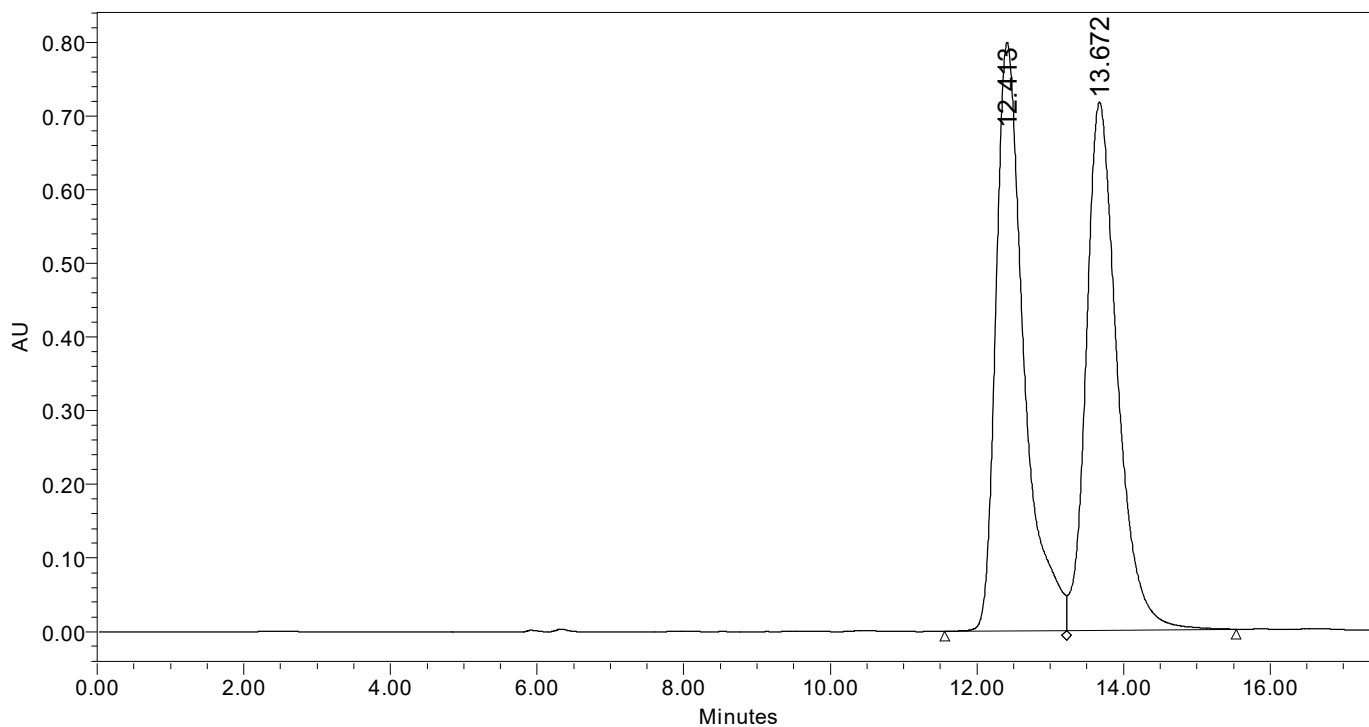
SAMPLE INFORMATION

Sample Name: PG-116-ODH
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 04-01-2023 15:55:06 IST
Date Processed: 04-01-2023 17:38:09 IST

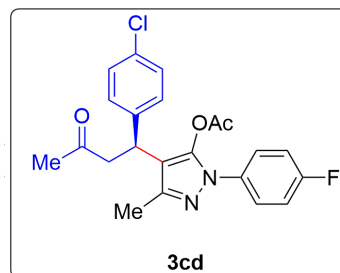


	RT	Area	% Area	Height
1	12.413	21312771	50.31	799331
2	13.672	21048474	49.69	717005

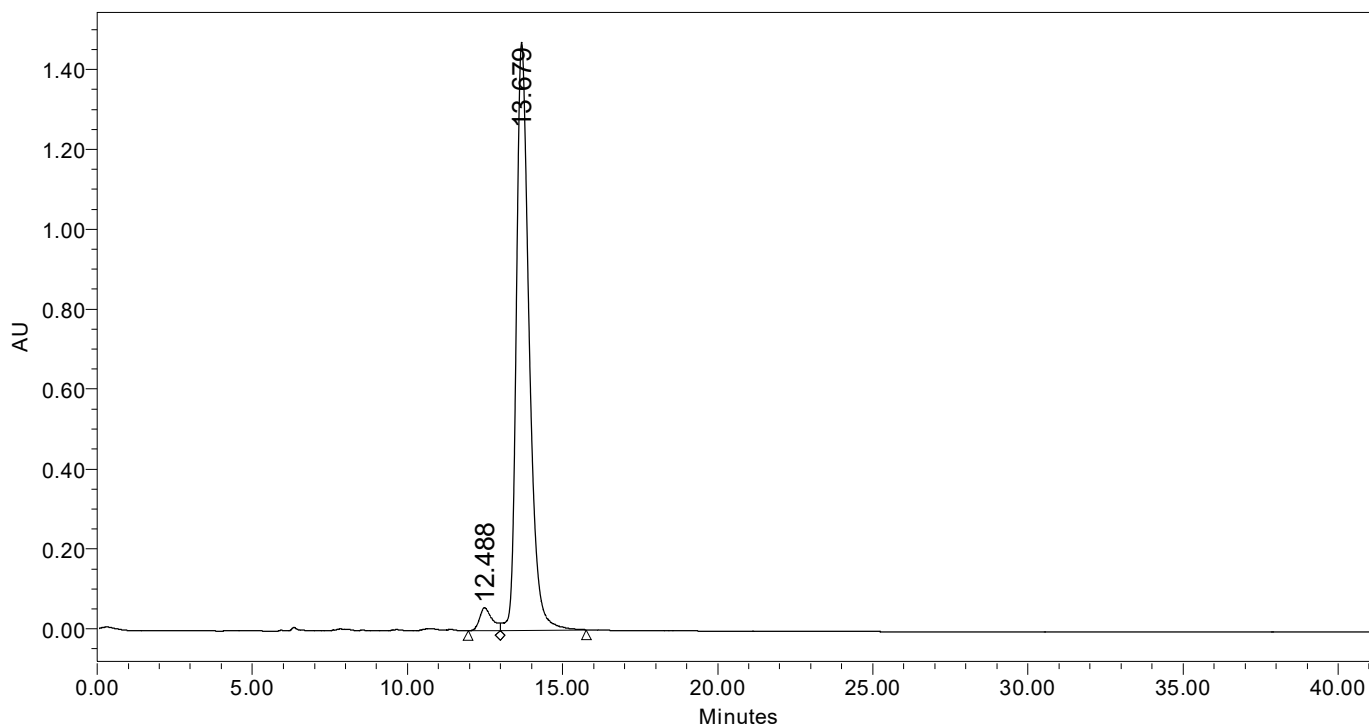
SAMPLE INFORMATION

Sample Name: PG-114-ODH
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 04-01-2023 16:13:23 IST
Date Processed: 04-01-2023 17:39:30 IST

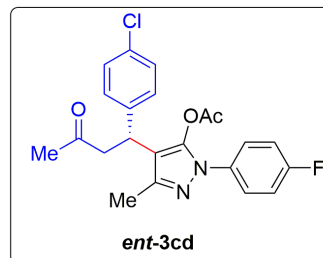


	RT	Area	% Area	Height
1	12.488	1596718	3.64	56505
2	13.679	42309384	96.36	1471717

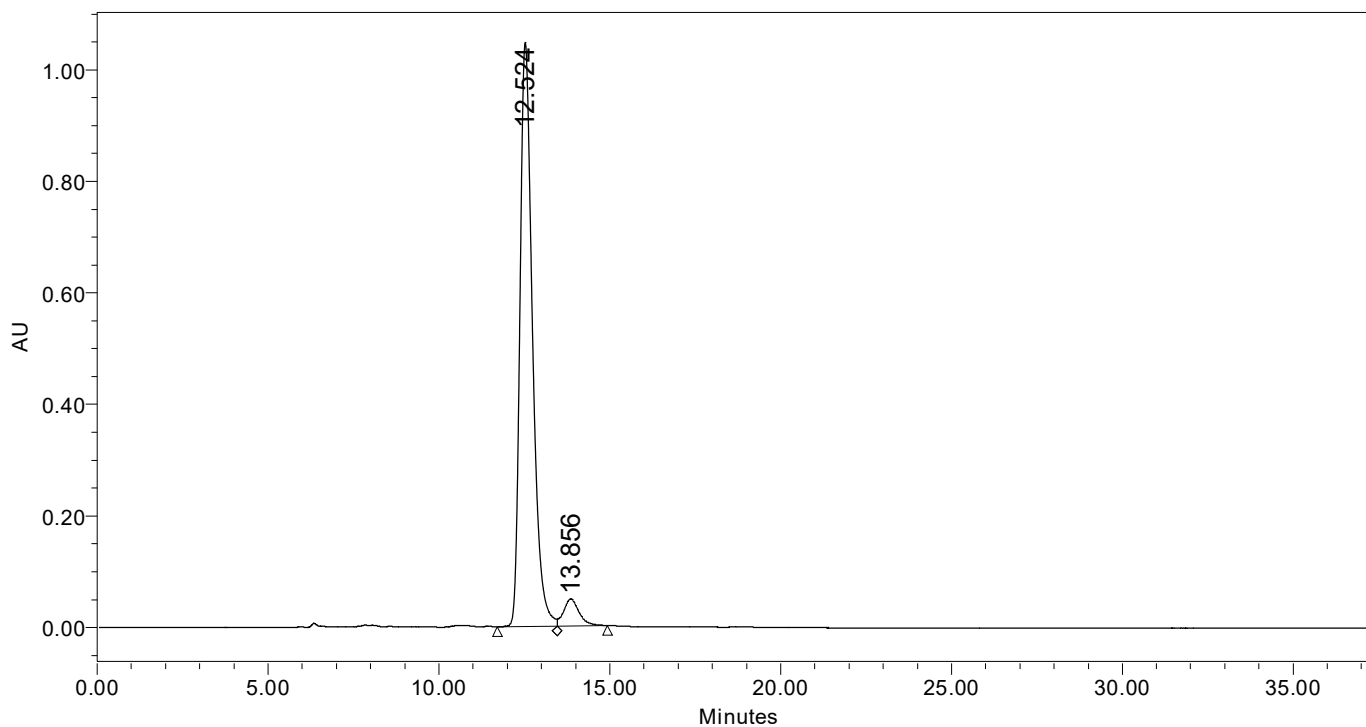
SAMPLE INFORMATION

Sample Name: PG-115-ODH
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 04-01-2023 16:55:08 IST
Date Processed: 04-01-2023 17:40:17 IST

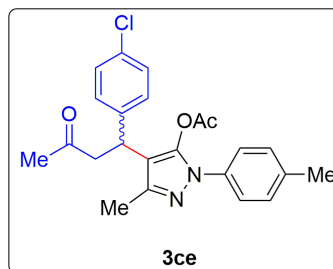


	RT	Area	% Area	Height
1	12.524	26617946	94.53	1047662
2	13.856	1539073	5.47	48556

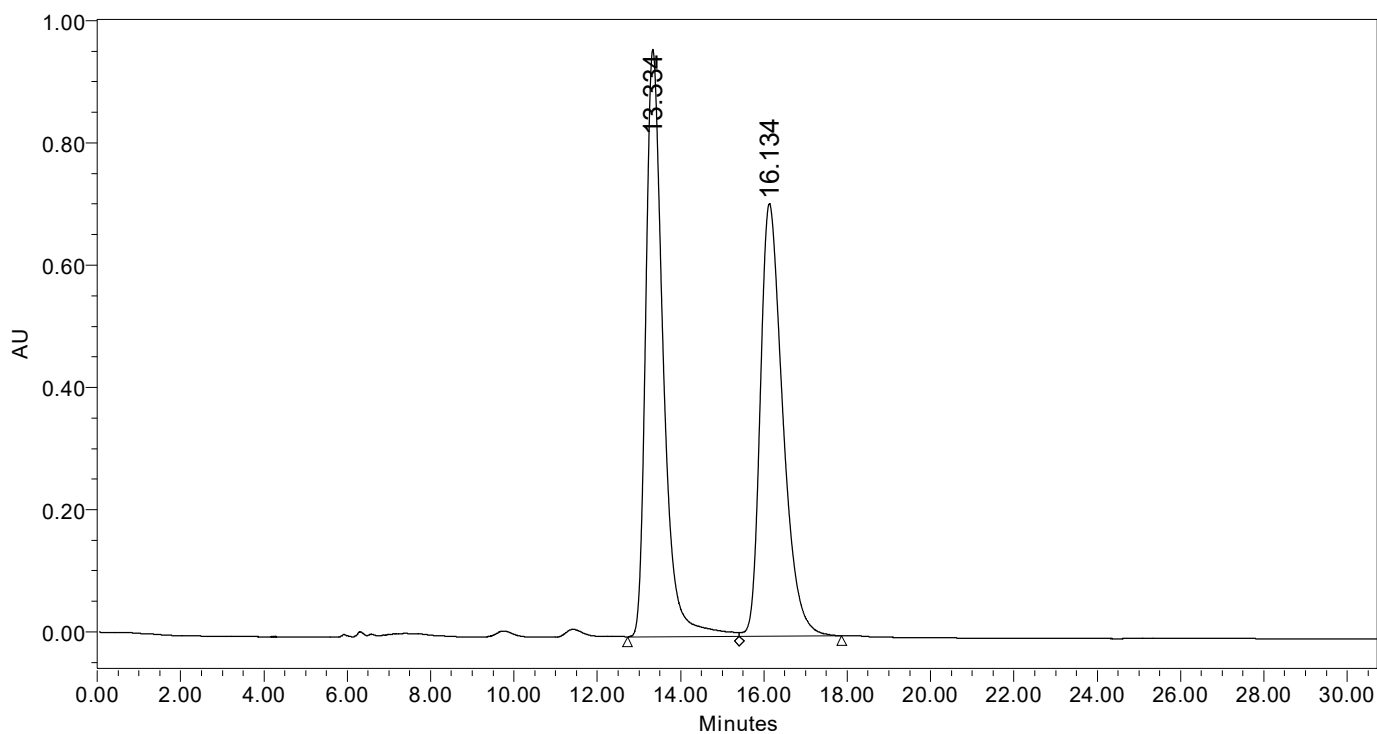
SAMPLE INFORMATION

Sample Name: AKD-642
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 29-12-2022 12:13:23 IST
Date Processed: 29-12-2022 15:05:27 IST

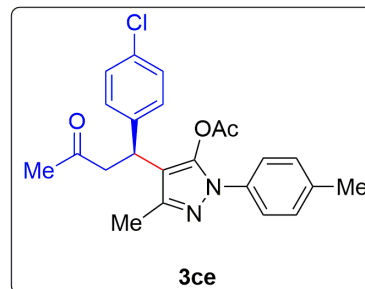


	RT	Area	% Area	Height
1	13.334	27937145	51.35	960801
2	16.134	26464101	48.65	707807

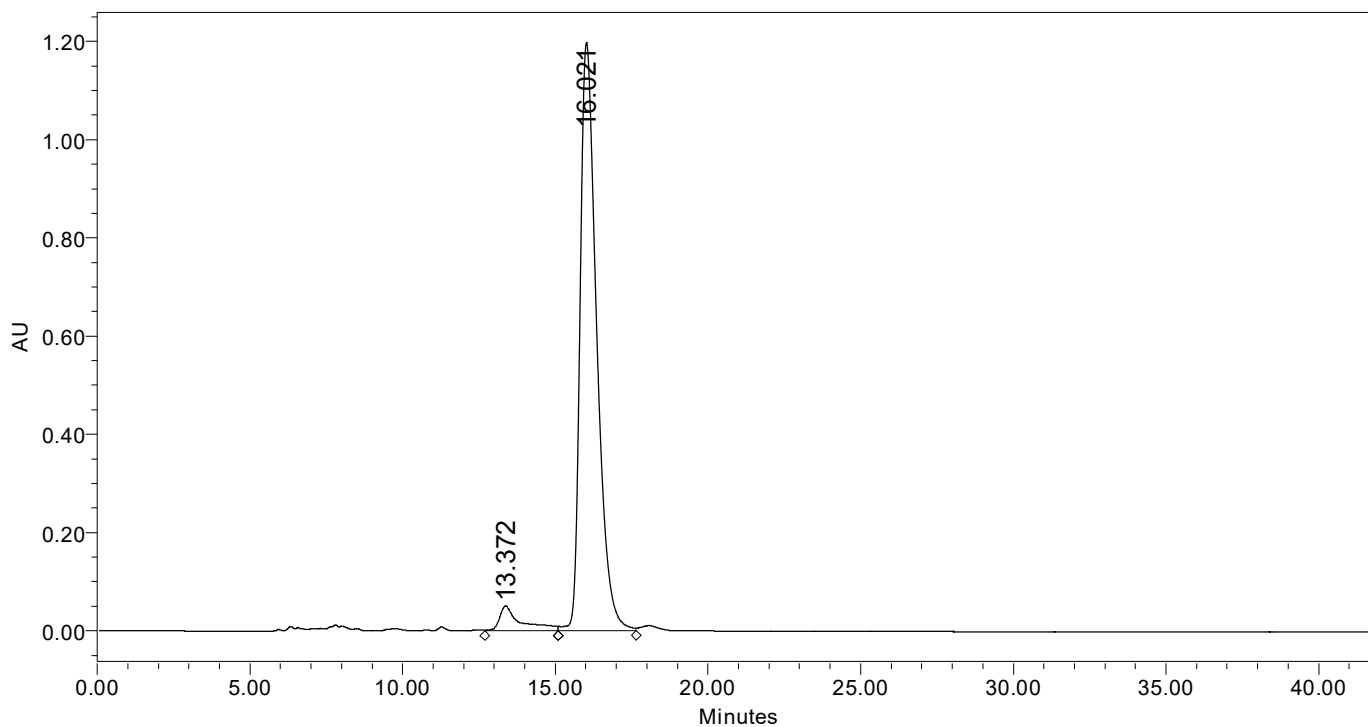
SAMPLE INFORMATION

Sample Name: PG104-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 29-12-2022 13:14:55 IST
Date Processed: 29-12-2022 15:04:03 IST

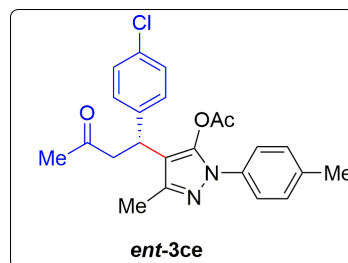


	RT	Area	% Area	Height
1	13.372	2507989	5.25	50485
2	16.021	45227068	94.75	1197961

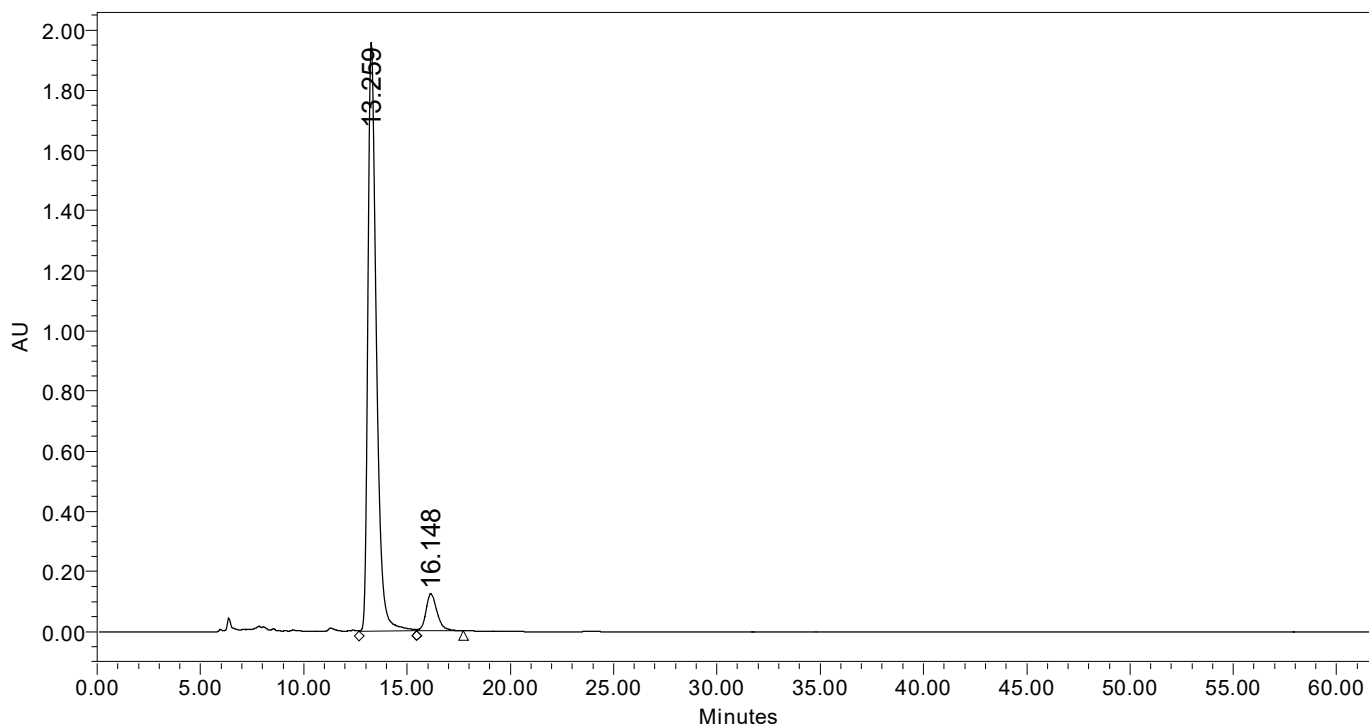
SAMPLE INFORMATION

Sample Name: PG105-OD-H
Sample Type: Unknown
Vial: 1
Injection #: 5
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 29-12-2022 13:57:27 IST
Date Processed: 29-12-2022 15:00:02 IST

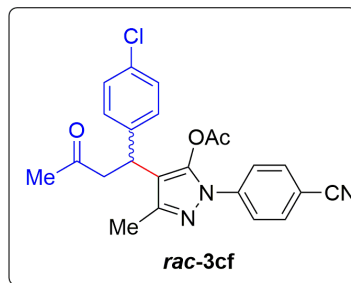


	RT	Area	% Area	Height
1	13.259	56063266	92.33	1957894
2	16.148	4660118	7.67	123711

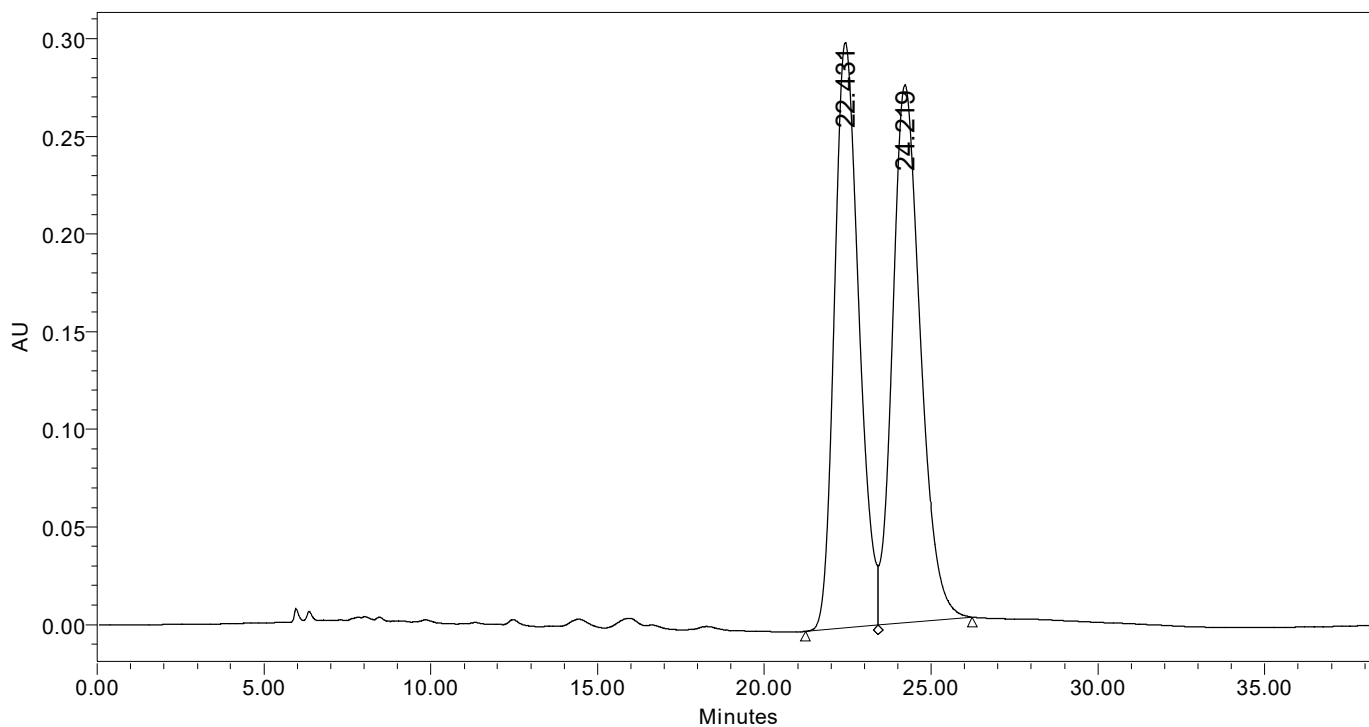
SAMPLE INFORMATION

Sample Name: AKD-646
Sample Type: Unknown
Vial: 1
Injection #: 6
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 17-01-2023 16:04:51 IST
Date Processed: 17-01-2023 16:36:04 IST

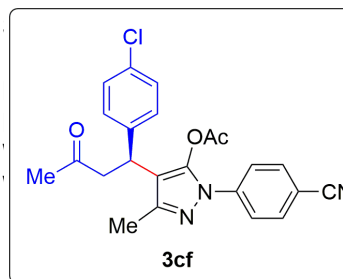


	RT	Area	% Area	Height
1	22.431	15282469	48.83	299864
2	24.219	16016144	51.17	275454

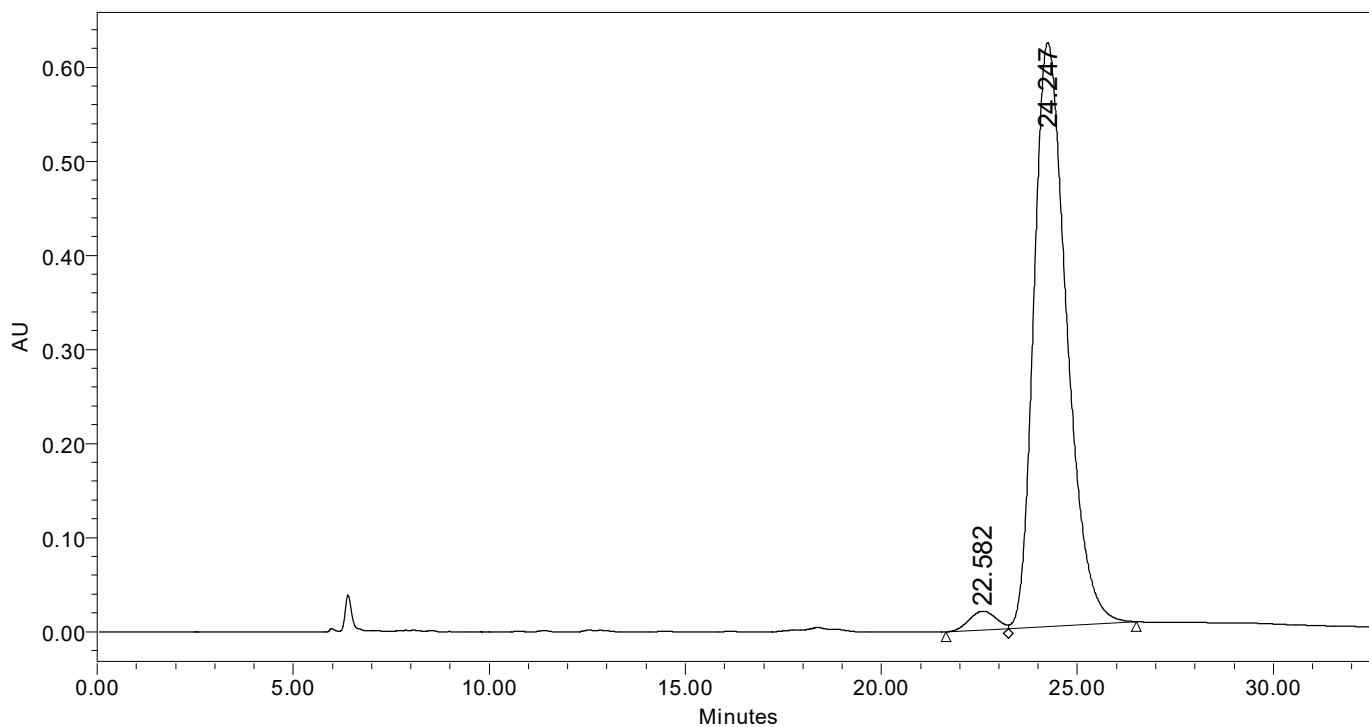
SAMPLE INFORMATION

Sample Name: PG129
Sample Type: Unknown
Vial: 1
Injection #: 5
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 17-01-2023 15:31:39 IST
Date Processed: 17-01-2023 16:44:49 IST



	RT	Area	% Area	Height
1	22.582	948660	2.57	19981
2	24.247	35945660	97.43	621059

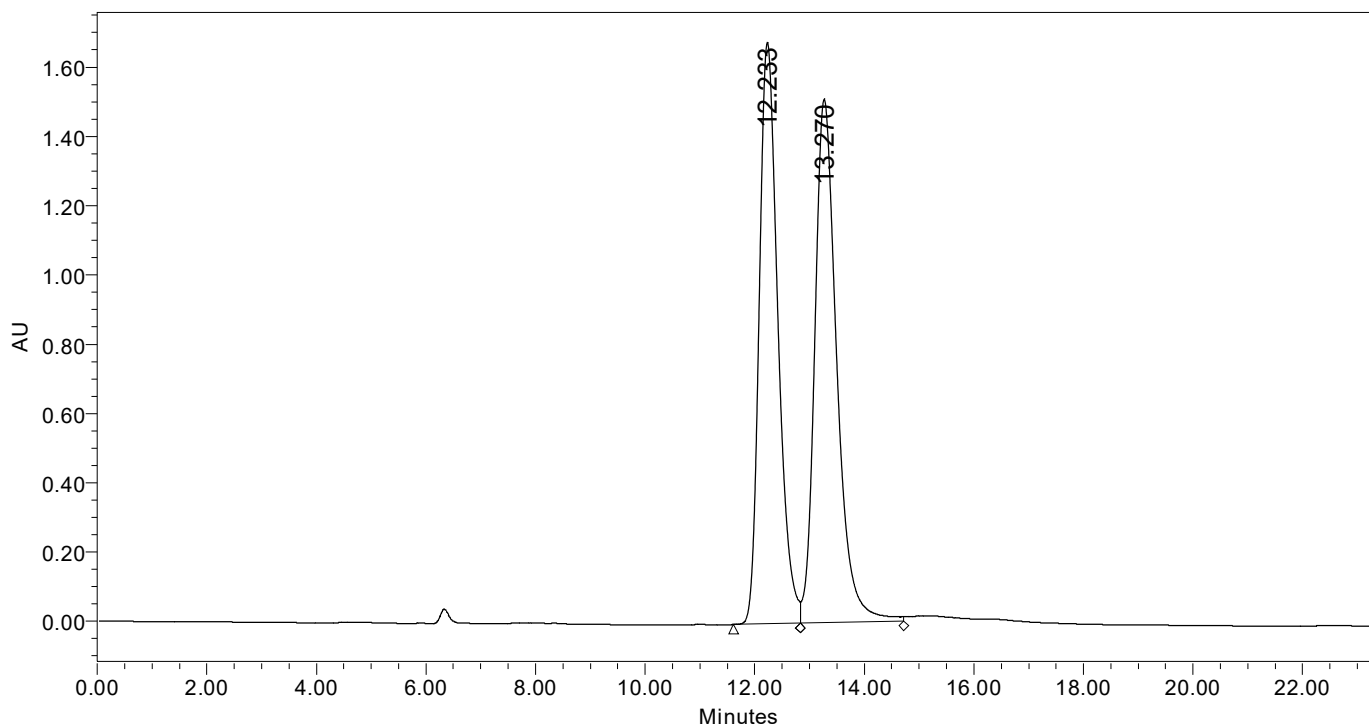
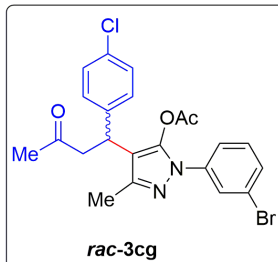
SAMPLE INFORMATION

Sample Name: PG-112-ODH
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Date Acquired: 02-01-2023 15:41:38 IST
Date Processed: 05-01-2023 18:18:21 IST

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

System

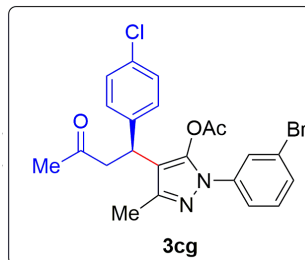


	RT	Area	% Area	Height
1	12.233	39764720	48.59	1678994
2	13.270	42073595	51.41	1511126

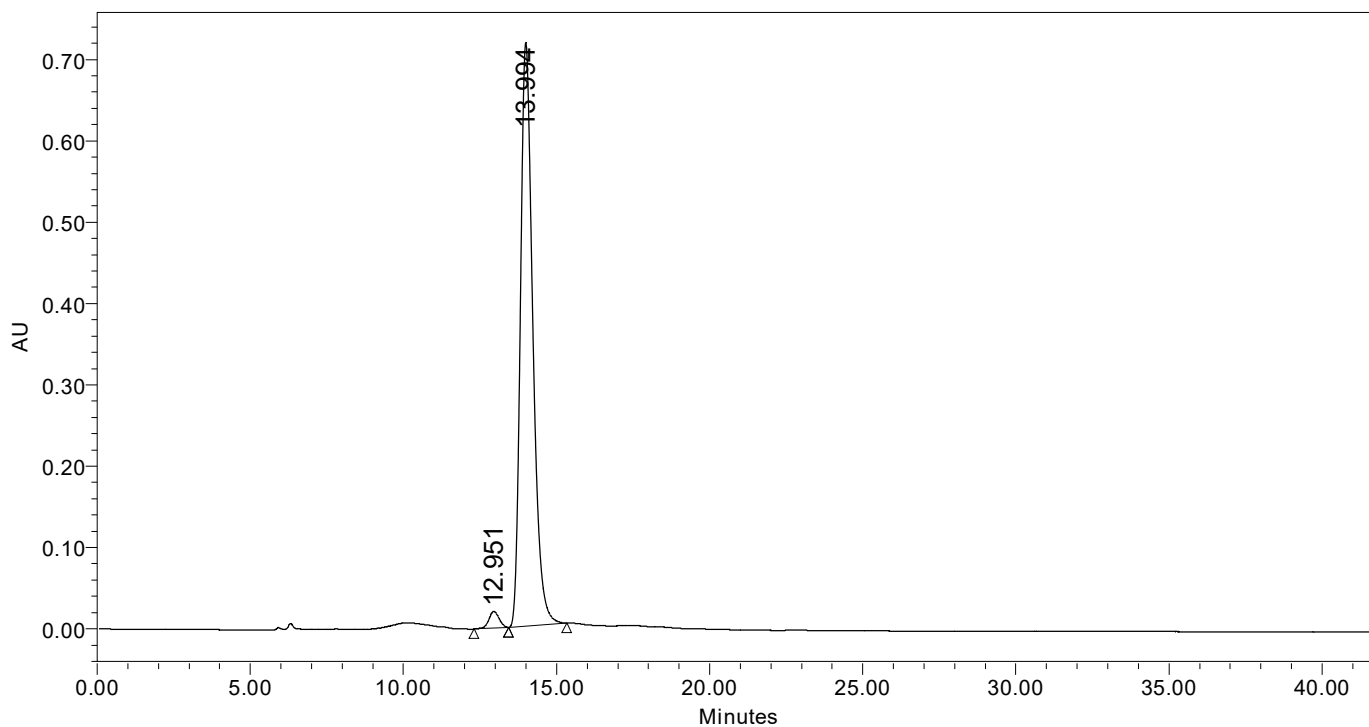
SAMPLE INFORMATION

Sample Name: PG-109-ODH
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 02-01-2023 16:05:20 IST
Date Processed: 05-01-2023 18:19:06 IST



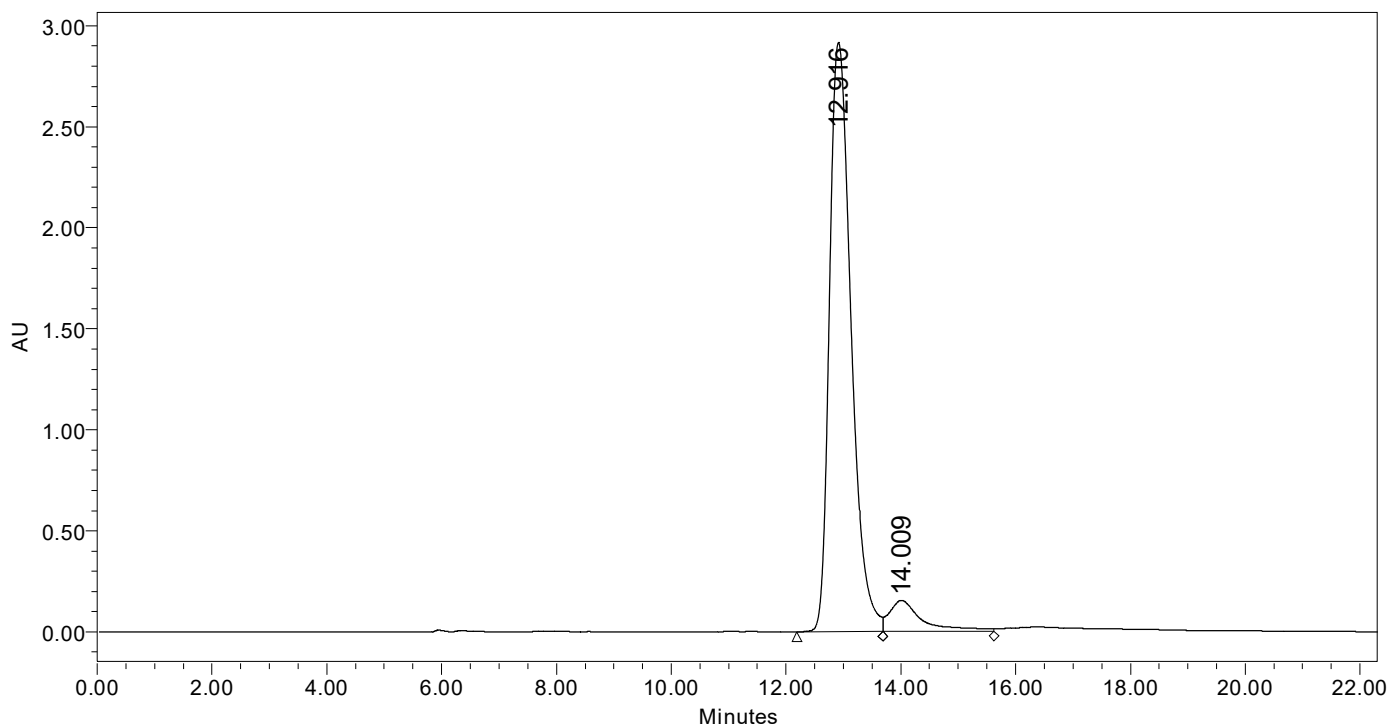
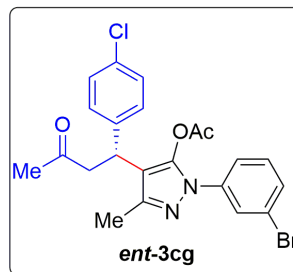
	RT	Area	% Area	Height
1	12.951	482089	2.33	20645
2	13.994	20175078	97.67	717992

SAMPLE INFORMATION

Sample Name: PG-110-ODH
Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Date Acquired: 02-01-2023 17:20:18 IST
Date Processed: 05-01-2023 18:19:59 IST

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

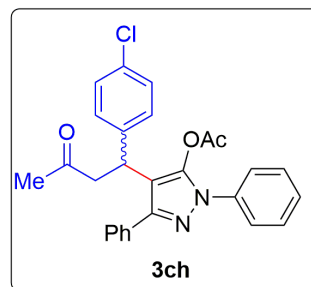


	RT	Area	% Area	Height
1	12.916	76334899	92.54	2916527
2	14.009	6152202	7.46	153622

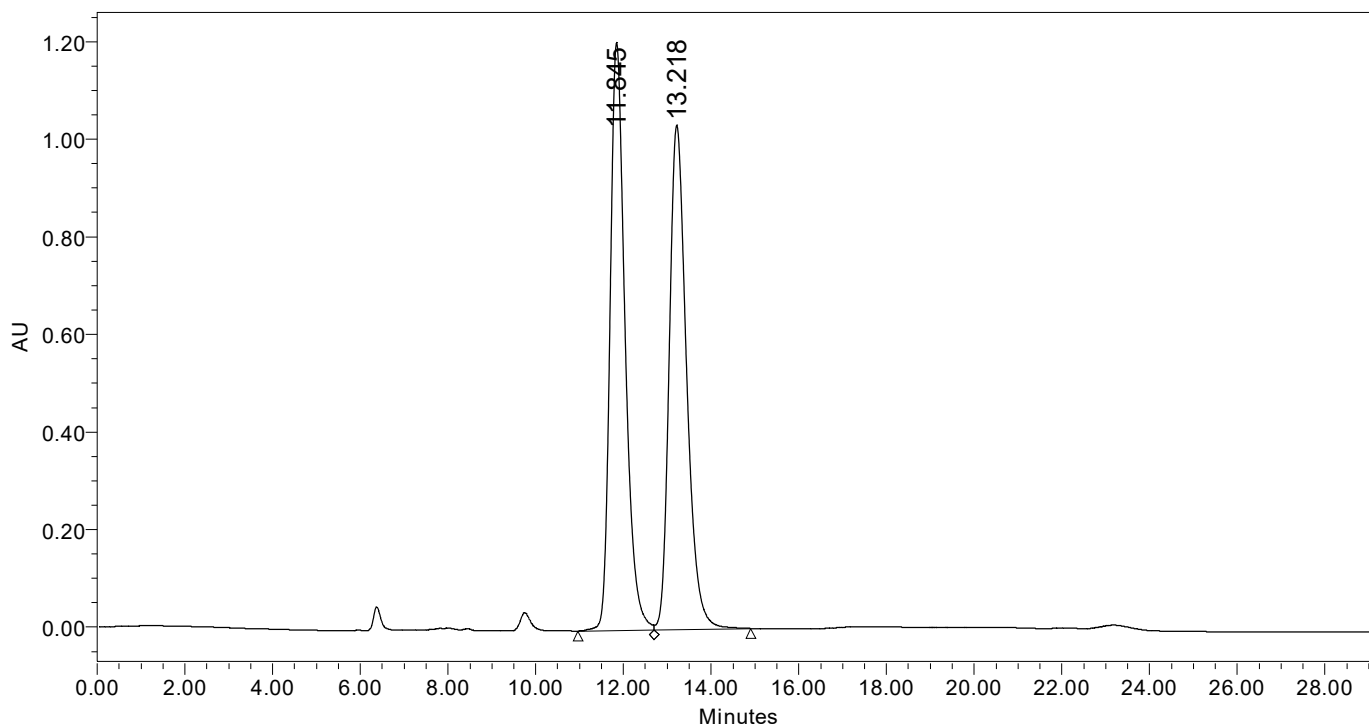
SAMPLE INFORMATION

Sample Name: PG-117
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 13-01-2023 11:36:38 IST
Date Processed: 13-01-2023 12:05:46 IST



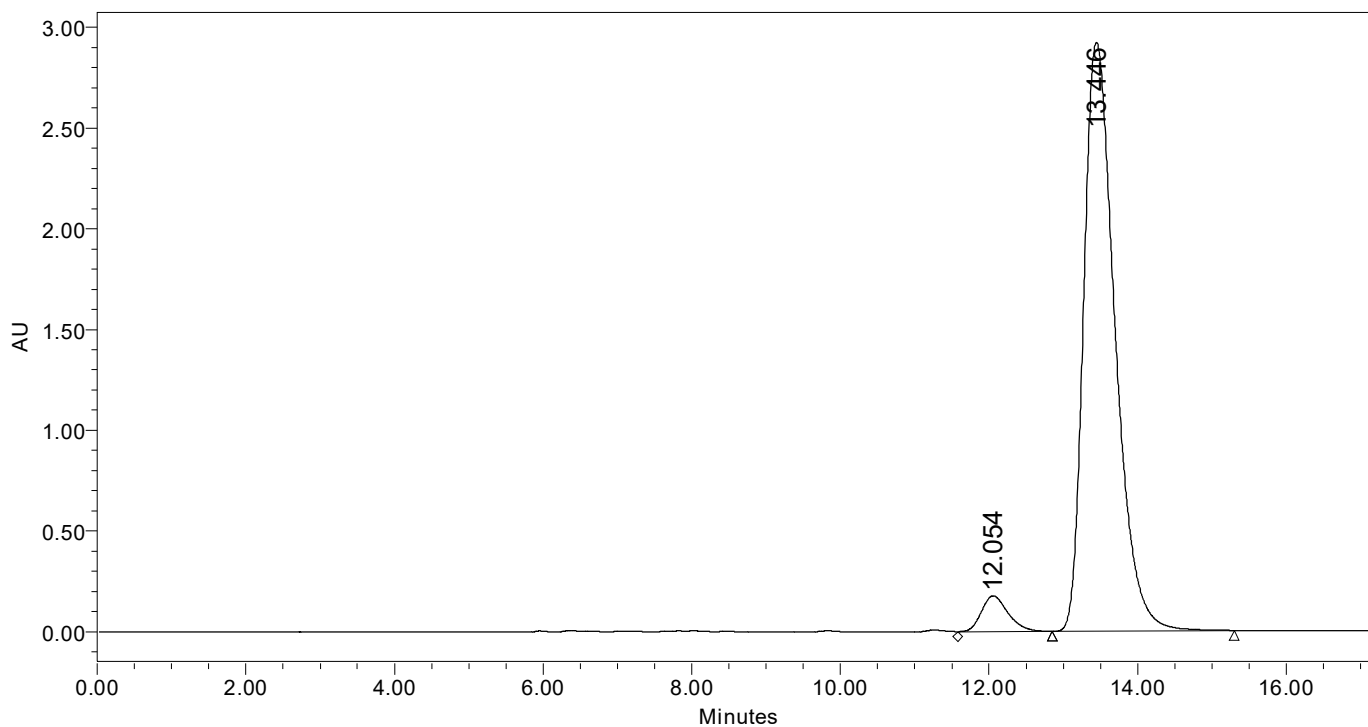
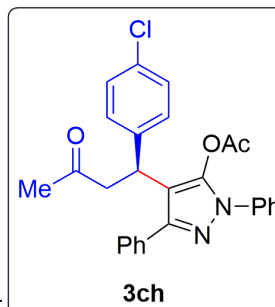
	RT	Area	% Area	Height
1	11.845	28733496	50.30	1205727
2	13.218	28392079	49.70	1034446

SAMPLE INFORMATION

Sample Name: PG-125
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Date Acquired: 13-01-2023 12:08:09 IST
Date Processed: 16-03-2023 18:37:11 IST

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

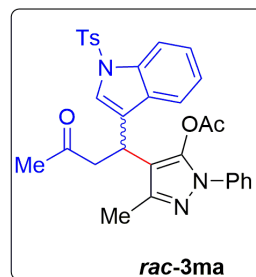


	RT	Area	% Area	Height
1	12.054	4438579	4.95	178103
2	13.446	85167103	95.05	2921835

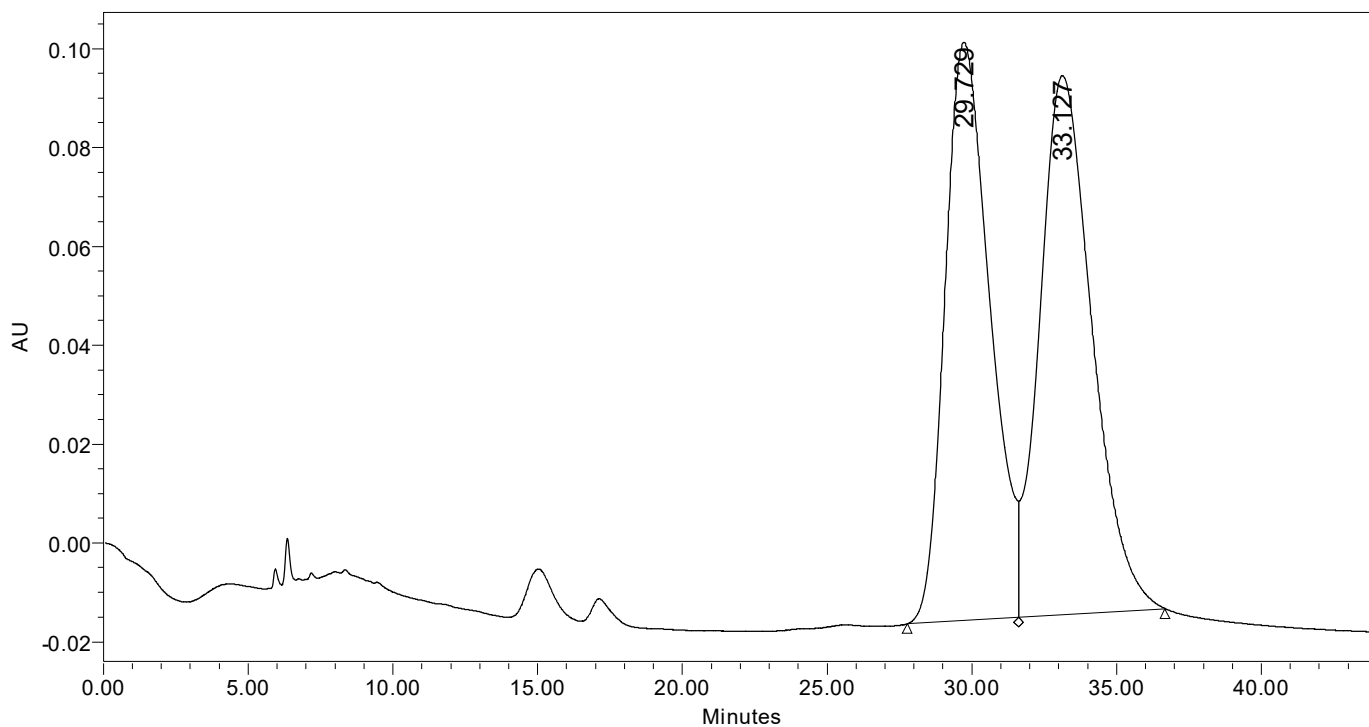
SAMPLE INFORMATION

Sample Name: PG126
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 18-01-2023 17:14:50 IST
Date Processed: 16-03-2023 18:47:49 IST

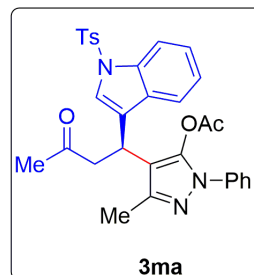


	RT	Area	% Area	Height
1	29.729	12712917	48.09	116985
2	33.127	13720371	51.91	109075

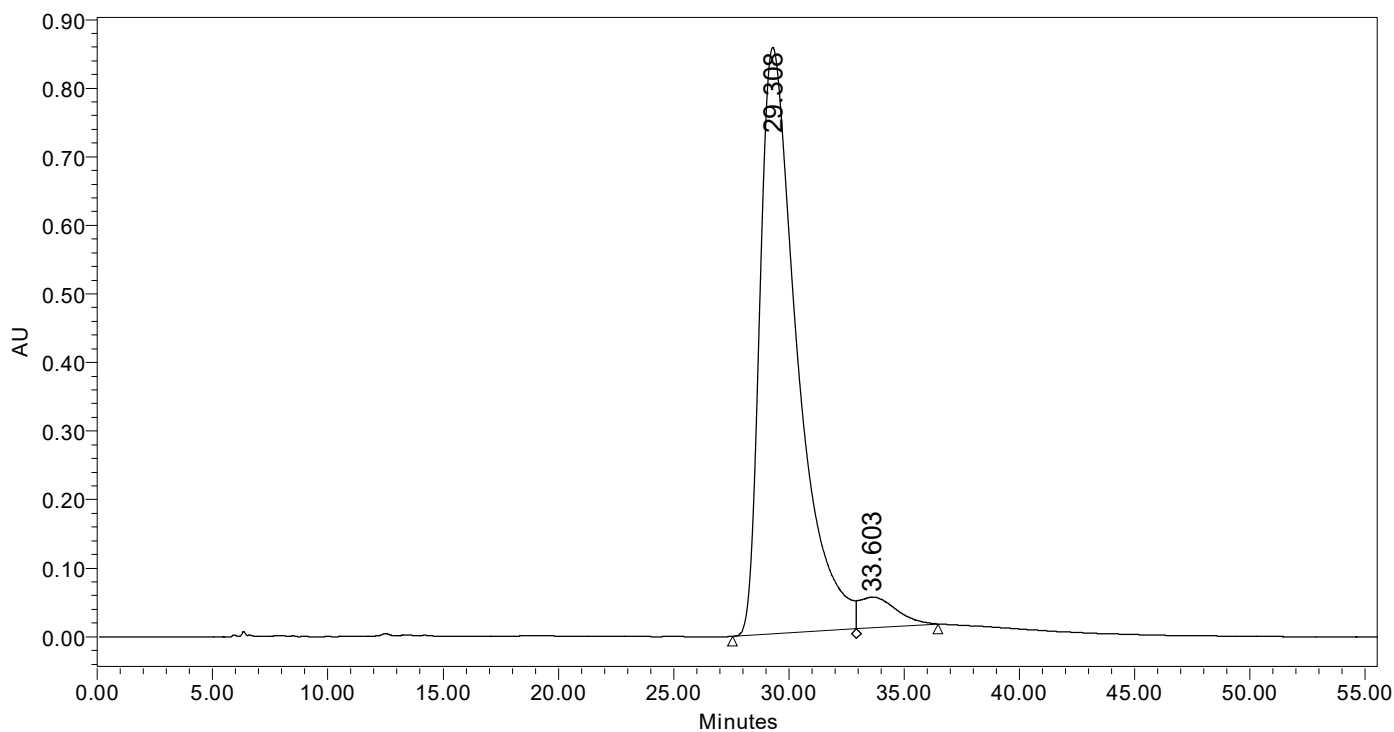
SAMPLE INFORMATION

Sample Name: PG131
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 19-01-2023 15:04:37 IST
Date Processed: 16-03-2023 18:50:57 IST



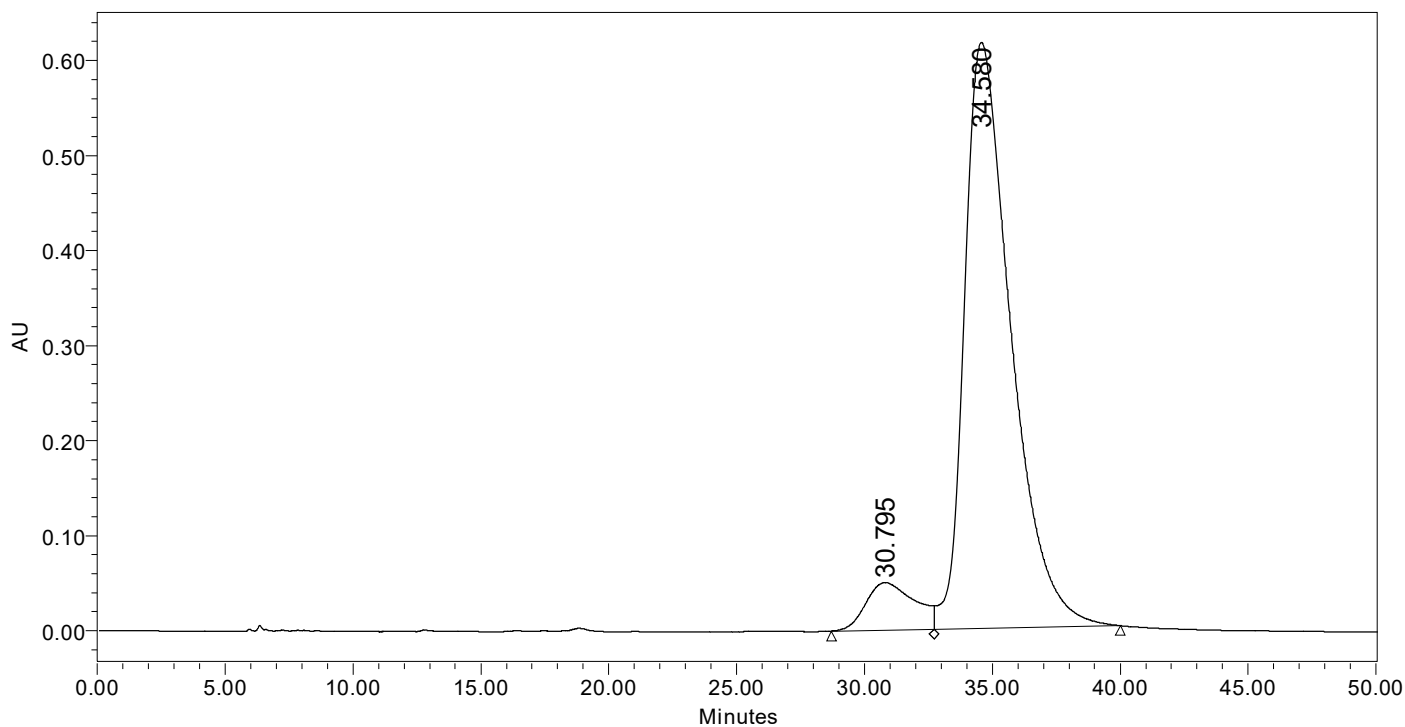
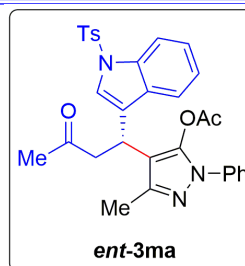
	RT	Area	% Area	Height
1	29.308	95690688	95.02	855863
2	33.603	5012813	4.98	44800

SAMPLE INFORMATION

Sample Name: PG132
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Date Acquired: 18-01-2023 17:59:13 IST
Date Processed: 16-03-2023 18:48:53 IST

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

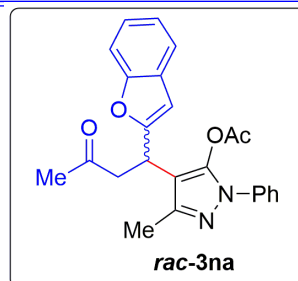


	RT	Area	% Area	Height
1	30.795	6683102	7.91	49908
2	34.580	77843218	92.09	616642

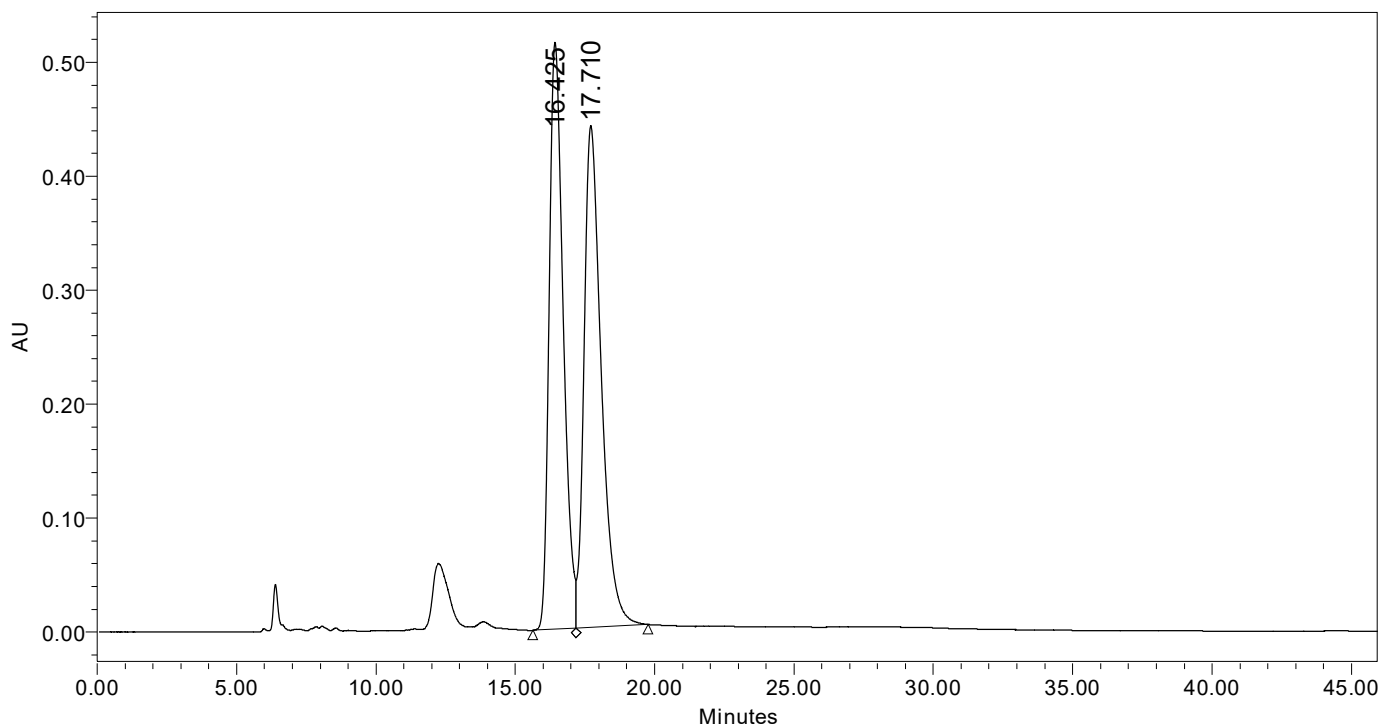
SAMPLE INFORMATION

Sample Name: PG123
Sample Type: Unknown
Vial: 1
Injection #: 7
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:



Date Acquired: 13-01-2023 14:33:05 IST
Date Processed: 16-01-2023 11:56:25 IST



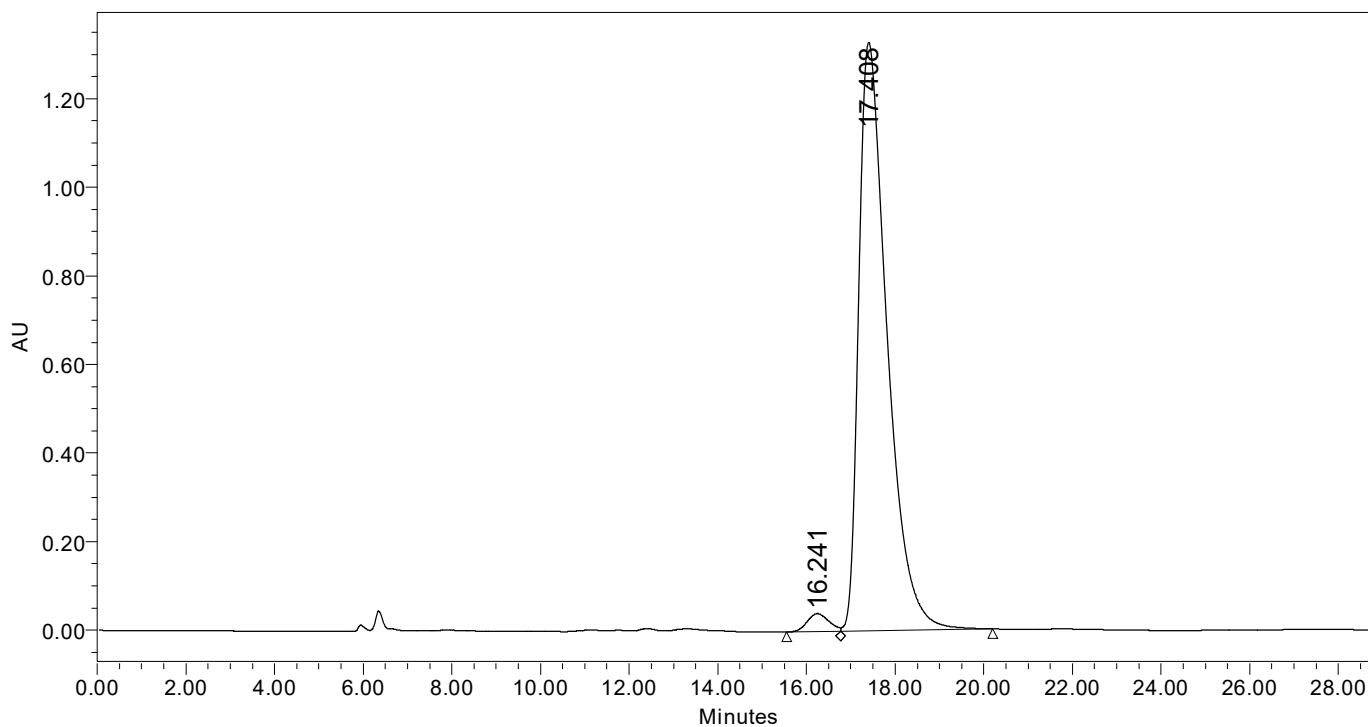
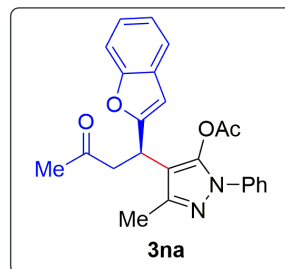
	RT	Area	% Area	Height
1	16.425	18060444	48.79	515128
2	17.710	18958230	51.21	440365

SAMPLE INFORMATION

Sample Name: PG127
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

Date Acquired: 16-01-2023 11:56:00 IST
Date Processed: 16-03-2023 18:41:01 IST

Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

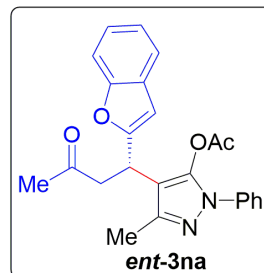


	RT	Area	% Area	Height
1	16.241	1374562	2.28	40318
2	17.408	59041896	97.72	1328807

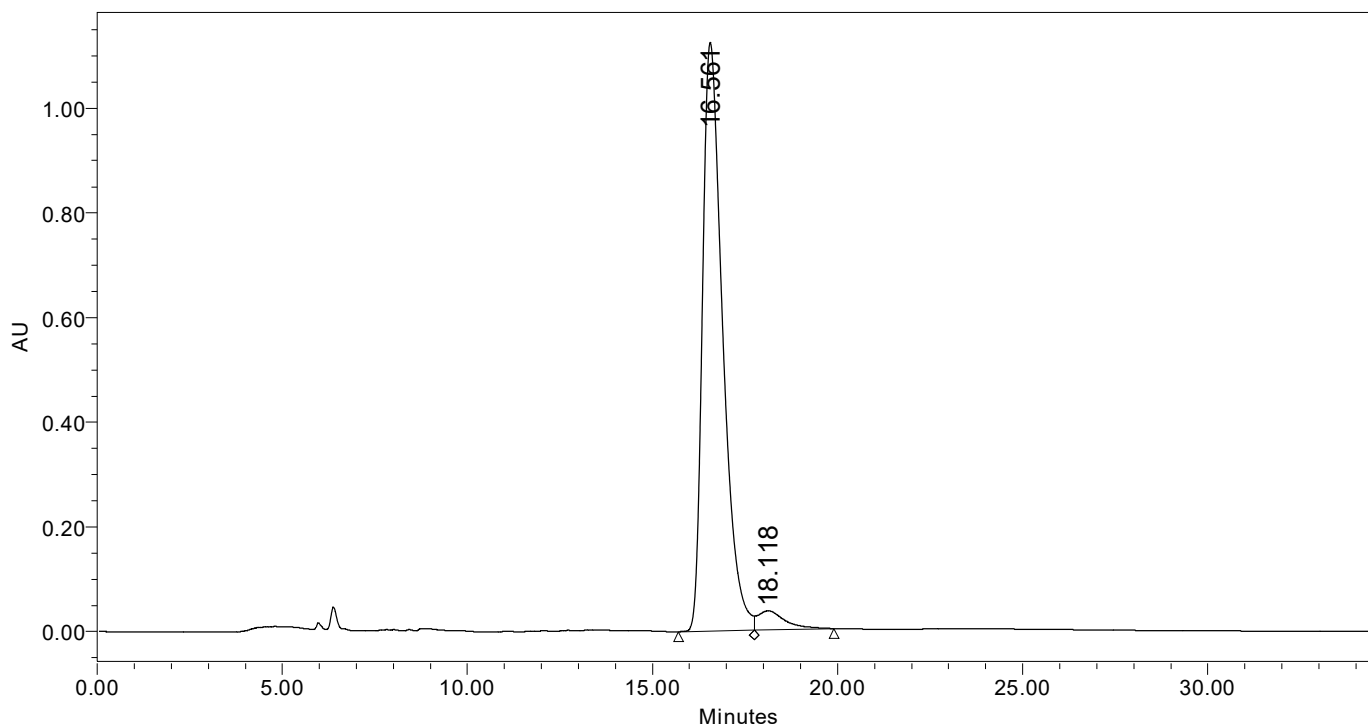
SAMPLE INFORMATION

Sample Name: PG128
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 10.00 ul
Run Time: 100.0 Minutes

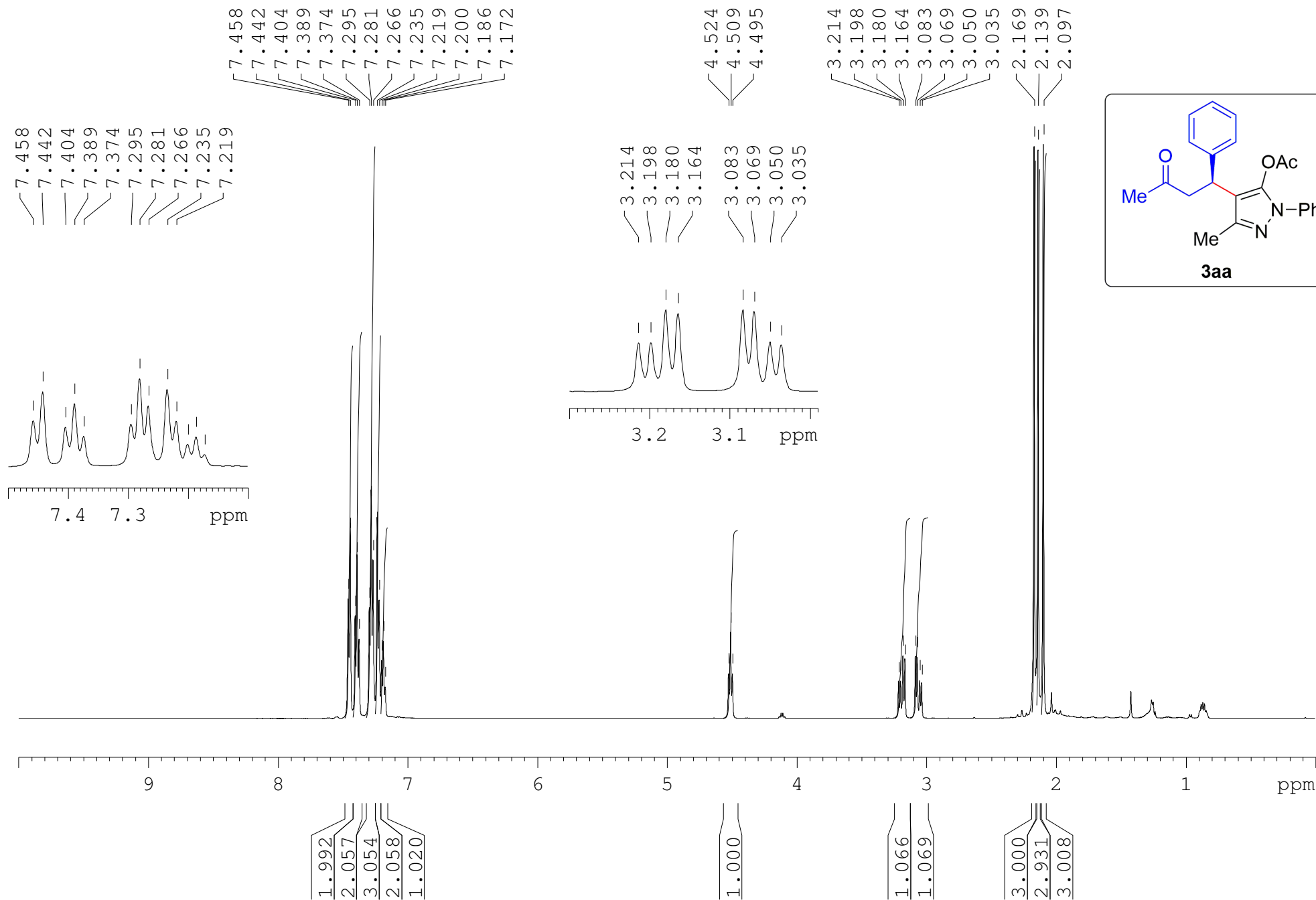
Acquired By:
Sample Set Name:
Acq. Method Set:
Processing Method
Channel Name:
Proc. Chnl. Descr.:

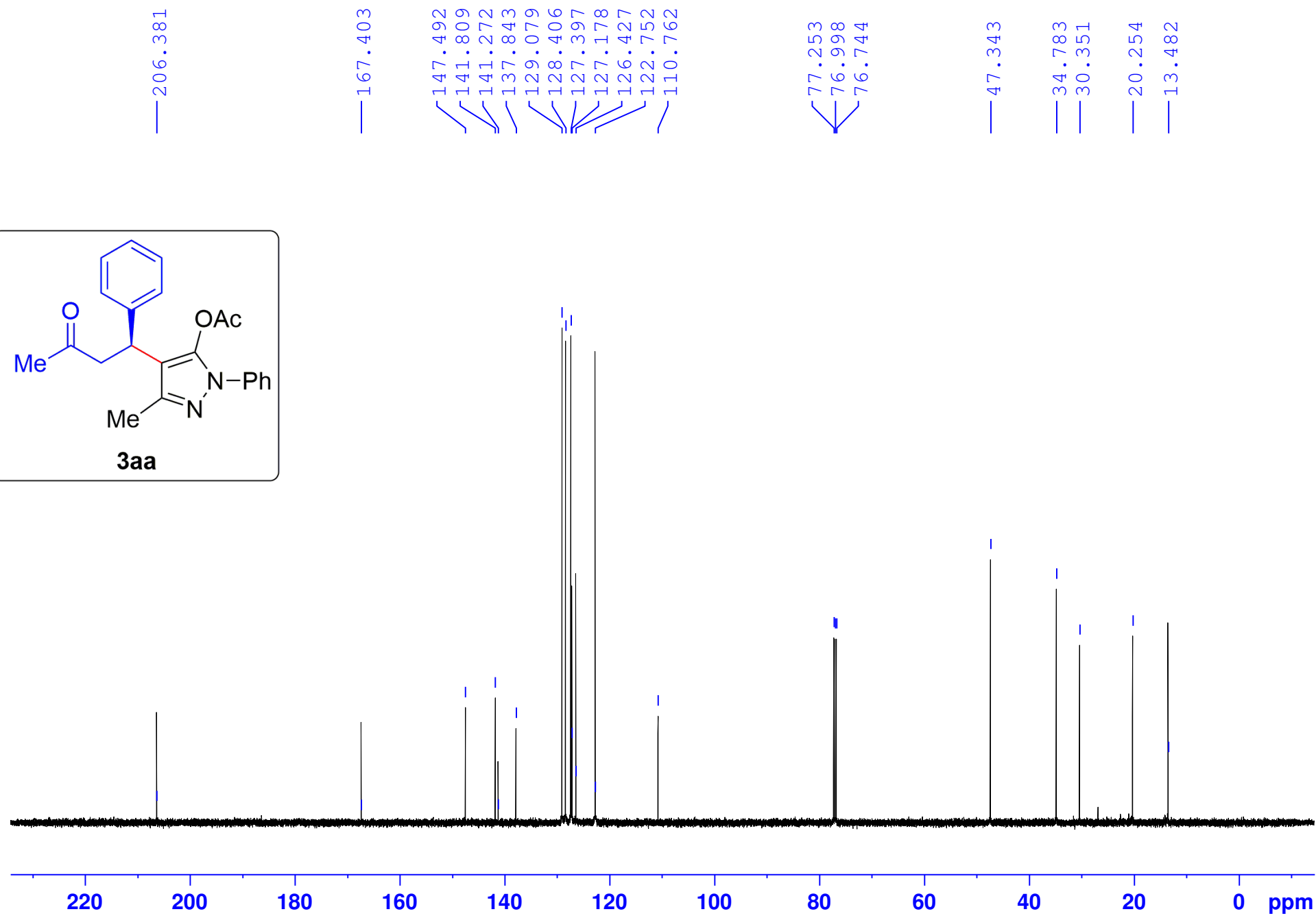
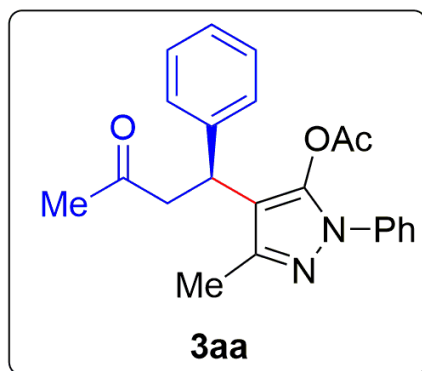


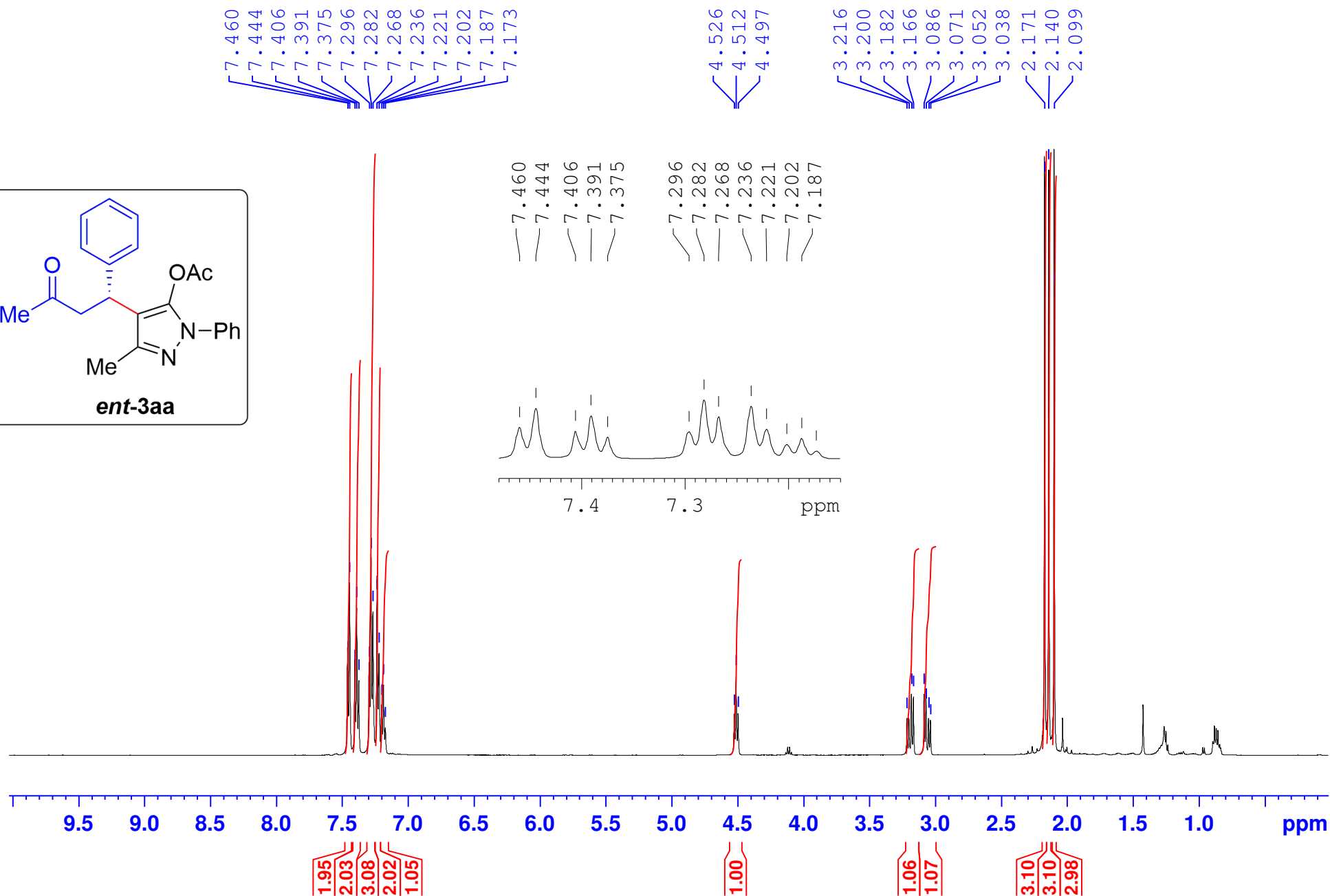
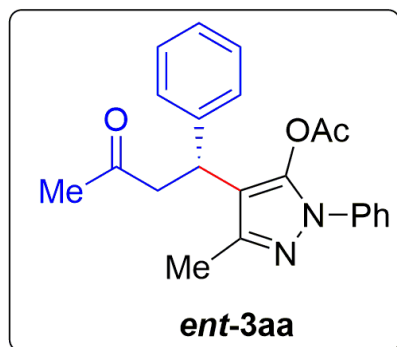
Date Acquired: 13-01-2023 18:41:08 IST
Date Processed: 16-01-2023 11:57:27 IST

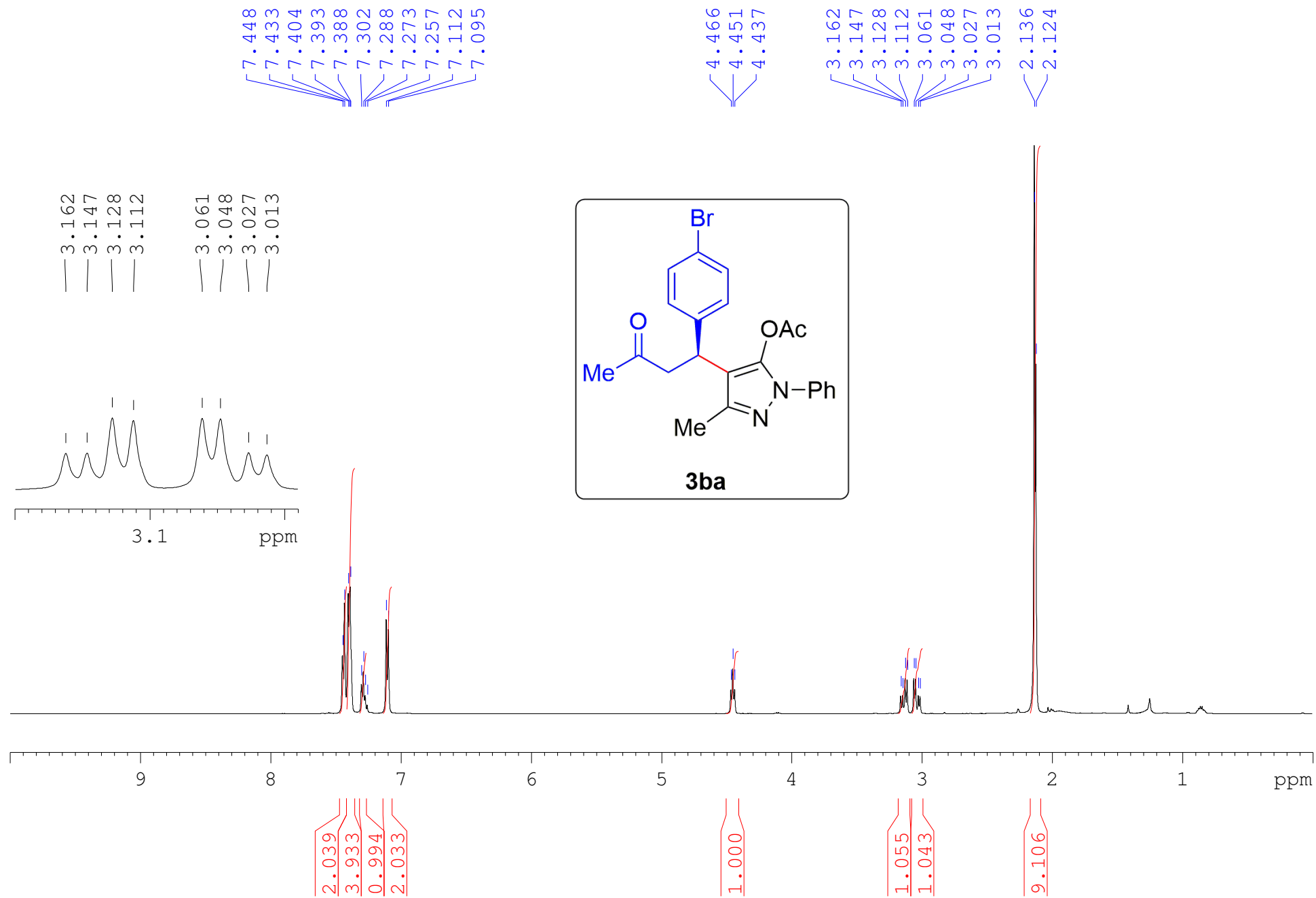


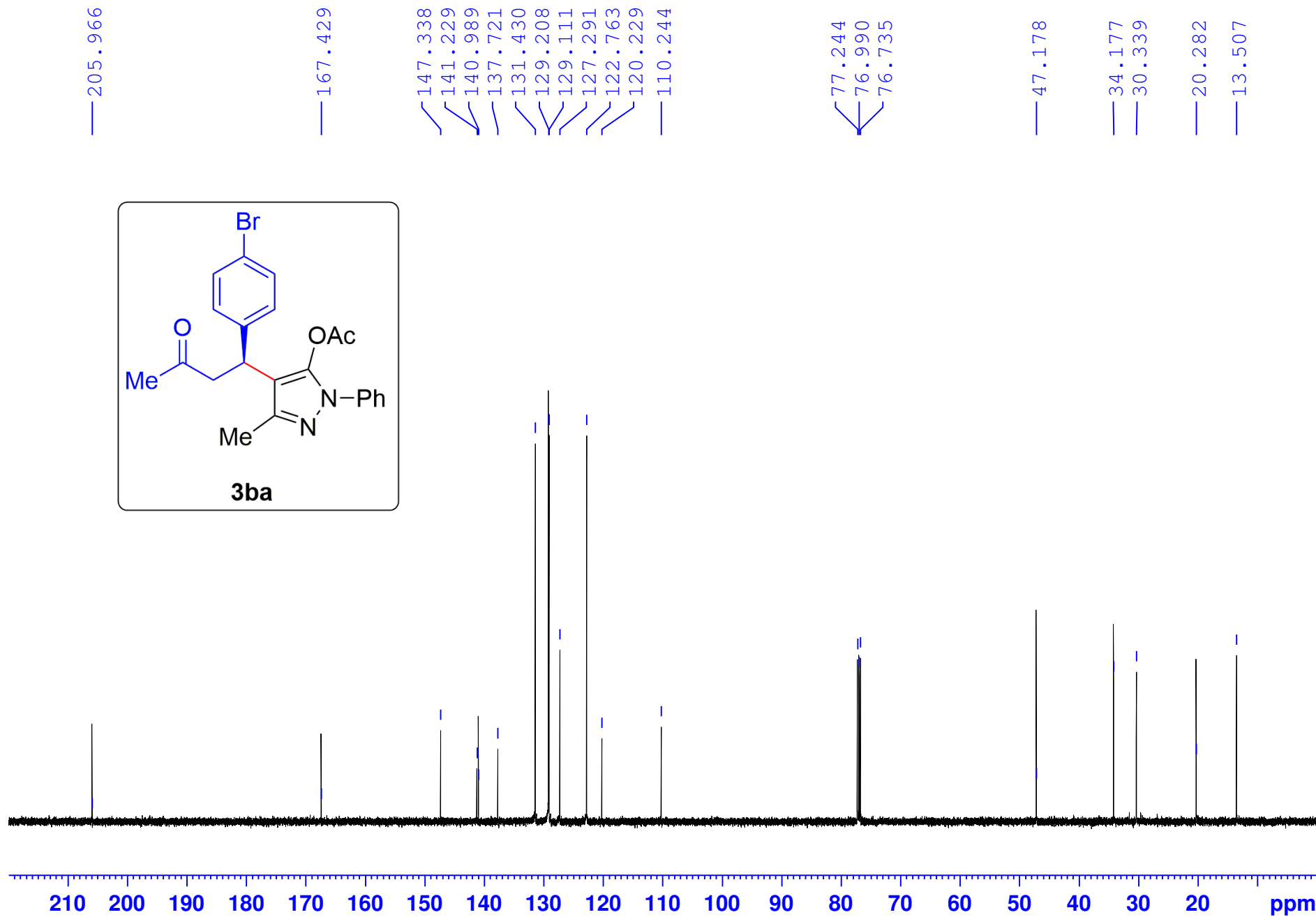
	RT	Area	% Area	Height
1	16.561	42604173	95.76	1125024
2	18.118	1884169	4.24	36487

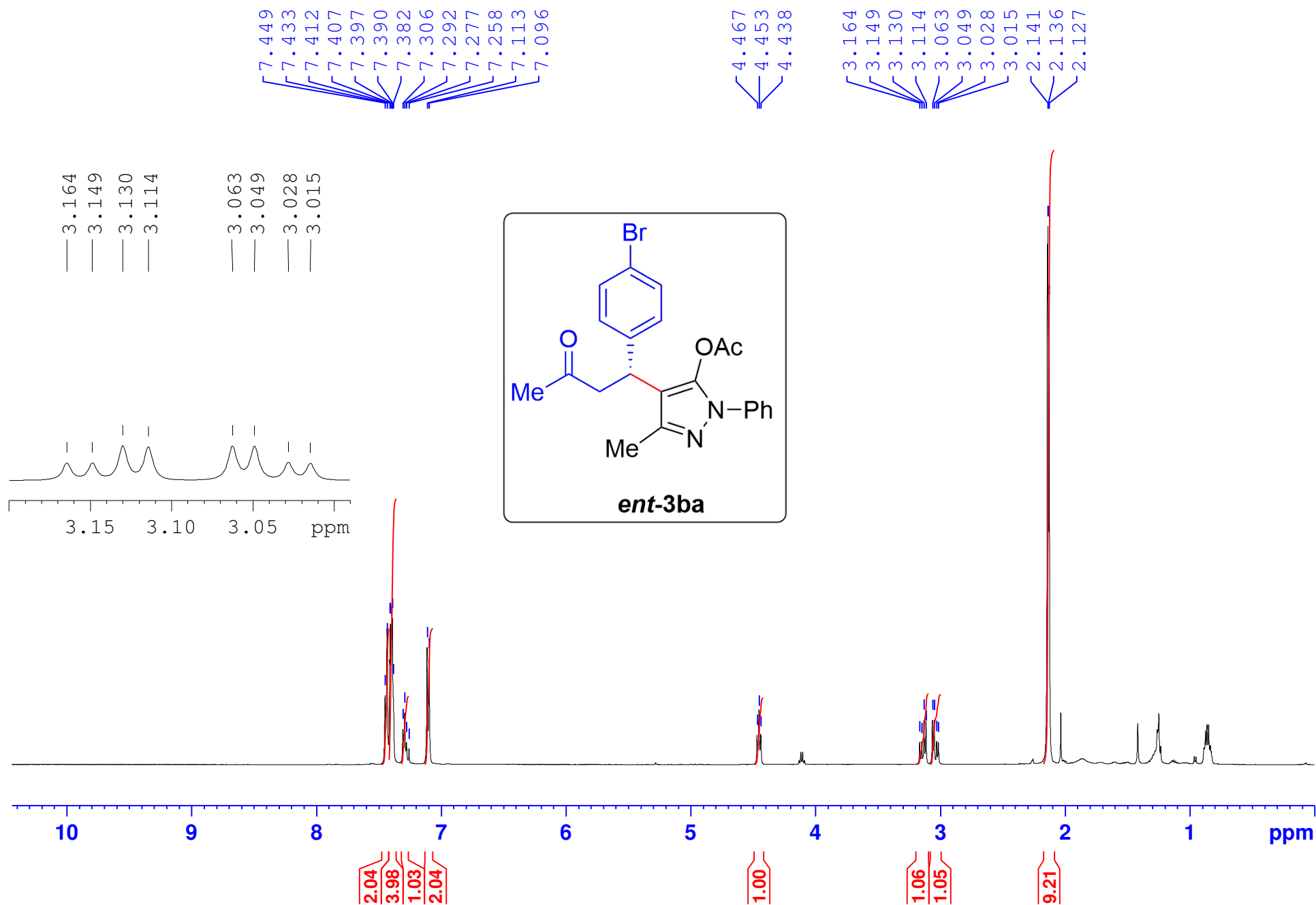


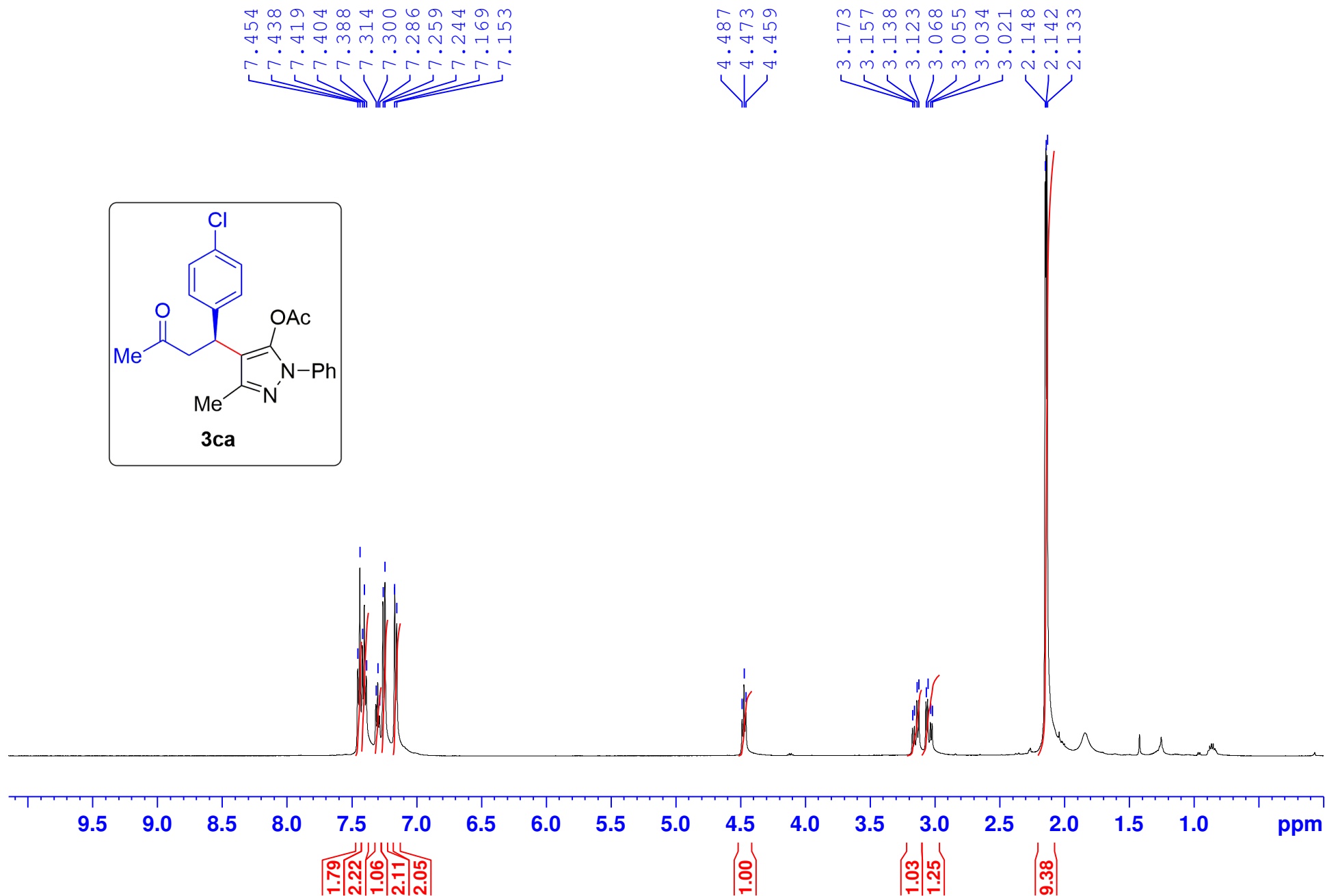


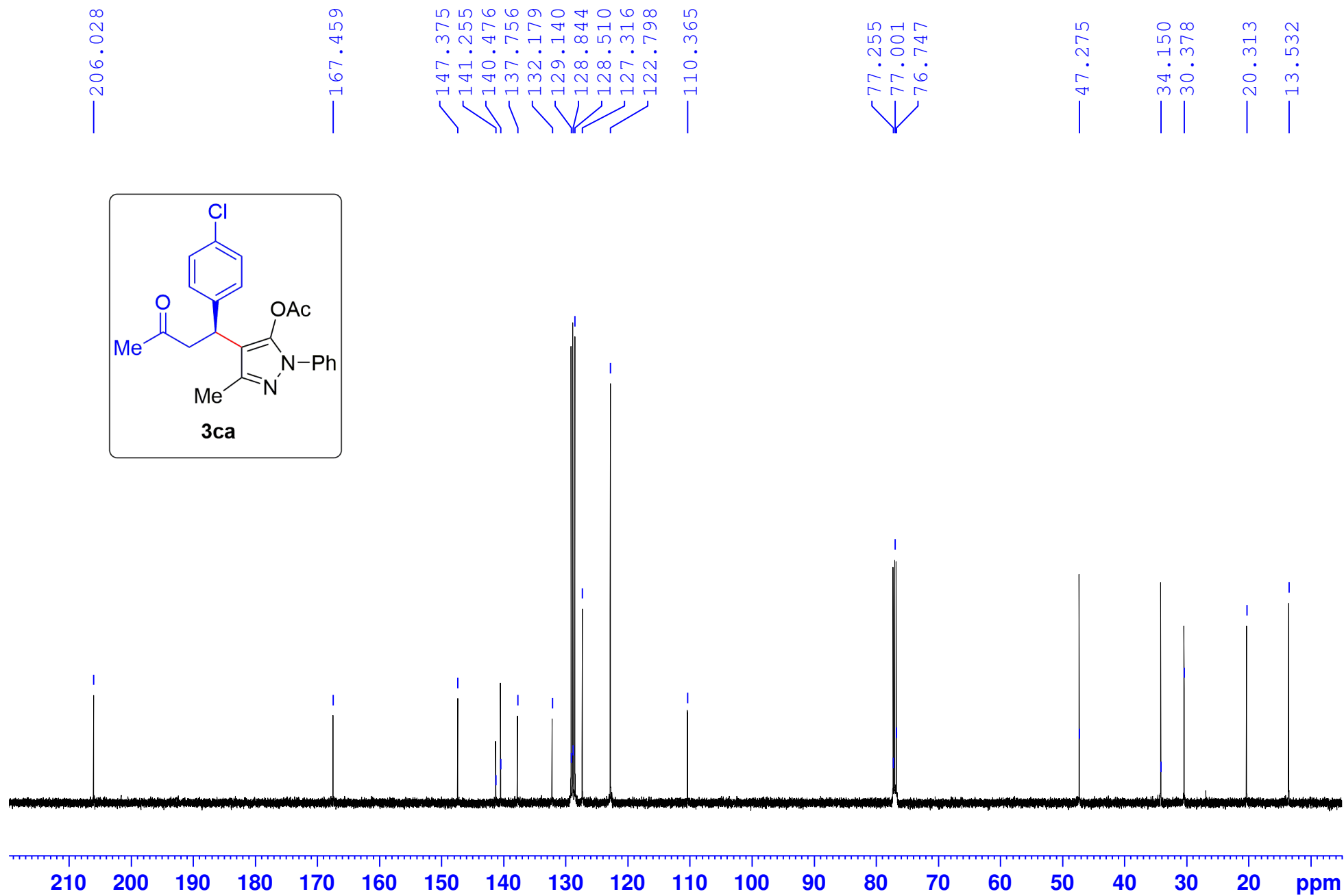
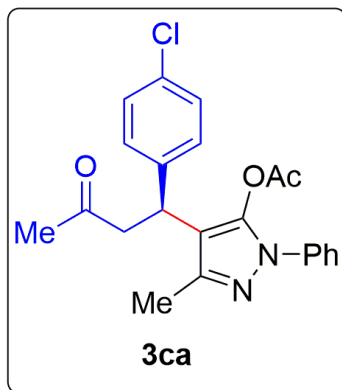


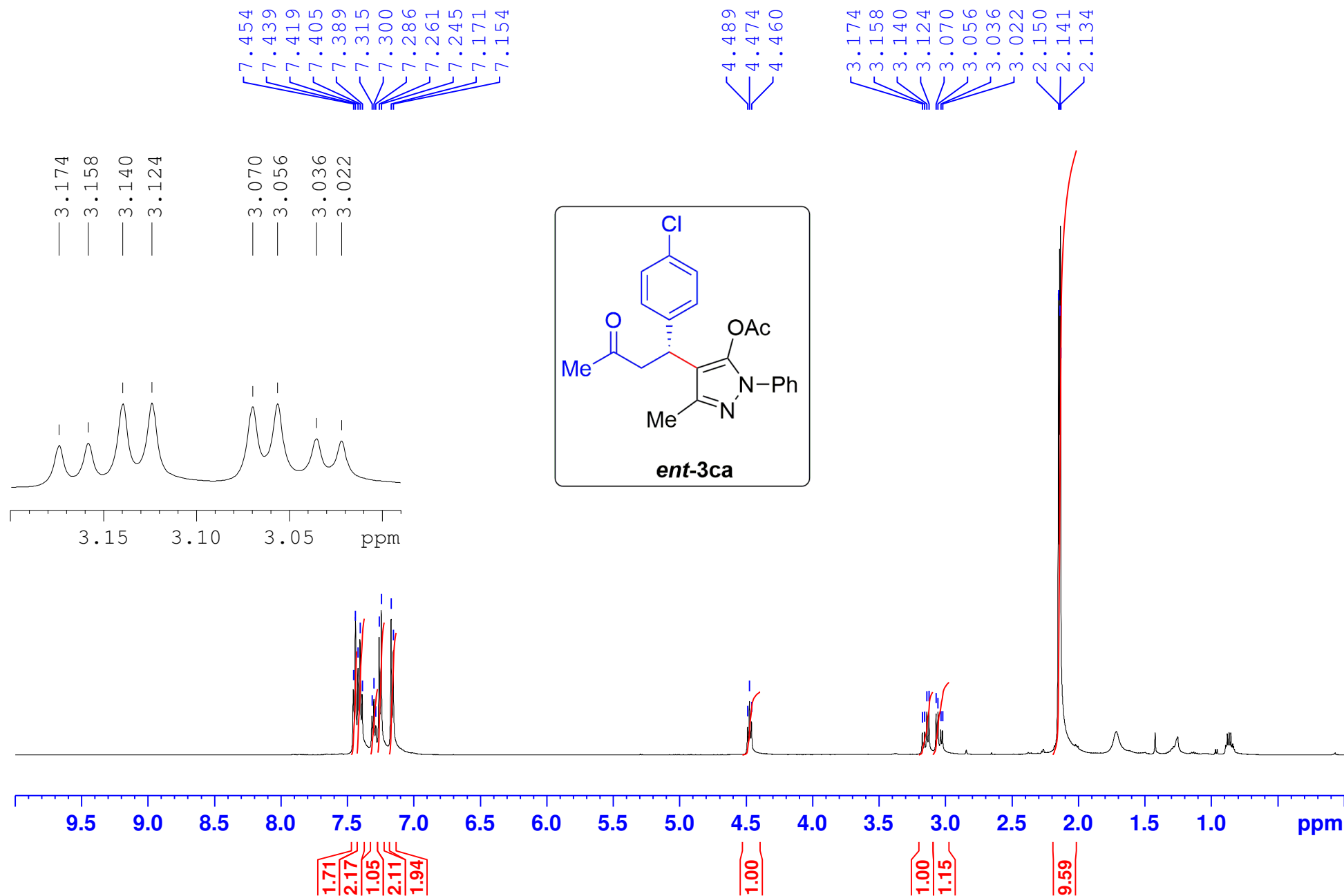


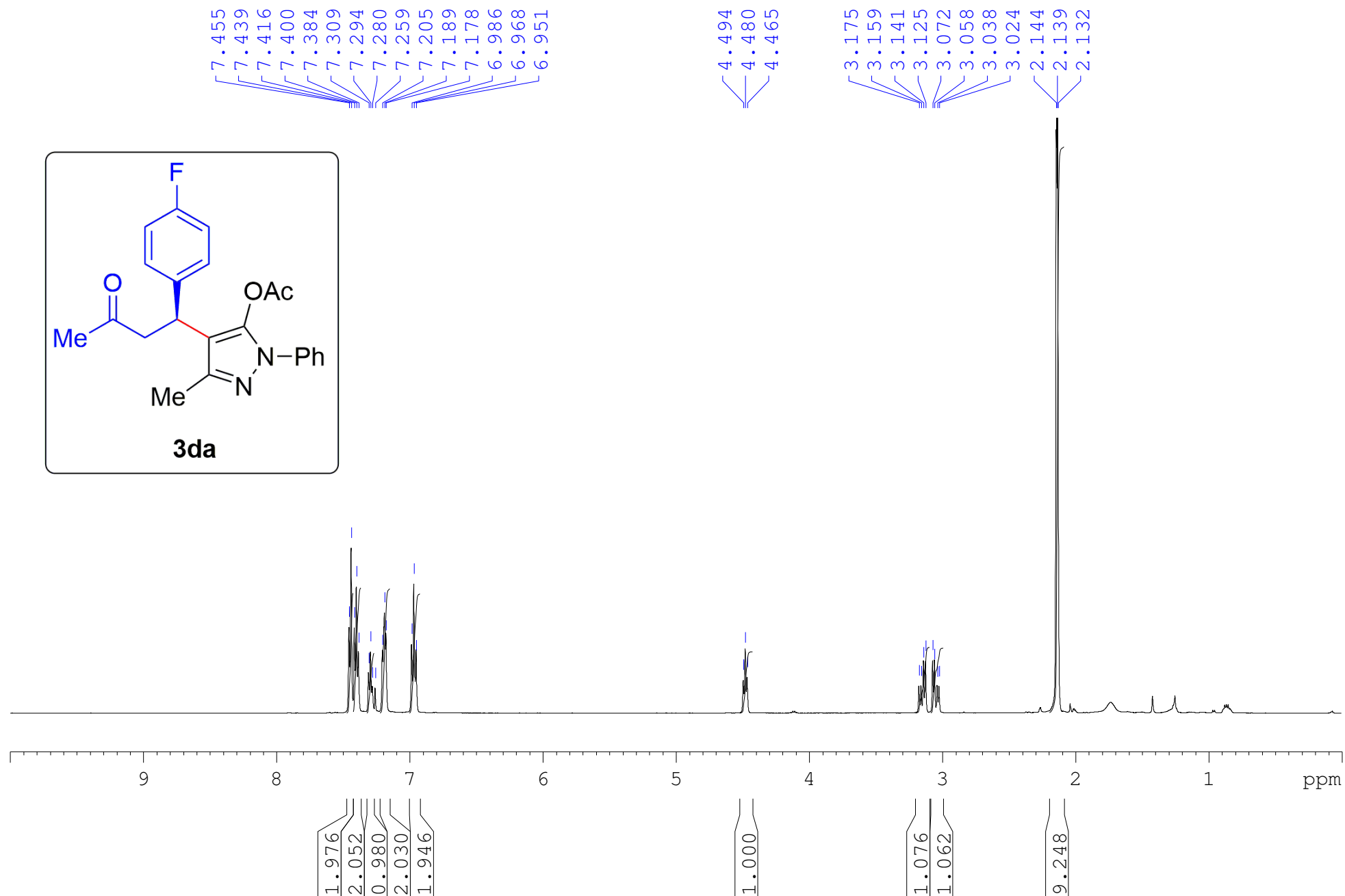


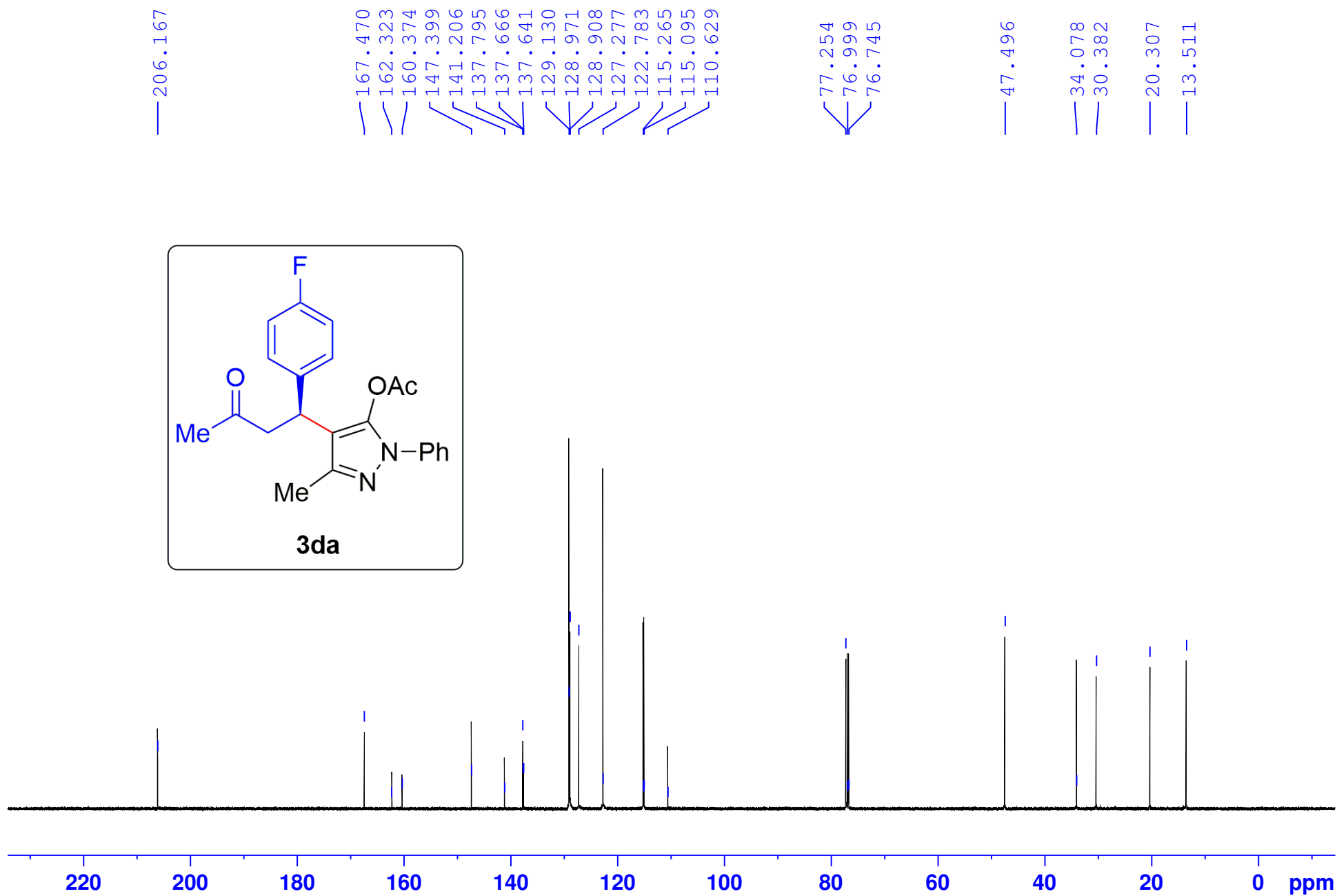


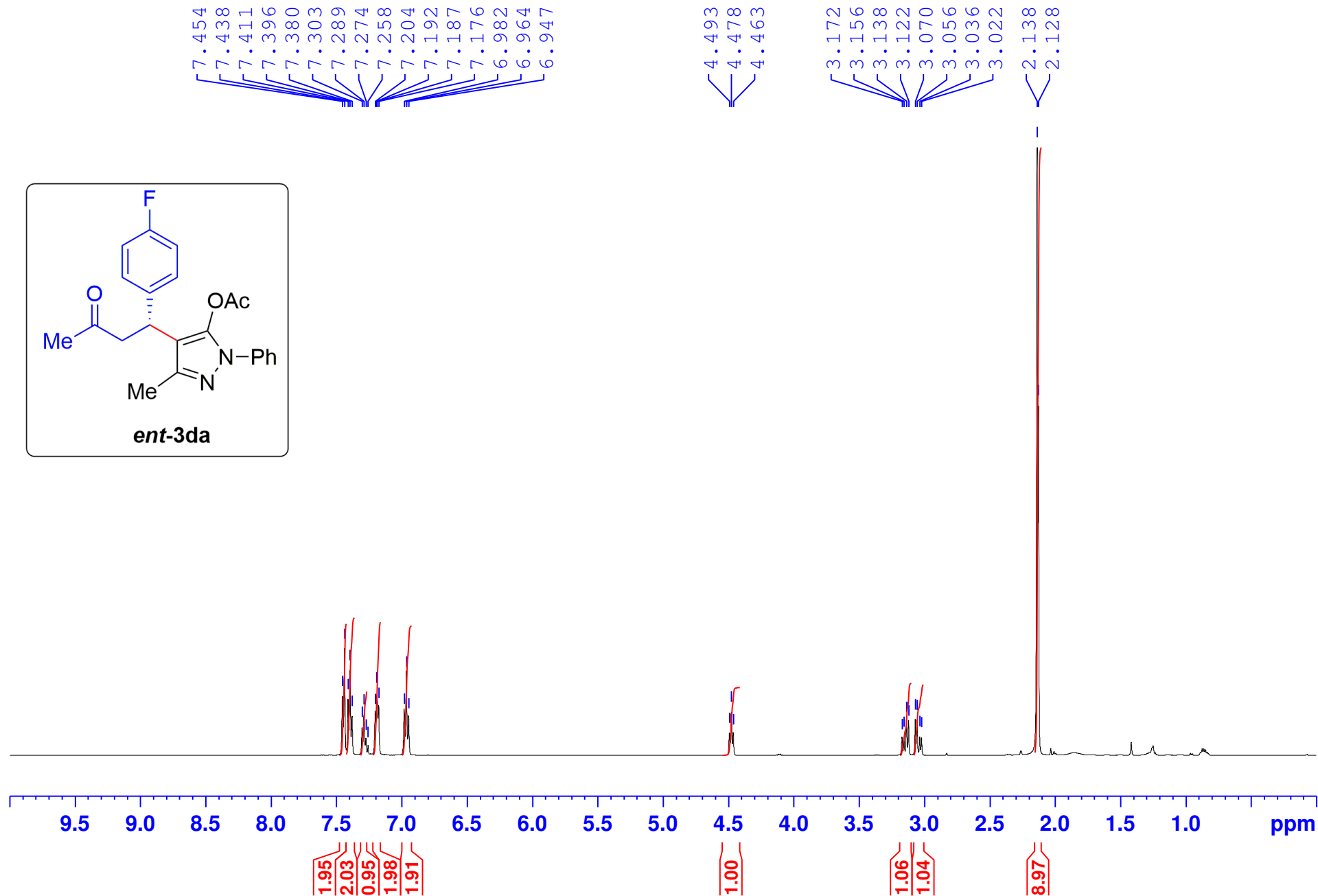


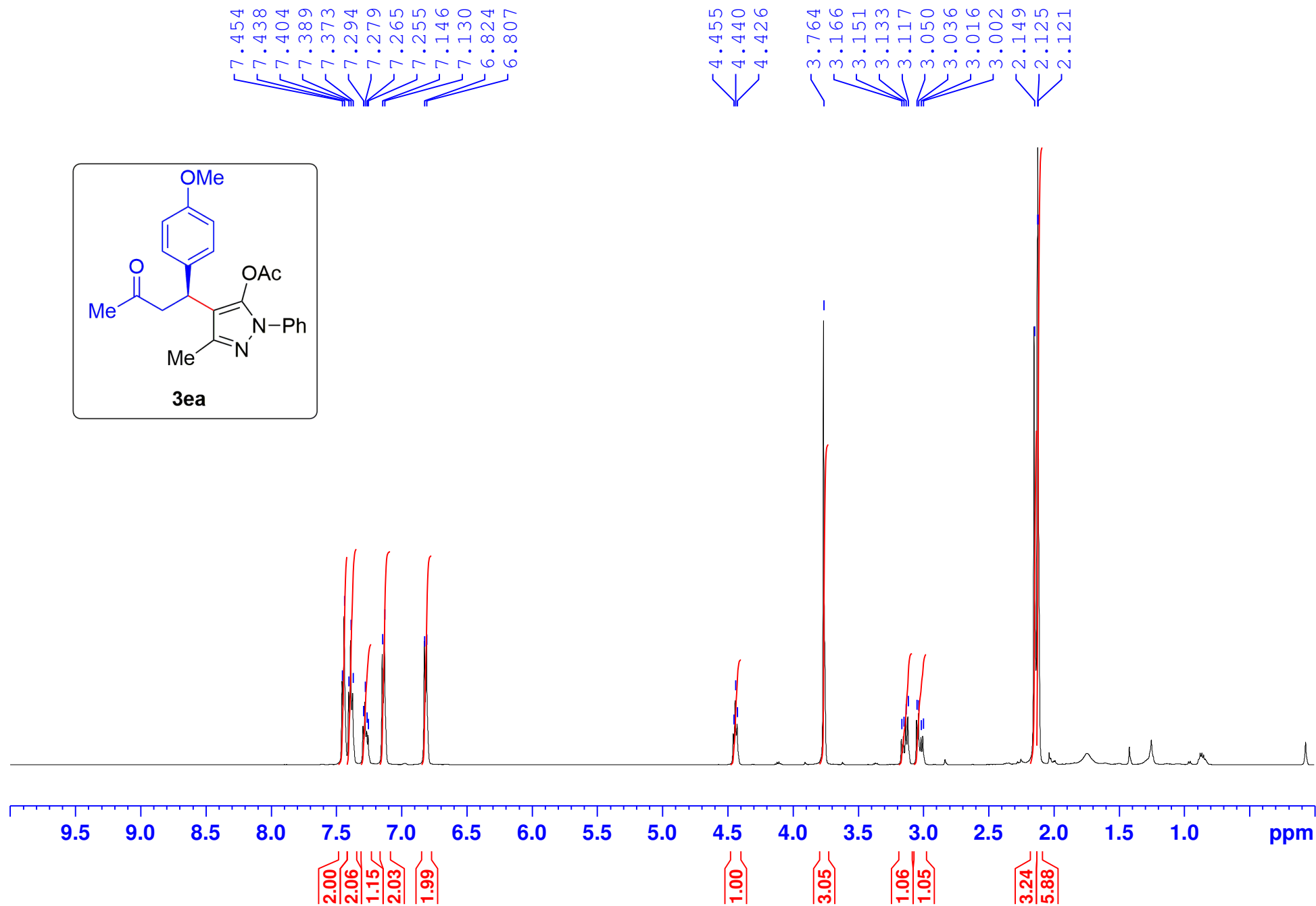


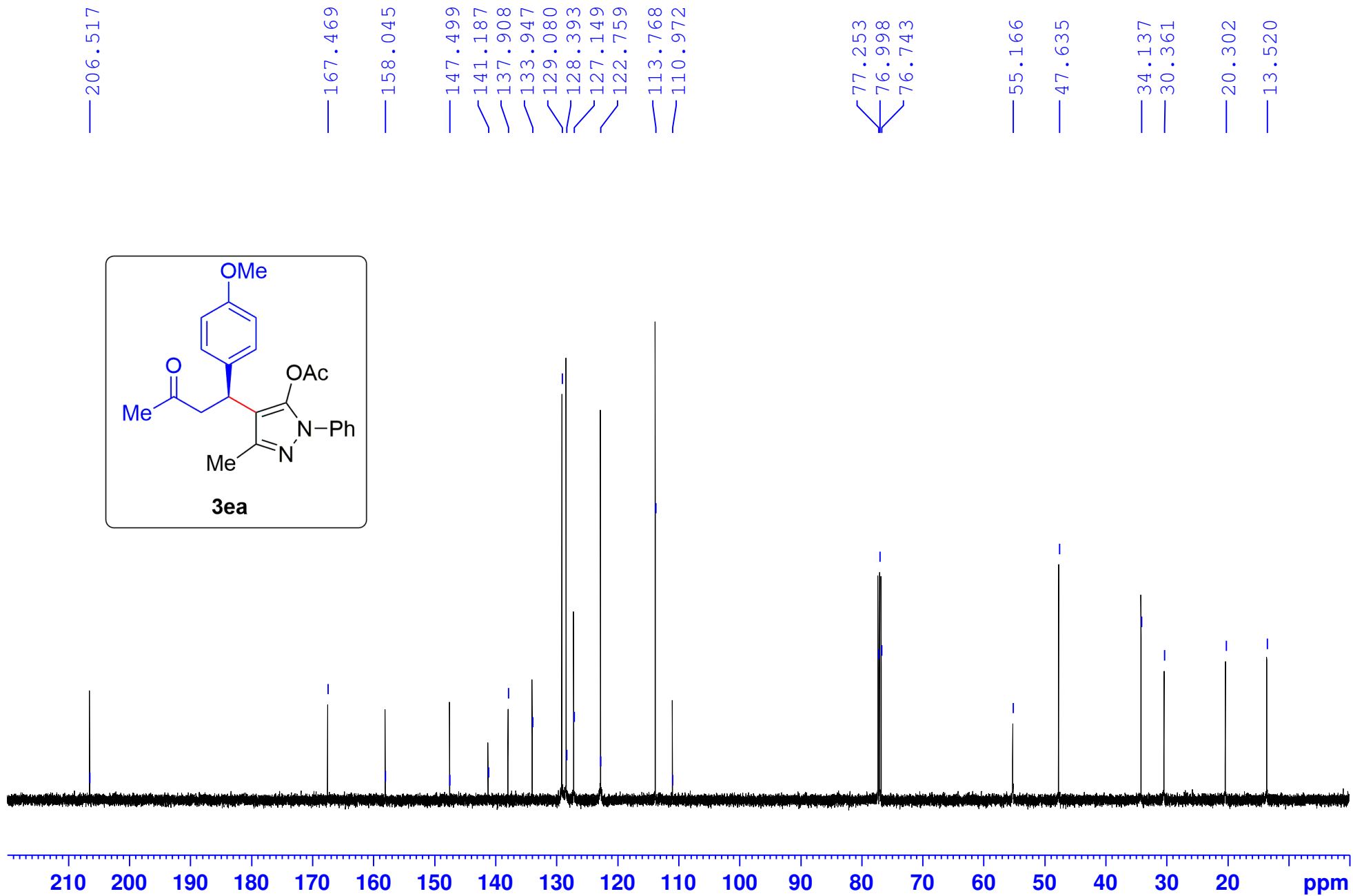


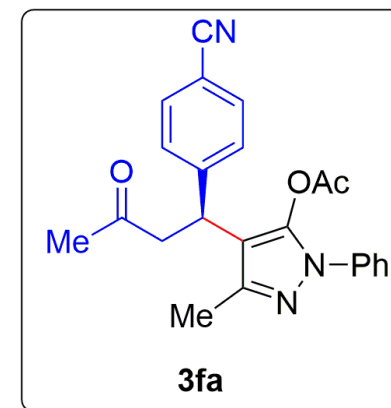
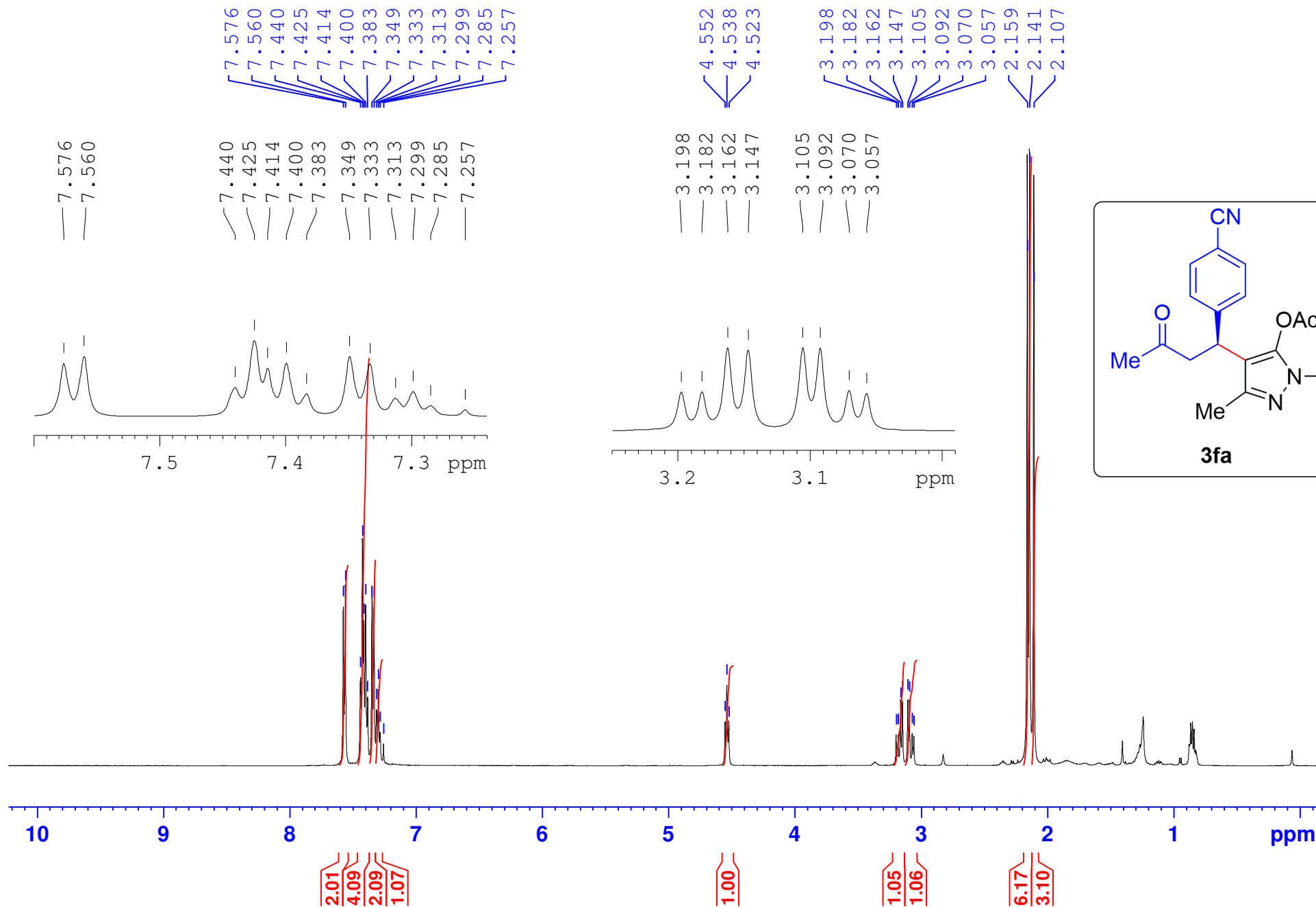


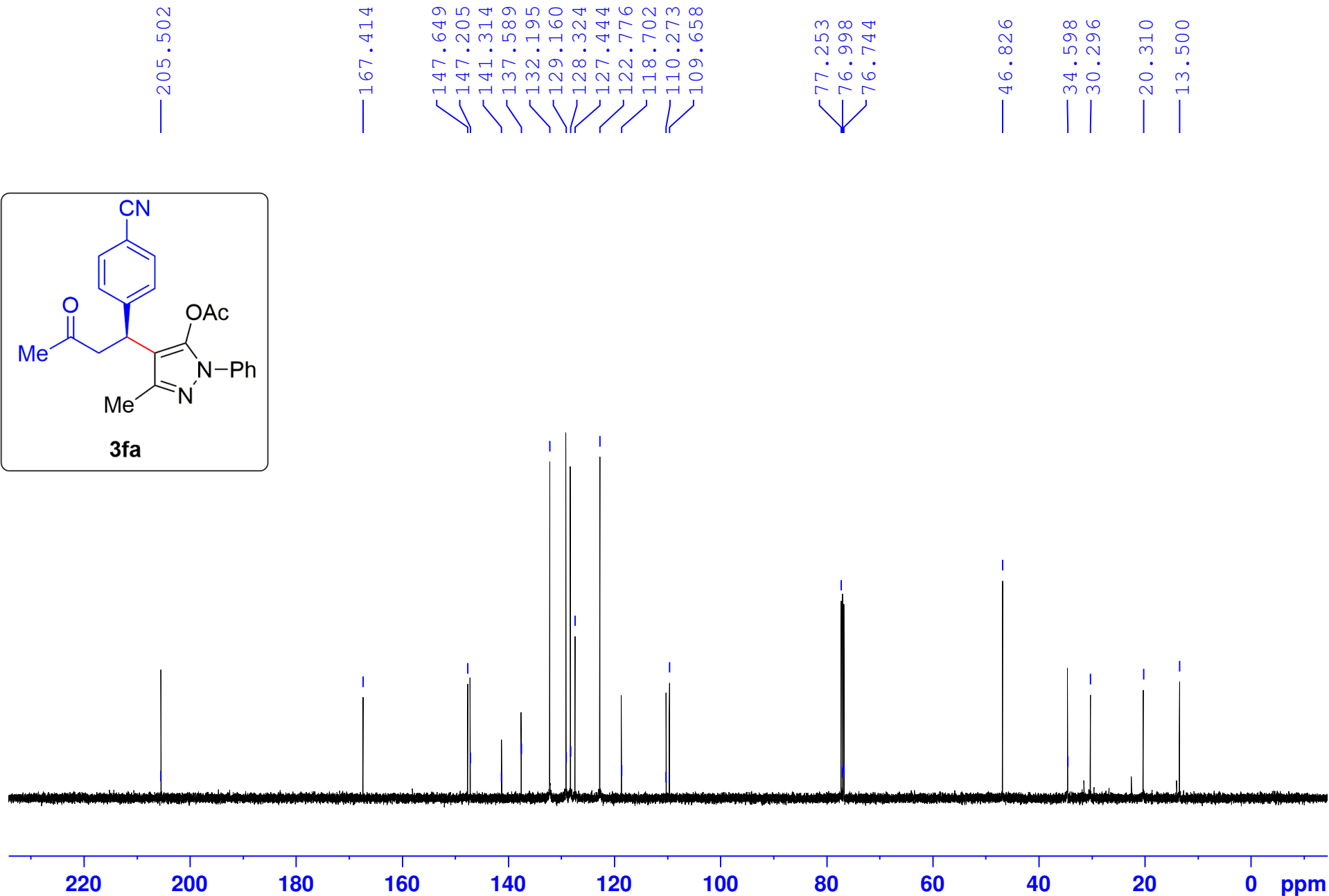
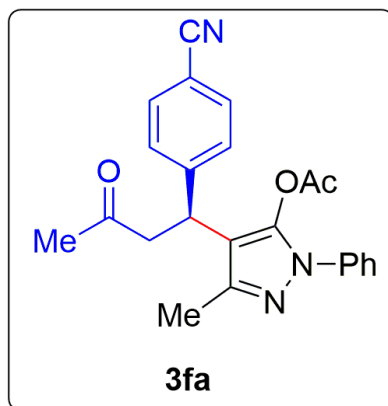


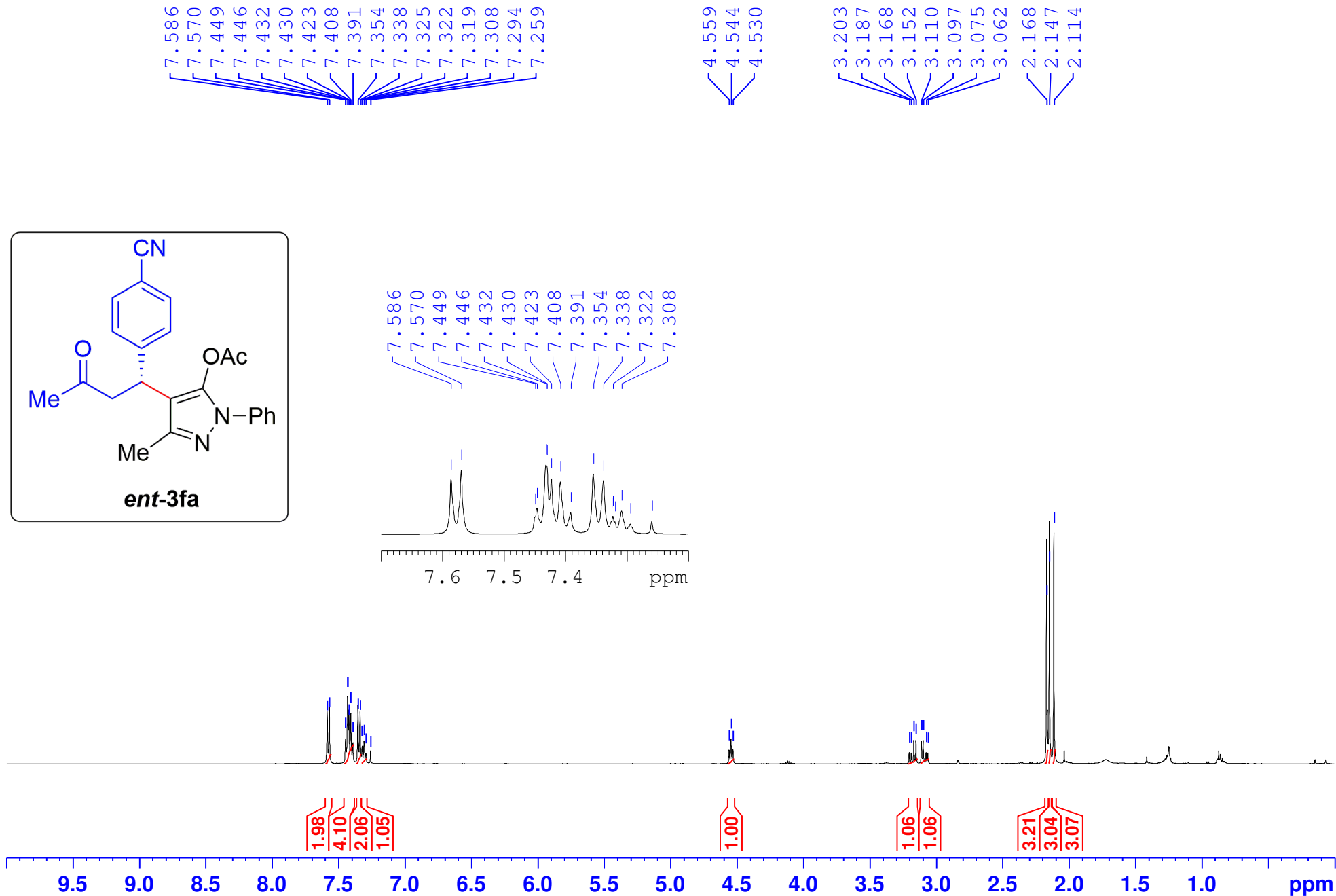


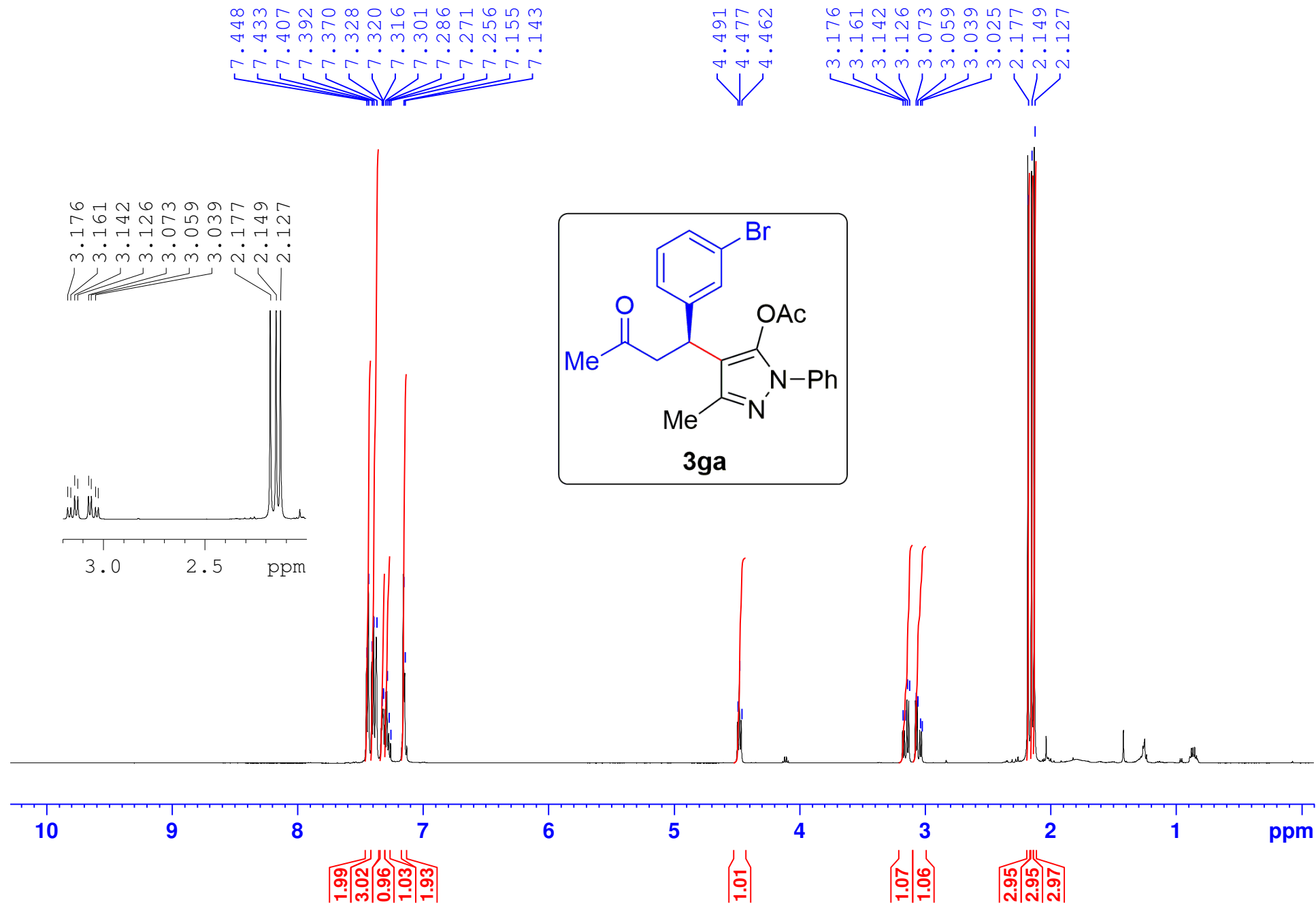


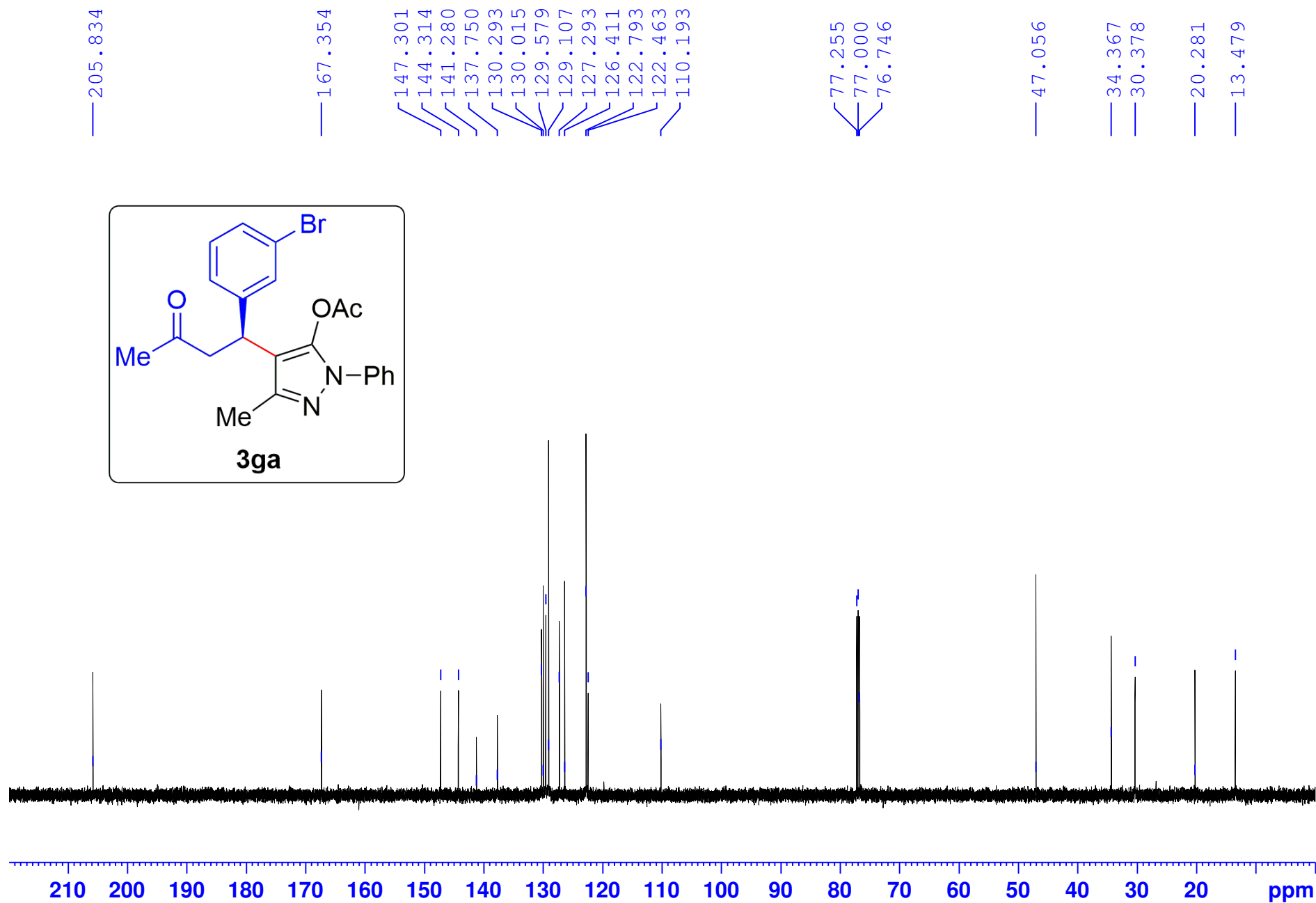
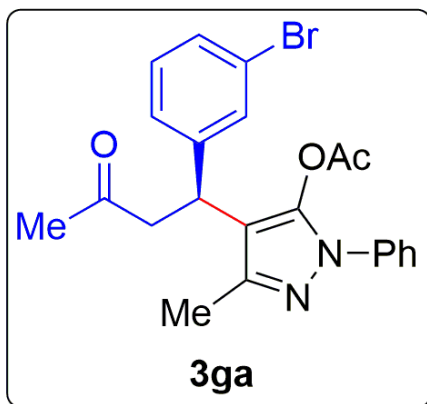


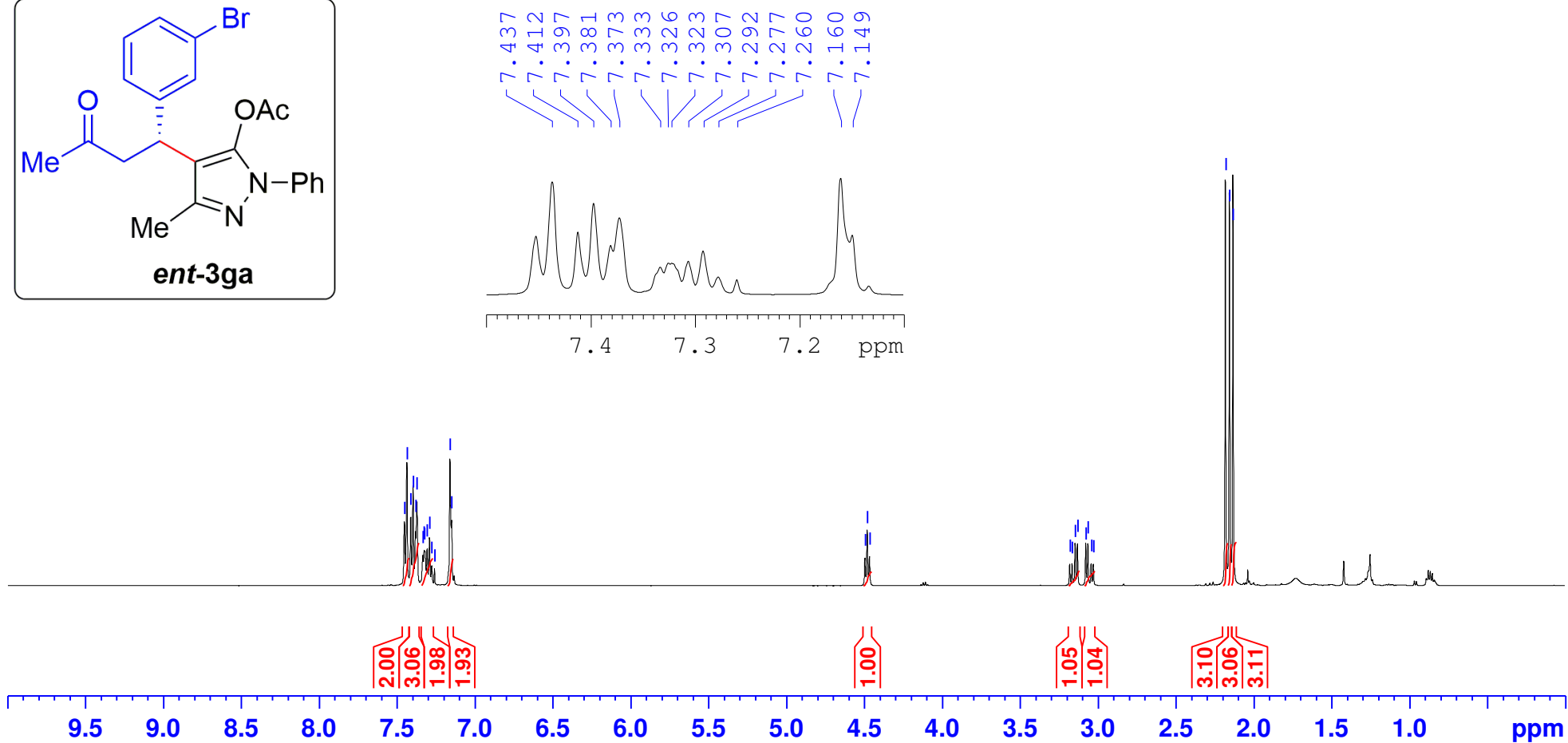
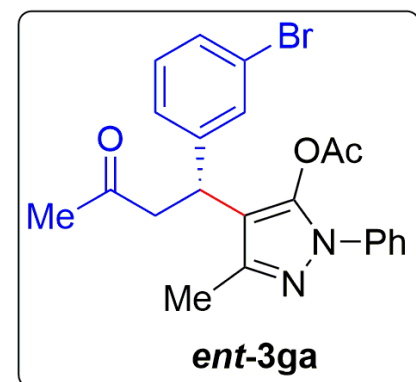


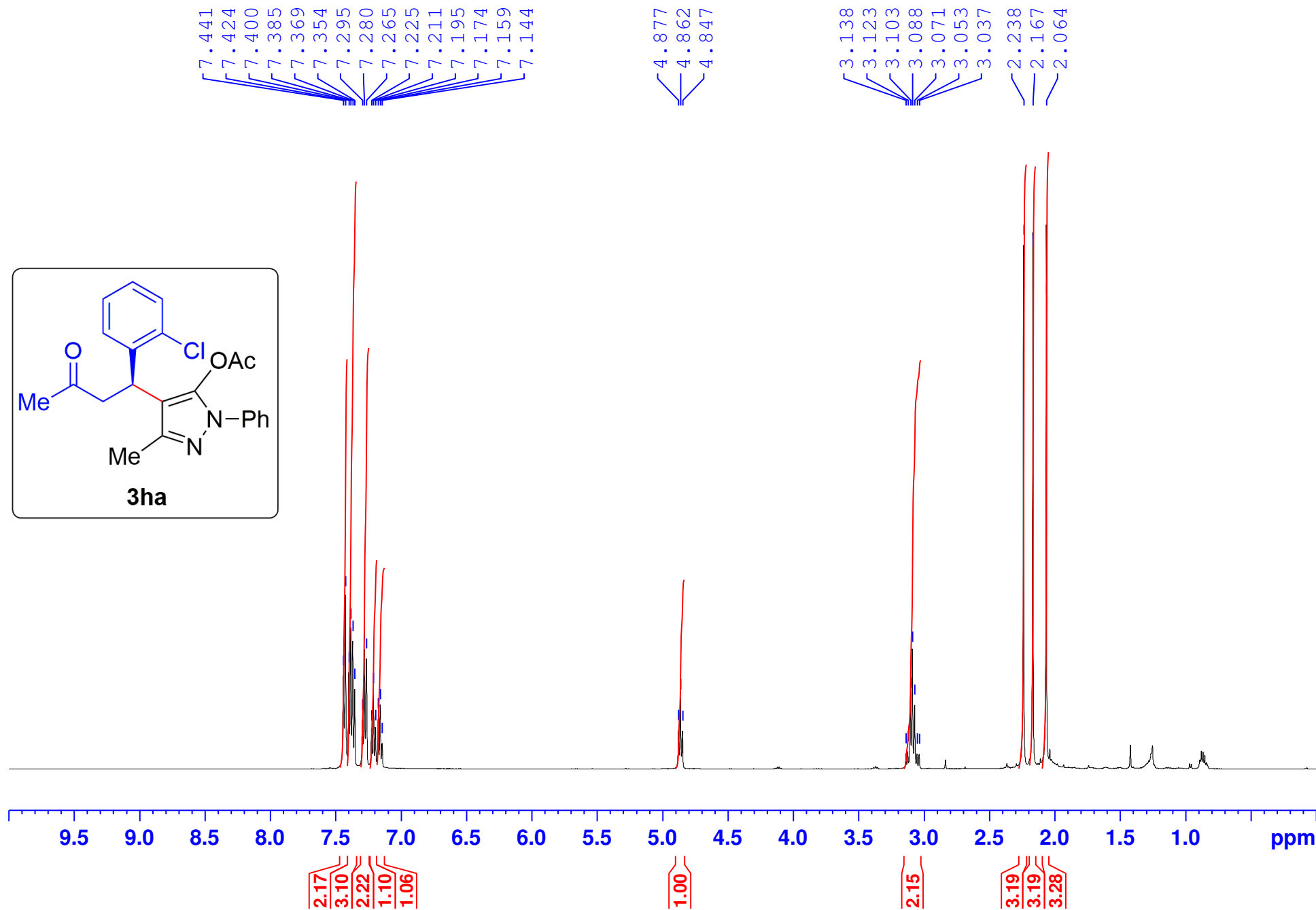
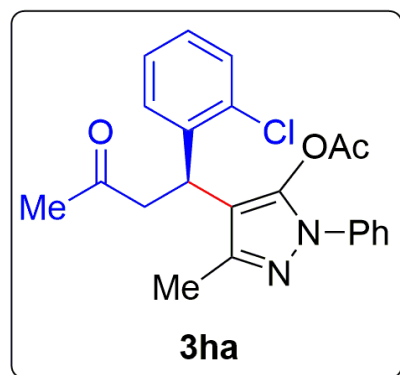


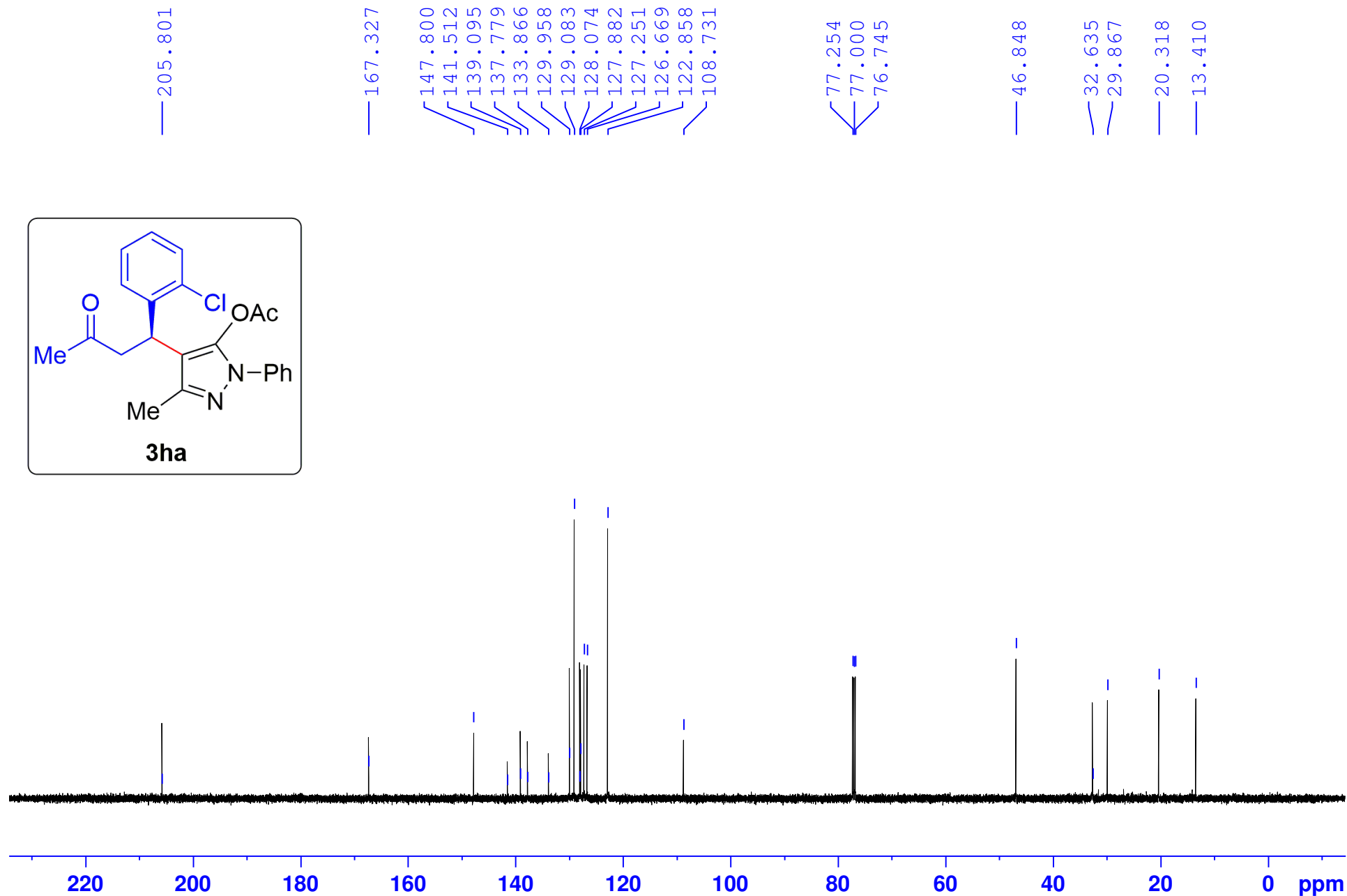
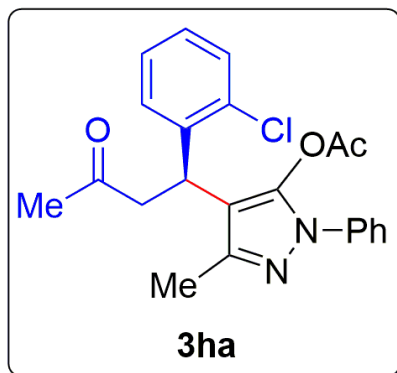


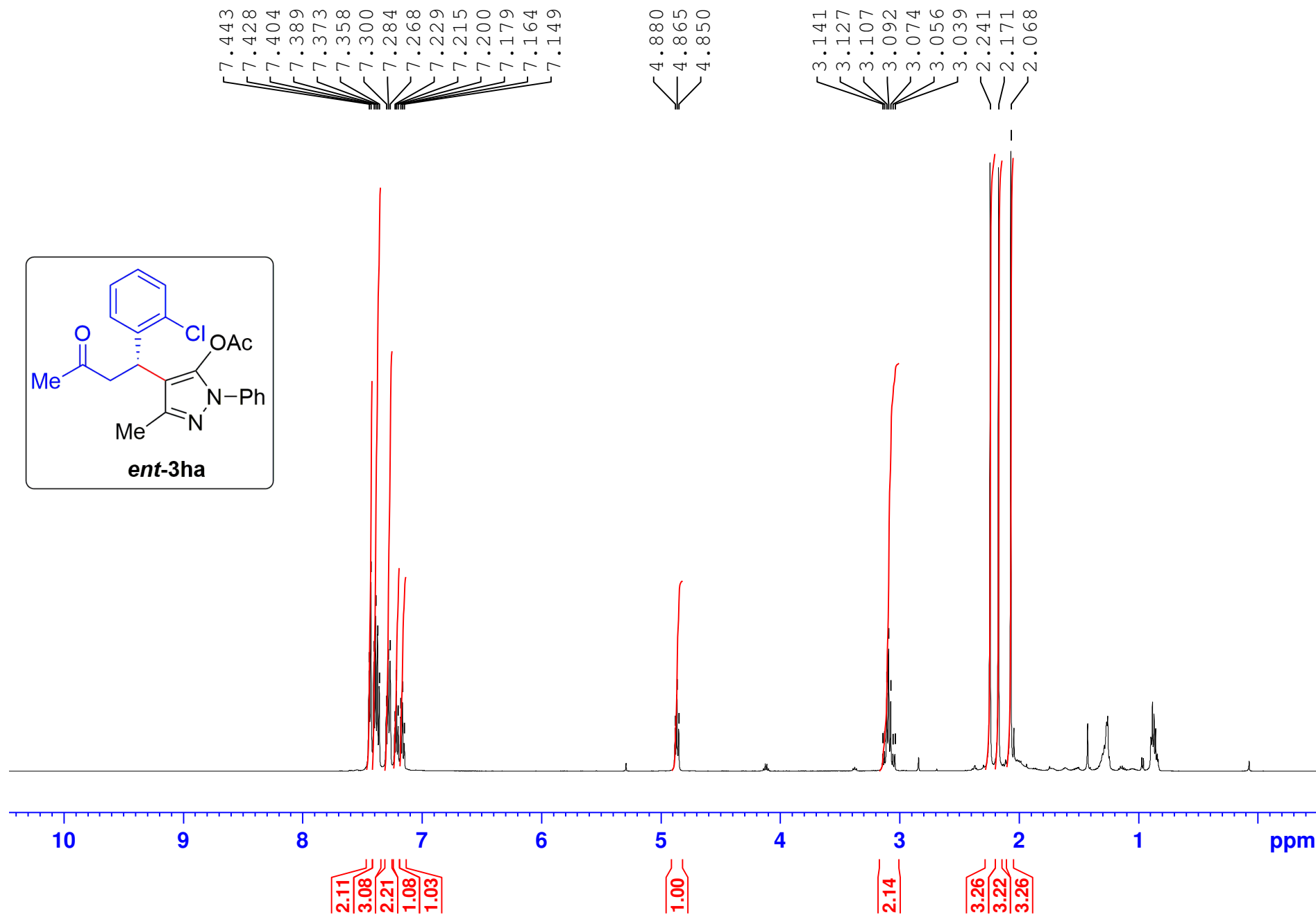


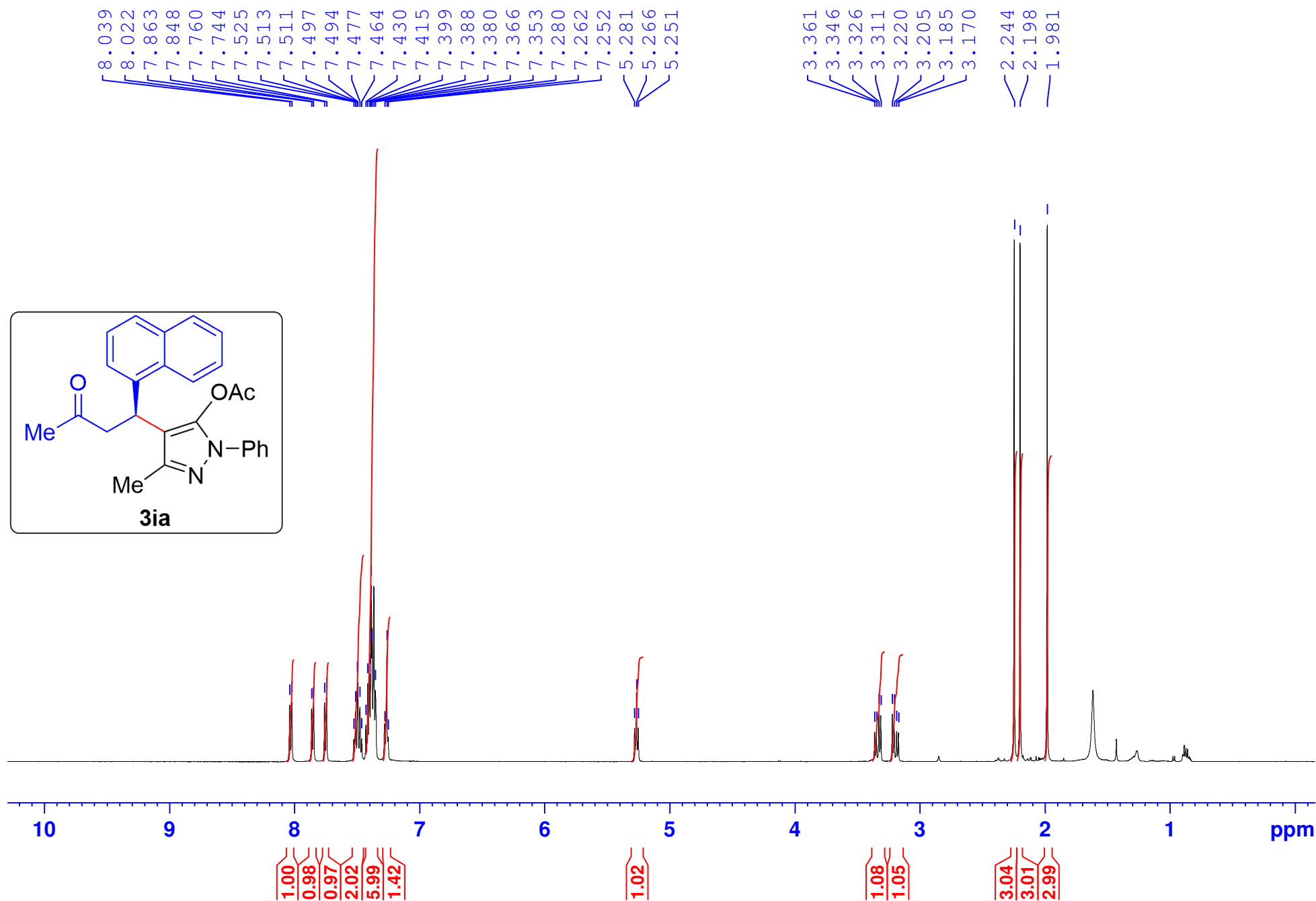


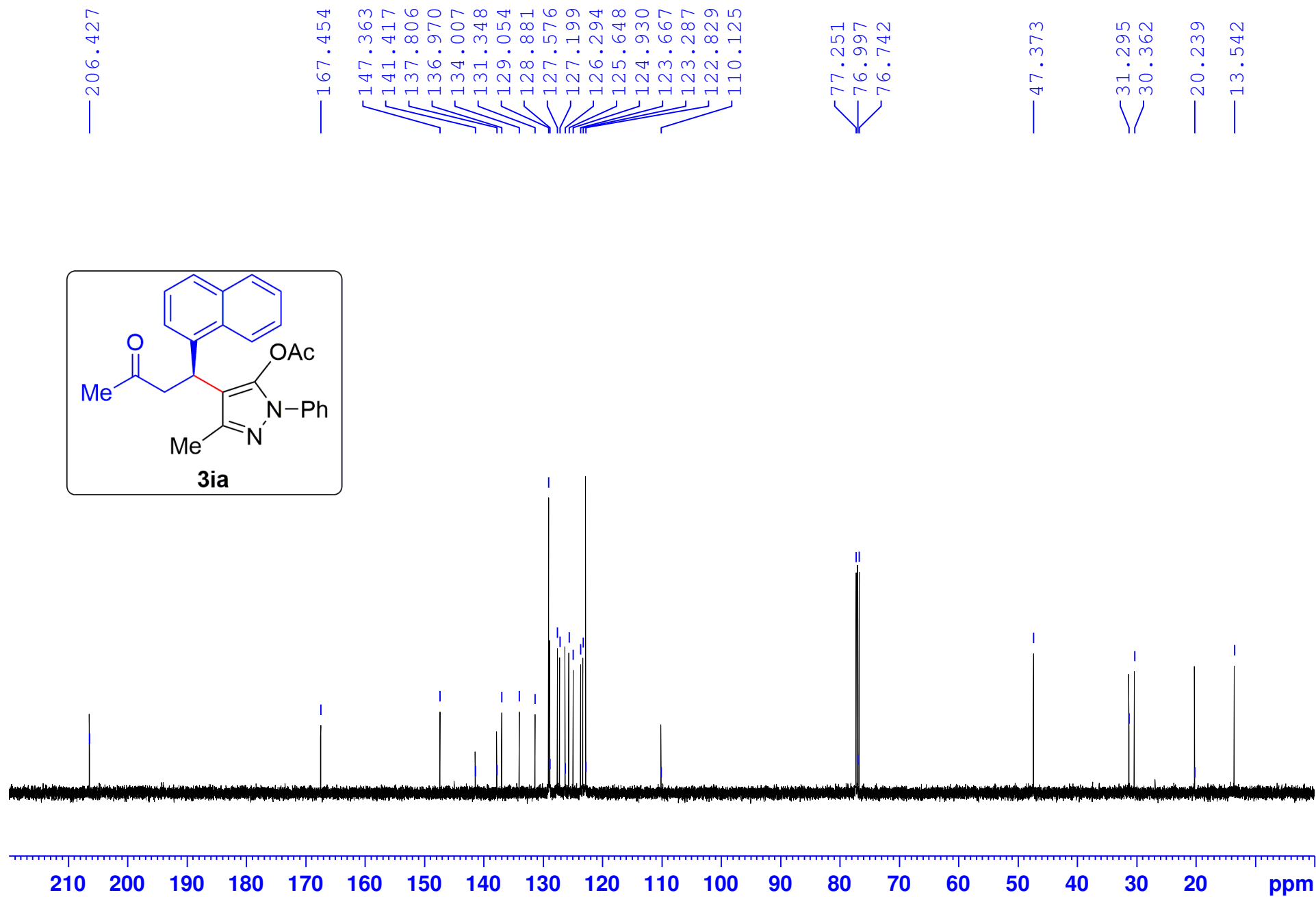
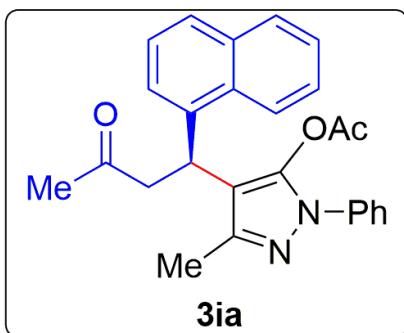


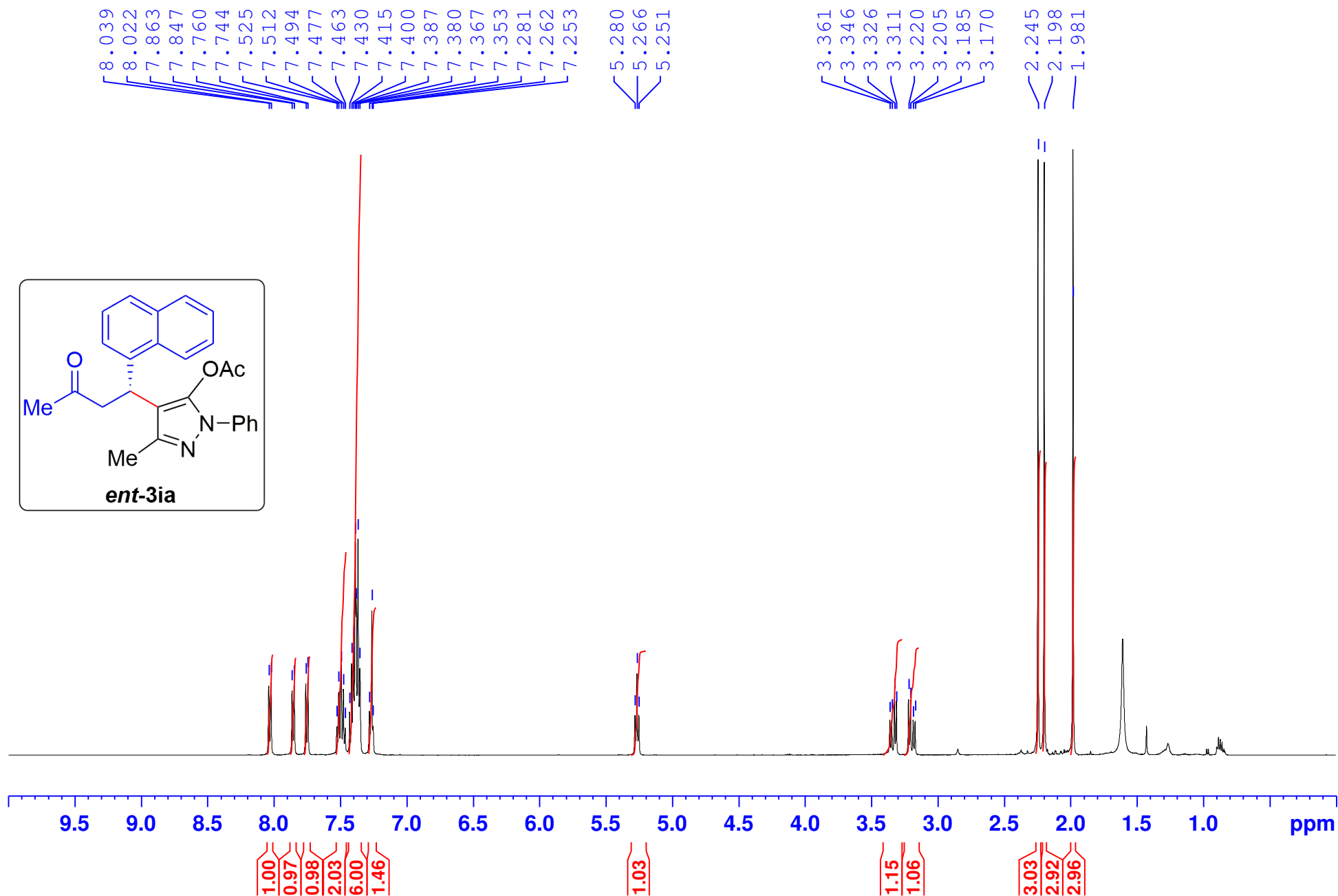


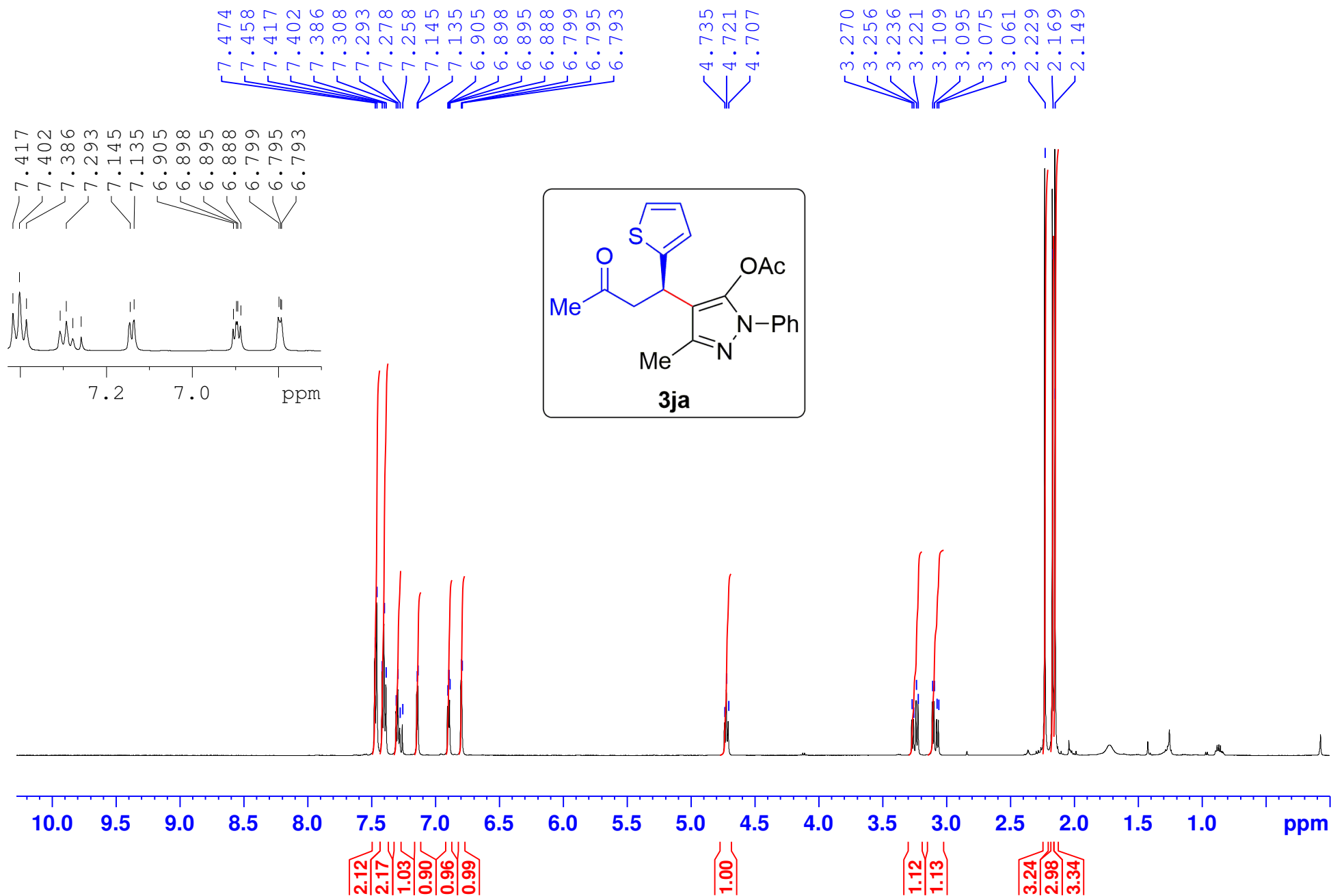


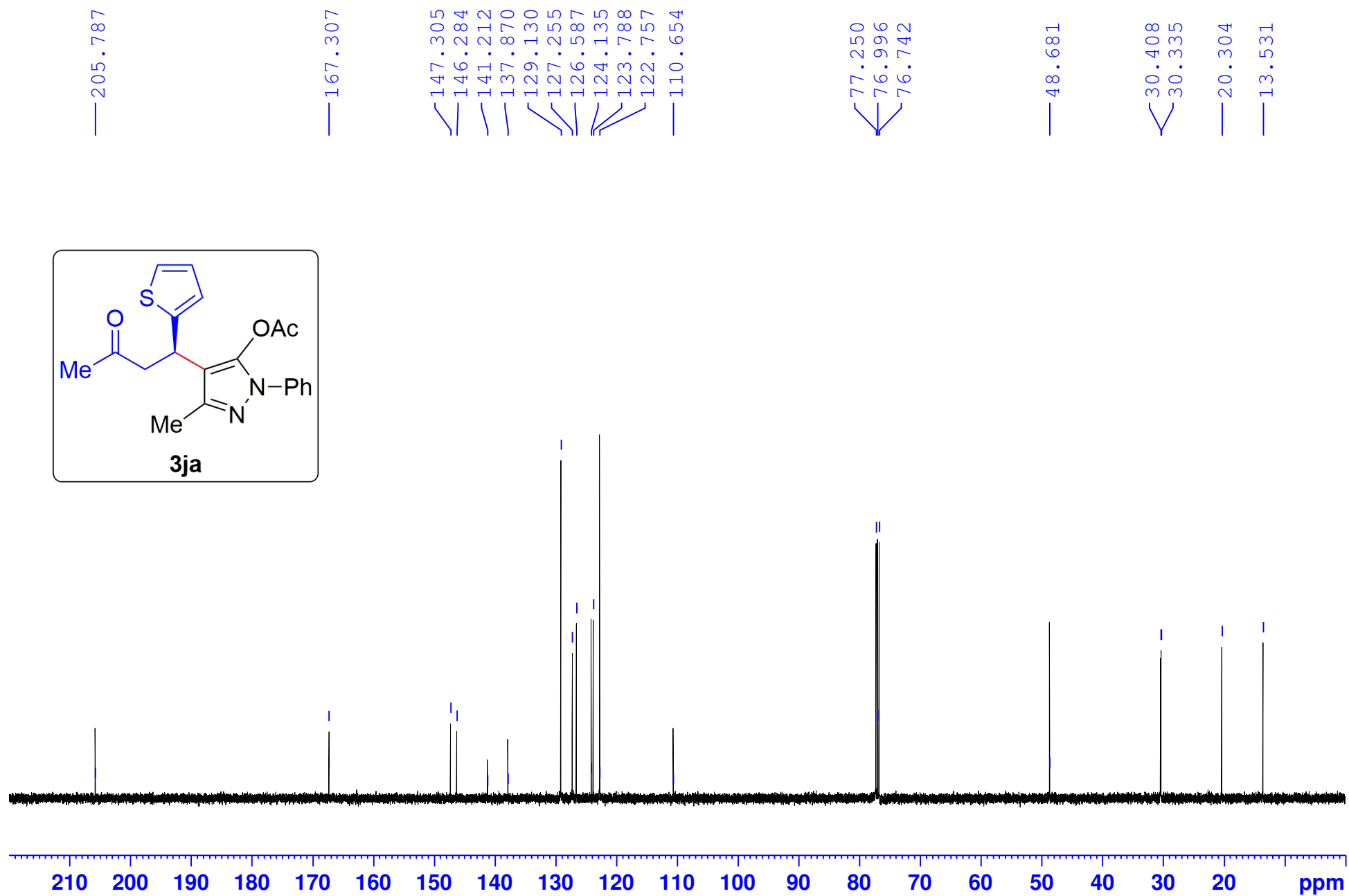


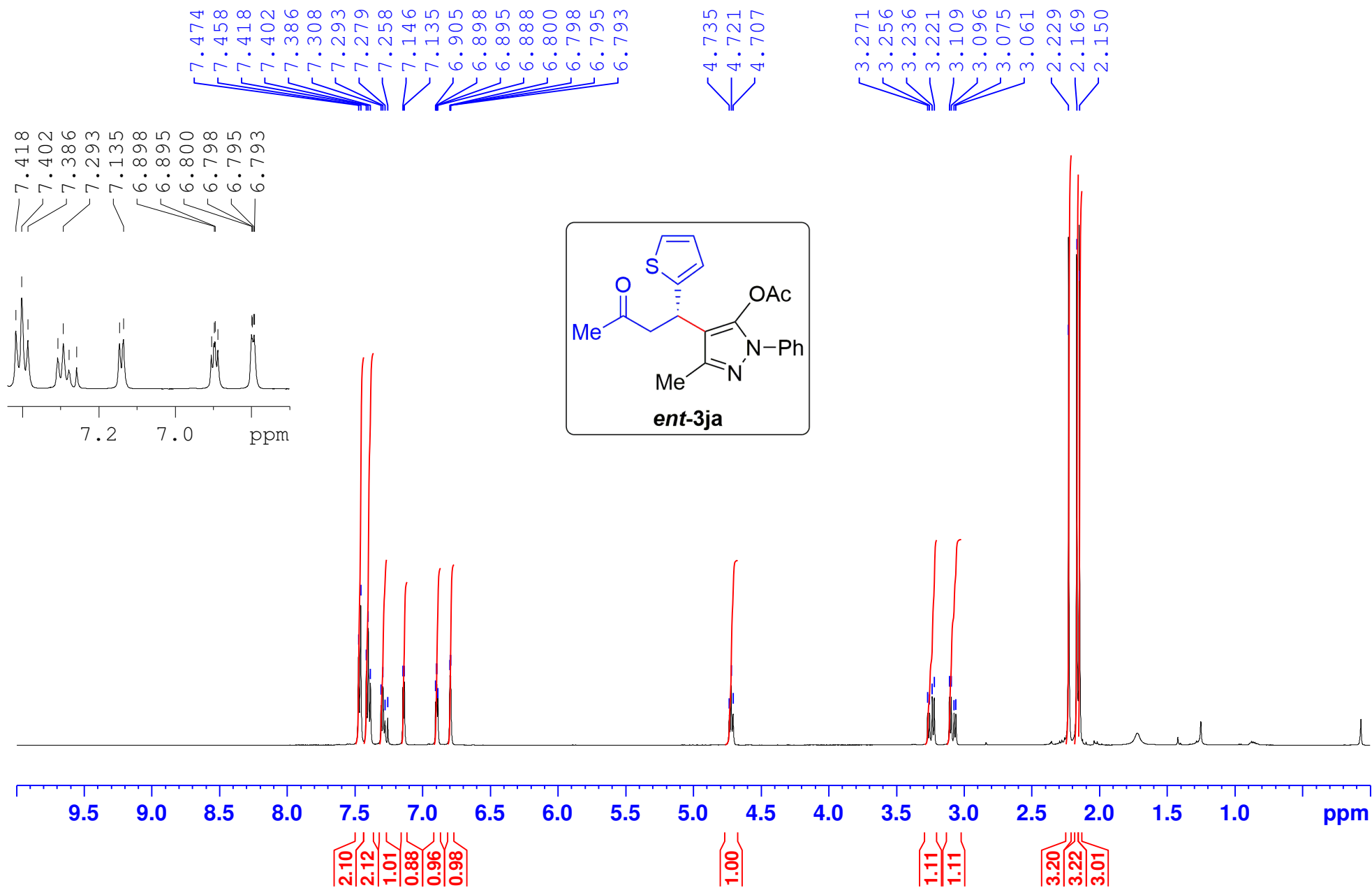


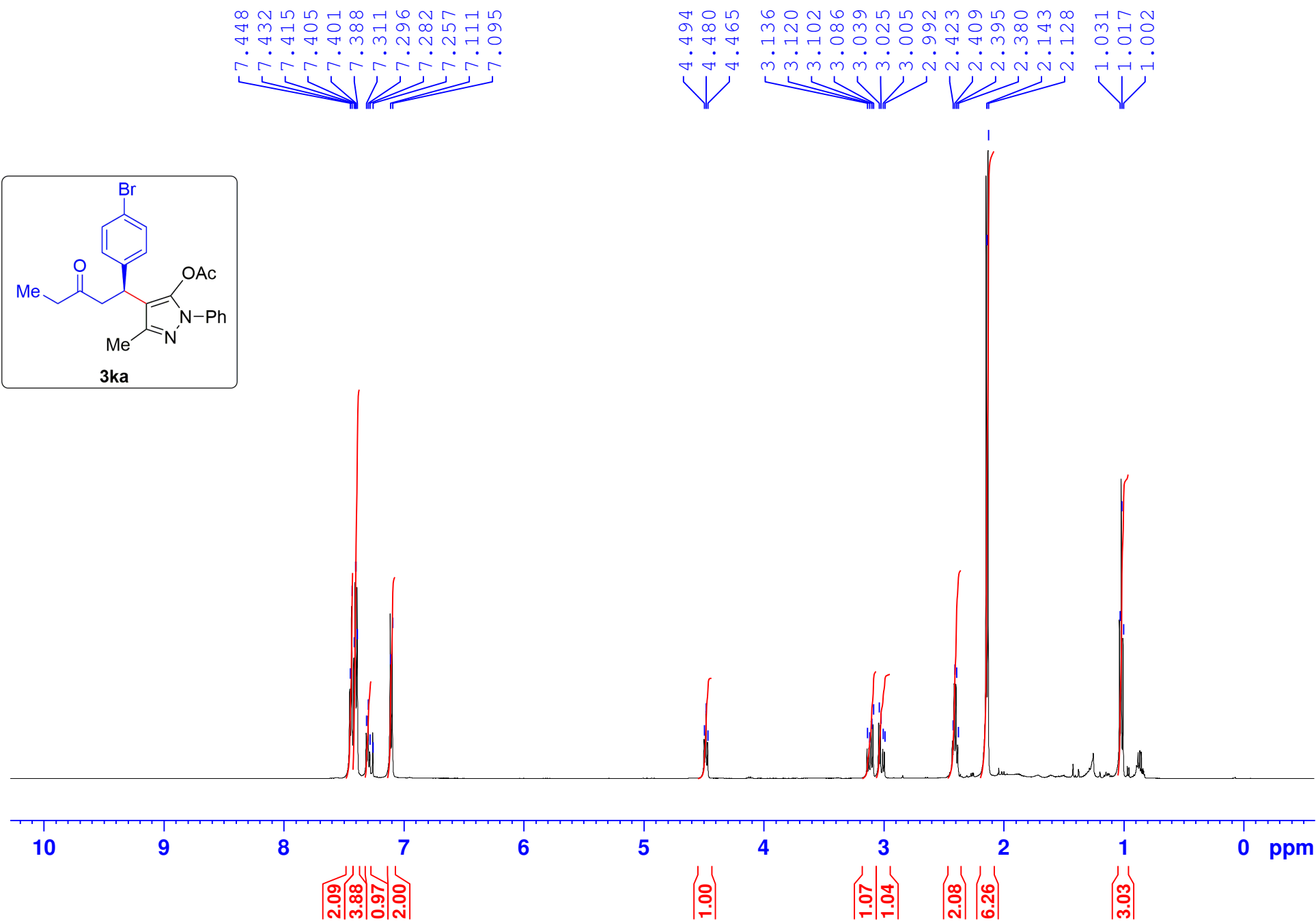
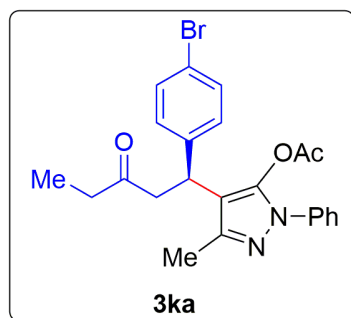


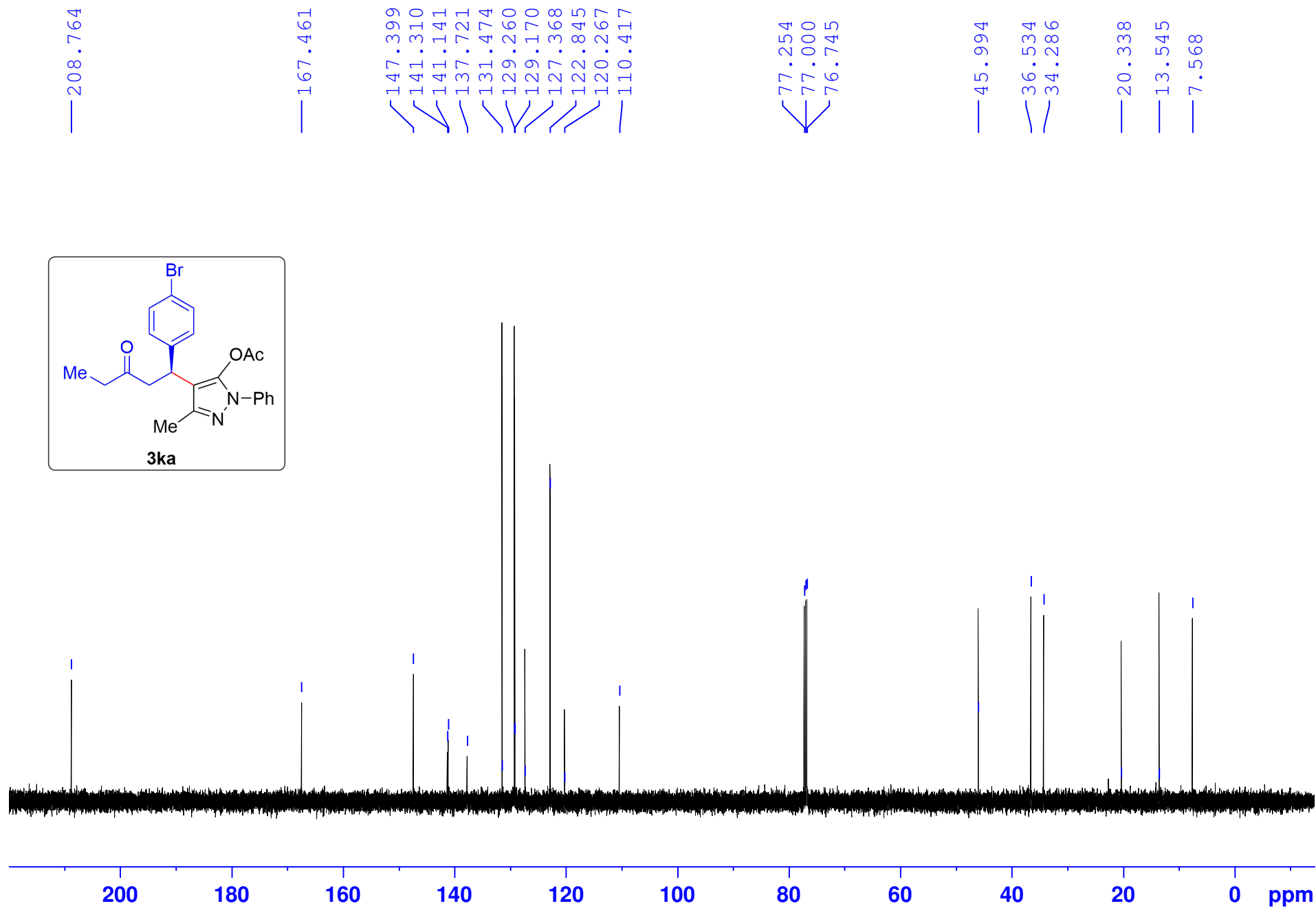
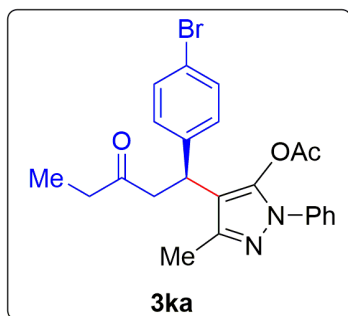


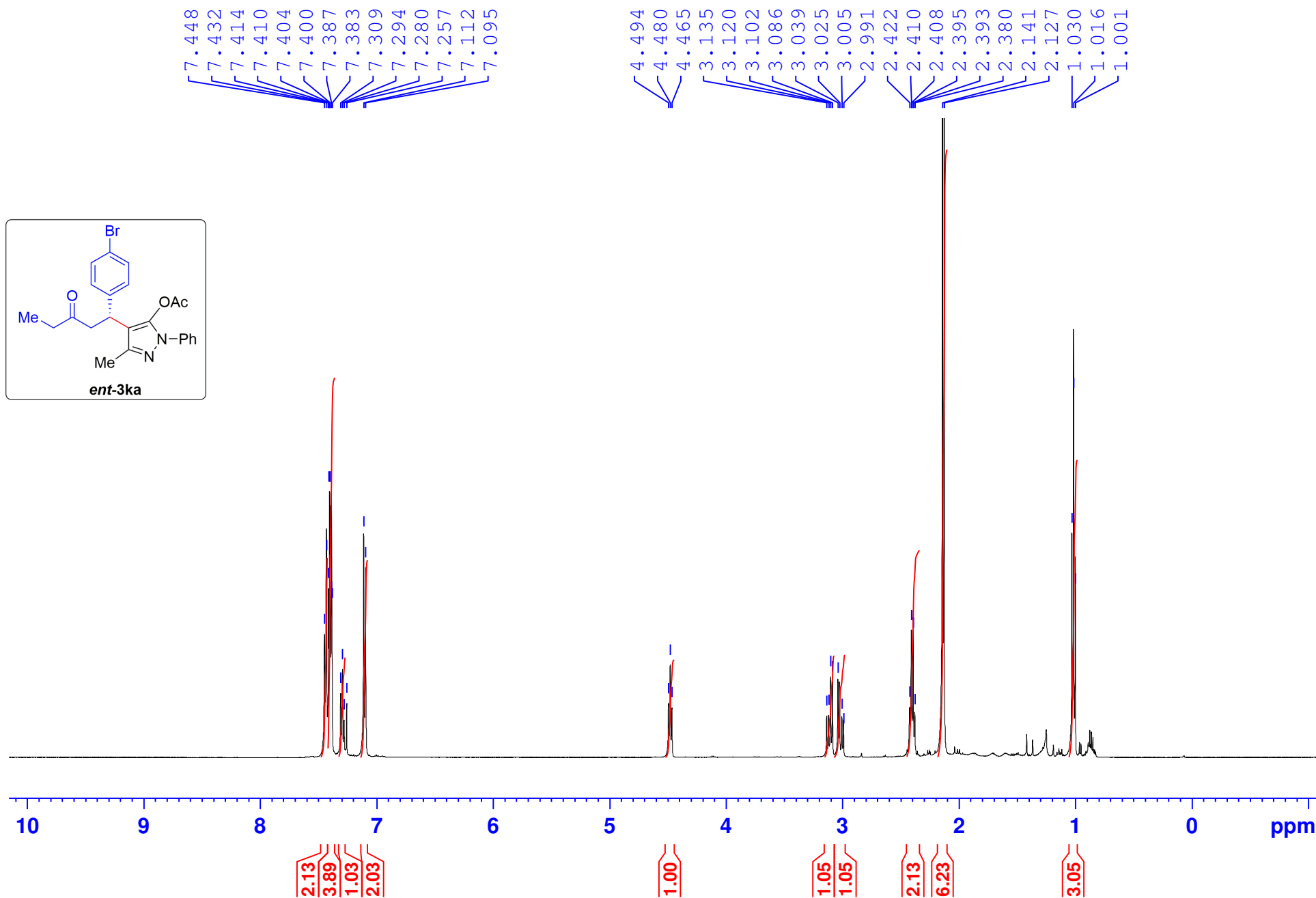
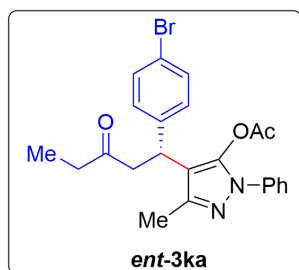


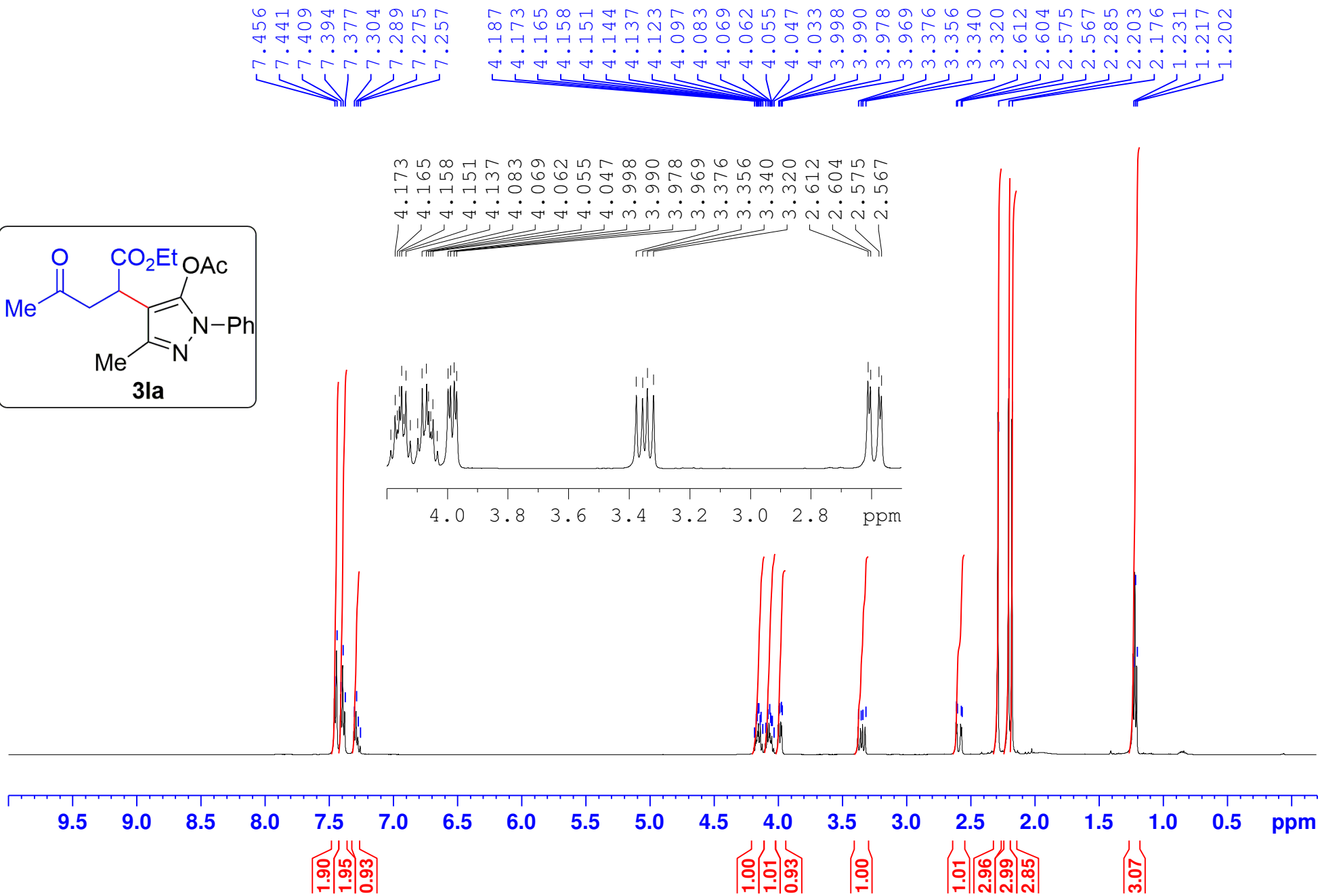
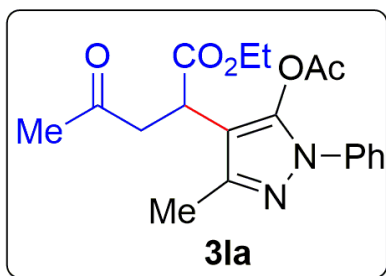


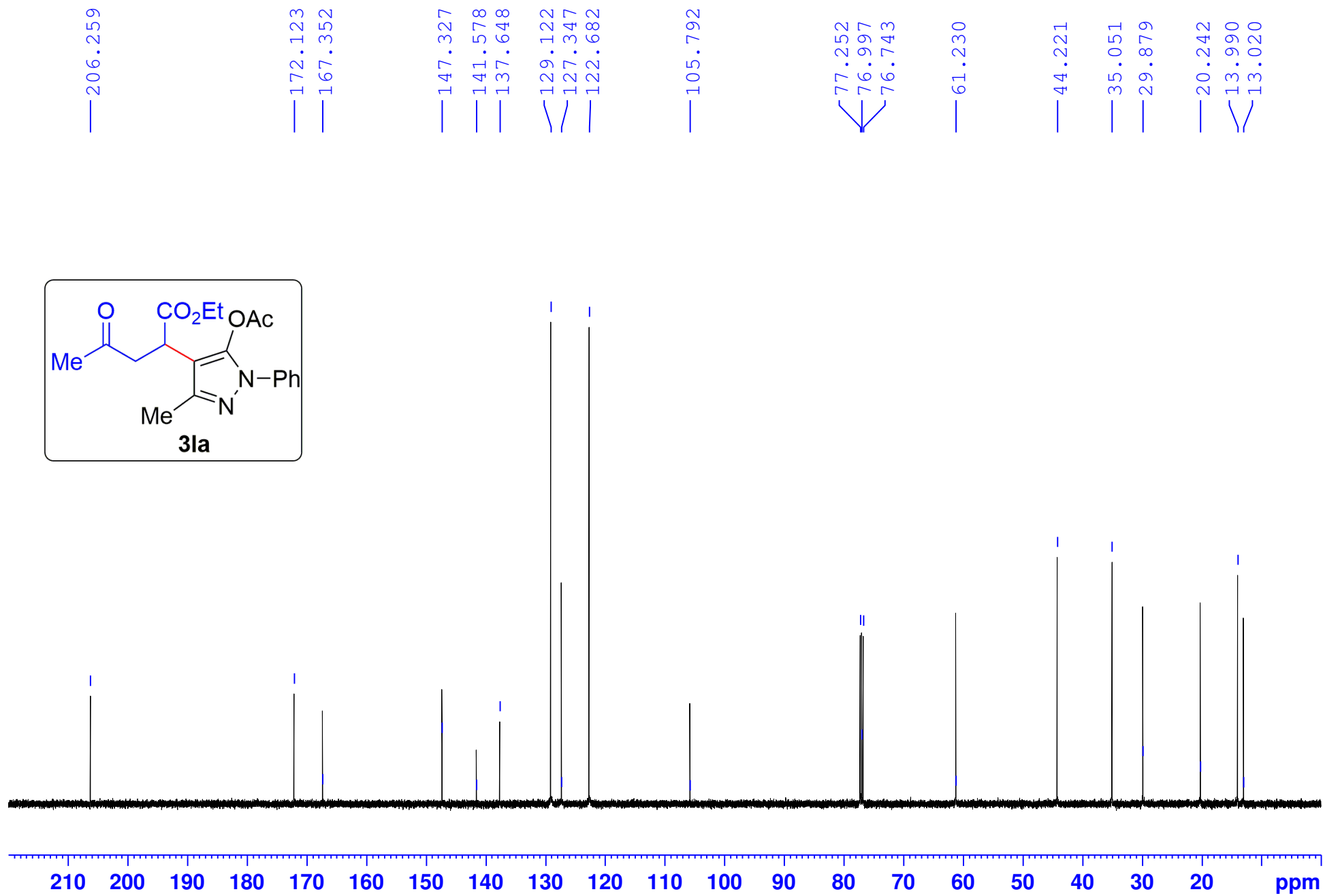


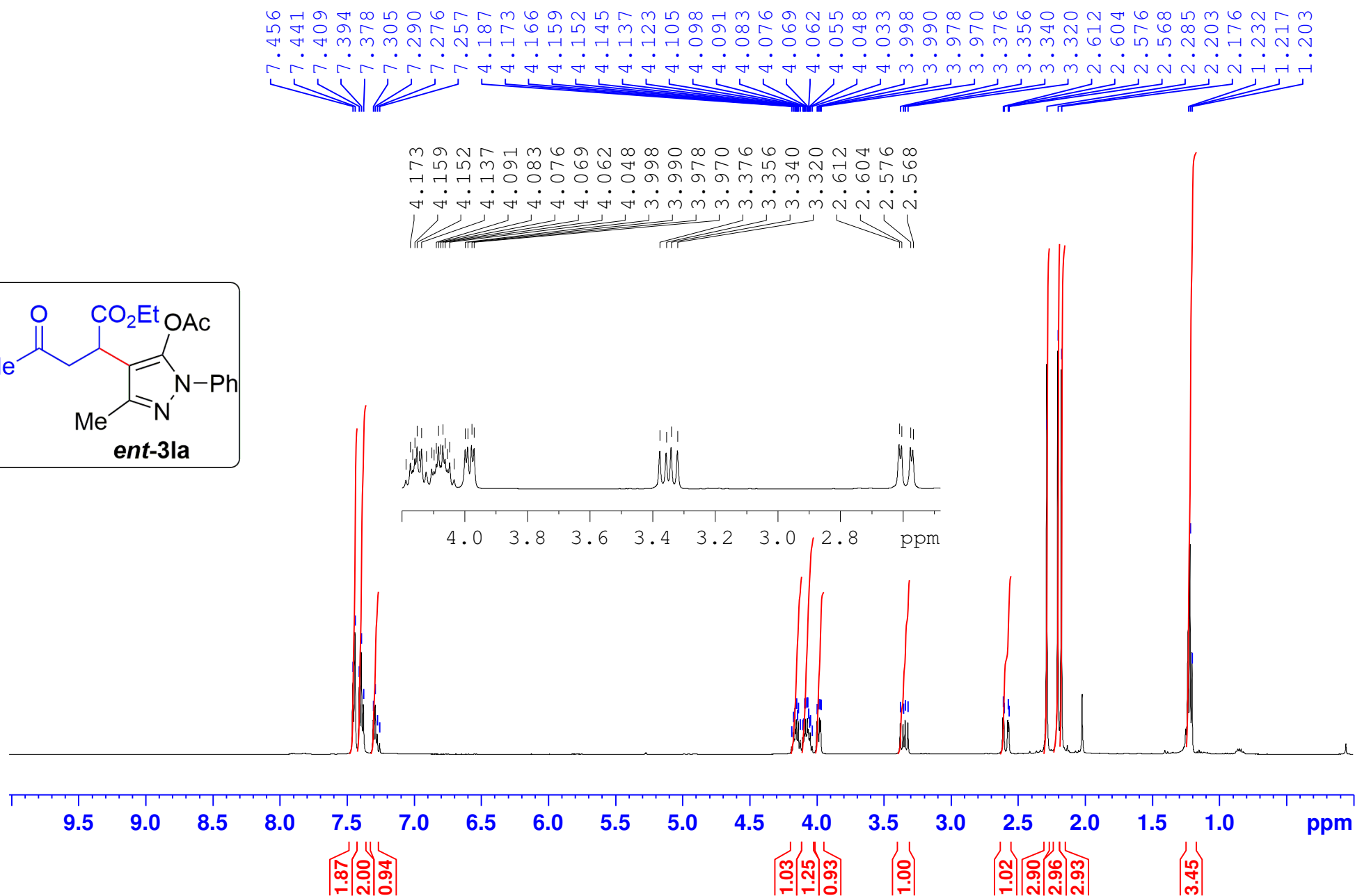
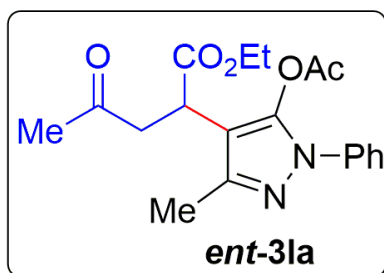


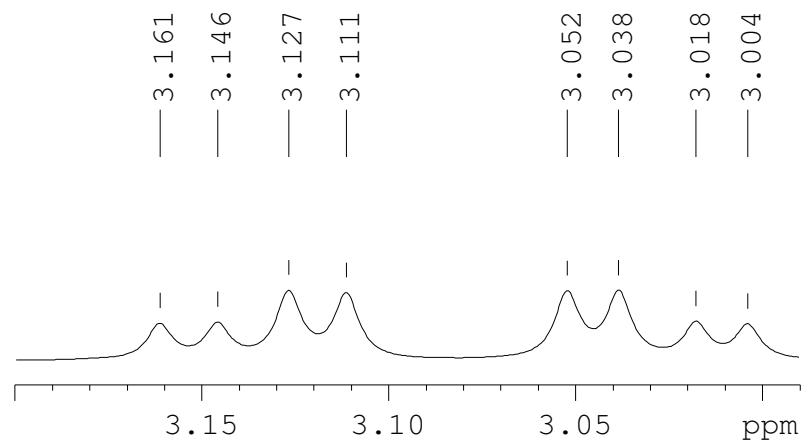
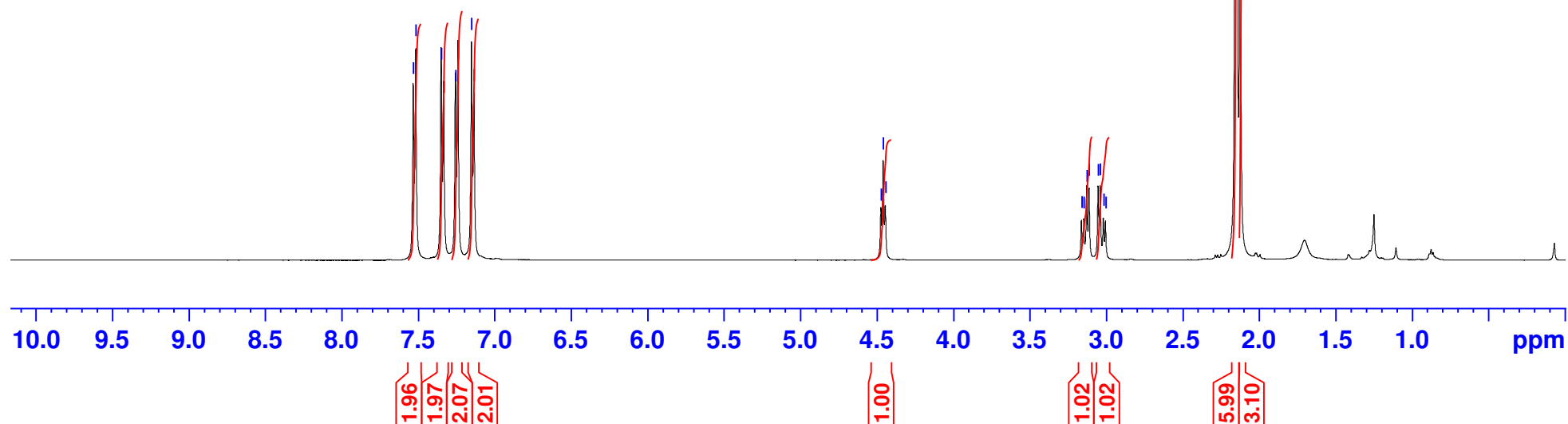
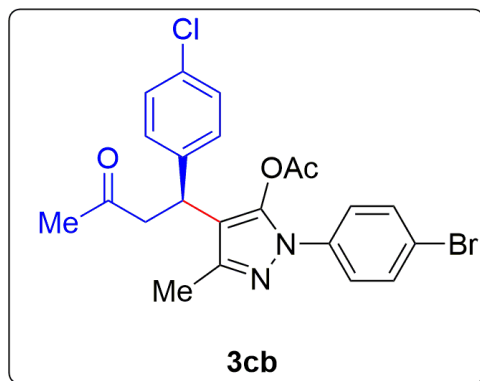








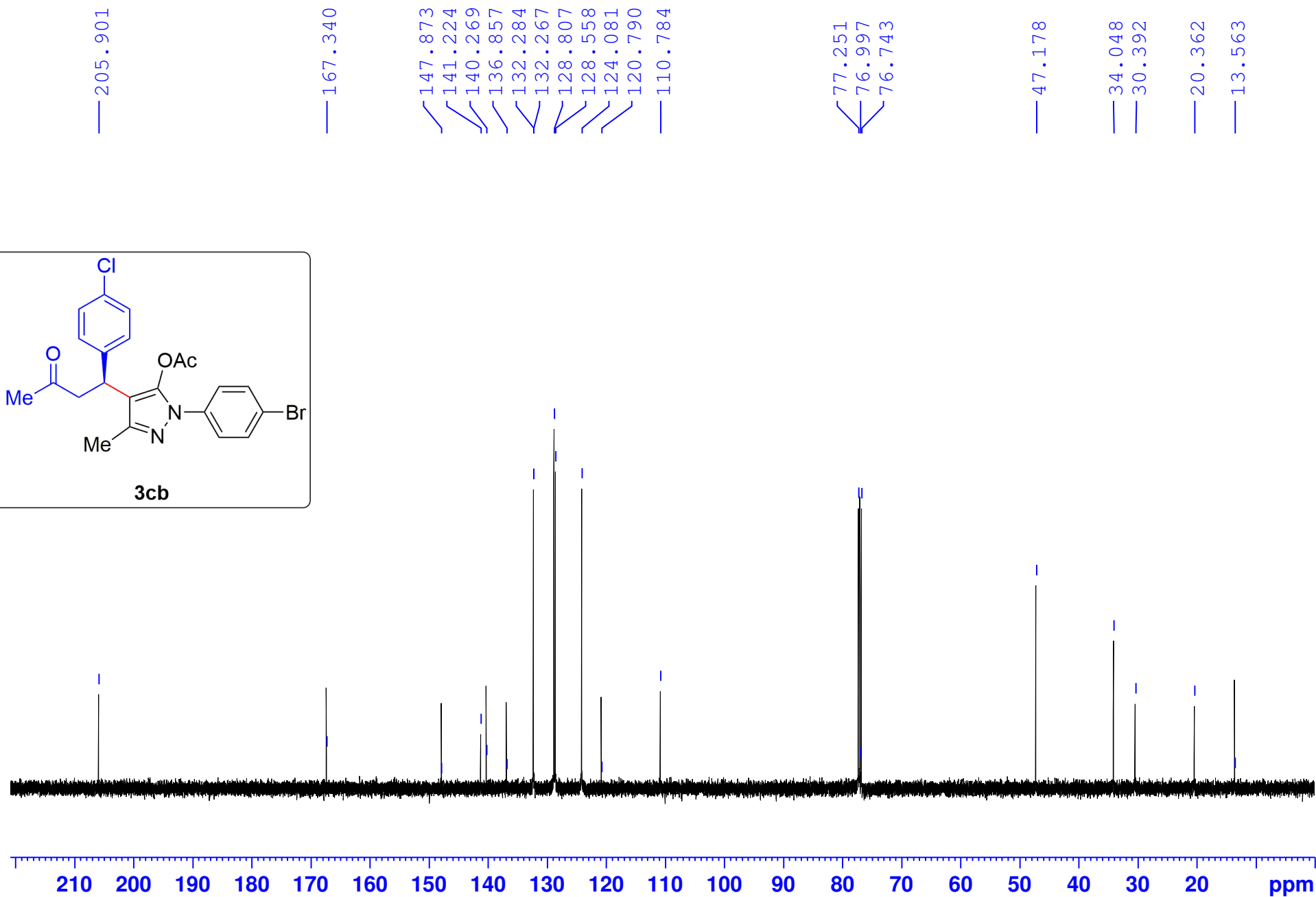
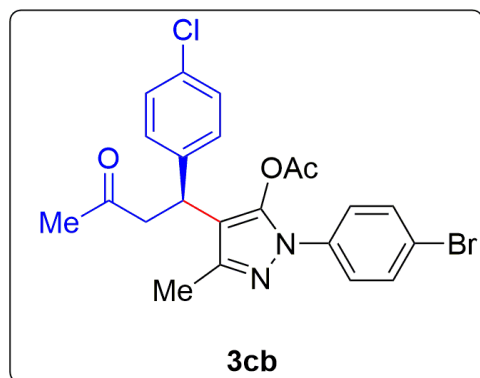


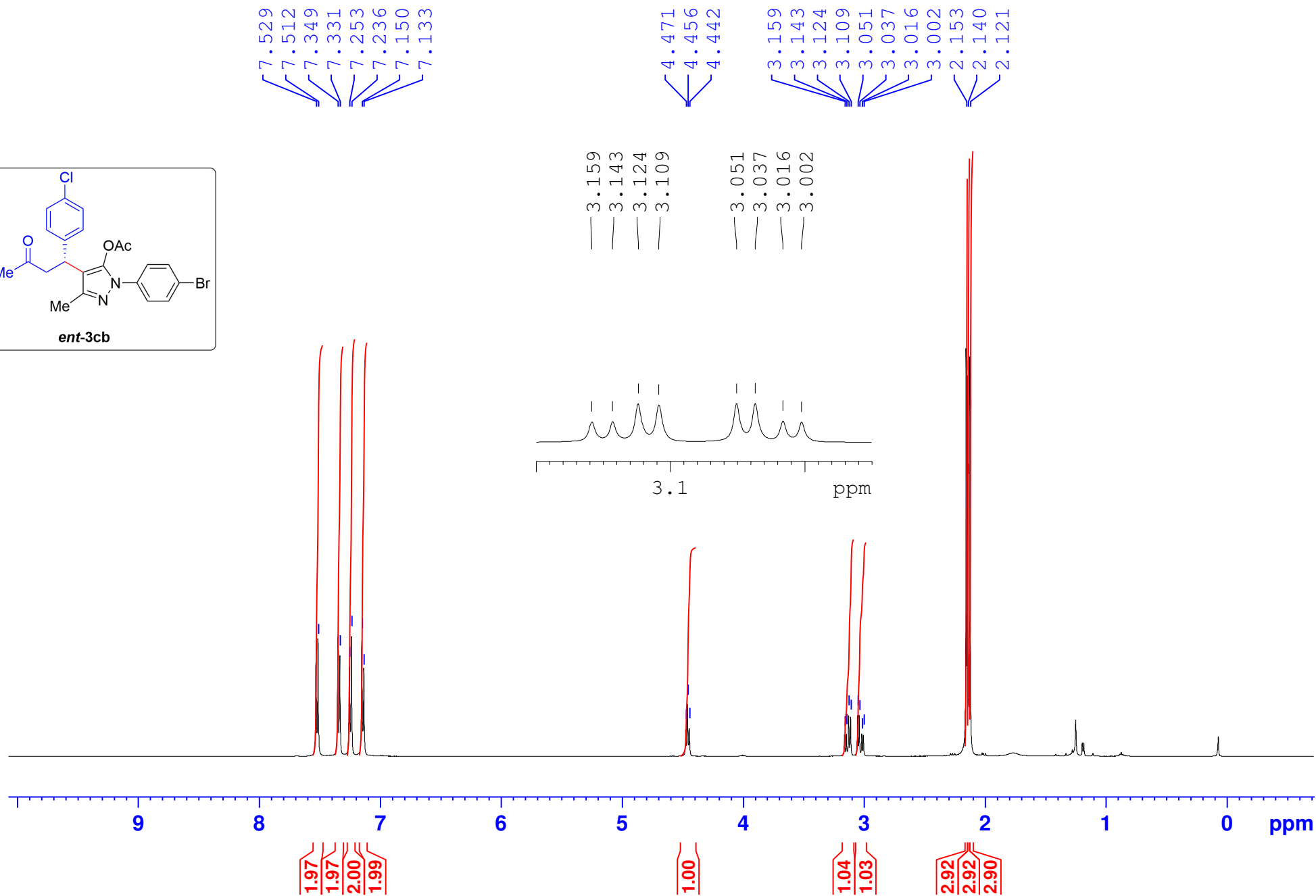
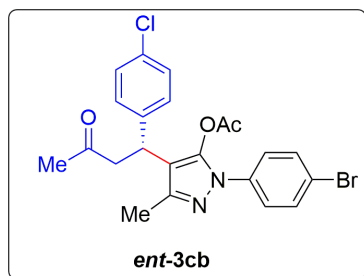


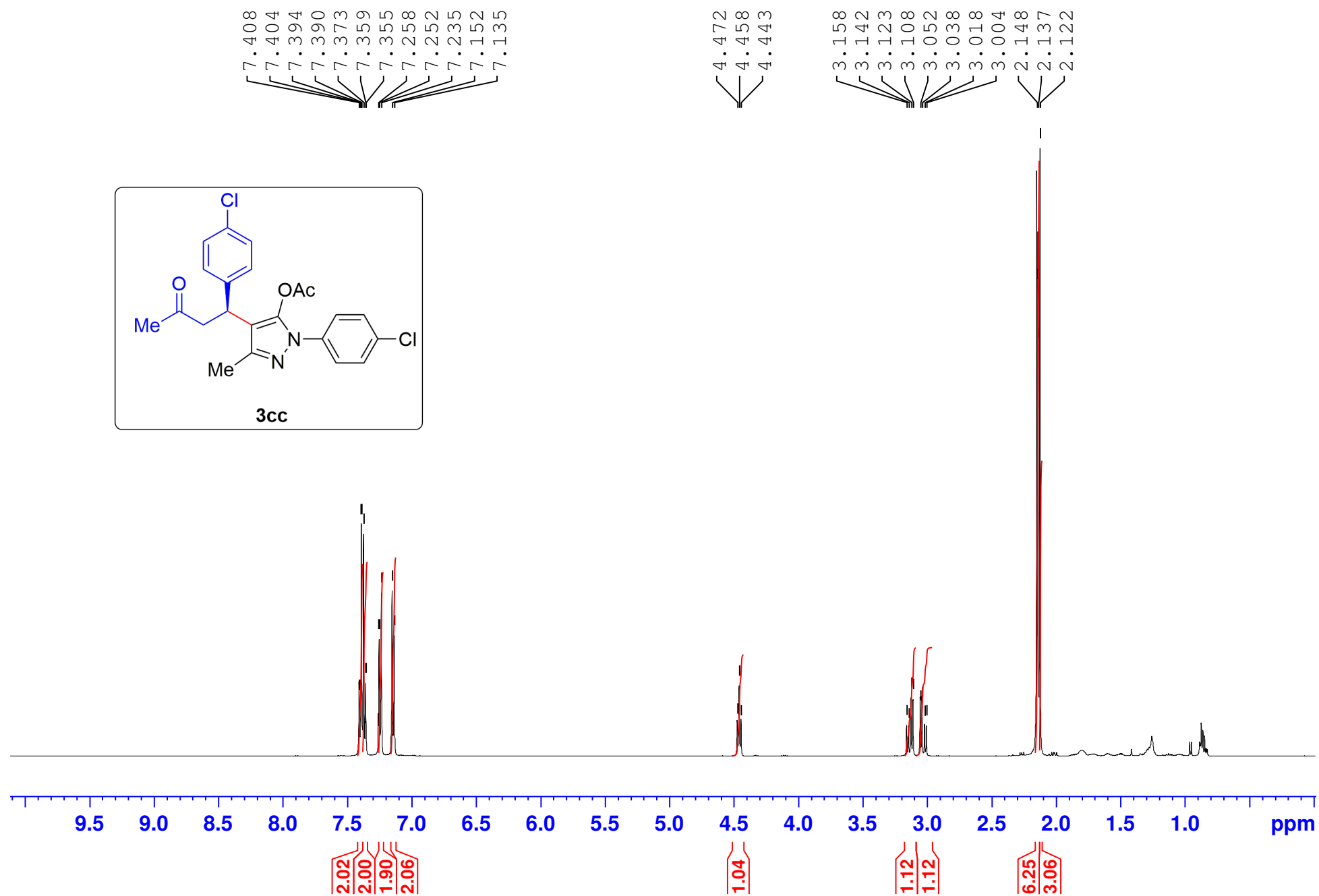
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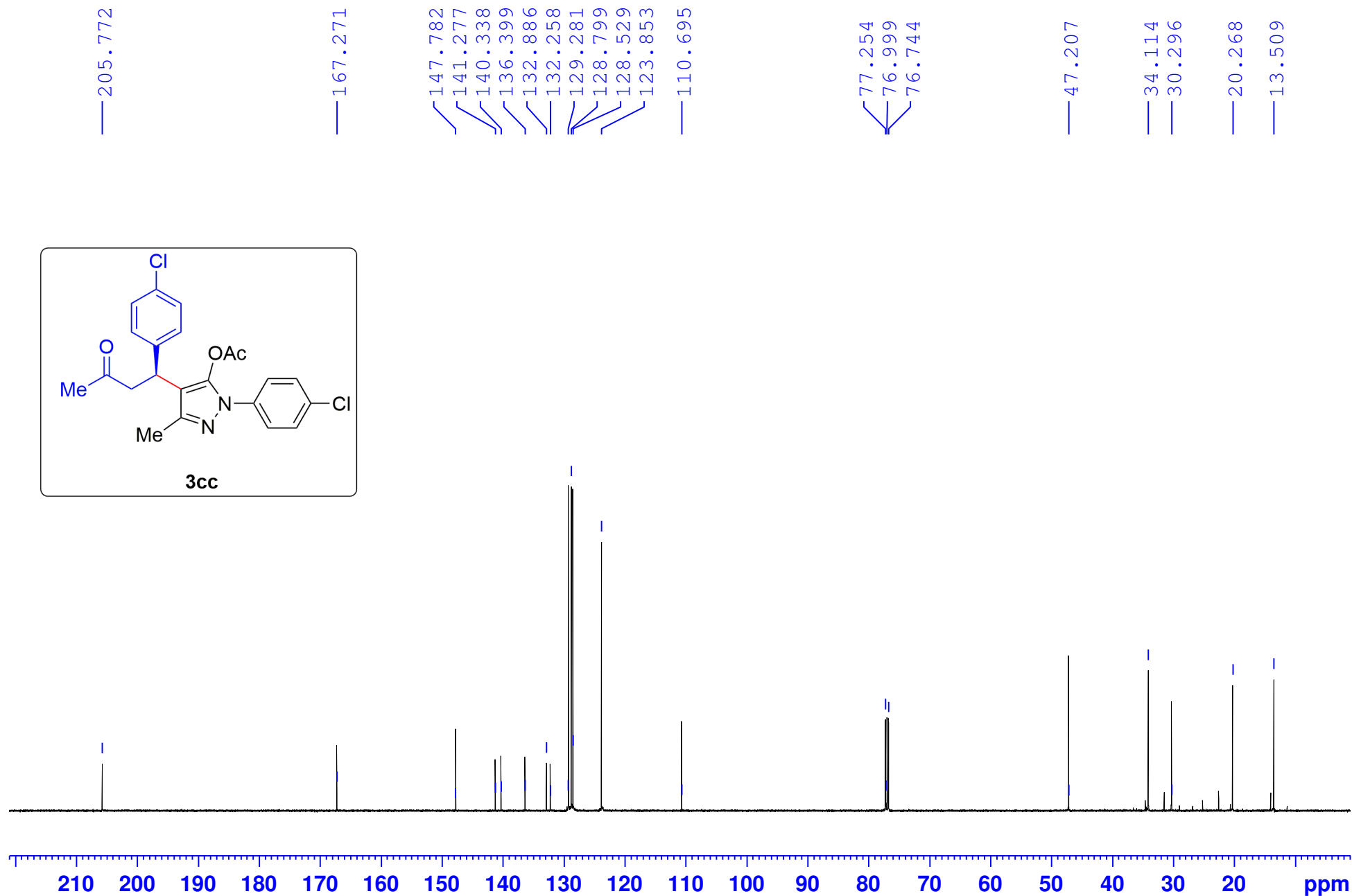
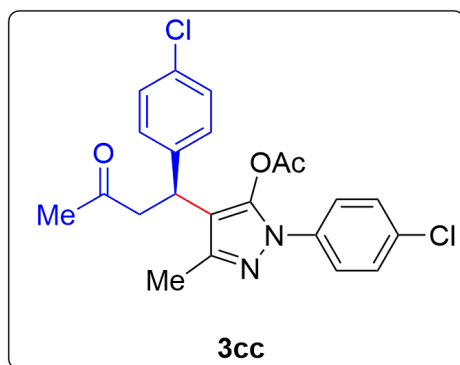
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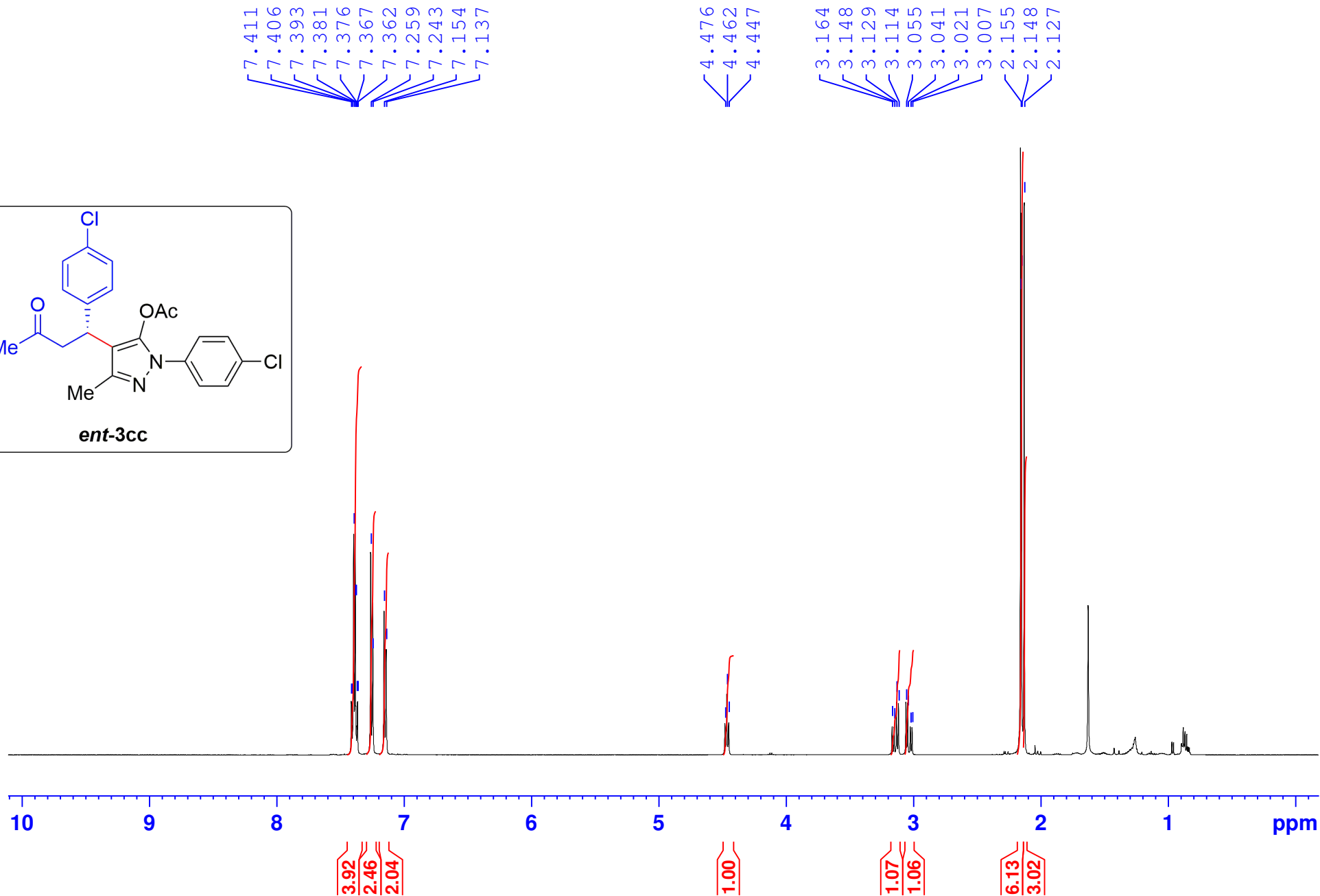
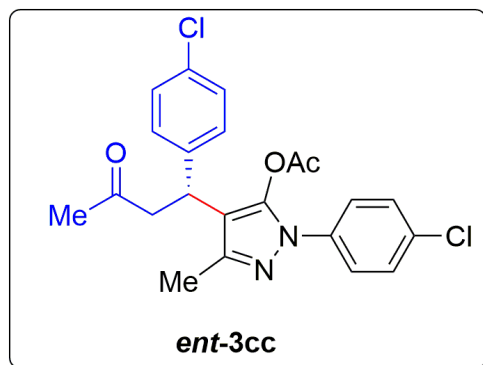
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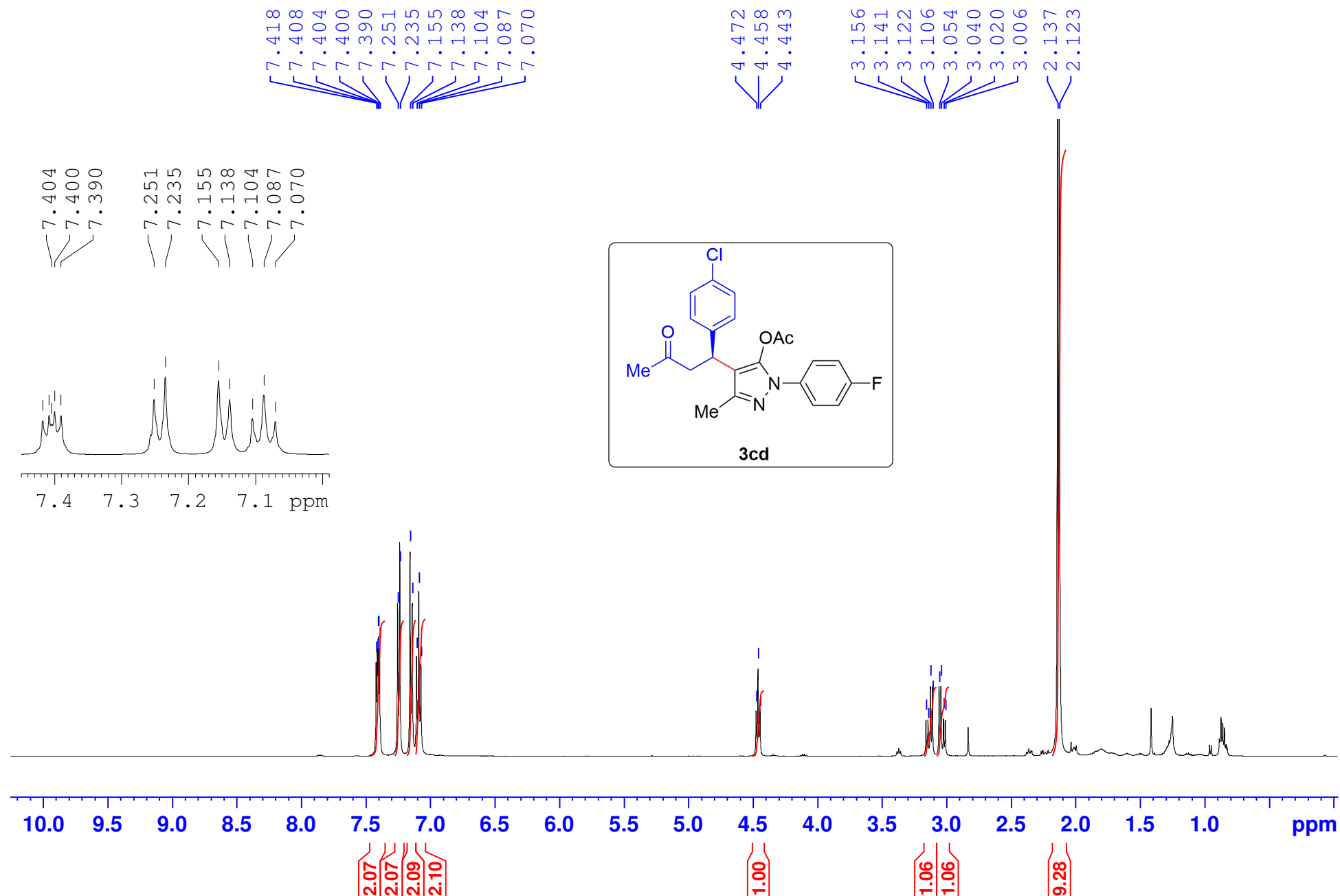


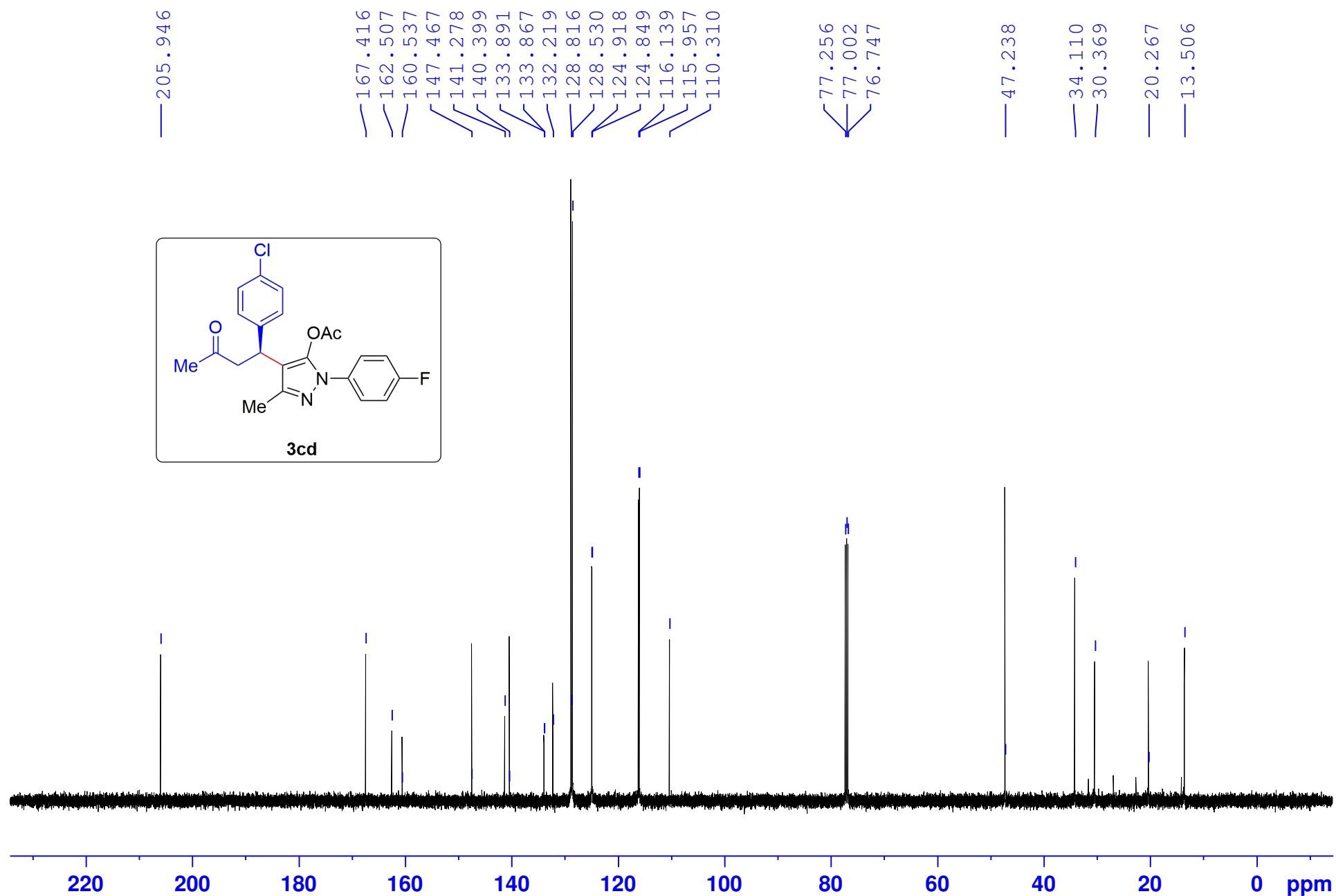


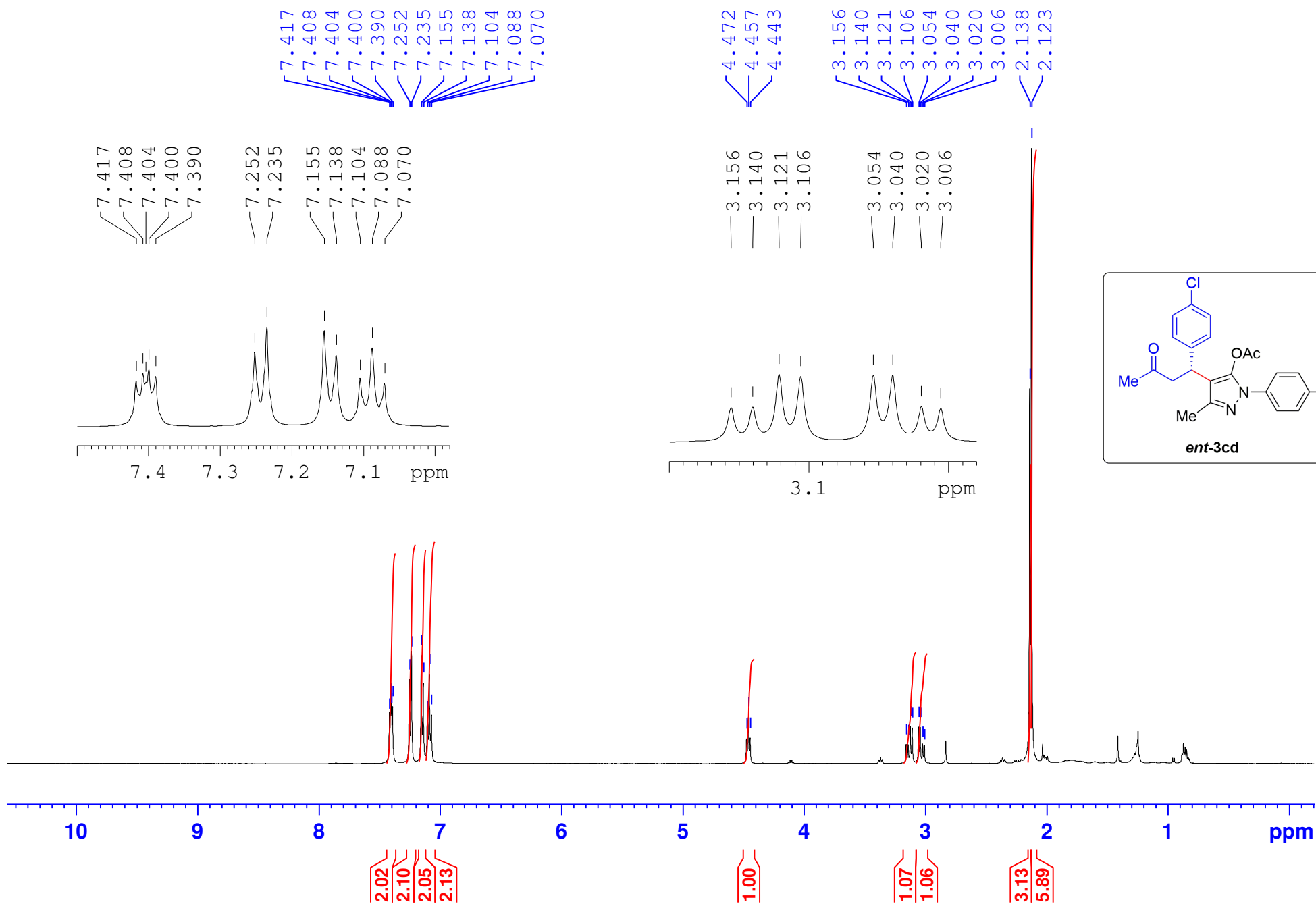


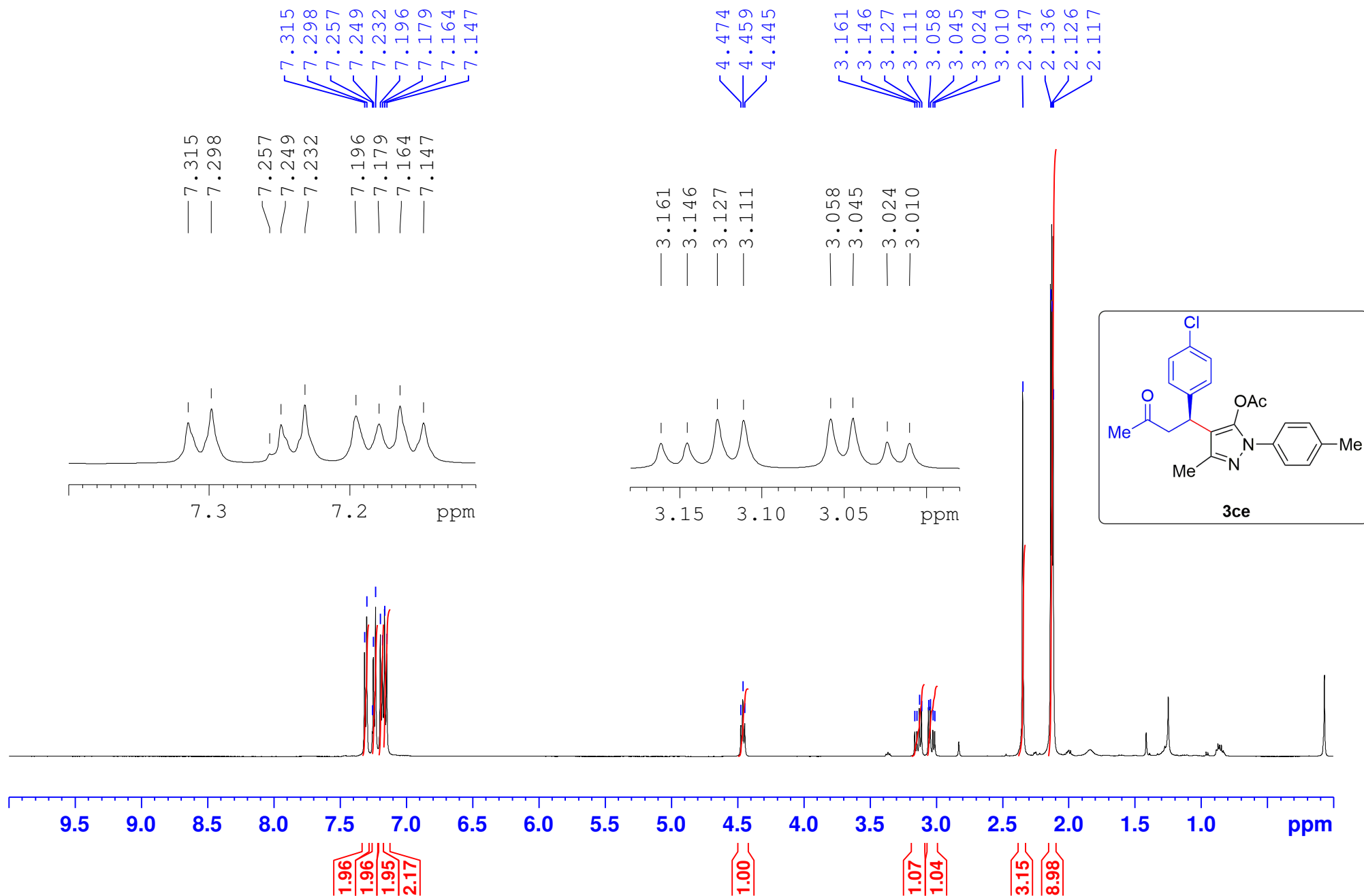


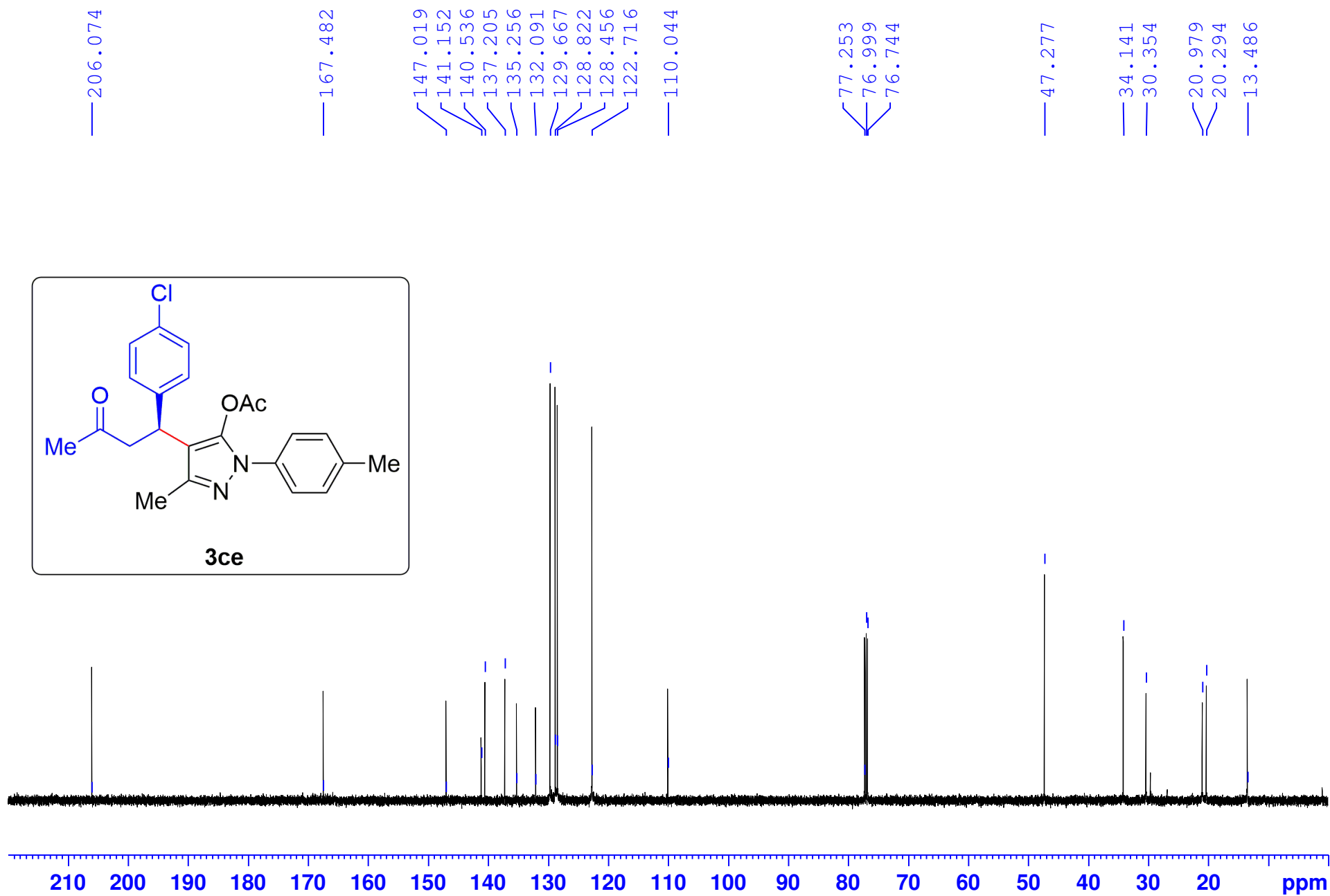


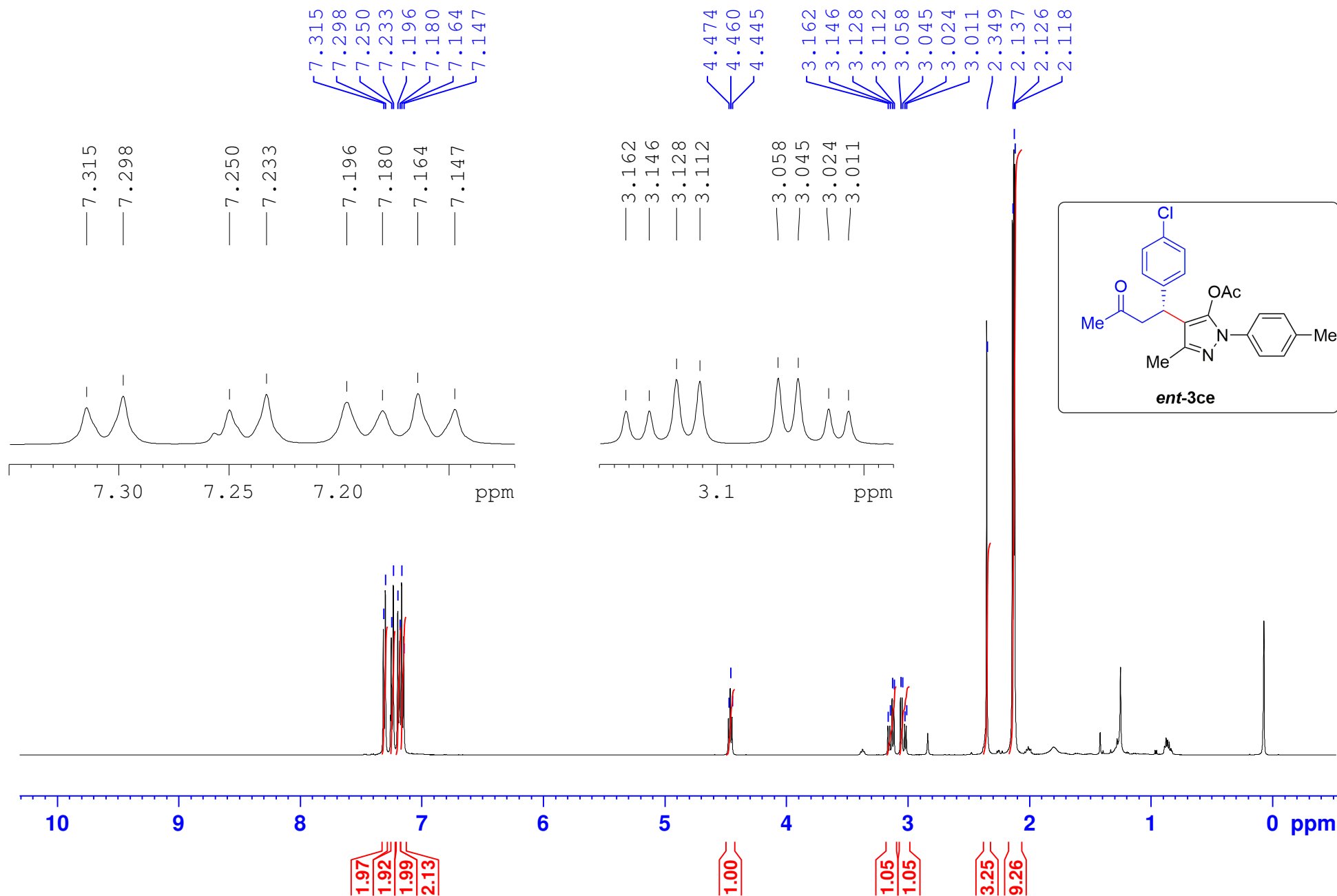


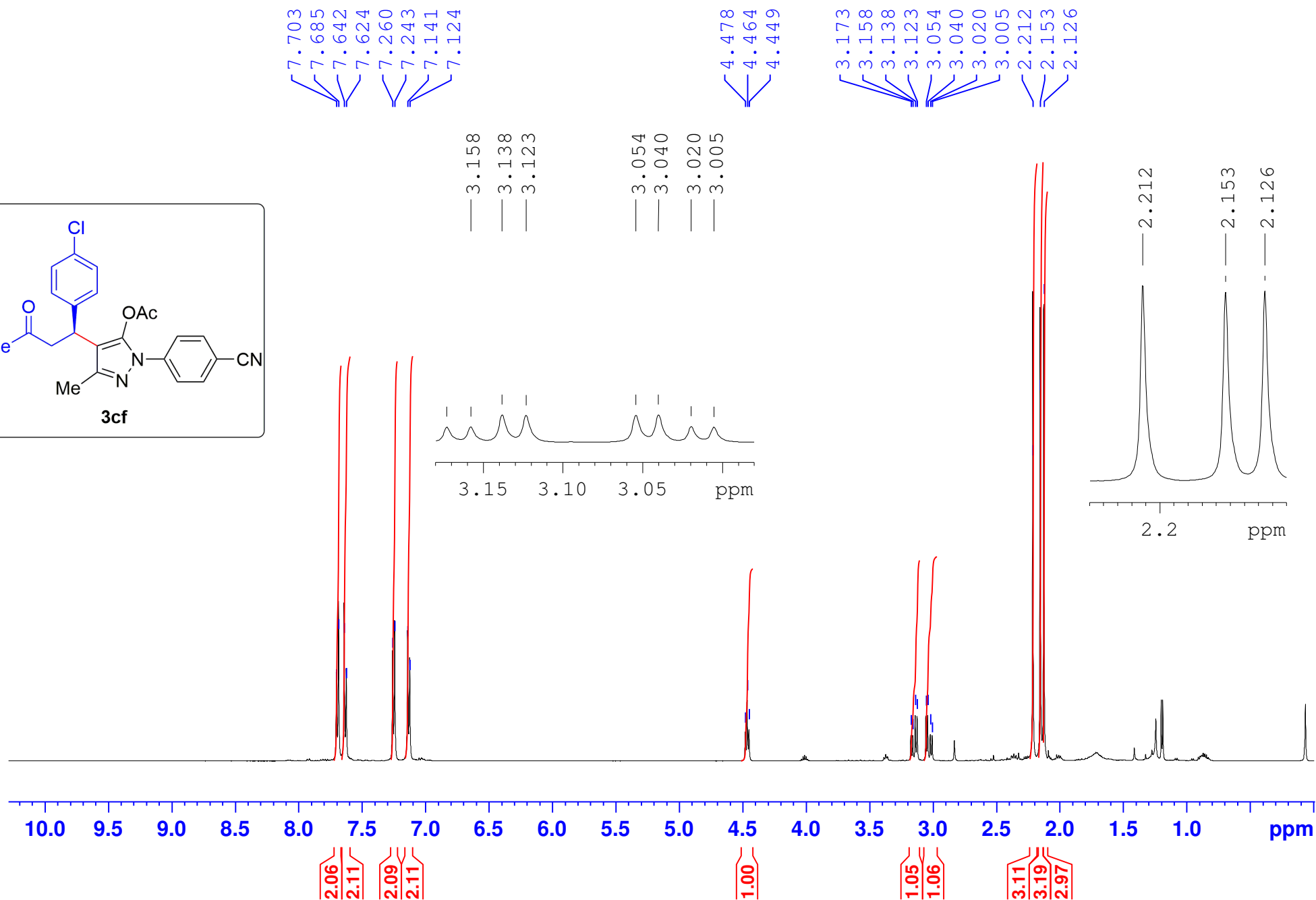
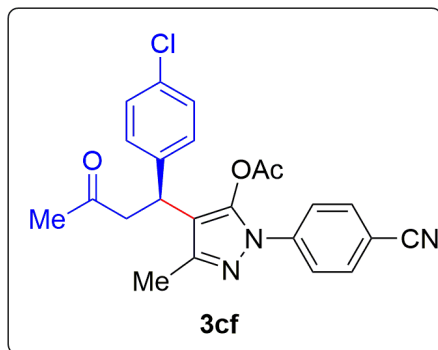


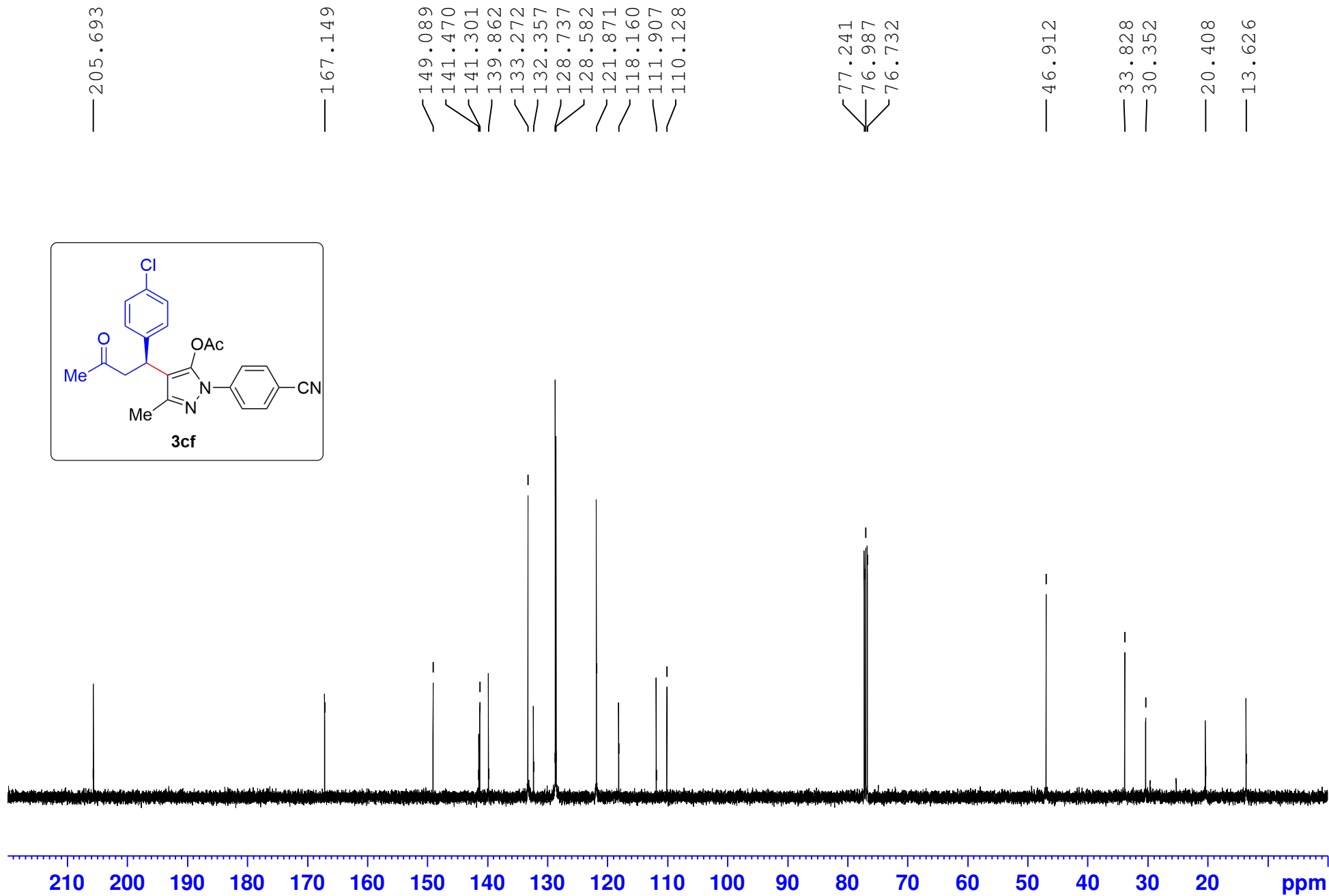


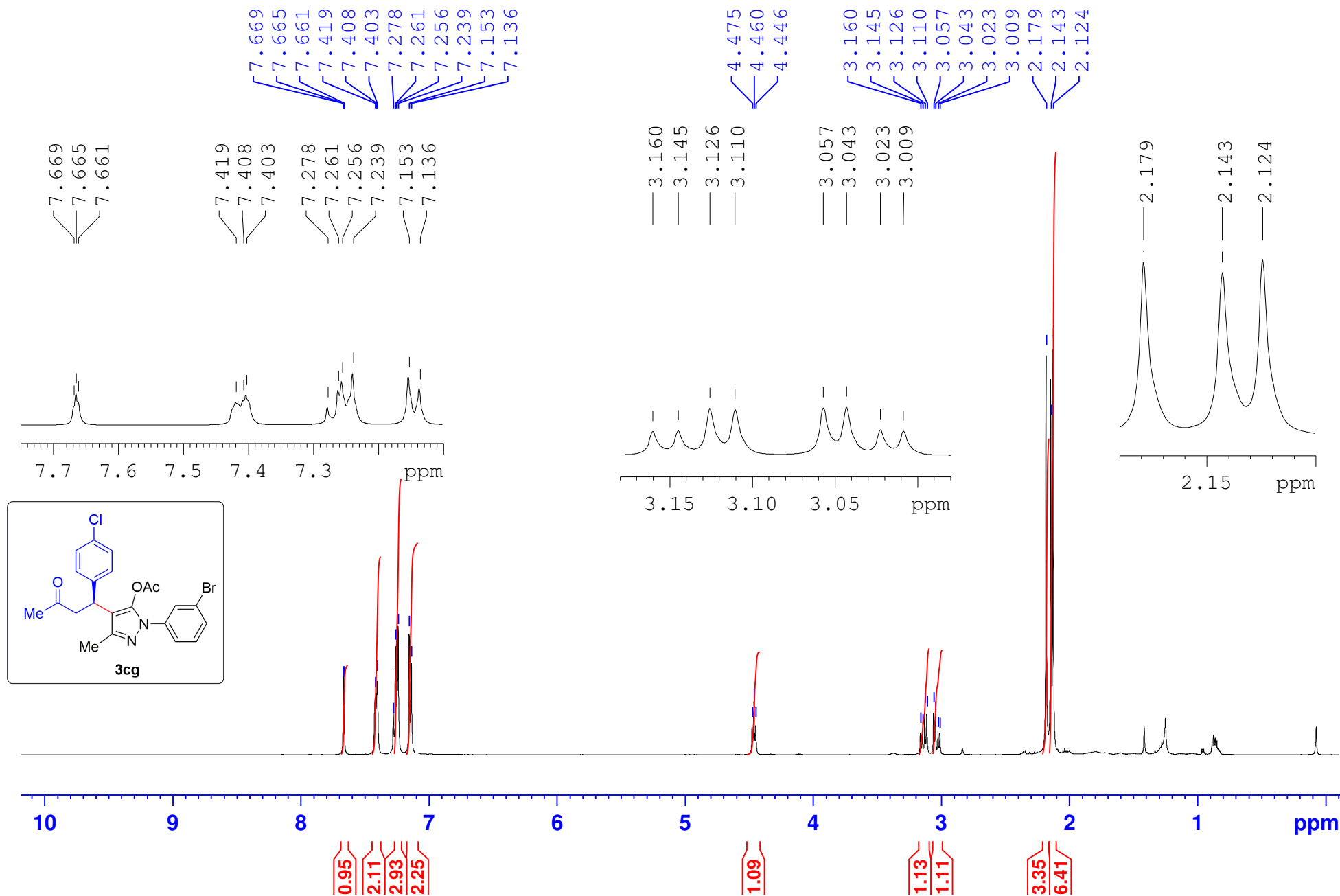


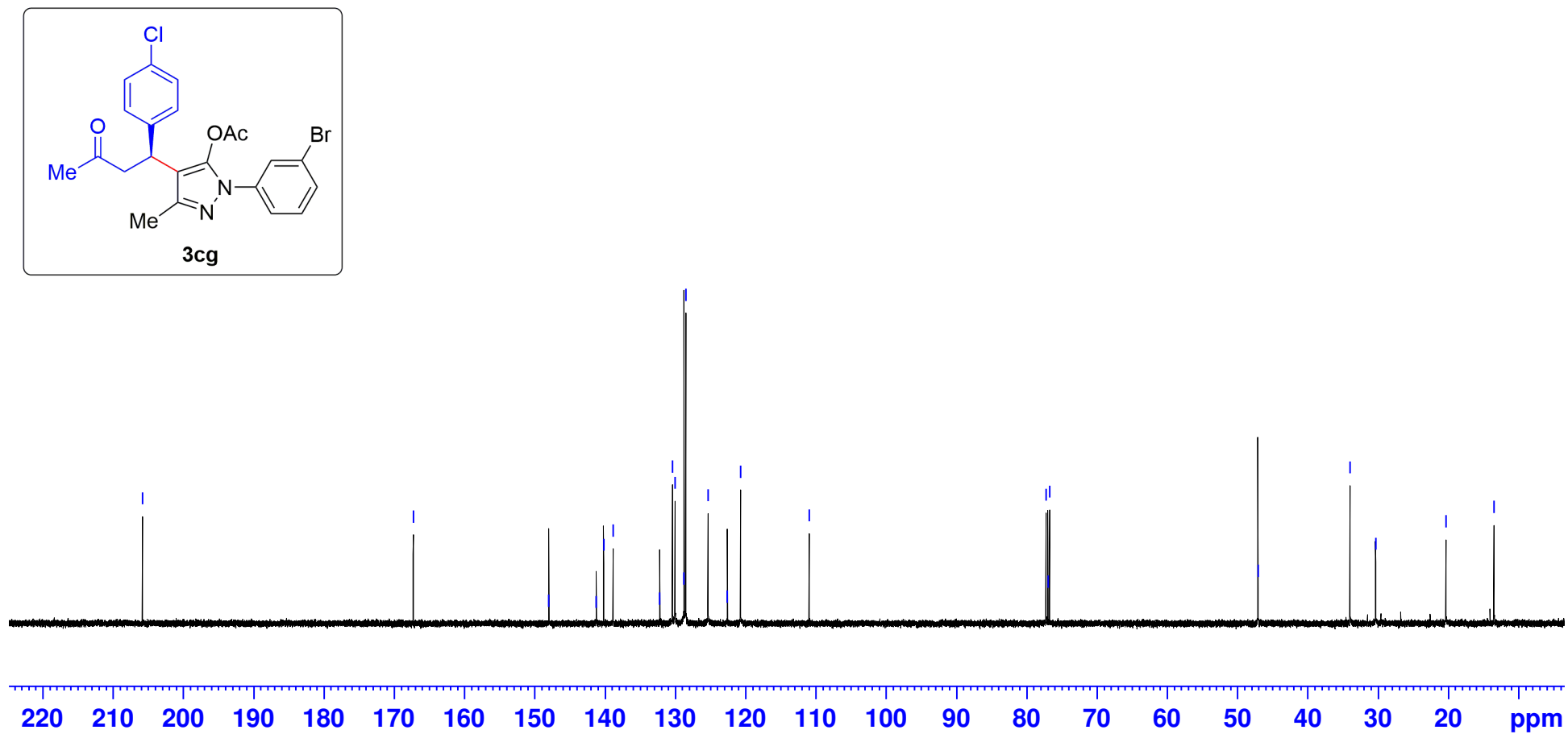


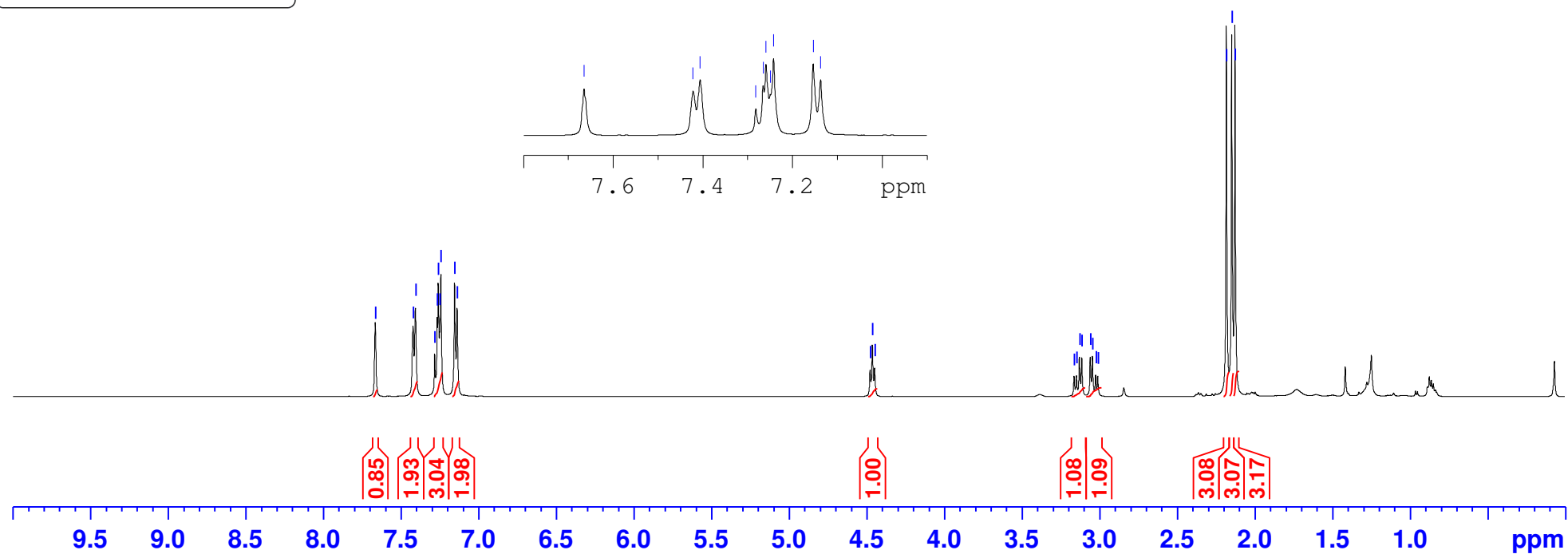
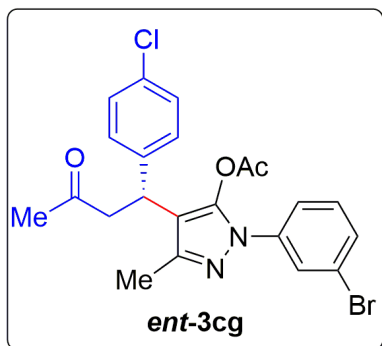












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