BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Azidophosphonium salt-directed chemoselective synthesis of (*E*)/(*Z*)-cinnamyl-1*H*-triazoles and regiospecific access to bromomethylcoumarins from Morita–Baylis–Hillman adducts

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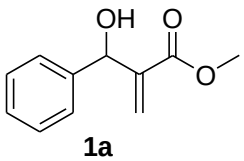
Compound characterization data and NMR spectra

Table of Contents

Structure of the Morita–Baylis–Hillman Adducts 1a–o

Morita–Baylis–Hillman adducts 1a–l utilised for the analysis



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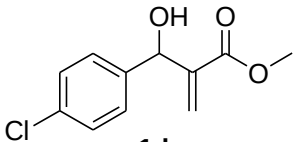

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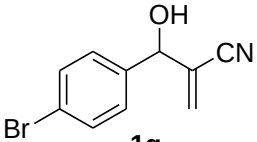

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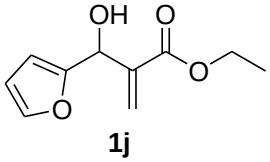

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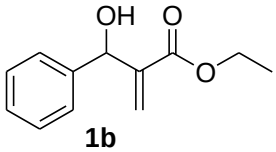

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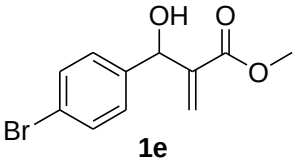

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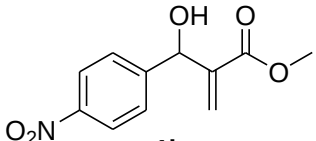

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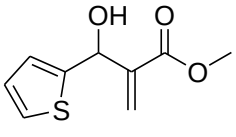

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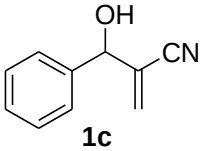

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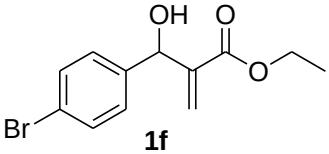

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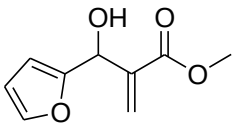

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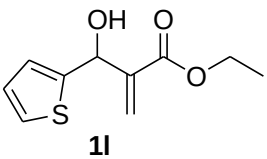

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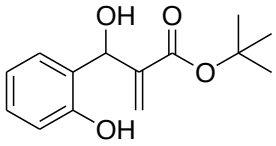
Morita–Baylis–Hillman adducts 1m–o utilised for the analysis



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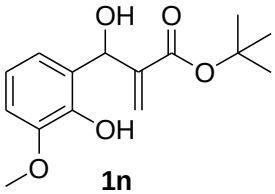

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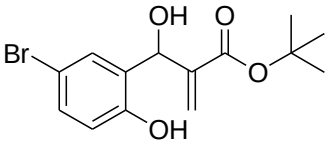

1o

Copies of ^{1}H NMR and ^{13}C NMR spectra for compounds 3a–q

Proton NMR spectrum of (*E*)-methyl 2-((4-hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylate (3a)

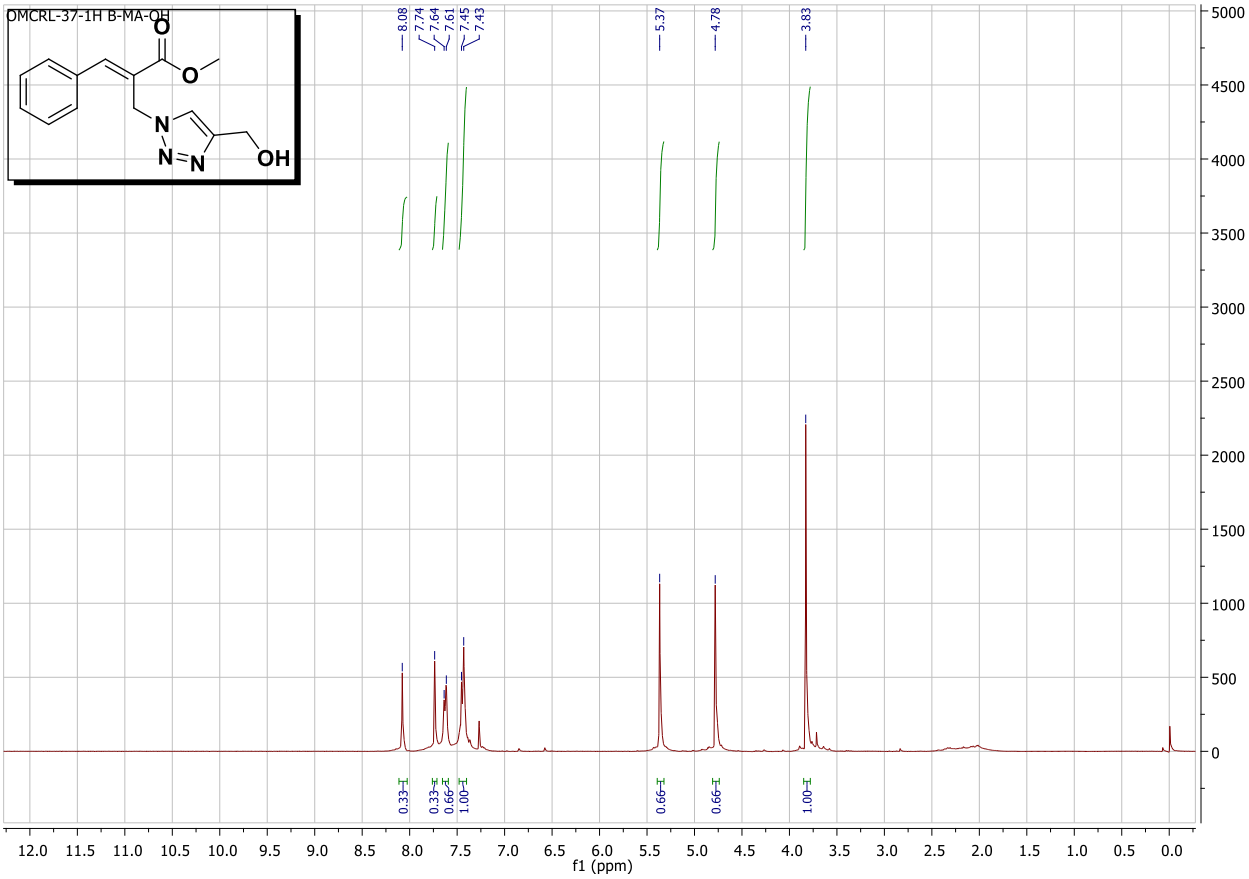

Figure S1 ^{1}H NMR spectrum of (*E*)-methyl 2-((4-hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylate (**3a**)

Carbon NMR spectrum of (*E*)-methyl 2-((4-hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylate (3a)

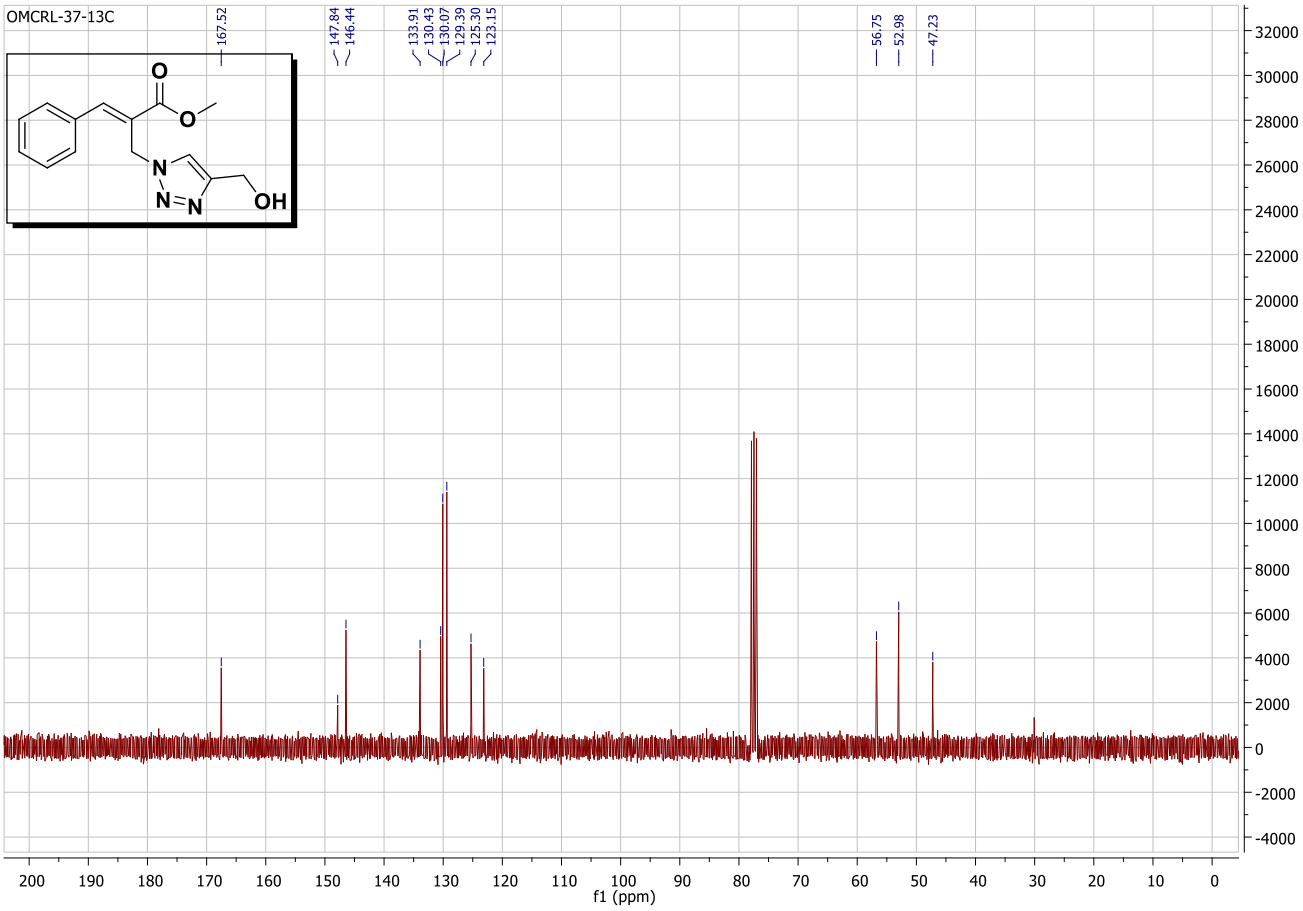

Figure S2 ^{13}C NMR spectrum of (*E*)-methyl 2-((4-hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylate (**3a**)

Proton NMR spectrum of (*E*)-methyl 3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3b)

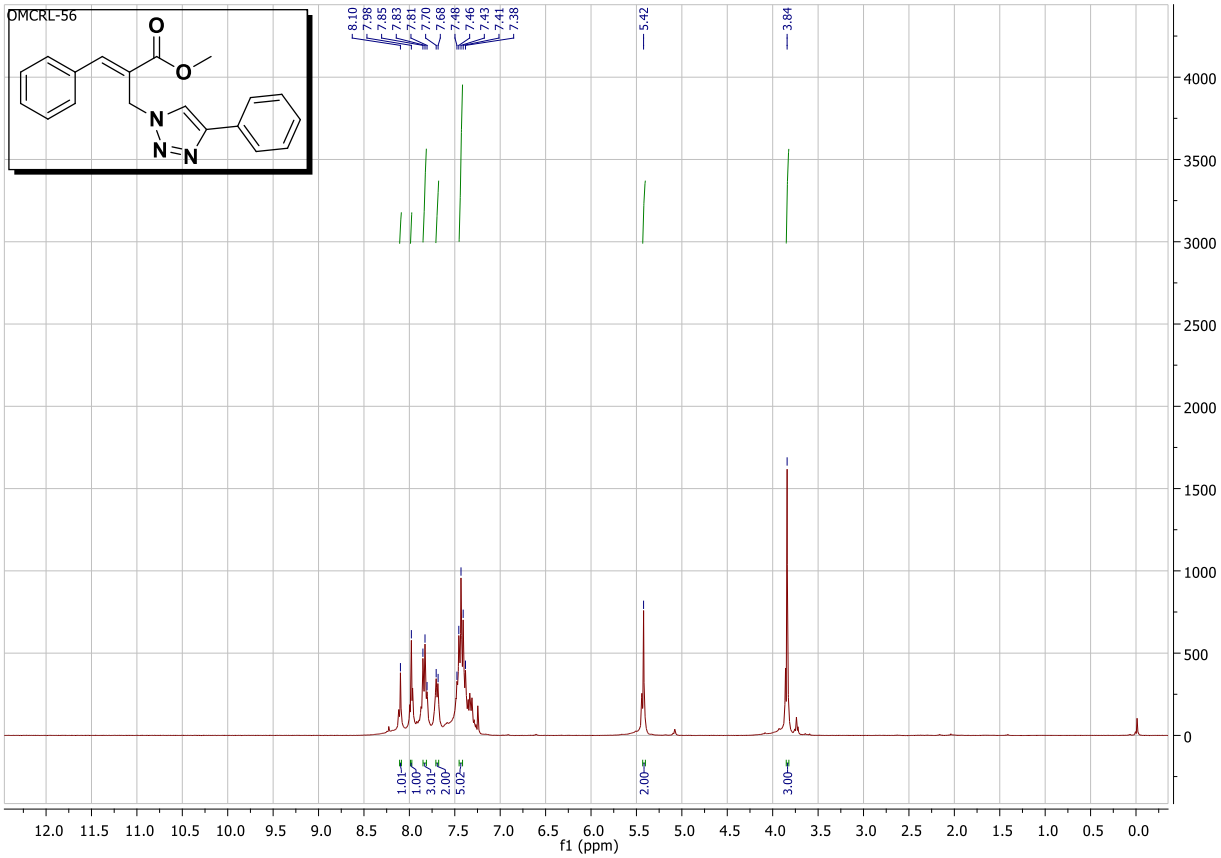

Figure S3 ^{1}H NMR spectrum of (*E*)-methyl 3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3b**)

Carbon NMR spectrum of (*E*)-methyl 3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3b)

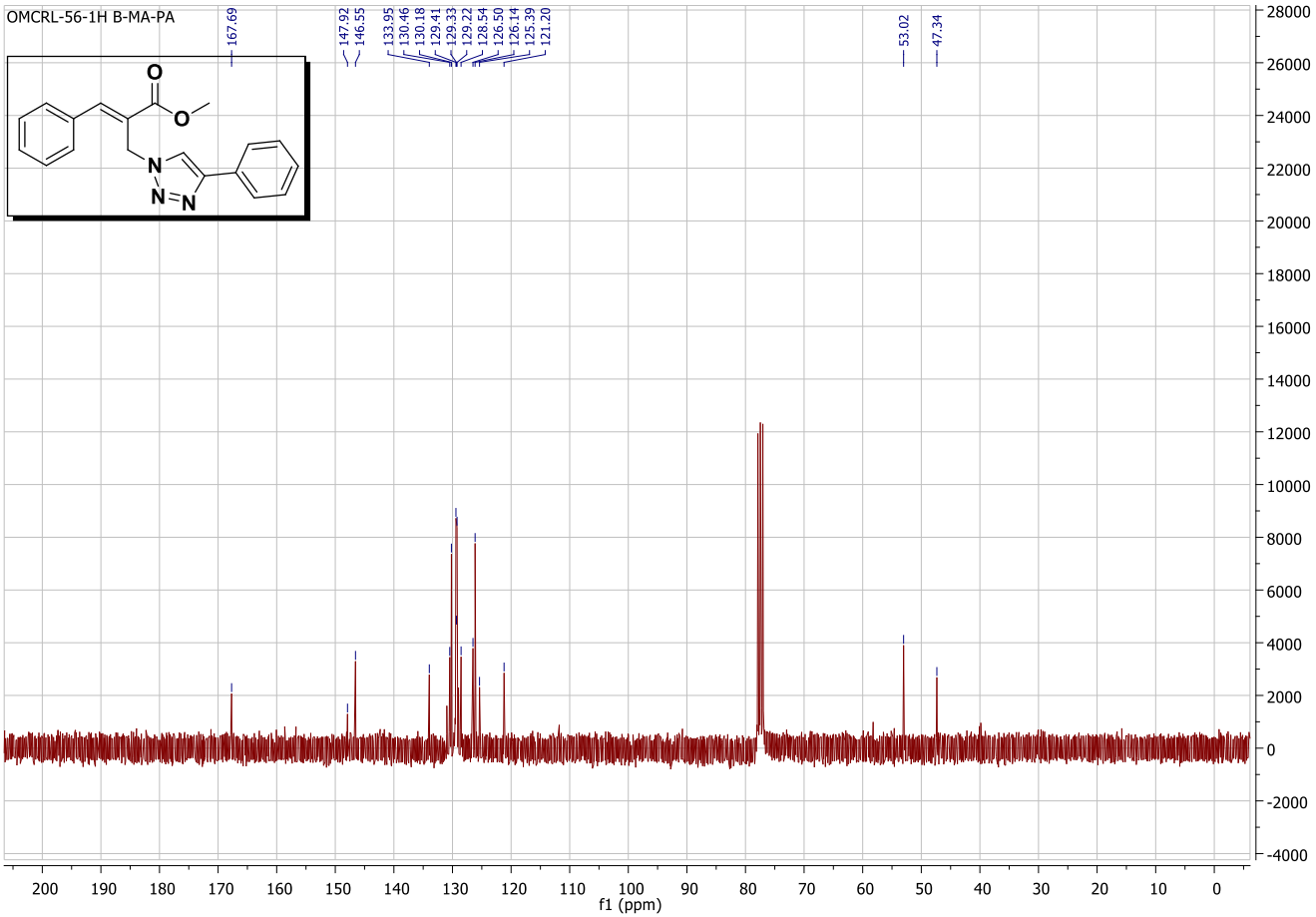

Figure S4 ^{13}C NMR spectrum of (*E*)-methyl 3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3b**)

Proton NMR spectrum of (*E*)-ethyl 2-((4-hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylate (3c)

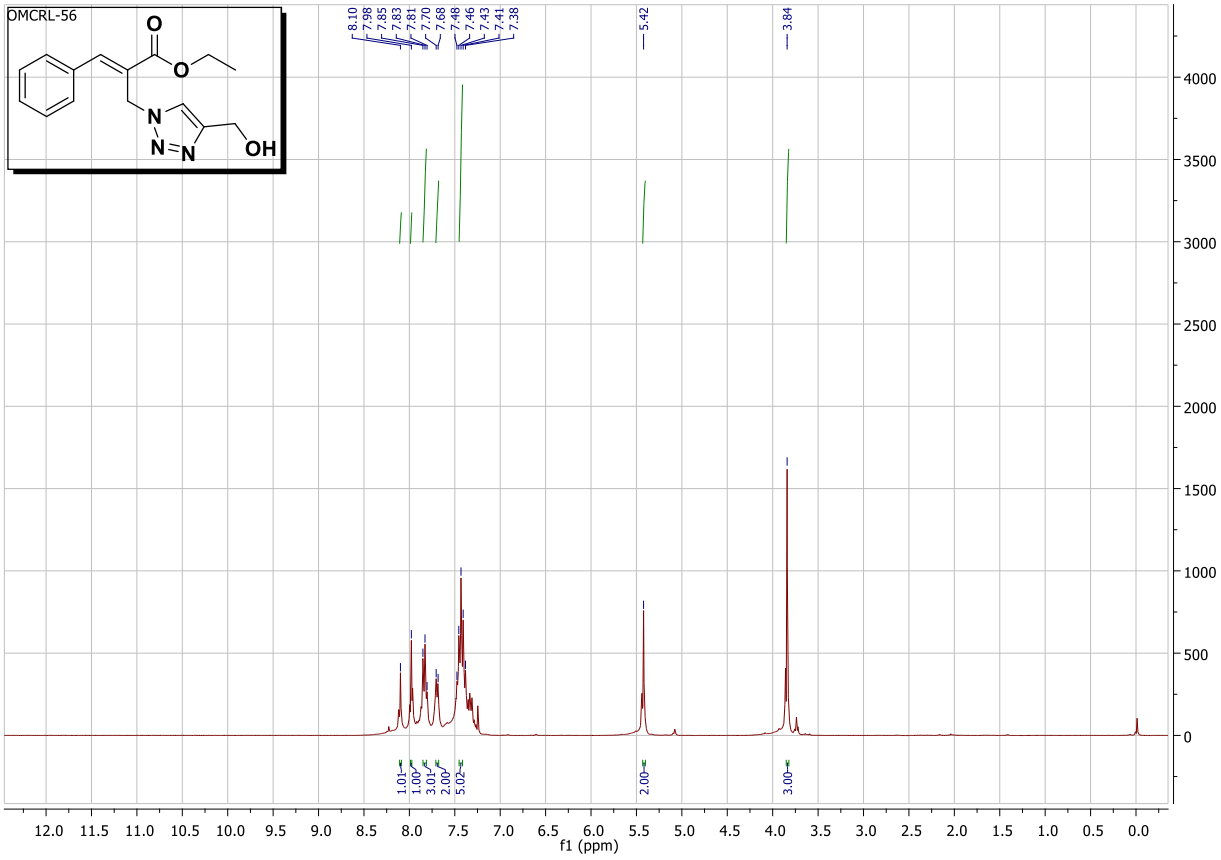

Figure S5 ^{1}H NMR spectrum of (*E*)-ethyl 2-((4-hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylate (**3c**)

Carbon NMR spectrum of (*E*)-ethyl 2-((4-hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylate (3c)

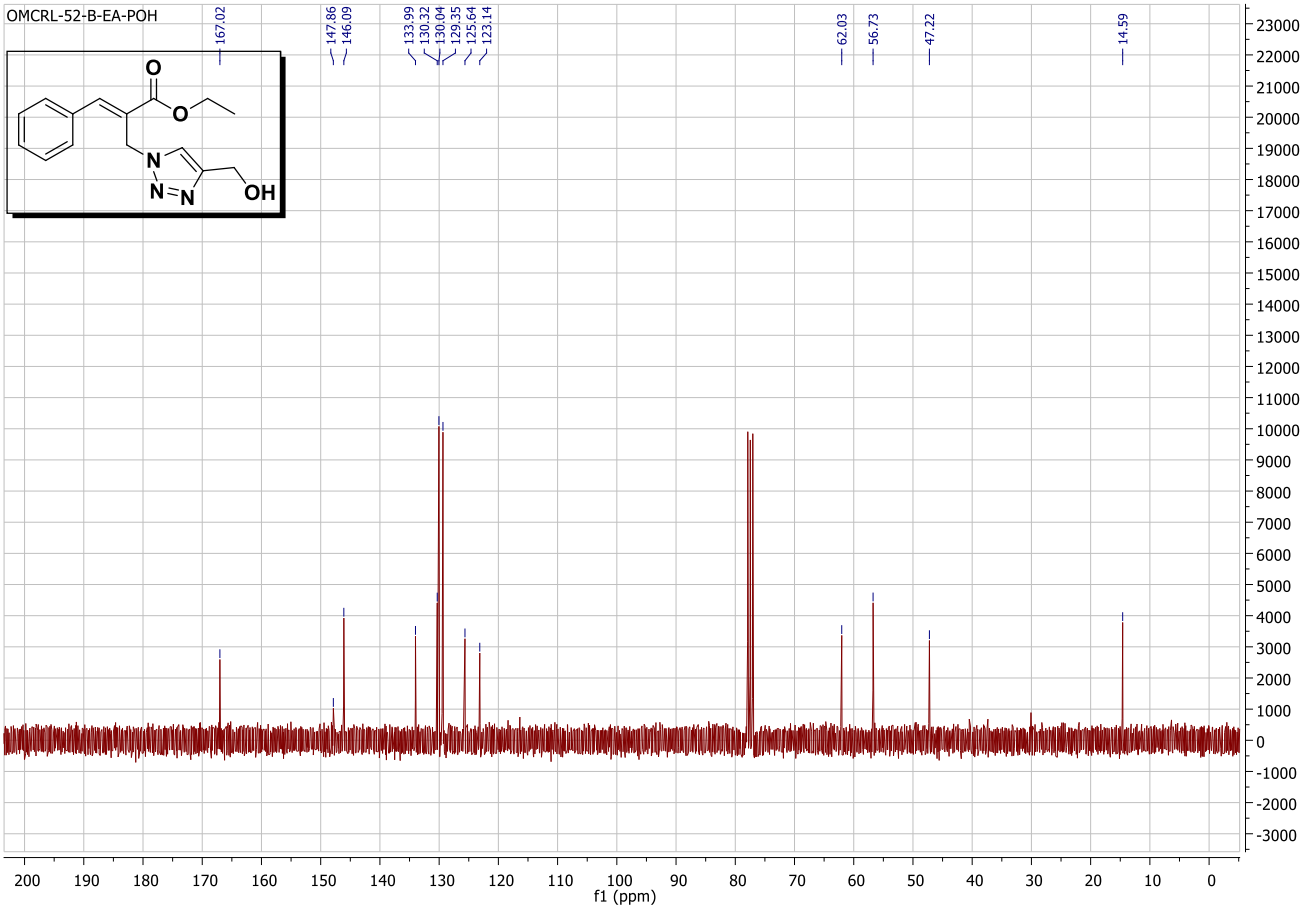

Figure S6 ^{13}C NMR spectrum of (*E*)-ethyl 2-((4-hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylate (**3c**)

Proton NMR spectrum of (*E*)-ethyl 3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3d)

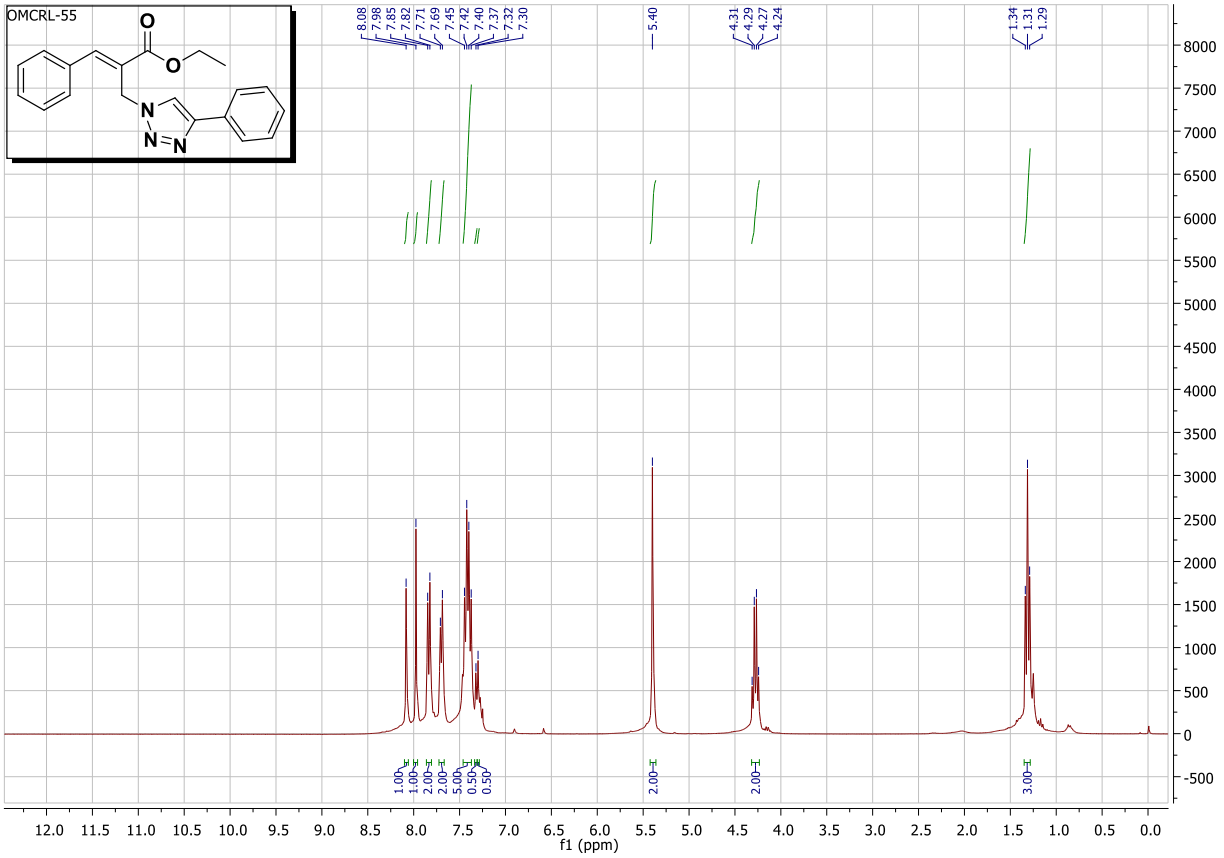

Figure S7 ^{1}H NMR spectrum of (*E*)-ethyl 3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3d**)

Carbon NMR spectrum of (*E*)-ethyl 3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3d)

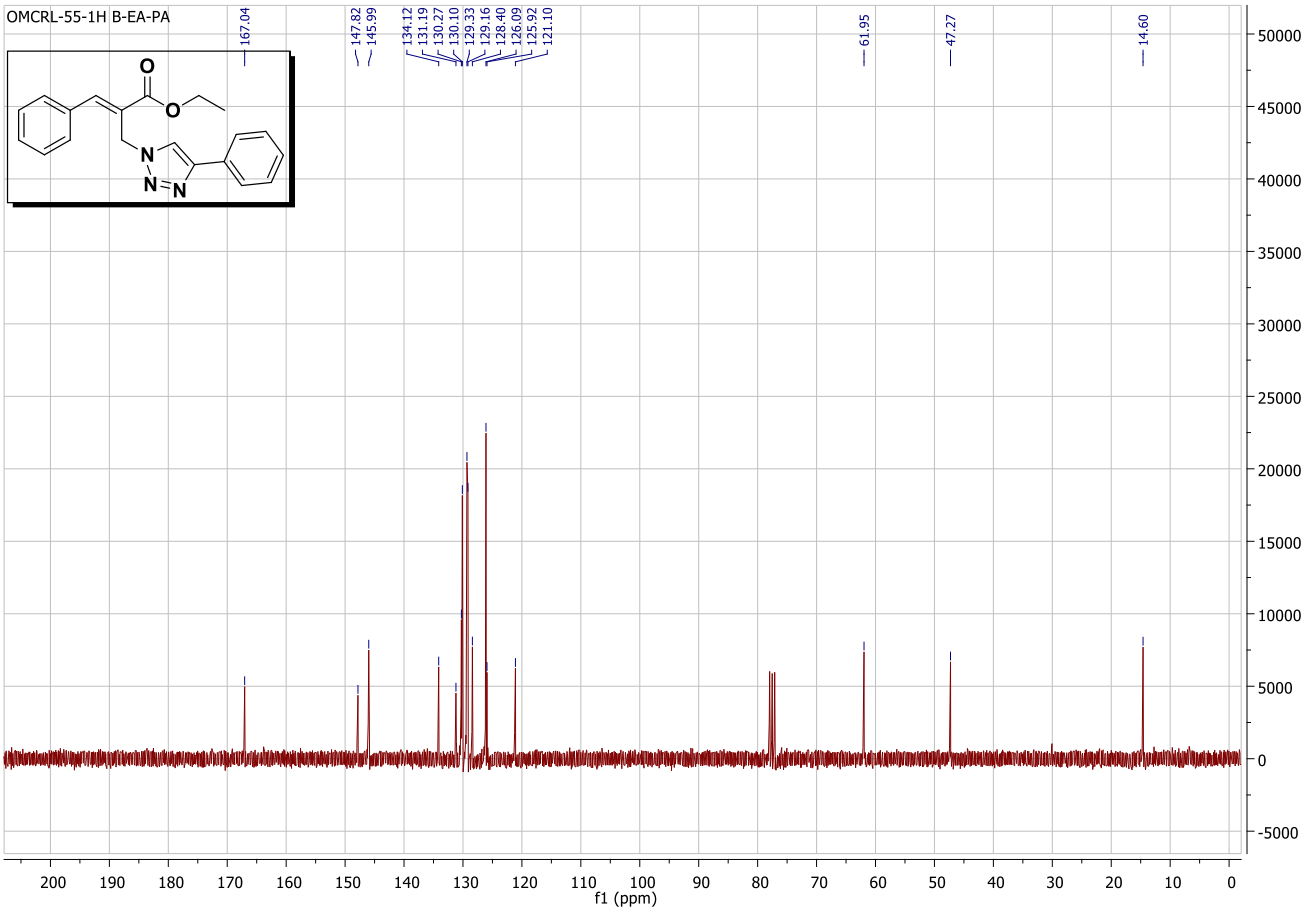

Figure S8 ^{13}C NMR spectrum of (*E*)-ethyl 3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3d**)

Proton NMR spectrum of (*Z*)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylonitrile (3e)

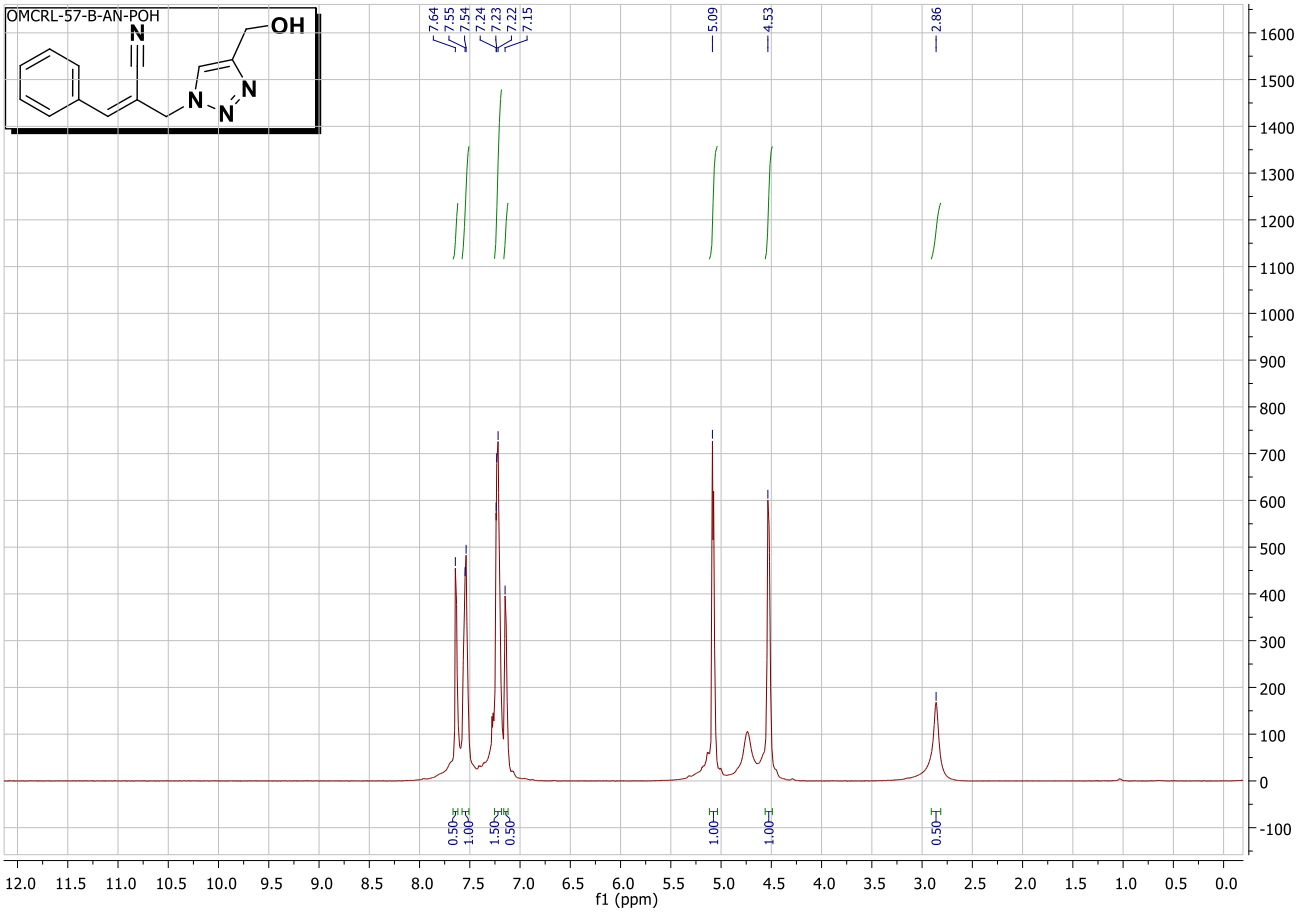

Figure S9 ^{1}H NMR spectrum of (*Z*)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylonitrile (**3e**)

Carbon NMR spectrum of (*Z*)-2-((4-(hydroxymethyl)-1H-1,2,3-triazol-1-yl)methyl)-3-phenylacrylonitrile (3e)

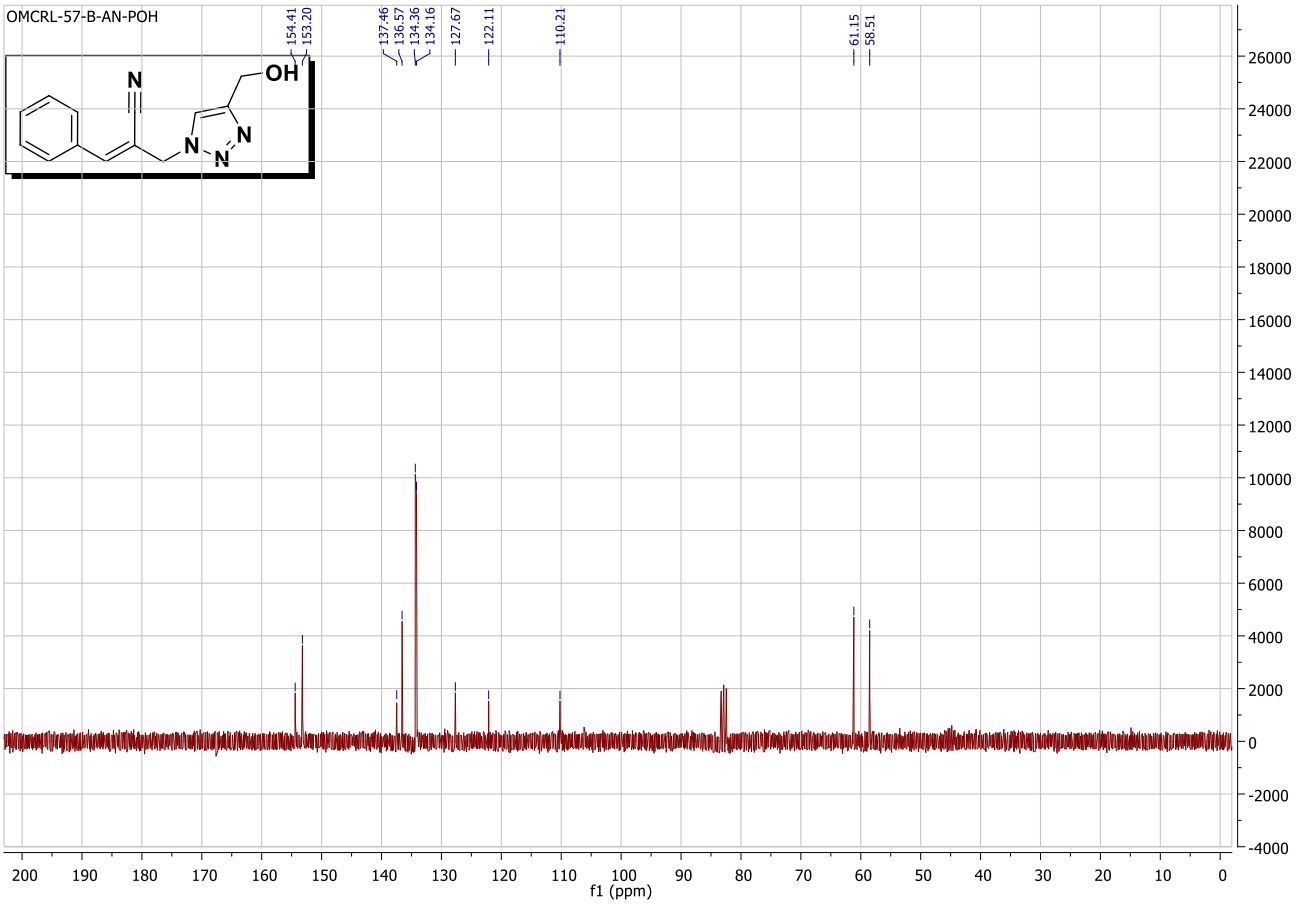

Figure S10 ^{13}C NMR spectrum of (*Z*)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylonitrile (**3e**)

Proton NMR spectrum of (*Z*)-3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylonitrile (3f)

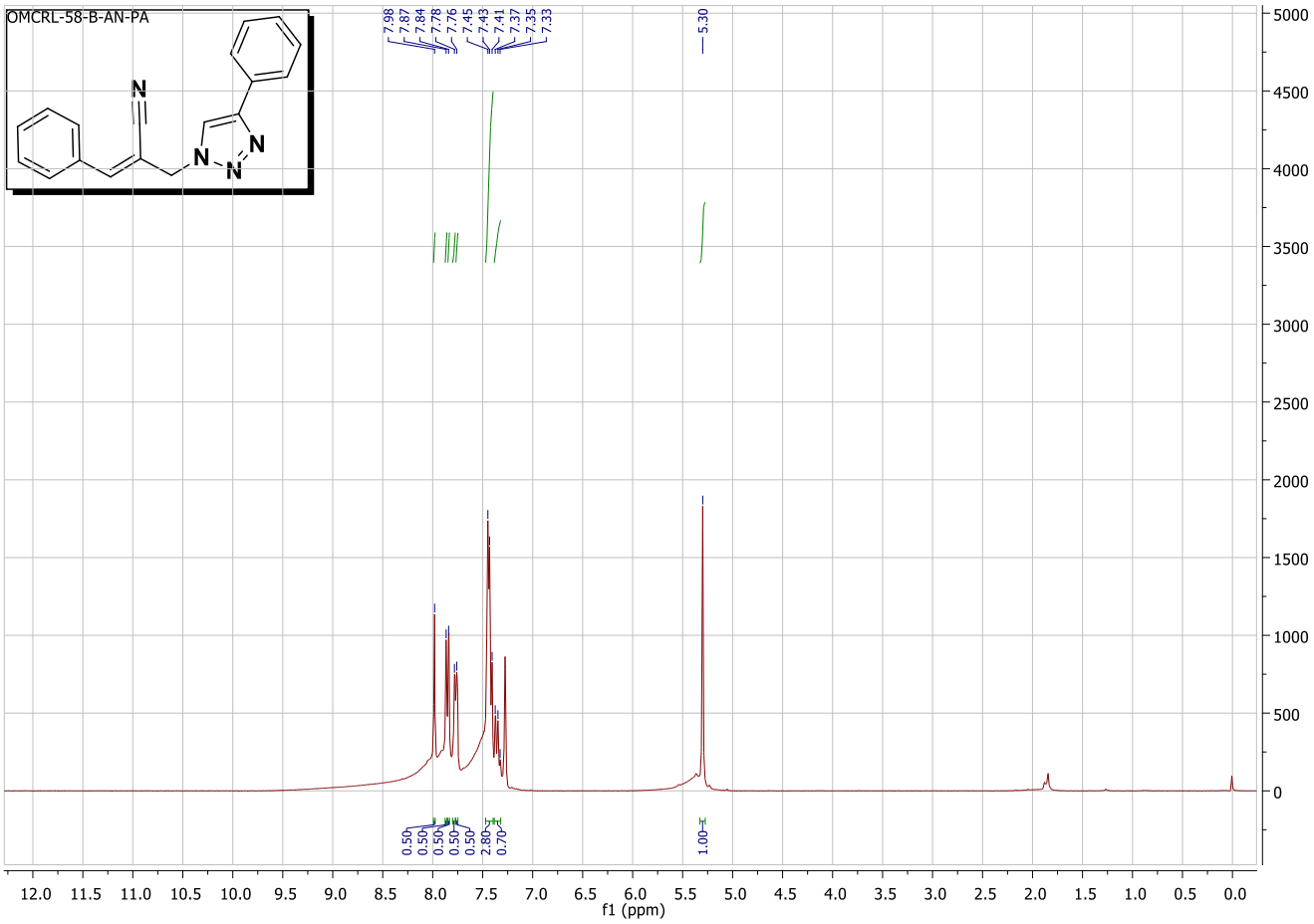

Figure S11 ^{1}H NMR spectrum of (*Z*)-3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylonitrile (**3f**)

Carbon NMR spectrum of (*Z*)-3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylonitrile (3f)

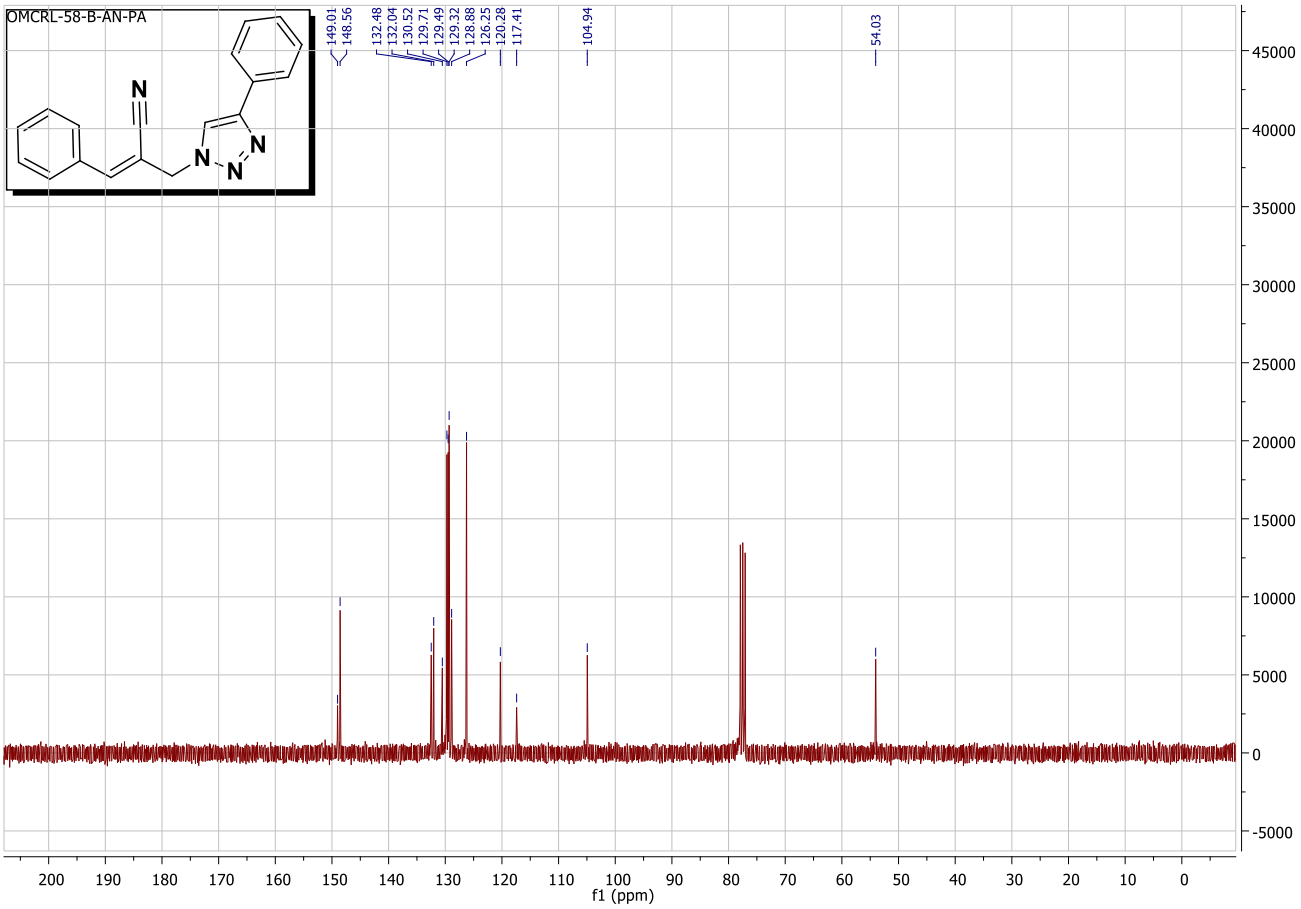

Figure S12 ^{13}C NMR spectrum of (*Z*)-3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylonitrile (**3f**)

Proton NMR spectrum of (*E*)-methyl 3-(4-chlorophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3g)

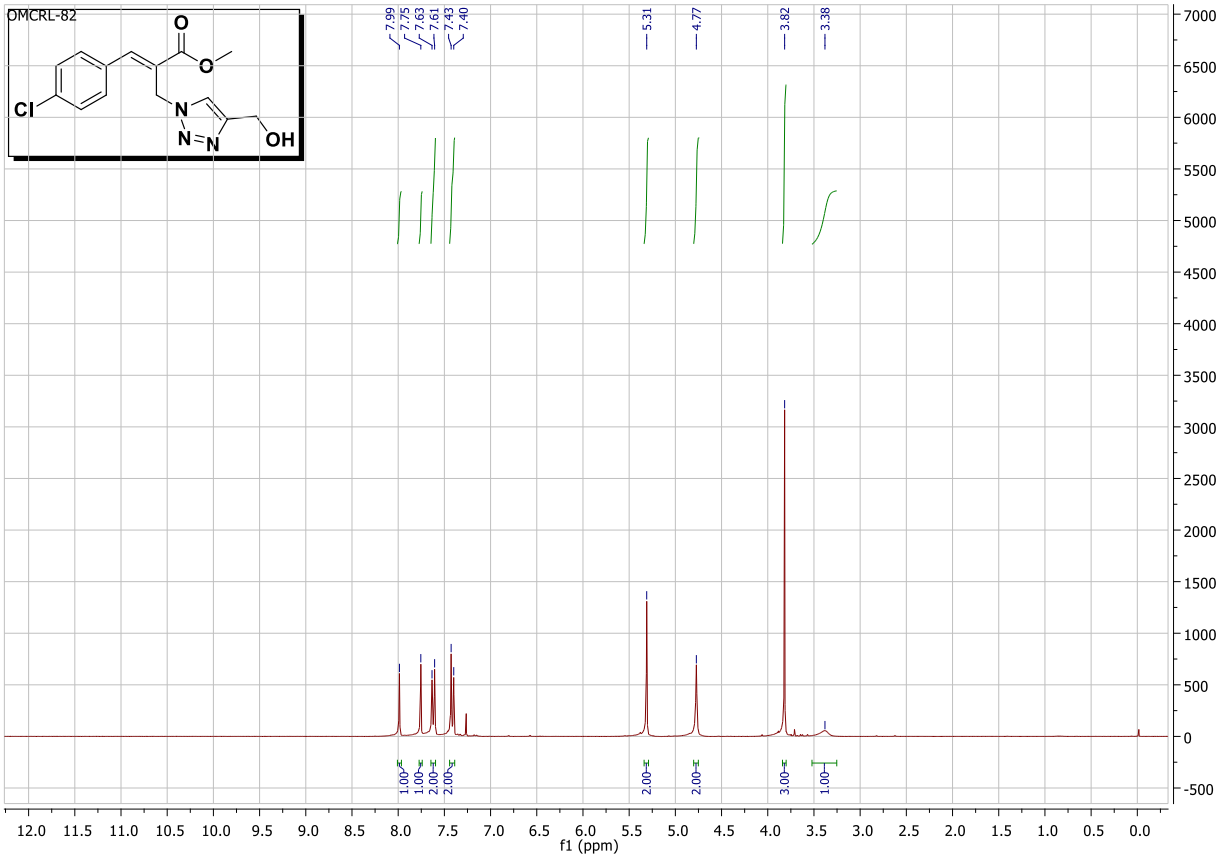

Figure S13 ^{1}H NMR spectrum of (*E*)-methyl 3-(4-chlorophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3g**)

Carbon NMR spectrum of (*E*)-methyl 3(4-chlorophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3g)

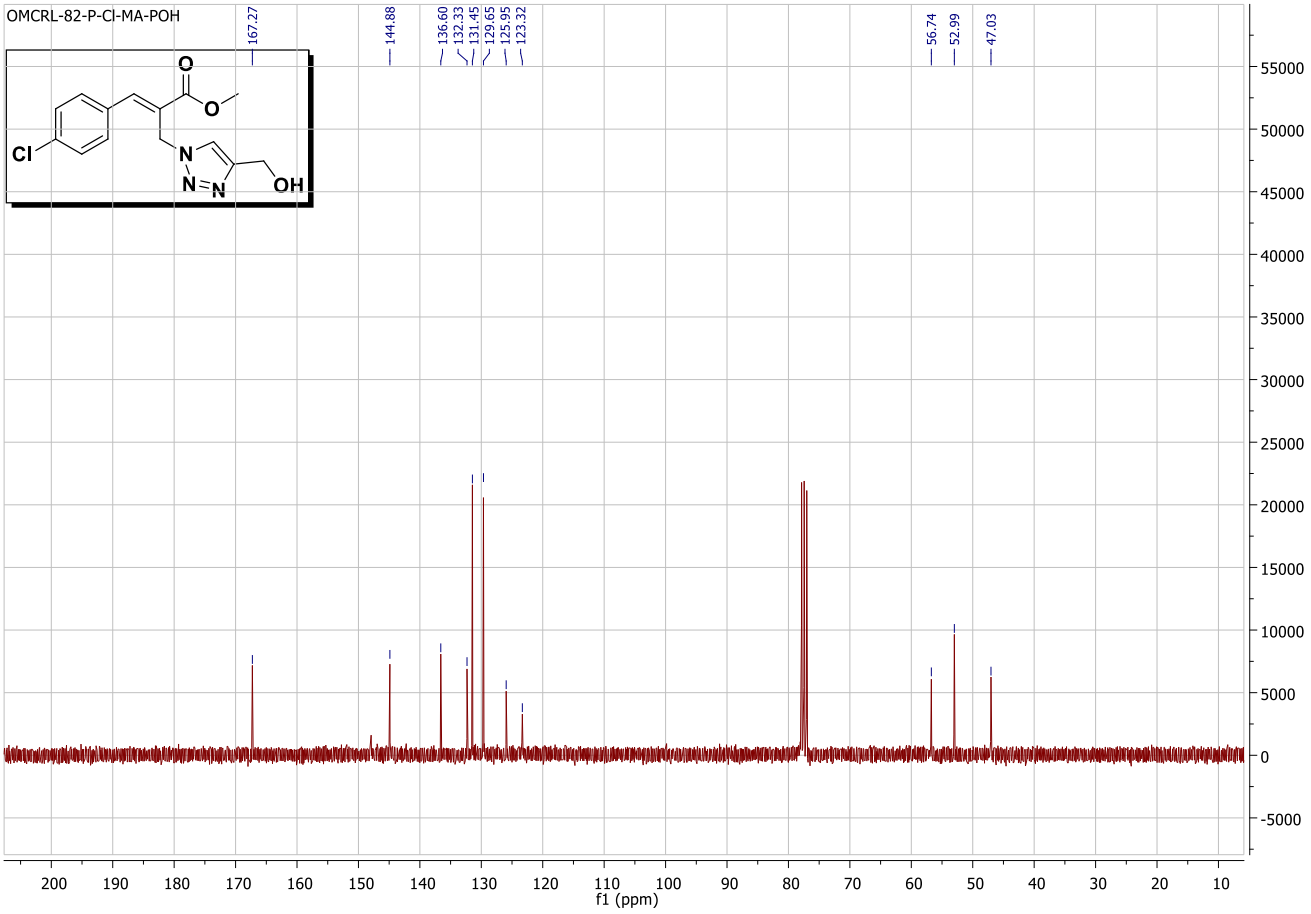

Figure S14 ^{13}C NMR spectrum of (*E*)-methyl 3(4-chlorophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3g**)

Proton NMR spectrum of (*E*)-methyl 3-(4-chlorophenyl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3h)

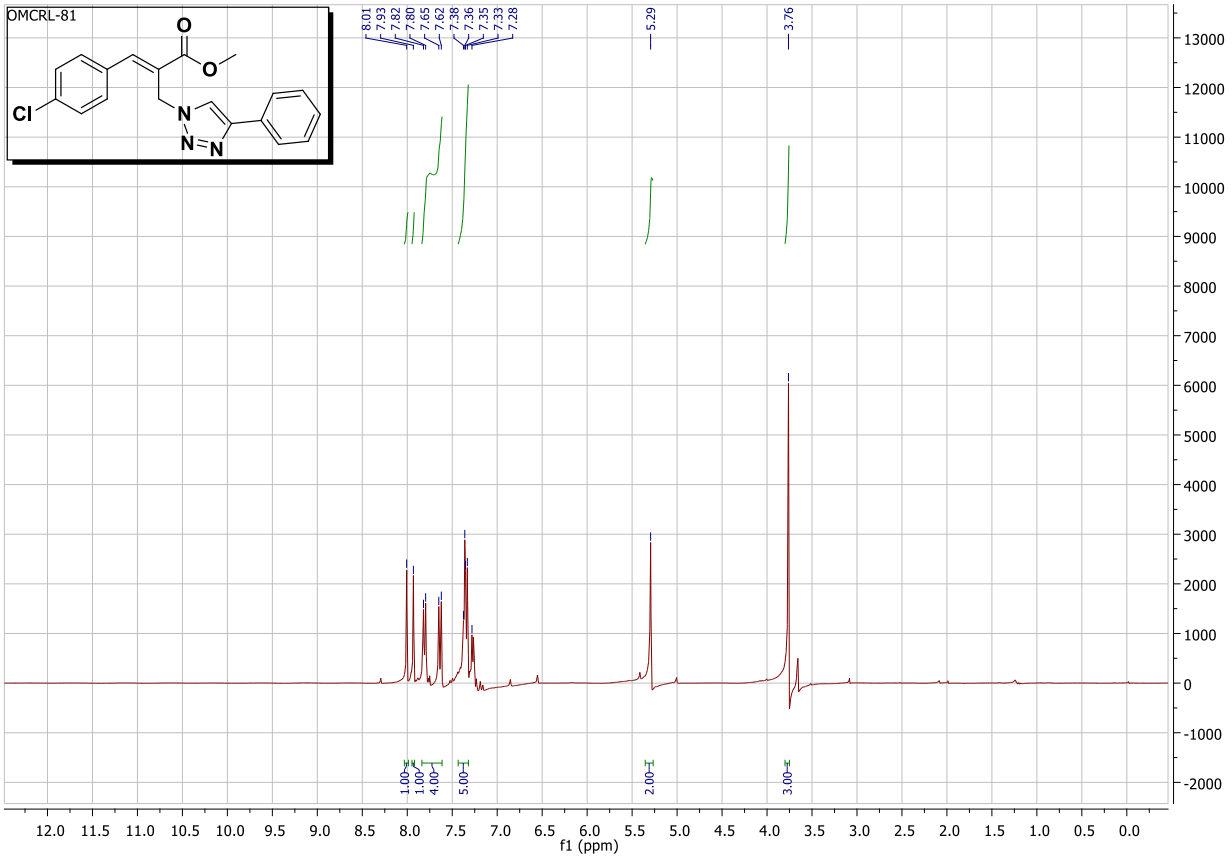

Figure S15 ^{1}H NMR spectrum of (*E*)-methyl 3-(4-chlorophenyl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3h**)

Carbon NMR spectrum of (*E*)-methyl 3-(4-chlorophenyl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3h)

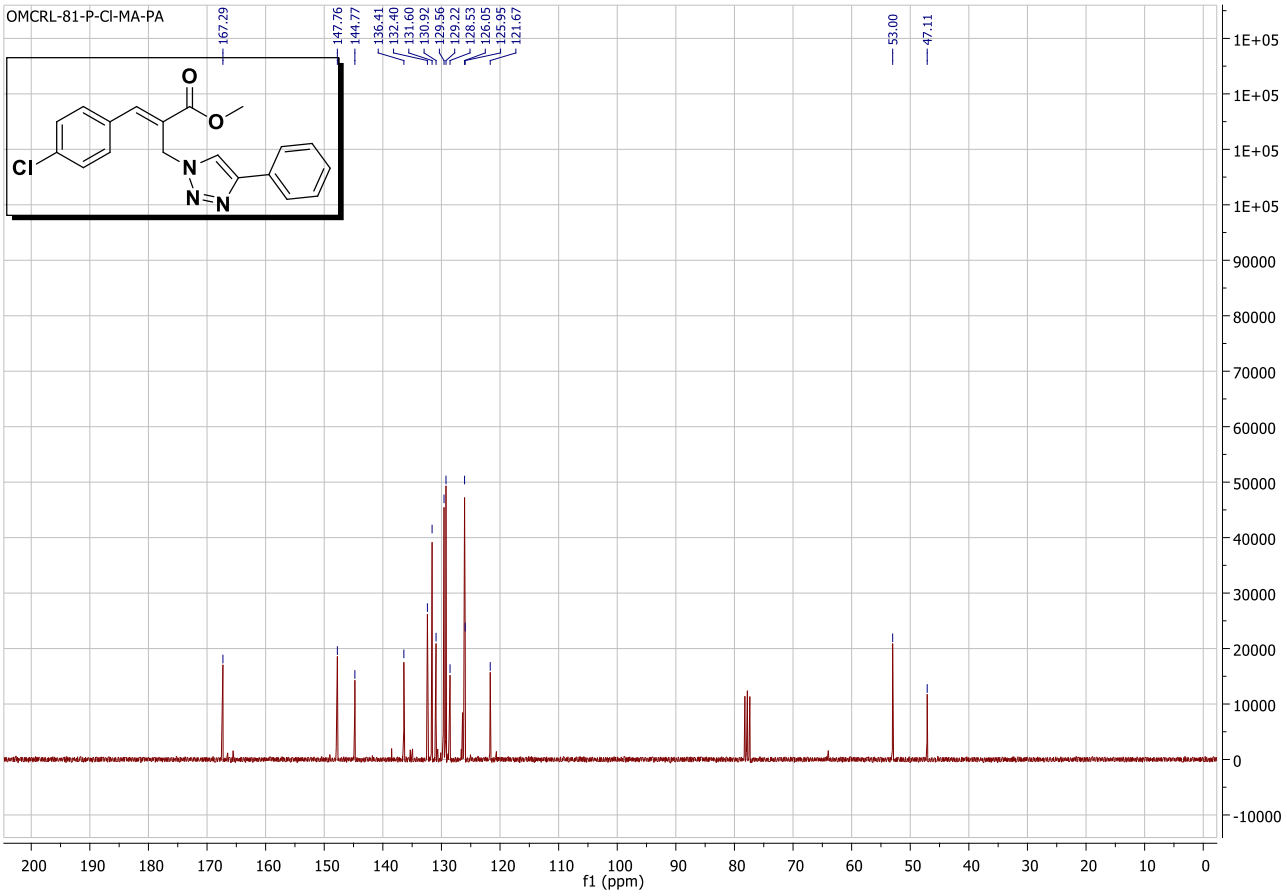

Figure S16 ^{13}C NMR spectrum of (*E*)-methyl 3-(4-chlorophenyl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3h**)

Proton NMR spectrum of (*E*)-methyl 3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3i)

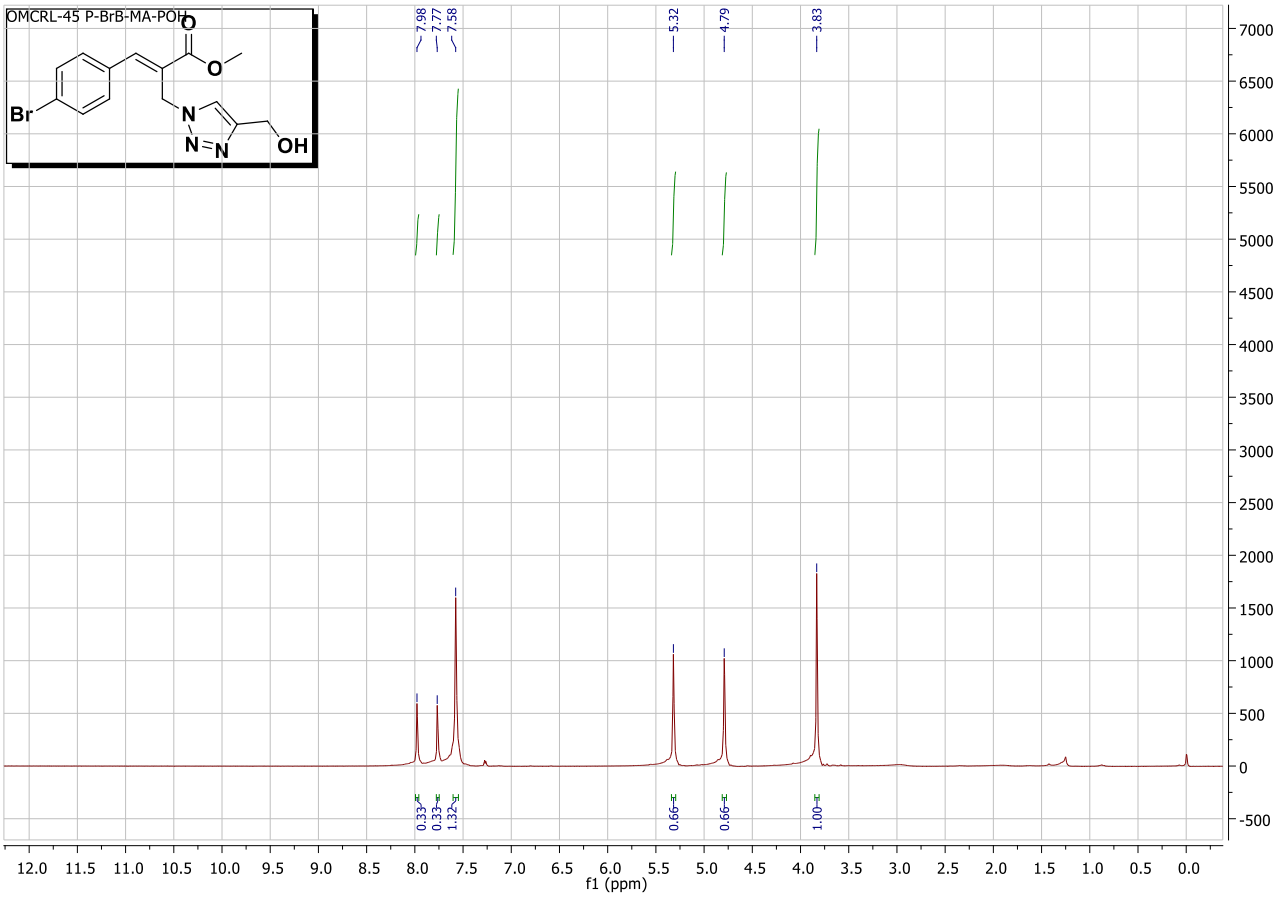

Figure S17 ^{1}H NMR spectrum of (*E*)-methyl 3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3i**)

Carbon NMR spectrum of (*E*)-methyl 3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3i)

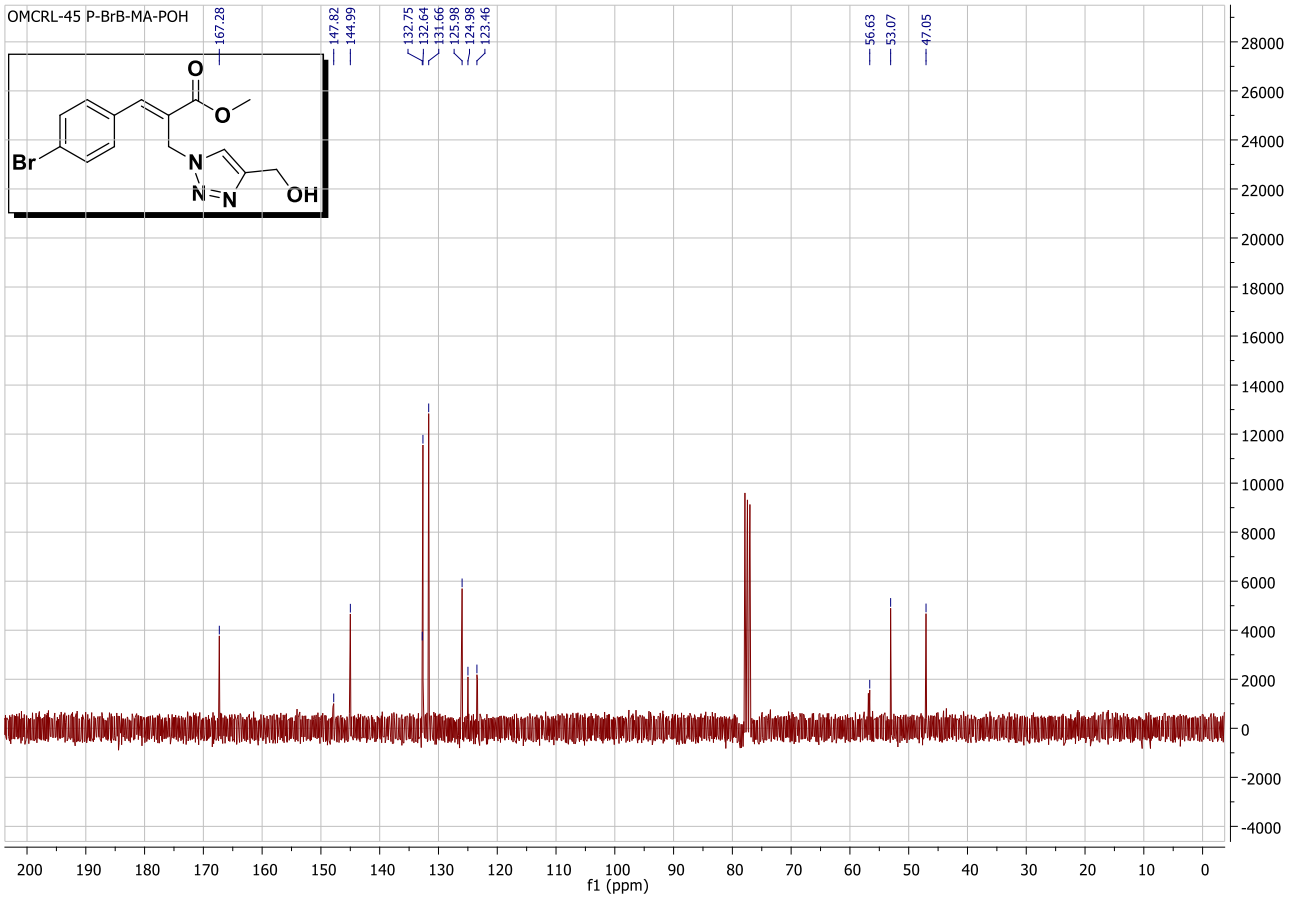

Figure S18 ^{13}C NMR spectrum of (*E*)-methyl 3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3i**)

Proton NMR spectrum of (*E*)-methyl 3-(4-bromophenyl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3j)

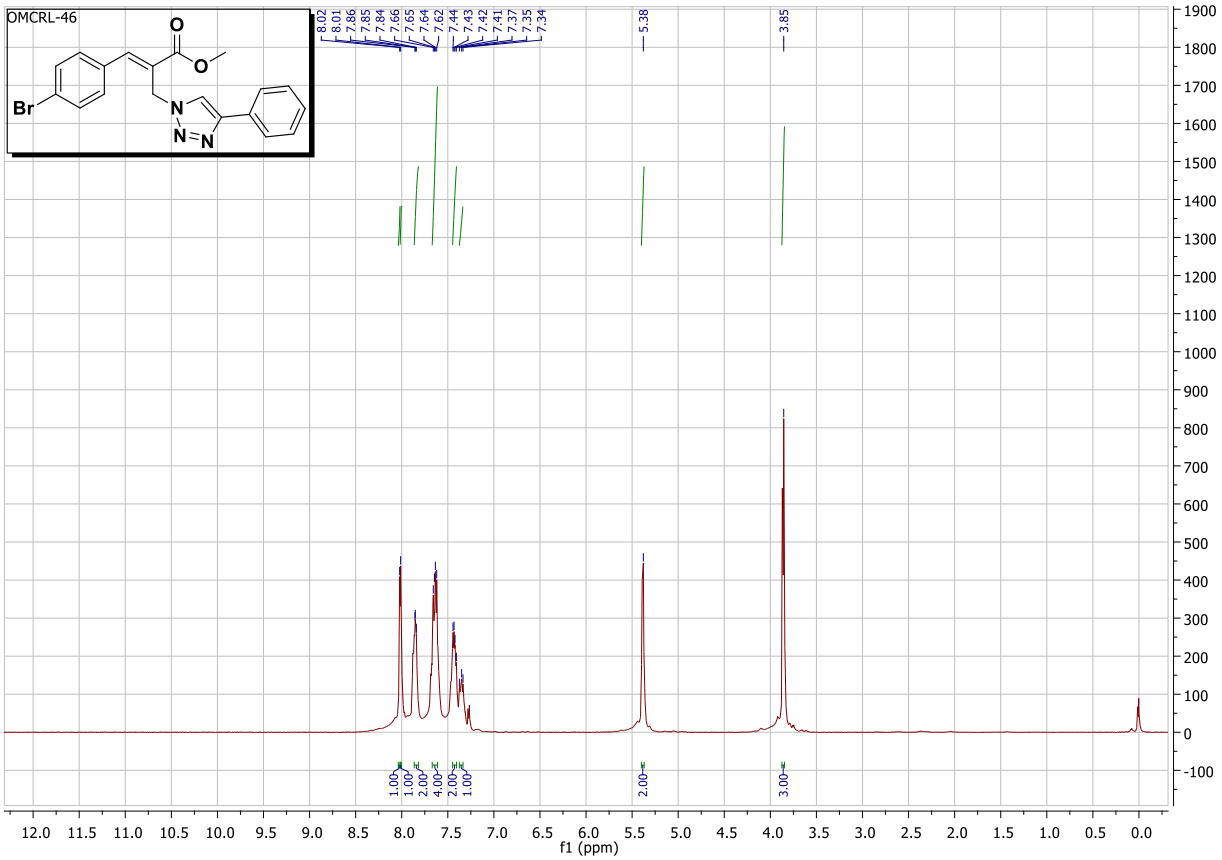

Figure S19 ^{1}H NMR spectrum of (*E*)-methyl 3-(4-bromophenyl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3j)**

Carbon NMR spectrum of (*E*)-methyl 3-(4-bromophenyl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3j)

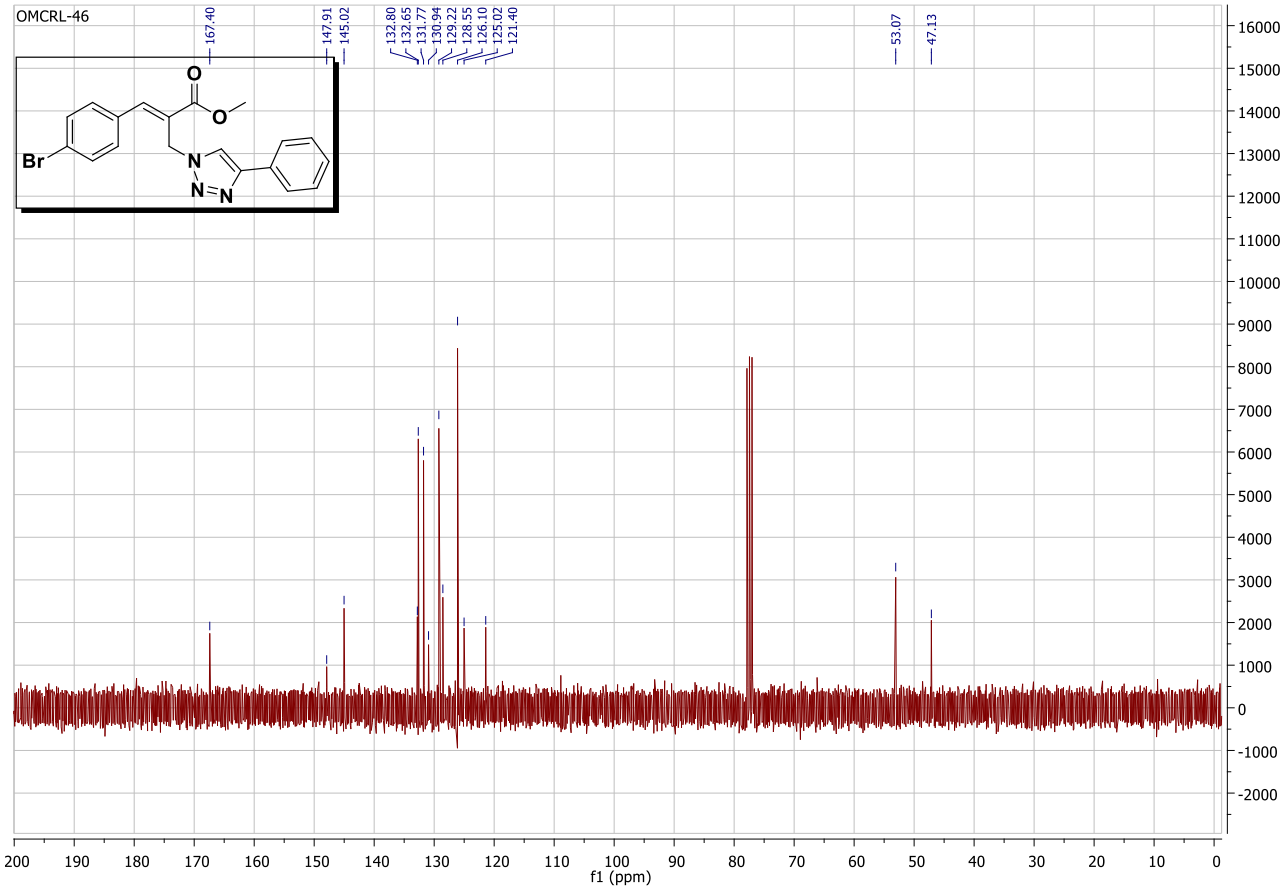

Figure S20 ^{13}C NMR spectrum of (*E*)-methyl 3-(4-bromophenyl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3j**)

Proton NMR spectrum of (*E*)-ethyl 3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3k)

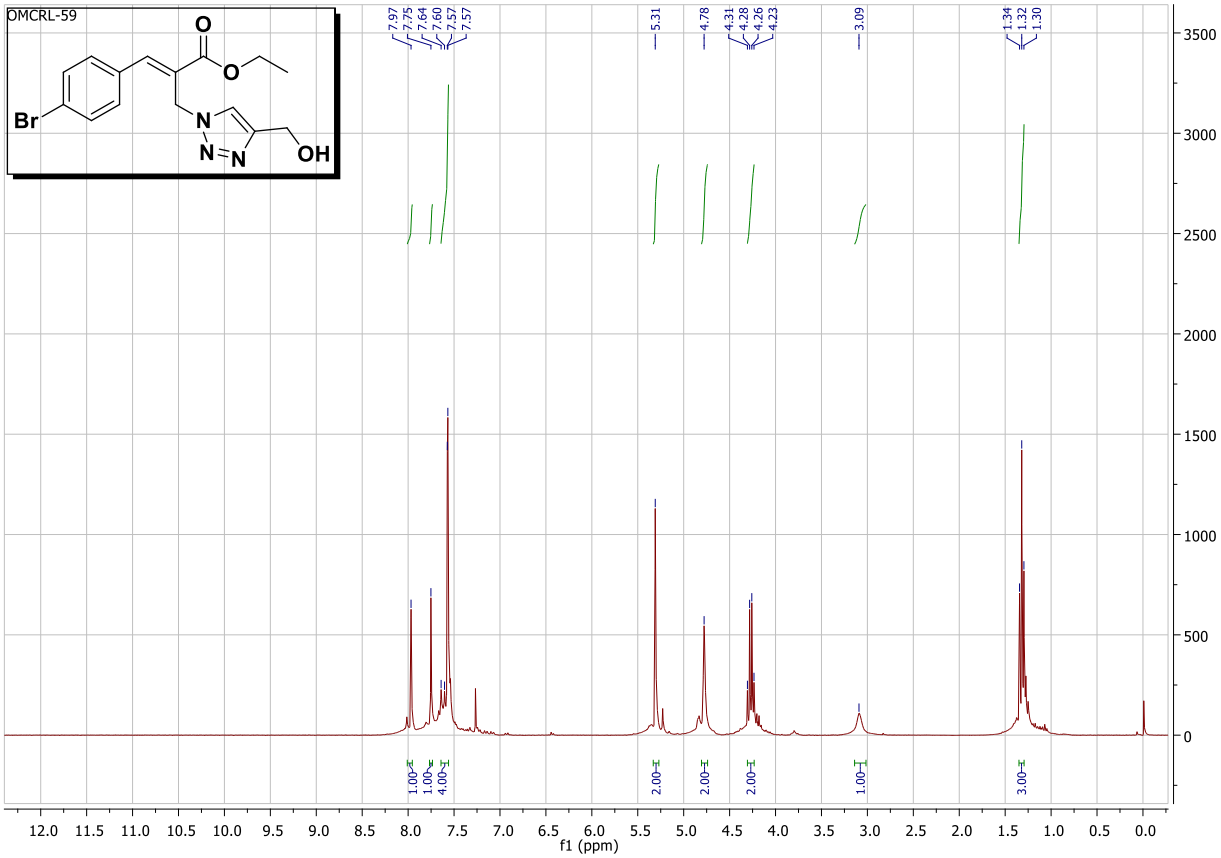

Figure S21 ^{1}H NMR spectrum of (*E*)-ethyl 3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3k**)

Carbon NMR spectrum of (*E*)-ethyl 3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3k)

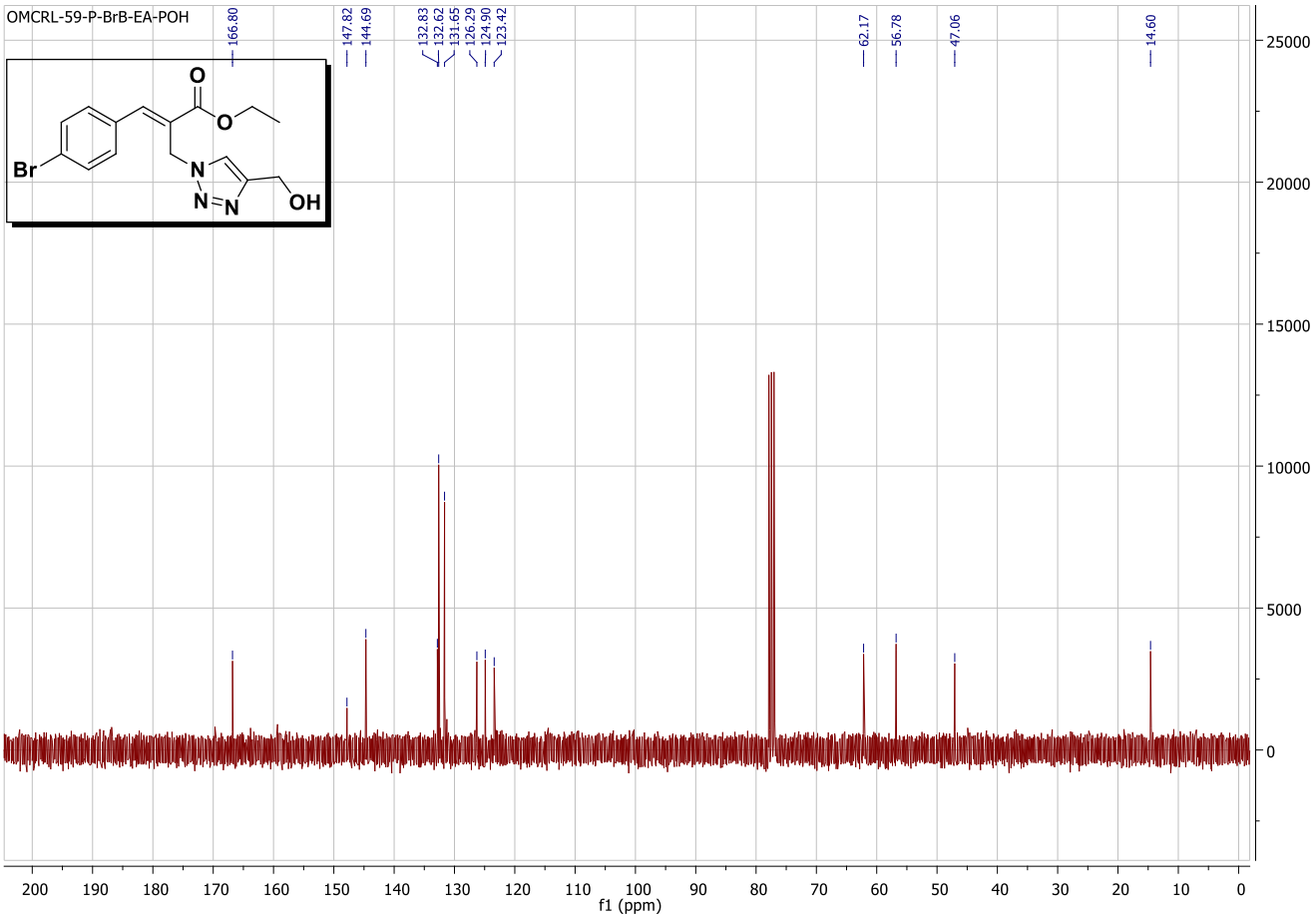

Figure S22 ^{13}C NMR spectrum of (*E*)-ethyl 3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3k**)

Proton NMR spectrum of (*Z*)-3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylonitrile (3l)

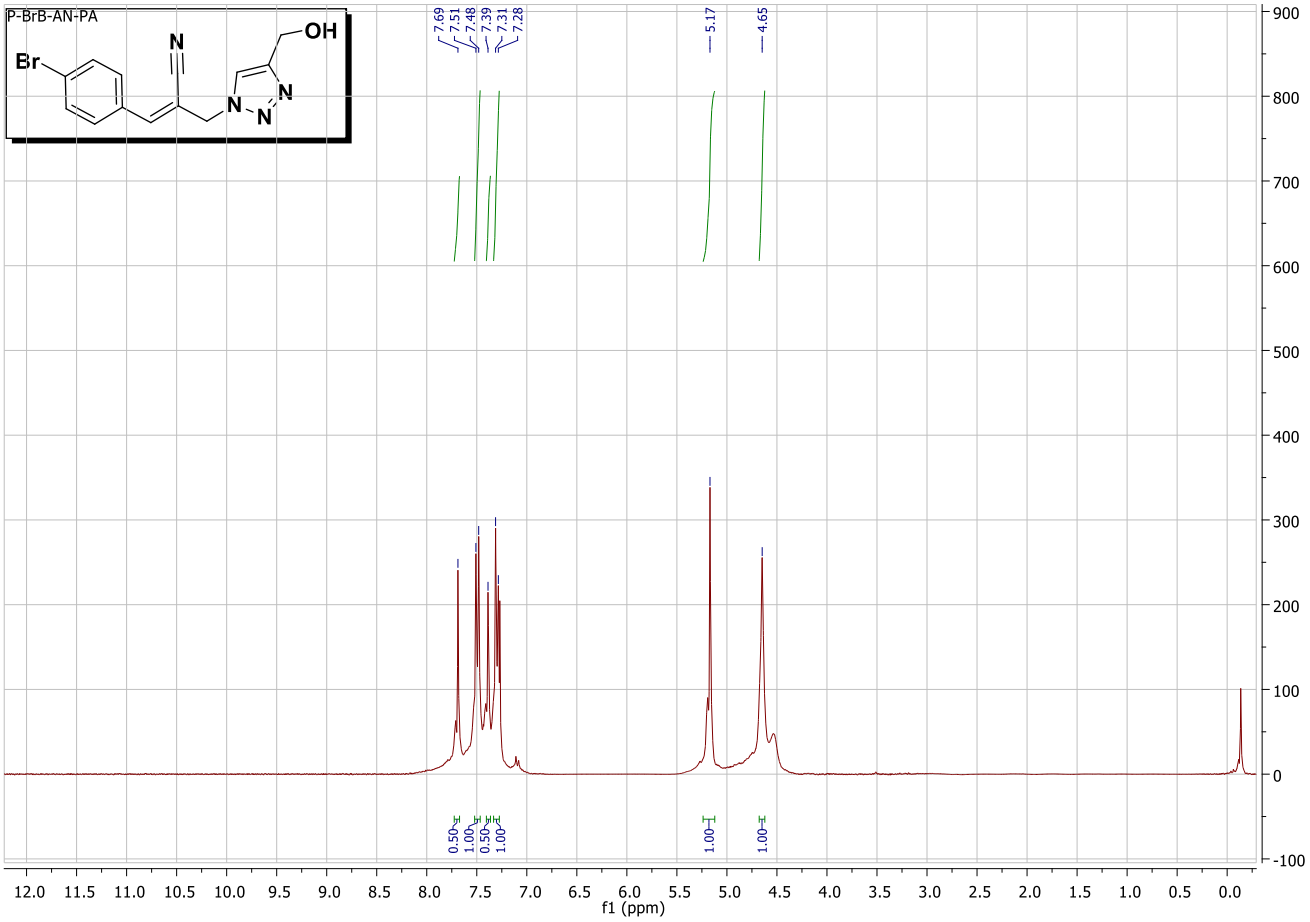

Figure S23 ^{1}H NMR spectrum of (*Z*)-3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylonitrile (**3l**)

Carbon NMR spectrum of (*Z*)-3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylonitrile (3l)

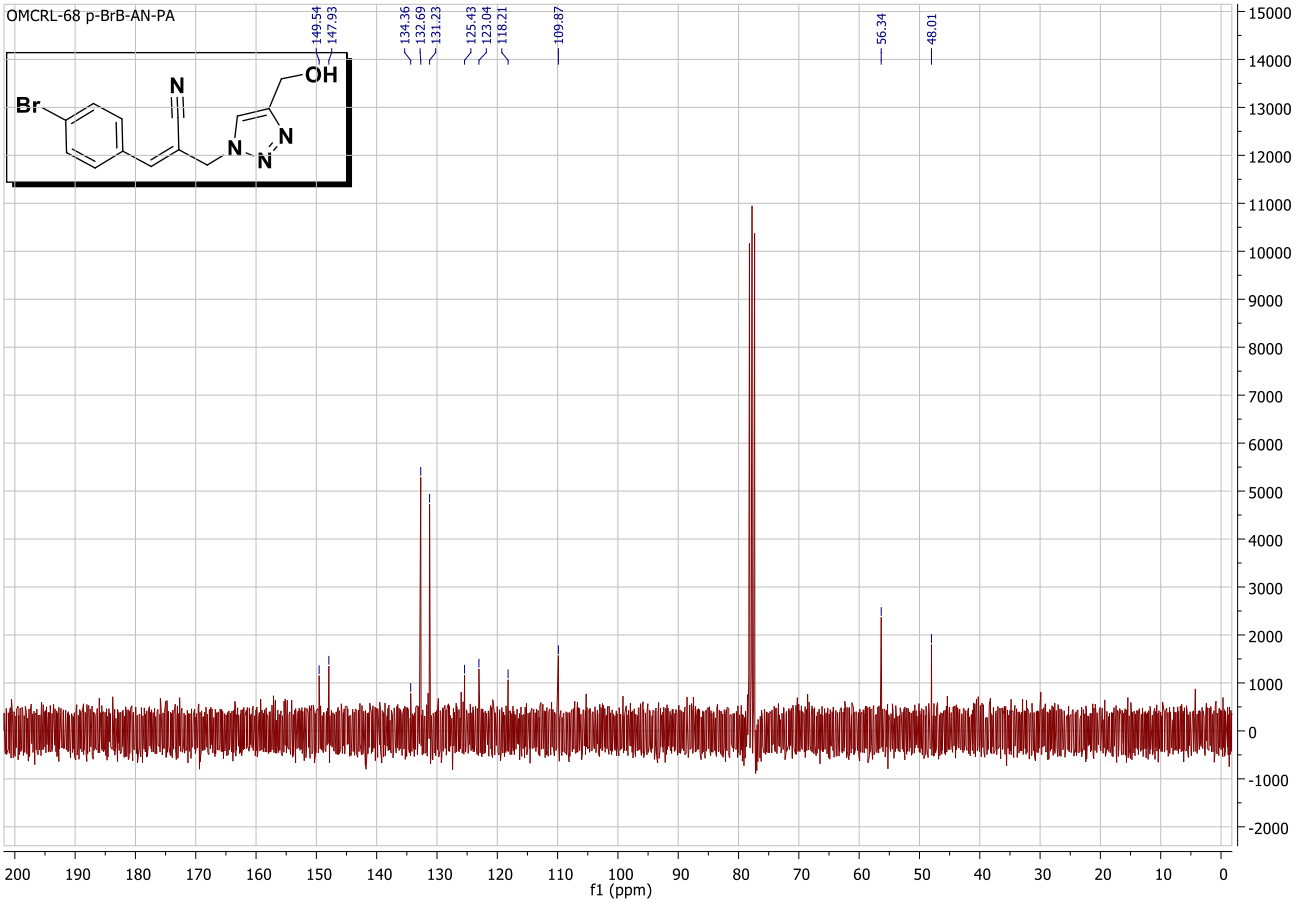

Figure S24 ^{13}C NMR spectrum of (*Z*)-3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylonitrile (**3l**)

Proton NMR spectrum of (*E*)-methyl 2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-(4-nitrophenyl)acrylate (3m)

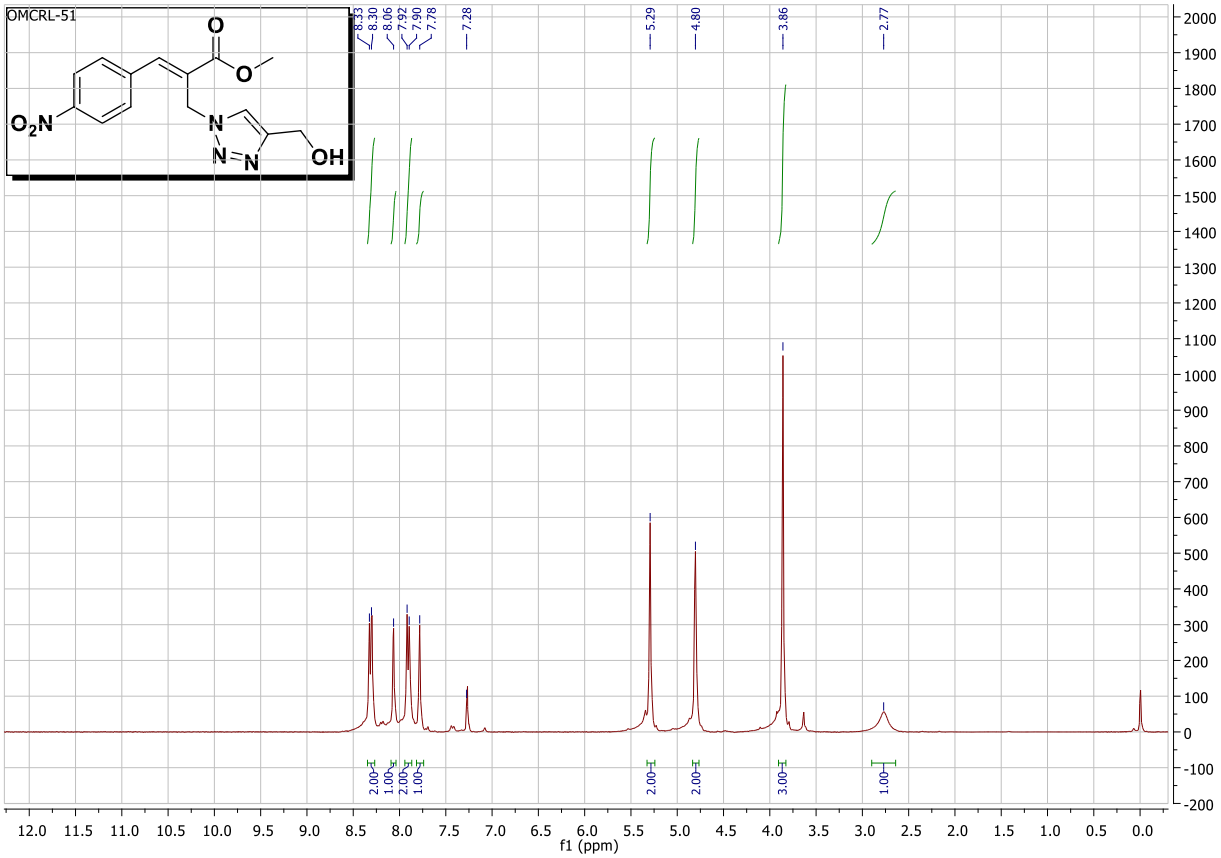

Figure S25 ^{1}H NMR spectrum of (*E*)-methyl 2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-(4-nitrophenyl)acrylate (**3m**)

Carbon NMR spectrum of (*E*)-methyl 2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-(4-nitrophenyl)acrylate (3m)

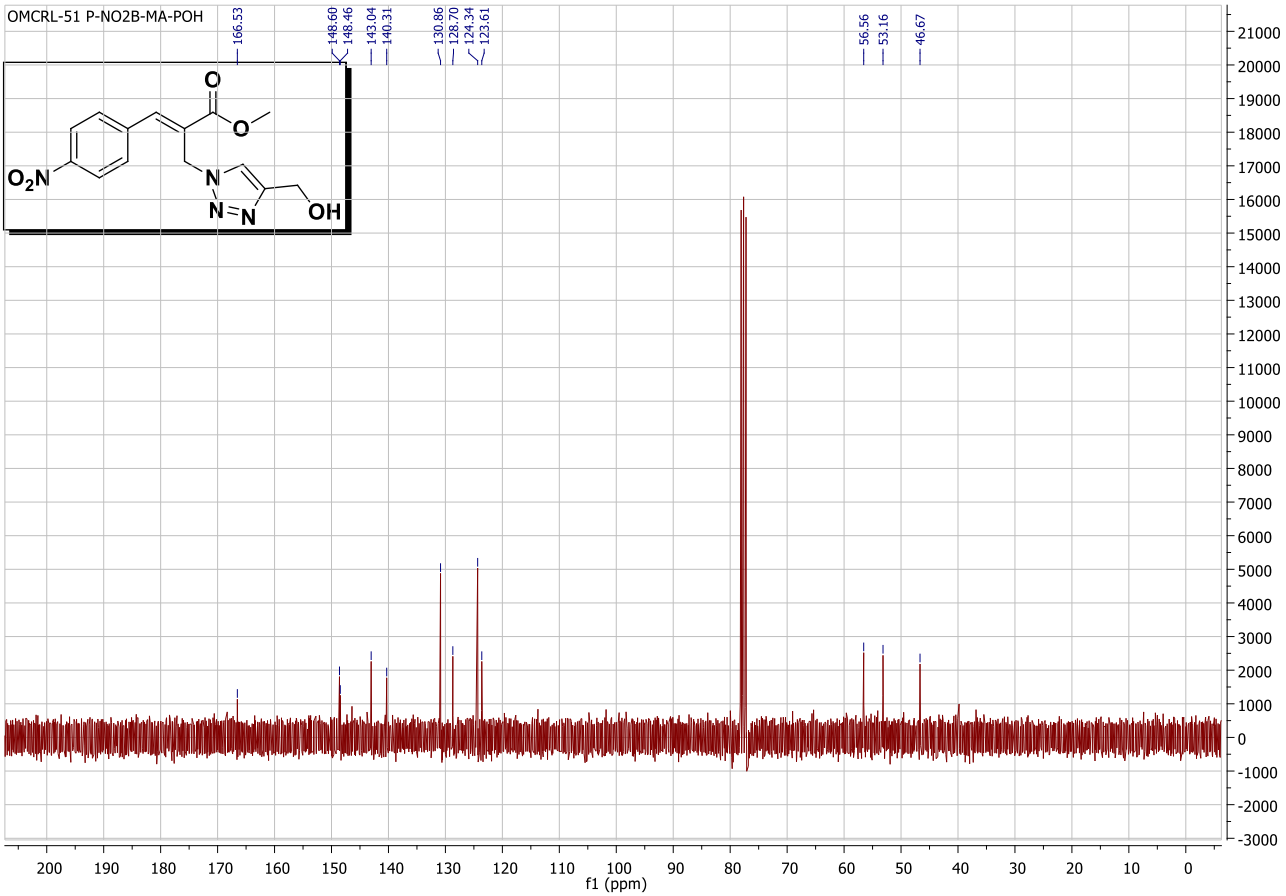

Figure S26 ^{13}C NMR spectrum of (*E*)-methyl 2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-(4-nitrophenyl)acrylate (**3m**)

Proton NMR spectrum of (*E*)-methyl 3-(furan-2-yl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3n)

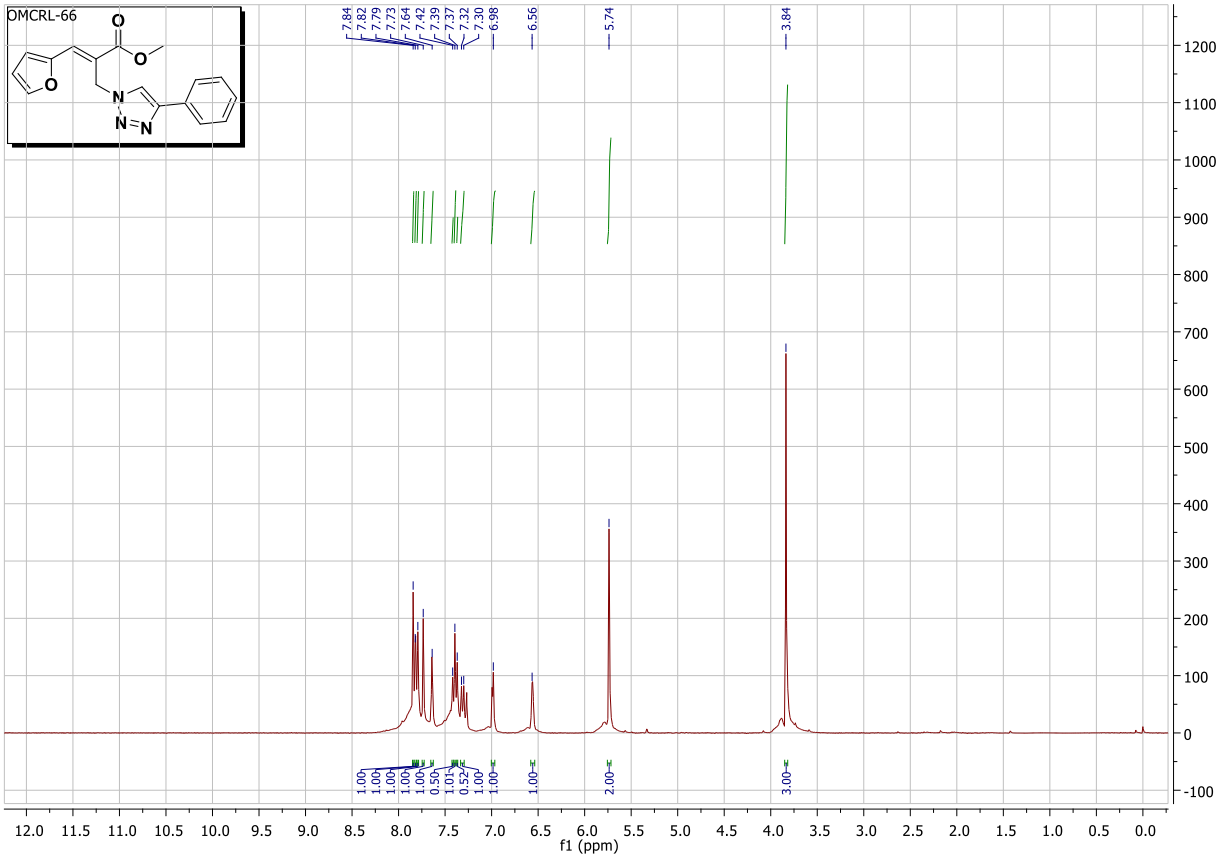

Figure S27 ^{1}H NMR spectrum of (*E*)-methyl 3-(furan-2-yl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3n**)

Carbon NMR spectrum of (*E*)-methyl 3-(furan-2-yl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3n)

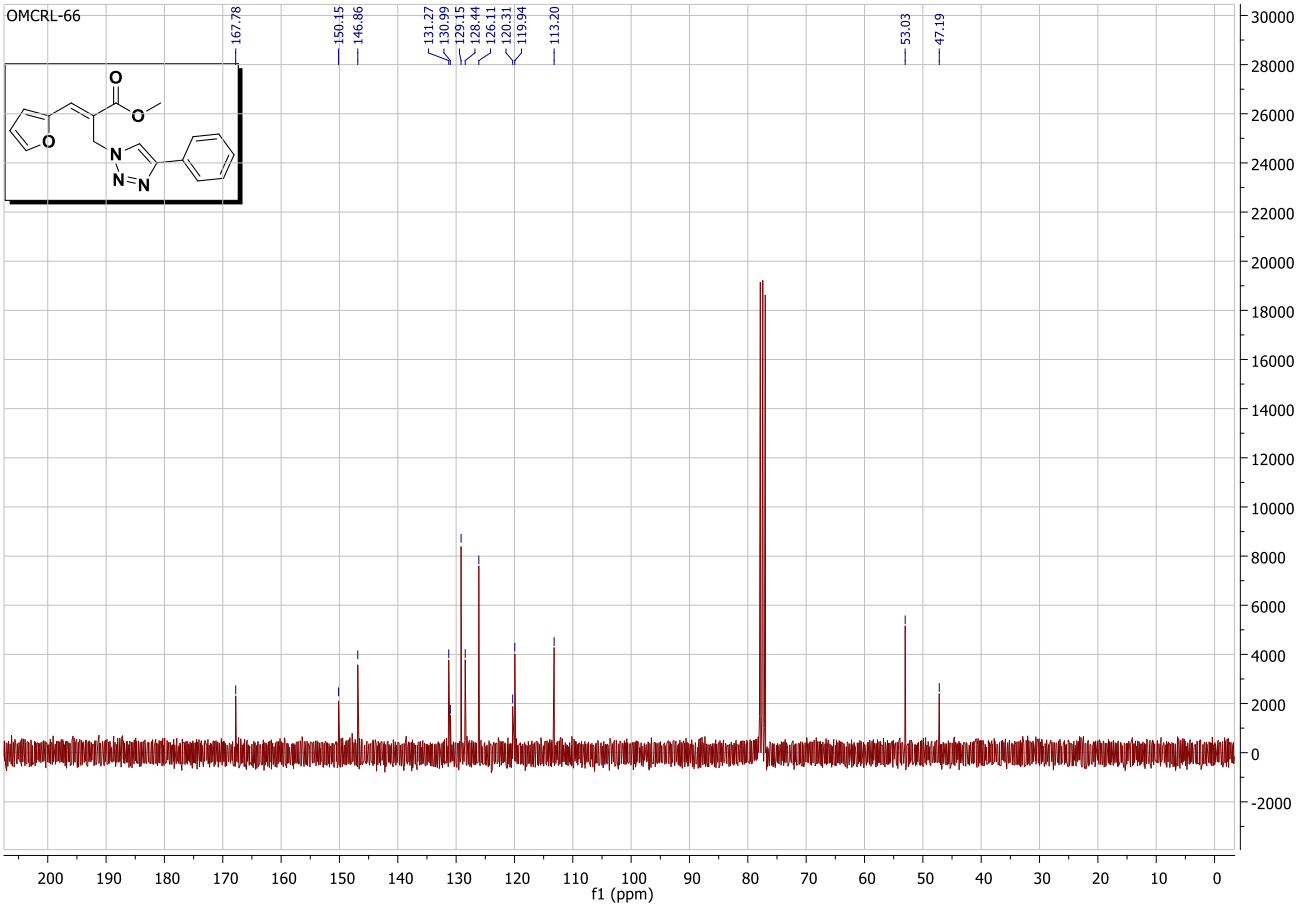

Figure S28 ^{13}C NMR spectrum of (*E*)-methyl 3-(furan-2-yl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3n**)

Proton NMR spectrum of (*E*)-ethyl 3-(furan-2-yl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3o)

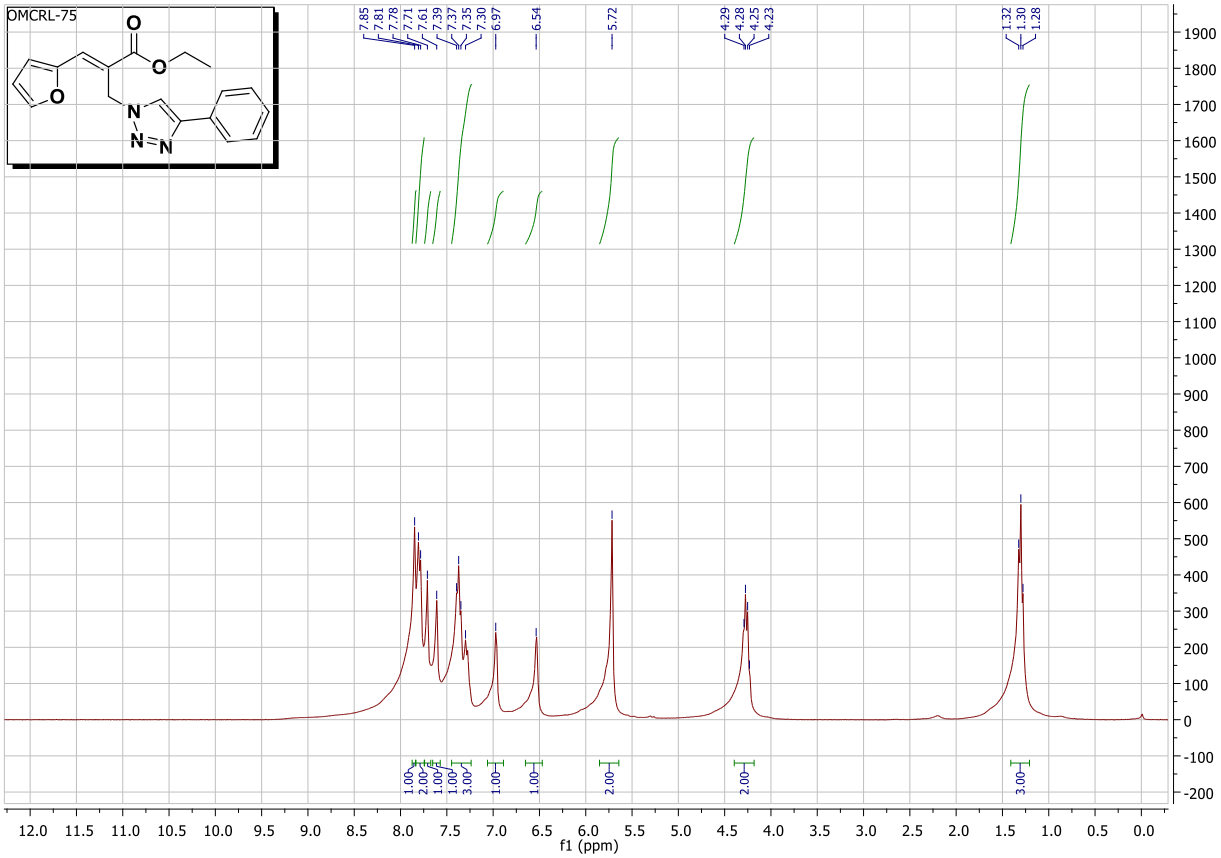

Figure S29 ^{1}H NMR spectrum of (*E*)-ethyl 3-(furan-2-yl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3o**)

Carbon NMR spectrum of (*E*)-ethyl 3-(furan-2-yl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3o)

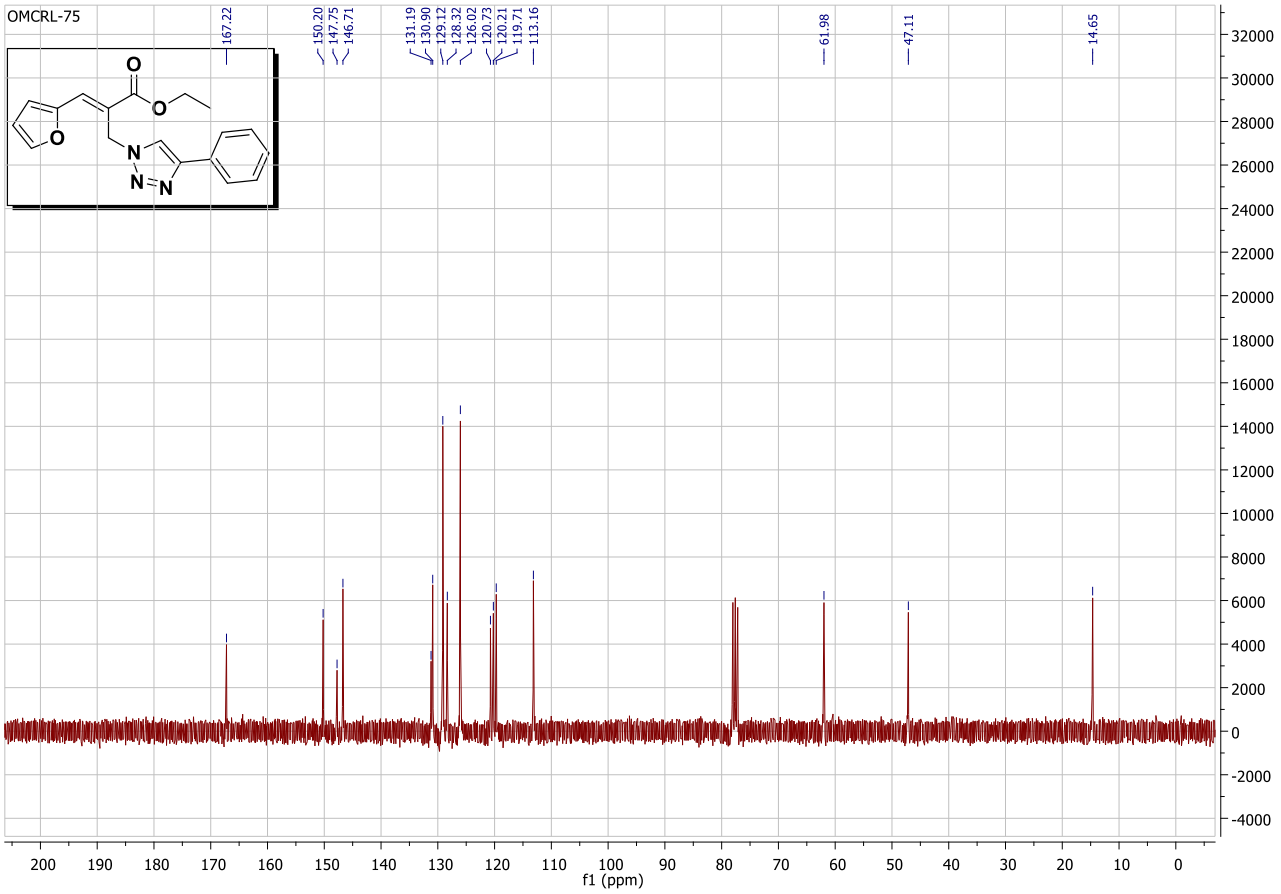

Figure S30 ^{13}C NMR spectrum of (*E*)-ethyl 3-(furan-2-yl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (**3o**)

Proton NMR spectrum of (*E*)-methyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-3-(thiophen-2-yl)acrylate (3p)

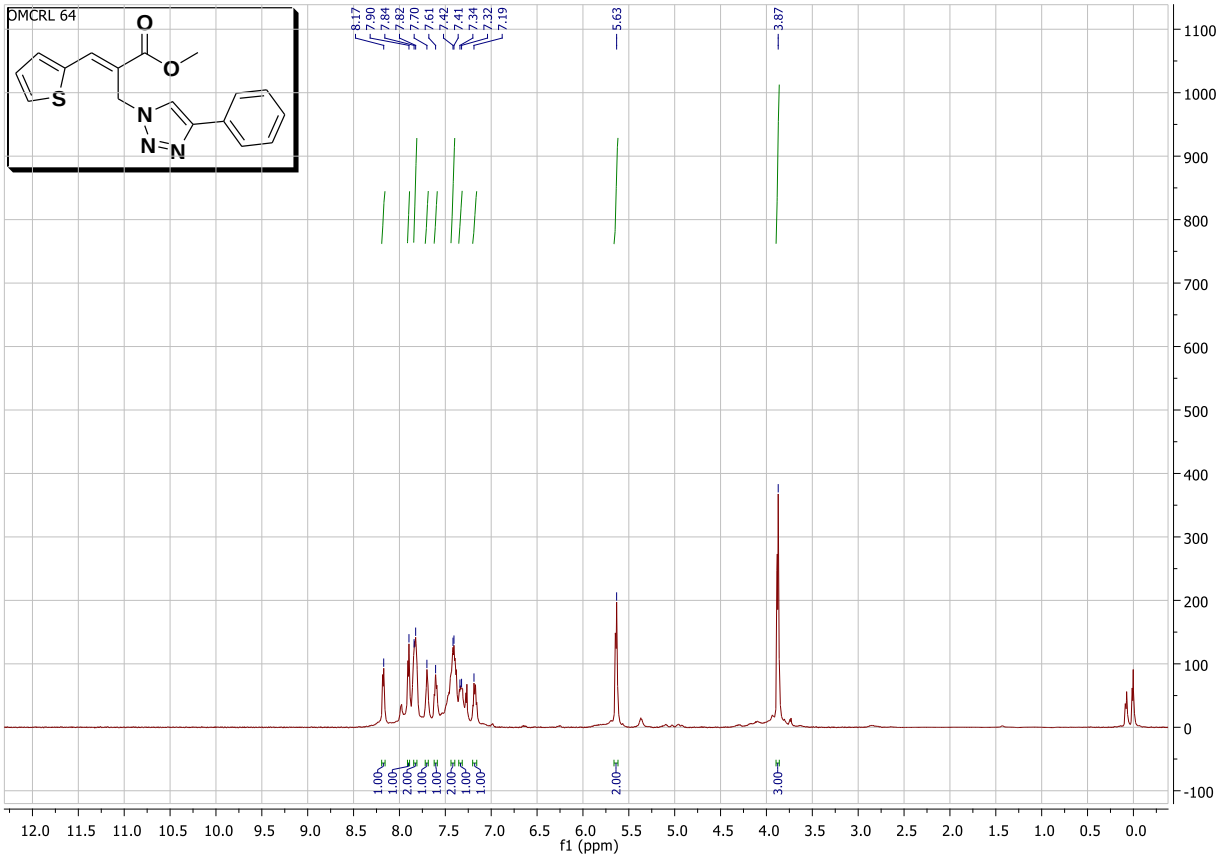

Figure S31 ^{1}H NMR spectrum of (*E*)-methyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-3-(thiophen-2-yl)acrylate (**3p**)

Carbon NMR spectrum of (*E*)-methyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-3-(thiophen-2-yl)acrylate (3p)

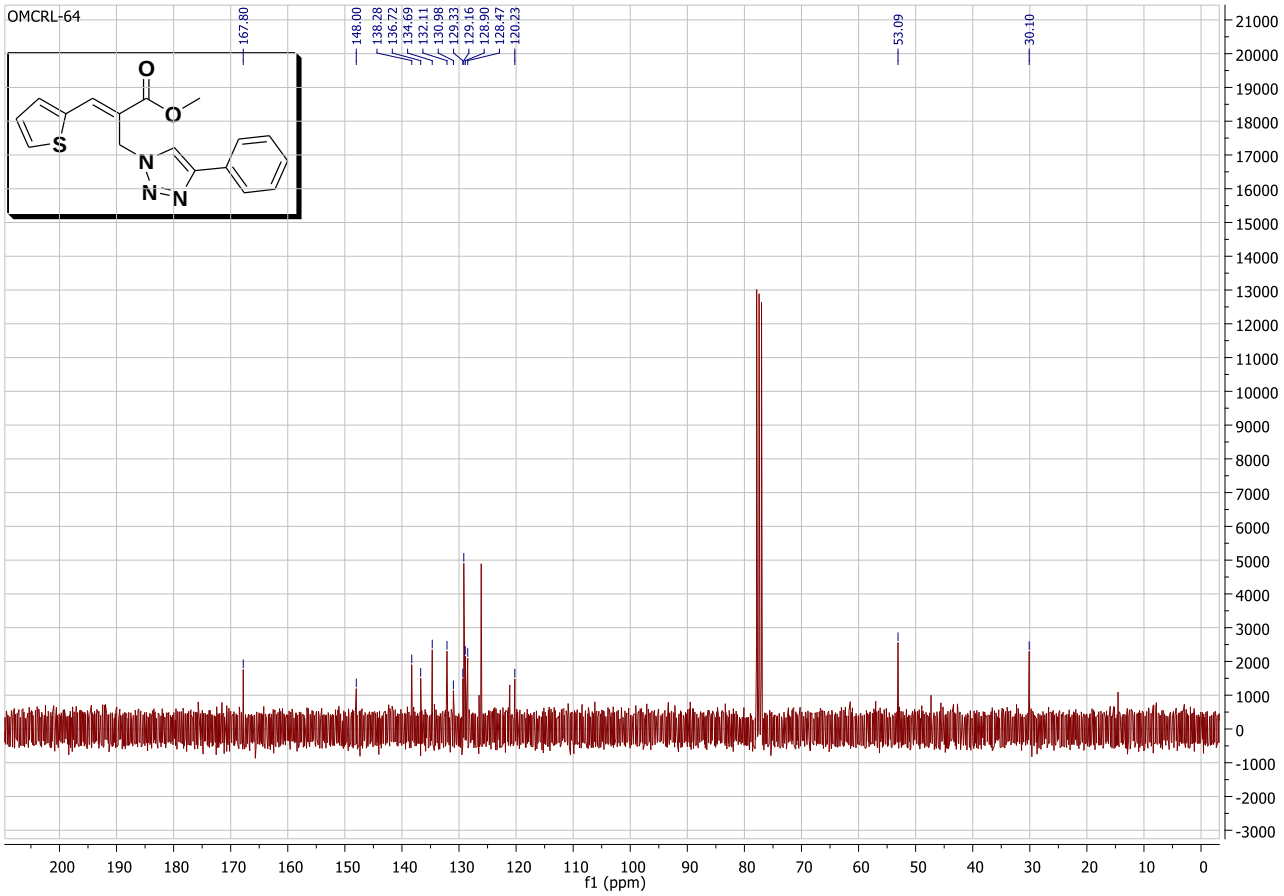

Figure S32 ^{13}C NMR spectrum of (*E*)-methyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-3-(thiophen-2-yl)acrylate (**3p**)

Proton NMR spectrum of (*E*)-ethyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-3-(thiophen-2-yl)acrylate (3q)

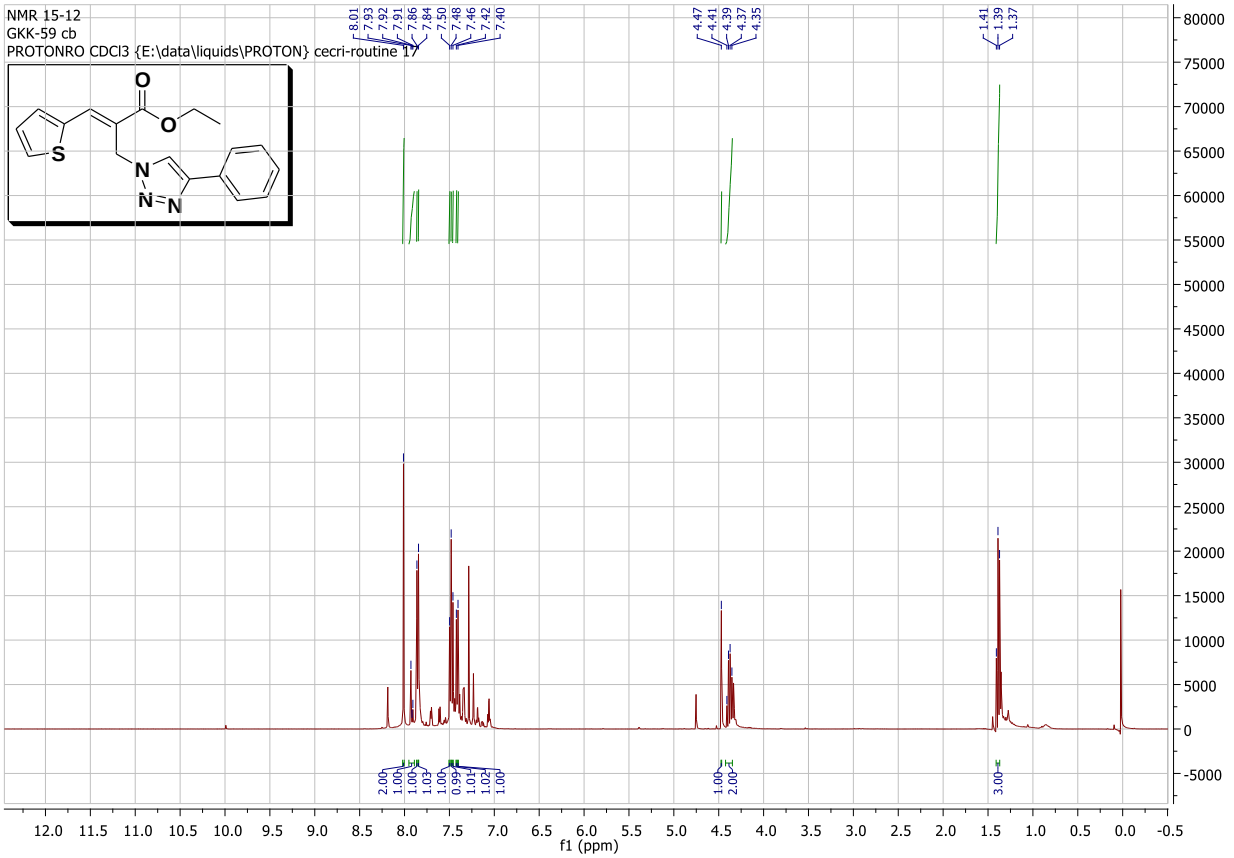

Figure S33 ^{1}H NMR spectrum of (*E*)-ethyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-3-(thiophen-2-yl)acrylate (**3q**)

Carbon NMR spectrum of (*E*)-ethyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-3-(thiophen-2-yl)acrylate (3q)

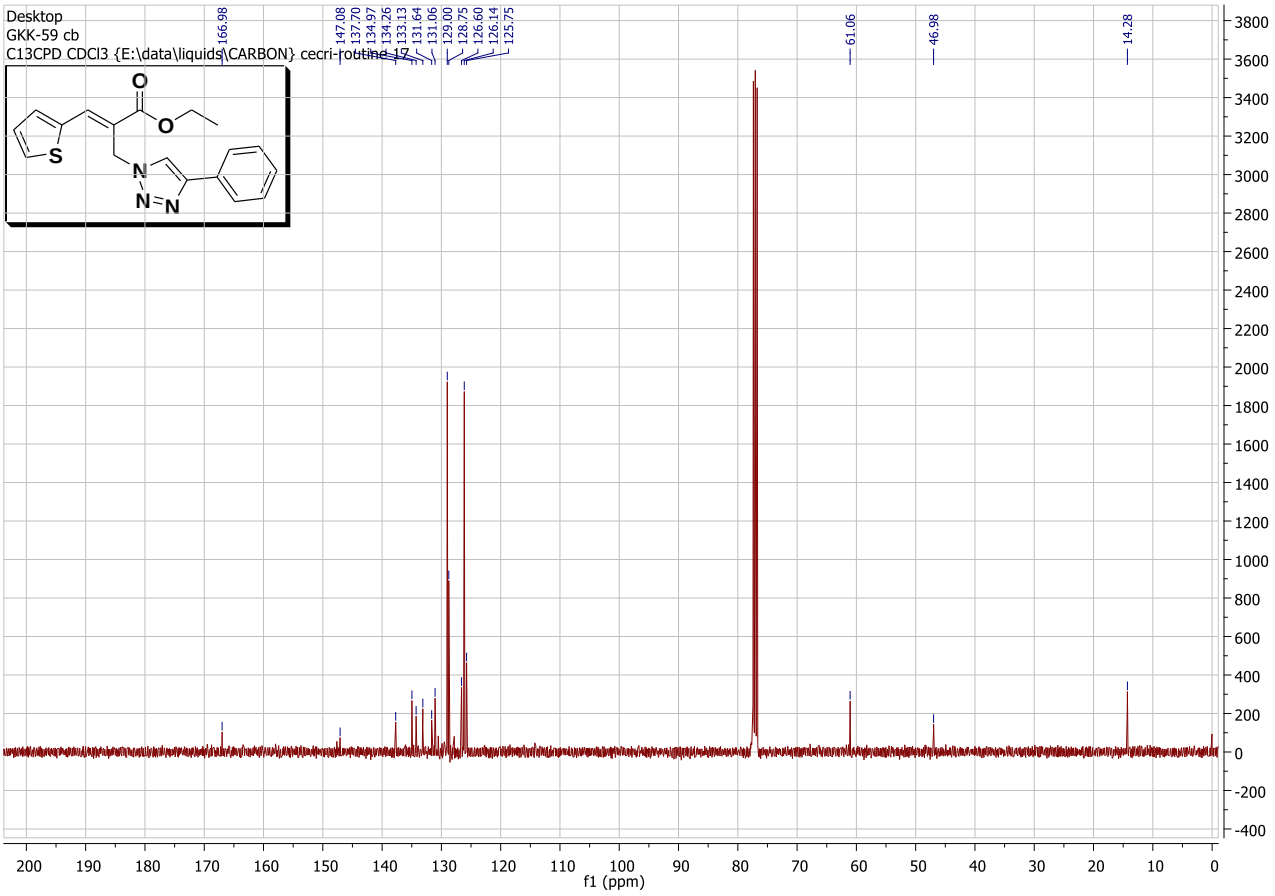

Figure S34 ^{13}C NMR spectrum of (*E*)-ethyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-3-(thiophen-2-yl)acrylate (**3q**)

Copies of ^{1}H NMR and ^{13}C NMR spectra for compounds 4a–c

Proton NMR spectrum of 3-(bromomethyl)-2*H*-chromen-2-one (4a)

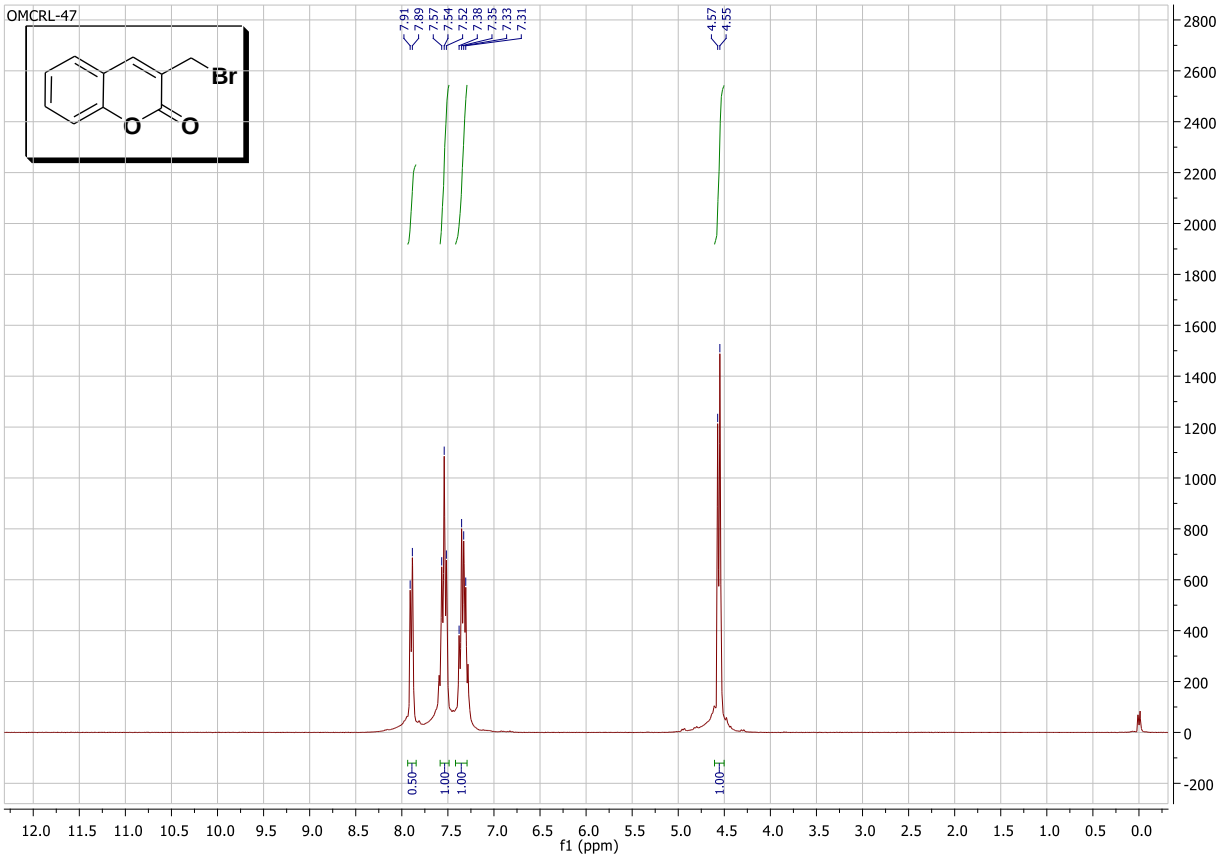

Figure S35 ^{1}H NMR spectrum of 3-(bromomethyl)-2*H*-chromen-2-one (**4a**)

Carbon NMR spectrum of 3-(bromomethyl)-2*H*-chromen-2-one (4a)

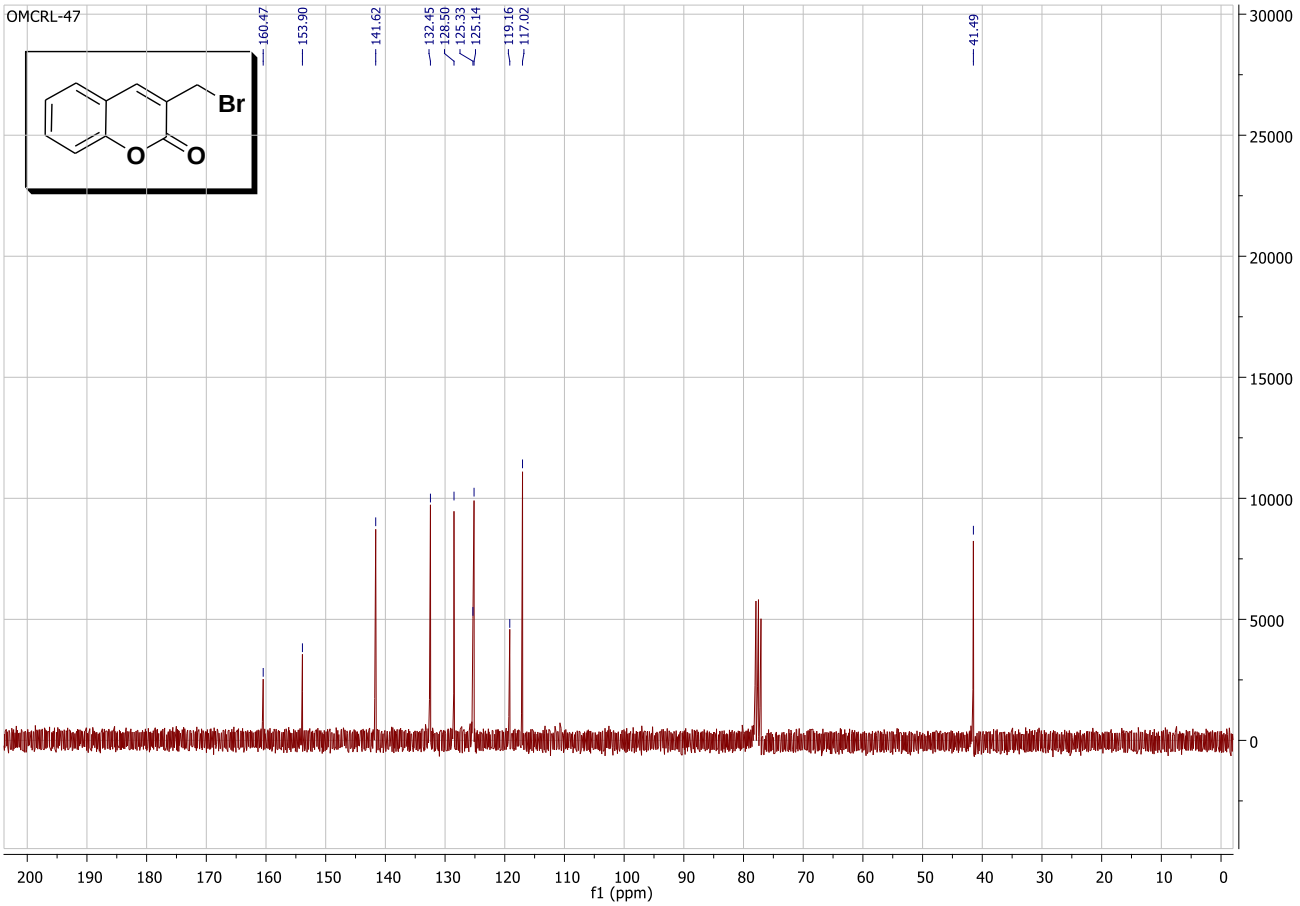

Figure S36 ^{13}C NMR spectrum of 3-(bromomethyl)-2*H*-chromen-2-one (**4a**)

Proton NMR spectrum of 3-(bromomethyl)-8-methoxy-2*H*-chromen-2-one (4b)

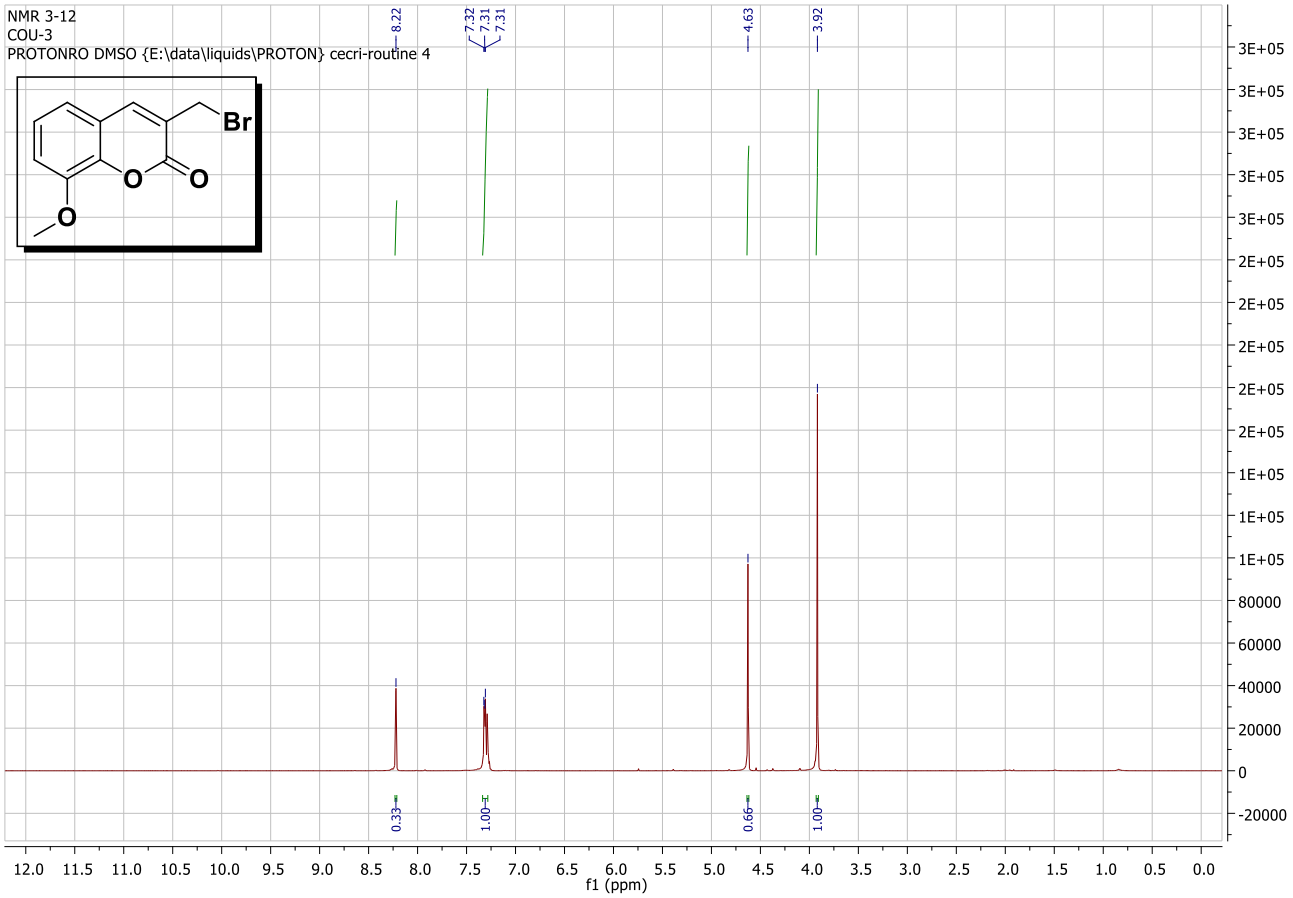

Figure S37 ^{1}H NMR spectrum of 3-(bromomethyl)-8-methoxy-2*H*-chromen-2-one (**4b**)

Carbon NMR spectrum of 3-(bromomethyl)-8-methoxy-2*H*-chromen-2-one (4b)

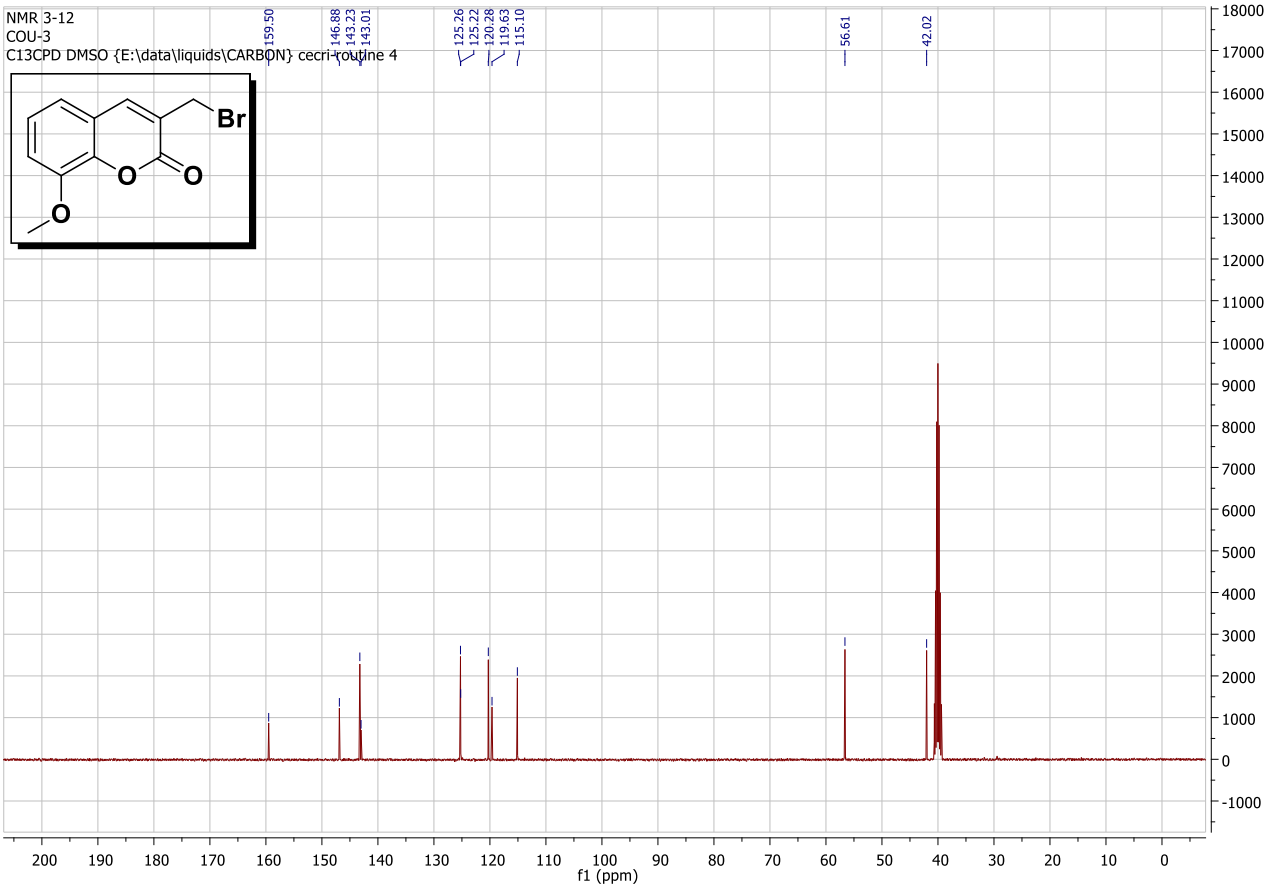

Figure S38 ^{13}C NMR spectrum of 3-(bromomethyl)-8-methoxy-2*H*-chromen-2-one (**4b**)

Proton NMR spectrum of 6-bromo-3-(bromomethyl)-2*H*-chromen-2-one (4c)

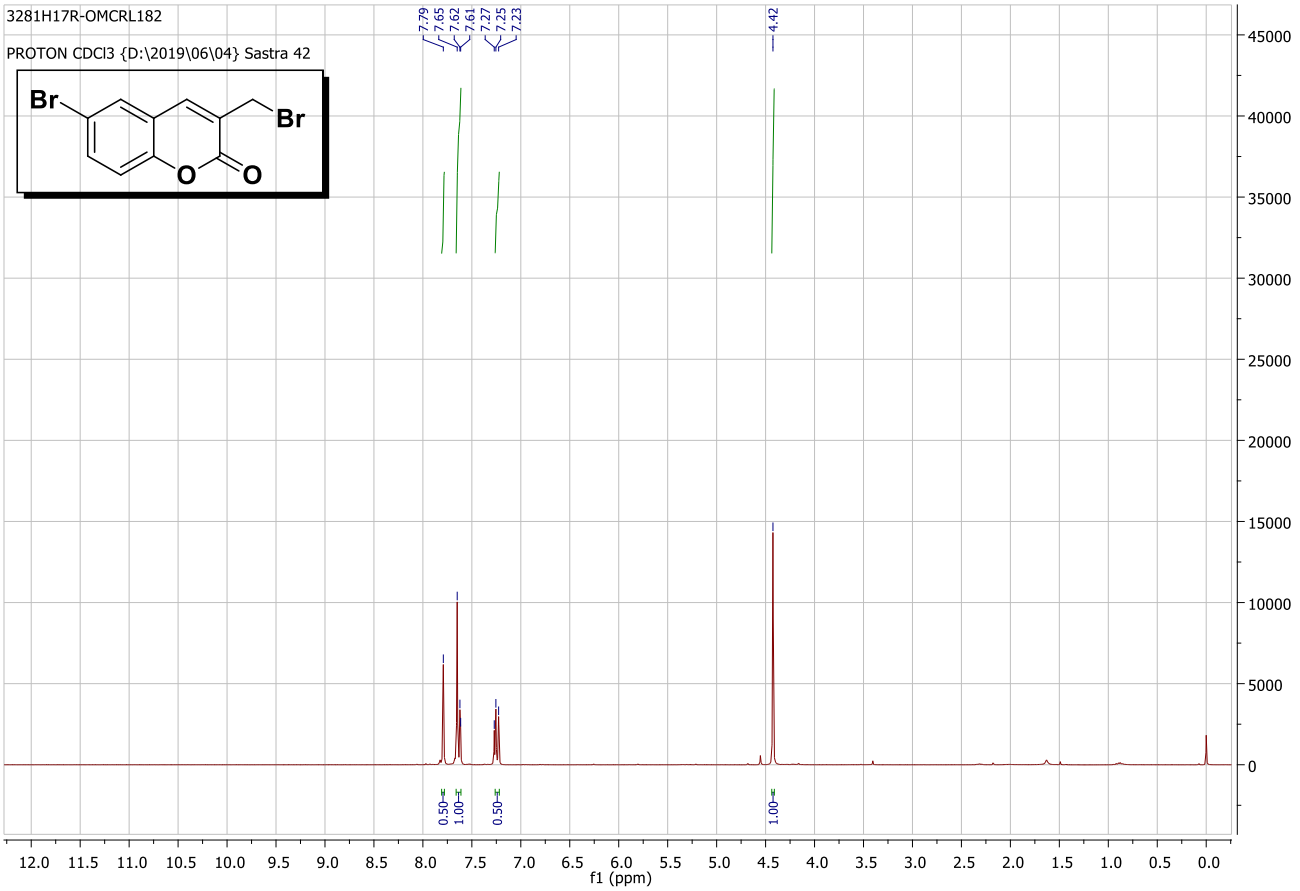

Figure S39 ^{1}H NMR spectrum of 6-bromo-3-(bromomethyl)-2*H*-chromen-2-one (**4c**)

Carbon NMR spectrum of 6-bromo-3-(bromomethyl)-2*H*-chromen-2-one (4c)

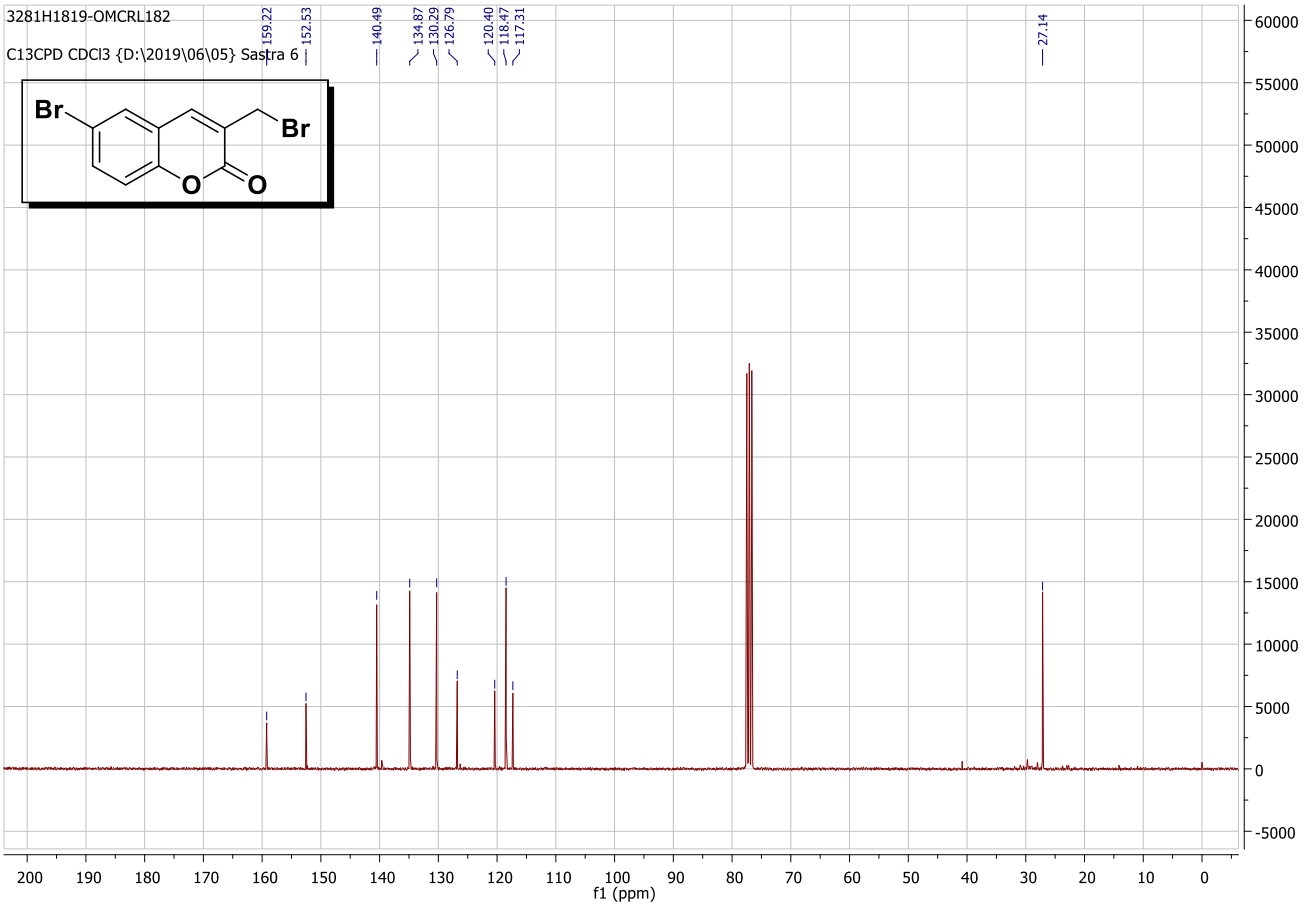

Figure S40 ^{13}C NMR spectrum of 6-bromo-3-(bromomethyl)-2*H*-chromen-2-one (**4c**)

Spectral data of (*E*)/(*Z*)-cinnamyl-1*H*-triazoles 3a–q

(*E*)-Methyl 2-((4-hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylate (3a)

Yield: 295 mg (83%); white solid; mp 92-94 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.83 (s, 3H, estr-CH_3), 4.78 (s, 2H, Trz-CH_2), 5.37 (s, 2H, Trz-CH_2OH), 7.43-7.45 (m, 3H, Aro-H), 7.61-7.64 (m, 2H, Aro-H), 7.74 (s, 1H, Trz-CH), 8.08 (s, 1H, Alkene-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 47.23, 52.98, 56.75, 123.15, 125.30, 129.39, 130.07, 130.43, 133.91, 146.44, 147.84, 167.52.

HRMS: m/z Calcd for $C_{14}H_{15}N_3O_3$ $[M+H]^+$: 274.1113; found: 274.1136.

(*E*)-Methyl 3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3b) [2]

Yield: 365 mg (88%); yellowish white solid; mp 114-116 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.84 (s, 3H, estr-CH_3), 5.42 (s, 2H, Trz-CH_2), 7.38-7.48 (m, 5H, Aro-H), 7.68-7.85 (m, 5H, Aro-H), 7.98 (s, 1H, Trz-CH), 8.10 (s, 1H, Alkene-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 47.34, 53.02, 121.20, 125.39, 126.14, 126.50, 128.54, 129.22, 129.33, 129.41, 130.18, 130.46, 133.95, 146.55, 147.92, 167.69.

HRMS: m/z Calcd for $C_{19}H_{17}N_3O_2$ $[M+H]^+$: 320.1321; found: 320.1311.

(*E*)-Ethyl 2-((4-hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylate (3c)

Yield: 278 mg (80%); white solid; mp 81-83 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 1.30-1.34 (t, *J* = 6 Hz, 3H, estr-CH_3), 3.50 (s, 1H, CH_2-OH), 4.24-4.31 (q, *J* = 6Hz, 2H, estr-CH_2), 4.78 (s, 2H, Trz-CH_2), 5.36 (s, 2H, Trz-CH_2OH), 7.41-7.61 (m, 5H, Aro-H), 7.74 (s, 1H, Trz-CH), 8.07 (s, 1H, Alkene-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 14.59, 47.22, 56.73, 62.03, 123.14, 125.64, 129.35, 130.04, 130.32, 133.99, 146.09, 147.86, 167.02.

HRMS: m/z Calcd for $C_{15}H_{17}N_3O_3$ $[M+H]^+$: 288.1270; found: 288.1258.

(*E*)-Ethyl 3-phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3d) [1]

Yield: 331 mg (82%); white crystals; mp 100-102 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 1.29-1.34 (t, *J* = 6 Hz, 3H, estr-CH_3), 4.24-4.31 (q, *J* = 6 Hz, 2H, estr-CH_2), 5.40 (s, 2H, Trz-CH_2), 7.30-7.85 (m, 10H, Aro-H), 7.98 (s, 1H, Trz-CH), 8.08 (s, 1H, Alkene-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 14.60, 47.27, 61.95, 121.10, 125.92, 126.09, 128.40, 129.16, 129.33, 130.10, 130.27, 131.19, 134.12, 145.99, 147.82, 167.04.

HRMS: m/z Calcd for $C_{20}H_{19}N_3O_2$ $[M+H]^+$: 334.1477; found: 334.1453.

(*Z*)-2-((4-(Hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-phenylacrylonitrile (3e) [2]

Yield: 339 mg (90%); yellowish solid; mp 103-105 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 2.86 (s, 1H, Trz-CH_2-OH), 4.53 (s, 2H, Trz-CH_2), 5.09 (s, 2H, Trz-CH_2-OH), 7.15 (s, 1H, Alkene-CH), 7.22-7.55 (m, 5H, Aro-H), 7.64 (s, 1H, Trz-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 58.51, 61.15, 110.21, 122.11, 127.67, 134.16, 134.36, 136.57, 137.46, 153.20, 154.41.

HRMS: m/z Calcd for $C_{13}H_{12}N_4O$ $[M+H]^+$: 241.1011; found: 241.1023.

(*Z*)-3-Phenyl-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylonitrile (3f) [2]

Yield: 413 mg (92%); white crystals; mp 128-130 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 5.30 (s, 2H, Trz-CH_2), 7.33-7.84 (m, 10H, Aro-H), 7.87 (s, 1H, Alkene-CH), 7.98 (s, 1H, Trz-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 54.03, 104.94, 117.41, 120.28, 126.25, 128.88, 129.32, 129.49, 129.71, 130.52, 132.04, 132.48, 148.56, 149.01.

HRMS: m/z Calcd for $C_{18}H_{14}N_4$ $[M+H]^+$: 287.1218; found: 287.1209.

(*E*)-Methyl 3-(4-chlorophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazole-1-yl)methyl)acrylate (3g)

Yield: 244 mg (72%); white solid; mp 125-127 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.38 (s, 1H, Trz-CH_2OH), 3.82 (s, 3H, estr-CH_3), 4.77 (s, 2H, Trz-CH_2), 5.31 (s, 2H, Trz-CH_2OH), 7.40-7.43 (d, *J* = 9 Hz, 2H, Aro-H), 7.61-7.63 (d, *J* = 6 Hz, 2H, Aro-H), 7.75 (s, 1H, Trz-CH), 7.99 (s, 1H, Alkene-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 47.03, 52.99, 56.74, 123.32, 125.95, 129.65, 131.45, 132.33, 136.60, 144.88, 167.27.

HRMS: m/z Calcd for $C_{14}H_{14}ClN_3O_3$ $[M+H]^+$: 308.0724; found: 308.0719.

(*E*)-Methyl 3-(4-chlorophenyl)-2-(4-phenyl-1*H*-1,2,3-triazole-1-yl)methyl)acrylate (3h) [2]

Yield: 304 mg (78%); white solid; mp 141-143 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.76 (s, 3H, estr-CH_3), 5.29 (s, 2H, Trz-CH_2), 7.33-7.38 (m, 5H, Aro-H), 7.62-7.65 (d, *J*= 9Hz, 2H, Aro-H), 7.80-7.82 (d, *J*= 6Hz, 2H, Aro-H), 7.93 (s, 1H, Trz-CH), 8.01 (s, 1H, Alkene-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 47.11, 53.00, 121.67, 125.95, 126.05, 128.53, 129.22, 129.56, 130.92, 131.60, 132.40, 136.41, 144.77, 147.76, 167.29.

HRMS: m/z Calcd for $C_{19}H_{16}ClN_3O_2$ $[M+H]^+$: 354.0931; found: 354.0928.

(*E*)-Methyl 3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3i)

Yield: 259 mg (80%); white solid; mp 116-118 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.83 (s, 3H, estr-CH_3), 4.79 (s, 2H, Trz-CH_2), 5.32 (s, 2H, Trz-CH_2OH), 7.58 (s, 4H, Aro-H), 7.77 (s, 1H, Trz-CH), 7.98 (s, 1H, Alkene-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 47.05, 53.07, 56.63, 123.46, 124.98, 125.98, 131.66, 132.64, 132.75, 144.99, 147.82, 167.28.

HRMS: m/z Calcd for $C_{14}H_{14}BrN_3O_3$ $[M+H]^+$: 352.0219; found: 352.0210.

(*E*)-Methyl 3-(4-bromophenyl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3j)

Yield: 308 mg (84%); yellow solid; mp 132-134 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.85 (s, 3H, estr-CH_3), 5.38 (s, 2H, Trz-CH_2), 7.34-7.86 (m, 9H, Aro-H), 8.01 (s, 1H, Trz-CH), 8.02 (s, 1H, Alkene-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 47.13, 53.07, 121.40, 125.02, 126.10, 128.55, 129.22, 130.94, 131.77, 132.65, 132.80, 145.02, 147.91, 167.40.

HRMS: m/z Calcd for $C_{19}H_{16}BrN_3O_2$ $[M+H]^+$: 398.0426; found: 398.0435.

(*E*)-Ethyl 3-(4-bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3k)

Yield: 250 mg (78%); white solid; mp 110-112 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 1.30-1.34 (t, *J* = 6 Hz, 3H, estr-CH_3), 3.09 (s, 1H, CH_2-OH), 4.23-4.31 (q, *J* = 9 Hz, 2H, estr-CH_2), 4.78 (s, 2H, Trz-CH_2), 5.31 (s, 2H, Trz-CH_2-OH), 7.57-7.64 (m, 4H, Aro-H), 7.75 (s, 1H, Trz-CH), 7.97 (s, 1H, Alkene-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 14.60, 47.06, 56.78, 62.17, 123.42, 124.90, 126.29, 131.65, 132.62, 132.83, 144.69, 147.82, 166.80.

HRMS: m/z Calcd for $C_{15}H_{16}BrN_3O_3$ $[M+H]^+$: 366.0375; found: 366.0383.

(*Z*)-3-(4-Bromophenyl)-2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)acrylonitrile(3l)

Yield: 274 mg (82%); white solid; mp 114-116 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 4.65 (s, 2H, Trz-CH_2), 5.17 (s, 2H, Trz-CH_2-OH), 7.28-7.31 (d, *J* = 9 Hz, 2H, Aro-H), 7.39 (s, 1H, Alkene-CH), 7.48-7.51, (d, *J* = 9 Hz, 2H, Aro-H), 7.69 (s, 1H, Trz-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 48.01, 56.34, 109.87, 118.21, 123.04, 125.43, 131.23, 132.69, 134.36, 147.93, 149.54.

HRMS: m/z Calcd for $C_{13}H_{11}BrN_4O$ $[M+H]^+$: 319.0116; found: 319.0125.

(*E*)-Methyl 2-((4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3-(4-nitrophenyl)acrylate (3m)

Yield: 291 mg (87%); yellow solid; mp 143-145 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 2.77 (s, 1H, Trz-CH_2OH), 3.86 (s, 3H, estr-CH_3), 4.80 (s, 2H, Trz-CH_2), 5.29 (s, 2H, Trz-CH_2-OH), 7.78 (s, 1H, Trz-CH), 7.90-7.92 (d, *J* = 6 Hz, 2H, Aro-H), 8.06 (s, 1H, Alkene-CH), 8.30-8.33 (d,*J* = 9 Hz, 2H, Aro-H).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 46.67, 53.16, 56.56, 123.61, 124.34, 128.70, 130.86, 140.31, 143.04, 148.46, 148.60, 166.53.

HRMS: m/z Calcd for $C_{14}H_{14}N_4O_5$ $[M+H]^+$: 319.0964; found: 319.0954.

(*E*)-Methyl 3-(furan-2-yl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3n)

Yield: 339 mg (80%); reddish oil.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.84 (s, 3H, estr-CH_3), 5.74 (s, 2H, Trz-CH_2), 6.56 (s, 1H, Het-H), 6.98 (s, 1H, Aro-H), 7.30-7.32 (d, *J* = 6Hz, 1H, Het-H), 7.37-7.42 (m, 2H, Aro-H), 7.64 (s, 1H, Trz-CH), 7.73 (s, 1H, Alkene-CH), 7.79-7.82 (m, 2H, Aro-H), 7.84 (s, broad, 1H, Het-H).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 47.19, 53.03, 113.20, 119.94, 120.31, 126.11, 128.44, 129.15, 130.99, 131.27, 146.86, 150.15, 167.78.

HRMS: m/z Calcd for $C_{17}H_{15}N_3O_3$ $[M+H]^+$: 310.1113; found: 310.1122.

(*E*)-Ethyl 3-(furan-2-yl)-2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)acrylate (3o)

Yield: 313 mg (76%); yellowish solid; mp 95-97 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 1.28-1.32 (t, *J* = 6Hz, 3H, estr-CH_3), 4.23-4.29 (q, *J* = 6Hz, 2H, estr-CH_2), 5.72 (s, 2H, Trz-CH_2), 6.54 (s, 1H, Het-H), 6.97 (s, 1H, Aro-H), 7.30-7.39 (m, 3H, Aro-H& Het-H), 7.61 (s, 1H, Trz-CH), 7.71 (s, 1H, Alkene-CH), 7.78-7.81 (m, 2H, Aro-H), 7.85 (s, broad, 1H, Het-H).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 14.65, 47.11, 61.98, 113.16, 119.71, 120.21, 120.73, 126.02, 128.32, 129.12, 130.90, 131.19, 146.71, 147.75, 150.20, 167.22.

HRMS: m/z Calcd for $C_{18}H_{17}N_3O_3$ $[M+H]^+$: 324.1270; found: 324.1256.

(*E*)-Methyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-3-(thiophen-2-yl)acrylate (3p)

Yield: 307 mg (75%); yellowish solid; mp 107-109 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.87 (s, 3H, estr-CH_3), 5.63 (s, 2H, Trz-CH_2), 7.19 (m, 1H, Aro-H), 7.34 (m, 1H, Het-H), 7.41-7.42 (m, 2H, Aro-H), 7.61 (s, 1H, Trz-CH), 7.70 (s, 1H,Alkene-CH), 7.82-7.84 (m, 2H, Aro-H), 7.90 (m, 1H, Het-H), 8.17 (s, 1H, Het-H).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 30.10, 53.09, 120.23, 128.47, 128.90, 129.16, 129.33, 130.98, 132.11, 134.69, 136.72, 138.28, 148.00, 167.80.

HRMS: m/z Calcd for $C_{17}H_{15}N_3O_2S$ $[M+H]^+$: 326.0885; found: 326.0879.

(*E*)-Ethyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-3-(thiophen-2-yl)acrylate (3q)

Yield: 279 mg (70%); yellow oil.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 1.37-1.41 (t, *J* = 6Hz, 3H, estr-CH_3), 4.35-4.41 (q,*J* = 6Hz, 2H, estr-CH_2), 4.47 (s, 2H, Trz-CH_2), 7.40 (s, 1H, Aro-H), 7.42 (s, 1H, Het-H), 7.46 (s, 1H, Aro-H), 7.48 (s, 1H, Aro-H), 7.50 (s, 1H, Het-H), 7.84 (s, 1H, Trz-CH), 7.86 (s, 1H, Alkene-CH), 7.91-7.93 (m, 1H, Aro-H), 8.01 (s, 2H, Aro-H& Het-H),

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 14.28, 46.98, 61.06, 125.75, 126.14, 126.60, 128.75, 129.00, 131.06, 131.64, 133.13, 134.26, 134.97, 137.70, 147.08, 166.98.

HRMS: m/z Calcd for $C_{18}H_{17}N_3O_2S$ $[M+H]^+$: 340.1041; found: 340.1029.

Spectral data of 3-(bromomethyl)-2*H*-chromen-2-one 4a–c

3-(Bromomethyl)-2*H*-chromen-2-one (4a) [3]

Yield: 186 mg (78%); White crystal; mp 112-114 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 4.55-4.57 (d, *J* = 6Hz, 2H, CH_2-Br), 7.31-7.57 (m,4H, Aro-H), 7.89-7.91 (d,*J* = 6Hz, 1H, Alkene-CH).

^{13}C NMR ($CDCl_3$, 300 MHz): δ = 41.49, 117.02, 119.16, 125.14, 125.33, 128.50, 132.45, 141.62, 153.90, 160.47.

HRMS: m/z Calcd for $C_{10}H_7BrO_2$ $[M+H]^+$: 238.9629; found: 238.9618.

3-(Bromomethyl)-8-methoxy-2*H*-chromen-2-one (4b)

Yield: 208 mg (87%); White crystals; mp 151-153 °C.

^{1}H NMR (DMSO-D_6, 300 MHz): δ = 3.92 (s, 3H, Aro-O-CH_3), 4.63 (s, 2H, CH_2-Br), 7.31-7.32 (m, 3H, Aro-H), 8.22 (s, 1H, Alkene-CH).

^{13}C NMR (DMSO-D_6, 300 MHz): δ = 42.02, 56.61, 115.10, 119.63, 120.28, 125.22, 125.26, 143.01, 143.23, 146.88, 159.50.

HRMS: m/z Calcd for $C_{11}H_9BrO_3$ $[M+H]^+$: 267.9735; found: 267.9724.

6-Bromo-3-(bromomethyl)-2*H*-chromen-2-one (4c)

Yield: 181 mg (75%); White crystals; mp 125-127 °C.

^{1}H NMR (CDCl3, 300 MHz,): δ = 4.42 (s, 2H, CH_2-Br), 7.23-7.25 (d, *J* = 6 Hz, 1H, Aro-H), 7.61-7.62 (d, *J* = 3Hz, 1H, Aro-H), 7.65 (s, 1H, Aro-H), 7.79 (s, 1H, Alkene-CH).

^{13}C NMR (CDCl3, 300 MHz,): δ = 27.14, 117.31, 118.47, 120.40, 126.79, 130.29, 134.87, 140.49, 152.53, 159.22.

HRMS: m/z Calcd for $C_{10}H_6Br_2O_2$ $[M+H]^+$: 317.8714; found: 317.8703.

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