Organocatalytic asymmetric halocyclization of allylic amides to chiral oxazolines using DTBM-SEGPHOS – Mechanistic implications from Hammett plots

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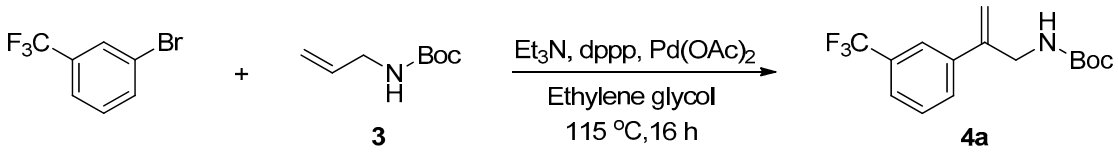
SUPPLEMENTARY INFORMATION

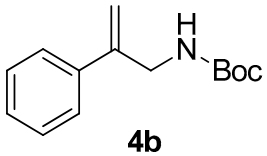
Synthesis of tert-butyl (2-(3-(trifluoromethyl)phenyl)allyl)carbamate (4a) – General procedure for Heck reaction



In an oven-dried 100 mL round-bottom flask equipped with a magnetic stir bar were added 500 mg *tert*-Butyl allylcarbamate (**3**) (3.18 mmol, 1eq), 535 μL 3-bromobenzotrifluoride (858 mg, 3.82 mmol, 1.2 eq), 21.4 mg palladium (II) acetate (3 mol%), 78.7 mg 1,3-Bis(diphenylphosphino)propane (6 mol%) and 7.5 mL degassed ethylene glycol (overall 0.42M). The reaction mixture was degassed under N_2 atmosphere. 881.5 μL (6.36 mmol, 2 eq) of triethylamine was added under N_2 atmosphere and the reaction was stirred at 115 ^oC for 16 h and monitored by HPLC. At completion, the solution was cooled to room temperature and 75 mL of water was added. The aqueous phase was extracted with EtOAc (3 × 15 mL). The organic phases were combined and washed with 0.1M HCl (2 × 12 mL), aq. $NaHCO_3$ 5% wt/wt (1 × 12 mL) and brine (1 × 12 mL). The organic phase was dried over Na_2SO_4. Charcoal (150 mg) was added and

the mixture was stirred at 60 °C for 2 h. After filtration through Celite™ the solvent was removed under reduced pressure to afford an oily residue.

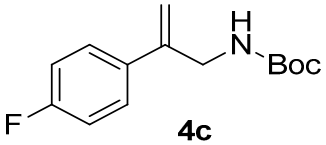
***tert*-butyl (2-phenylallyl)carbamate (4b)**



4b

Prepared according to the general procedure for the Heck reaction.

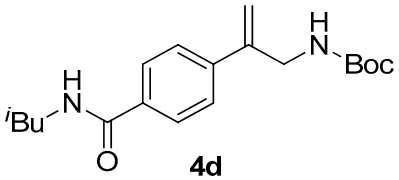
***tert*-butyl (2-(4-fluorophenyl)allyl)carbamate (4c)**



4c

Prepared according to the general procedure for the Heck reaction.

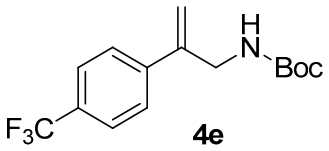
***tert*-butyl (2-(4-(isobutylcarbamoyl)phenyl)allyl)carbamate (4d)**



4d

Prepared according to the general procedure for the Heck reaction.

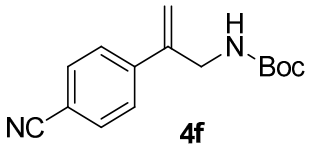
***tert*-butyl (2-(4-(trifluoromethyl)phenyl)allyl)carbamate (4e)**



4e

Prepared according to the general procedure for the Heck reaction.

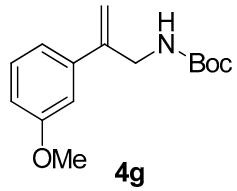
***tert*-butyl (2-(4-cyanophenyl)allyl)carbamate**



4f

Prepared according to the general procedure for the Heck reaction.

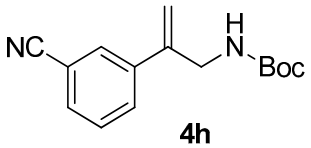
tert-butyl (2-(3-methoxyphenyl)allyl)carbamate



4g

Prepared according to the general procedure for the Heck reaction.

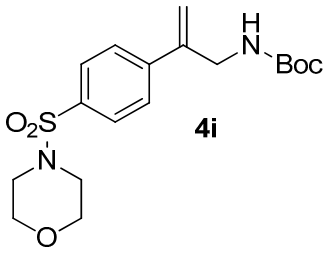
***tert*-butyl (2-(3-cyanophenyl)allyl)carbamate (4h)**



4h

Prepared according to the general procedure for the Heck reaction.

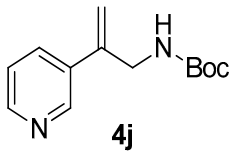
***tert*-butyl (2-(4-(morpholinosulfonyl)phenyl)allyl)carbamate (4i)**



4i

Prepared according to the general procedure for the Heck reaction.

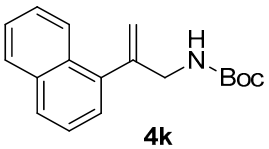
***tert*-butyl (2-(pyridin-3-yl)allyl)carbamate (4j)**



4j

Prepared according to the general procedure for the Heck reaction.

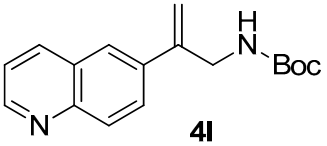
***tert*-butyl (2-(naphthalen-1-yl)allyl)carbamate (4k)**



4k

Prepared according to the general procedure for the Heck reaction.

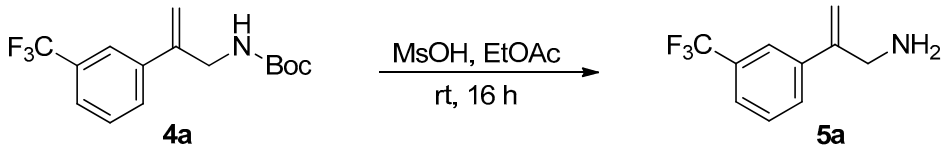
***tert*-butyl (2-(quinolin-6-yl)allyl)carbamate (4l)**



4l

Prepared according to the general procedure for the Heck reaction.

2-(3-(trifluoromethyl)phenyl)prop-2-en-1-amine (5a) – General procedure for Boc deprotection



4a **5a**

In a 10 mL round-bottom flask equipped with magnetic stir bar were added 318.4 mg *tert*-butyl (2-(3-(trifluoromethyl)phenyl)allyl)carbamate (**4a**) (1.0567 mmol, 1 eq) and dissolved in 1.9 mL EtOAc (0.56M). Next, 82.3 µL methanesulfonic acid (121.85 mg, 1.268 mmol, 1.2 eq) were added in the flask and the reaction was stirred for 16 h at room temperature and monitored by HPLC. The solvent was removed under reduced pressure and the residue was dissolved in 3 mL TBME (0.35 M) and extracted with 1M HCl (3 × 4 mL). The aqueous phases were combined and the pH was adjusted to 11-12. The aqueous phase was then extracted with DCM (3 × 4 mL). The organic phases were combined and dried over Na_2SO_4. The solvent was removed under reduced pressure to afford the product as an oil.

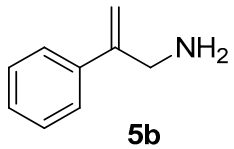
Overall yield for the Heck reaction and Boc deprotection: 192 mg (30%)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (s, 1H), 7.59 (d, J = 7.7 Hz, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.46 (t, J = 7.8 Hz, 1H), 5.41 (d, J = 0.5 Hz, 1H), 5.34 (d, J = 0.5 Hz, 1H), 3.73 (s, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 148.52, 140.69, 130.76 (q, J = 33.2 Hz), 129.39, 128.91, 124.32 (q, J = 3.02 Hz), 123.20 (q, J = 272.5 Hz), 122.96 (q, J = 3.9 Hz), 112.92, 45.95

(ESI) calculated for $C_{11}H_{15}F_3NO_3S$ $[M+H]^+$ requires 202.0765, found 202.0780

2-phenylprop-2-en-1-amine (5b)



5b

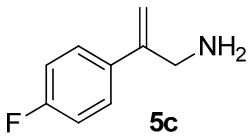
Prepared according to the general procedure for Boc deprotection.

Overall yield from Heck procedure and Boc deprotection: 40%

The product could not be fully purified; The corresponding cyclized derivative however has been purified and the characterization is provided below.

(ESI) calculated for $C_9H_{12}N$ $[M+H]^+$ requires 134.0891, found 134.0887

2-(4-fluorophenyl)prop-2-en-1-amine (5c)



5c

Prepared according to the general procedure for Boc deprotection.

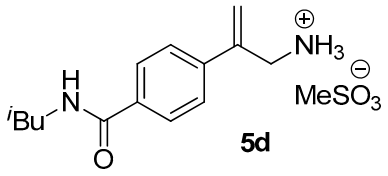
Overall yield from Heck procedure and Boc deprotection: 31%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 – 7.36 (m, 2H), 7.05 – 7.01 (m, 2H), 5.30 (s, 1H), 5.22 (s, 1H), 3.68 (d, J = 7.9 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 160.83 (d, J = 242.1 Hz), 130.66 (d, J = 9.06 Hz), 128.64 (d, J = 12.08 Hz), 127.78, 115.42 (d, J = 22.65 Hz), 114.33, 41.80

(ESI) calculated for $C_9H_{11}FN$ $[M+H]^+$ requires 151.0797, found 151.0802

2-(4-(isobutylcarbamoyl)phenyl)prop-2-en-1-aminium methanesulfonate (5d)



5d

Prepared according to the general procedure for Boc deprotection. The product was isolated as its mesylate salt by filtration from the reaction without further purification.

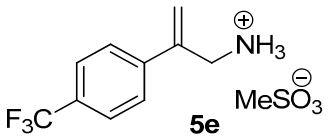
Overall yield for the Heck reaction and Boc deprotection: 40%

^{1}H NMR (600 MHz, DMSO) δ 8.48 (t, J = 5.7 Hz, 1H), 8.11 (s, 3H), 7.87 (d, J = 8.4 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H), 5.77 (s, 1H), 5.43 (s, 1H), 3.96 (d, J = 5.5 Hz, 2H), 3.07 (dd, J = 13.3, 7.0 Hz, 2H), 1.83 (dt, J = 13.5, 6.8 Hz, 1H), 0.87 (d, J = 6.7 Hz, 6H)

^{13}C NMR (151 MHz, DMSO) δ 166.05, 140.63, 140.30, 134.88, 127.95, 126.21, 116.94, 47.15, 41.64, 40.20, 28.55, 20.65

(ESI) calculated for $C_{15}H_{25}N_2O_4S$ $[M+H]^+$ requires 328.1452, found 328.1449

2-(4-(trifluoromethyl)phenyl)prop-2-en-1-aminium mesylate (5e)



5e

Prepared according to the general procedure for Boc deprotection. The product was isolated as its mesylate salt by filtration from the reaction without further purification.

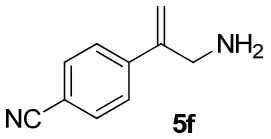
Overall yield for the Heck reaction and Boc deprotection: 35%

^{1}H NMR (600 MHz, DMSO) δ 8.17 (s, 3H), 7.76 (q, J = 8.5 Hz, 4H), 5.82 (s, 1H), 5.53 (s, 1H), 4.00 (s, 2H), 2.35 (s, 3H)

^{13}C NMR (151 MHz, DMSO) δ 142.07, 140.24, 128.99 (q, J = 32.01 Hz), 127.32, 125.93 (q, J = 4.53 Hz), 125.52 (q, J = 271.8 Hz), 118.37, 41.62

(ESI) calculated for $C_{10}H_{11}F_3N$ $[M+H]^+$ requires 329.0539, found 329.0555

4-(3-aminoprop-1-en-2-yl)benzonitrile (5f)



5f

Prepared according to the general procedure for Boc deprotection.

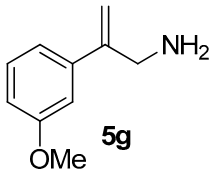
Overall yield for the Heck reaction and Boc deprotection: 43%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, 2H), 7.52 (d, 2H), 5.46 (s, 1H), 5.39 (s, 1H), 3.72 (d, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 148.05, 144.44, 132.28, 126.79, 118.80, 114.36, 111.24, 45.67

(ESI) calculated for $C_{10}H_{11}N_2$ $[M+H]^+$ requires 159.0844, found 159.0841

2-(3-methoxyphenyl)prop-2-en-1-amine (5g)



5g

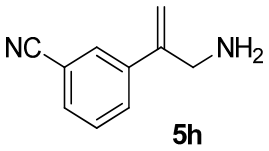
Prepared according to the general procedure for Boc deprotection.

Overall yield for the Heck reaction and Boc deprotection: 25%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.26 (dd, J = 9.0, 6.9 Hz, 1H), 7.00 (d, J = 7.7 Hz, 1H), 6.96 – 6.93 (m, 1H), 6.84 (dt, J = 8.1, 4.0 Hz, 1H), 5.34 (s, 1H), 5.22 (s, 1H), 3.82 (s, J = 4.9 Hz, 2H), 3.70 (s, 2H)

(ESI) calculated for $C_{10}H_{14}NO$ $[M+H]^+$ requires 163.0997, found 163.0988

3-(3-aminoprop-1-en-2-yl)benzonitrile (5h)



5h

Prepared according to the general procedure for Boc deprotection.

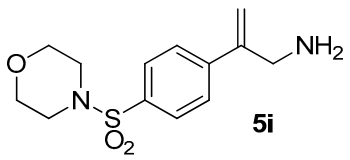
Overall yield for the Heck reaction and Boc deprotection: 55%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.64 (d, J = 7.9 Hz, 1H), 7.56 (d, J = 7.7 Hz, 1H), 7.45 (t, J = 7.8 Hz, 1H), 5.41 (s, 1H), 5.36 (s, 1H), 3.71 (s, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 147.64, 141.15, 131.06, 130.48, 129.85, 129.27, 118.77, 113.64, 112.69, 45.80

(ESI) calculated for $C_{10}H_{11}N_2$ $[M+H]^+$ requires 159.0844, found 159.0839

2-(4-(morpholinosulfonyl)phenyl)prop-2-en-1-amine (5i)



5i

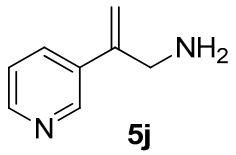
Prepared according to the general procedure for Boc deprotection.

Overall yield for the Heck reaction and Boc deprotection: 30%

^{1}H NMR (600 MHz, CDCl3) δ 7.72 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 8.3 Hz, 2H), 5.49 (s, 1H), 5.41 (s, 1H), 3.77 – 3.73 (m, 6H), 3.04 – 3.00 (m, 4H)

(ESI) calculated for $C_{13}H_{19}N_2O_3S$ $[M+H]^+$ requires 283.1038, found 283.1035

2-(pyridin-3-yl)prop-2-en-1-amine (5j)



5j

Prepared according to general procedure for Boc deprotection.

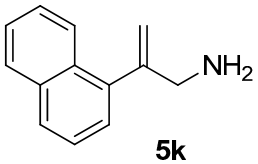
Overall yield from for the Heck reaction and Boc deprotection: 60%

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (d, *J* = 2.0 Hz, 1H), 8.53 (dd, *J* = 4.8, 1.4 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.30 – 7.27 (m, 1H), 5.42 (s, 1H), 5.36 (s, 1H), 3.73 (s, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 160.97, 149.09, 147.40, 141.21, 133.53, 123.37, 115.96, 41.36

(ESI) calculated for $C_8H_{11}N_2$ $[M+H]^+$ requires 135.0844, found 135.0849

2-(naphthalen-1-yl)prop-2-en-1-amine



5k

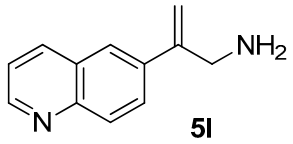
Prepared according to the general procedure for Boc deprotection.

The product could not be fully purified; Derivatives thereof characterized by NMR are provided below.

Overall yield for the Heck reaction and Boc deprotection: 65%

(ESI) calculated for $C_{13}H_{14}N$ $[M+H]^+$ requires 184.1048, found 184.1045

2-(quinolin-6-yl)prop-2-en-1-amine (5l)



5l

Prepared according to general procedure for Boc deprotection.

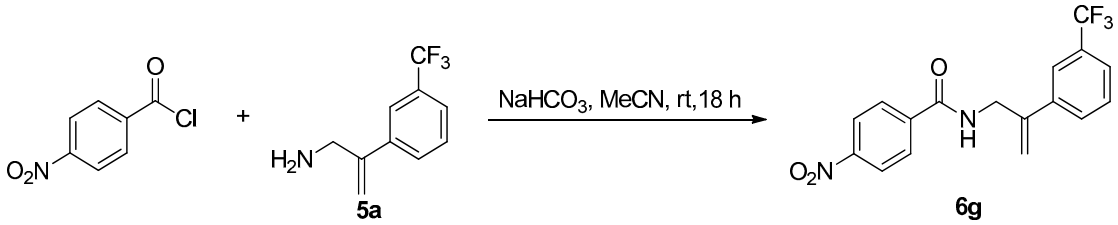
Overall yield from Heck procedure and Boc deprotection: 40%

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.88 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 8.7 Hz, 1H), 7.82 (dd, *J* = 10.9, 2.1 Hz, 2H), 7.38 (dd, *J* = 8.2, 4.2 Hz, 1H), 5.53 (s, 1H), 5.38 (s, 1H), 3.83 (s, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 150.35, 148.80, 147.93, 137.78, 136.20, 129.55, 128.22, 126.53, 124.41, 121.40, 112.84, 46.07

(ESI) calculated for $C_{12}H_{13}N_2$ $[M+H]^+$ requires 185.1000, found 185.1007

Synthesis of 4-nitro-N-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6g) – General procedure A for amide formation from benzoyl chlorides



5a **6g**

In a 10 mL round-bottom flask equipped with magnetic stir bar were added 50 mg 2-(3-(trifluoromethyl)phenyl)prop-2-en-1-amine (**5a**) (0.2485 mmol, 1 eq) and dissolved in 0.3 mL MeCN (0.08 M). Next, 27.2 mg $NaHCO_3$ (0.323 mmol, 1.3 eq) and 46 mg 4-nitrobenzyl chloride (0.2485 mmol, 1 eq) were added in the

flask and the reaction was stirred for 16 h at room temperature and monitored by HPLC. At completion, the solvent was removed under reduced pressure and the crude was dissolved in 2 mL EtOAc. The organic phase was washed with 0.1M HCl (2 × 0.5 mL), aq. $NaHCO_3$ 5% wt/wt (0.5 mL) and brine (0.5 mL). The organic phase was dried over Na_2SO_4. The solvent was removed under reduced pressure to afford an oil residue.

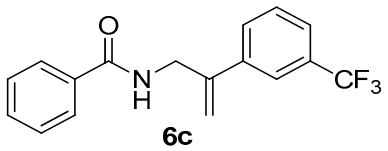
Isolated yield: 51 mg (59%)

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.27 (d, J = 8.8 Hz, 2H), 7.89 (d, J = 8.7 Hz, 2H), 7.73 (s, 1H), 7.67 (d, J = 7.8 Hz, 1H), 7.60 (d, J = 7.7 Hz, 1H), 7.51 (t, J = 7.8 Hz, 1H), 6.38 (s, 1H), 5.62 (s, 1H), 5.44 (s, 1H), 4.60 (d, J = 5.7 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 165.48, 149.63, 142.84, 139.74, 138.91, 130.96 (q, J = 33.22 Hz), 129.30, 129.18, 128.11, 124.92 (q, J = 4.53 Hz), 123.83, 123.05 (q, J = 271.8 Hz), 122.92 (q, J = 4.53 Hz), 115.91, 43.70

(ESI) calculated for $C_{17}H_{14}F_3N_2O_3$ $[M+H]^+$ requires 350.0878, found 350.0881

<u>*N*-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6c)</u>



6c

Prepared according to the general procedure for amide formation A.

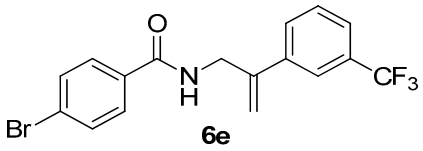
Isolated yield: 71%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 3H), 7.68 (d, J = 7.8 Hz, 1H), 7.58 (d, J = 7.7 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.43 (t, J = 7.7 Hz, 2H), 6.28 (s, J = 31.2 Hz, 1H), 5.59 (s, 1H), 5.43 (s, 1H), 4.58 (d, J = 5.8 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 167.41, 143.37, 139.22, 134.25, 131.63, 130.91 (q, *J* = 33.22 Hz), 129.35, 129.08, 128.62, 126.85, 124.74 (q, *J* = 4.53 Hz), 123.12 (q, *J* = 270.3 Hz), 122.97 (q, *J* = 4.53 Hz), 115.41, 43.42

(ESI) calculated for $C_{17}H_{15}F_3NO$ $[M+H]^+$ requires 306.1027, found 306.1030

4-bromo-*N*-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6e)



6e

Prepared according to general procedure for amide formation A.

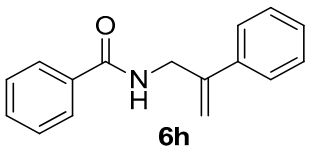
Isolated yield: 63%

^{1}H NMR (600 MHz, $CDCl_3$) *δ* 7.72 (s, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.60 – 7.53 (m, 5H), 7.47 (t, *J* = 7.8 Hz, 1H), 6.17 (s, 1H), 5.57 (s, 1H), 5.40 (s, 1H), 4.54 (d, *J* = 5.7 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) *δ* 166.46, 143.17, 139.08, 133.01, 131.87, 130.93 (q, *J* = 33.22 Hz), 129.32, 129.12, 128.48, 126.36, 124.81 (q, *J* = 4.53 Hz), 123.08 (q, *J* = 272.3 Hz), 122.96 (q, *J* = 4.53 Hz), 115.59, 43.50

(ESI) calculated for $C_{17}H_{14}BrF_3NO$ $[M+H]^+$ requires 384.0133, found 384.0129

***N*-(2-phenylallyl)benzamide (6h)**



6h

Prepared according to general procedure for amide formation A.

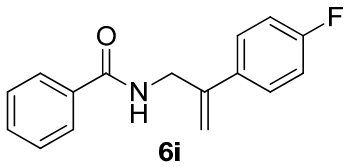
Isolated yield: 70%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, 2H), 7.48 (t, 3H), 7.40 (t, J = 7.6 Hz, 2H), 7.36 (t, J = 10.2, 4.7 Hz, 2H), 7.31 (t, 1H), 6.20 (s, 1H), 5.52 (s, 1H), 5.32 (s, 1H), 4.54 (d, J = 5.5 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 167.34, 144.25, 138.29, 134.45, 131.49, 128.60, 128.57, 128.13, 126.87, 126.09, 114.11, 43.75

(ESI) calculated for $C_{16}H_{16}NO$ $[M+H]^+$ requires 238.1154, found 238.1149

<u>*N*-(2-(4-fluorophenyl)allyl)benzamide (6i)</u>



6i

Prepared according to general procedure for amide formation A.

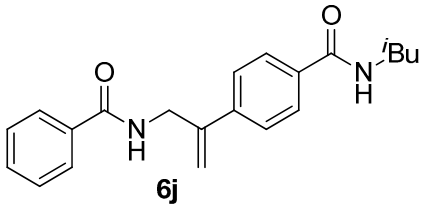
Isolated yield: 75%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 – 7.70 (m, 2H), 7.53 (t, J = 7.8 Hz, 1H), 7.48 – 7.45 (m, 2H), 7.41 (t, J = 7.6 Hz, 2H), 7.06 – 7.01 (m, 2H), 6.28 – 6.14 (m, 1H), 5.46 (s, 1H), 5.30 (s, 1H), 4.52 (d, J = 5.7 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 161.82 (d, J = 241.6 Hz), 143.38 (d, J = 4.53 Hz), 134.35, 131.57, 130.56, 128.87, 128.59, 127.78 (d, J = 7.55 Hz), 126.86, 115.38 (d, J = 21.14 Hz), 113.97, 43.73

(ESI) calculated for $C_{16}H_{15}FNO$ $[M+H]^+$ requires 255.1059, found 255.1063

4-(3-benzamidoprop-1-en-2-yl)-*N*-isobutylbenzamide (6j)



6j

Prepared according to general procedure for amide formation A.

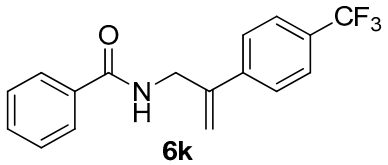
Isolated yield: 85%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (t, J = 7.1 Hz, 4H), 7.50 (d, J = 8.1 Hz, 2H), 7.47 (d, J = 7.3 Hz, 1H), 7.39 (t, J = 7.5 Hz, 2H), 6.40 (s, 1H), 6.29 (s, 1H), 5.56 (s, 1H), 5.37 (s, 1H), 4.52 (d, J = 5.4 Hz, 2H), 3.26 (t, J = 6.3 Hz, 2H), 1.89 (dt, J = 13.3, 6.6 Hz, 1H), 0.96 (d, J = 6.6 Hz, 7H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 167.40, 167.14, 143.55, 141.26, 134.34, 134.23, 131.60, 128.59, 127.15, 126.90, 126.22, 115.38, 47.36, 43.47, 28.61, 20.16

(ESI) calculated for $C_{21}H_{25}N_2O_2$ $[M+H]^+$ requires 336.1838, found 336.1841

***N*-(2-(4-(trifluoromethyl)phenyl)allyl)benzamide (6k)**



6k

Prepared according to general procedure for amide formation A.

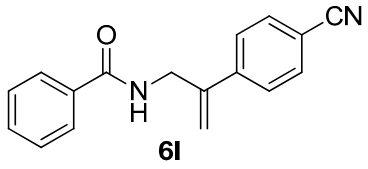
Isolated yield: 55%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 7.4 Hz, 2H), 7.62 (d, J = 2.6 Hz, 4H), 7.52 (t, J = 7.2 Hz, 1H), 7.44 (t, J = 7.5 Hz, 2H), 6.25 (s, 1H), 5.61 (s, 1H), 5.45 (s, 1H), 4.58 (d, J = 5.4 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 167.36, 143.43, 141.89, 134.18, 131.67, 129.98 (q, *J* = 31.71 Hz), 128.64, 126.86, 126.44, 125.52 (q, *J* = 3.02 Hz), 123.14 (q, *J* = 271.8 Hz), 116.01, 43.44

(ESI) calculated for $C_{17}H_{15}F_3NO$ $[M+H]^+$ requires 306.1027, found 306.1032

<u>*N*-(2-(4-cyanophenyl)allyl)benzamide (6i)</u>



6l

Prepared according to general procedure for amide formation A.

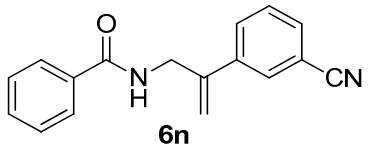
Isolated yield: 80%

^{1}H NMR (600 MHz, $CDCl_3$) *δ* 7.71 (d, *J* = 7.5 Hz, 2H), 7.61 (dd, *J* = 28.9, 8.3 Hz, 4H), 7.49 (d, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 3H), 6.21 (s, 1H), 5.62 (s, 1H), 5.47 (s, 1H), 4.55 (d, *J* = 5.7 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) *δ* 167.33, 143.25, 142.83, 134.05, 132.39, 131.76, 128.67, 126.83, 126.79, 118.64, 116.98, 111.72, 43.20

(ESI) calculated for $C_{17}H_{15}N_2O$ $[M+H]^+$ requires 263.1106, found 263.1103

<u>*N*-(2-(3-cyanophenyl)allyl)benzamide (6n)</u>



6n

Prepared according to general procedure for amide formation A.

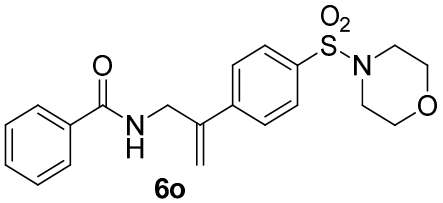
Isolated yield: 70%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.72 (t, J = 7.3 Hz, 3H), 7.58 (d, J = 7.7 Hz, 1H), 7.50 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.8 Hz, 1H), 7.42 (t, J = 7.7 Hz, 2H), 6.28 (s, 1H), 5.55 (s, 1H), 5.43 (s, 1H), 4.53 (d, J = 5.8 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 178.35, 167.34, 142.85, 142.16, 131.74, 131.51, 131.49, 130.44, 129.85, 129.46, 128.68, 126.84, 116.14, 112.88, 43.25

(ESI) calculated for $C_{17}H_{15}N_2O$ $[M+H]^+$ requires 263.1106, found 263.1111

<u>*N*-(2-(4-(morpholinosulfonyl)phenyl)allyl)benzamide (6o)</u>



6o

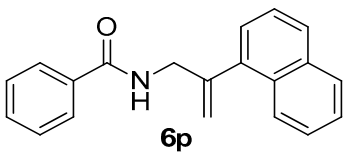
Prepared according to general procedure for amide formation A.

Isolated yield: 51%

^{1}H NMR (600 MHz, CDCl3) δ 7.72 (t, J = 6.8 Hz, 4H), 7.65 (d, J = 8.2 Hz, 2H), 7.51 – 7.48 (m, 1H), 7.42 (t, J = 7.6 Hz, 2H), 5.63 (s, 1H), 5.48 (s, 1H), 4.56 (d, J = 5.6 Hz, 2H), 3.79 – 3.67 (m, 6H), 3.21 (s, 2H)

(ESI) calculated for $C_{20}H_{23}N_2O_4S$ $[M+H]^+$ requires 387.1300, found 387.1310

<u>*N*-(2-(naphthalen-1-yl)allyl)benzamide (6p)</u>



6p

Prepared according to general procedure for amide formation A.

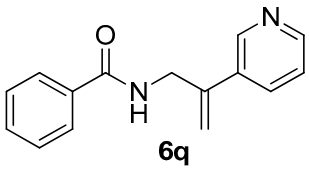
Isolated yield: 55%

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 – 8.11 (m, 1H), 7.88 – 7.85 (m, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.70 – 7.67 (m, 2H), 7.50 (ddd, *J* = 8.0, 3.5, 1.6 Hz, 2H), 7.48 – 7.43 (m, 2H), 7.39 (t, *J* = 7.7 Hz, 2H), 7.36 (dd, *J* = 6.9, 1.0 Hz, 1H), 6.40 (s, 1H), 5.64 (d, *J* = 1.4 Hz, 1H), 5.27 (d, *J* = 1.1 Hz, 1H), 4.46 (d, *J* = 5.9 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 167.42, 144.59, 138.38, 134.45, 133.69, 131.49, 131.44, 130.57, 128.88, 128.57, 128.36, 127.97, 126.87, 126.34, 125.95, 125.58, 125.41, 125.26, 116.06, 46.01

(ESI) calculated for $C_{20}H_{18}NO$ $[M+H]^+$ requires 288.1310, found 288.1307

<u>*N*-(2-(pyridin-3-yl)allyl)benzamide (6q)</u>



6q

Prepared according to general procedure for amide formation A. During this work up, the organic phase was not washed with 0.1M HCl.

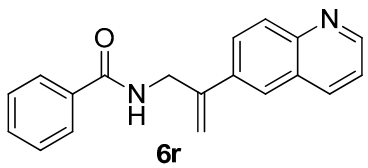
Isolated yield: 60%

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.72 (d, *J* = 1.9 Hz, 1H), 8.52 (d, *J* = 4.7 Hz, 1H), 7.77 (d, *J* = 7.9 Hz, 1H), 7.72 (d, *J* = 7.4 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.27 (dd, *J* = 8.7, 3.9 Hz, 1H), 6.41 (s, 1H), 5.55 (s, 1H), 5.41 (s, 1H), 4.53 (d, *J* = 5.8 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 167.41, 149.15, 147.50, 141.77, 134.16, 134.10, 133.45, 131.65, 128.61, 126.89, 123.34, 115.57, 43.28

(ESI) calculated for $C_{15}H_{15}N_2O$ $[M+H]^+$ requires 239.1106, found 239.1110

<u>*N*-(2-(quinolin-6-yl)allyl)benzamide (6r)</u>



6r

Prepared according to general procedure for amide formation A.

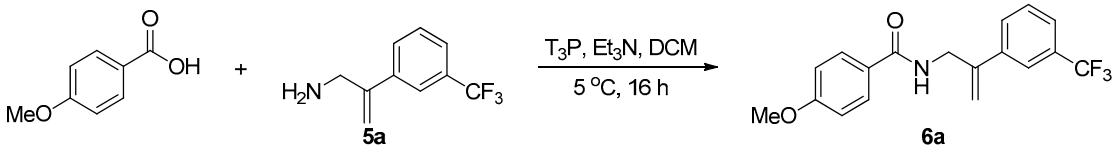
Isolated yield: 88%

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.89 (d, J = 3.9 Hz, 1H), 8.16 (d, J = 7.7 Hz, 2H), 8.09 (d, J = 8.8 Hz, 1H), 7.91 (s, 1H), 7.72 (d, J = 7.8 Hz, 2H), 7.53 (t, J = 7.6 Hz, 1H), 7.41 – 7.37 (m, 3H), 6.30 (s, 1H), 5.70 (s, 1H), 5.48 (s, 1H), 4.67 (d, J = 5.6 Hz, 2H)

^{13}C NMR (151 MHz, CDCl3) δ 167.42, 162.35, 150.46, 143.57, 136.56, 136.25, 134.52, 134.30, 131.58, 130.56, 129.58, 128.86, 128.60, 127.96, 126.86, 124.78, 121.52, 115.62, 43.69

(ESI) calculated for $C_{19}H_{17}N_2O$ $[M+H]^+$ requires 289.1263, found 289.1270

<u>Synthesis of 4-methoxy-N-(2-(3-(trifluoromethyl)phenyl) allyl) benzamide (6a) – General procedure for amide formation B from aryl carboxylic acids</u>



In a 10 mL round-bottom flask equipped with magnetic stir bar, 100 mg 2-(3-(trifluoromethyl) phenyl) prop-2-en-1-amine (**5a**) (0.497 mmol, 1.1 eq), 68.7 mg 4-methoxy benzoic acid (0.4518 mmol, 1 eq) and 470 µL triethylamine (342.9 mg, 3.388 mmol, 7.5 eq) were dissolved in 0.75 mL DCM (0.60M). The mixture was stirred for 15 minutes at -15 °C. Next, 226 µL T_3P of a 50% wt/wt solution in EtOAc (244 mg, 0.768 mmol, 1.7 eq) were diluted in 0.25 mL DCM (1.81 M) and added to the reaction mixture in 3 portions during 1h. The mixture was stirred at 4 °C for 16 h and monitored by HPLC. At completion, the reaction mixture was washed with HCl 0.1 M (2 × 1 mL), aq $NaHCO_3$ 5% wt/wt (1 mL)

and brine (1 mL). The organic phase was dried over Na_2SO_4. The solvent was removed under reduced pressure to afford a white solid.

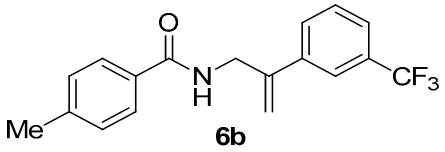
Isolated yield: 75%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.69 (d, *J* = 8.8 Hz, 2H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.47 (d, *J* = 7.8 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.16 (s, 1H), 5.56 (s, 1H), 5.39 (s, 1H), 4.53 (d, *J* = 5.8 Hz, 2H), 3.83 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.89, 162.31, 143.52, 139.30, 130.85 (q, *J* = 31.7 Hz), 129.36, 129.06, 128.68, 126.46, 124.69 (q, *J* = 4.53 Hz), 123.13 (q, *J* = 271.8 Hz), 122.97 (q, *J* = 4.53 Hz), 115.27, 113.80, 55.38, 43.36

(ESI) calculated for $C_{18}H_{17}F_3NO_2$ $[M+H]^+$ requires 335.1133, found 335.1129

4-methyl-N-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6b)



6b

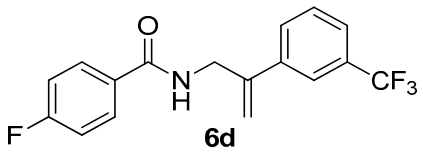
Prepared according to general procedure for amide formation B.

Isolated yield: 82%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (s, 1H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.19 (s, 1H), 5.56 (s, 1H), 5.40 (s, 1H), 4.54 (d, *J* = 5.8 Hz, 2H), 2.38 (s, 3H)

(ESI) calculated for $C_{18}H_{17}F_3NO$ $[M+H]^+$ requires 320.1184, found 320.1193

4-fluoro-N-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6d)



6d

Prepared according to general procedure for amide formation B.

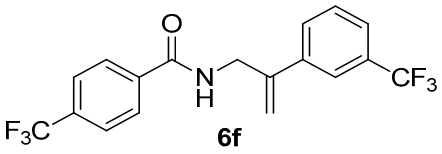
Isolated yield: 80%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (dd, J = 8.6, 5.7 Hz, 3H), 7.64 (d, J = 7.5 Hz, 1H), 7.56 (d, J = 7.5 Hz, 1H), 7.47 (t, J = 7.6 Hz, 1H), 7.07 (t, J = 8.5 Hz, 2H), 6.26 (s, 1H), 5.56 (s, 1H), 5.39 (s, 1H), 4.53 (d, J = 5.5 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.37, 163.95 (d, J = 250.66 Hz), 143.27, 139.16, 130.89 (q, J = 31.71 Hz), 130.37 (d, J = 3.02 Hz), 129.32, 129.19 (d, J = 7.55 Hz), 129.09, 124.77 (q, J = 4.53 Hz), 123.10 (q, J = 273.31 Hz), 122.97 (q, J = 4.53 Hz), 115.57 (d, J = 22.65 Hz), 115.46, 43.47

(ESI) calculated for $C_{17}H_{14}F_4NO$ $[M+H]^+$ requires 324.0933, found 324.0942

4-(trifluoromethyl)-*N*-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6f)



6f

Prepared according to general procedure for amide formation B.

Isolated yield: 92%

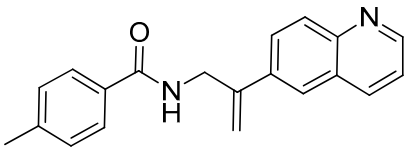
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, J = 8.1 Hz, 2H), 7.72 (s, 1H), 7.67 (d, J = 8.2 Hz, 2H), 7.65 (d, J = 7.6 Hz, 1H), 7.57 (d, J = 7.7 Hz, 1H), 7.48 (t, J = 7.9 Hz, 1H), 6.34 (s, J = 20.3 Hz, 1H), 5.58 (s,12H), 5.41 (s, 1H), 4.57 (d, J = 5.8 Hz, 2H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.15, 143.07, 139.04, 137.49, 133.26 (q, J = 31.71 Hz), 130.95 (q, J = 33.22 Hz), 129.32, 129.13, 127.37, 126.63 (q, J = 270.3 Hz), 125.65

(q, *J* = 4.53 Hz), 124.84 (q, *J* = 3.02 Hz), 123.08 (q, *J* = 271.2 Hz), 122.96 (q, *J* = 4.53 Hz), 115.70, 43.57

(ESI) calculated for $C_{18}H_{14}F_6NO$ $[M+H]^+$ requires 374.0901, found 374.0913

4-methyl-N-(2-(quinolin-6-yl)allyl)benzamide (6s)



6s

Prepared according to general procedure for amide formation B.

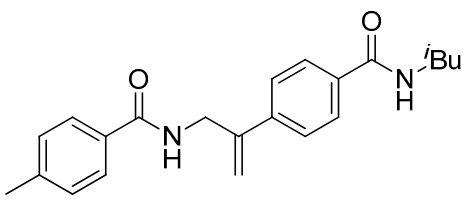
Isolated yield: 90%

^{1}H NMR (600 MHz, DMSO) δ 8.93 – 8.87 (m, 2H), 8.41 (d, *J* = 8.2 Hz, 1H), 8.16 (s, 1H), 8.01 (s, 2H), 7.80 (d, *J* = 8.2 Hz, 2H), 7.56 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 5.72 (s, 1H), 5.35 (s, 1H), 4.45 (d, *J* = 5.8 Hz, 2H), 2.33 (s, 3H)

^{13}C NMR (151 MHz, DMSO) δ 166.59, 150.63, 144.06, 141.51, 137.34, 137.06, 132.00, 129.24, 128.85, 128.56, 128.31, 127.75, 125.00, 122.27, 114.11, 79.75, 42.62, 21.38

(ESI) calculated for $C_{18}H_{14}F_6NO$ $[M+H]^+$ requires 302.1419, found 302.1450

N-isobutyl-4-(3-(4-methylbenzamido)prop-1-en-2-yl)benzamide



7t

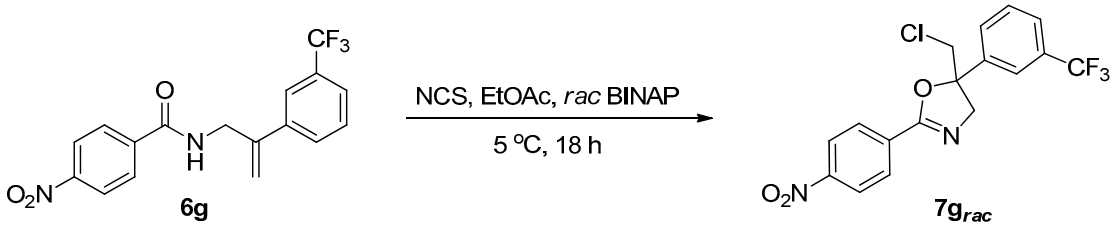
Prepared according to general procedure for amide formation.

Isolated yield: 92%

The product could not be fully purified; The corresponding cyclized derivative however has been purified and the characterization is provided below.

(ESI) calculated for $C_{22}H_{26}N_2O_2$ $[M+H]^+$ requires 350.1994, found 350.1920

Synthesis of 5-(chloromethyl)-2-(4-nitrophenyl)-5-(3-(trifluoromethyl) phenyl)-4,5-dihydrooxazole ($7g_{rac}$)– General procedure for the preparation of racemic oxazolines



In a flamed-dried 1 mL vial equipped with magnetic stir bar, 17.9 mg 4-nitro-N-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (0.0511 mmol, 1 eq) were dissolved in 0.179 mL EtOAc (0.29M). Next, 6.3 mg *rac* BINAP (20 mol %) were added under N_2 atmosphere. The mixture was stirred for 15-20 min at 5 °C before 10.9 mg *N*-chlorosuccinimide (0.0817 mmol, 1.6 eq) were added to the vial under N_2 atmosphere. The reaction mixture was stirred for 16 h at 5 °C and monitored by HPLC. At completion, the organic phase was washed with 0.2M NaOH (2 × 0.2 mL), deionized water (0.2 mL) and brine (0.2 mL). The organic phase was dried over Na_2SO_4 and the solvent was removed under reduced pressure to afford an oil. The product was purified by column chromatography (Hexane/EtOAc: 65/35).

Isolated yield: 84%

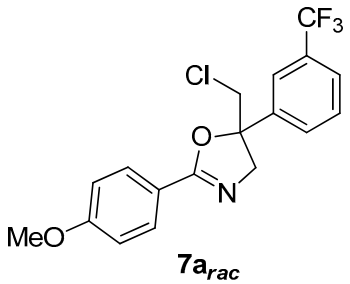
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.33 (d, J = 8.8 Hz, 2H), 8.23 (d, J = 8.8 Hz, 2H), 7.68 (s, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.62 (d, J = 7.9 Hz, 1H), 7.57 (t, J = 7.7 Hz,

1H), 4.61 (d, *J* = 15.4 Hz, 1H), 4.30 (d, *J* = 15.4 Hz, 1H), 3.95 (d, *J* = 12.2 Hz, 1H), 3.88 (d, *J* = 12.2 Hz, 1H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 161.13, 149.78, 142.01, 132.75, 131.35 (q, *J* = 31.71 Hz), 129.57, 129.34, 128.40, 125.52 (q, *J* = 3.02 Hz), 123.74, 122.82 (q, *J* = 271.8 Hz), 121.79 (q, *J* = 3.02 Hz), 88.08, 65.20, 50.64

(ESI) calculated for $C_{17}H_{13}ClF_3N_2O_3$ $[M+H]^+$ requires 385.0489, found 385.0492

5-(chloromethyl)-2-(4-methoxyphenyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole ($7a_{rac}$)



$7a_{rac}$

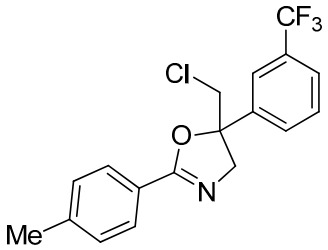
Prepared according to the general procedure for racemic oxazoline formation.

Isolated yield: 91%

(ESI) calculated for $C_{18}H_{16}ClF_3NO_2$ $[M+H]^+$ requires 370.0743, found 370.0752

The oxazoline product was decomposed when tried to be purified by column chromatography. This phenomenon was observed with *p*-OMe group only, probably because of its electron donating effect, enhancing its N-protonation and subsequent hydrolysis of the oxazoline ring.

5-(chloromethyl)-2-(p-tolyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7b$_{rac}$)



7b$_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The crude residue was treated with chilled diethyl ether which caused BINAP to precipitate as a white solid. The diethyl ether liquors were evaporated and the product was isolated as a yellow oil.

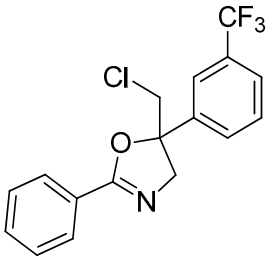
Isolated yield: 93%

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (d, J = 7.9 Hz, 2H), 7.69 (s, 1H), 7.64 – 7.61 (m, 2H), 7.57 – 7.53 (m, 1H), 7.29 (d, J = 7.9 Hz, 2H), 4.55 (d, J = 14.7 Hz, 1H), 4.25 (d, J = 14.6 Hz, 1H), 3.94 (d, J = 12.1 Hz, 1H), 3.88 (d, J = 12.1 Hz, 1H), 2.43 (s, 3H)

(ESI) calculated for $C_{18}H_{16}ClF_3NO$ $[M+H]^+$ requires 354.0794, found 154.0786

Inseparable from the 6-*endo* isomer (**8b**); 13% present in the ^{1}H/^{13}C NMR spectra.

5-(chloromethyl)-2-phenyl-5-(3-(trifluoromethyl)phenyl)-4,5-dihydro-oxazole (7c$_{rac}$)



7c$_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 70/30).

Isolated yield: 76%

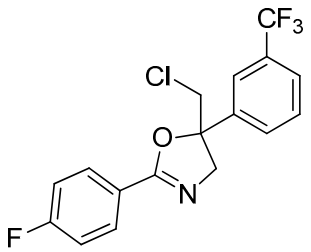
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.2 Hz, 1H), 7.70 (s, 1H), 7.63 (t, *J* = 6.5 Hz, 2H), 7.54 (dd, *J* = 13.7, 7.5 Hz, 2H), 7.47 (t, *J* = 7.6 Hz, 2H), 4.54 (d, *J* = 14.9 Hz, 1H), 4.23 (d, *J* = 14.9 Hz, 1H), 3.93 (d, *J* = 12.0 Hz, 1H), 3.87 (d, *J* = 12.0 Hz, 1H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 162.93, 142.55, 131.79, 129.36, 128.57 (q, *J* = 33.2 Hz), 128.53, 128.28, 127.06, 126.91, 125.23 (q, *J* = 3.02 Hz), 122.92 (q, *J* = 271 Hz), 121.94 (q, *J* = 3.02 Hz), 87.23, 65.10, 50.60

(ESI) calculated for $C_{17}H_{14}ClF_3NO$ $[M+H]^+$ requires 340.0638, found 340.0635

Inseparable from the 6-*endo* isomer (**8c**); 3% present in the ^{1}H/^{13}C NMR spectra.

5-(chloromethyl)-2-(4-fluorophenyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7d$_{rac}$)



7d*rac*

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 70/30).

Isolated yield: 90%

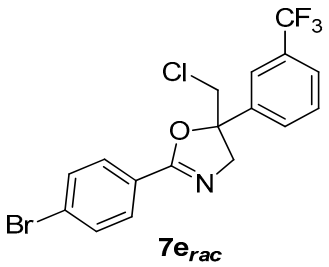
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 – 8.02 (m, 2H), 7.68 (s, 1H), 7.62 (t, *J* = 8.1 Hz, 2H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.17 – 7.13 (m, 2H), 4.53 (d, *J* = 14.9 Hz, 1H), 4.22 (d, *J* = 14.9 Hz, 1H), 3.92 (d, *J* = 12.0 Hz, 1H), 3.87 (d, *J* = 12.0 Hz, 1H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 165.80 (d, *J* = 252.9 Hz), 162.00, 142.42, 131.18 (q, *J* = 31.71 Hz), 130.54 (d, *J* = 9.06 Hz), 129.40, 128.51, 125.28 (q, *J* = 3.02 Hz), 123.31 (d, *J* = 3.02 Hz), 122.90 (q, *J* = 271.9 Hz), 121.89 (q, *J* = 3.02 Hz), 115.65 (d, *J* = 22.65 Hz), 87.44, 65.11, 50.60

(ESI) calculated for $C_{17}H_{14}ClF_4NO$ $[M+H]^+$ requires 358.0544, found 358.0551

Inseparable from the 6-*endo* isomer (**8d**); 10% present in the ^{1}H/^{13}C NMR spectra.

<u>2-(4-bromophenyl)-5-(chloromethyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole ($7e_{rac}$)</u>



$7e_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 80/20).

Isolated yield: 86%

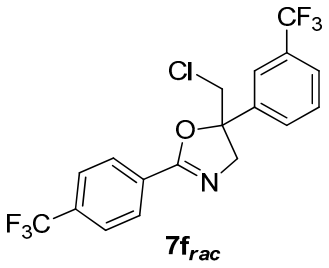
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.3 Hz, 2H), 7.70 (s, 1H), 7.68 – 7.60 (m, 4H), 7.60 – 7.57 (m, 1H), 4.56 (d, *J* = 15.0 Hz, 1H), 4.25 (d, *J* = 15.0 Hz, 1H), 3.95 (d, *J* = 12.0 Hz, 1H), 3.88 (d, *J* = 12.0 Hz, 1H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 142.31, 132.00, 131.86, 131.22 (q, J = 33.22 Hz), 129.79, 129.43, 128.49, 126.59, 125.94, 125.34 (q, J = 4.53 Hz), 122.88 (q, J = 271.8 Hz), 121.89 (q, J = 4.53 Hz), 87.55, 65.05, 50.58

(ESI) calculated for $C_{17}H_{13}BrClF_3NO$ $[M+H]^+$ requires 417.9743, found 417.9739

Inseparable from the 6-*endo* isomer (**8e**); 7% present in the ^{1}H/^{13}C NMR spectra.

5-(chloromethyl)-5-(3-(trifluoromethyl)phenyl)-2-(4(trifluoromethyl) phenyl)-4,5-dihydrooxazole ($7f_{rac}$)



$7f_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 70/30).

Isolated yield: 90%

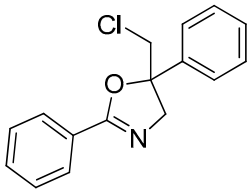
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.17 (d, J = 8.0 Hz, 2H), 7.74 (d, J = 8.1 Hz, 2H), 7.69 (s, 1H), 7.63 (dd, J = 13.1, 7.8 Hz, 2H), 7.56 (t, J = 7.7 Hz, 1H), 4.59 (d, J = 15.2 Hz, 1H), 4.27 (d, J = 15.2 Hz, 1H), 3.94 (d, J = 12.1 Hz, 1H), 3.87 (d, 1H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 142.22, 133.31 (q, J = 31.71 Hz), 131.28 (q, J = 33.22 Hz), 130.38, 129.49, 128.67, 128.45, 125.53 (q, J = 4.53 Hz), 125.41 (q, J = 3.02 Hz), 122.85 (q, J = 273.31 Hz), 122.80 (q, J = 273.31 Hz), 121.84 (q, J = 3.02 Hz), 87.73, 65.10, 50.61

(ESI) calculated for $C_{18}H_{13}ClF_6NO$ $[M+H]^+$ requires 408.0512, found 408.0521

Inseparable from the 6-*endo* isomer (**8f**); 3% present in the ^{1}H/^{13}C NMR spectra.

5-(chloromethyl)-2,5-diphenyl-4,5-dihydrooxazole ($7h_{rac}$)



$7h_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 70/30).

Isolated yield: 50%

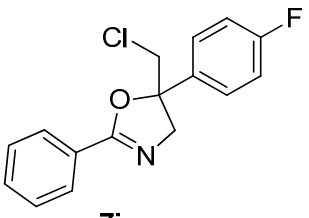
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, J = 7.2 Hz, 2H), 7.52 (t, J = 7.4 Hz, 1H), 7.48 – 7.38 (m, 6H), 7.34 (t, J = 6.4 Hz, 1H), 4.52 (d, J = 14.8 Hz, 1H), 4.25 (d, J = 14.8 Hz, 1H), 3.95 (d, J = 12.0 Hz, 1H), 3.87 (d, J = 12.0 Hz, 1H)

^{13}C NMR (151 MHz, CDCl3) δ 142.59, 132.38, 128.91, 128.70, 128.64, 128.60, 126.97, 125.08, 124.84, 50.87, 40.31, 29.68

(ESI) calculated for $C_{16}H_{15}ClNO$ $[M+H]^+$ requires 272.0764, found 272.0770

Inseparable from the 6-*endo* isomer (**8h**); 7% present in the ^{1}H/^{13}C NMR spectra.

5-(chloromethyl)-5-(4-fluorophenyl)-2-phenyl-4,5-dihydrooxazole ($7i_{rac}$)



$7i_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 70/30).

Isolated yield: 95%

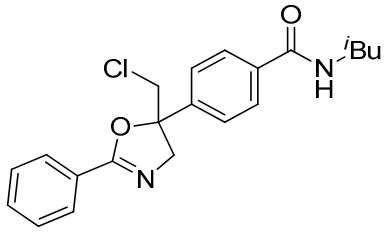
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, J = 7.4 Hz, 2H), 7.52 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.5 Hz, 2H), 7.43 – 7.40 (m, 2H), 7.10 (dd, J = 12.0, 5.2 Hz, 2H), 4.50 (d, J = 14.8 Hz, 1H), 4.22 (d, J = 14.8 Hz, 1H), 3.91 (d, 1H), 3.84 (d, J = 12.0 Hz, 1H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 161.69 (d, J = 243.11 Hz), 137.30 (d, J = 3.02 Hz), 131.66, 128.72, 128.47, 128.25, 127.24, 126.87 (d, J = 9.06 Hz), 115.64 (d, J = 22.65 Hz), 87.26, 65.03, 50.83

(ESI) calculated for $C_{16}H_{14}ClFNO$ $[M+H]^+$ requires 290.0670, found 290.0674

Inseparable from the 6-*endo* isomer (**8i**); 9% present in the ^{1}H/^{13}C NMR spectra.

4-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)-*N*-isobutylbenzamide ($7j_{rac}$)



$7j_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 70/30).

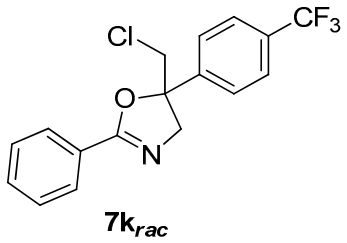
Isolated yield: 90%

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, J = 7.4 Hz, 2H), 7.80 (d, J = 8.4 Hz, 2H), 7.54 (t, J = 7.4 Hz, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.47 (t, J = 7.6 Hz, 2H), 6.18 (s, J = 20.8 Hz, 1H), 4.52 (d, J = 14.8 Hz, 1H), 4.23 (d, 1H), 3.93 (d, J = 12.0 Hz, 1H), 3.87 (d, J = 12.0 Hz, 1H), 3.29 (t, J = 6.4 Hz, 2H), 1.90 (dt, J = 13.4, 6.7 Hz, 1H), 0.98 (d, J = 6.7 Hz, 6H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.83, 135.01, 131.90, 128.54, 128.36, 127.37, 126.93, 125.29, 50.59, 47.38, 30.90, 29.68, 28.61, 20.14, 14.09

(ESI) calculated for $C_{21}H_{24}ClN_2O_2$ $[M+H]^+$ requires 371.1448, found 371.1451

5-(chloromethyl)-2-phenyl-5-(4-(trifluoromethyl)phenyl)-4,5-dihydro-oxazole ($7k_{rac}$)



$7k_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 70/30).

Isolated yield: 45%

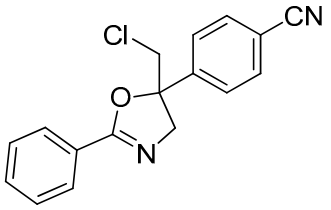
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.4 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.57 (d, *J* = 8.1 Hz, 2H), 7.53 (d, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 4.53 (d, *J* = 14.6 Hz, 1H), 4.22 (d, *J* = 14.6 Hz, 1H), 3.94 (d, *J* = 12.0 Hz, 1H), 3.88 (d, *J* = 12.0 Hz, 1H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 162.96, 145.36, 131.82, 130.53 (q, *J* = 31.71 Hz), 128.53, 128.30, 127.02, 125.78 (q, *J* = 3.02 Hz), 125.58, 122.92 (q, *J* = 271.8 Hz), 87.33, 65.16, 50.51

(ESI) calculated for $C_{17}H_{14}ClF_3NO$ $[M+H]^+$ requires 340.0638, found 340.0641

Inseparable from the 6-*endo* isomer (**8k**); 3% present in the ^{1}H/^{13}C NMR spectra.

4-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)benzonitrile (7l$_{rac}$)



7l$_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 50/50).

Isolated yield: 67%

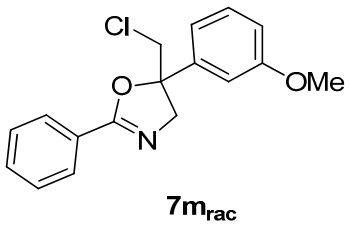
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, J = 7.2 Hz, 2H), 7.71 (d, J = 8.5 Hz, 2H), 7.57 (d, J = 8.5 Hz, 2H), 7.54 (d, J = 7.5 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 4.51 (d, J = 15.0 Hz, 1H), 4.20 (d, J = 15.0 Hz, 1H), 3.92 (d, J = 12.0 Hz, 1H), 3.87 (d, J = 12.0 Hz, 1H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 162.85, 146.53, 132.60, 131.91, 128.56, 128.27, 126.89, 126.01, 118.24, 112.43, 87.21, 65.20, 50.20

(ESI) calculated for $C_{17}H_{14}ClN_2O$ $[M+H]^+$ requires 297.0716, found 297.0725

Inseparable from the 6-*endo* isomer (**8l**); 3% present in the ^{1}H/^{13}C NMR spectra.

5-(chloromethyl)-5-(3-methoxyphenyl)-2-phenyl-4,5-dihydrooxazole (7m$_{rac}$)



7m$_{rac}$

Prepared according to general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 70/30).

Isolated yield: 90%

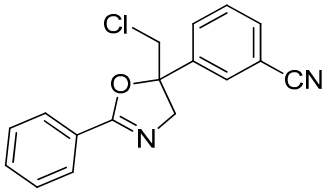
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (d,*J* = 7.2, 2H), 7.53 (dd, *J* = 11.8, 4.3 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.34 (dd, *J* = 9.8, 6.2 Hz, 1H), 7.02 – 6.98 (m, 2H), 6.90 – 6.86 (m, 1H), 4.53 (d, *J* = 15 Hz, 1H), 4.26 (d, *J* = 15 Hz, 1H), 3.95 (d, *J* = 12 Hz, 1H), 3.87 (d, *J* = 12 Hz, 1H), 3.83 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 159.85, 143.06, 131.71, 129.96, 128.69, 128.48, 128.33, 127.15, 126.93, 124.94, 117.15, 113.14, 111.33, 87.72, 64.63, 55.31, 50.98

(ESI) calculated for $C_{17}H_{17}ClNO_2$ $[M+H]^+$ requires 301.0870, found 301.0864

Inseparable from the 6-*endo* isomer (**8m**); 5% present in the ^{1}H/^{13}C NMR spectra.

3-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)benzonitrile ($7n_{rac}$)



$7n_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 60/40).

Isolated yield: 93%

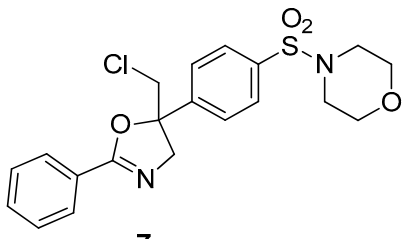
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.1 Hz, 2H), 7.78 (s, *J* = 1.4 Hz, 1H), 7.67 – 7.64 (m, 2H), 7.56 – 7.52 (m, 2H), 7.48 (t, *J* = 7.6 Hz, 2H), 4.51 (d, *J* = 15.0 Hz, 1H), 4.20 (d, *J* = 15.0 Hz, 1H), 3.93 – 3.89 (m, 1H), 3.86 (d, *J* = 12.0 Hz, 1H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.08, 131.97, 131.93, 129.68, 129.56, 129.02, 128.96, 128.58, 128.29, 128.21, 126.85, 113.11, 86.92, 65.18, 50.30

(ESI) calculated for $C_{17}H_{14}ClN_2O$ $[M+H]^+$ requires 297.0716, found 297.0722

Inseparable from the 6-*endo* isomer (**8n**); 4% present in the ^{1}H/^{13}C NMR spectra.

4-((4-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)phenyl)sulfonyl) morpholine ($7o_{rac}$)



$7o_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 50/50).

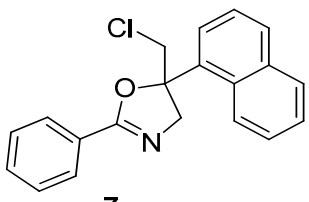
Isolated yield: 74%

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, J = 7.5 Hz, 2H), 7.81 (d, J = 8.4 Hz, 2H), 7.64 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 7.4 Hz, 1H), 7.48 (t, J = 7.5 Hz, 2H), 4.55 (d, J = 14.9 Hz, 1H), 4.24 (d, J = 14.8 Hz, 1H), 3.95 (d, J = 12.0 Hz, 1H), 3.89 (d, J = 12.0 Hz, 1H), 3.76 – 3.72 (m, 4H), 3.04 – 3.00 (m, 4H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 131.89, 128.56, 128.33, 128.28, 126.03, 66.06, 50.29, 45.92, 31.91, 29.68, 29.64, 29.34, 22.67, 14.09

(ESI) calculated for $C_{20}H_{22}ClN_2O_4S$ $[M+H]^+$ requires 421.0911, found 421.0907

5-(chloromethyl)-5-(naphthalen-1-yl)-2-phenyl-4,5-dihydrooxazole ($7p_{rac}$)



$7p_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 70/30).

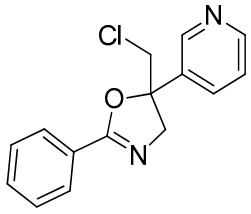
Isolated yield: 72%

^{1}H NMR (600 MHz, CD_3CN) δ 8.13 – 8.08 (m, 2H), 7.97 (dd, J = 19.4, 7.6 Hz, 2H), 7.92 (t, J = 9.0 Hz, 2H), 7.65 – 7.61 (m, 1H), 7.59 (dd, J = 8.1, 5.0 Hz, 2H), 7.53 (t, J = 7.6 Hz, 3H), 4.84 (d, J = 15.2 Hz, 1H), 4.40 (d, J = 15.1 Hz, 1H), 4.33 (d, J = 12.5 Hz, 1H), 4.17 (d, J = 12.5 Hz, 1H)

^{13}C NMR (151 MHz, CD_3CN) δ 161.73, 137.05, 134.52, 131.66, 129.53, 129.47, 128.65, 128.03, 127.55, 126.65, 125.83, 125.29, 124.19, 123.97, 88.55, 78.16, 77.95, 77.73, 64.58, 51.49

(ESI) calculated for $C_{20}H_{17}ClNO$ $[M+H]^+$ requires 322.0920, found 322.0917

5-(chloromethyl)-2-phenyl-5-(pyridin-3-yl)-4,5-dihydrooxazole ($7q_{rac}$)



$7q_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 70/30).

Isolated yield: 31%

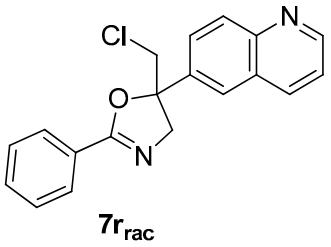
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.73 (d, J = 1.8 Hz, 1H), 8.64 – 8.59 (m, 1H), 8.04 (d, J = 7.2 Hz, 2H), 7.81 – 7.74 (m, 1H), 7.53 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 7.35 (dd, J = 7.9, 4.8 Hz, 1H), 4.53 (d, J = 15.0 Hz, 1H), 4.24 (d, J = 15.0 Hz, 1H), 3.94 (d, J = 11.9 Hz, 1H), 3.88 (d, J = 11.9 Hz, 1H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 162.88, 149.66, 146.77, 133.03, 131.82, 128.52, 128.29, 126.96, 123.43, 86.19, 64.97, 50.38, 29.68

(ESI) calculated for $C_{15}H_{14}ClN_2O$ $[M+H]^+$ requires 273.0716, found 273.0721

Inseparable from the 6-*endo* isomer (**8q**); 5% present in the $^{1}H/^{13}C$ NMR spectra.

5-(chloromethyl)-2-phenyl-5-(quinolin-6-yl)-4,5-dihydrooxazole ($7r_{rac}$)



$7r_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 60/40).

Isolated yield: 58%

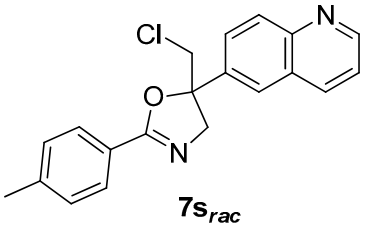
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (s, 1H), 8.23 – 8.19 (m, 2H), 8.10 (d, J = 7.5 Hz, 2H), 7.95 (d, J = 5.6 Hz, 1H), 7.75 (dd, J = 8.8, 1.7 Hz, 1H), 7.54 (d, J = 7.3 Hz, 1H), 7.51 – 7.47 (m, 3H), 4.60 (d, J = 14.9 Hz, 1H), 4.34 (d, 1H), 4.03 (d, J = 12.0 Hz, 1H), 3.99 (d, J = 12.0 Hz, 1H)

^{13}C NMR (151 MHz, CDCl3) δ 139.67, 136.68, 131.97, 131.76, 130.13, 128.79, 128.72, 128.62, 128.53, 128.33, 127.22, 126.92, 126.85, 126.55, 124.19, 121.81, 87.58, 50.67, 31.91, 29.34

(ESI) calculated for $C_{19}H_{16}ClN_2O$ $[M+H]^+$ requires 323.0873, found 323.0868

Inseparable from the 6-*endo* isomer (**8r**); 10% present in the $^{1}H/^{13}C$ NMR spectra.

5-(chloromethyl)-5-(quinolin-6-yl)-2-(p-tolyl)-4,5-dihydrooxazole ($7s_{rac}$)



$7s_{rac}$

Prepared according to general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 40/60).

Isolated yield: 90%

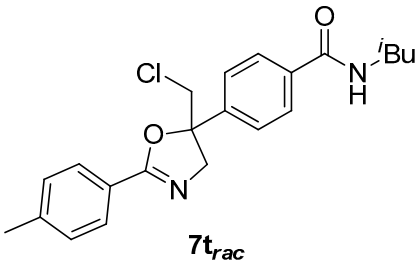
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.96 (s, 1H), 8.22 – 8.16 (m, 2H), 8.00 (d, J = 8.0 Hz, 2H), 7.94 (s, 1H), 7.74 (dd, J = 8.7, 1.9 Hz, 1H), 7.48-7.45 (m, 1H), 7.30 (d, J = 7.9 Hz, 2H), 4.59 (d, J = 14.8 Hz, 1H), 4.33 (d, J = 14.9 Hz, 1H), 4.04 (d, J = 12.0 Hz,1H), 3.99 (d, J = 12.0 Hz, 1H), 2.45 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 142.22, 139.61, 136.37, 130.36, 129.36, 129.24, 129.02, 128.29, 126.93, 126.41, 124.45, 124.18, 121.78, 65.11, 50.69, 29.68, 21.62

(ESI) calculated for $C_{20}H_{17}ClN_2O$ $[M+H]^+$ requires 336.1029, found 336.1050

Inseparable from the 6-*endo* isomer (**8s**); 5% present in the ^{1}H/^{13}C NMR spectra.

4-(5-(chloromethyl)-2-(p-tolyl)-4,5-dihydrooxazol-5-yl)-N-isobutyl benzamide ($7t_{rac}$)



$7t_{rac}$

Prepared according to the general procedure for racemic oxazoline formation. The product was purified by column chromatography (Hexane/EtOAc: 40/60).

Isolated yield: 88%

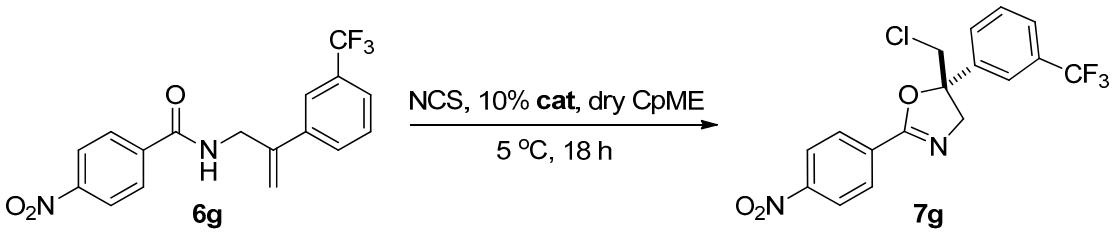
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (d, J = 7.4 Hz, 2H), 7.81 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 8.3 Hz, 2H), 7.28 (d, J = 7.4 Hz, 2H), 6.15 (s, 1H), 4.51 (d, J = 14.7 Hz, 1H), 4.21 (d, J = 15.2 Hz, 1H), 3.94 (d, J = 12.0 Hz, 1H), 3.88 (d, J = 11.9 Hz, 1H),

3.31 (t, *J* = 6.4 Hz, 2H), 2.43 (s, 3H), 1.91 (dt, *J* = 13.5, 6.7 Hz, 1H), 0.99 (d, *J* = 6.7 Hz, 9H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.66, 135.42, 129.90, 129.60, 129.38, 129.04, 127.56, 127.38, 127.05, 126.07, 125.45, 125.18, 125.02, 50.36, 47.41, 29.68, 29.64, 29.34, 28.61, 21.79, 20.15

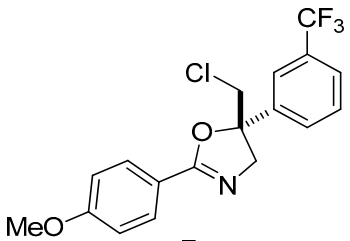
(ESI) calculated for $C_{22}H_{25}ClN_2O_2$ $[M+H]^+$ requires 384.1605, found 384.1642

<u>Synthesis of 5-(chloromethyl)-2-(4-nitrophenyl)-5-(3-(trifluoromethyl) phenyl)-4,5-dihydrooxazole (7g) – General procedure for the asymmetric halocyclisation</u>



In a flamed-dried 1 mL vial equipped with magnetic stir bar 57.3 mg 4-nitro-N-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (**6g**) (0.1635 mmol, 1 eq) were dissolved in 0.57 mL dry CpME (0.29M). 19.2 mg (*S*)-DTBM-SEGPHOS (10 mol%) were added under N_2 atmosphere. The mixture was stirred for 15-20 min at 5 °C before 28.4 mg N-Chlorosuccinimide (0.2125 mmol, 1.3 eq) was added to the vial under N_2 atmosphere. The reaction mixture was stirred for 16 h at 5 °C and monitored by HPLC. At completion, the organic phase was washed with NaOH 0.2 M (2 × 0.5 mL), deionized water (0.5 mL) and brine (0.5 mL). The organic phase was dried over Na_2SO_4 and the solvent was removed under reduced pressure to afford an oil.

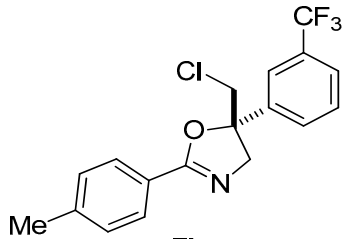
5-(chloromethyl)-2-(4-methoxyphenyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7a)



7a

Prepared according to the general procedure for asymmetric halocyclisation.

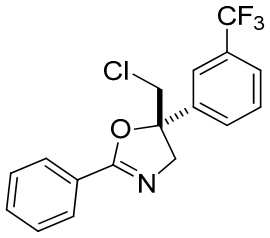
5-(chloromethyl)-2-(p-tolyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7b)



7b

Prepared according to the general procedure for asymmetric halocyclisation.

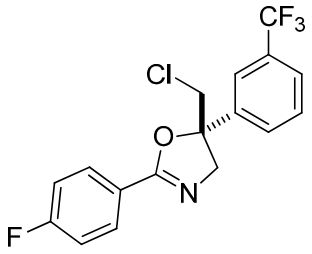
5-(chloromethyl)-2-phenyl-5-(3-(trifluoromethyl)phenyl)-4,5-dihydro-oxazole (7c)



7c

Prepared according to the general procedure for asymmetric halocyclisation.

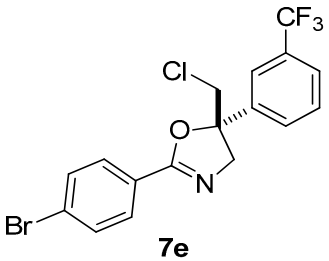
5-(chloromethyl)-2-(4-fluorophenyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7d)



7d

Prepared according to the general procedure for asymmetric halocyclisation.

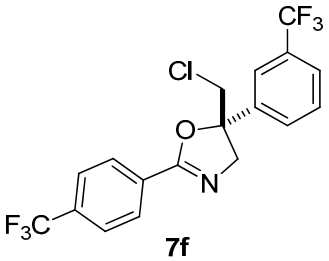
2-(4-bromophenyl)-5-(chloromethyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7e)



7e

Prepared according to the general procedure for asymmetric halocyclisation.

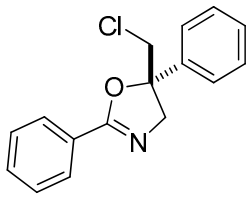
(R)-5-(chloromethyl)-5-(3-(trifluoromethyl)phenyl)-2-(4-(trifluoromethyl) phenyl)-4,5-dihydrooxazole (7f)



7f

Prepared according to the general procedure for asymmetric halocyclisation.

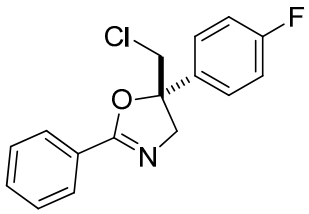
5-(chloromethyl)-2,5-diphenyl-4,5-dihydrooxazole (7h)



7h

Prepared according to the general procedure for asymmetric halocyclisation.

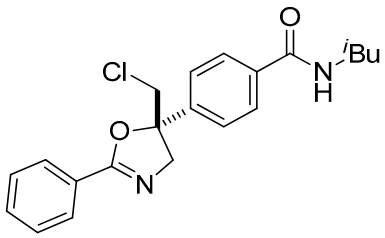
5-(chloromethyl)-5-(4-fluorophenyl)-2-phenyl-4,5-dihydrooxazole (7i)



7i

Prepared according to the general procedure for asymmetric halocyclisation.

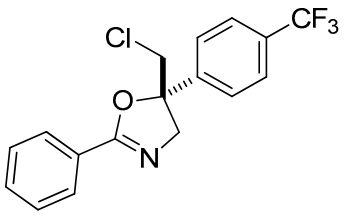
4-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)-N-isobutylbenzamide (7j)



7j

Prepared according to the general procedure for asymmetric halocyclisation.

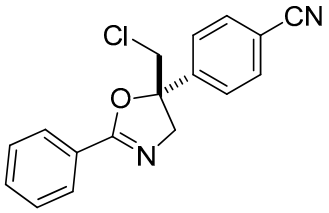
5-(chloromethyl)-2-phenyl-5-(4-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7k)



7k

Prepared according to the general procedure for asymmetric halocyclisation.

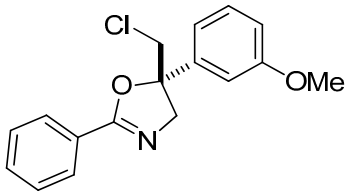
4-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)benzonitrile (7l)



7l

Prepared according to the general procedure for asymmetric halocyclisation.

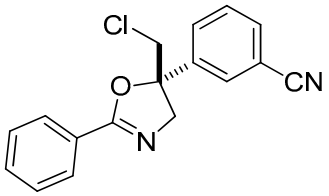
5-(chloromethyl)-5-(3-methoxyphenyl)-2-phenyl-4,5-dihydrooxazole (7m)



7m

Prepared according to the general procedure for asymmetric halocyclisation.

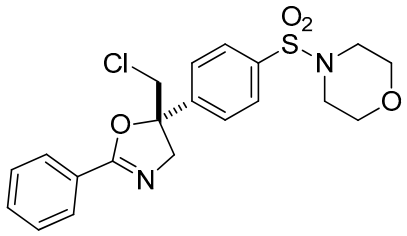
3-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)benzonitrile (7n)



7n

Prepared according to the general procedure for asymmetric halocyclisation.

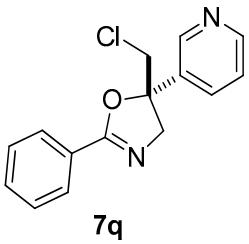
4-((4-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)phenyl)sulfonyl) morpholine (7o)



7o

Prepared according to the general procedure for asymmetric halocyclisation.

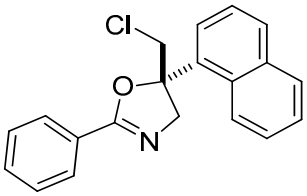
5-(chloromethyl)-2-phenyl-5-(pyridin-3-yl)-4,5-dihydrooxazole (7q)



7q

Prepared according to the general procedure for asymmetric halocyclisation.

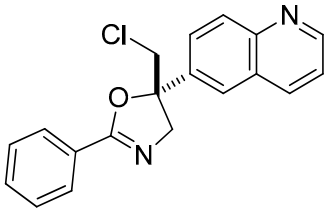
5-(chloromethyl)-5-(naphthalen-1-yl)-2-phenyl-4,5-dihydrooxazole (7p)



7p

Prepared according to the general procedure for asymmetric halocyclisation.

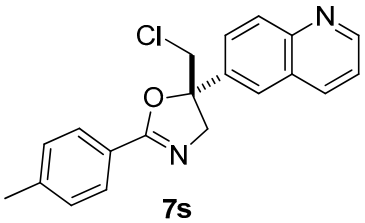
5-(chloromethyl)-2-phenyl-5-(quinolin-6-yl)-4,5-dihydrooxazole (7r)



7r

Prepared according to the general procedure for asymmetric halocyclisation.

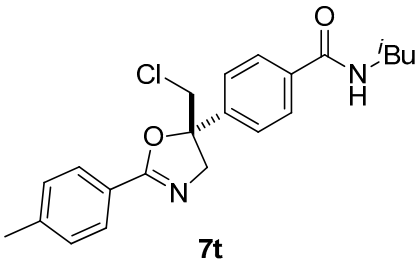
5-(chloromethyl)-5-(quinolin-6-yl)-2-(p-tolyl)-4,5-dihydrooxazole (7s)



7s

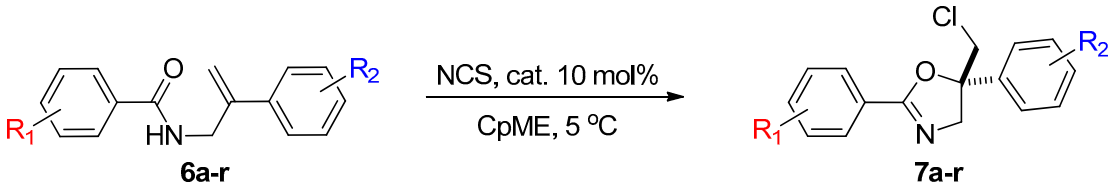
Prepared according to the general procedure for asymmetric halocyclisation.

4-(5-(chloromethyl)-2-(p-tolyl)-4,5-dihydrooxazol-5-yl)-N-isobutyl benzamide (7t)



7t

Prepared according to the general procedure for asymmetric halocyclisation.



6a-r **7a-r**

Table S1 Chiral HPLC methods for racemic oxazolines.

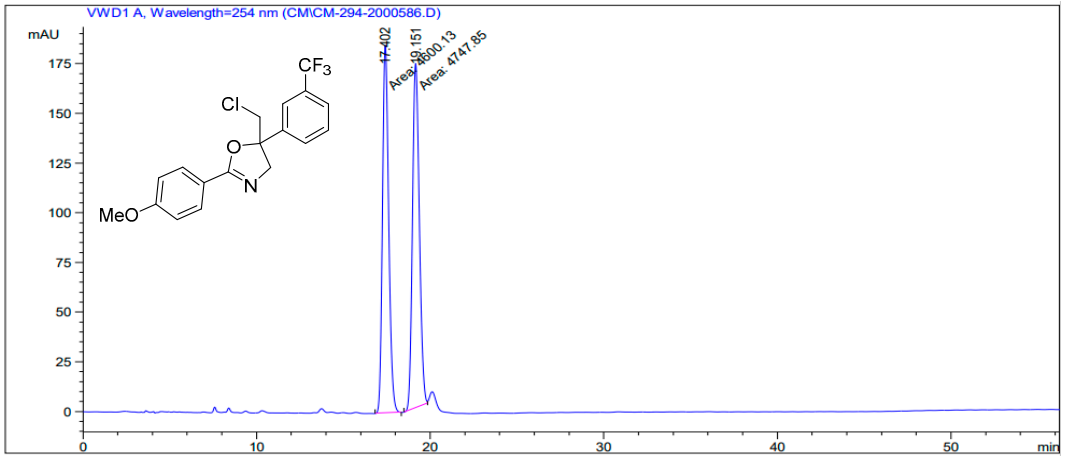
Product	R_1	R_2	Column type	HPLC settings	Retention Times
7a	4-OMeC_6H_4	3-$CF_3C_6H_4$	PHENOMENEX Lux® Cellulose-1 250x4.6 mm, 5µm	Hexane/IPA: 97/3, 0.9 mL/min, 25 °C, 254 nm	17.564 min 19.906 min
7b	4-Me-C_6H_4	3-$CF_3C_6H_4$	PHENOMENEX Lux® Cellulose-3 250x4.6 mm, 5µm	MeCN/H_2O: 60/40, 0.8 mL/min, 25 °C, 254 nm	8.367 min 10.956 min
7c	C_6H_5	3-$CF_3C_6H_4$	PHENOMENEX Lux® Cellulose-1 250x4.6 mm, 5µm	Hexane/IPA: 97/3, 0.9 mL/min, 25 °C, 254 nm	9.817 min 10.965 min
7d	4-FC_6H_4	3-$CF_3C_6H_4$	PHENOMENEX Lux® Cellulose-3 250x4.6 mm, 5µm	MeCN/H_2O: 60/40, 0.8 mL/min, 25 °C, 254 nm	7.858 min 9.449 min
7e	4-BrC_6H_4	3-$CF_3C_6H_4$	PHENOMENEX Lux® Cellulose-3 250x4.6 mm, 5µm	MeCN/H_2O: 60/40, 0.8 mL/min, 25 °C, 254 nm	11.300 min 12.794 min

7f	4-$CF_3C_6H_4$	3-$CF_3C_6H_4$	PHENOMENEX Lux® i-Amylose-1 250x4.6 mm, 5µm	Hexane/IPA: 92/8, 0.6 mL/min, 25 °C, 254 nm	13.117 min 14.031 min
7g	4-$NO_2C_6H_4$	3-$CF_3C_6H_4$	PHENOMENEX Lux® Cellulose-1 250x4.6 mm, 5µm	Hexane/IPA: 97/3, 0.9 mL/min, 25 °C, 254 nm	27.172 min 39.547 min
7h	C_6H_5	C_6H_5	PHENOMENEX Lux® i-Amylose-1 250x4.6 mm, 5µm	Hexane/IPA: 93/7, 1.0 mL/min, 25 °C, 254 nm	10.767 min 14.331 min
7i	C_6H_5	4-FC_6H_4	PHENOMENEX Lux® i-Amylose-1 250x4.6 mm, 5µm	Hexane/IPA:80/20, 0.8 mL/min, 25 °C, 254 nm	7.619 min 8.625 min
7j	C_6H_5	4-CONH-^{i}BuC_6H_4	PHENOMENEX Lux® i-Amylose-1 250x4.6 mm, 5µm	Hexane/IPA:80/20, 0.8 mL/min, 25 °C, 254 nm	21.608 min 26.333 min
7k	C_6H_5	4-$CF_3C_6H_4$	PHENOMENEX Lux® Cellulose-1 250x4.6 mm, 5µm	Hexane/IPA: 95/5, 1.0 mL/min, 25 °C, 254 nm	8.366 min 10.229 min
7l	C_6H_5	4-NCC_6H_4	PHENOMENEX Lux® Cellulose-1 250x4.6 mm, 5µm	Hexane/IPA: 92/8, 1.0 mL/min, 25 °C, 254 nm	19.966 min 24.267 min
7m	C_6H_5	3-$OMeC_6H_4$	PHENOMENEX Lux® Cellulose-1 250x4.6 mm, 5µm	Hexane/IPA:90/10, 0.9 mL/min, 25 °C, 254 nm	10.789 min 11.356 min
7n	C_6H_5	3-NCC_6H_4	PHENOMENEX Lux® Cellulose-1 250x4.6 mm, 5µm	Hexane/IPA: 95/5, 1.0 mL/min, 25 °C, 254 nm	24,407 min 33.363 min
7o	C_6H_5	4-(SO_2-morpholine) C_6H_4	PHENOMENEX Lux® i-Amylose-1 250x4.6 mm, 5µm	Hexane/IPA:80/20, 0.7 mL/min, 25 °C, 254 nm	36.560 min 45.888 min
7p	C_6H_5	1-naphthyl	PHENOMENEX Lux® Cellulose-1 250x4.6 mm, 5µm	Hexane/IPA: 95/5, 1.0 mL/min, 25 °C, 254 nm	11.647 min 12.936 min

7q	C_6H_5	3-C_5H_5N	PHENOMENEX Lux® i-Amylose-1 250x4.6 mm, 5µm	Hexane/IPA:80/20, 0.7 mL/min, 25 °C, 254 nm	14.234 min 21.243 min
7r	C_6H_5	6-quinoline	PHENOMENEX Lux® i-Amylose-1 250x4.6 mm, 5µm	Hexane/IPA:80/20, 0.5 mL/min, 25 °C, 254 nm	26.782 min 28.188 min
7s	4-Me-C_6H_4	6-quinoline	PHENOMENEX Lux® Cellulose-3 250x4.6 mm, 5µm	MeCN/H_2O: 60/40, 0.8 mL/min, 25 °C, 254 nm	6.932 min 9.696 min
7t	4-Me-C_6H_4	4-CONH-^{i}BuC_6H_4	PHENOMENEX Lux® Cellulose-3 250x4.6 mm, 5µm	MeCN/H_2O: 60/40, 0.8 mL/min, 25 °C, 254 nm	6.387 min 3.774 min

HPLC

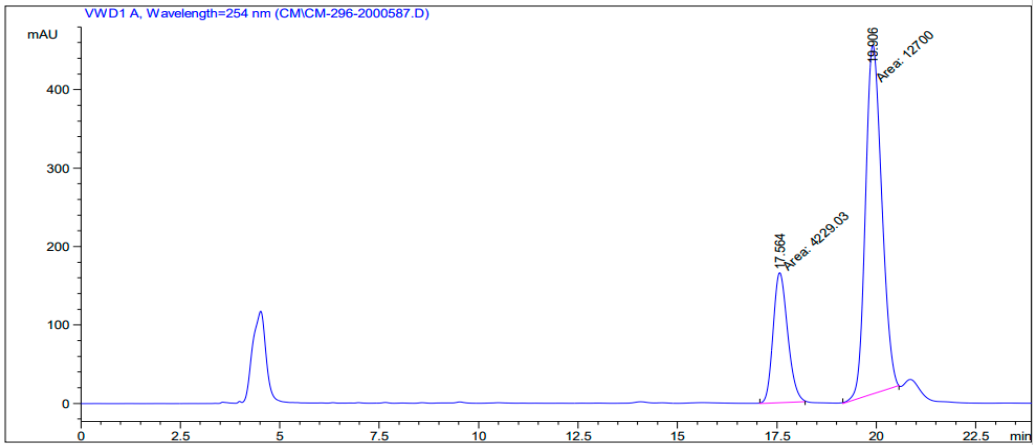
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	17.402	MM	0.4146	4600.13232	184.92120	49.2099
2	19.151	MM	0.4570	4747.84961	173.15601	50.7901

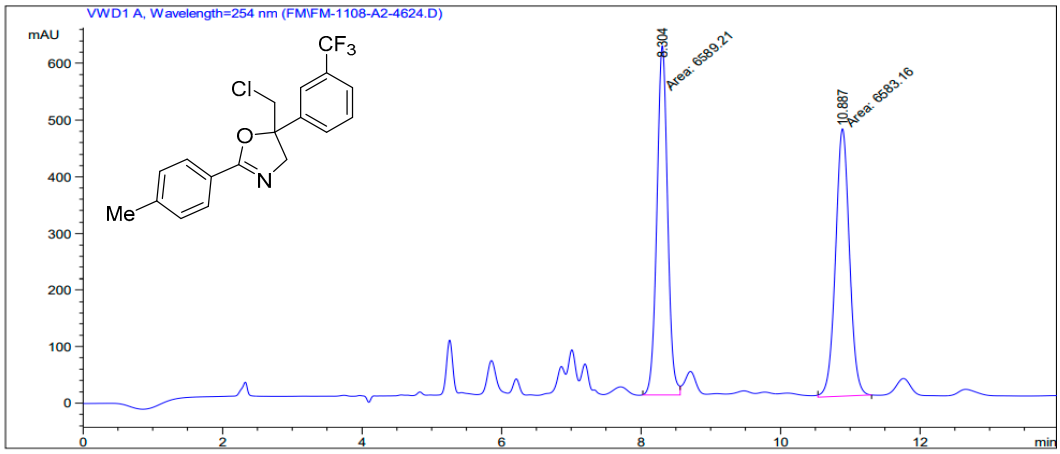
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	17.564	MM	0.4247	4229.03320	165.95943	24.9810
2	19.906	MM	0.4751	1.27000e4	445.50519	75.0190

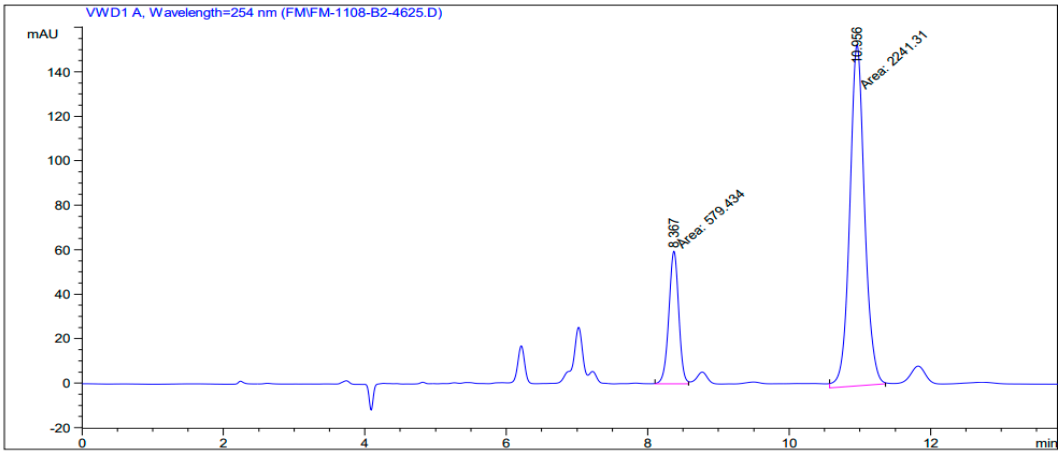
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.304	MM	0.1778	6589.20605	617.57483	50.0230
2	10.887	MM	0.2324	6583.15869	472.19656	49.9770

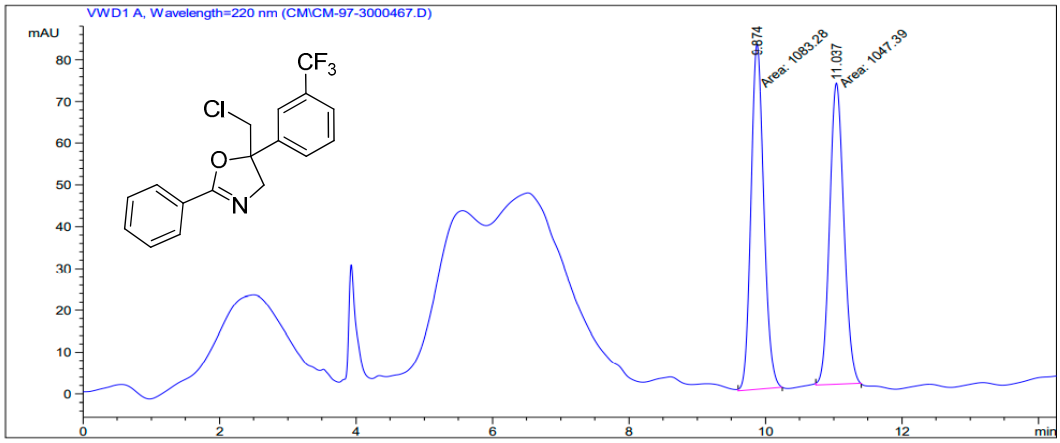
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.367	MM	0.1618	579.43427	59.67440	20.5419
2	10.956	MM	0.2433	2241.30933	153.52629	79.4581

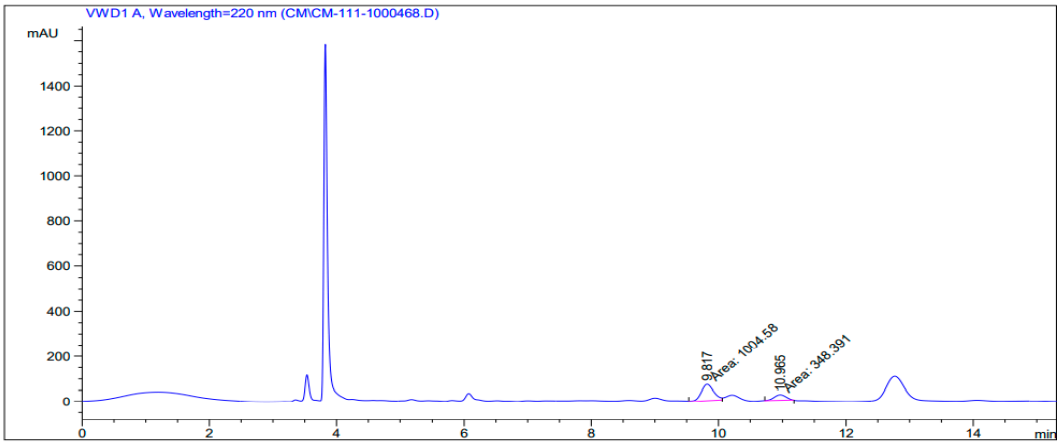
Racemic product



Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.874	MM	0.2181	1083.27563	82.76808	50.8420
2	11.037	MM	0.2417	1047.39490	72.22694	49.1580

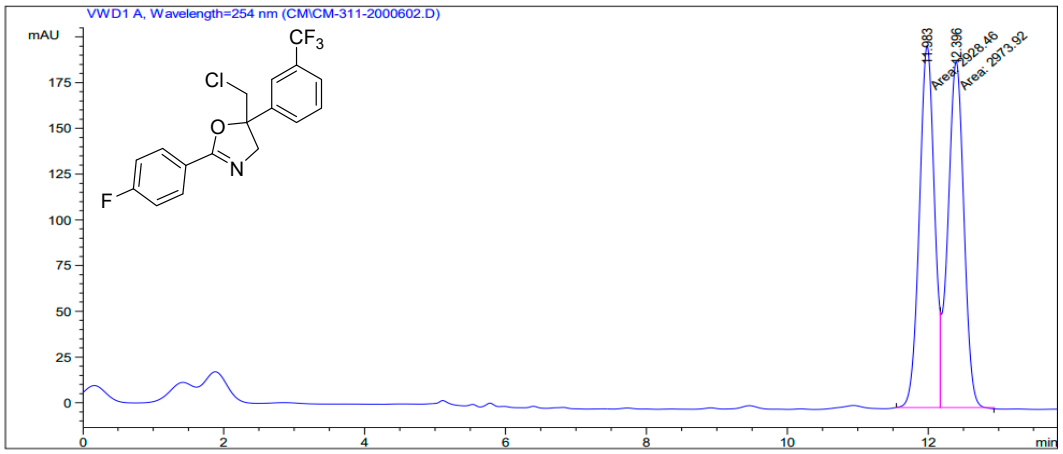
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.817	MM	0.2298	1004.58484	72.84771	74.2500
2	10.965	MM	0.2278	348.39081	25.48541	25.7500

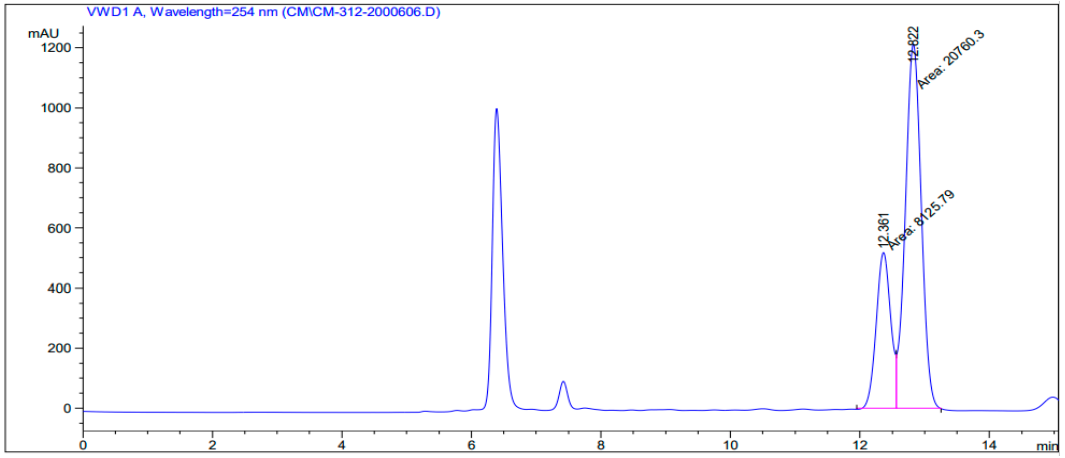
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.983	MF	0.2467	2928.46094	197.84641	49.6149
2	12.396	FM	0.2619	2973.92017	189.27411	50.3851

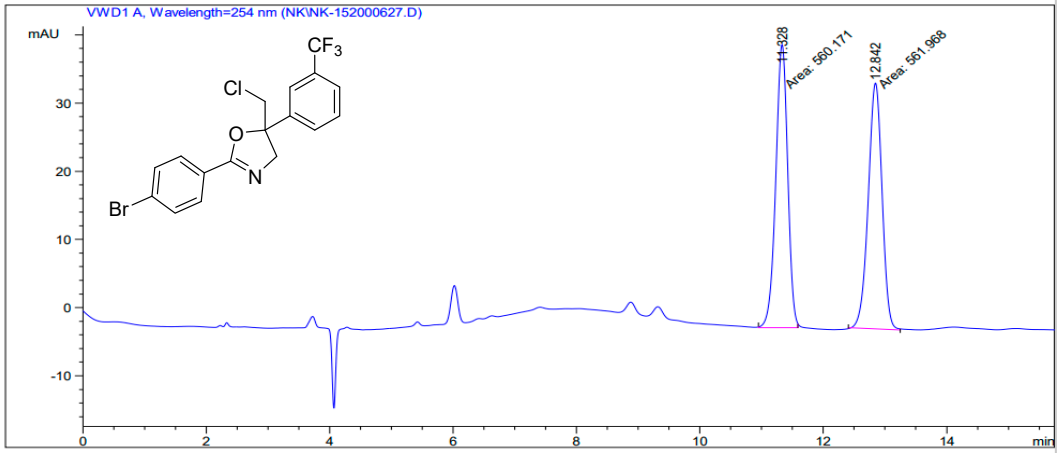
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	12.361	MF	0.2614	8125.78711	518.11908	28.1304
2	12.822	FM	0.2852	2.07603e4	1213.21680	71.8696

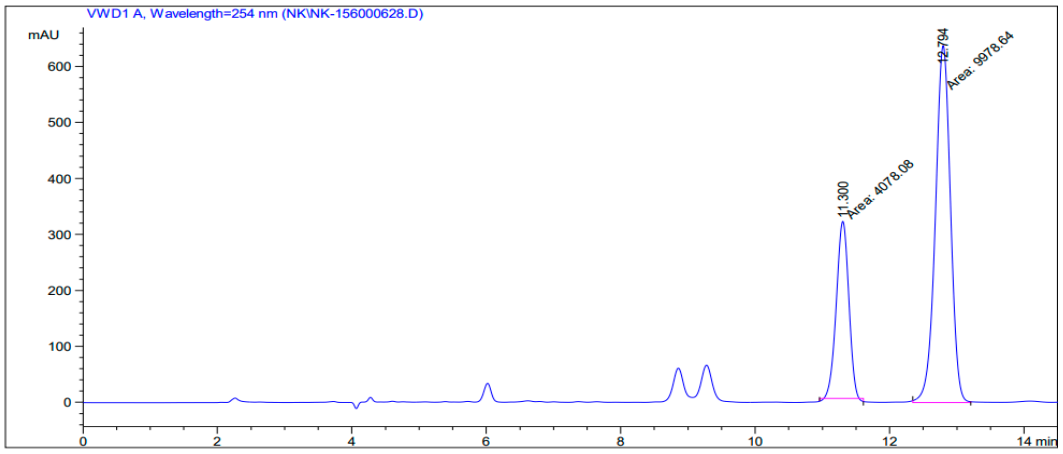
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.328	MM	0.2245	560.17059	41.58200	49.9199
2	12.842	MM	0.2596	561.96759	36.07897	50.0801

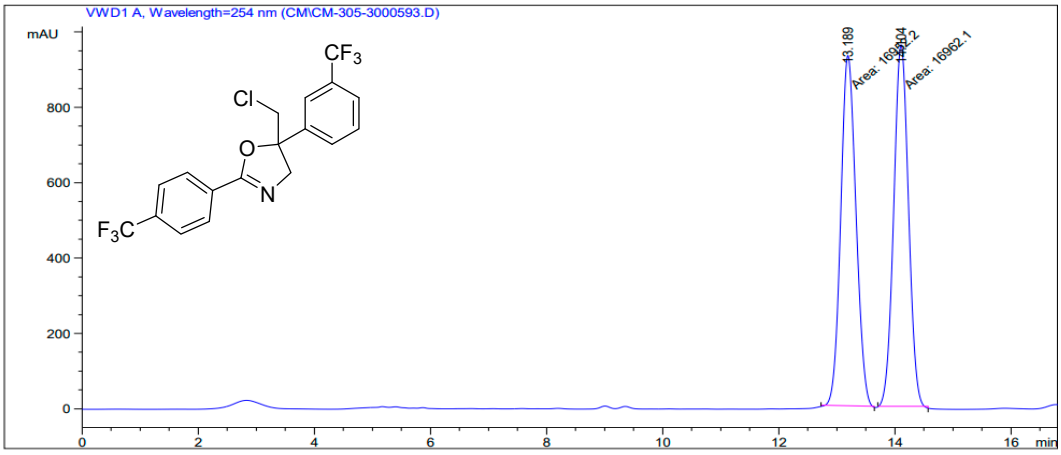
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.300	MM	0.2146	4078.07690	316.65405	29.0116
2	12.794	MM	0.2607	9978.64258	637.86646	70.9884

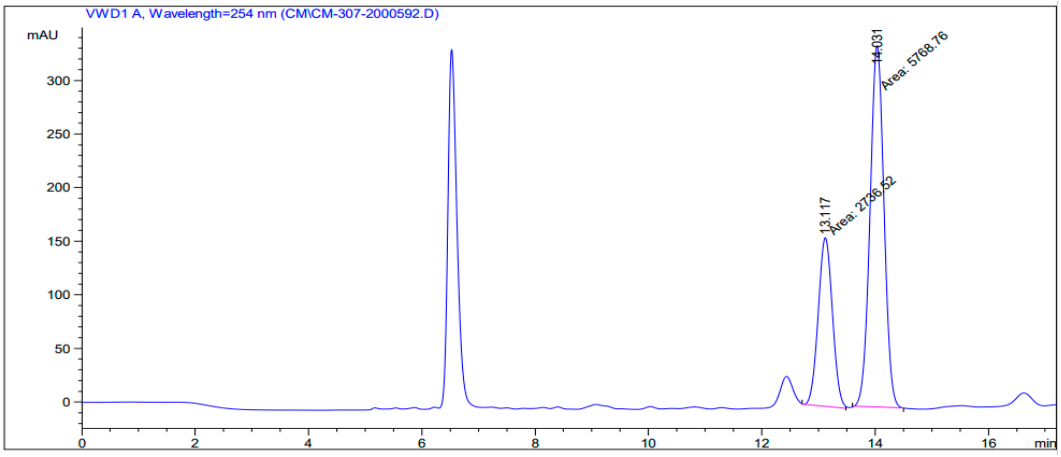
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.189	MM	0.3039	1.69522e4	929.75256	49.9853
2	14.104	MM	0.2944	1.69621e4	960.14893	50.0147

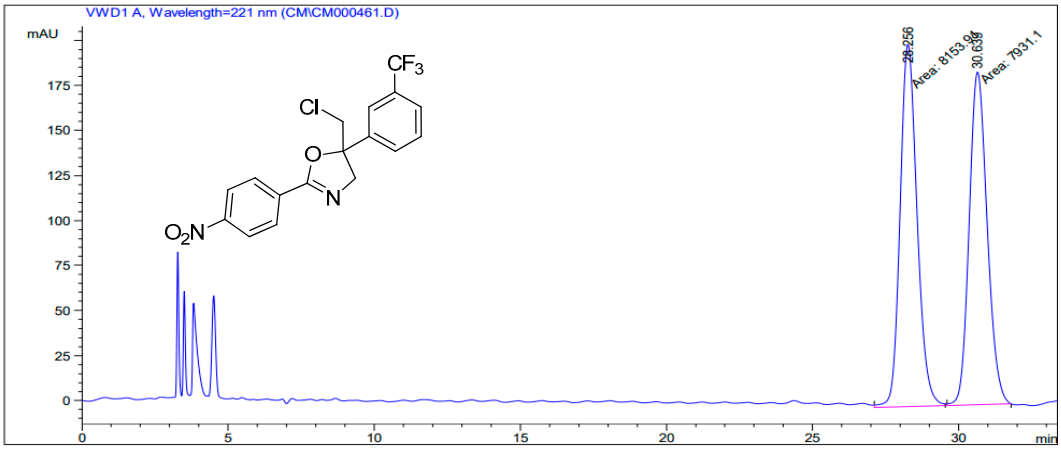
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.117	MM	0.2900	2736.51831	157.27640	32.1744
2	14.031	MM	0.2853	5768.75635	337.04285	67.8256

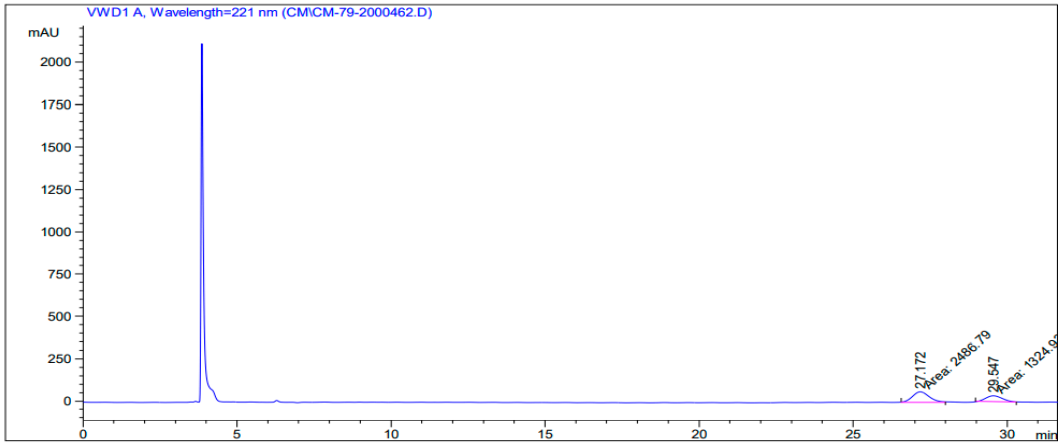
Racemic product



Signal 1: VWD1 A, Wavelength=221 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	28.256	MM	0.6744	8153.91260	201.51906	50.6926
2	30.639	MM	0.7151	7931.10010	184.83716	49.3074

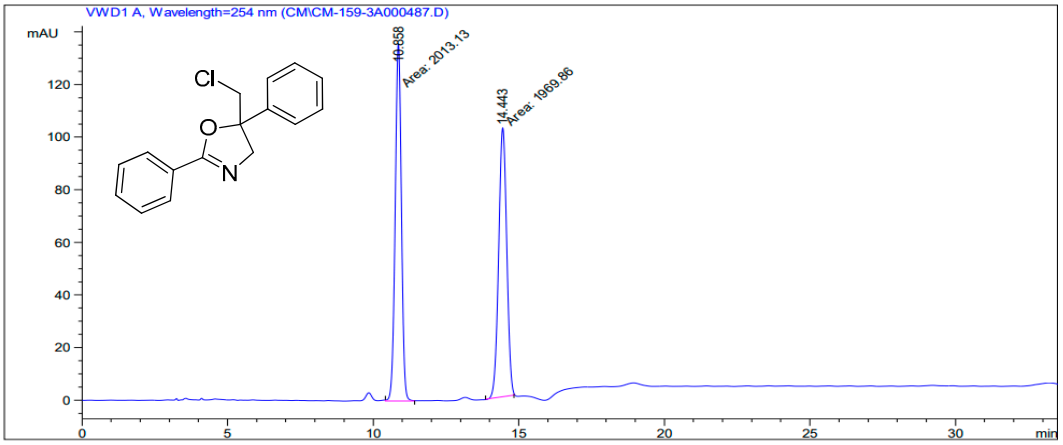
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=221 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	27.172	MM	0.6520	2486.78882	63.57108	65.2406
2	29.547	MM	0.6284	1324.92944	35.14028	34.7594

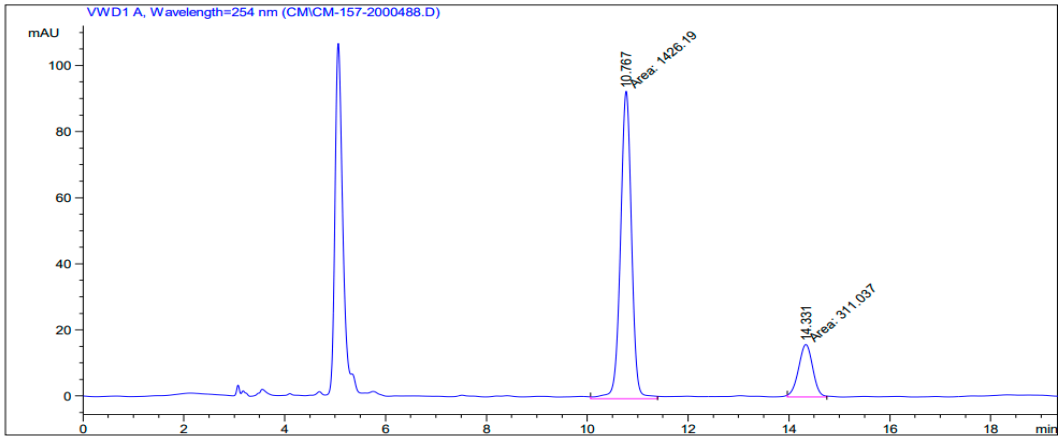
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.858	MM	0.2470	2013.12927	135.84595	50.5431
2	14.443	MM	0.3211	1969.86279	102.23176	49.4569

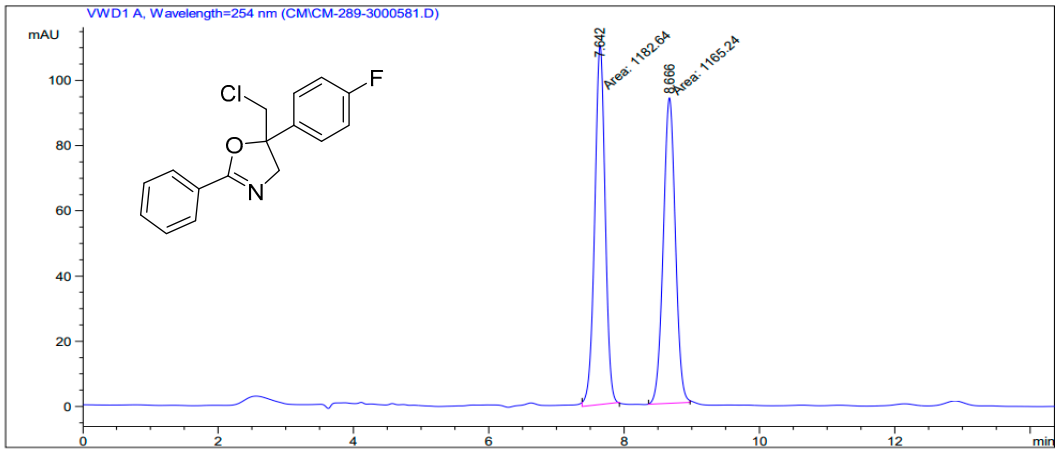
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.767	MM	0.2552	1426.18823	93.12705	82.0958
2	14.331	MM	0.3261	311.03683	15.89640	17.9042

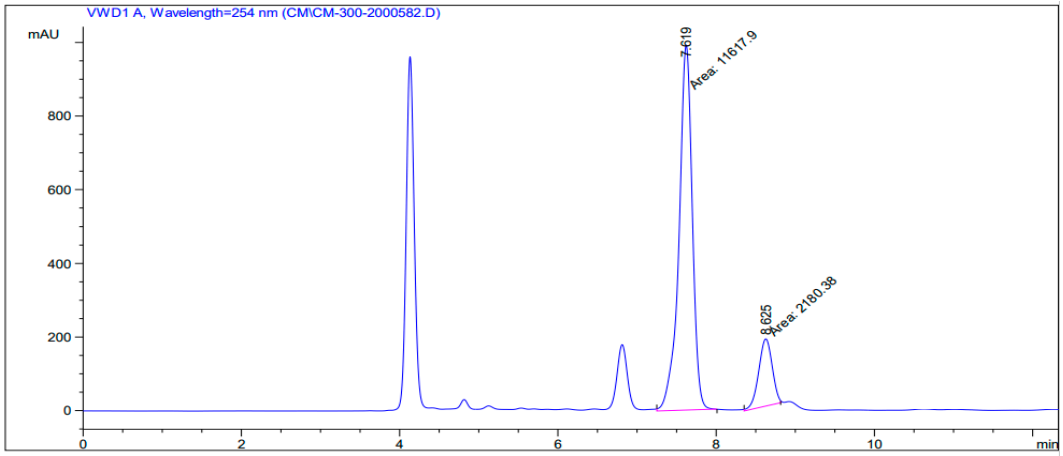
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.642	MM	0.1788	1182.64307	110.26910	50.3707
2	8.666	MM	0.2071	1165.23511	93.76143	49.6293

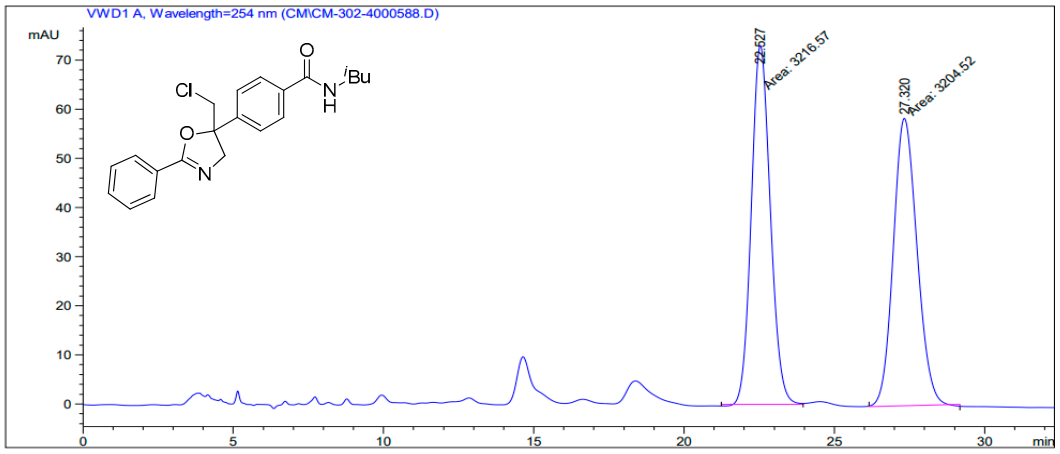
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.619	MM	0.1952	1.16179e4	992.18384	84.1981
2	8.625	MM	0.1980	2180.38379	183.56395	15.8019

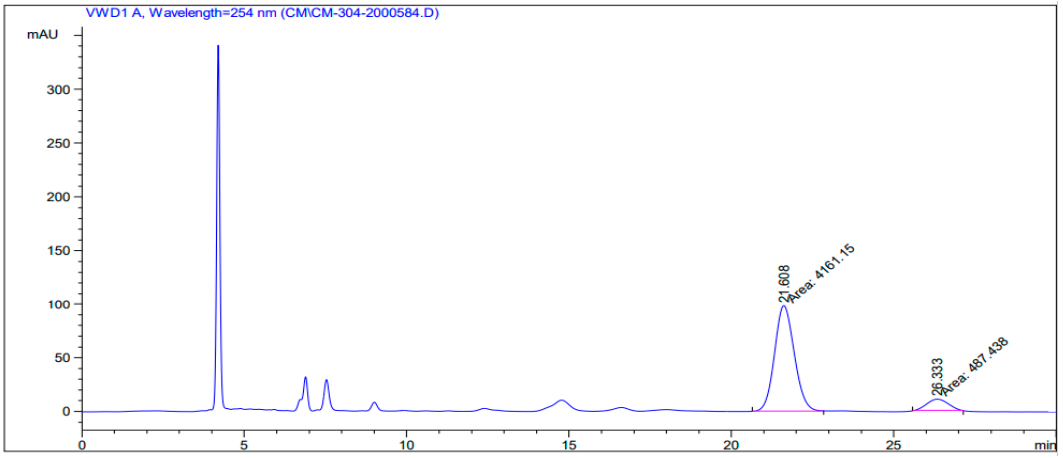
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	22.527	MM	0.7335	3216.56738	73.08369	50.0938
2	27.320	MM	0.9131	3204.52124	58.49326	49.9062

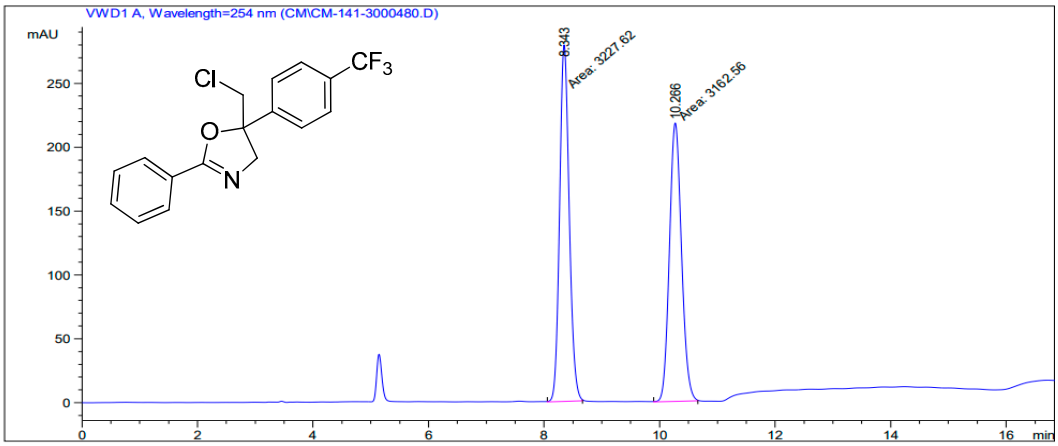
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.608	MM	0.7056	4161.14600	98.28674	89.5143
2	26.333	MM	0.7678	487.43768	10.58071	10.4857

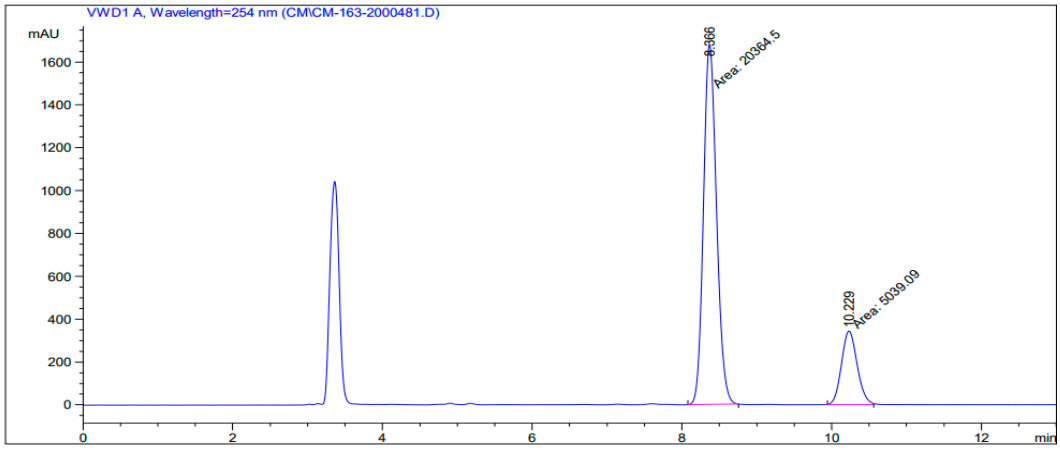
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.343	MM	0.1926	3227.61914	279.24811	50.5091
2	10.266	MM	0.2417	3162.56055	218.05081	49.4909

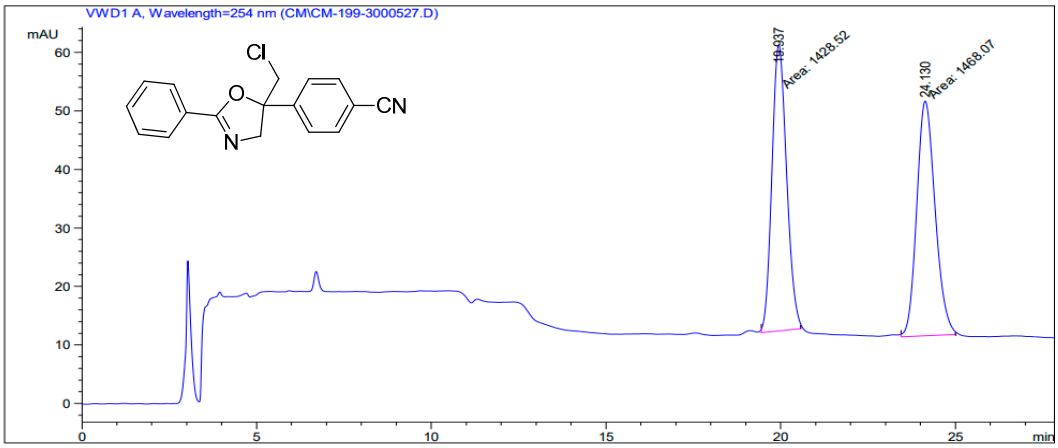
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.366	MM	0.2019	2.03645e4	1681.23145	80.1638
2	10.229	MM	0.2439	5039.09277	344.33011	19.8362

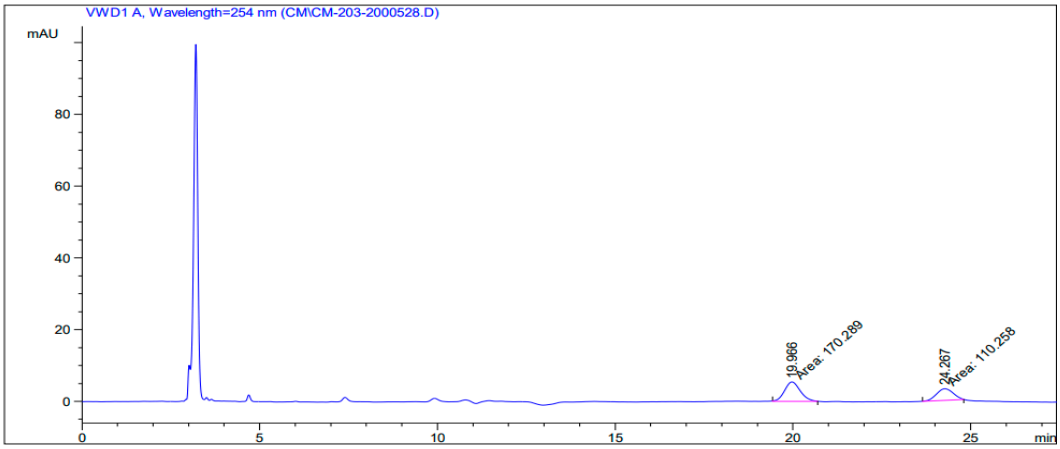
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.937	MM	0.4868	1428.52417	48.90645	49.3173
2	24.130	MM	0.6099	1468.07251	40.11523	50.6827

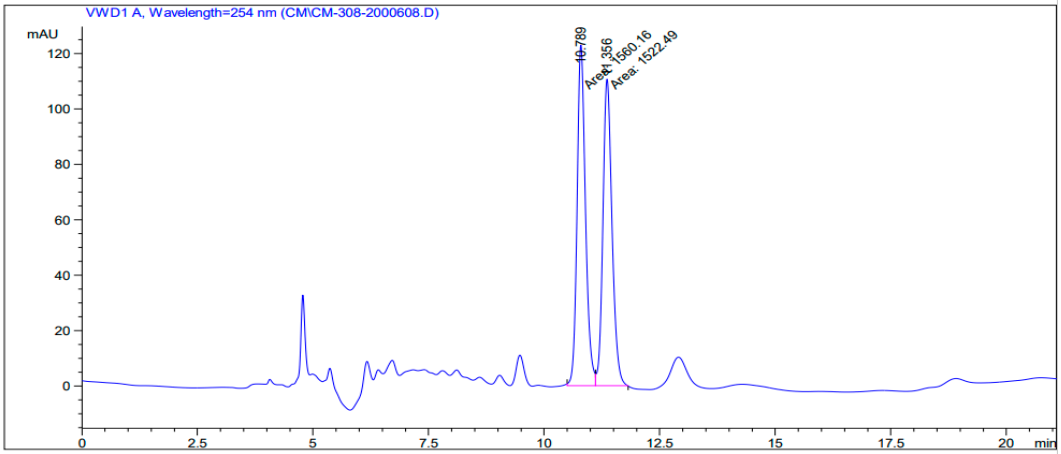
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.966	MM	0.5195	170.28851	5.46335	60.6989
2	24.267	MM	0.5579	110.25771	3.29400	39.3011

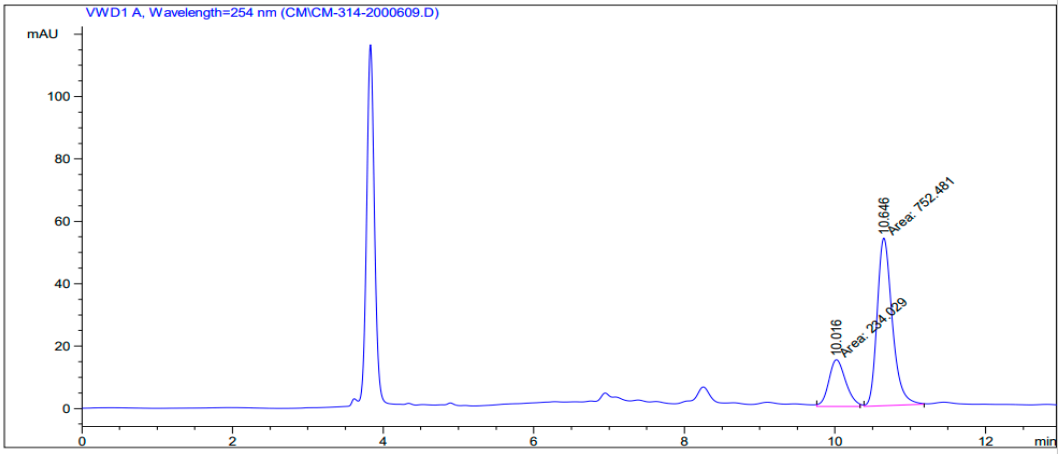
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.789	MF	0.2111	1560.15967	123.17421	50.6110
2	11.356	FM	0.2290	1522.48779	110.79945	49.3890

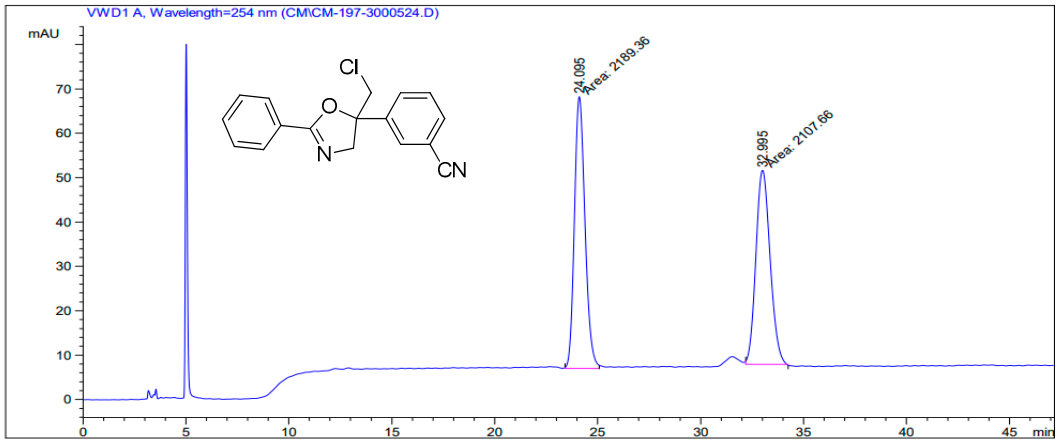
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.016	MM	0.2599	234.02852	15.00996	23.7229
2	10.646	MM	0.2332	752.48132	53.77718	76.2771

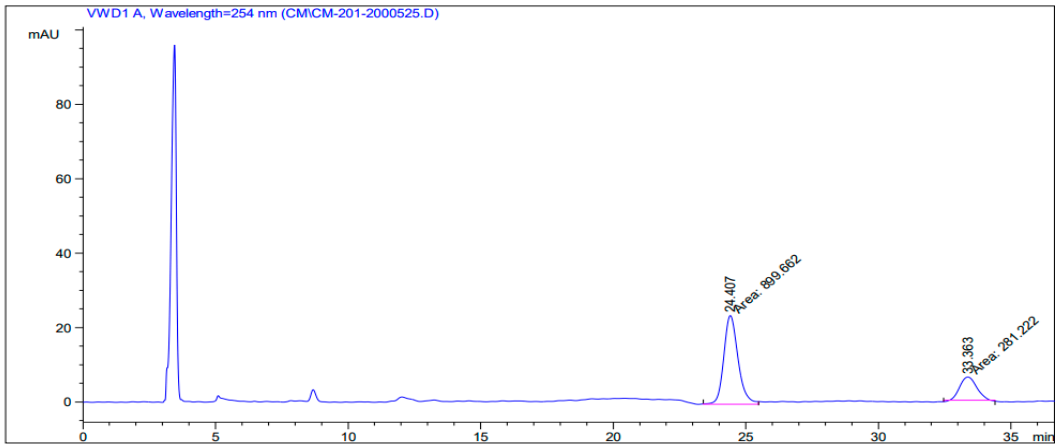
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	24.095	MM	0.5960	2189.35815	61.22585	50.9506
2	32.995	MM	0.8028	2107.66235	43.75399	49.0494

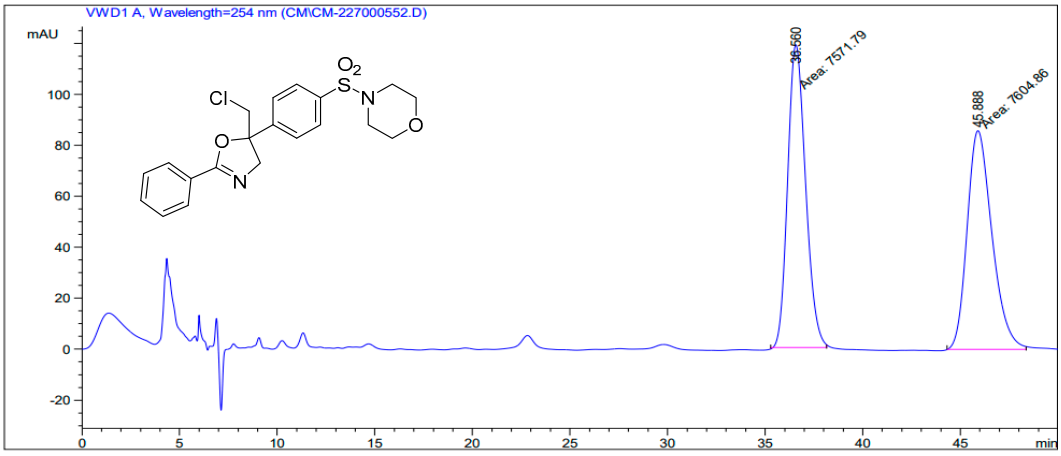
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	24.407	MM	0.6279	899.66211	23.87840	76.1854
2	33.363	MM	0.7444	281.22244	6.29643	23.8146

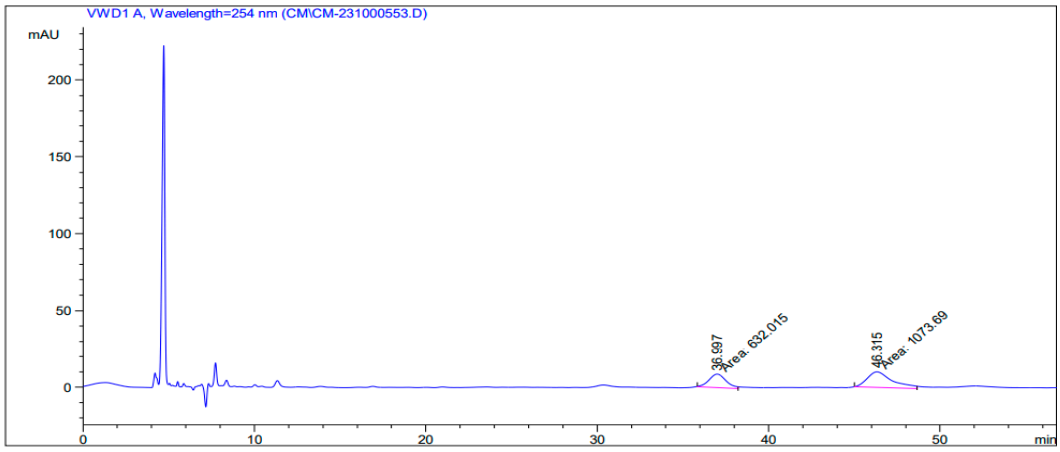
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	36.560	MM	1.0624	7571.79395	118.78789	49.8911
2	45.888	MM	1.4756	7604.85645	85.89352	50.1089

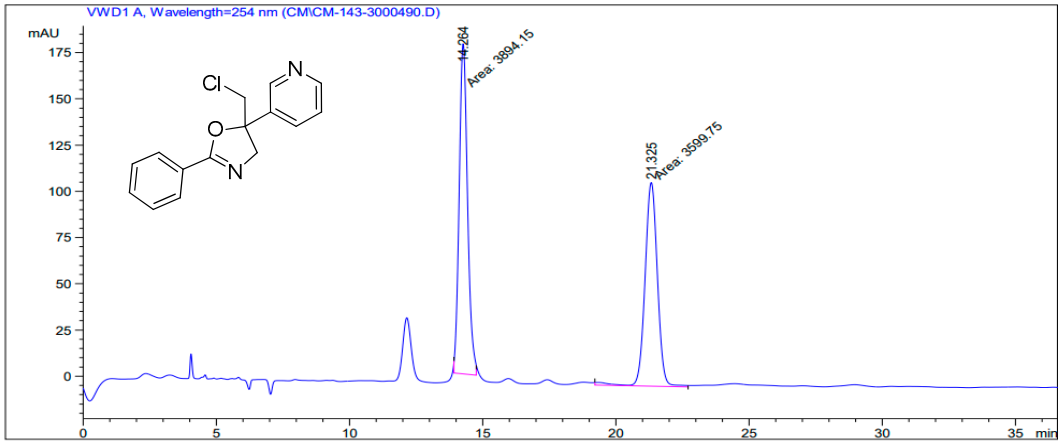
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	36.997	MM	1.1764	632.01465	8.95406	37.0529
2	46.315	MM	1.7400	1073.69421	10.28434	62.9471

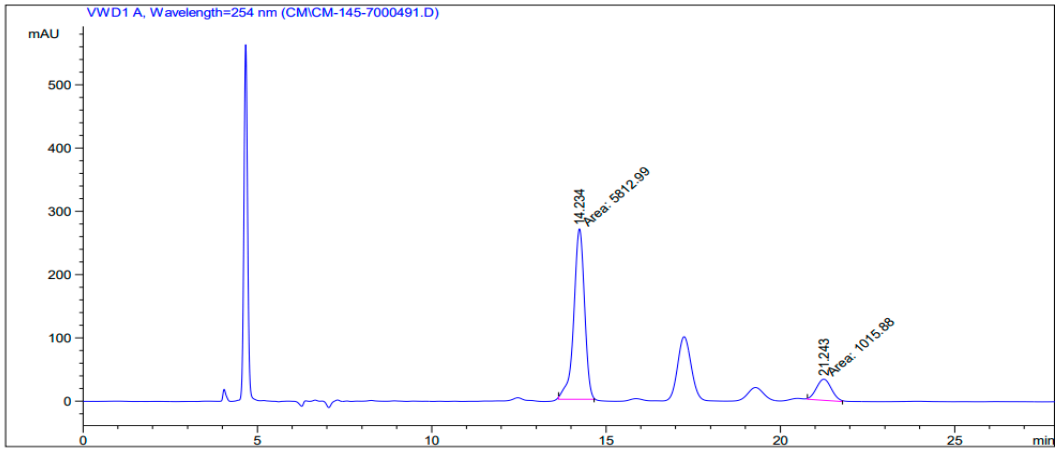
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.264	MM	0.3632	3894.15430	178.69928	51.9643
2	21.325	MM	0.5443	3599.74878	110.21660	48.0357

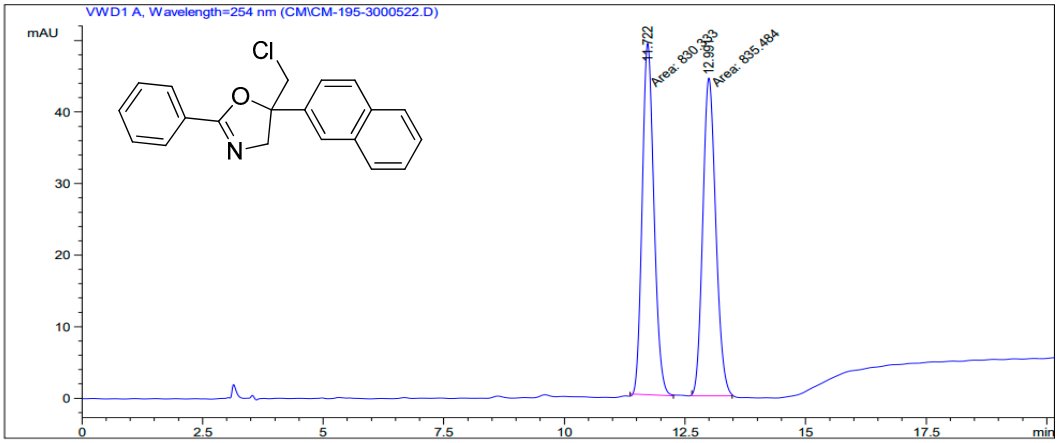
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.234	MM	0.3588	5812.99170	269.99182	85.1237
2	21.243	MM	0.5011	1015.88348	33.78618	14.8763

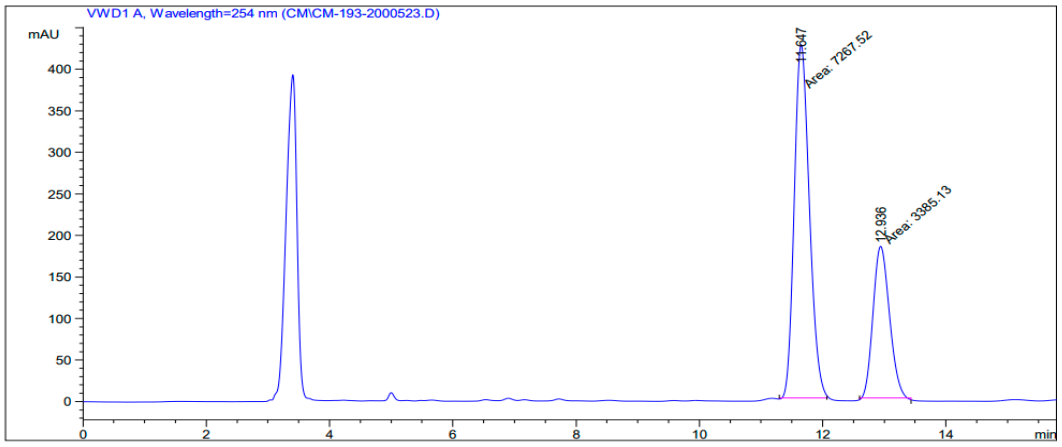
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.722	MM	0.2817	830.33325	49.11953	49.8454
2	12.991	MM	0.3133	835.48376	44.43855	50.1546

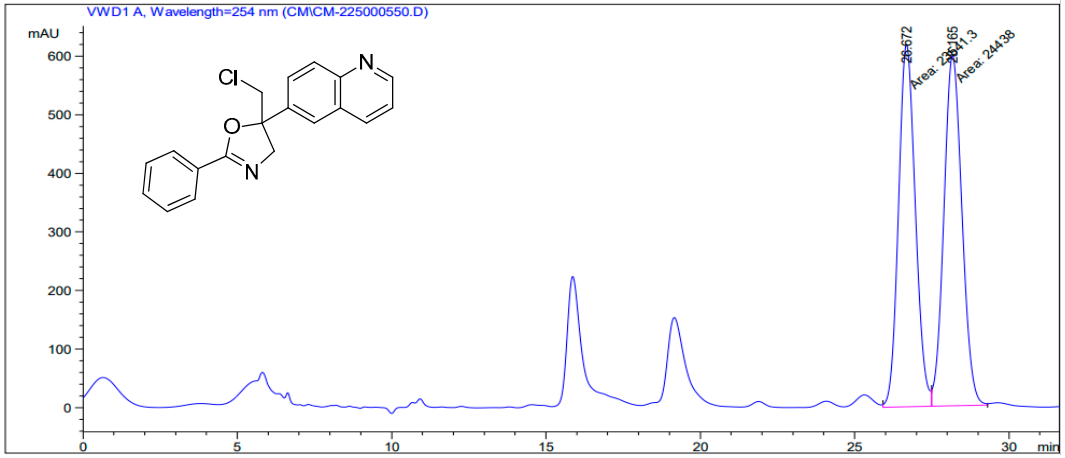
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.647	MM	0.2848	7267.52148	425.29709	68.2227
2	12.936	MM	0.3088	3385.12573	182.72333	31.7773

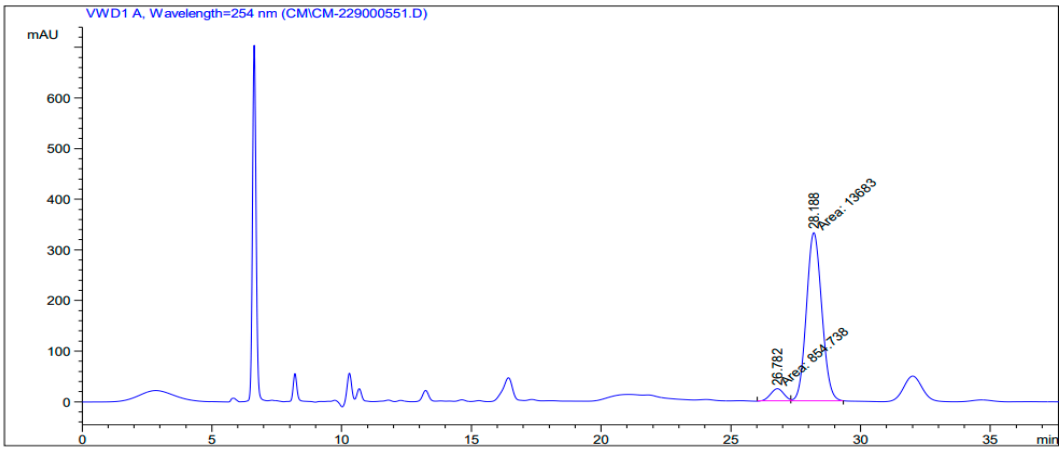
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	26.672	MF	0.6340	2.35413e4	618.88348	49.0655
2	28.165	FM	0.6808	2.44380e4	598.27405	50.9345

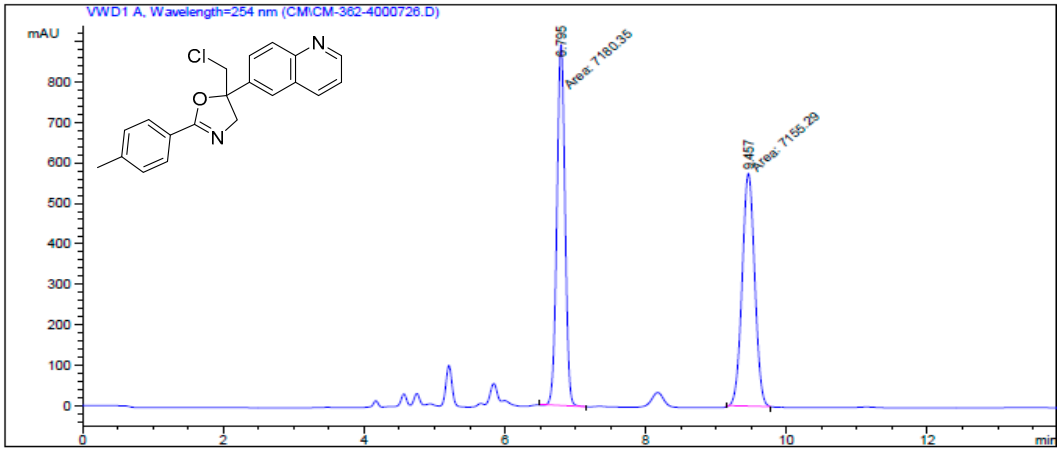
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	26.782	MF	0.5923	854.73798	24.04999	5.8794
2	28.188	FM	0.6865	1.36830e4	332.20920	94.1206

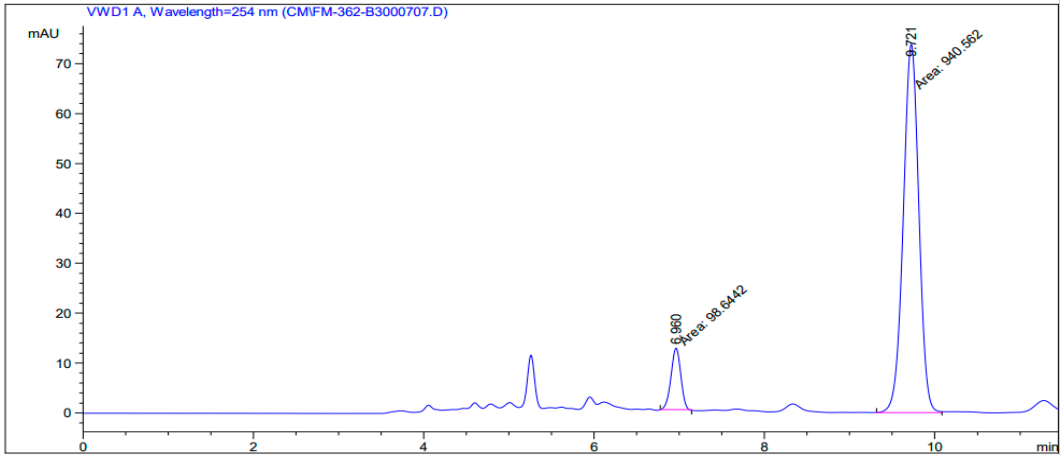
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.795	MM	0.1338	7180.35449	894.50604	50.0874
2	9.457	MM	0.2069	7155.29102	576.28223	49.9126

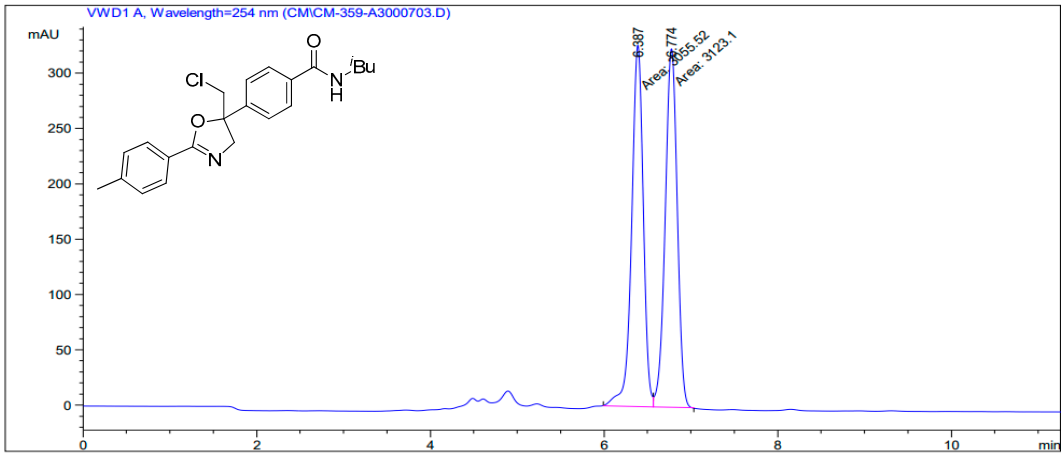
Product from enantioselective reaction



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.960	MM	0.1332	98.64417	12.34398	9.4923
2	9.721	MM	0.2123	940.56232	73.83438	90.5077

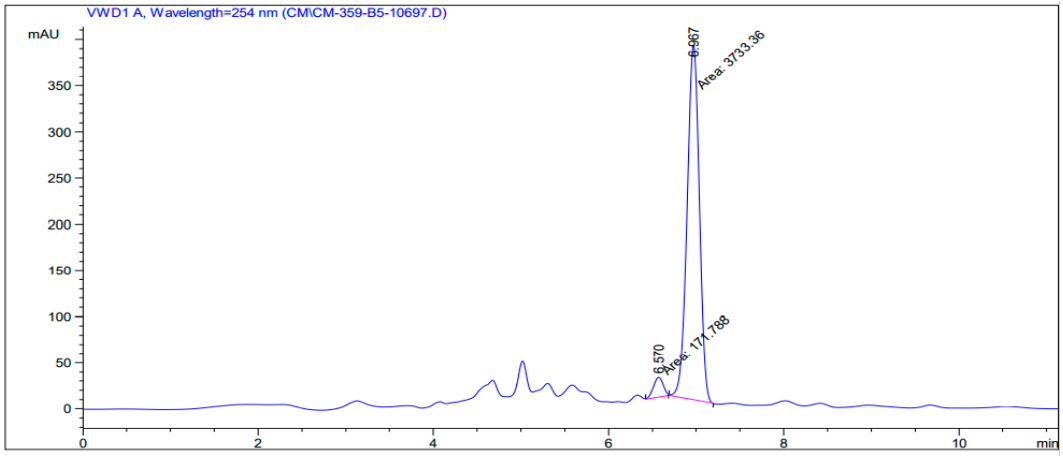
Racemic product



Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.387	MF	0.1558	3055.51514	326.81030	49.4531
2	6.774	FM	0.1605	3123.10034	324.29355	50.5469

Product from enantioselective reaction

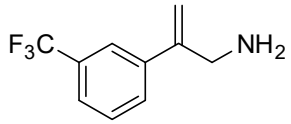


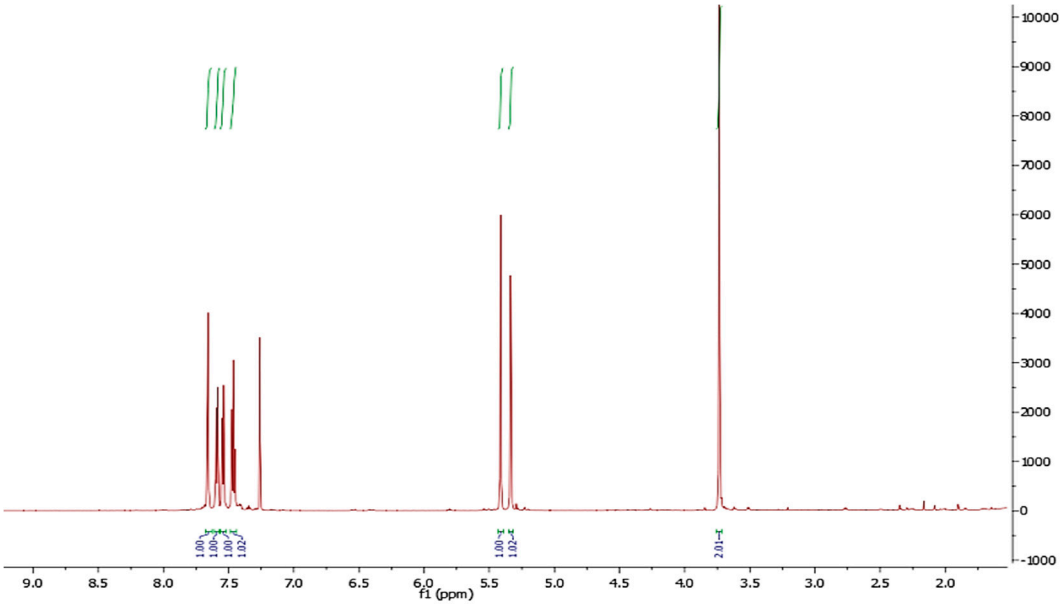
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.570	MM	0.1313	171.78766	21.81222	4.3990
2	6.967	MM	0.1618	3733.36353	384.60712	95.6010

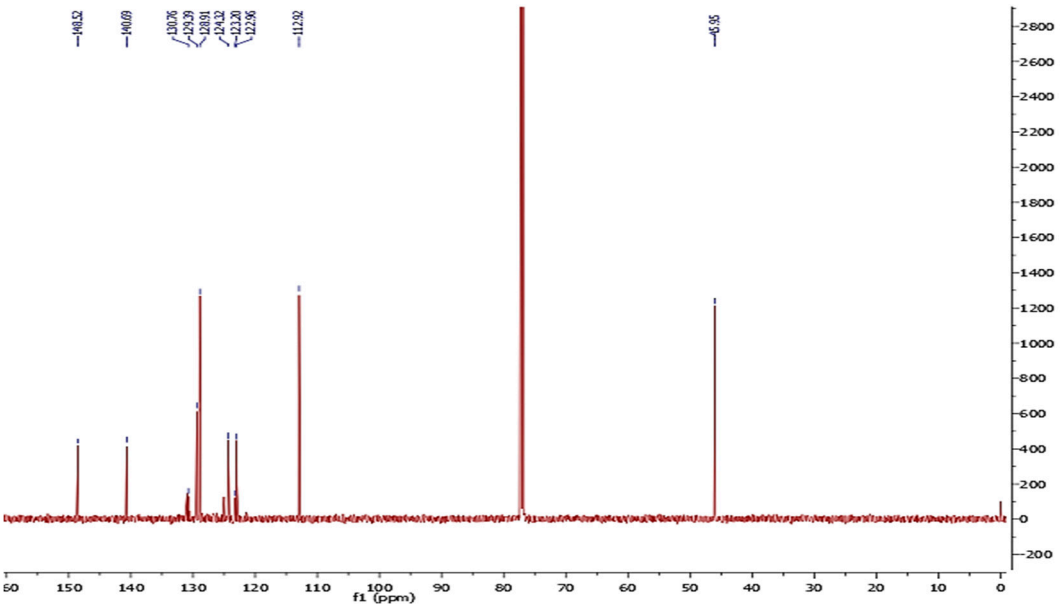
NMR Sectra

2-(3-(trifluoromethyl)phenyl)prop-2-en-1-aminium mesylate (5a)



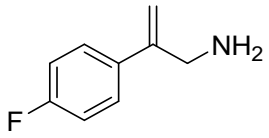


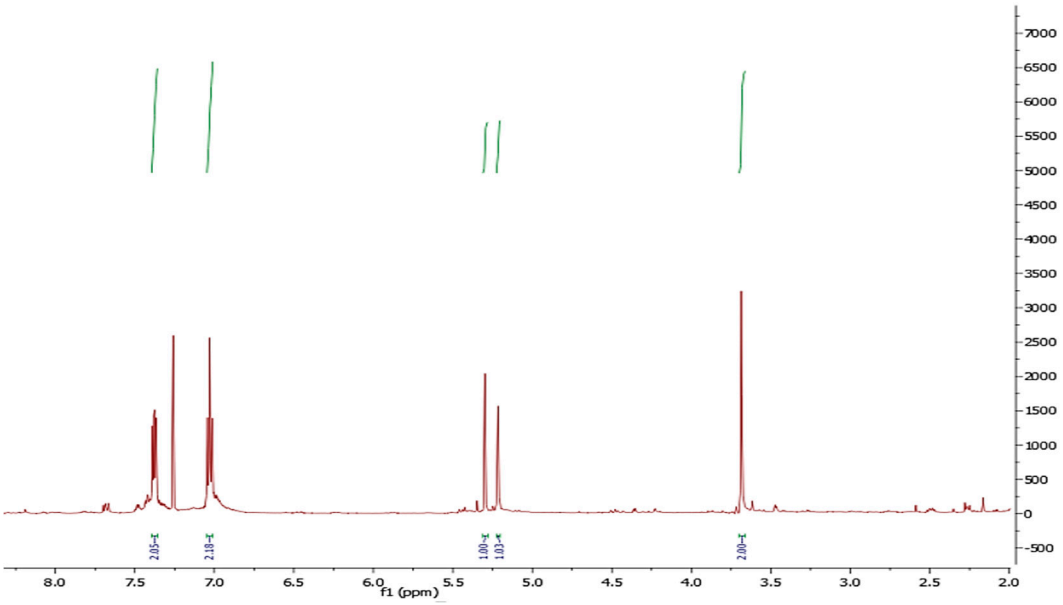
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (s, 1H), 7.59 (d, J = 7.7 Hz, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.46 (t, J = 7.8 Hz, 1H), 5.41 (d, J = 0.5 Hz, 1H), 5.34 (d, J = 0.5 Hz, 1H), 3.73 (s, 2H)



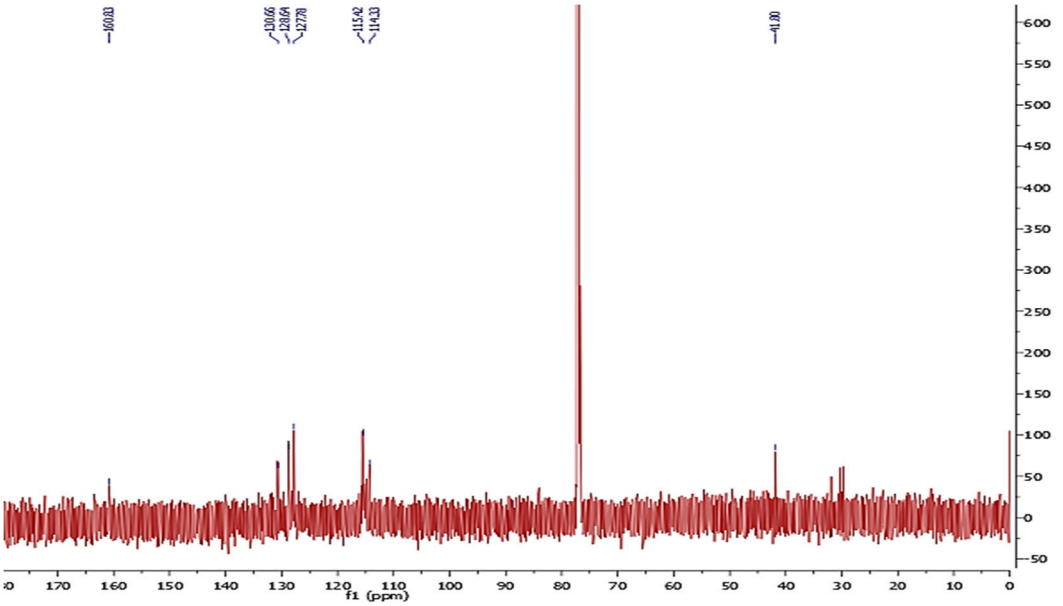
^{13}C NMR (151 MHz, $CDCl_3$) δ 148.52, 140.69, 130.76 (q, J = 33.2 Hz), 129.39, 128.91, 124.32 (q, J = 3.02 Hz), 123.20 (q, J = 272.5 Hz), 122.96 (q, J = 3.9 Hz), 112.92, 45.95

2-(4-fluorophenyl)prop-2-en-1-amine (5c)



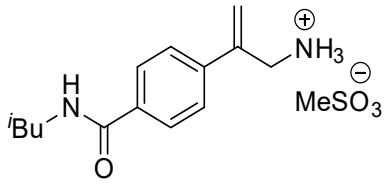


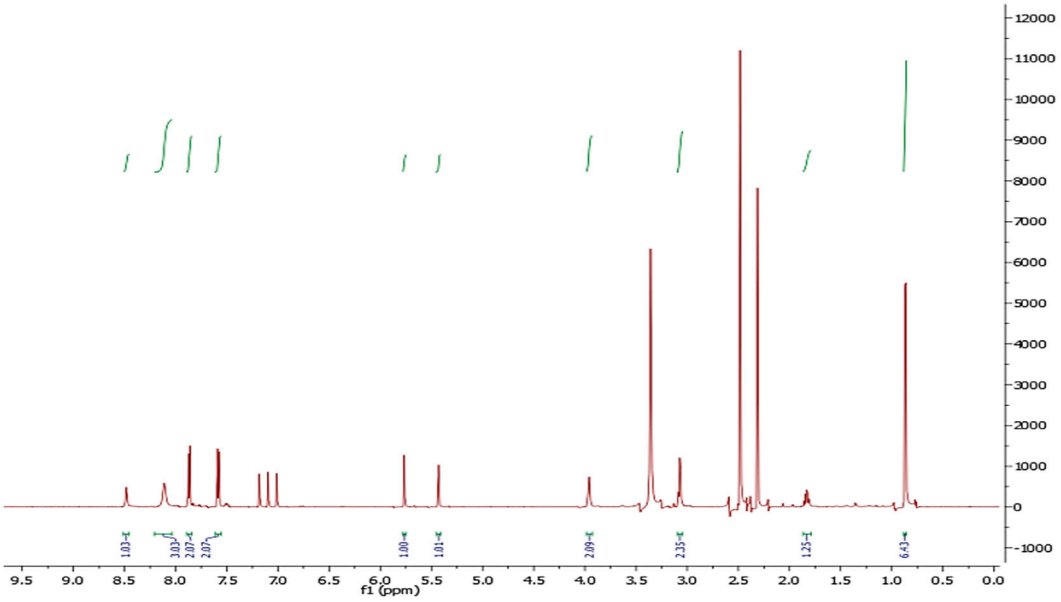
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 – 7.36 (m, 2H), 7.05 – 7.01 (m, 2H), 5.30 (s, 1H), 5.22 (s, 1H), 3.68 (d, *J* = 7.9 Hz, 2H)



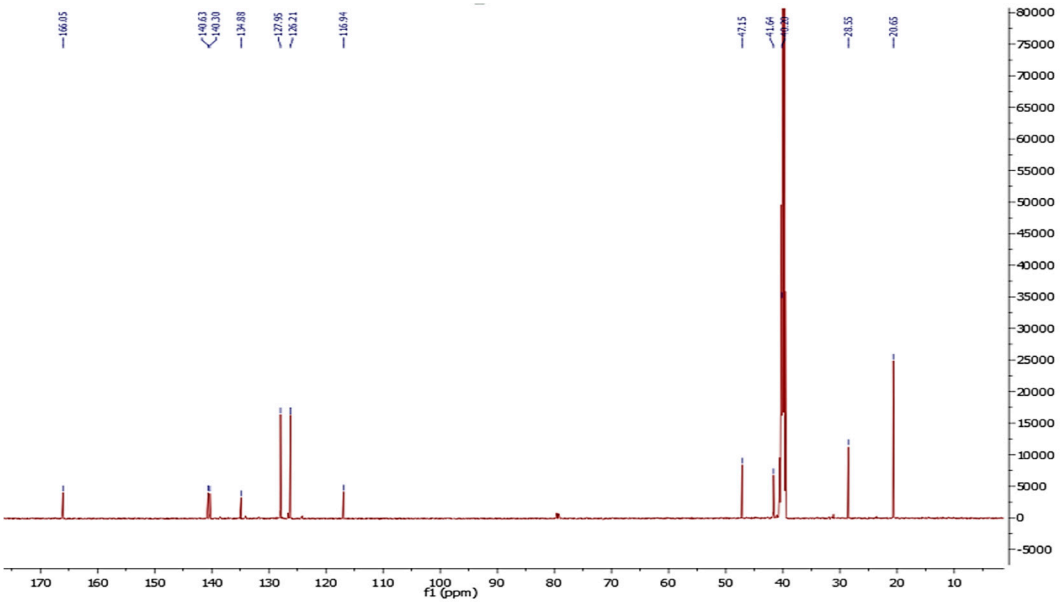
^{13}C NMR (151 MHz, $CDCl_3$) δ 160.83 (d, *J* = 242.1 Hz), 130.66 (d, *J* = 9.06 Hz), 128.64 (d, *J* = 12.08 Hz), 127.78, 115.42 (d, *J* = 22.65 Hz), 114.33, 41.80

2-(4-(isobutylcarbamoyl)phenyl)prop-2-en-1-aminium methanesulfonate (5d)



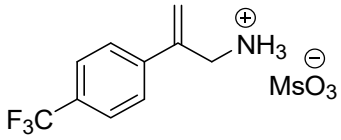


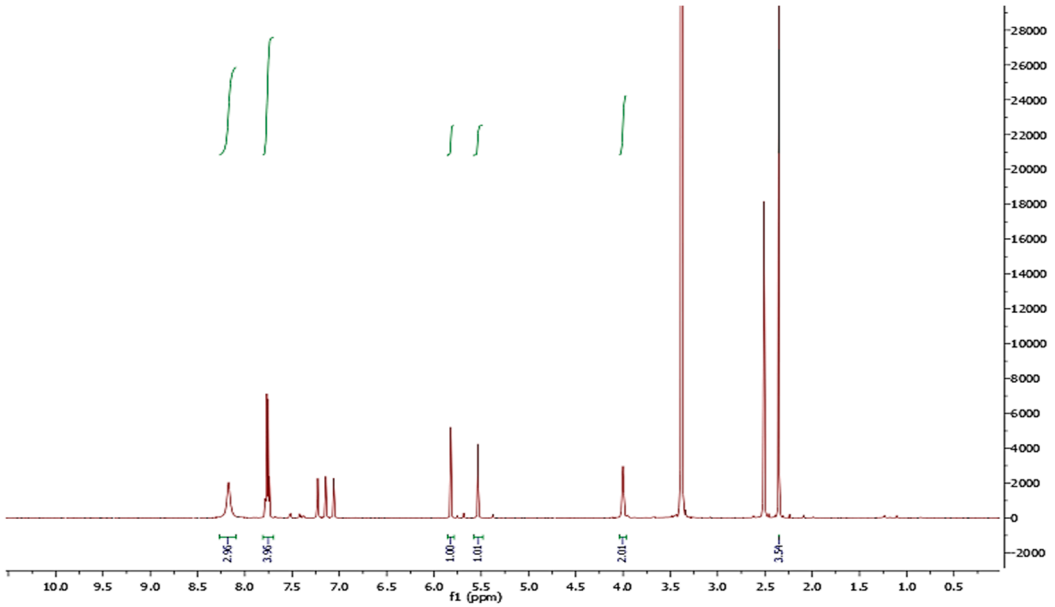
^{1}H NMR (600 MHz, DMSO) δ 8.48 (t, J = 5.7 Hz, 1H), 8.11 (s, 3H), 7.87 (d, J = 8.4 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H), 5.77 (s, 1H), 5.43 (s, 1H), 3.96 (d, J = 5.5 Hz, 2H), 3.07 (dd, J = 13.3, 7.0 Hz, 2H), 1.83 (dt, J = 13.5, 6.8 Hz, 1H), 0.87 (d, J = 6.7 Hz, 6H)



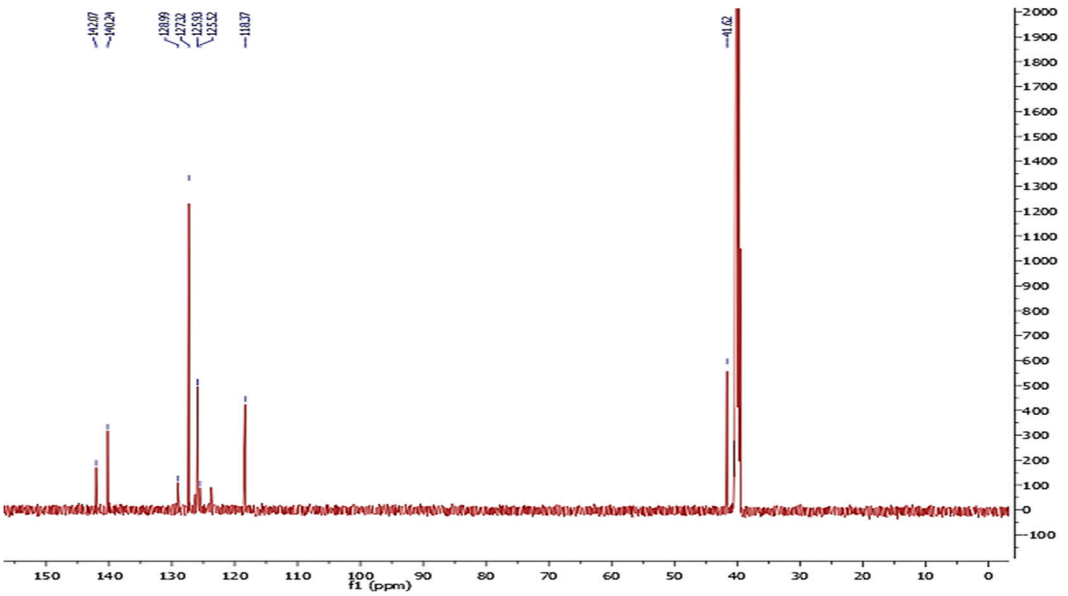
^{13}C NMR (151 MHz, DMSO) δ 166.05, 140.63, 140.30, 134.88, 127.95, 126.21, 116.94, 47.15, 41.64, 40.20, 28.55, 20.65

2-(4-(trifluoromethyl)phenyl)prop-2-en-1-amine (5e)



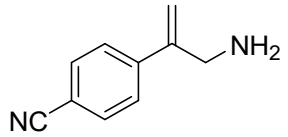


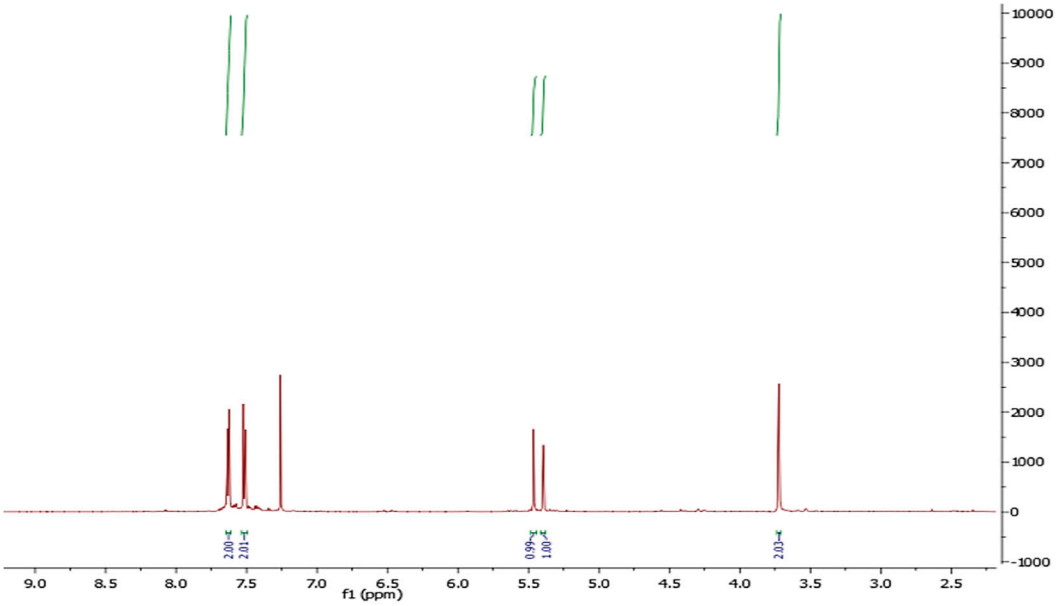
^{1}H NMR (600 MHz, DMSO) δ 8.17 (s, 3H), 7.76 (q, J = 8.5 Hz, 4H), 5.82 (s, 1H), 5.53 (s, 1H), 4.00 (s, 2H), 2.35 (s, 3H)



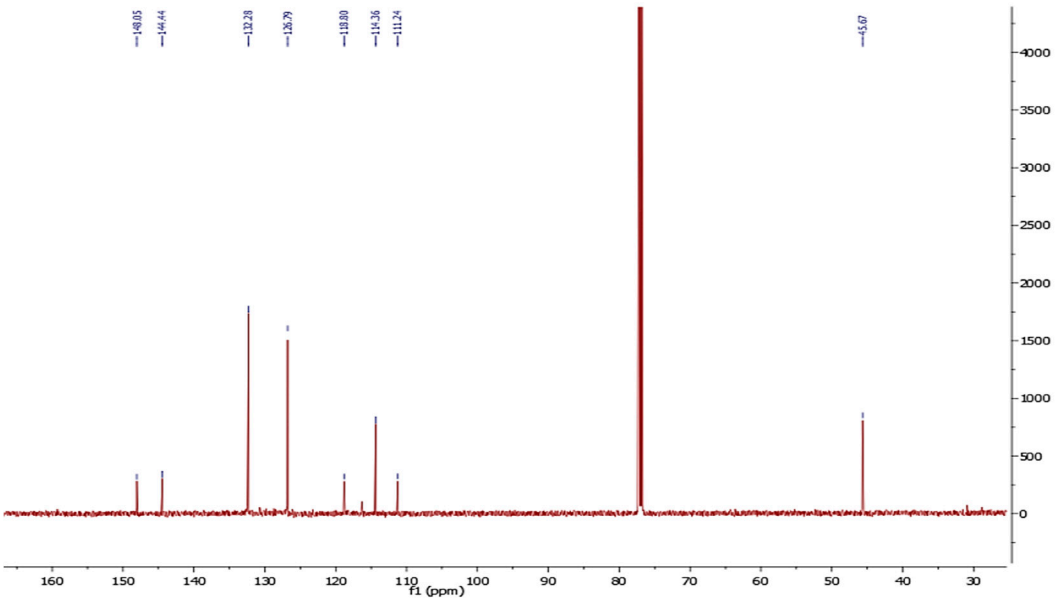
^{13}C NMR (151 MHz, DMSO) δ 142.07, 140.24, 128.99 (q, J = 32.01 Hz), 127.32, 125.93 (q, J = 4.53 Hz), 125.52 (q, J = 271.8 Hz), 118.37, 41.62

4-(3-aminoprop-1-en-2-yl)benzonitrile (5f)



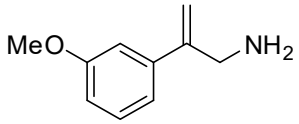


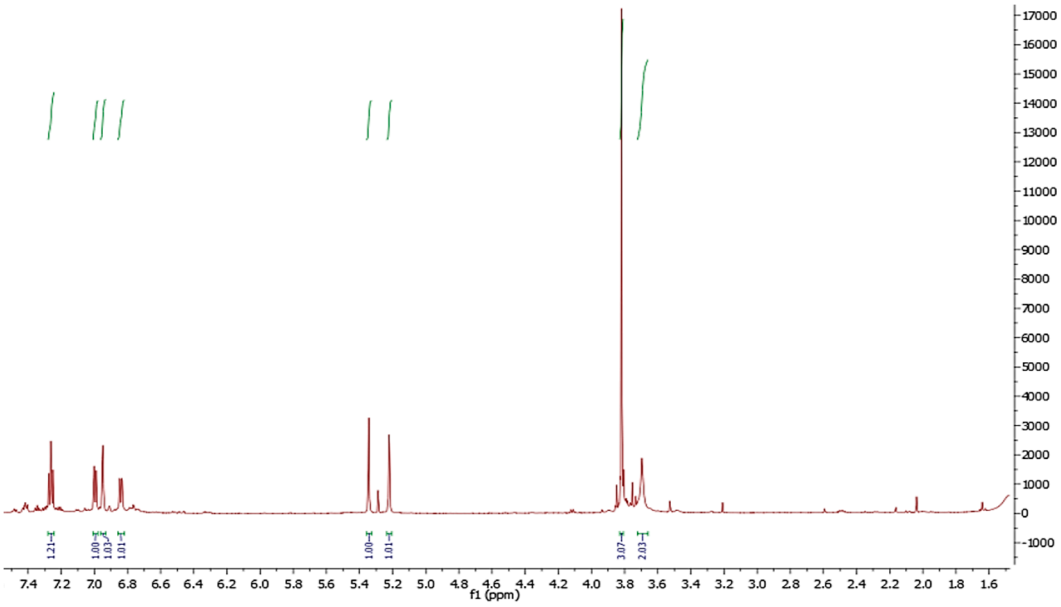
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, 2H), 7.52 (d, 2H), 5.46 (s, 1H), 5.39 (s, 1H), 3.72 (d, 2H)



^{13}C NMR (151 MHz, $CDCl_3$) δ 148.05, 144.44, 132.28, 126.79, 118.80, 114.36, 111.24, 45.67

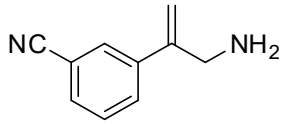
2-(3-methoxyphenyl)prop-2-en-1-amine (5g)

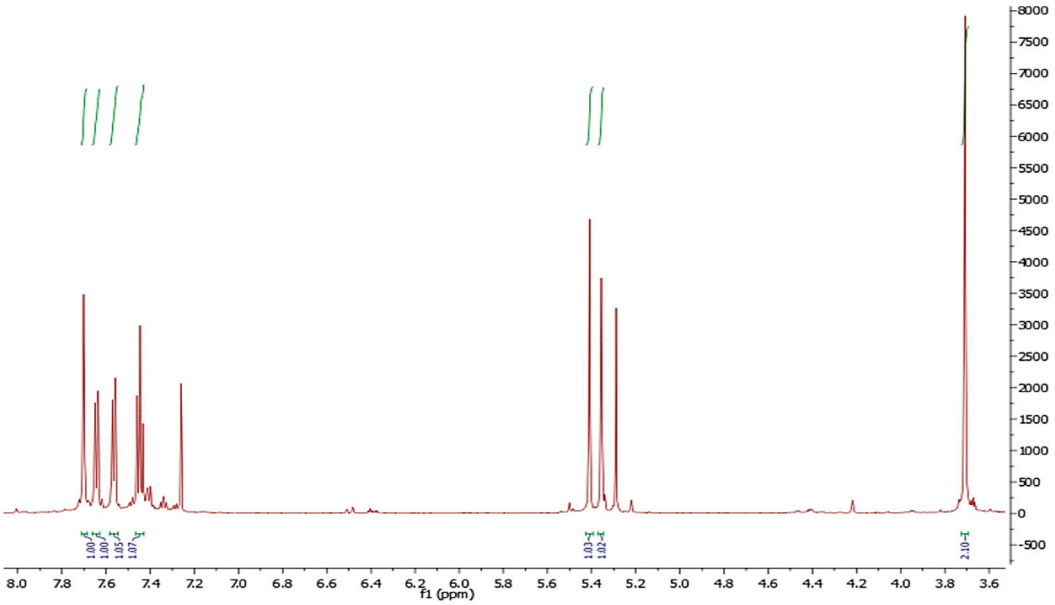




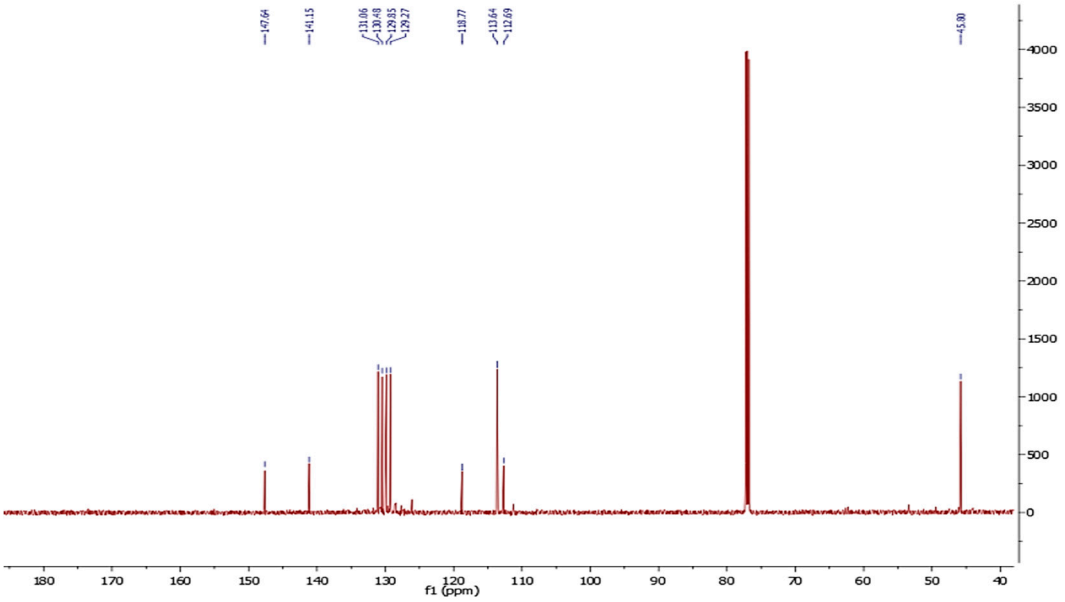
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.26 (dd, J = 9.0, 6.9 Hz, 1H), 7.00 (d, J = 7.7 Hz, 1H), 6.96 – 6.93 (m, 1H), 6.84 (dt, J = 8.1, 4.0 Hz, 1H), 5.34 (s, 1H), 5.22 (s, 1H), 3.82 (s, J = 4.9 Hz, 2H), 3.70 (s, 2H)

3-(3-aminoprop-1-en-2-yl)benzonitrile (5h)



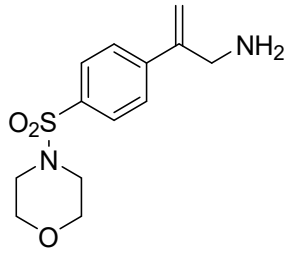


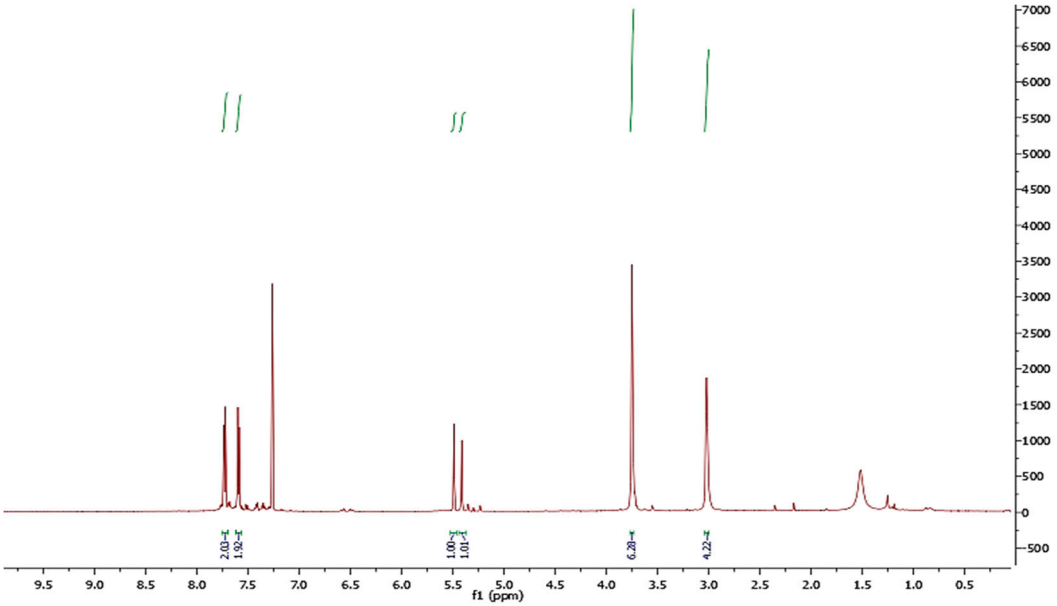
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.64 (d, J = 7.9 Hz, 1H), 7.56 (d, J = 7.7 Hz, 1H), 7.45 (t, J = 7.8 Hz, 1H), 5.41 (s, 1H), 5.36 (s, 1H), 3.71 (s, 2H)



^{13}C NMR (151 MHz, $CDCl_3$) δ 147.64, 141.15, 131.06, 130.48, 129.85, 129.27, 118.77, 113.64, 112.69, 45.80

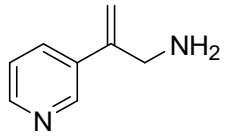
2-(4-(morpholinosulfonyl)phenyl)prop-2-en-1-amine (5i)

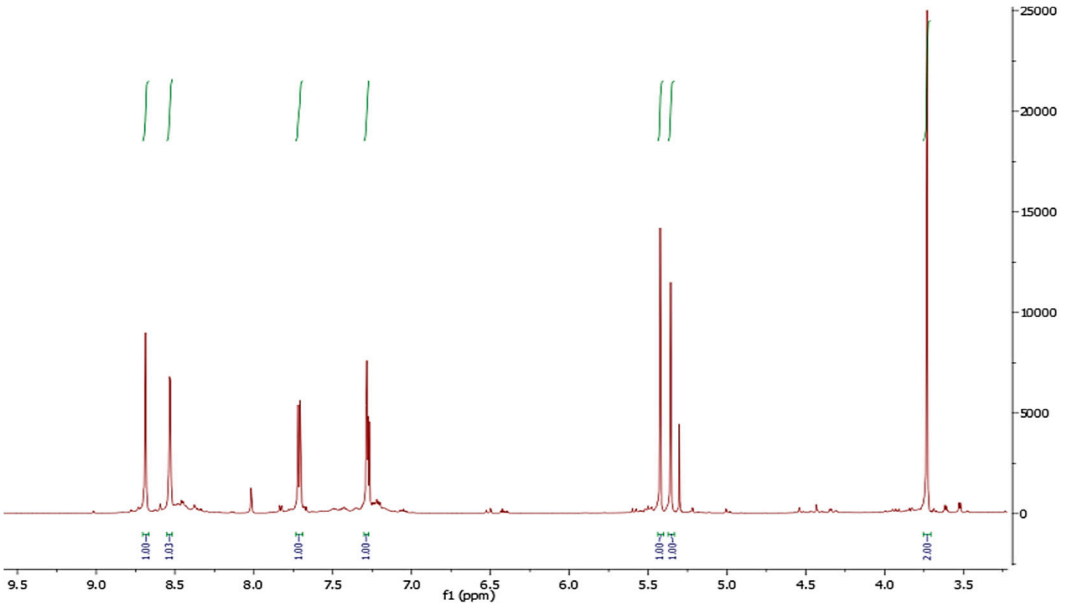




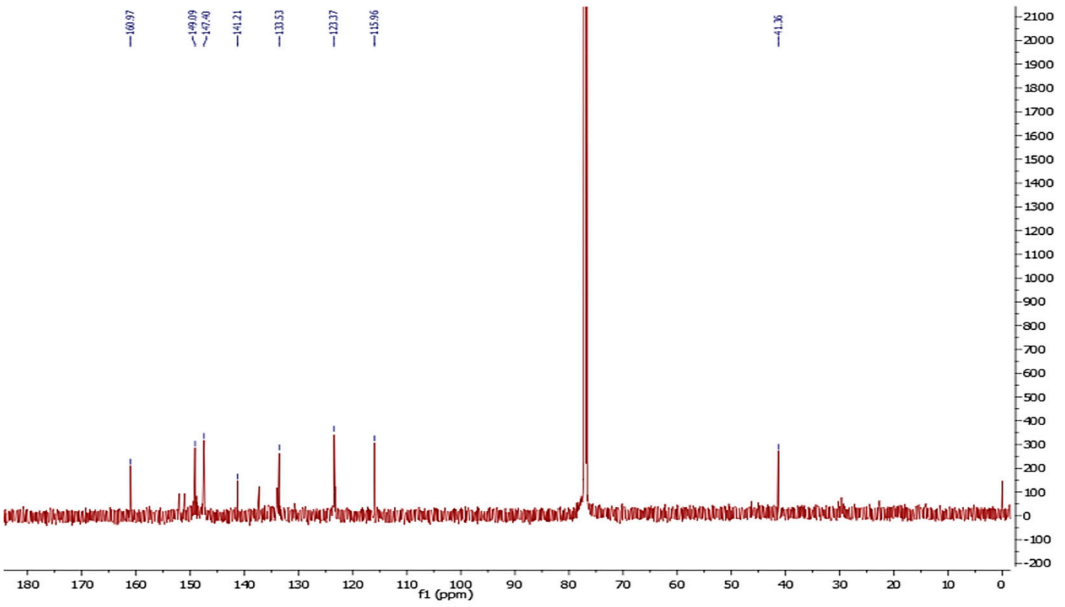
^{1}H NMR (600 MHz, CDCl3) δ 7.72 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 8.3 Hz, 2H), 5.49 (s, 1H), 5.41 (s, 1H), 3.77 – 3.73 (m, 6H), 3.04 – 3.00 (m, 4H)

2-(pyridin-3-yl)prop-2-en-1-amine (5j)



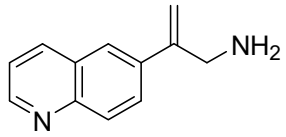


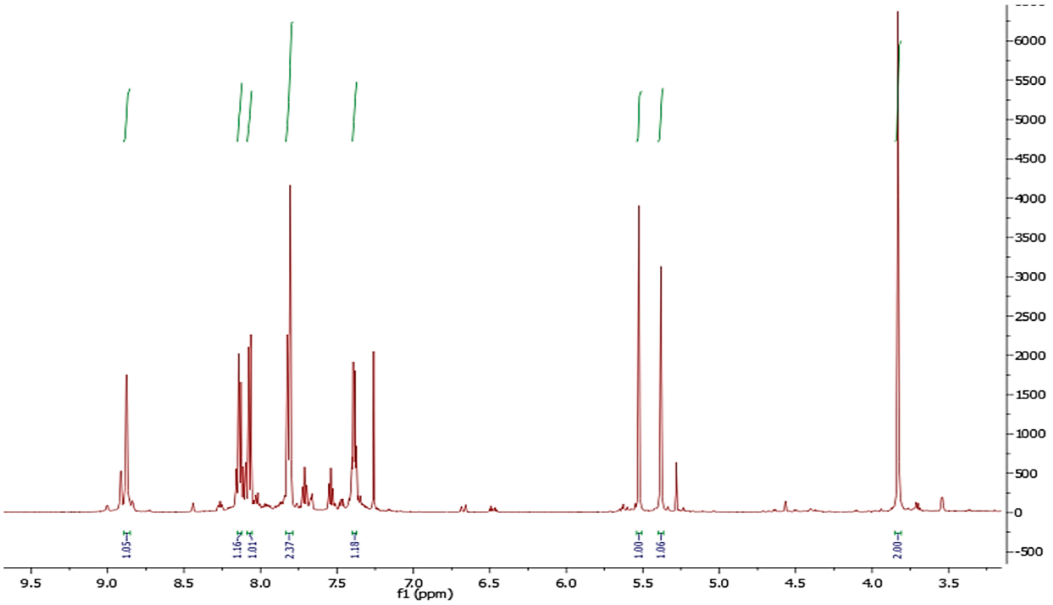
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (d, J = 2.0 Hz, 1H), 8.53 (dd, J = 4.8, 1.4 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.30 – 7.27 (m, 1H), 5.42 (s, 1H), 5.36 (s, 1H), 3.73 (s, 2H)



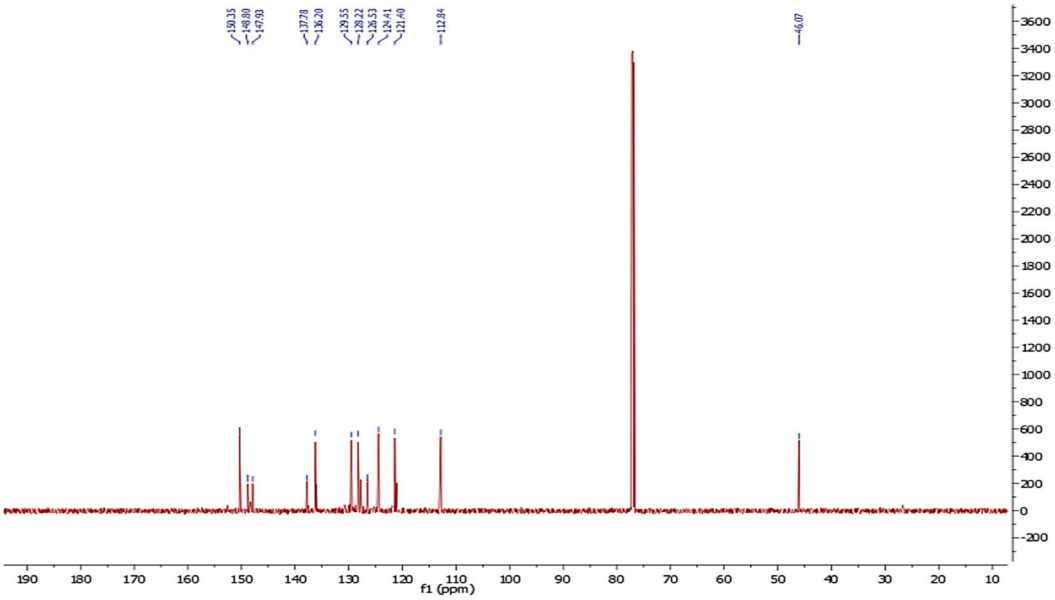
^{13}C NMR (151 MHz, $CDCl_3$) δ 160.97, 149.09, 147.40, 141.21, 133.53, 123.37, 115.96, 41.36

2-(quinolin-6-yl)prop-2-en-1-amine (5l)



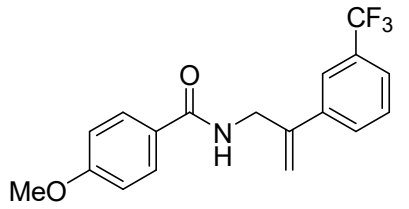


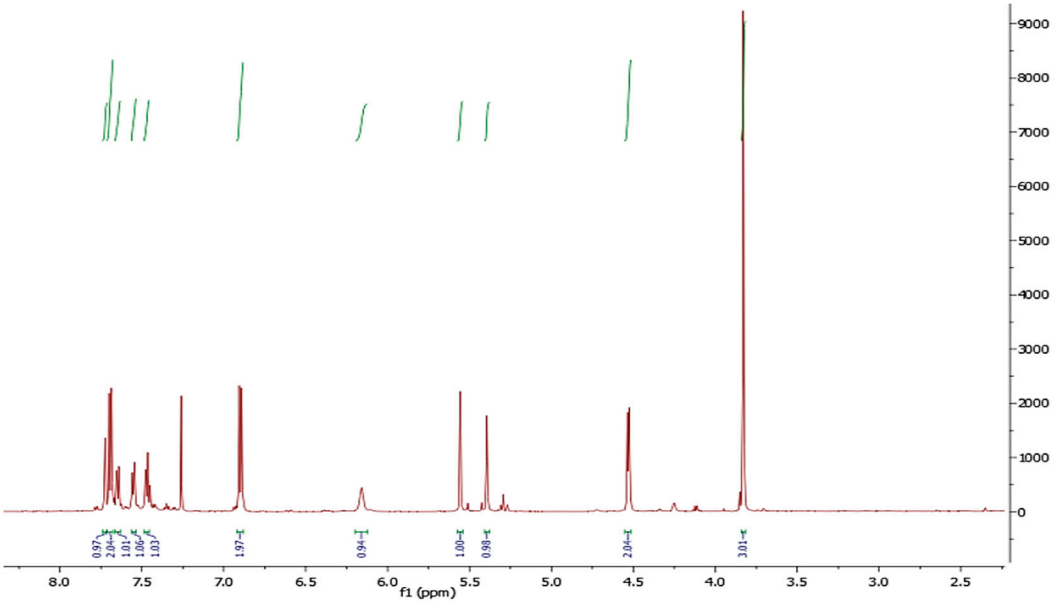
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.88 (dd, J = 4.2, 1.6 Hz, 1H), 8.14 (d, J = 8.4 Hz, 1H), 8.07 (d, J = 8.7 Hz, 1H), 7.82 (dd, J = 10.9, 2.1 Hz, 2H), 7.38 (dd, J = 8.2, 4.2 Hz, 1H), 5.53 (s, 1H), 5.38 (s, 1H), 3.83 (s, 2H)



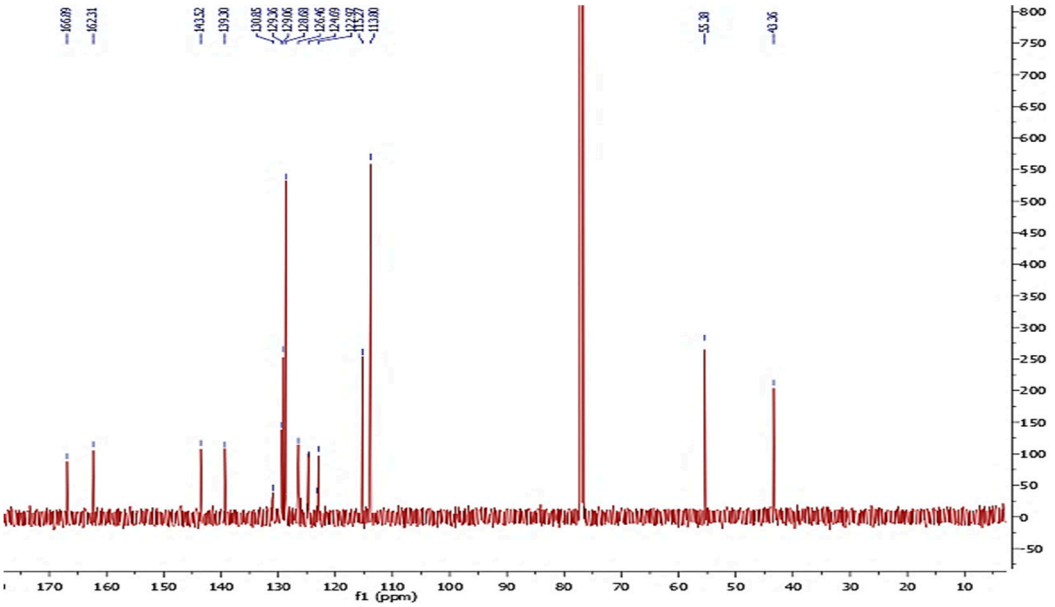
^{13}C NMR (151 MHz, $CDCl_3$) δ 150.35, 148.80, 147.93, 137.78, 136.20, 129.55, 128.22, 126.53, 124.41, 121.40, 112.84, 46.07

4-methoxy-*N*-(2-(3-(trifluoromethyl)phenyl) allyl) benzamide (6a)



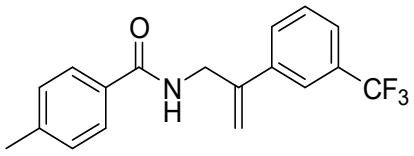


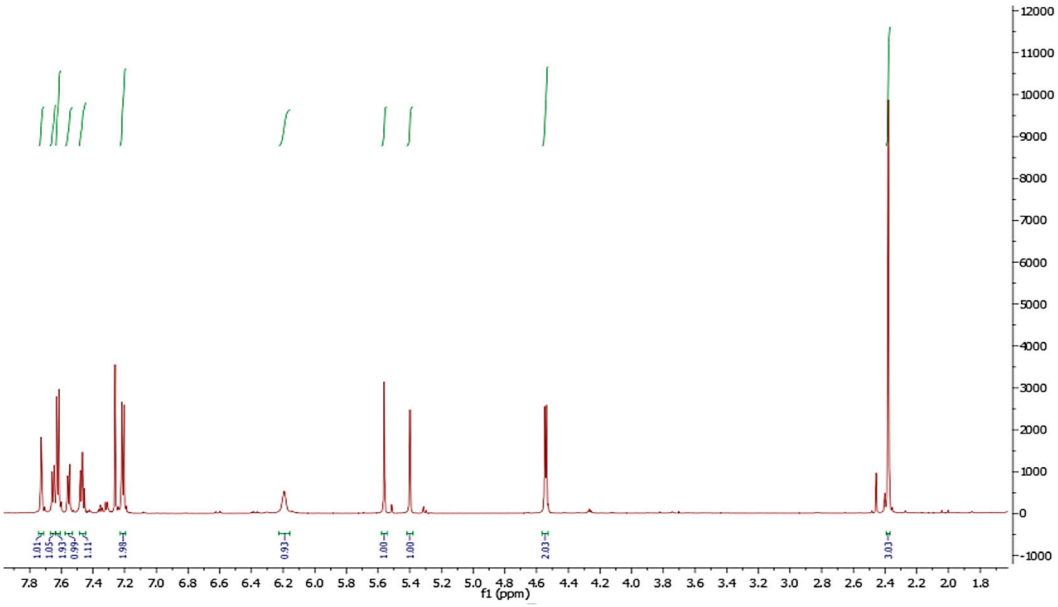
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.69 (d, J = 8.8 Hz, 2H), 7.65 (d, J = 7.9 Hz, 1H), 7.55 (d, J = 7.7 Hz, 1H), 7.47 (d, J = 7.8 Hz, 1H), 6.90 (d, J = 8.8 Hz, 2H), 6.16 (s, 1H), 5.56 (s, 1H), 5.39 (s, 1H), 4.53 (d, J = 5.8 Hz, 2H), 3.83 (s, 3H)



^{13}C NMR (151 MHz, $CDCl_3$) δ 166.89, 162.31, 143.52, 139.30, 130.85 (q, J = 31.7 Hz), 129.36, 129.06, 128.68, 126.46, 124.69 (q, J = 4.53 Hz), 123.13 (q, J = 271.8 Hz), 122.97 (q, J = 4.53 Hz), 115.27, 113.80, 55.38, 43.36

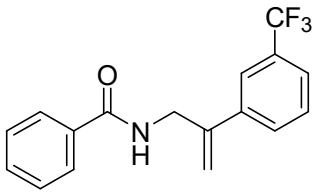
4-methyl-N-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6b)

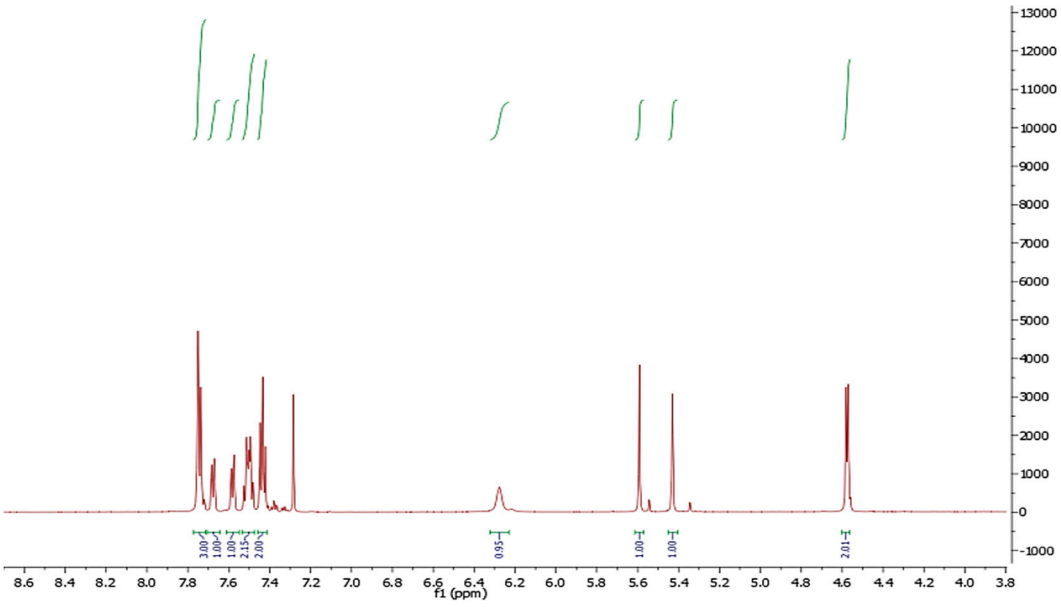




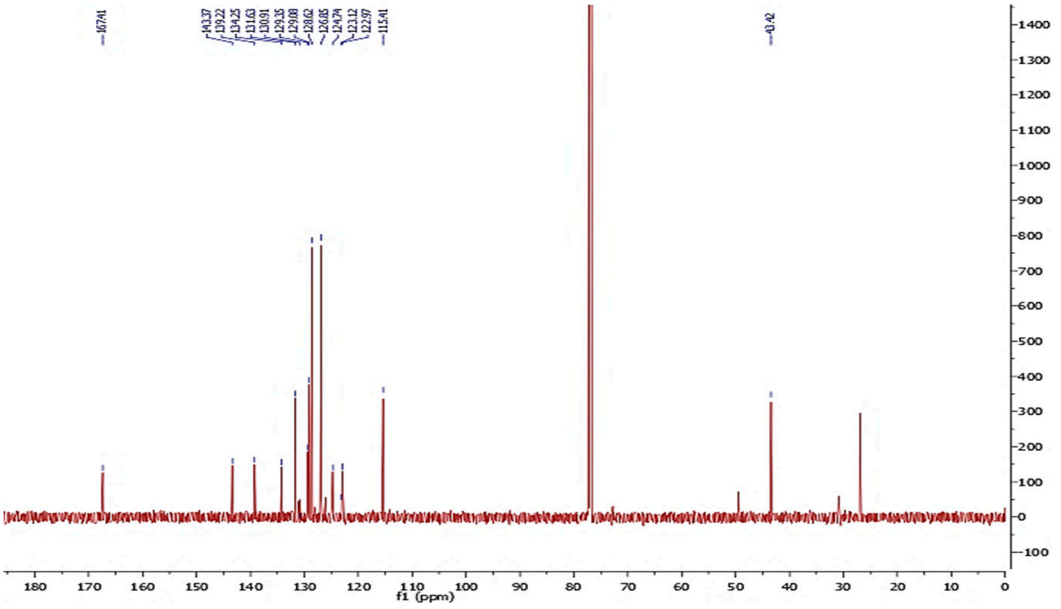
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (s, 1H), 7.65 (d, J = 7.8 Hz, 1H), 7.62 (d, J = 8.1 Hz, 2H), 7.55 (d, J = 7.7 Hz, 1H), 7.47 (t, J = 7.8 Hz, 1H), 7.21 (d, J = 8.0 Hz, 2H), 6.19 (s, 1H), 5.56 (s, 1H), 5.40 (s, 1H), 4.54 (d, J = 5.8 Hz, 2H), 2.38 (s, 3H)

_N_-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6c)



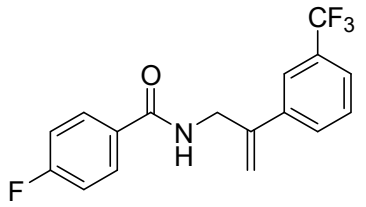


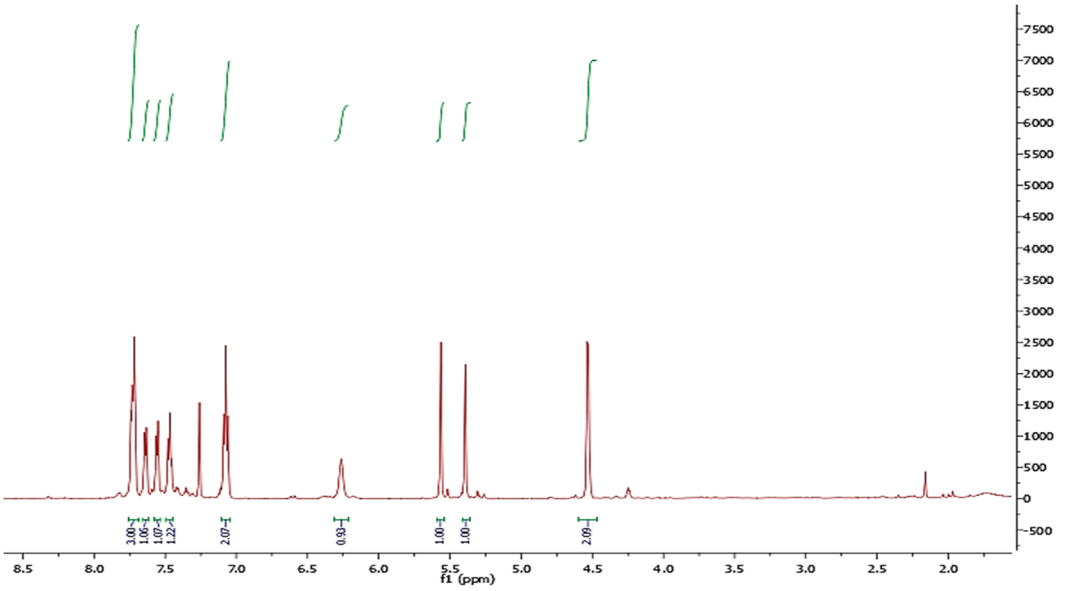
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 3H), 7.68 (d, J = 7.8 Hz, 1H), 7.58 (d, J = 7.7 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.43 (t, J = 7.7 Hz, 2H), 6.28 (s, J = 31.2 Hz, 1H), 5.59 (s, 1H), 5.43 (s, 1H), 4.58 (d, J = 5.8 Hz, 2H)



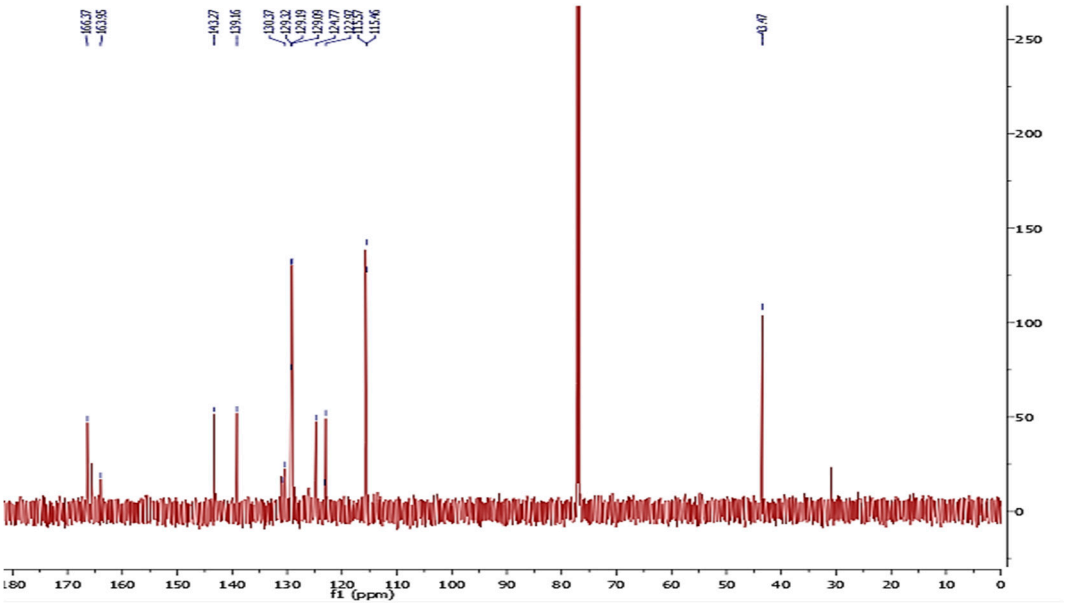
^{13}C NMR (151 MHz, $CDCl_3$) δ 167.41, 143.37, 139.22, 134.25, 131.63, 130.91 (q, J = 33.22 Hz), 129.35, 129.08, 128.62, 126.85, 124.74 (q, J = 4.53 Hz), 123.12 (q, J = 270.3 Hz), 122.97 (q, J = 4.53 Hz), 115.41, 43.42

4-fluoro-*N*-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6d)



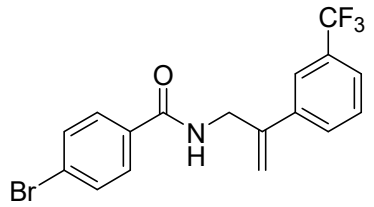


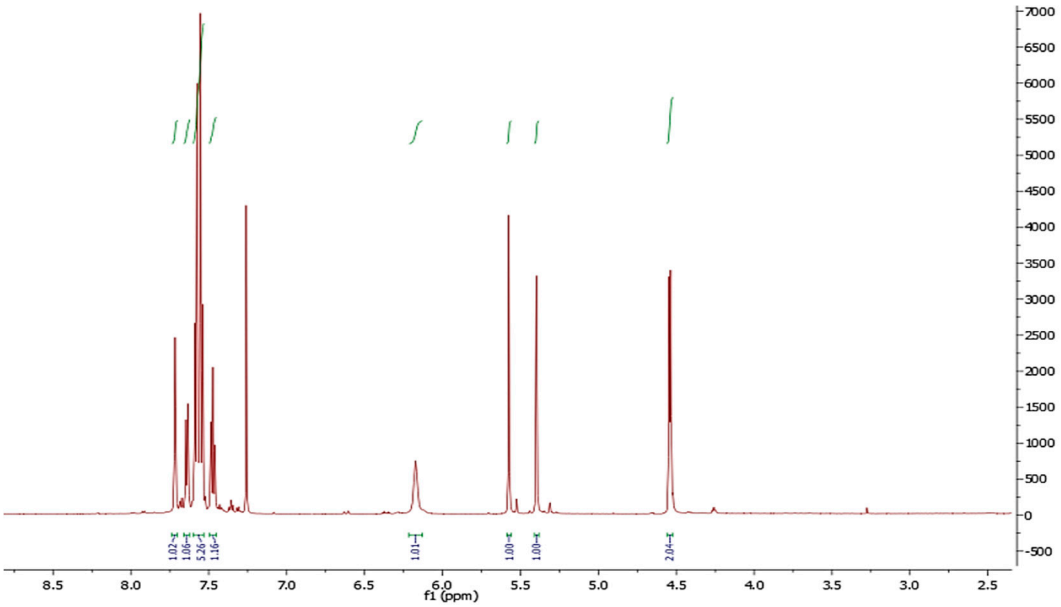
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (dd, J = 8.6, 5.7 Hz, 3H), 7.64 (d, J = 7.5 Hz, 1H), 7.56 (d, J = 7.5 Hz, 1H), 7.47 (t, J = 7.6 Hz, 1H), 7.07 (t, J = 8.5 Hz, 2H), 6.26 (s, 1H), 5.56 (s, 1H), 5.39 (s, 1H), 4.53 (d, J = 5.5 Hz, 2H)



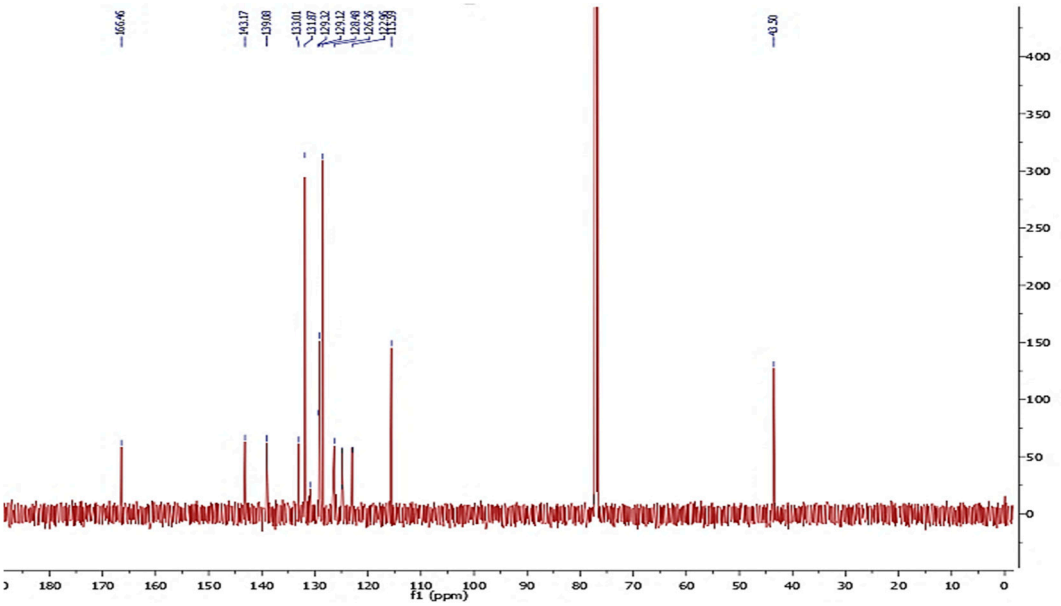
^{13}C NMR (151 MHz, $CDCl_3$) δ 166.37, 143.27, 139.16, 131.11, 130.39, 129.32, 129.25, 129.19, 129.09 (d, J = 3.8 Hz), 124.77 (dd, J = 3.6 Hz), 122.97, 115.72 (dd, J = 3.6 Hz), 115.57, 115.46, 43.47

4-bromo-N-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6e)



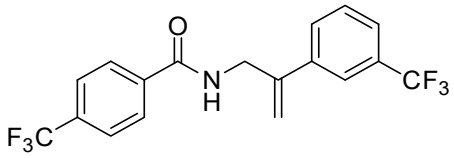


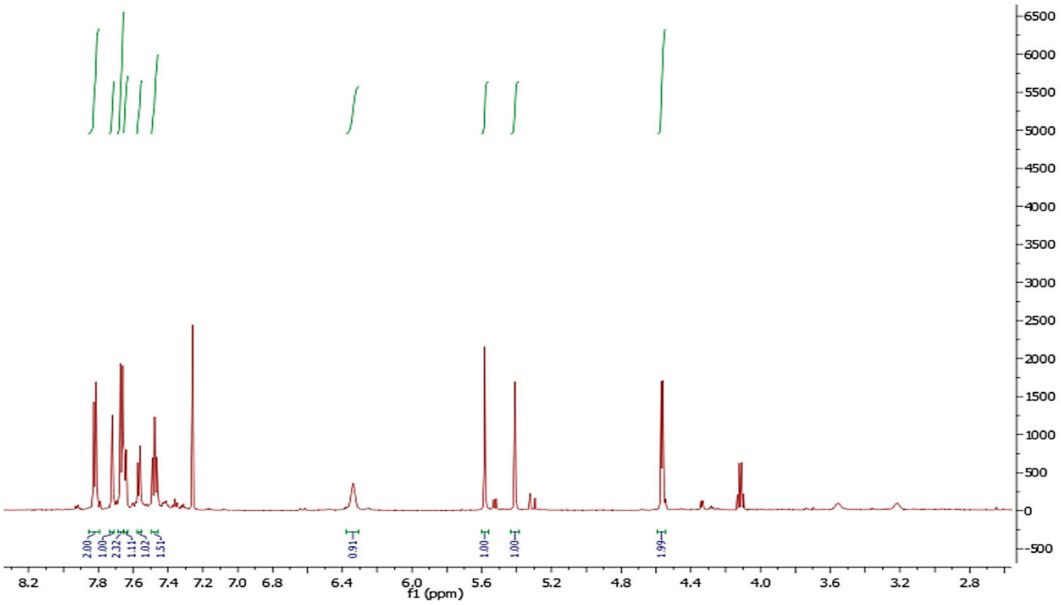
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.64 (d, J = 7.8 Hz, 1H), 7.60 – 7.53 (m, 5H), 7.47 (t, J = 7.8 Hz, 1H), 6.17 (s, 1H), 5.57 (s, 1H), 5.40 (s, 1H), 4.54 (d, J = 5.7 Hz, 2H)



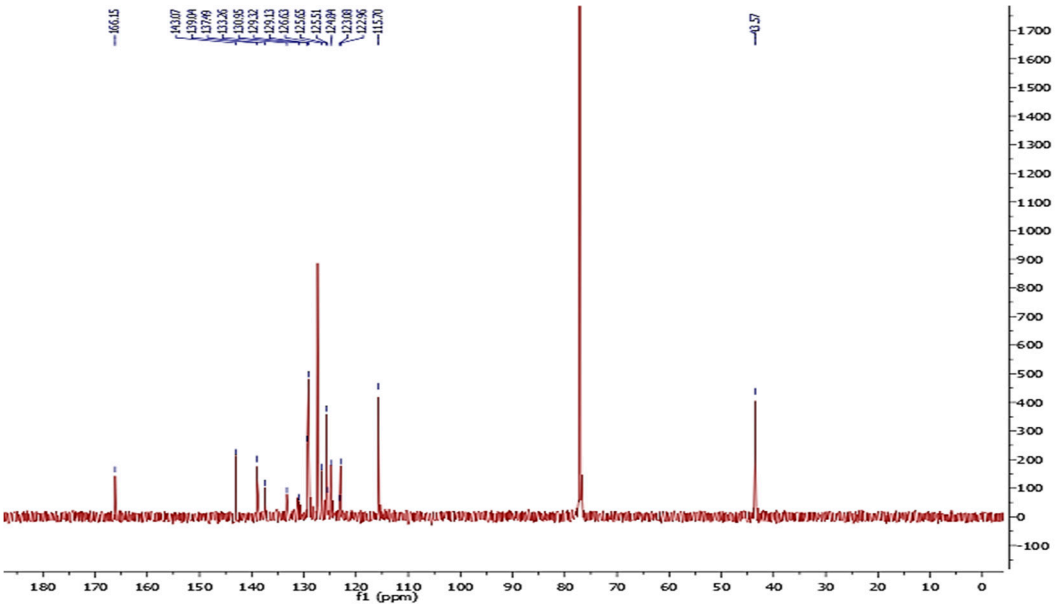
^{13}C NMR (151 MHz, $CDCl_3$) δ 166.46, 143.17, 139.08, 133.01, 131.87, 130.93 (q, J = 33.22 Hz), 129.32, 129.12, 128.48, 126.36, 124.81 (q, J = 4.53 Hz), 123.08 (q, J = 272.3 Hz), 122.96 (q, J = 4.53 Hz), 115.59, 43.50

4-(trifluoromethyl)-*N*-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6f)



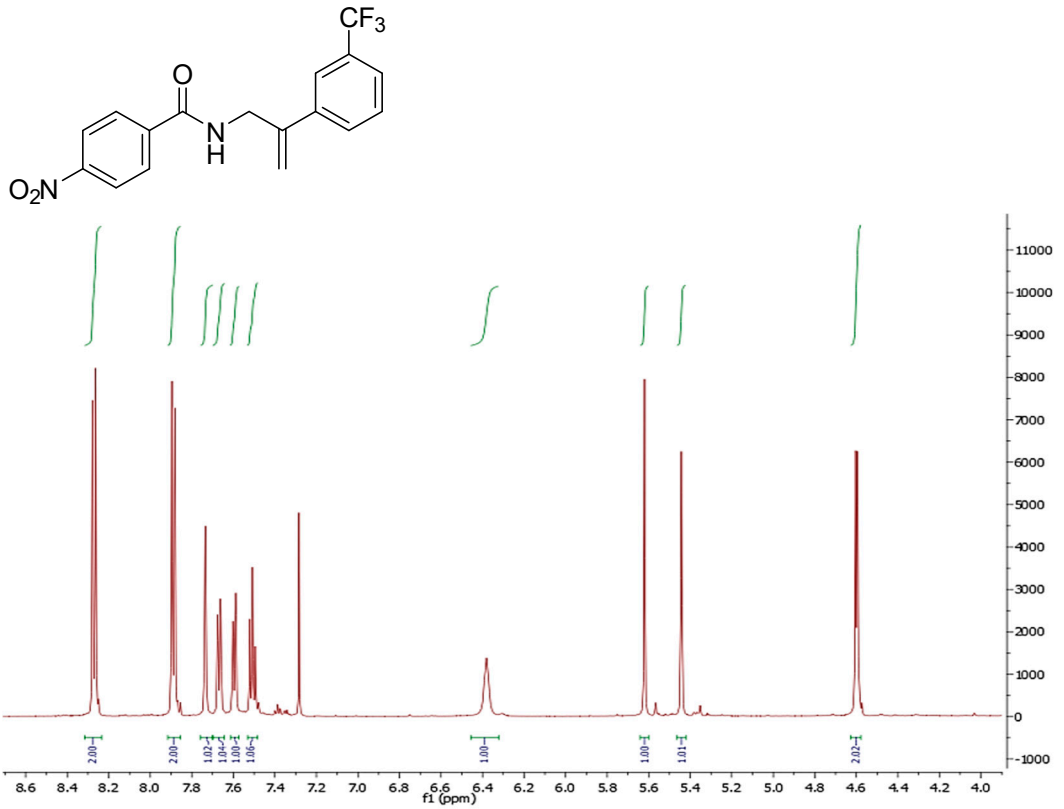


^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.1 Hz, 2H), 7.72 (s, 1H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.48 (t, *J* = 7.9 Hz, 1H), 6.34 (s, *J* = 20.3 Hz, 1H), 5.58 (s,12H), 5.41 (s, 1H), 4.57 (d, *J* = 5.8 Hz, 2H)

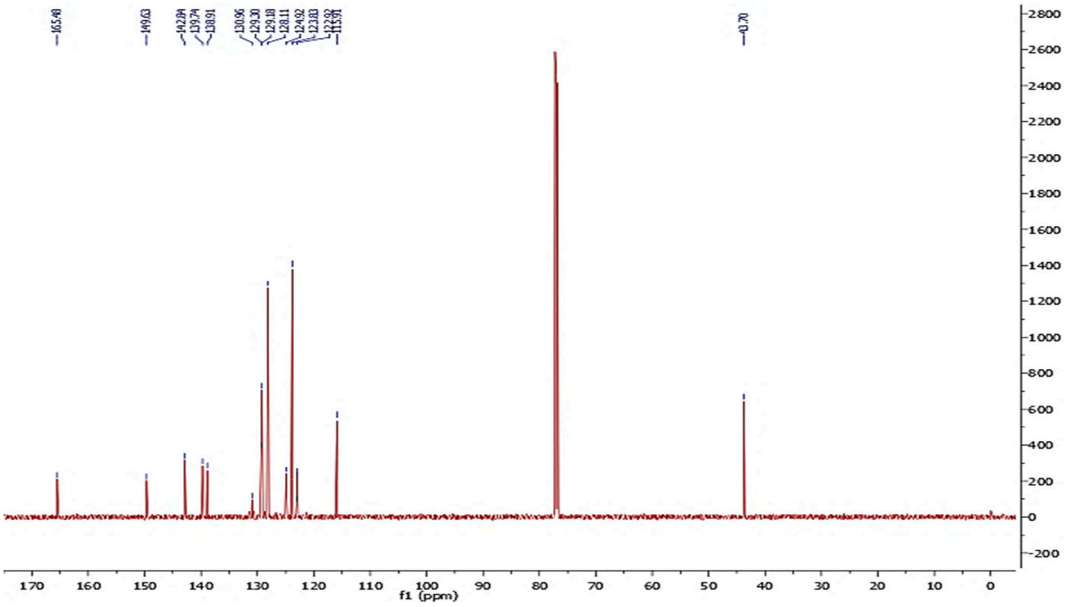


^{13}C NMR (151 MHz, $CDCl_3$) δ 166.15, 143.07, 139.04, 137.49, 133.26 (q, *J* = 31.71 Hz), 130.95 (q, *J* = 33.22 Hz), 129.32, 129.13, 127.37, 126.63 (q, *J* = 270.3 Hz), 125.65 (q, *J* = 4.53 Hz), 124.84 (q, *J* = 3.02 Hz), 123.08 (q, *J* = 271.2 Hz), 122.96 (q, *J* = 4.53 Hz), 115.70, 43.57

4-nitro-*N*-(2-(3-(trifluoromethyl)phenyl)allyl)benzamide (6g)

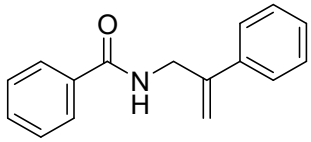


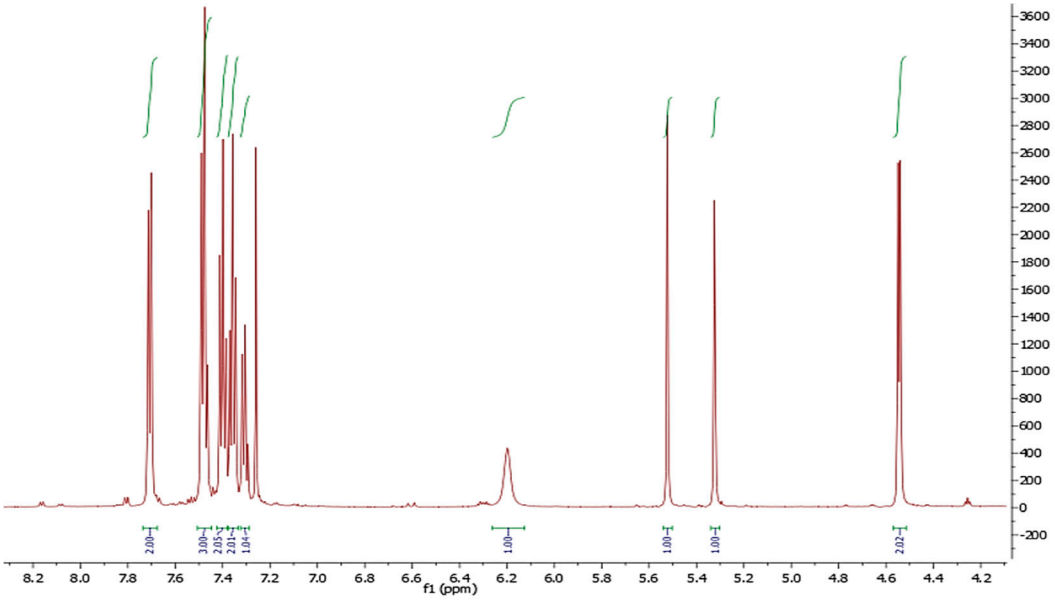
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.27 (d, J = 8.8 Hz, 2H), 7.89 (d, J = 8.7 Hz, 2H), 7.73 (s, 1H), 7.67 (d, J = 7.8 Hz, 1H), 7.60 (d, J = 7.7 Hz, 1H), 7.51 (t, J = 7.8 Hz, 1H), 6.38 (s, 1H), 5.62 (s, 1H), 5.44 (s, 1H), 4.60 (d, J = 5.7 Hz, 2H)



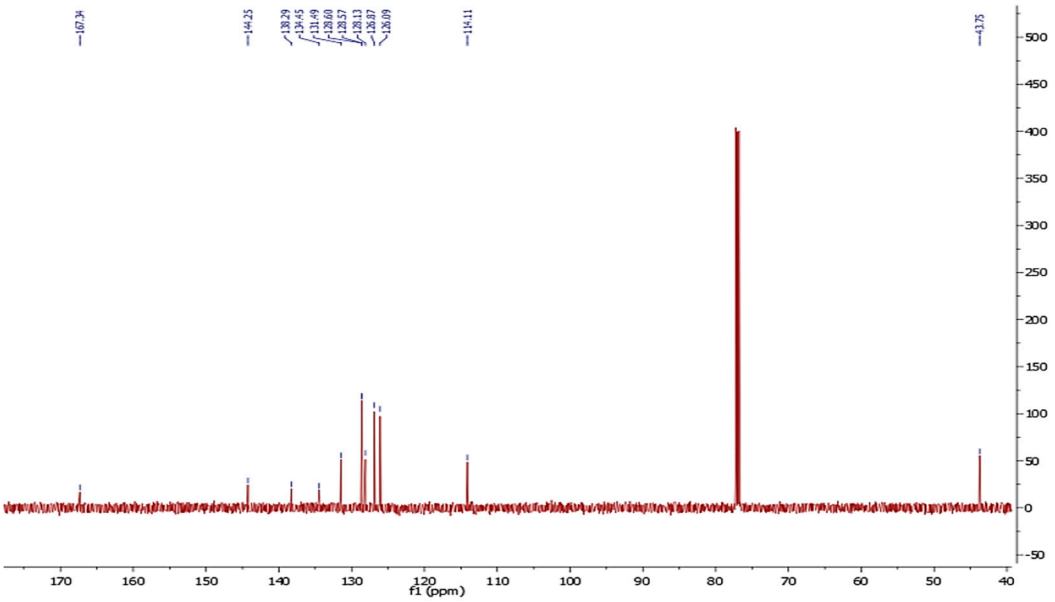
^{13}C NMR (151 MHz, $CDCl_3$) δ 165.48, 149.63, 142.84, 139.74, 138.91, 130.96 (q, J = 33.22 Hz), 129.30, 129.18, 128.11, 124.92 (q, J = 4.53 Hz), 123.83, 123.05 (q, J = 271.8 Hz), 122.92 (q, J = 4.53 Hz), 115.91, 43.70

<u>*N*-(2-phenylallyl)benzamide (6h)</u>



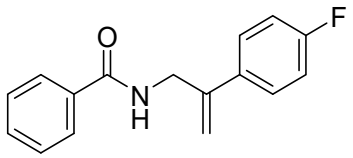


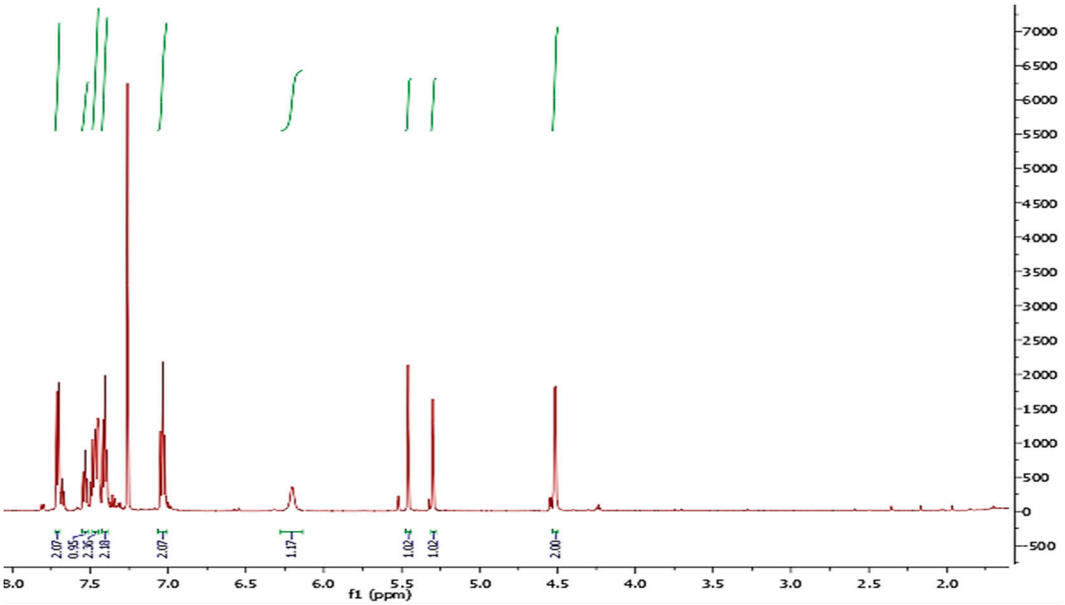
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, 2H), 7.48 (t, 3H), 7.40 (t, J = 7.6 Hz, 2H), 7.36 (t, J = 10.2, 4.7 Hz, 2H), 7.31 (t, 1H), 6.20 (s, 1H), 5.52 (s, 1H), 5.32 (s, 1H), 4.54 (d, J = 5.5 Hz, 2H)



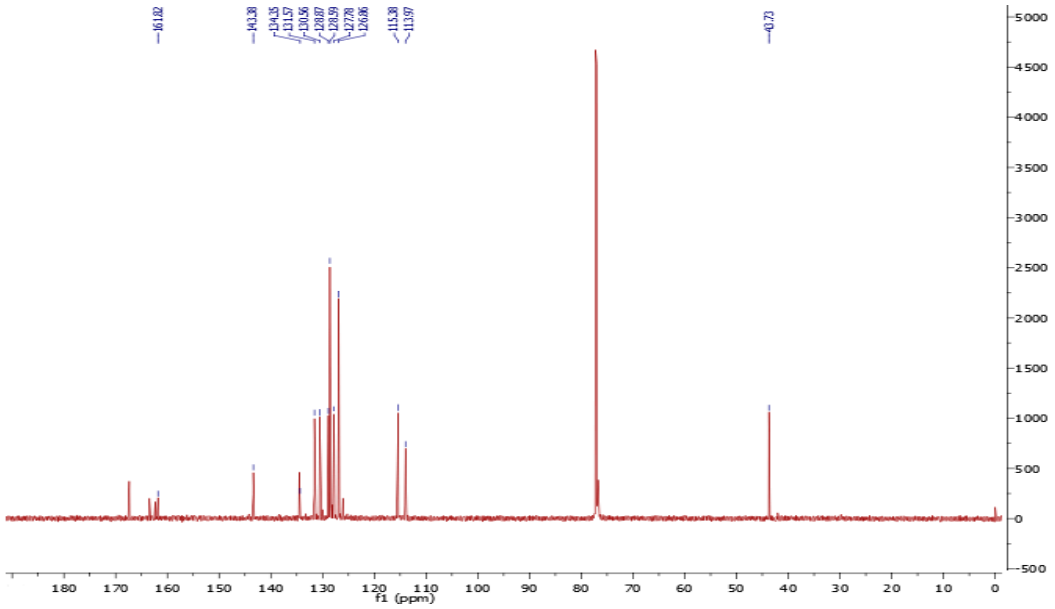
^{13}C NMR (151 MHz, $CDCl_3$) δ 167.34, 144.25, 138.29, 134.45, 131.49, 128.60, 128.57, 128.13, 126.87, 126.09, 114.11, 43.75

<u>*N*-(2-(4-fluorophenyl)allyl)benzamide (6i)</u>



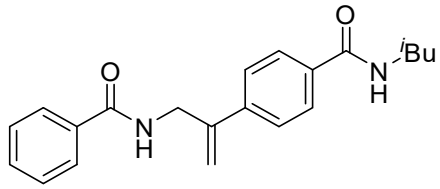


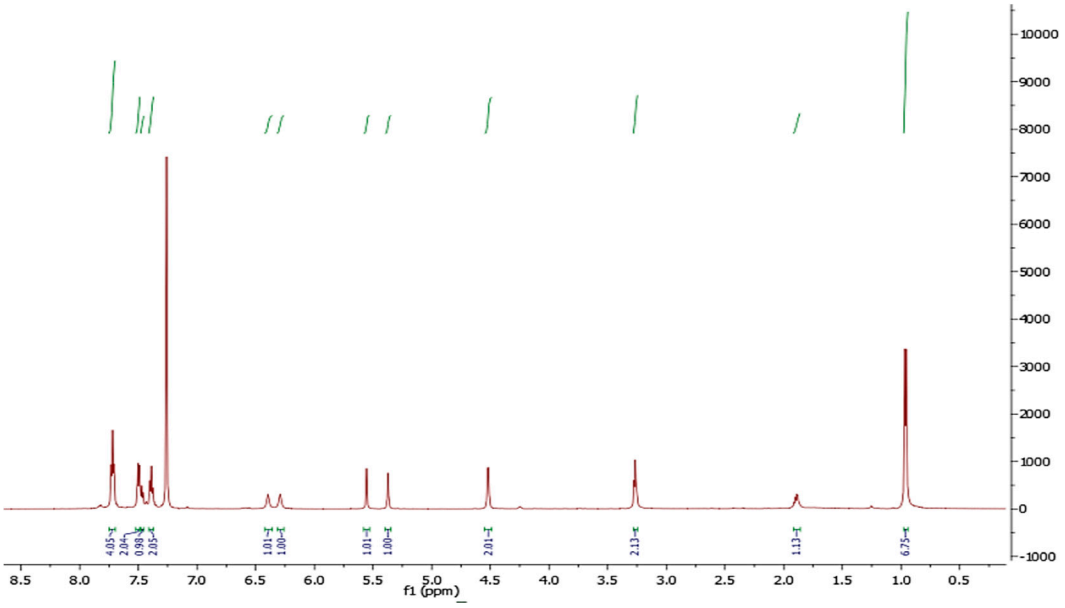
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 – 7.70 (m, 2H), 7.53 (t, J = 7.8 Hz, 1H), 7.48 – 7.45 (m, 2H), 7.41 (t, J = 7.6 Hz, 2H), 7.06 – 7.01 (m, 2H), 6.28 – 6.14 (m, 1H), 5.46 (s, 1H), 5.30 (s, 1H), 4.52 (d, J = 5.7 Hz, 2H)



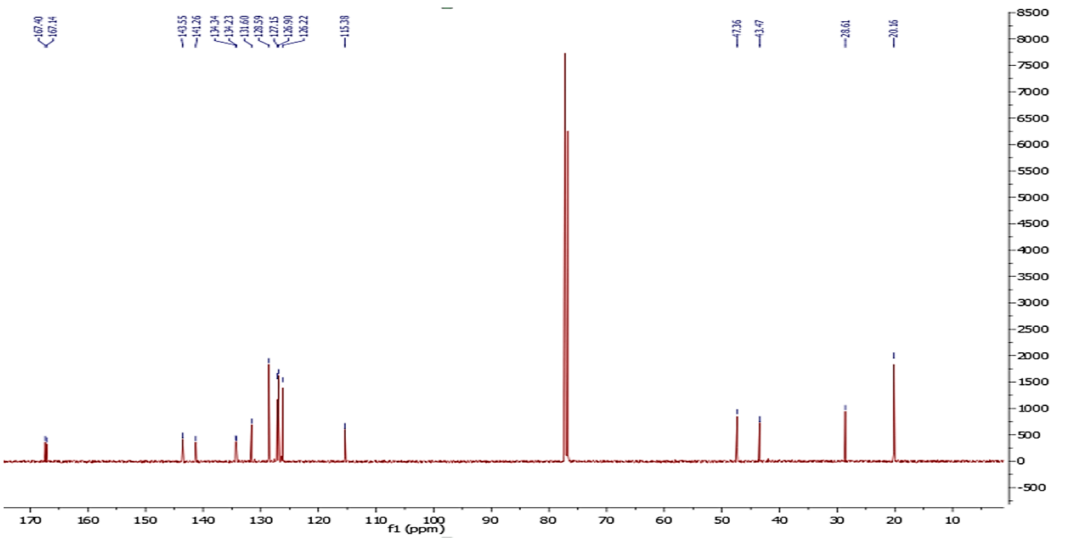
^{13}C NMR (151 MHz, $CDCl_3$) δ 161.82 (d, J = 241.6 Hz), 143.38 (d, J = 4.53 Hz), 134.35, 131.57, 130.56, 128.87, 128.59, 127.78 (d, J = 7.55 Hz), 126.86, 115.38 (d, J = 21.14 Hz), 113.97, 43.73

4-(3-benzamidoprop-1-en-2-yl)-*N*-isobutylbenzamide (6j)



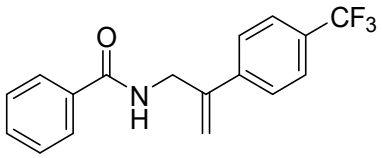


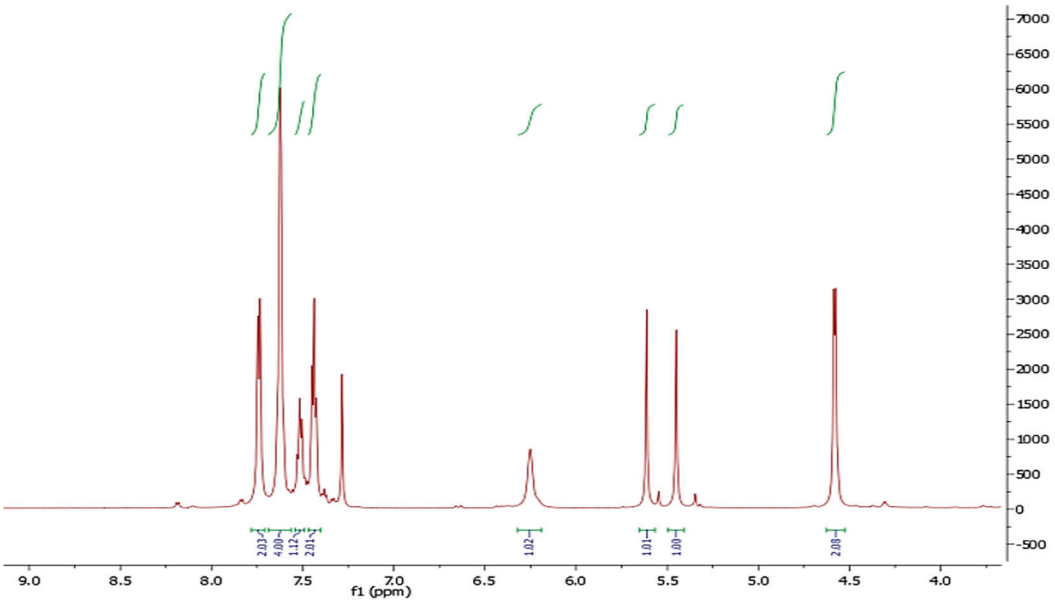
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (t, J = 7.1 Hz, 4H), 7.50 (d, J = 8.1 Hz, 2H), 7.47 (d, J = 7.3 Hz, 1H), 7.39 (t, J = 7.5 Hz, 2H), 6.40 (s, 1H), 6.29 (s, 1H), 5.56 (s, 1H), 5.37 (s, 1H), 4.52 (d, J = 5.4 Hz, 2H), 3.26 (t, J = 6.3 Hz, 2H), 1.89 (dt, J = 13.3, 6.6 Hz, 1H), 0.96 (d, J = 6.6 Hz, 7H)



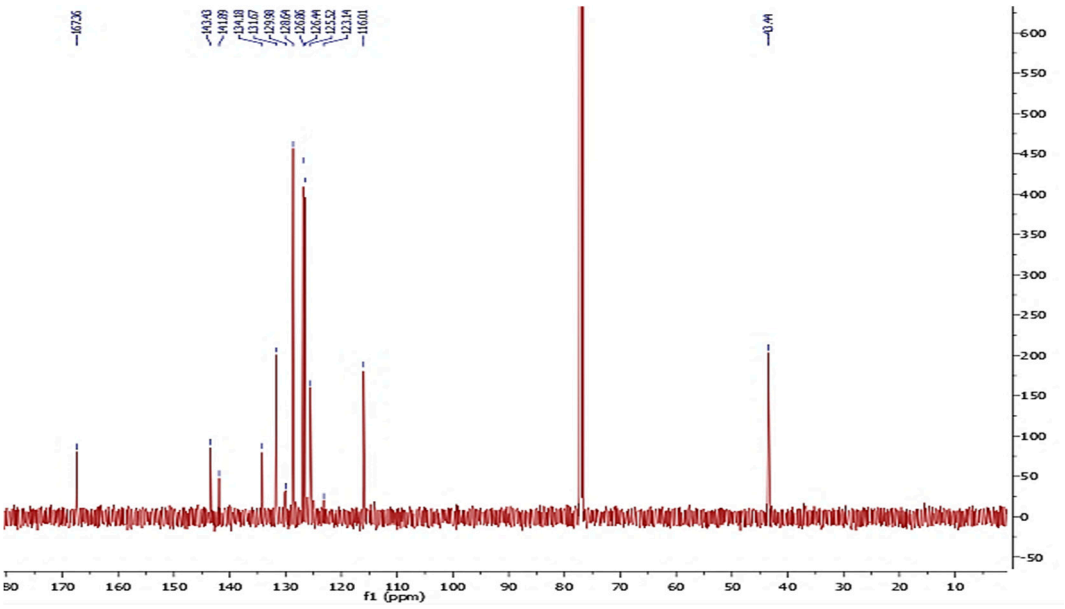
^{13}C NMR (151 MHz, $CDCl_3$) δ 167.40, 167.14, 143.55, 141.26, 134.34, 134.23, 131.60, 128.59, 127.15, 126.90, 126.22, 115.38, 47.36, 43.47, 28.61, 20.16

***N*-(2-(4-(trifluoromethyl)phenyl)allyl)benzamide (6k)**



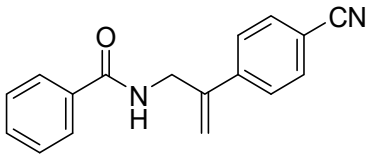


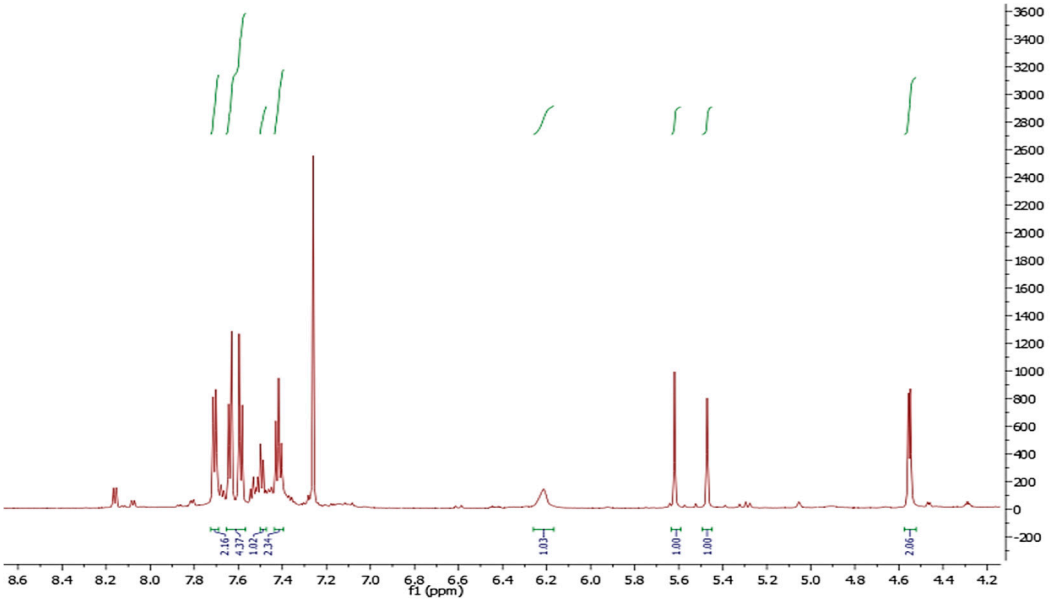
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 7.4 Hz, 2H), 7.62 (d, J = 2.6 Hz, 4H), 7.52 (t, J = 7.2 Hz, 1H), 7.44 (t, J = 7.5 Hz, 2H), 6.25 (s, 1H), 5.61 (s, 1H), 5.45 (s, 1H), 4.58 (d, J = 5.4 Hz, 2H)



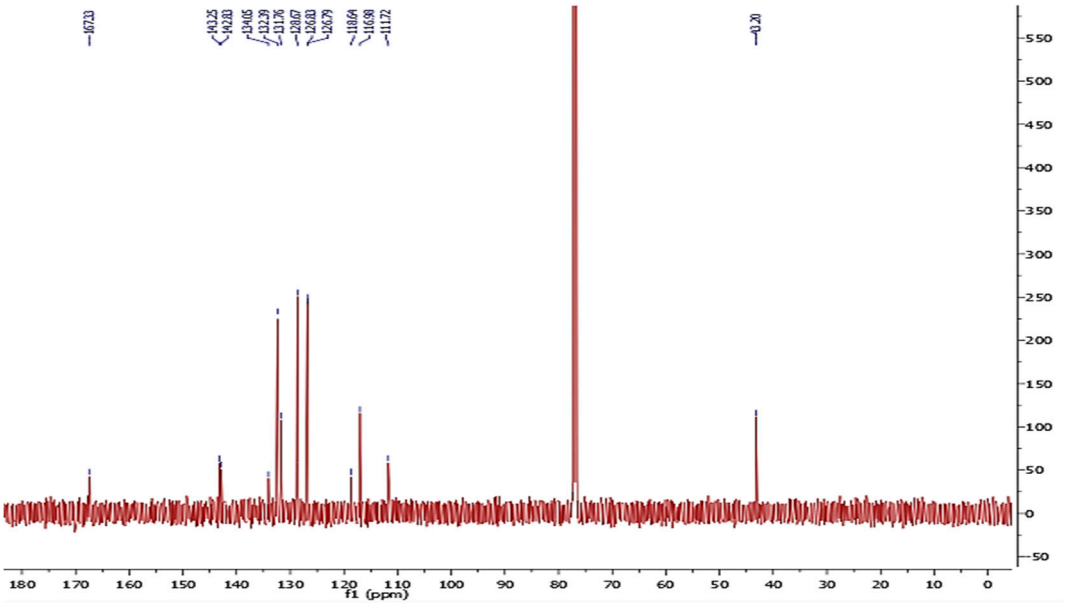
^{13}C NMR (151 MHz, $CDCl_3$) δ 167.36, 143.43, 141.89, 134.18, 131.67, 129.98 (q, J = 31.71 Hz), 128.64, 126.86, 126.44, 125.52 (q, J = 3.02 Hz), 123.14 (q, J = 271.8 Hz), 116.01, 43.44

<u>*N*-(2-(4-cyanophenyl)allyl)benzamide (6l)</u>



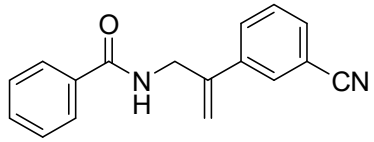


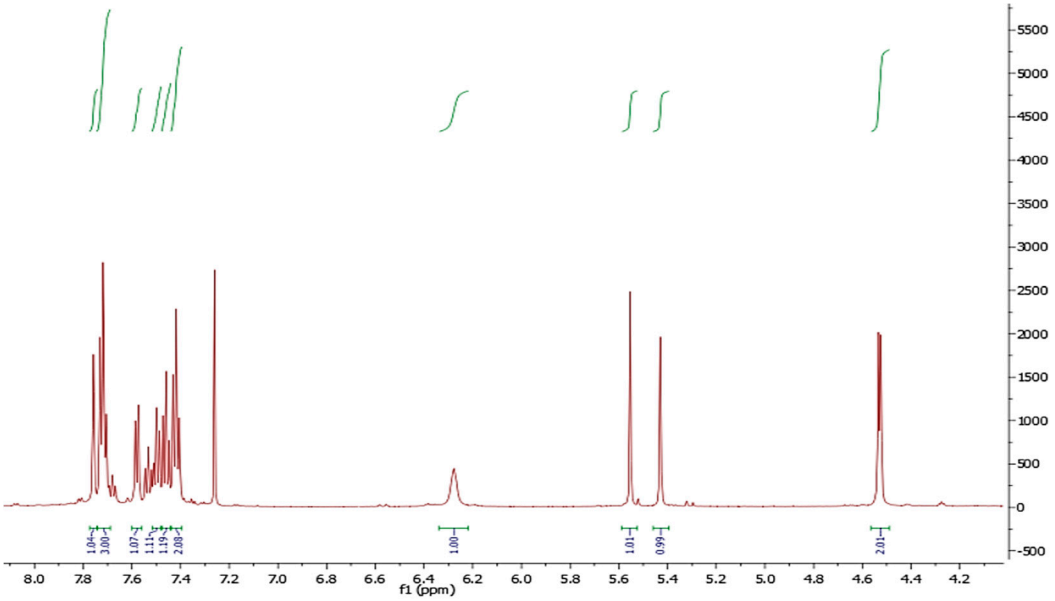
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 (d, J = 7.5 Hz, 2H), 7.61 (dd, J = 28.9, 8.3 Hz, 4H), 7.49 (d, J = 7.4 Hz, 1H), 7.42 (t, J = 7.7 Hz, 3H), 6.21 (s, 1H), 5.62 (s, 1H), 5.47 (s, 1H), 4.55 (d, J = 5.7 Hz, 2H)



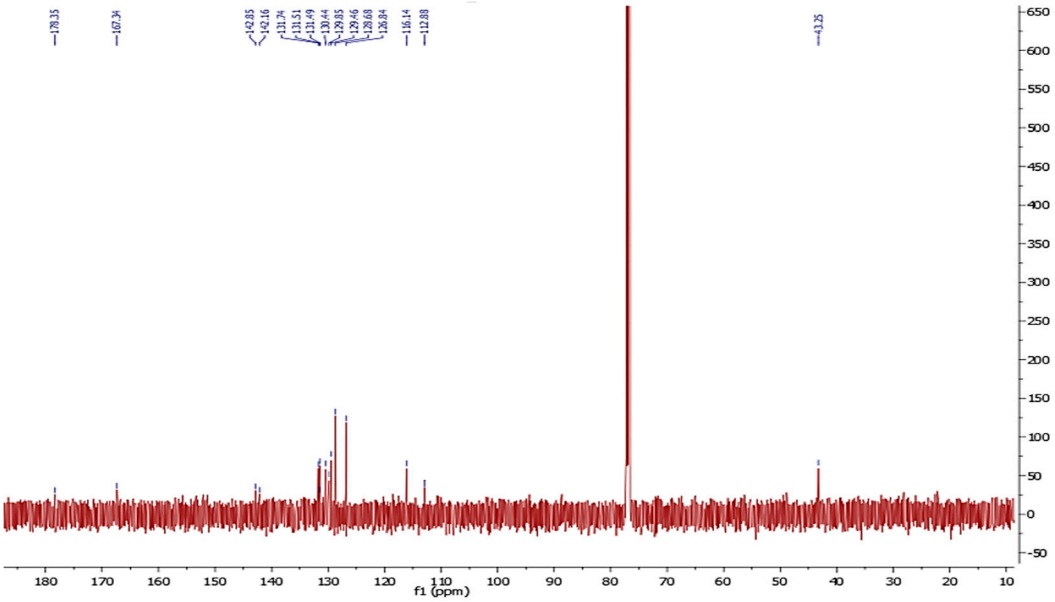
^{13}C NMR (151 MHz, $CDCl_3$) δ 167.33, 143.25, 142.83, 134.05, 132.39, 131.76, 128.67, 126.83, 126.79, 118.64, 116.98, 111.72, 43.20

<u>*N*-(2-(3-cyanophenyl)allyl)benzamide (6n)</u>



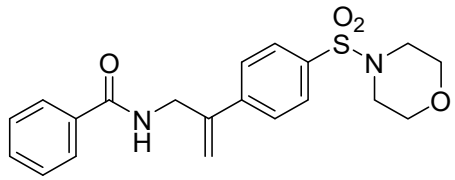


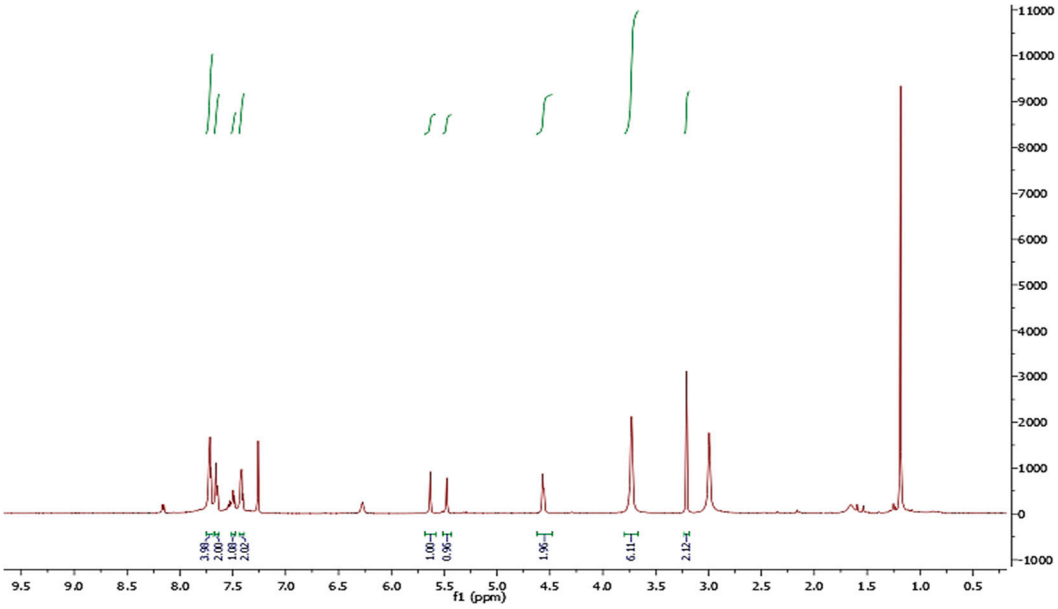
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.72 (t, J = 7.3 Hz, 3H), 7.58 (d, J = 7.7 Hz, 1H), 7.50 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.8 Hz, 1H), 7.42 (t, J = 7.7 Hz, 2H), 6.28 (s, 1H), 5.55 (s, 1H), 5.43 (s, 1H), 4.53 (d, J = 5.8 Hz, 2H)



^{13}C NMR (151 MHz, $CDCl_3$) δ 178.35, 167.34, 142.85, 142.16, 131.74, 131.51, 131.49, 130.44, 129.85, 129.46, 128.68, 126.84, 116.14, 112.88, 43.25

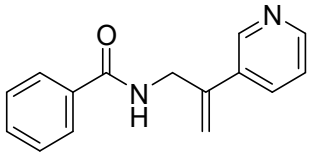
***N*-(2-(4-(morpholinosulfonyl)phenyl)allyl)benzamide (6o)**

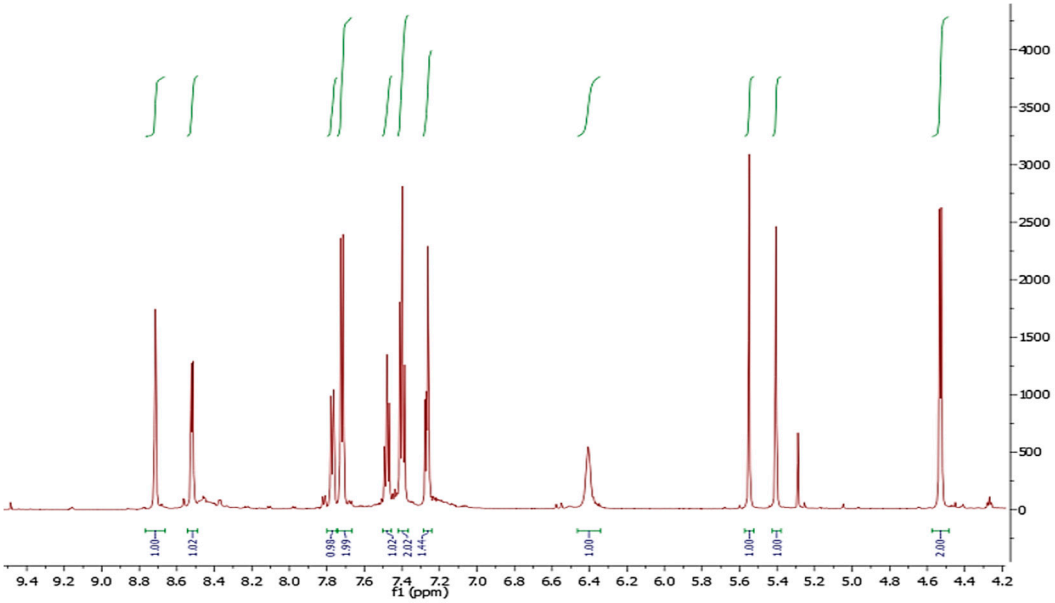




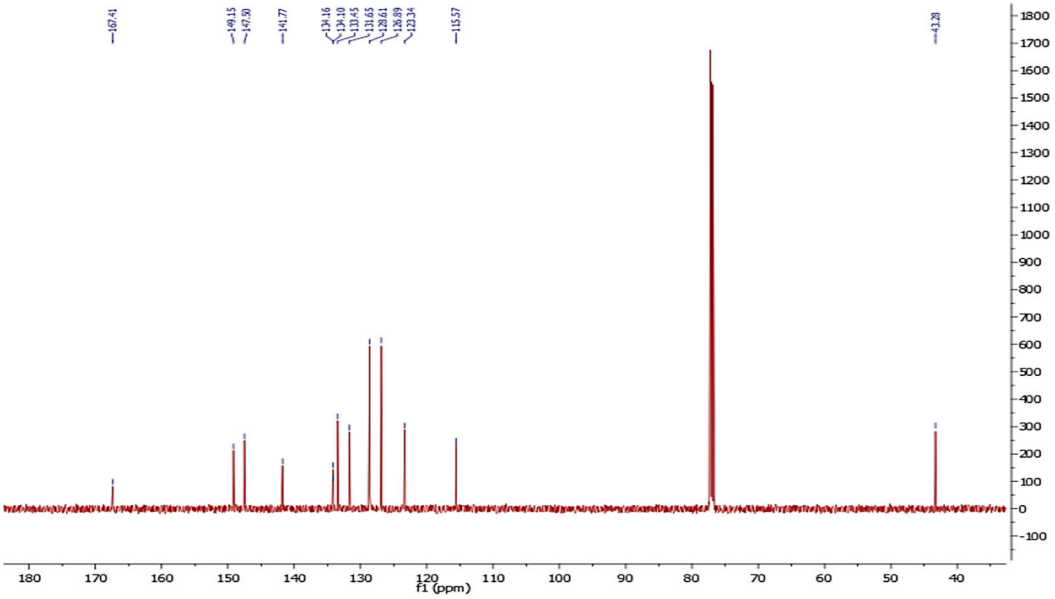
^{1}H NMR (600 MHz, CDCl3) δ 7.72 (t, J = 6.8 Hz, 4H), 7.65 (d, J = 8.2 Hz, 2H), 7.51 – 7.48 (m, 1H), 7.42 (t, J = 7.6 Hz, 2H), 5.63 (s, 1H), 5.48 (s, 1H), 4.56 (d, J = 5.6 Hz, 2H), 3.79 – 3.67 (m, 6H), 3.21 (s, 2H)

<u>*N*-(2-(pyridin-3-yl)allyl)benzamide (6q)</u>



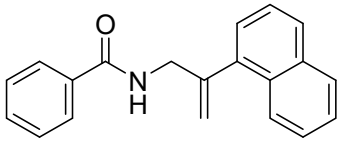


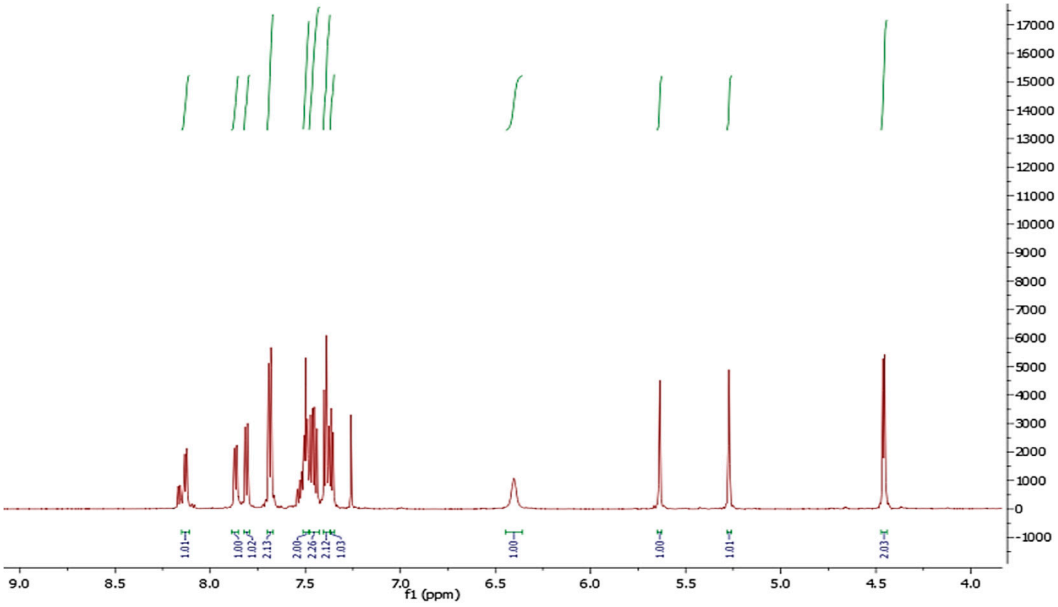
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.72 (d, J = 1.9 Hz, 1H), 8.52 (d, J = 4.7 Hz, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.72 (d, J = 7.4 Hz, 2H), 7.48 (t, J = 7.4 Hz, 1H), 7.40 (t, J = 7.7 Hz, 2H), 7.27 (dd, J = 8.7, 3.9 Hz, 1H), 6.41 (s, 1H), 5.55 (s, 1H), 5.41 (s, 1H), 4.53 (d, J = 5.8 Hz, 2H)



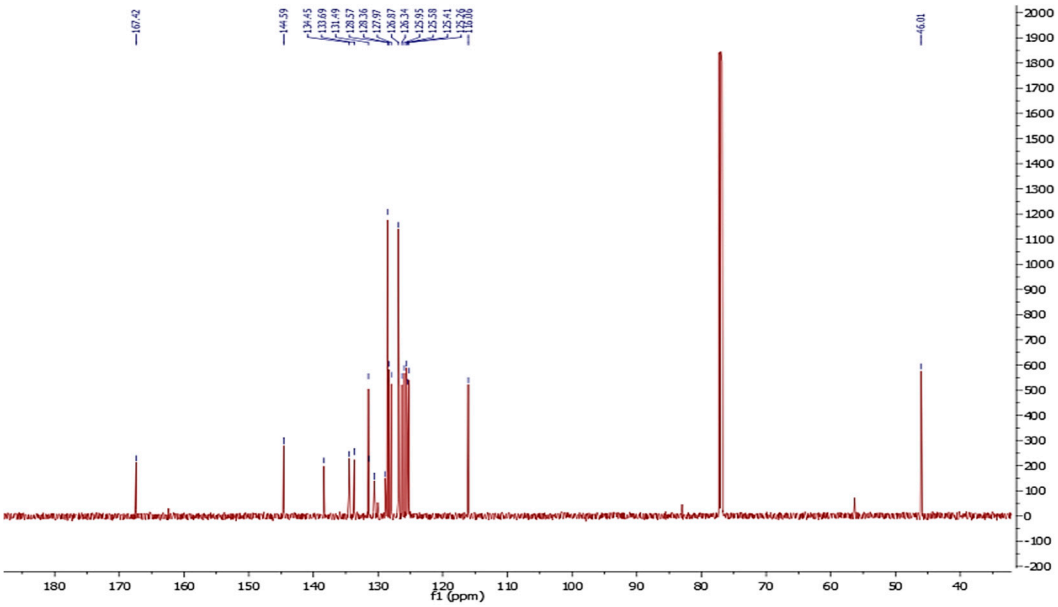
^{13}C NMR (151 MHz, $CDCl_3$) δ 167.41, 149.15, 147.50, 141.77, 134.16, 134.10, 133.45, 131.65, 128.61, 126.89, 123.34, 115.57, 43.28

<u>*N*-(2-(naphthalen-1-yl)allyl)benzamide (6p)</u>



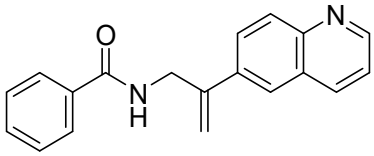


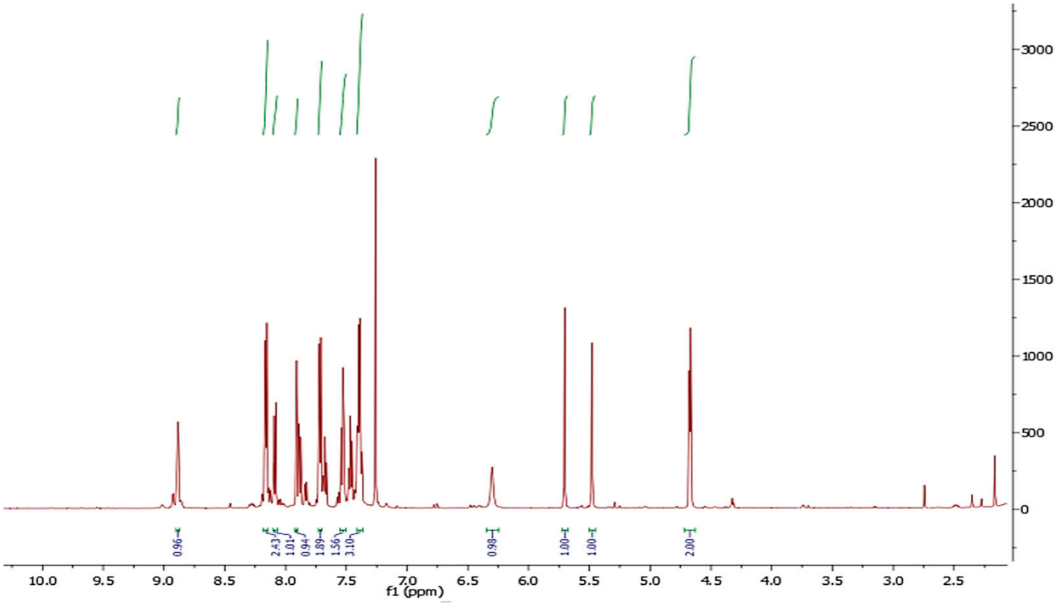
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 – 8.11 (m, 1H), 7.88 – 7.85 (m, 1H), 7.81 (d, J = 8.2 Hz, 1H), 7.70 – 7.67 (m, 2H), 7.50 (ddd, J = 8.0, 3.5, 1.6 Hz, 2H), 7.48 – 7.43 (m, 2H), 7.39 (t, J = 7.7 Hz, 2H), 7.36 (dd, J = 6.9, 1.0 Hz, 1H), 6.40 (s, 1H), 5.64 (d, J = 1.4 Hz, 1H), 5.27 (d, J = 1.1 Hz, 1H), 4.46 (d, J = 5.9 Hz, 2H)



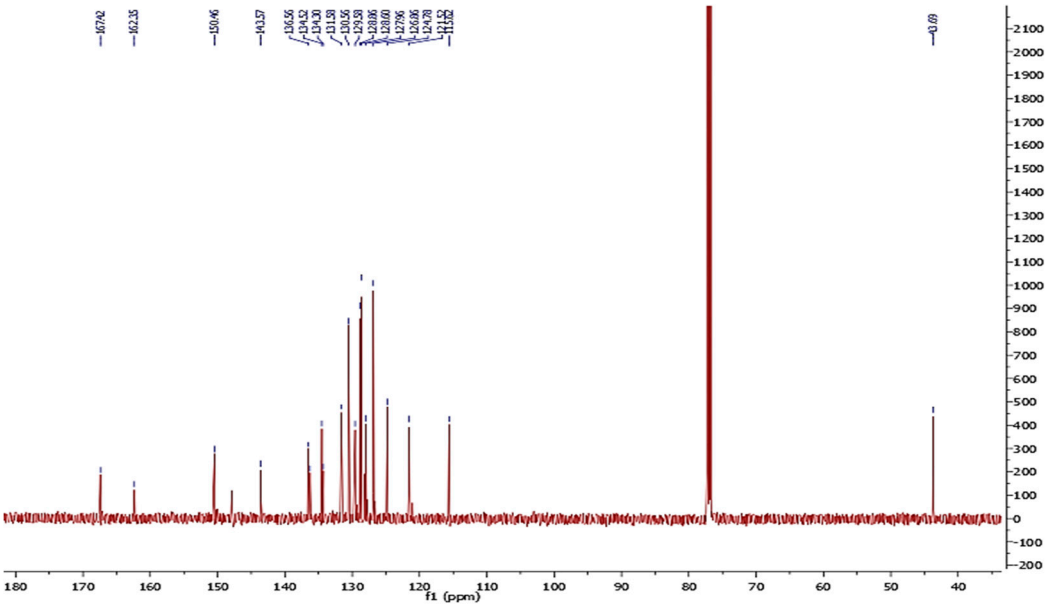
^{13}C NMR (151 MHz, $CDCl_3$) δ 167.42, 144.59, 138.38, 134.45, 133.69, 131.49, 131.44, 130.57, 128.88, 128.57, 128.36, 127.97, 126.87, 126.34, 125.95, 125.58, 125.41, 125.26, 116.06, 46.01

<u>*N*-(2-(quinolin-6-yl)allyl)benzamide (6r)</u>



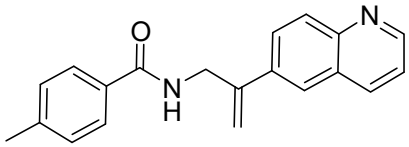


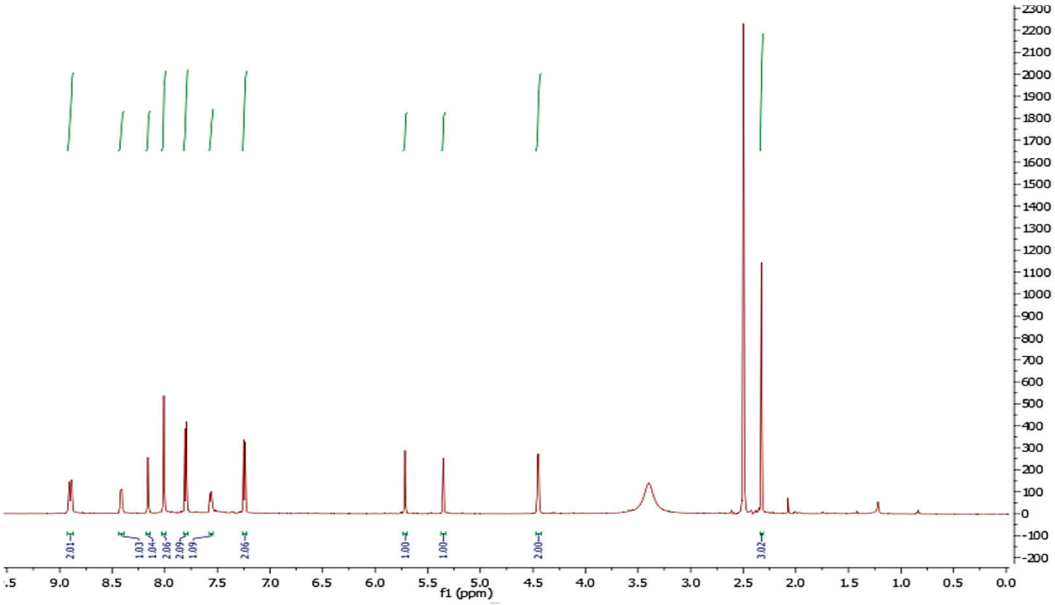
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.89 (d, J = 3.9 Hz, 1H), 8.16 (d, J = 7.7 Hz, 2H), 8.09 (d, J = 8.8 Hz, 1H), 7.91 (s, 1H), 7.72 (d, J = 7.8 Hz, 2H), 7.53 (t, J = 7.6 Hz, 1H), 7.41 – 7.37 (m, 3H), 6.30 (s, 1H), 5.70 (s, 1H), 5.48 (s, 1H), 4.67 (d, J = 5.6 Hz, 2H)



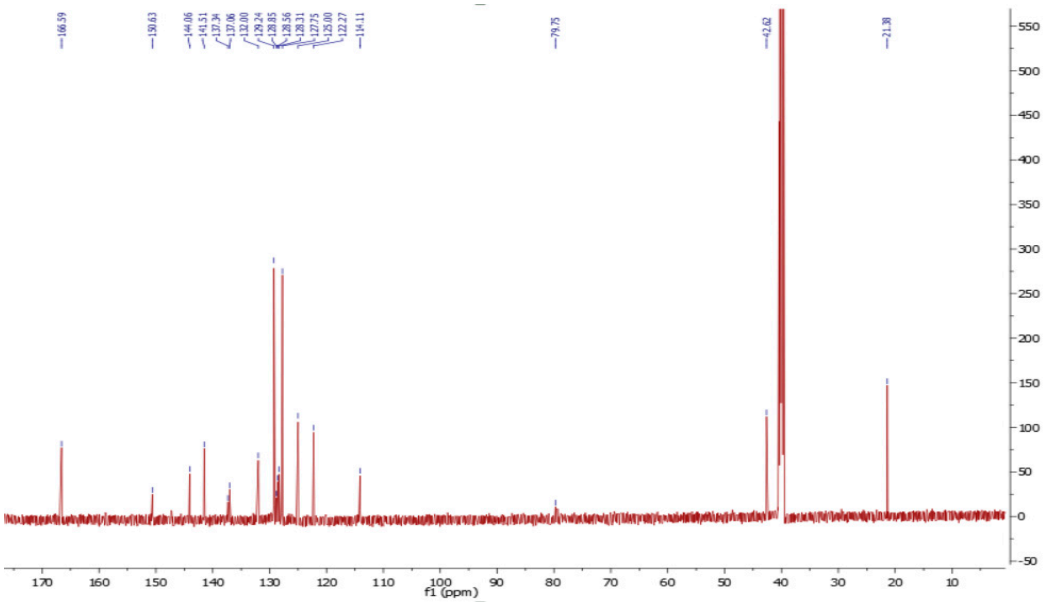
^{13}C NMR (151 MHz, CDCl3) δ 167.42, 162.35, 150.46, 143.57, 136.56, 136.25, 134.52, 134.30, 131.58, 130.56, 129.58, 128.86, 128.60, 127.96, 126.86, 124.78, 121.52, 115.62, 43.69

4-methyl-N-(2-(quinolin-6-yl)allyl)benzamide (6s)



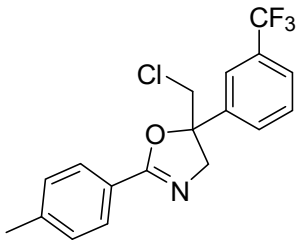


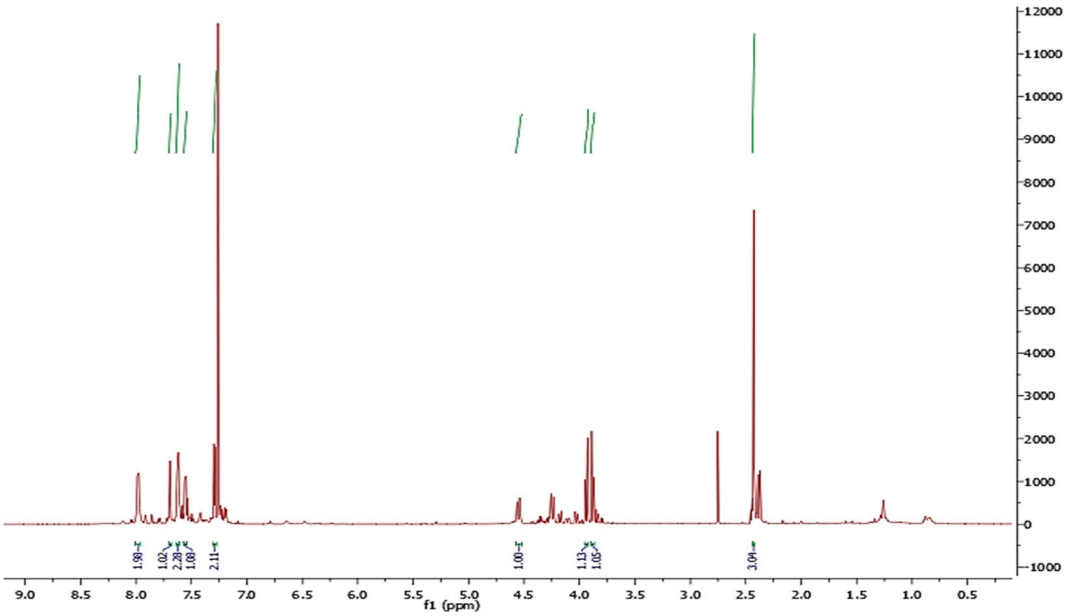
^{1}H NMR (600 MHz, DMSO) δ 8.93 – 8.87 (m, 2H), 8.41 (d, J = 8.2 Hz, 1H), 8.16 (s, 1H), 8.01 (s, 2H), 7.80 (d, J = 8.2 Hz, 2H), 7.56 (dd, J = 8.2, 4.2 Hz, 1H), 7.24 (d, J = 8.0 Hz, 2H), 5.72 (s, 1H), 5.35 (s, 1H), 4.45 (d, J = 5.8 Hz, 2H), 2.33 (s, 3H)



^{13}C NMR (151 MHz, DMSO) δ 166.59, 150.63, 144.06, 141.51, 137.34, 137.06, 132.00, 129.24, 128.85, 128.56, 128.31, 127.75, 125.00, 122.27, 114.11, 79.75, 42.62, 21.38

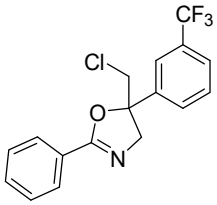
5-(chloromethyl)-2-(p-tolyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7b)

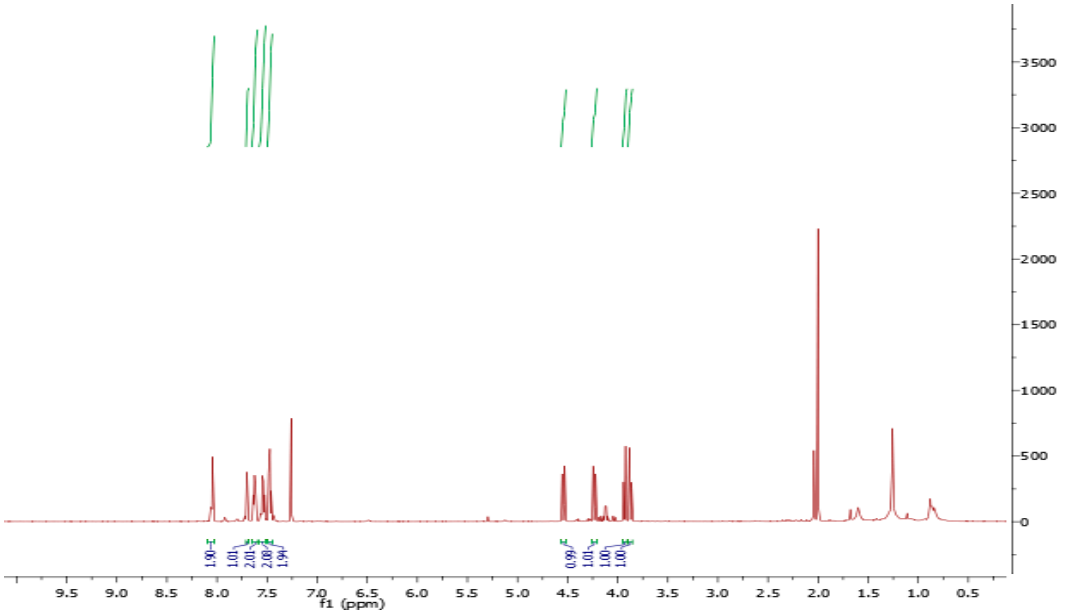




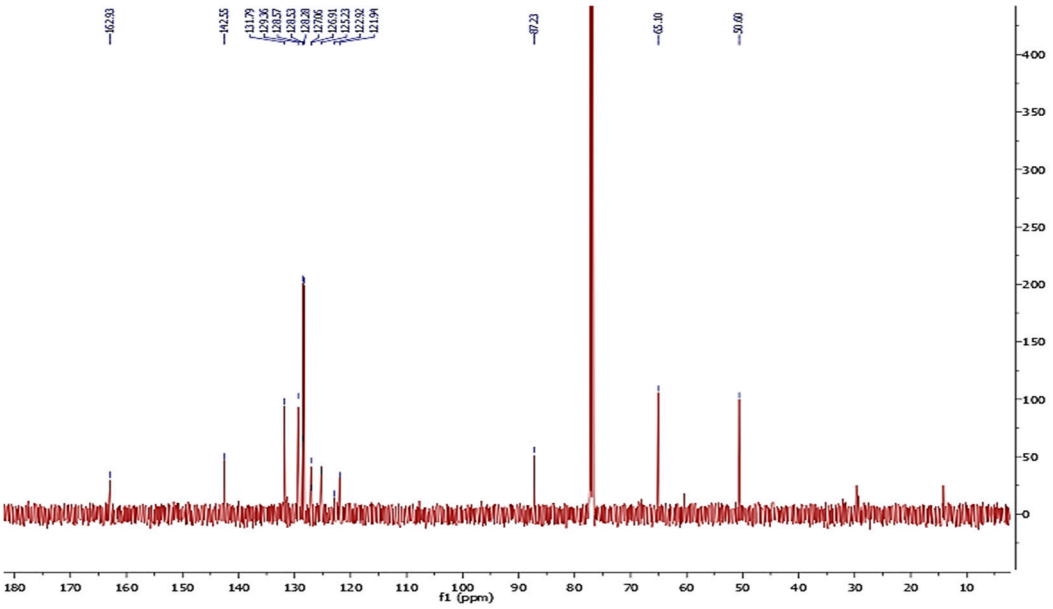
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (d, J = 7.9 Hz, 2H), 7.69 (s, 1H), 7.64 – 7.61 (m, 2H), 7.57 – 7.53 (m, 1H), 7.29 (d, J = 7.9 Hz, 2H), 4.55 (d, J = 14.7 Hz, 1H), 4.25 (d, J = 14.6 Hz, 1H), 3.94 (d, J = 12.1 Hz, 1H), 3.88 (d, J = 12.1 Hz, 1H), 2.43 (s, 3H)

5-(chloromethyl)-2-phenyl-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7c)



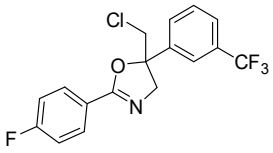


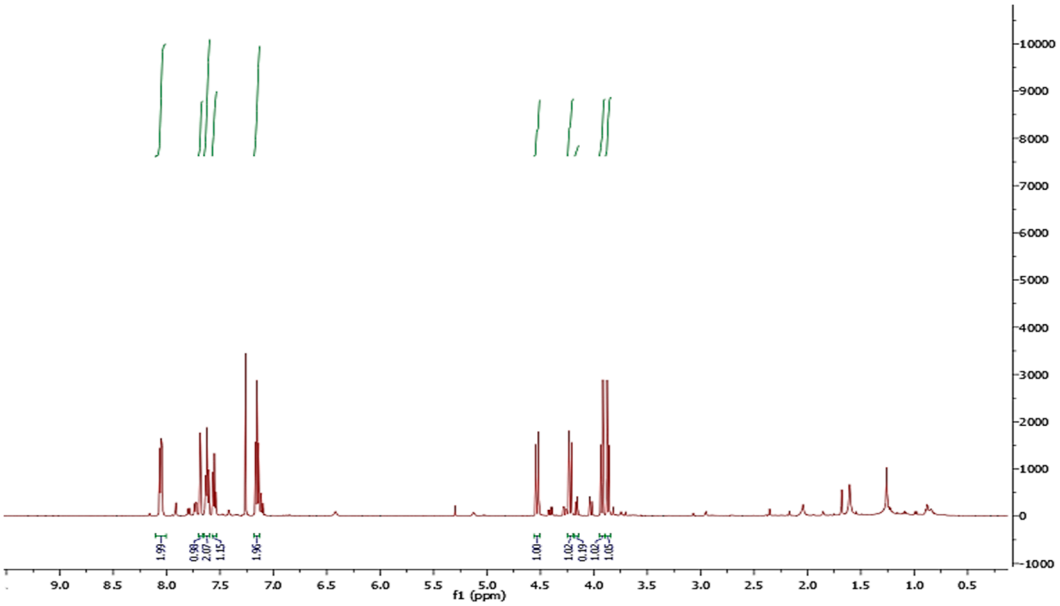
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, J = 7.2 Hz, 1H), 7.70 (s, 1H), 7.63 (t, J = 6.5 Hz, 2H), 7.54 (dd, J = 13.7, 7.5 Hz, 2H), 7.47 (t, J = 7.6 Hz, 2H), 4.54 (d, J = 14.9 Hz, 1H), 4.23 (d, J = 14.9 Hz, 1H), 3.93 (d, J = 12.0 Hz, 1H), 3.87 (d, J = 12.0 Hz, 1H)



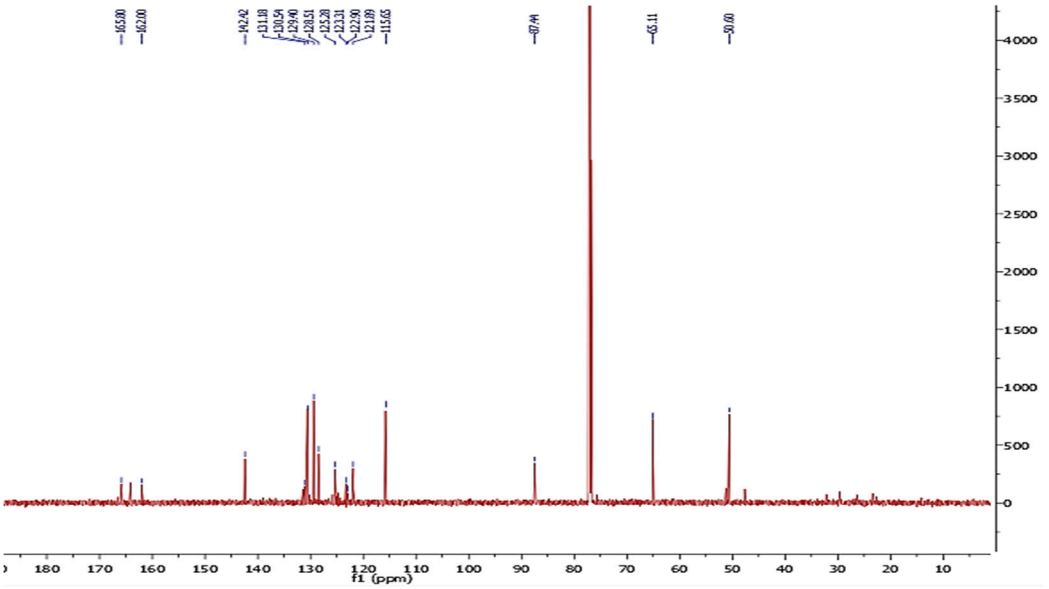
^{13}C NMR (151 MHz, $CDCl_3$) δ 162.93, 142.55, 131.79, 129.36, 128.57 (q, J = 33.2 Hz), 128.53, 128.28, 127.06, 126.91, 125.23 (q, J = 3.02 Hz), 122.92 (q, J = 271 Hz), 121.94 (q, J = 3.02 Hz), 87.23, 65.10, 50.60

5-(chloromethyl)-2-(4-fluorophenyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7d)



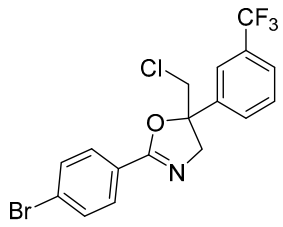


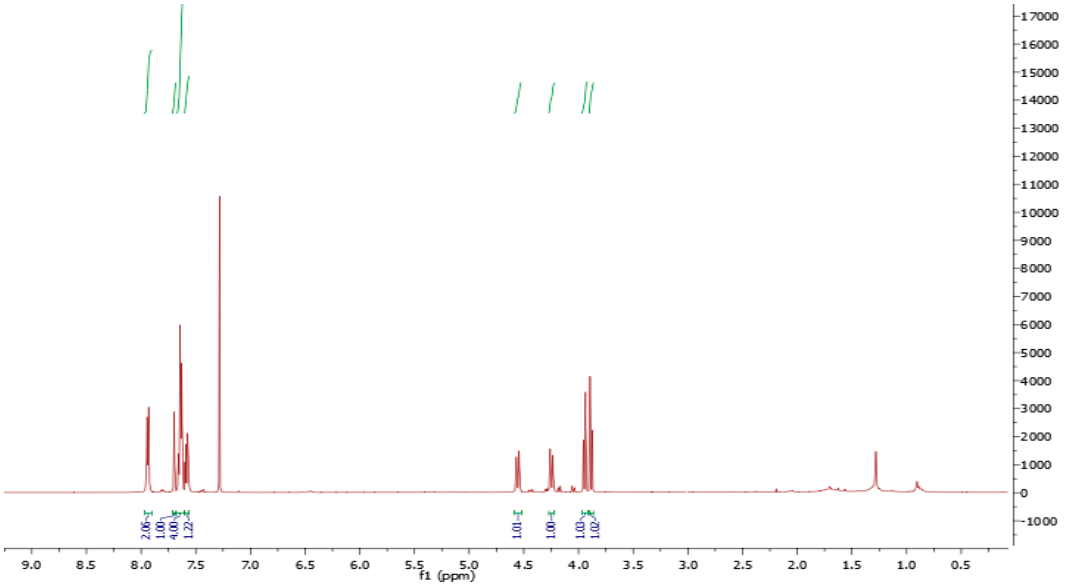
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 – 8.02 (m, 2H), 7.68 (s, 1H), 7.62 (t, *J* = 8.1 Hz, 2H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.17 – 7.13 (m, 2H), 4.53 (d, *J* = 14.9 Hz, 1H), 4.22 (d, *J* = 14.9 Hz, 1H), 3.92 (d, *J* = 12.0 Hz, 1H), 3.87 (d, *J* = 12.0 Hz, 1H)



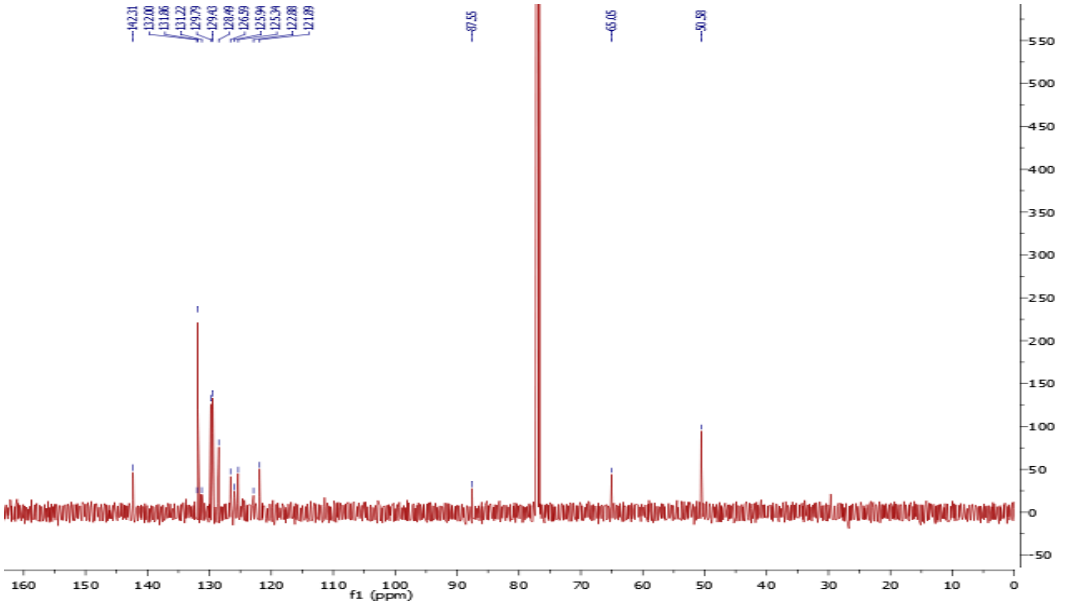
^{13}C NMR (151 MHz, $CDCl_3$) δ 165.80 (d, *J* = 252.9 Hz), 162.00, 142.42, 131.18 (q, *J* = 31.71 Hz), 130.54 (d, *J* = 9.06 Hz), 129.40, 128.51, 125.28 (q, *J* = 3.02 Hz), 123.31 (d, *J* = 3.02 Hz), 122.90 (q, *J* = 271.9 Hz), 121.89 (q, *J* = 3.02 Hz), 115.65 (d, *J* = 22.65 Hz), 87.44, 65.11, 50.60

2-(4-bromophenyl)-5-(chloromethyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7e)



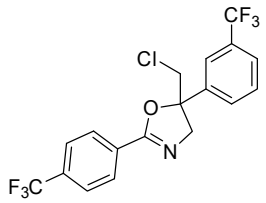


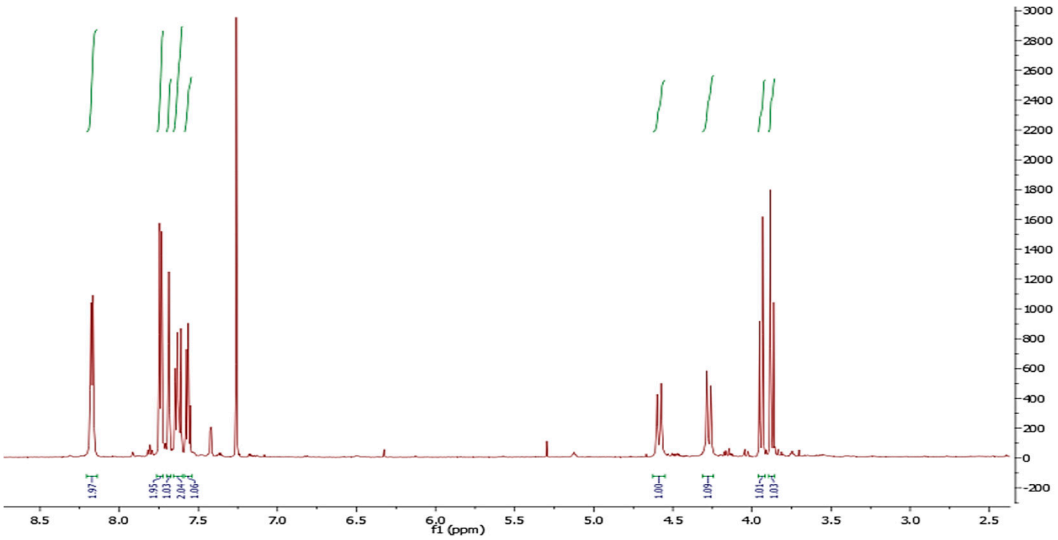
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, J = 8.3 Hz, 2H), 7.70 (s, 1H), 7.68 – 7.60 (m, 4H), 7.60 – 7.57 (m, 1H), 4.56 (d, J = 15.0 Hz, 1H), 4.25 (d, J = 15.0 Hz, 1H), 3.95 (d, J = 12.0 Hz, 1H), 3.88 (d, J = 12.0 Hz, 1H)



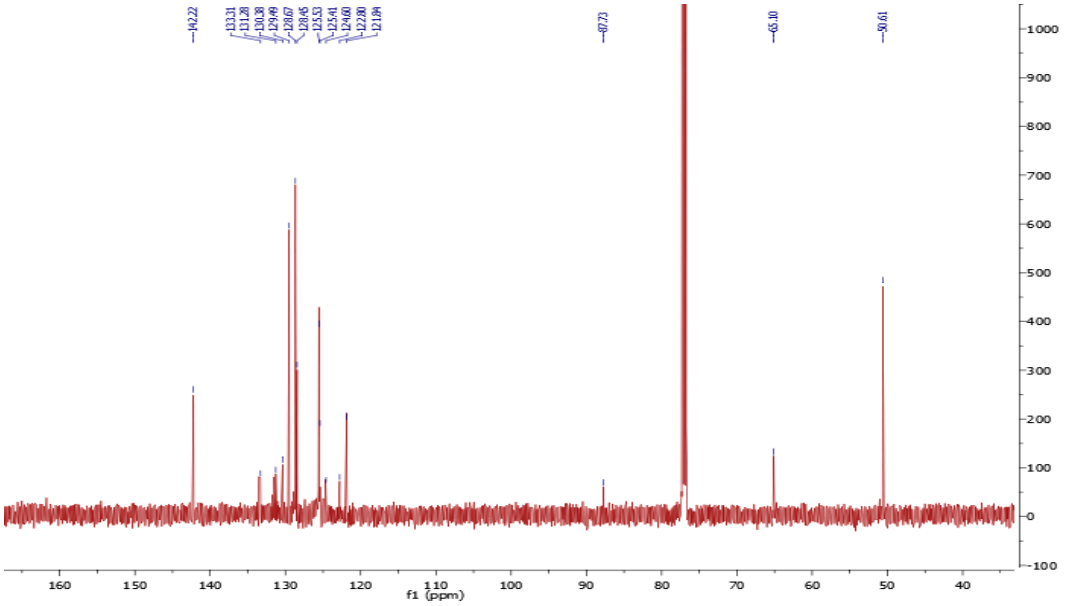
^{13}C NMR (151 MHz, $CDCl_3$) δ 142.31, 132.00, 131.86, 131.22 (q, J = 33.22 Hz), 129.79, 129.43, 128.49, 126.59, 125.94, 125.34 (q, J = 4.53 Hz), 122.88 (q, J = 271.8 Hz), 121.89 (q, J = 4.53 Hz), 87.55, 65.05, 50.58

5-(chloromethyl)-5-(3-(trifluoromethyl)phenyl)-2-(4(trifluoromethyl) phenyl)-4,5-dihydrooxazole (7f)



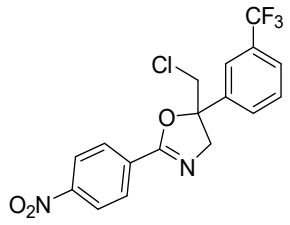


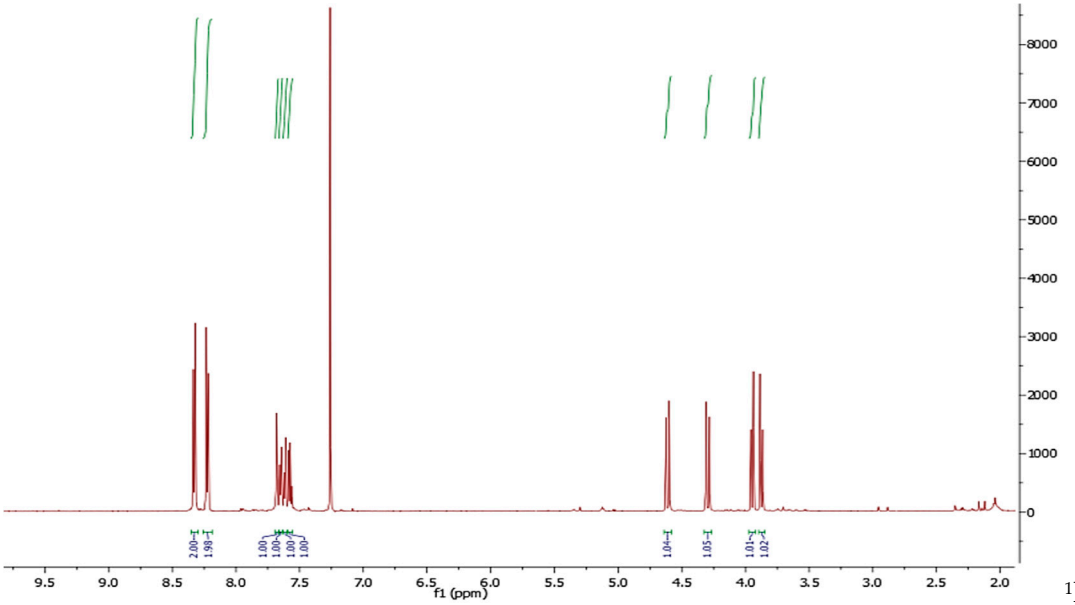
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.0 Hz, 2H), 7.74 (d, *J* = 8.1 Hz, 2H), 7.69 (s, 1H), 7.63 (dd, *J* = 13.1, 7.8 Hz, 2H), 7.56 (t, *J* = 7.7 Hz, 1H), 4.59 (d, *J* = 15.2 Hz, 1H), 4.27 (d, *J* = 15.2 Hz, 1H), 3.94 (d, *J* = 12.1 Hz, 1H), 3.87 (d, 1H)



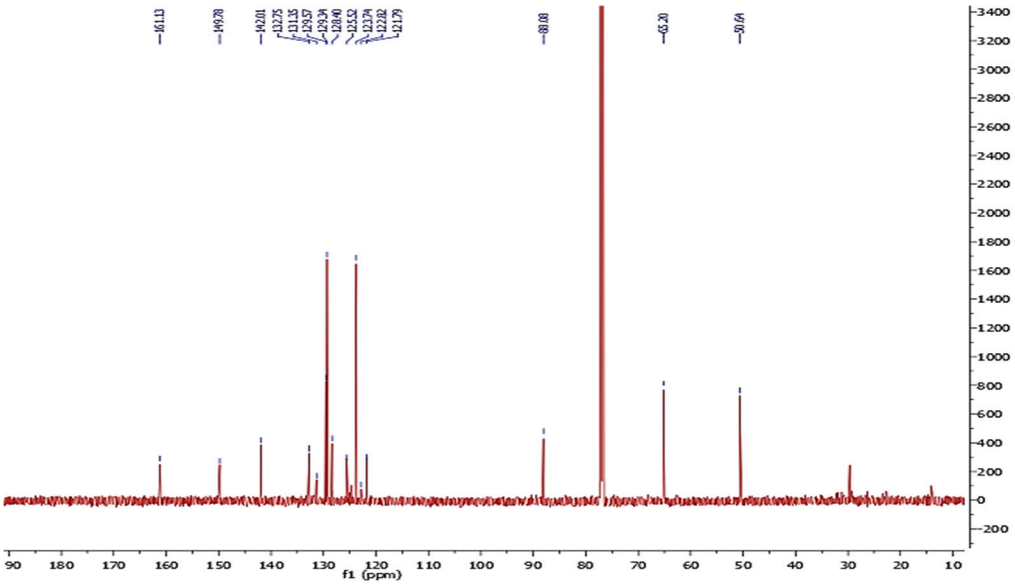
^{13}C NMR (151 MHz, $CDCl_3$) δ 142.22, 133.31 (q, *J* = 31.71 Hz), 131.28 (q, *J* = 33.22 Hz), 130.38, 129.49, 128.67, 128.45, 125.53 (q, *J* = 4.53 Hz), 125.41 (q, *J* = 3.02 Hz), 122.85 (q, *J* = 273.31 Hz), 122.80 (q, *J* = 273.31 Hz), 121.84 (q, *J* = 3.02 Hz), 87.73, 65.10, 50.61

5-(chloromethyl)-2-(4-nitrophenyl)-5-(3-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7g)



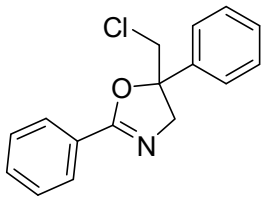


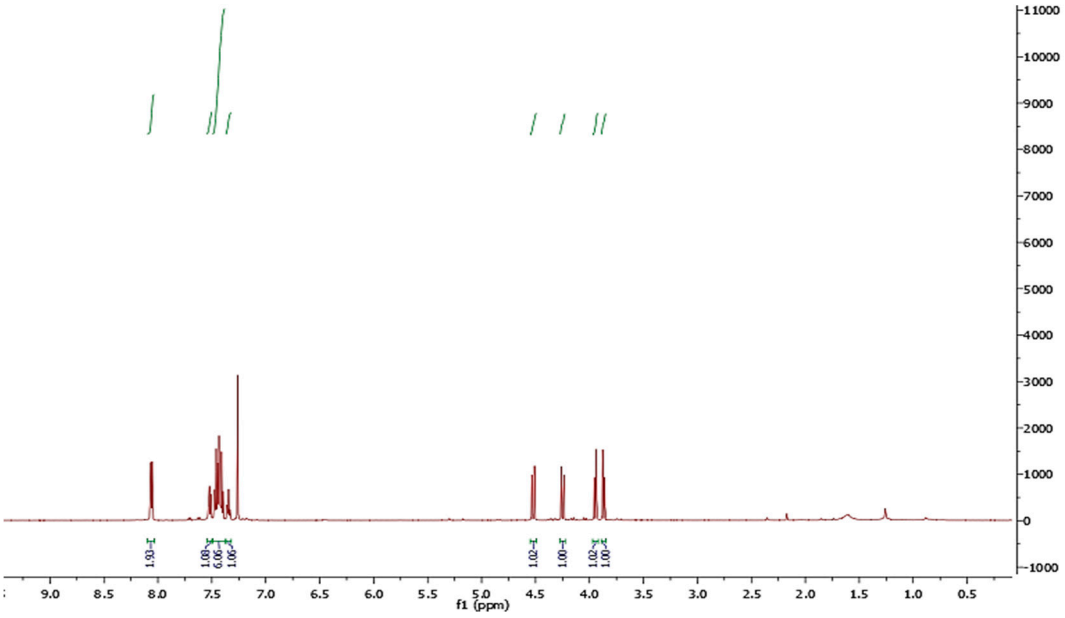
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.33 (d, J = 8.8 Hz, 2H), 8.23 (d, J = 8.8 Hz, 2H), 7.68 (s, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.62 (d, J = 7.9 Hz, 1H), 7.57 (t, J = 7.7 Hz, 1H), 4.61 (d, J = 15.4 Hz, 1H), 4.30 (d, J = 15.4 Hz, 1H), 3.95 (d, J = 12.2 Hz, 1H), 3.88 (d, J = 12.2 Hz, 1H)



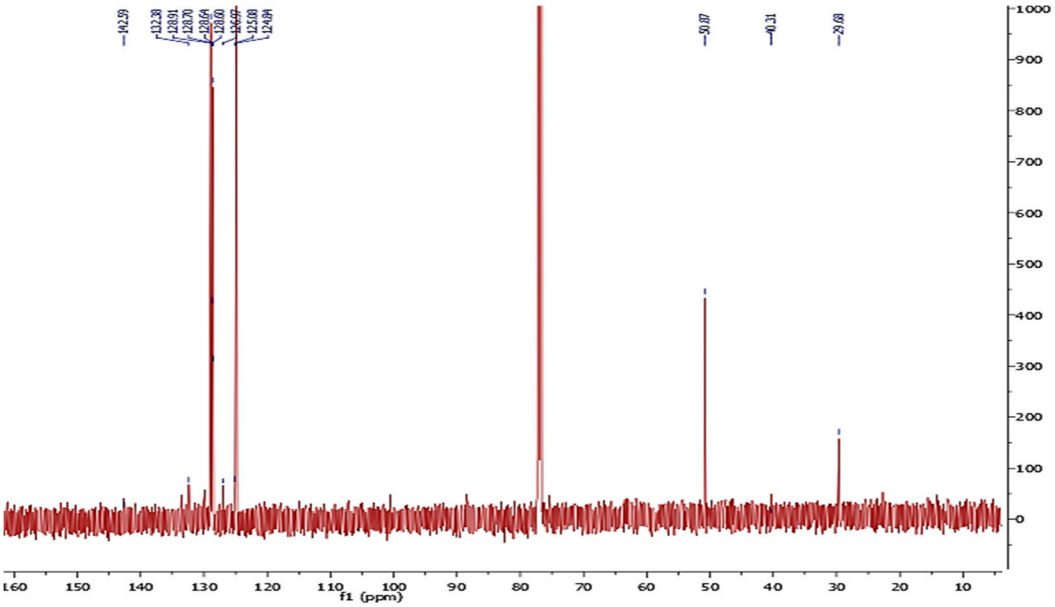
^{13}C NMR (151 MHz, $CDCl_3$) δ 161.13, 149.78, 142.01, 132.75, 131.35 (q, J = 31.71 Hz), 129.57, 129.34, 128.40, 125.52 (q, J = 3.02 Hz), 123.74, 122.82 (q, J = 271.8 Hz), 121.79 (q, J = 3.02 Hz), 88.08, 65.20, 50.64

5-(chloromethyl)-2,5-diphenyl-4,5-dihydrooxazole (7h)



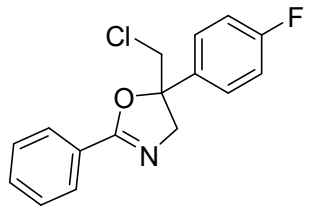


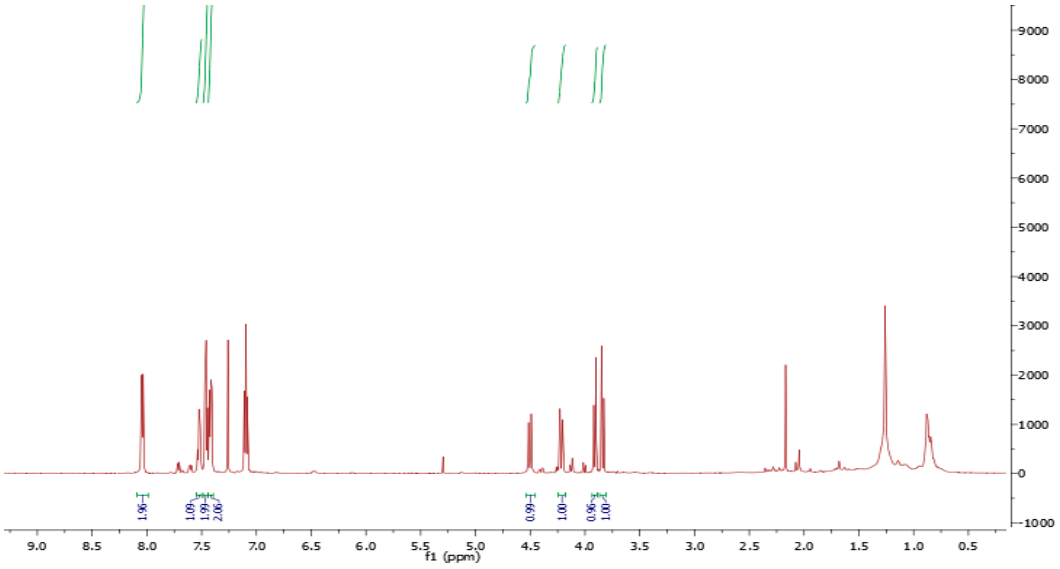
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, J = 7.2 Hz, 2H), 7.52 (t, J = 7.4 Hz, 1H), 7.48 – 7.38 (m, 6H), 7.34 (t, J = 6.4 Hz, 1H), 4.52 (d, J = 14.8 Hz, 1H), 4.25 (d, J = 14.8 Hz, 1H), 3.95 (d, J = 12.0 Hz, 1H), 3.87 (d, J = 12.0 Hz, 1H)



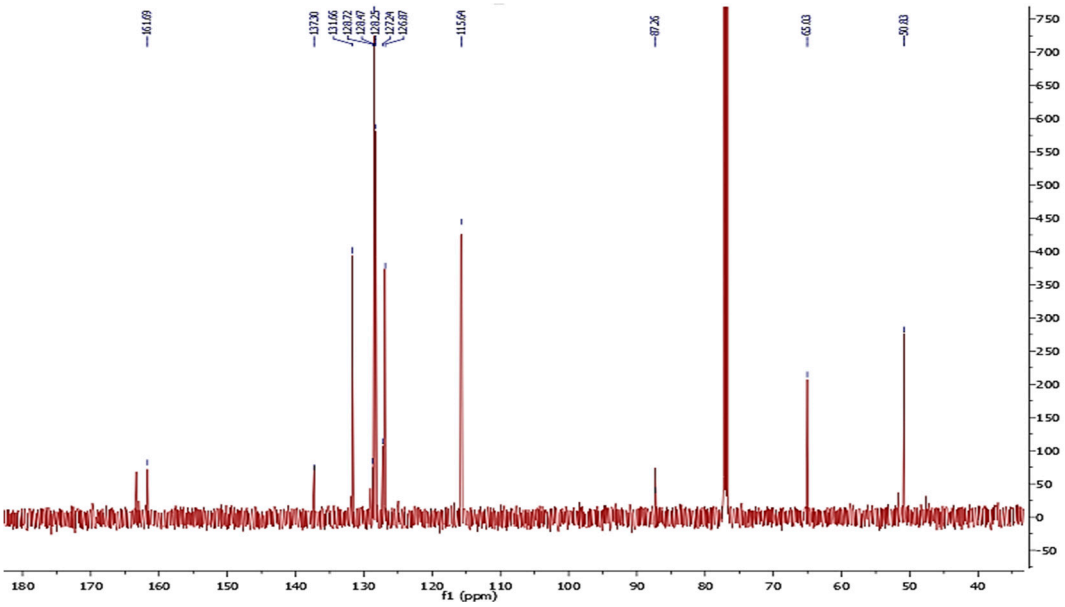
^{13}C NMR (151 MHz, CDCl3) δ 142.59, 132.38, 128.91, 128.70, 128.64, 128.60, 126.97, 125.08, 124.84, 50.87, 40.31, 29.68

5-(chloromethyl)-5-(4-fluorophenyl)-2-phenyl-4,5-dihydrooxazole (7i)



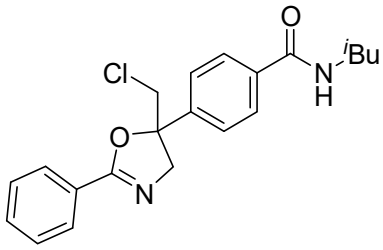


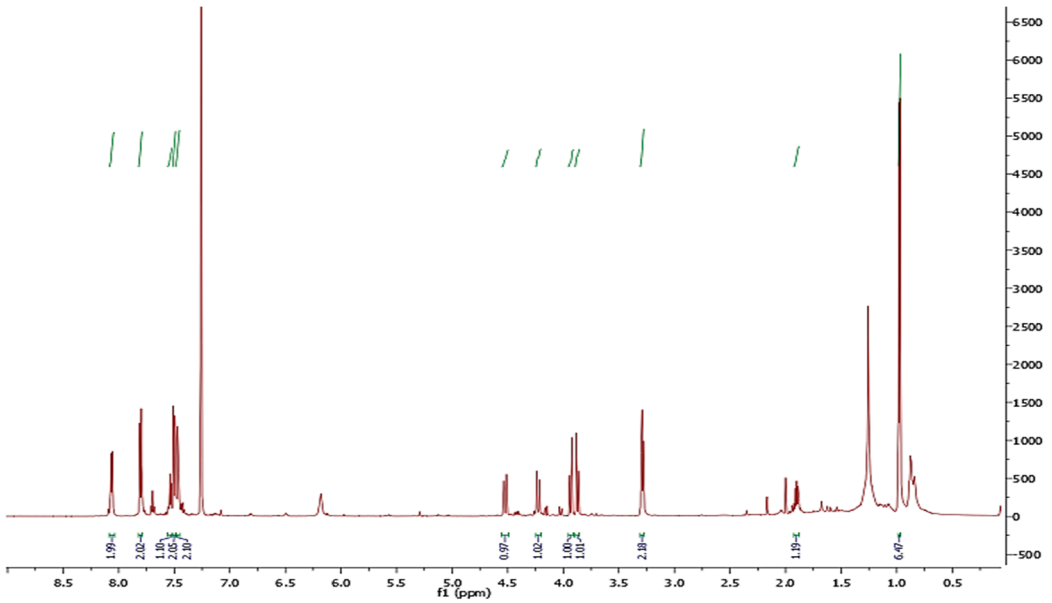
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, J = 7.4 Hz, 2H), 7.52 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.5 Hz, 2H), 7.43 – 7.40 (m, 2H), 7.10 (dd, J = 12.0, 5.2 Hz, 2H), 4.50 (d, J = 14.8 Hz, 1H), 4.22 (d, J = 14.8 Hz, 1H), 3.91 (d, 1H), 3.84 (d, J = 12.0 Hz, 1H)



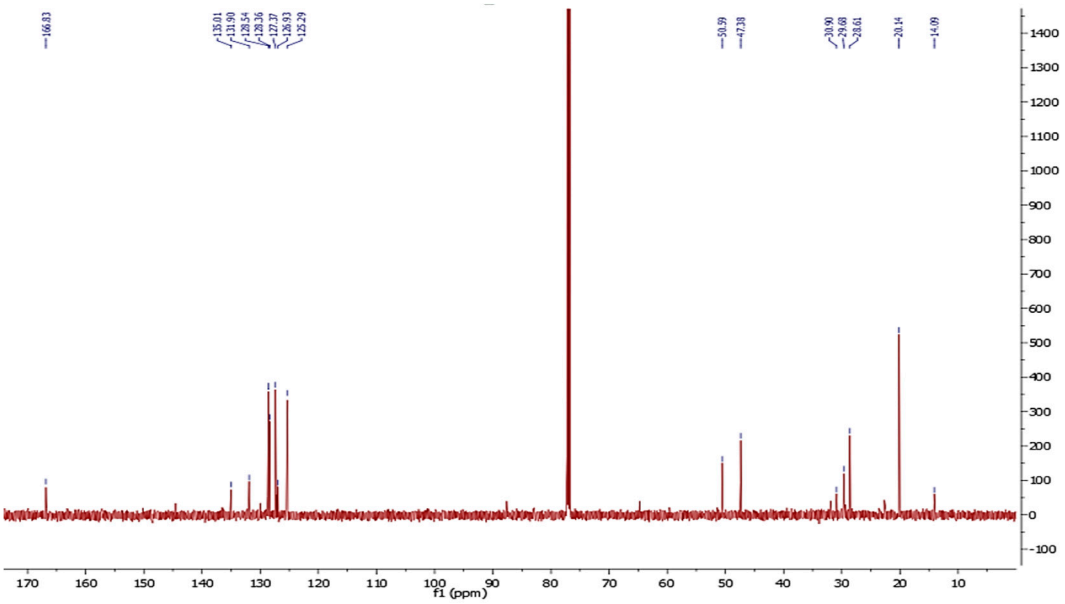
^{13}C NMR (151 MHz, $CDCl_3$) δ 161.69 (d, J = 243.11 Hz), 137.30 (d, J = 3.02 Hz), 131.66, 128.72, 128.47, 128.25, 127.24, 126.87 (d, J = 9.06 Hz), 115.64 (d, J = 22.65 Hz), 87.26, 65.03, 50.83

4-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)-*N*-isobutylbenzamide (7j)



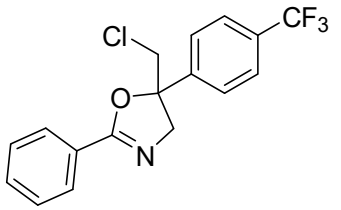


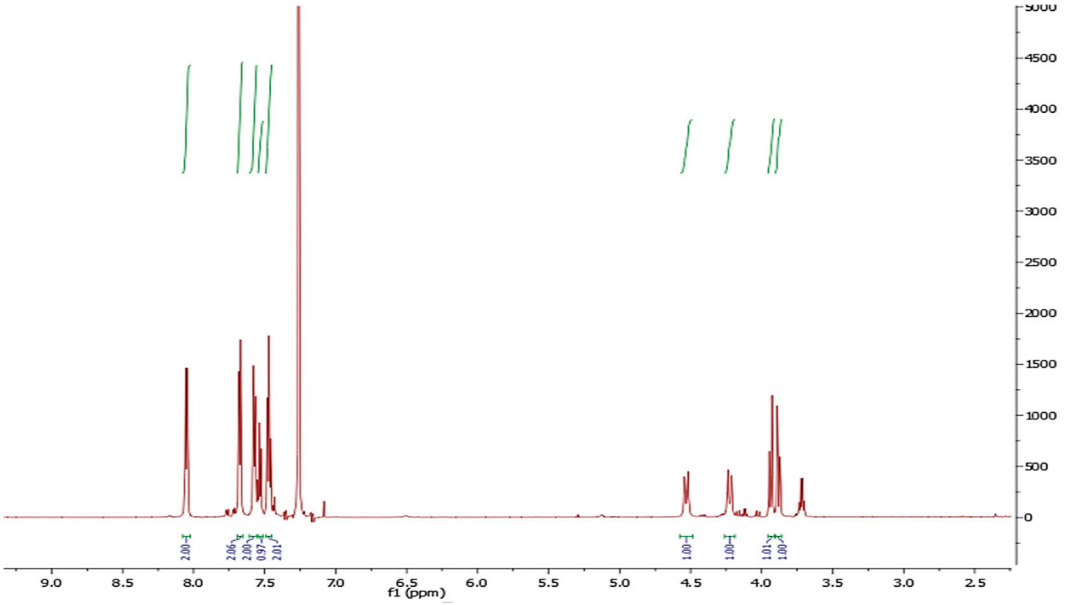
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, J = 7.4 Hz, 2H), 7.80 (d, J = 8.4 Hz, 2H), 7.54 (t, J = 7.4 Hz, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.47 (t, J = 7.6 Hz, 2H), 6.18 (s, J = 20.8 Hz, 1H), 4.52 (d, J = 14.8 Hz, 1H), 4.23 (d, 1H), 3.93 (d, J = 12.0 Hz, 1H), 3.87 (d, J = 12.0 Hz, 1H), 3.29 (t, J = 6.4 Hz, 2H), 1.90 (dt, J = 13.4, 6.7 Hz, 1H), 0.98 (d, J = 6.7 Hz, 6H)



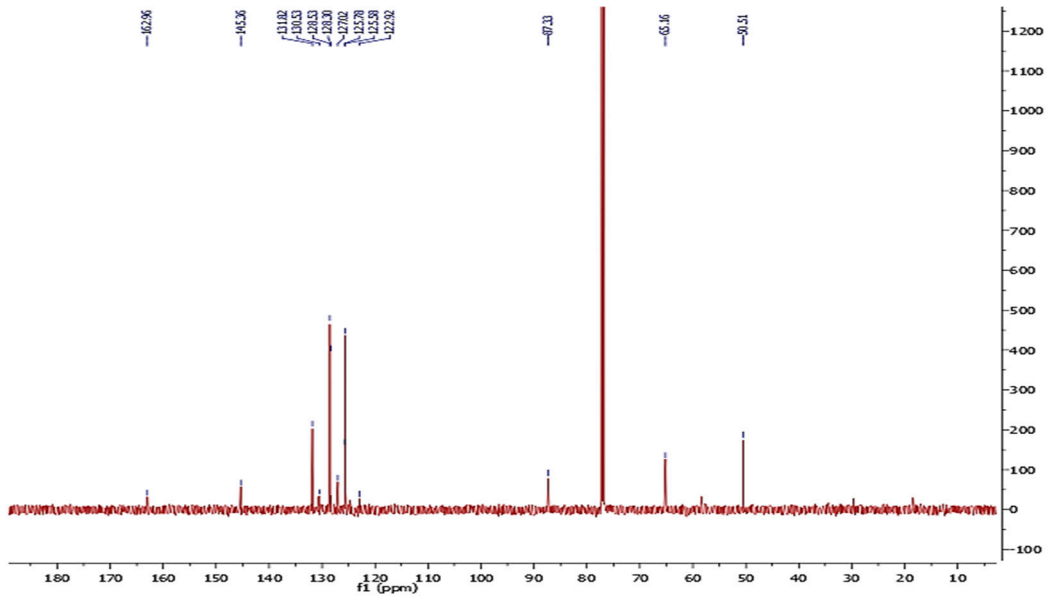
^{13}C NMR (151 MHz, $CDCl_3$) δ 166.83, 135.01, 131.90, 128.54, 128.36, 127.37, 126.93, 125.29, 50.59, 47.38, 30.90, 29.68, 28.61, 20.14, 14.09

5-(chloromethyl)-2-phenyl-5-(4-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (7k)



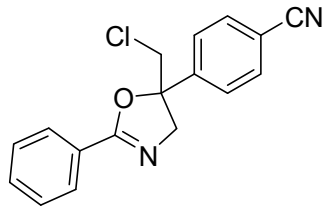


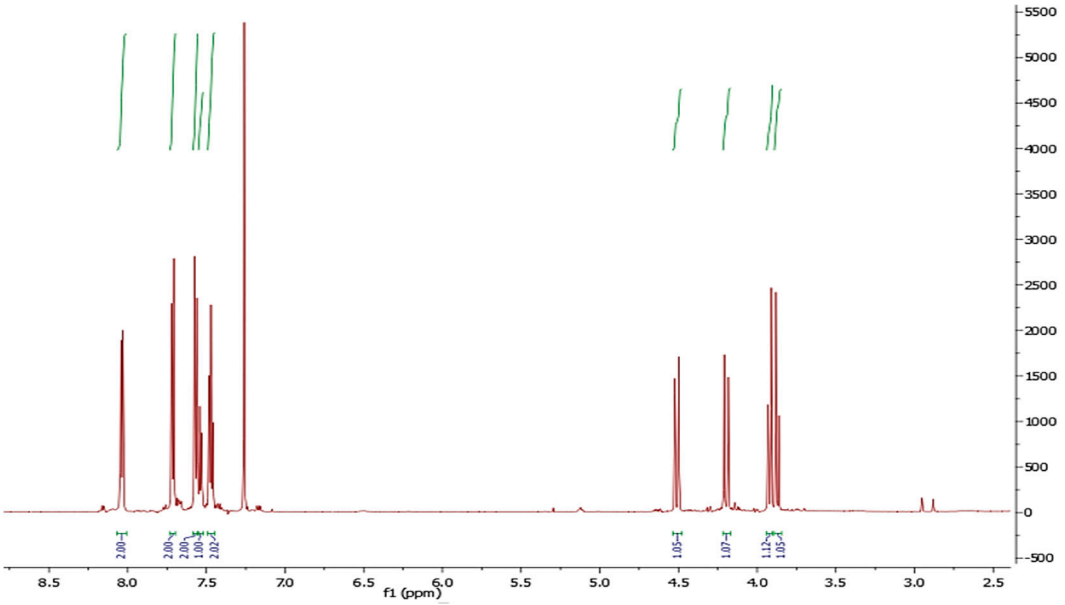
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, J = 7.4 Hz, 2H), 7.68 (d, J = 8.0 Hz, 2H), 7.57 (d, J = 8.1 Hz, 2H), 7.53 (d, J = 7.4 Hz, 1H), 7.47 (t, J = 7.5 Hz, 2H), 4.53 (d, J = 14.6 Hz, 1H), 4.22 (d, J = 14.6 Hz, 1H), 3.94 (d, J = 12.0 Hz, 1H), 3.88 (d, J = 12.0 Hz, 1H)



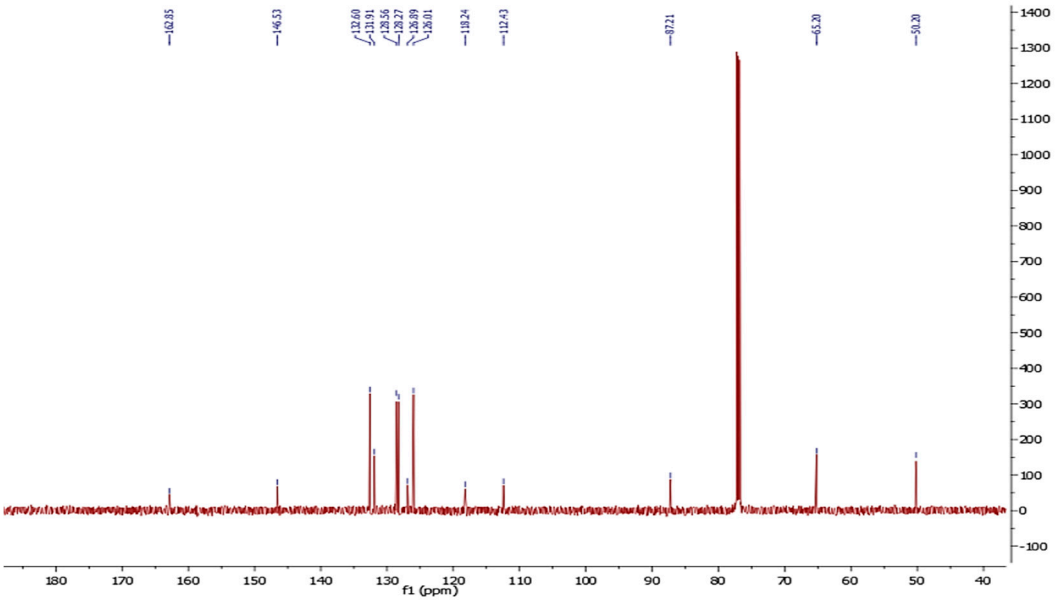
^{13}C NMR (151 MHz, $CDCl_3$) δ 162.96, 145.36, 131.82, 130.53 (q, J = 31.71 Hz), 128.53, 128.30, 127.02, 125.78 (q, J = 3.02 Hz), 125.58, 122.92 (q, J = 271.8 Hz), 87.33, 65.16, 50.51

4-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)benzonitrile (7l)



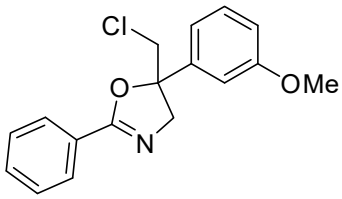


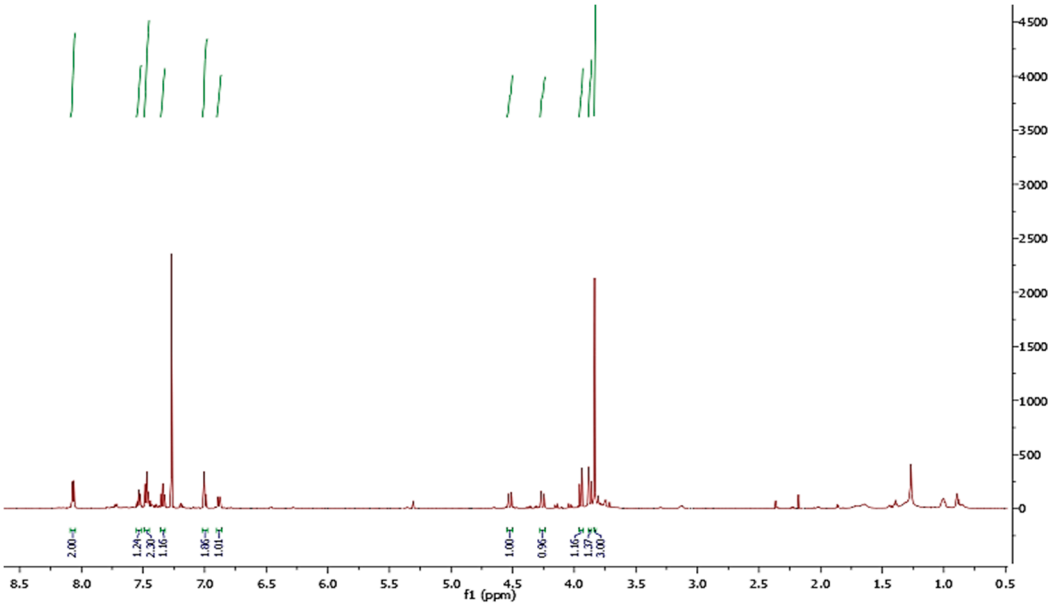
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, J = 7.2 Hz, 2H), 7.71 (d, J = 8.5 Hz, 2H), 7.57 (d, J = 8.5 Hz, 2H), 7.54 (d, J = 7.5 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 4.51 (d, J = 15.0 Hz, 1H), 4.20 (d, J = 15.0 Hz, 1H), 3.92 (d, J = 12.0 Hz, 1H), 3.87 (d, J = 12.0 Hz, 1H)



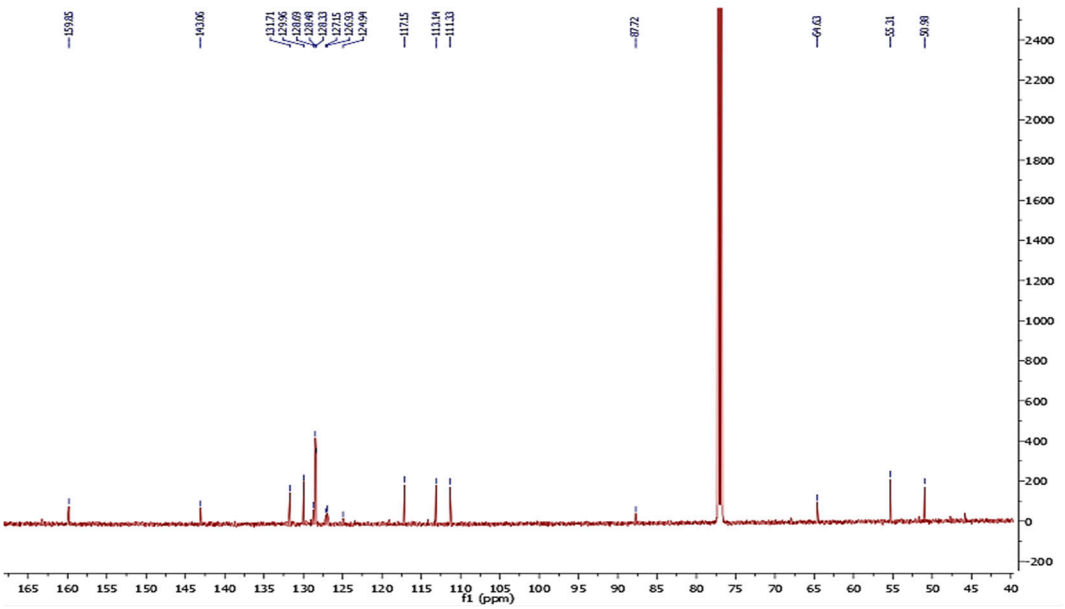
^{13}C NMR (151 MHz, $CDCl_3$) δ 162.85, 146.53, 132.60, 131.91, 128.56, 128.27, 126.89, 126.01, 118.24, 112.43, 87.21, 65.20, 50.20

5-(chloromethyl)-5-(3-methoxyphenyl)-2-phenyl-4,5-dihydrooxazole (7m)



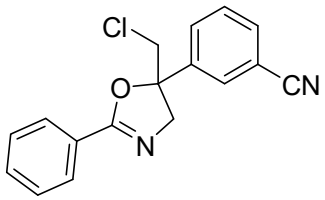


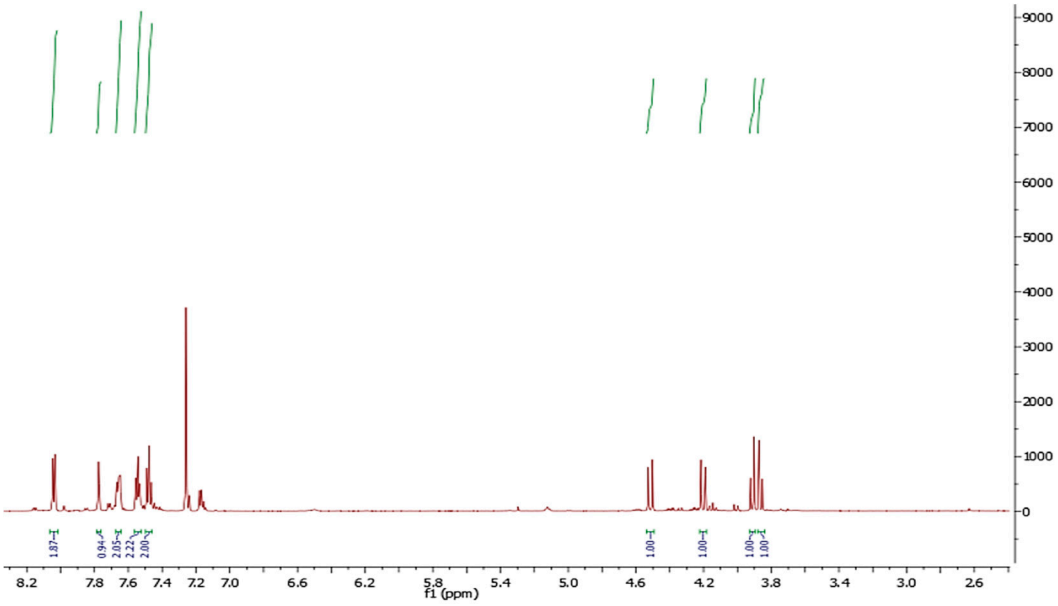
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (d,*J* = 7.2, 2H), 7.53 (dd, *J* = 11.8, 4.3 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.34 (dd, *J* = 9.8, 6.2 Hz, 1H), 7.02 – 6.98 (m, 2H), 6.90 – 6.86 (m, 1H), 4.53 (d, *J* = 15 Hz, 1H), 4.26 (d, *J* = 15 Hz, 1H), 3.95 (d, *J* = 12 Hz, 1H), 3.87 (d, *J* = 12 Hz, 1H), 3.83 (s, 3H)



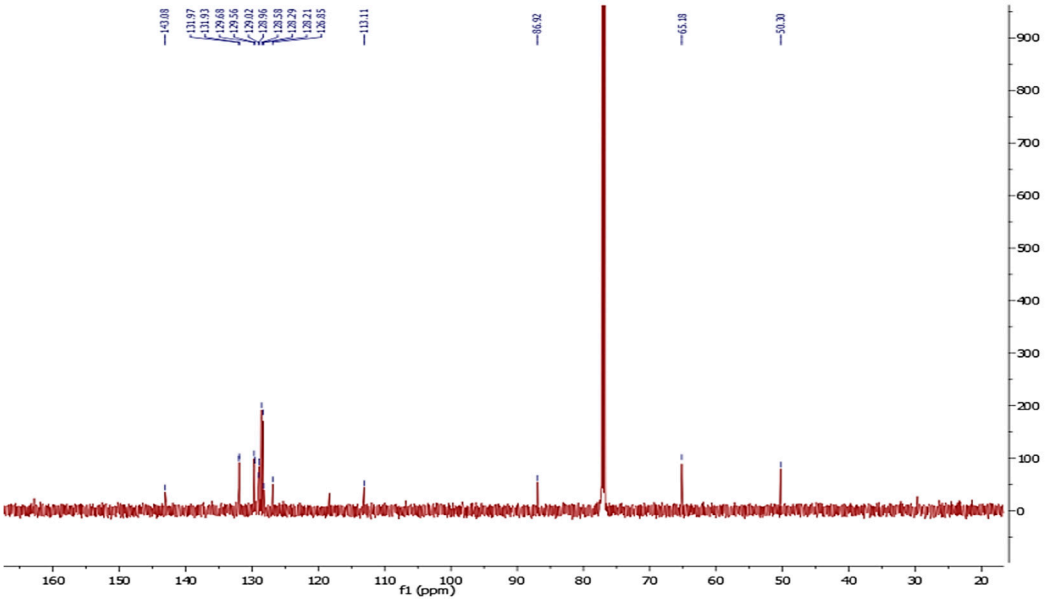
^{13}C NMR (151 MHz, $CDCl_3$) δ 159.85, 143.06, 131.71, 129.96, 128.69, 128.48, 128.33, 127.15, 126.93, 124.94, 117.15, 113.14, 111.33, 87.72, 64.63, 55.31, 50.98

3-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl)benzonitrile (7n)



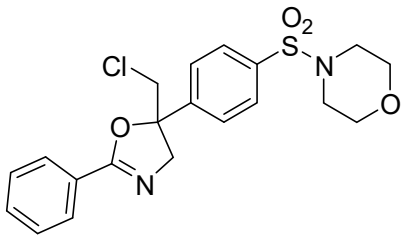


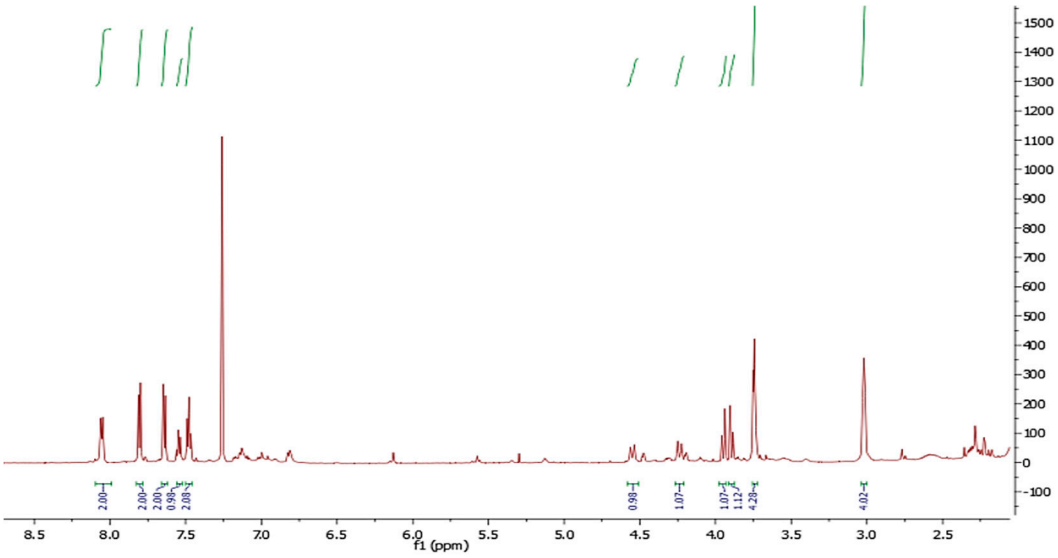
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, J = 7.1 Hz, 2H), 7.78 (s, J = 1.4 Hz, 1H), 7.67 – 7.64 (m, 2H), 7.56 – 7.52 (m, 2H), 7.48 (t, J = 7.6 Hz, 2H), 4.51 (d, J = 15.0 Hz, 1H), 4.20 (d, J = 15.0 Hz, 1H), 3.93 – 3.89 (m, 1H), 3.86 (d, J = 12.0 Hz, 1H)



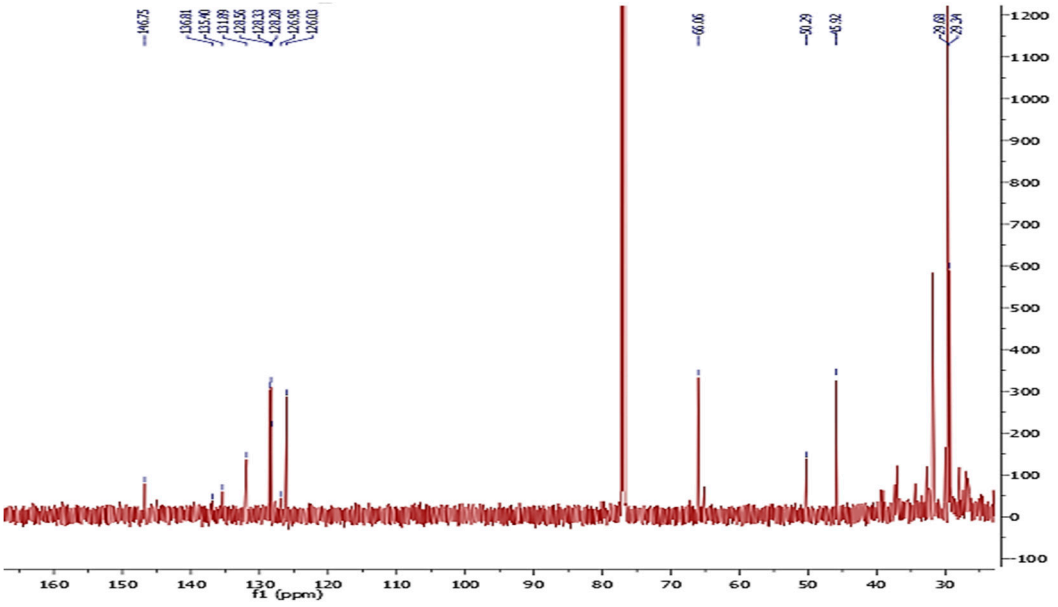
^{13}C NMR (151 MHz, $CDCl_3$) δ 143.08, 131.97, 131.93, 129.68, 129.56, 129.02, 128.96, 128.58, 128.29, 128.21, 126.85, 113.11, 86.92, 65.18, 50.30

4-((4-(5-(chloromethyl)-2-phenyl-4,5-dihydrooxazol-5-yl) phenyl) sulfonyl) morpholine (7o)



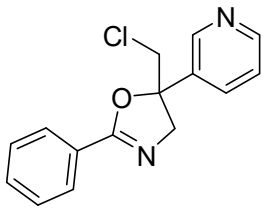


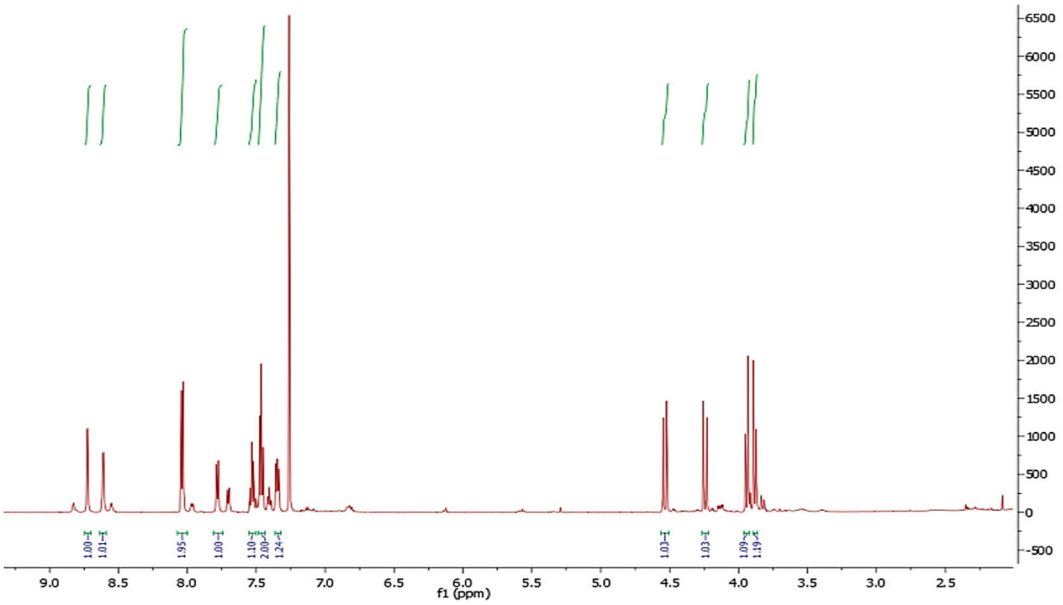
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, J = 7.5 Hz, 2H), 7.81 (d, J = 8.4 Hz, 2H), 7.64 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 7.4 Hz, 1H), 7.48 (t, J = 7.5 Hz, 2H), 4.55 (d, J = 14.9 Hz, 1H), 4.24 (d, J = 14.8 Hz, 1H), 3.95 (d, J = 12.0 Hz, 1H), 3.89 (d, J = 12.0 Hz, 1H), 3.76 – 3.72 (m, 4H), 3.04 – 3.00 (m, 4H)



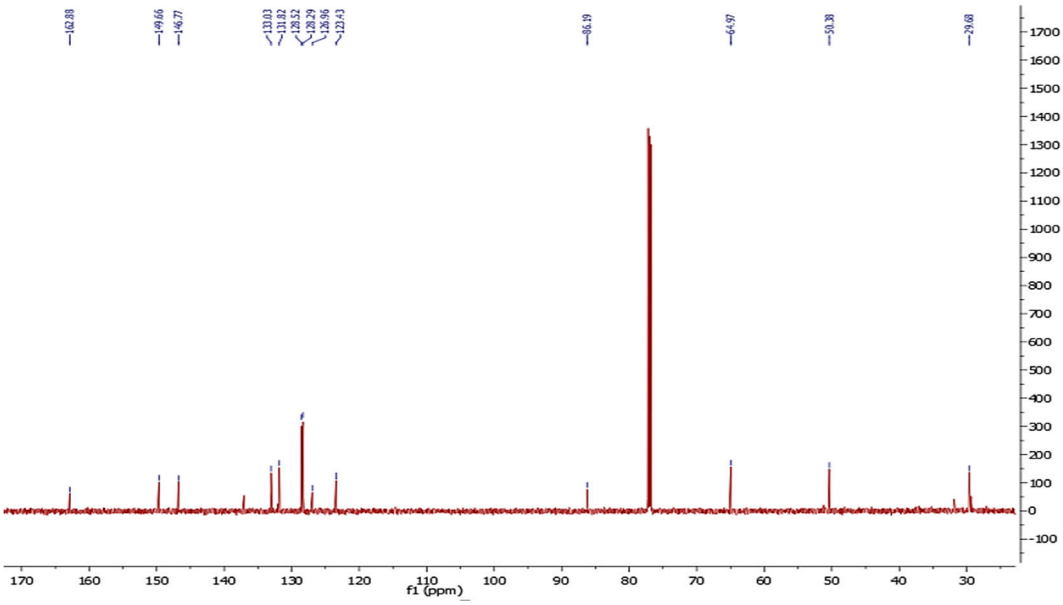
^{13}C NMR (151 MHz, $CDCl_3$) δ 146.75, 136.81, 135.40, 131.89, 128.56, 128.33, 128.28, 126.95, 126.03, 66.06, 50.29, 45.92, 29.68, 29.34

5-(chloromethyl)-2-phenyl-5-(pyridin-3-yl)-4,5-dihydrooxazole (7q)



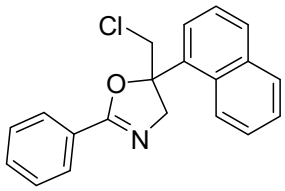


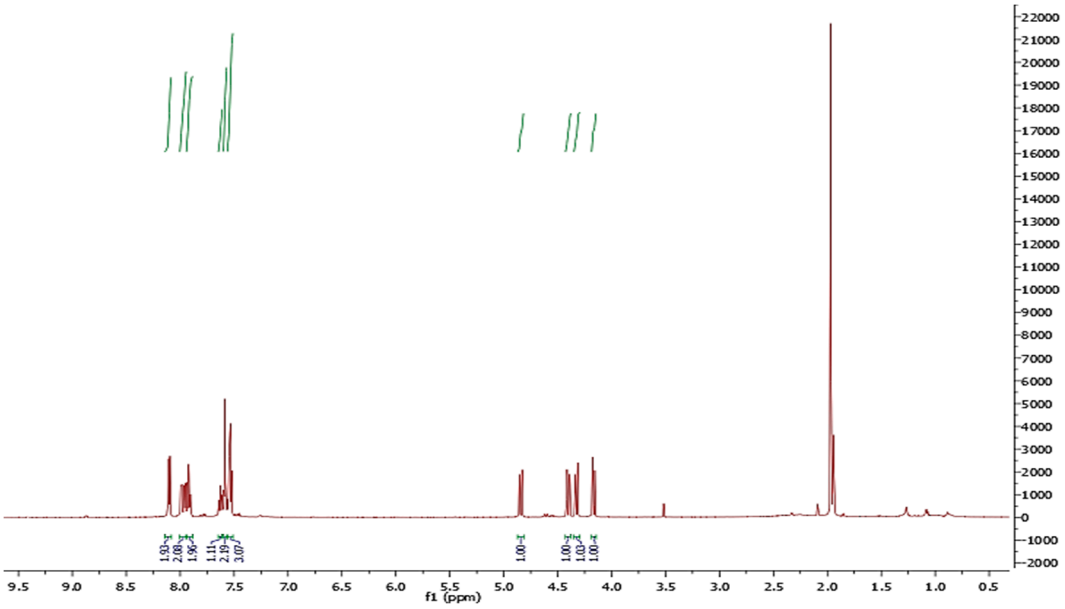
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.73 (d, J = 1.8 Hz, 1H), 8.64 – 8.59 (m, 1H), 8.04 (d, J = 7.2 Hz, 2H), 7.81 – 7.74 (m, 1H), 7.53 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 7.35 (dd, J = 7.9, 4.8 Hz, 1H), 4.53 (d, J = 15.0 Hz, 1H), 4.24 (d, J = 15.0 Hz, 1H), 3.94 (d, J = 11.9 Hz, 1H), 3.88 (d, J = 11.9 Hz, 1H)



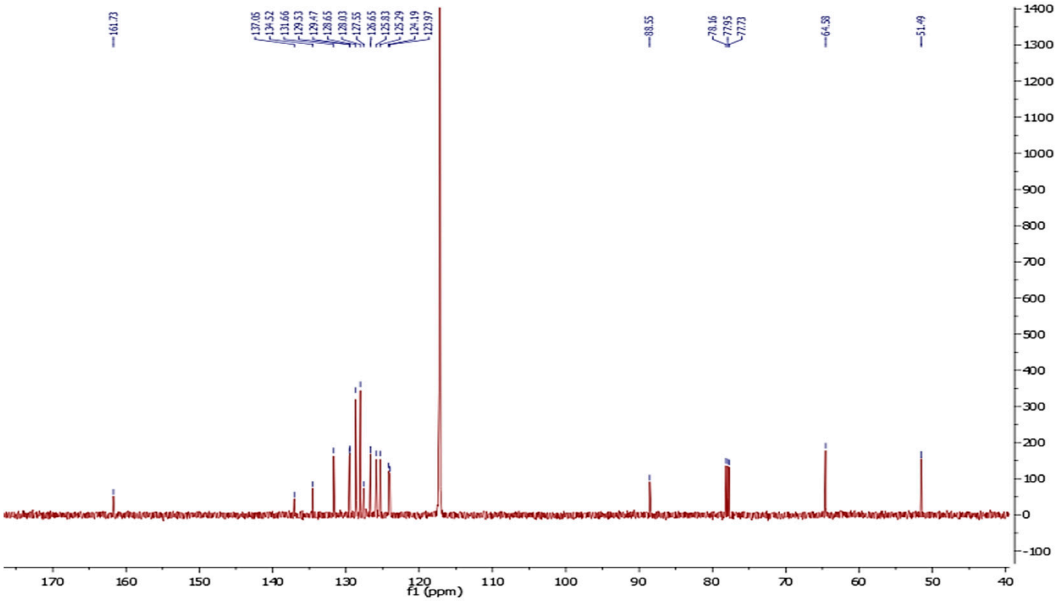
^{13}C NMR (151 MHz, $CDCl_3$) δ 162.88, 149.66, 146.77, 133.03, 131.82, 128.52, 128.29, 126.96, 123.43, 86.19, 64.97, 50.38, 29.68

5-(chloromethyl)-5-(naphthalen-1-yl)-2-phenyl-4,5-dihydrooxazole (7p)



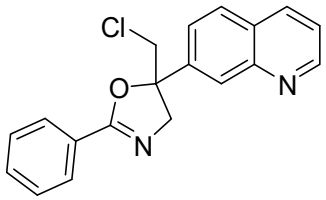


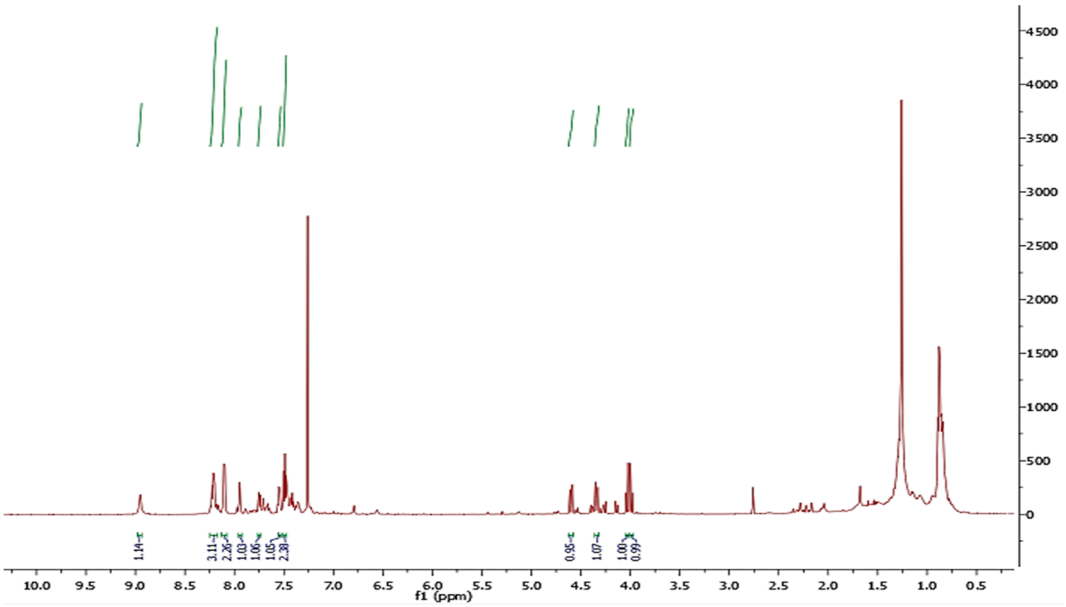
^{1}H NMR (600 MHz, CD_3CN) δ 8.13 – 8.08 (m, 2H), 7.97 (dd, J = 19.4, 7.6 Hz, 2H), 7.92 (t, J = 9.0 Hz, 2H), 7.65 – 7.61 (m, 1H), 7.59 (dd, J = 8.1, 5.0 Hz, 2H), 7.53 (t, J = 7.6 Hz, 3H), 4.84 (d, J = 15.2 Hz, 1H), 4.40 (d, J = 15.1 Hz, 1H), 4.33 (d, J = 12.5 Hz, 1H), 4.17 (d, J = 12.5 Hz, 1H)



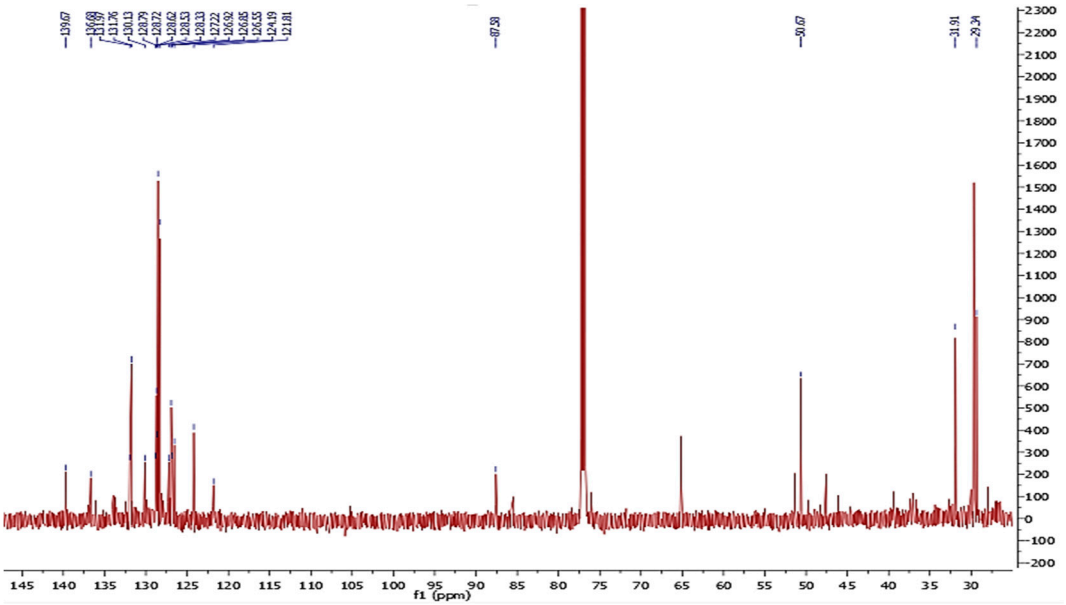
^{13}C NMR (151 MHz, CD_3CN) δ 161.73, 137.05, 134.52, 131.66, 129.53, 129.47, 128.65, 128.03, 127.55, 126.65, 125.83, 125.29, 124.19, 123.97, 88.55, 78.16, 77.95, 77.73, 64.58, 51.49

5-(chloromethyl)-2-phenyl-5-(quinolin-6-yl)-4,5-dihydrooxazole (7r)



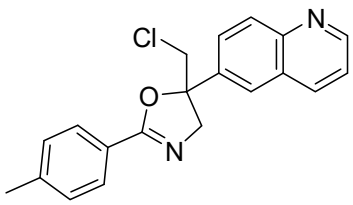


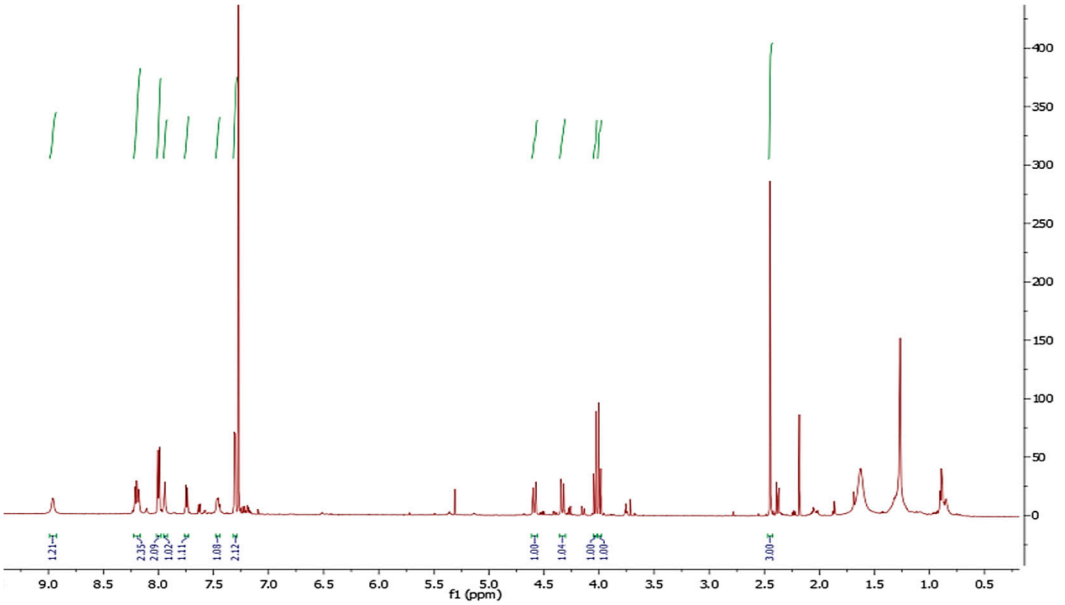
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (s, 1H), 8.23 – 8.19 (m, 2H), 8.10 (d, J = 7.5 Hz, 2H), 7.95 (d, J = 5.6 Hz, 1H), 7.75 (dd, J = 8.8, 1.7 Hz, 1H), 7.54 (d, J = 7.3 Hz, 1H), 7.51 – 7.47 (m, 3H), 4.60 (d, J = 14.9 Hz, 1H), 4.34 (d, 1H), 4.03 (d, J = 12.0 Hz, 1H), 3.99 (d, J = 12.0 Hz, 1H)



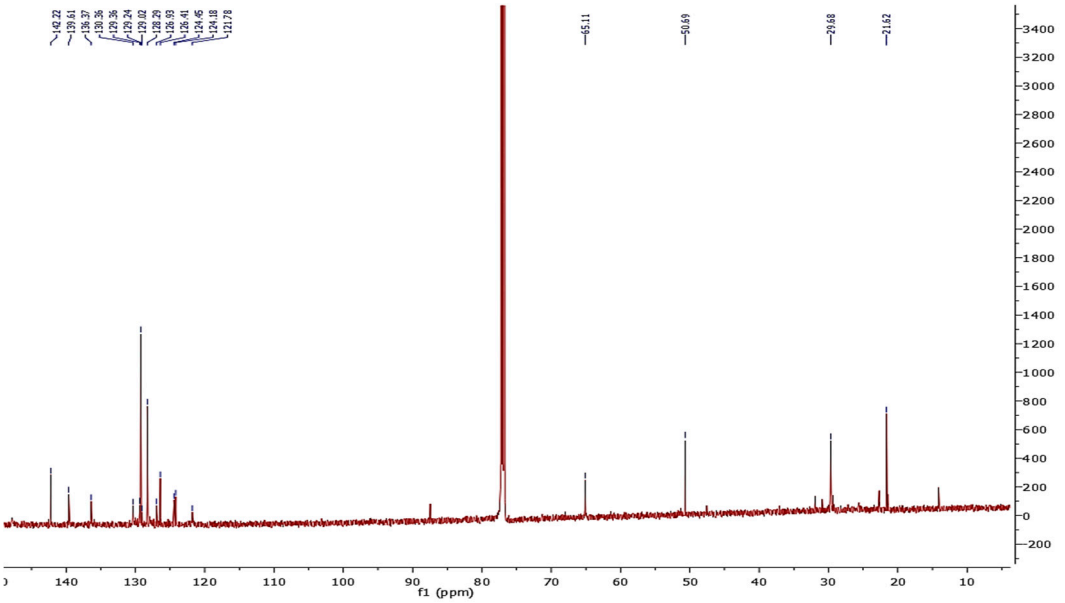
^{13}C NMR (151 MHz, CDCl3) δ 139.67, 136.68, 131.97, 131.76, 130.13, 128.79, 128.72, 128.62, 128.53, 128.33, 127.22, 126.92, 126.85, 126.55, 124.19, 121.81, 87.58, 50.67, 31.91, 29.34

5-(chloromethyl)-5-(quinolin-6-yl)-2-(p-tolyl)-4,5-dihydrooxazole (7s)



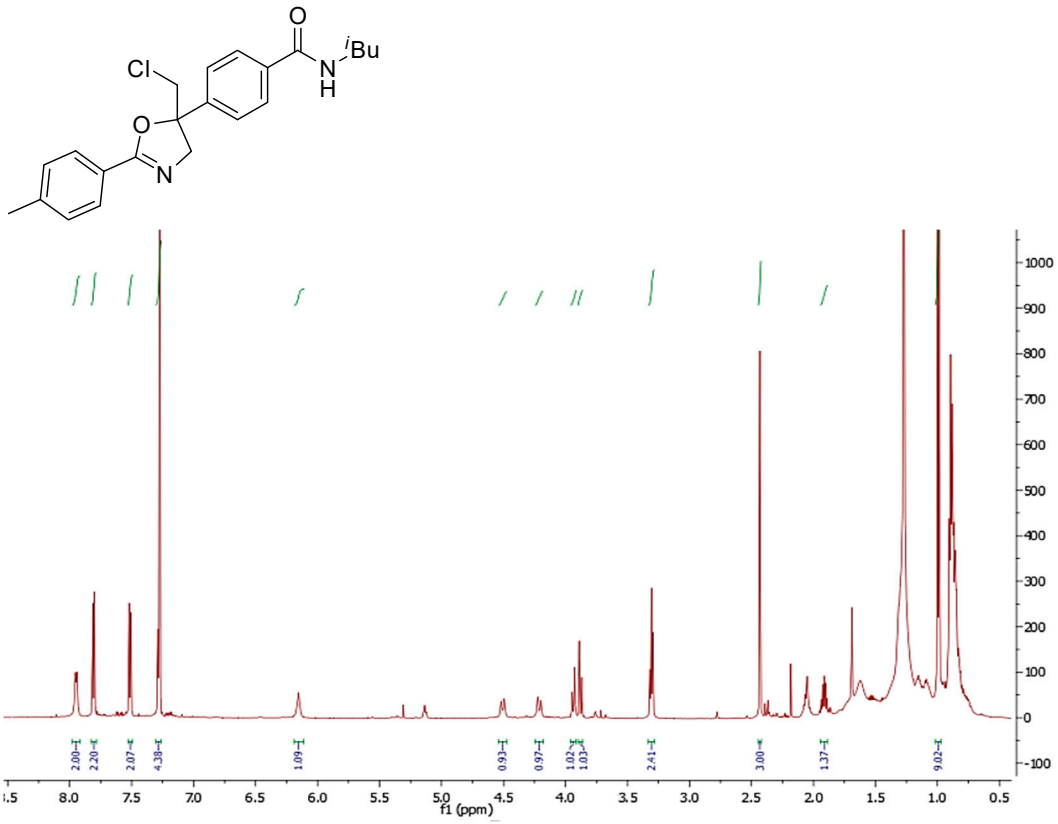


^{1}H NMR (600 MHz, $CDCl_3$) δ 8.96 (s, 1H), 8.22 – 8.16 (m, 2H), 8.00 (d, J = 8.0 Hz, 2H), 7.94 (s, 1H), 7.74 (dd, J = 8.7, 1.9 Hz, 1H), 7.48-7.45 (m, 1H), 7.30 (d, J = 7.9 Hz, 2H), 4.59 (d, J = 14.8 Hz, 1H), 4.33 (d, J = 14.9 Hz, 1H), 4.04 (d, J = 12.0 Hz,1H), 3.99 (d, J = 12.0 Hz, 1H), 2.45 (s, 3H)

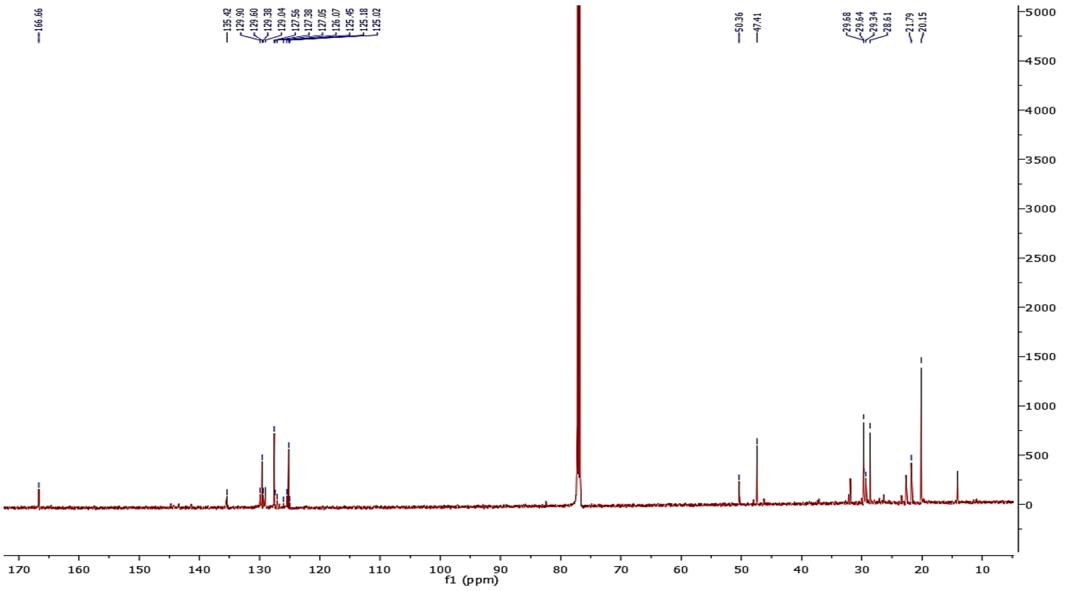


^{13}C NMR (151 MHz, $CDCl_3$) δ 142.22, 139.61, 136.37, 130.36, 129.36, 129.24, 129.02, 128.29, 126.93, 126.41, 124.45, 124.18, 121.78, 65.11, 50.69, 29.68, 21.62

4-(5-(chloromethyl)-2-(p-tolyl)-4,5-dihydrooxazol-5-yl)-N-isobutyl benzamide (7t)



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (d, J = 7.4 Hz, 2H), 7.81 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 8.3 Hz, 2H), 7.28 (d, J = 7.4 Hz, 2H), 6.15 (s, 1H), 4.51 (d, J = 14.7 Hz, 1H), 4.21 (d, J = 15.2 Hz, 1H), 3.94 (d, J = 12.0 Hz, 1H), 3.88 (d, J = 11.9 Hz, 1H), 3.31 (t, J = 6.4 Hz, 2H), 2.43 (s, 3H), 1.91 (dt, J = 13.5, 6.7 Hz, 1H), 0.99 (d, J = 6.7 Hz, 9H)



^{13}C NMR (151 MHz, $CDCl_3$) δ 166.66, 135.42, 129.90, 129.60, 129.38, 129.04, 127.56, 127.38, 127.05, 126.07, 125.45, 125.18, 125.02, 50.36, 47.41, 29.68, 29.64, 29.34, 28.61, 21.79, 20.15