crystals

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Article

Design, Synthesis, and Evaluation of X-ray Crystal Structure, Biological Activities, DFT Calculations, and Molecular Docking of Phenyl Imidazolidin-2-One Derivatives

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Supplementary Materials

Table S1. Dihedral angles of phenyl or substituted phenyl ring and imidazolinone ring of calculated structures of compound **3a–h.**

Compounds	Angle (°)	Compounds	Angle (°)
3a	22.96	**3e**	26.21
3b	23.88	**3f**	21.69
3c	16.25	**3g**	21.36
3d	26.18	**3h**	23.81

Table S2. Hydrogen bond geometry.

Compounds	D–H···A	d(D–H)/(Å)	d(D···A)/(Å)	<(DHA)/(°)
3a	ASP84(C)–ASP84(O)···**3a** (H–N)	1.01	2.91	171.2
	TYR269(C)–TYR269(O)···**3a** (H–C)	1.08	3.24	153.0
3f	**3f**(C)–**3f**(O) ··· (H–C) ASN61	1.01	2.84	159.4
	ASN81(C)–ASN81(O)···**3f** (H–C)	1.08	3.07	119.3
3c	ASN81(C)–ASN81(O)···**3c**(H–C)	1.08	3.16	122.3
	3c(C)–**3c**(O)···ASN61 (H–C)	1.01	2.80	158.7
	3c(C)–**3c**(O)···PHE290 (H–C)	1.08	3.43	121.7
DPMF	ASP84(C)–ASP84(O)···DPMF (H–N)	1.02	2.84	172.0
	TYR269(C)–TYR269(O)···DPMF (H–C)	1.07	3.00	94.3

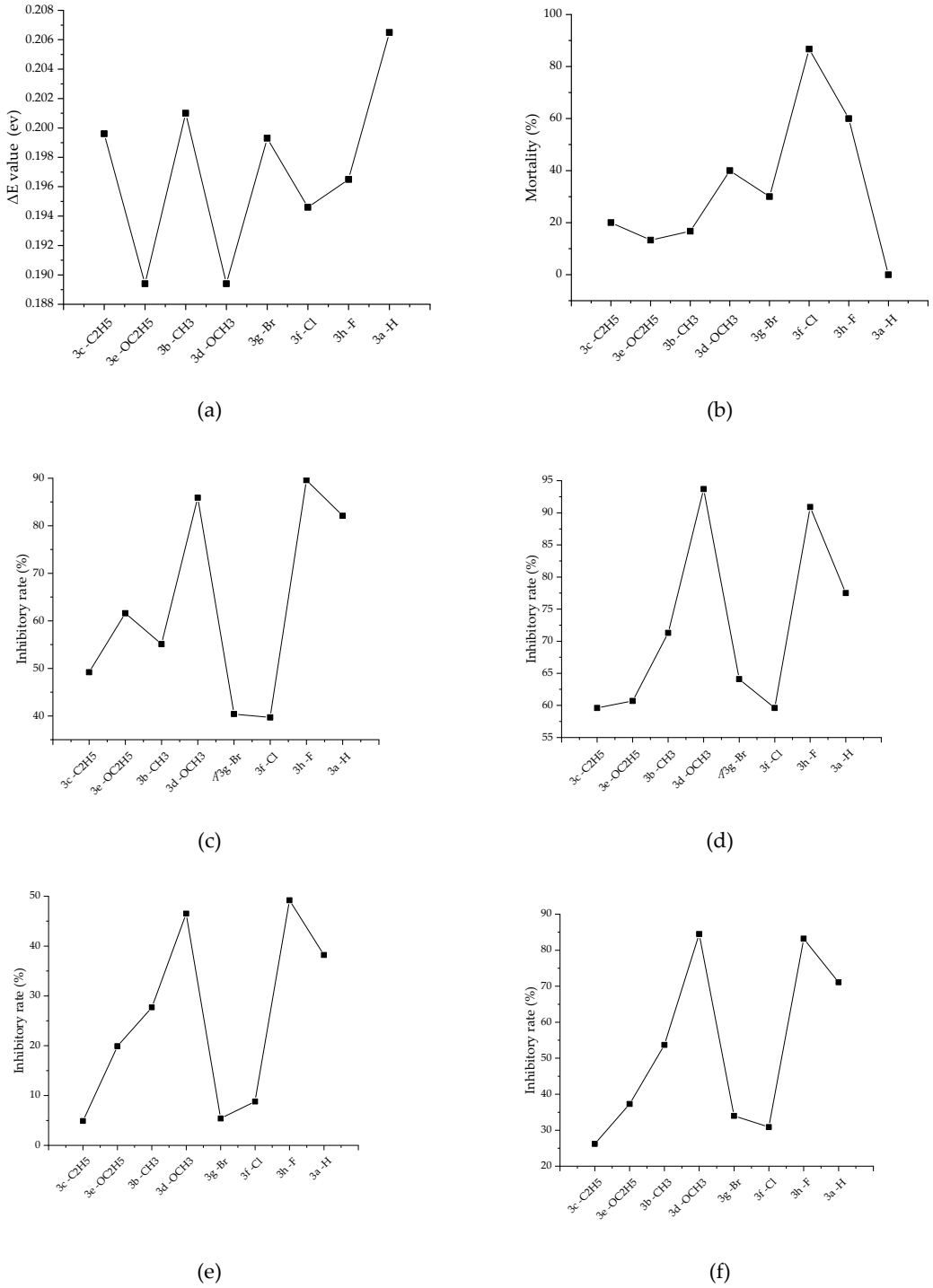


Figure S1. Steric effects of **3a–h** influencing the *Δ*E values (**a**), insecticidal activities against *P. xylostella* (**b**), and fungicidal activities against *P. infestans* (**c**), *P. capsic* (**d**), *P. litchi* (**e**), and *P. sojae* (**f**). (Steric effects show the following pattern: -C_2H_5 > -OC_2H_5 >-CH_3>-OCH_3; -Br >-Cl >-F >-H).

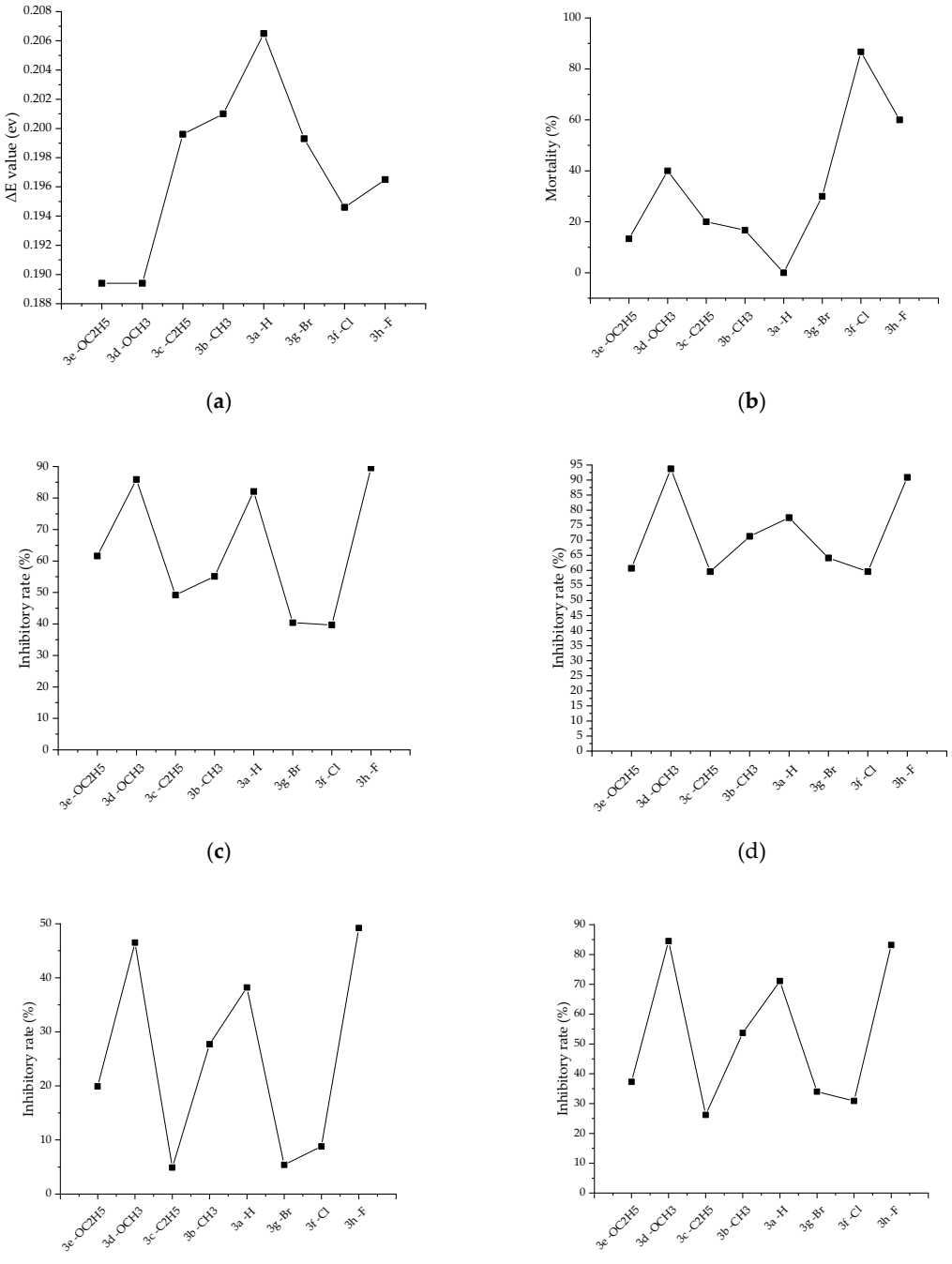
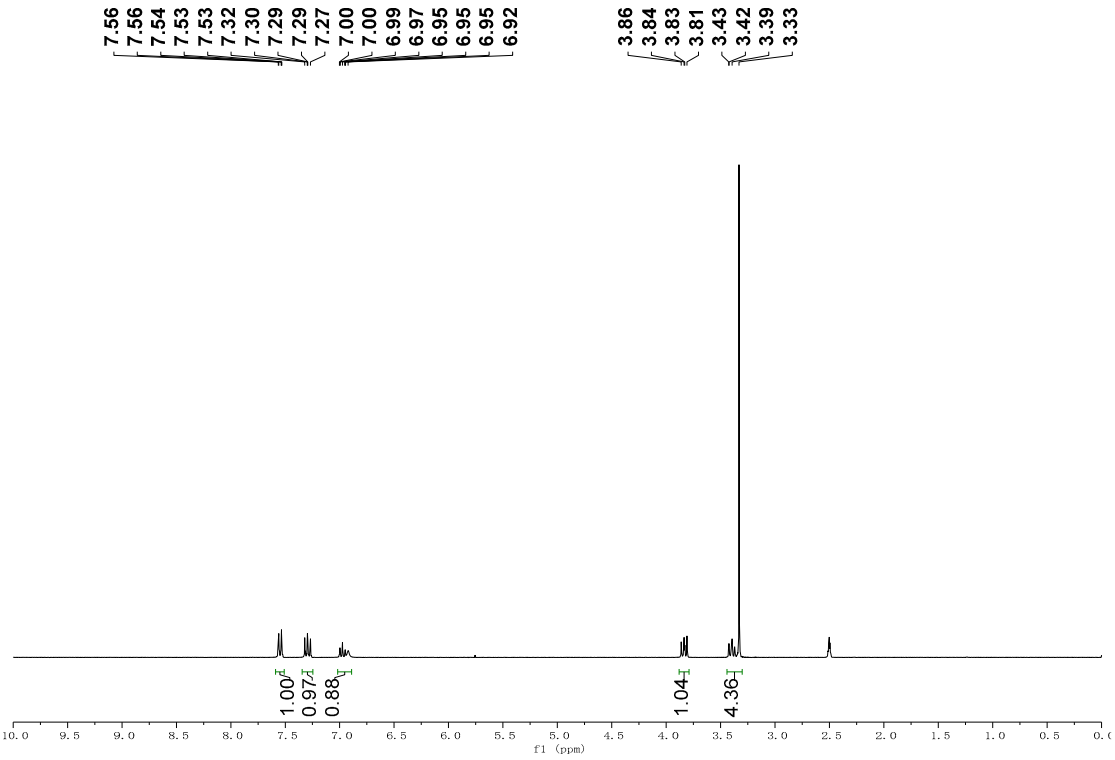


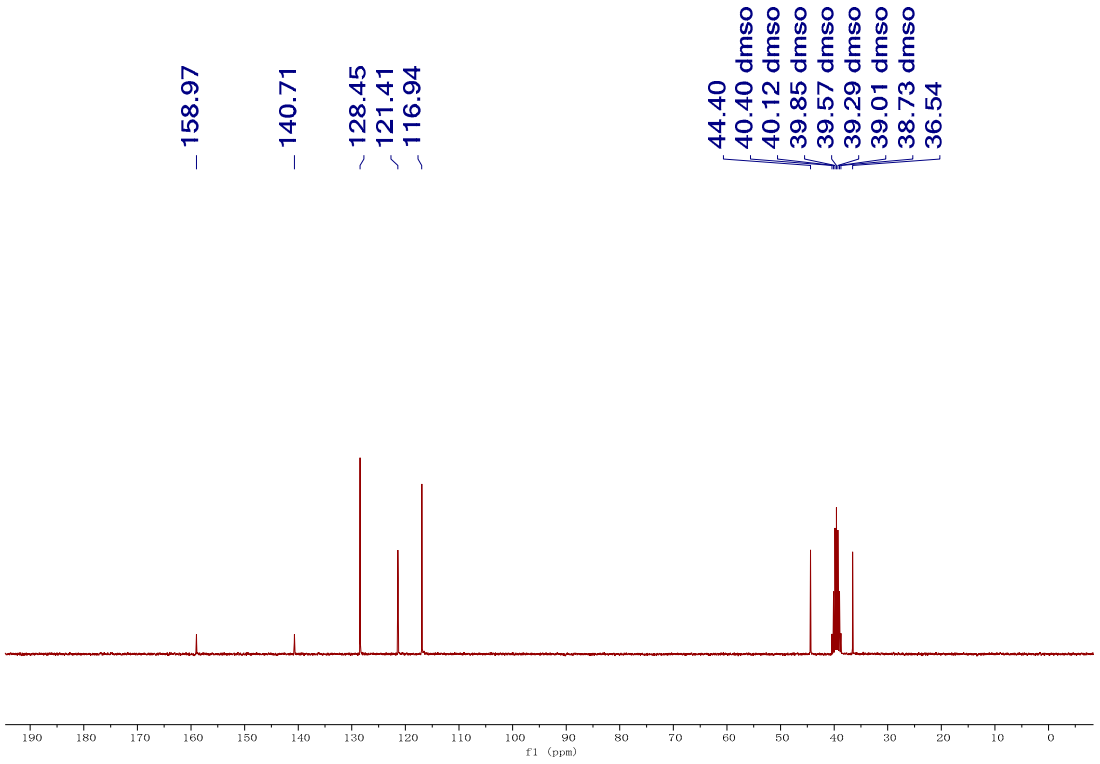
Figure S2. Electron donation/withdrawing properties of **3a–h** influencing the *Δ*E values (**a**), insecticidal activities against *P. xylostella* (**b**), and fungicidal activities against *P. infestans* (**c**), *P. capsic* (**d**), *P. litchi* (**e**), and *P. sojae* (**f**). (Electron donation property shows the following pattern: -OC_2H_5 > -OCH_3 > -C_2H_5 > -CH_3; Electron withdrawing property shows the following pattern: -Br < -Cl < -F).

1-phenylimidazolidin-2-one (**3a**)

^{1}H NMR spectrum

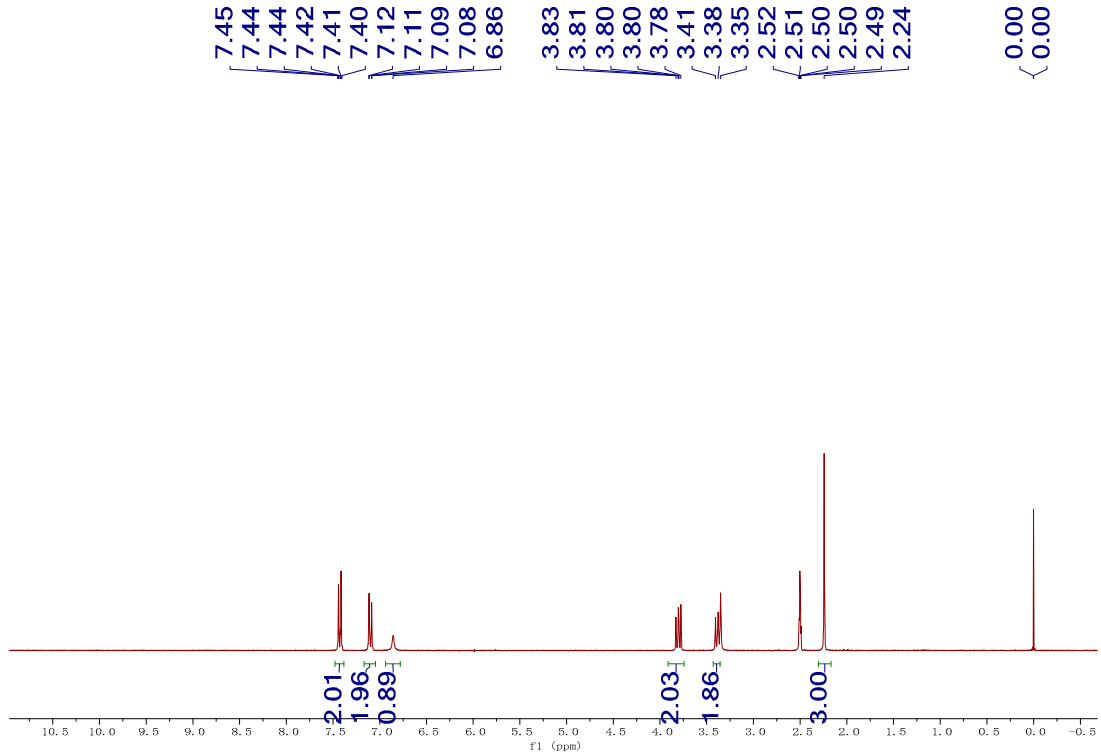


^{13}C NMR spectrum

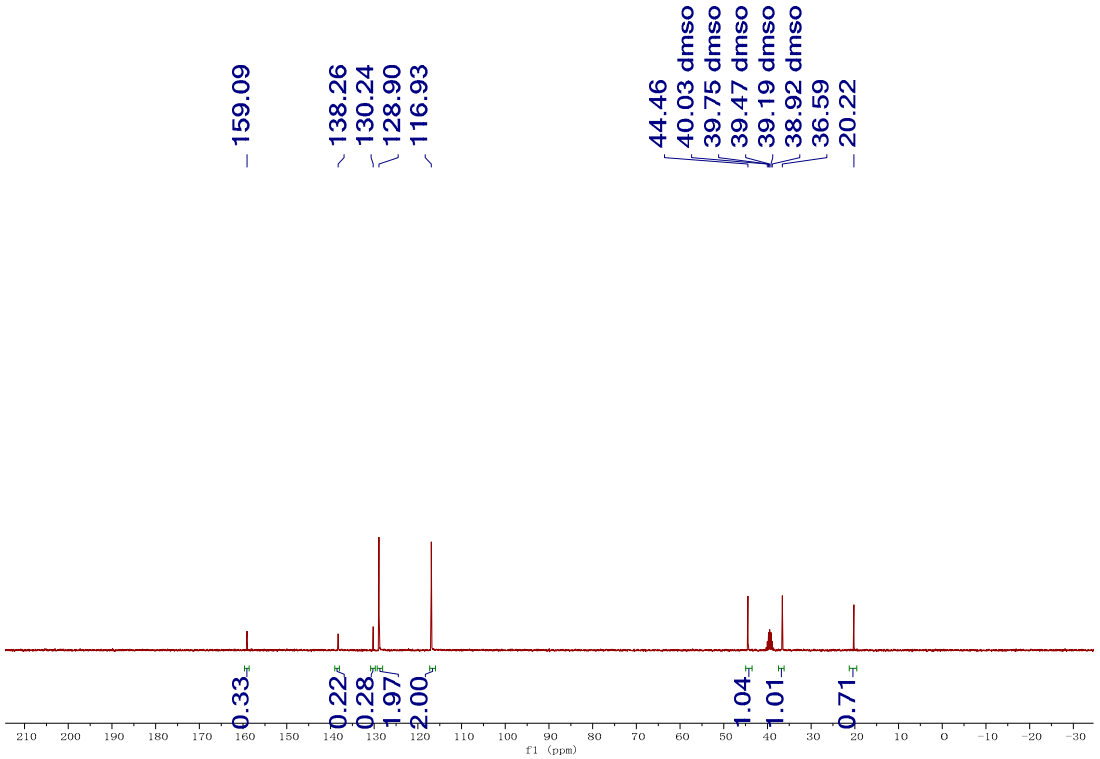


1-(4-methyl)imidazolidin-2-one (**3b**)

^{1}H NMR spectrum

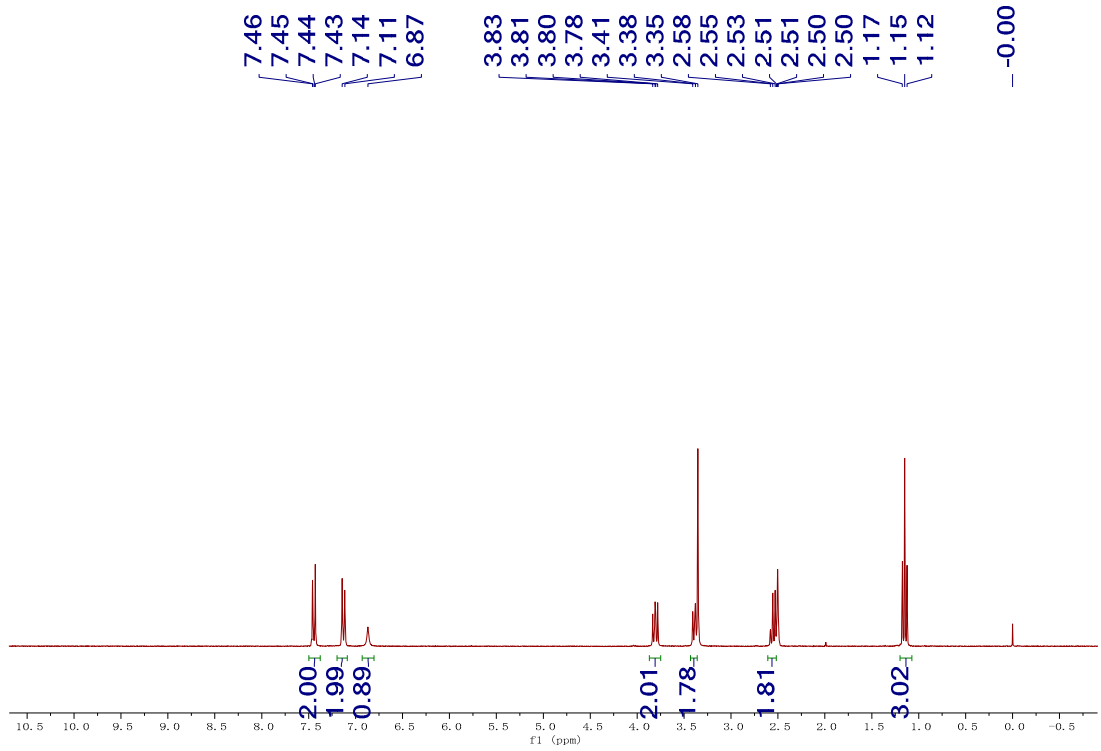


^{13}C NMR spectrum

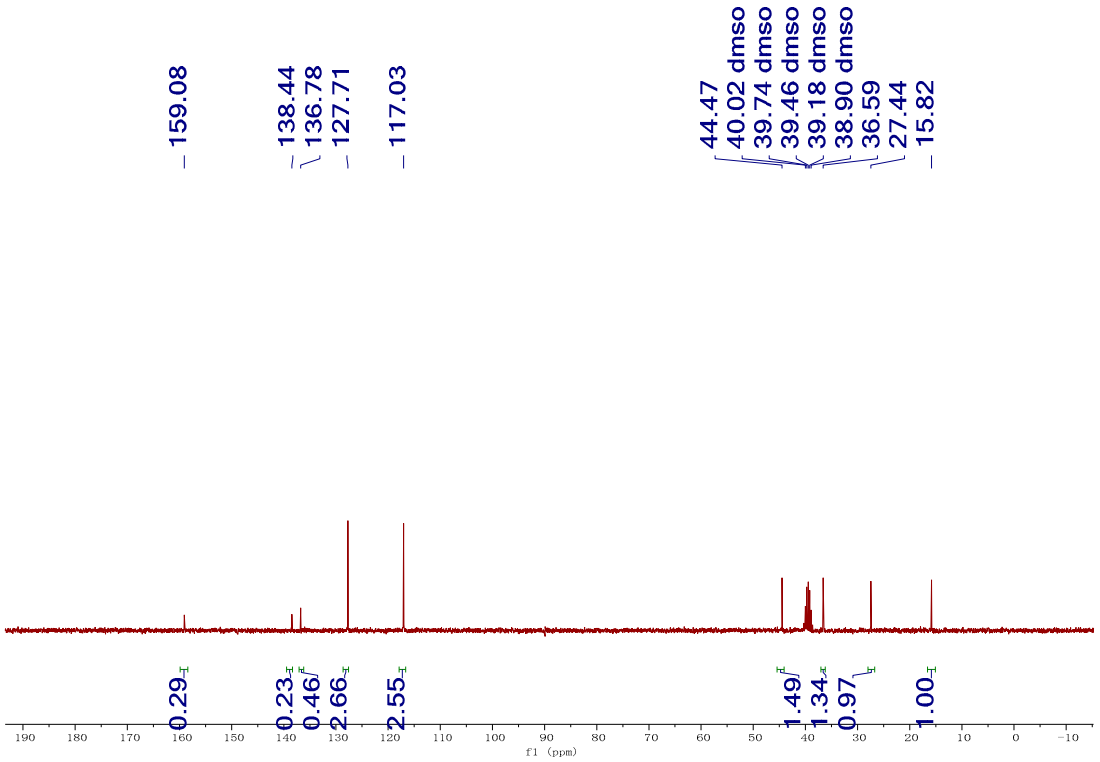


1-(4-ethylphenyl)imidazolidin-2-one (**3c**)

^{1}H NMR spectrum

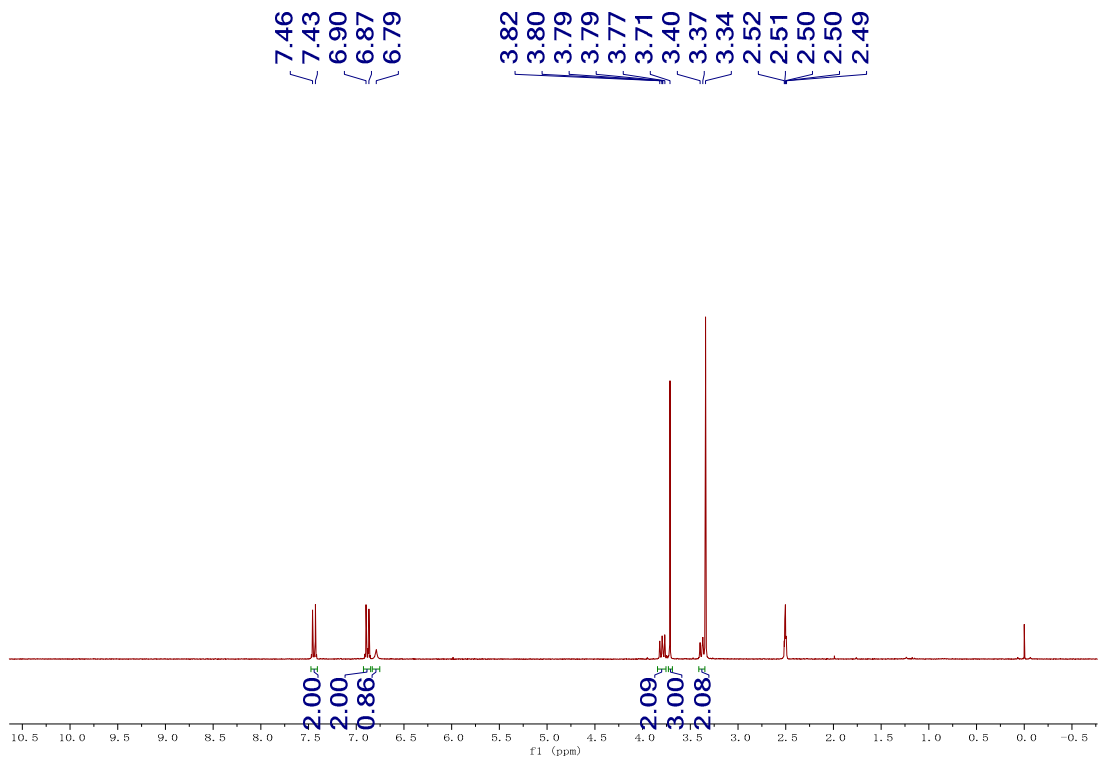


^{13}C NMR spectrum

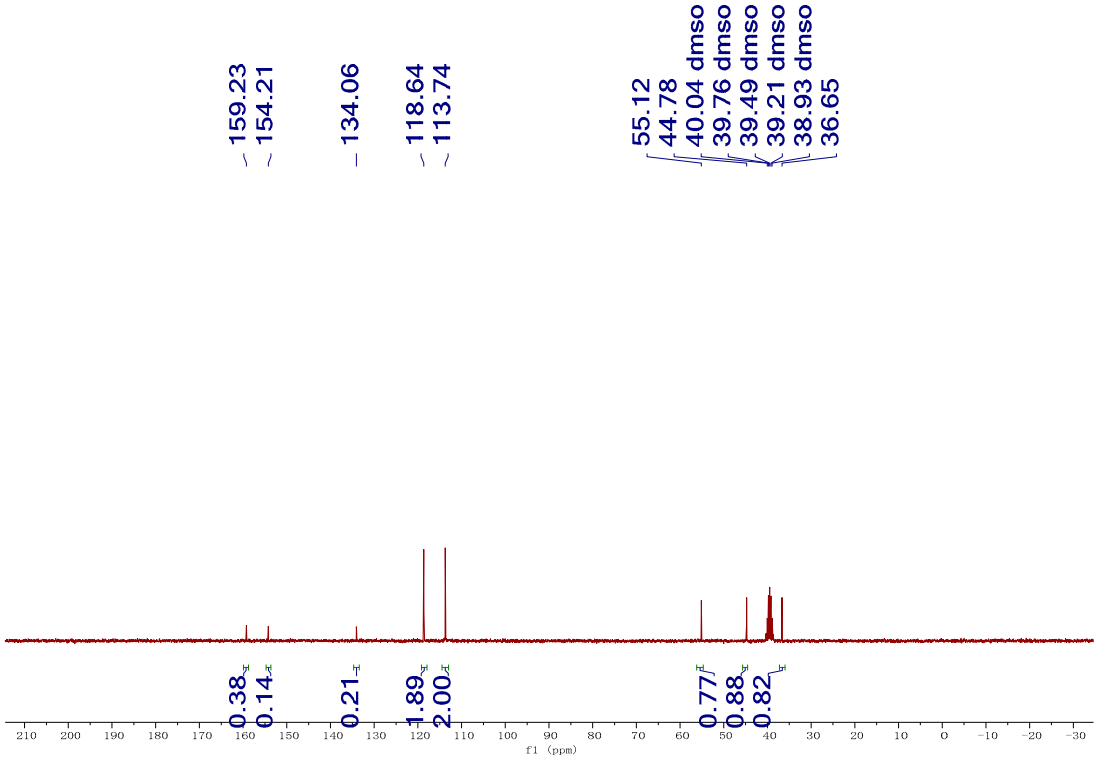


1-(4-methoxyphenyl)imidazolidin-2-one (**3d**)

^{1}H NMR spectrum

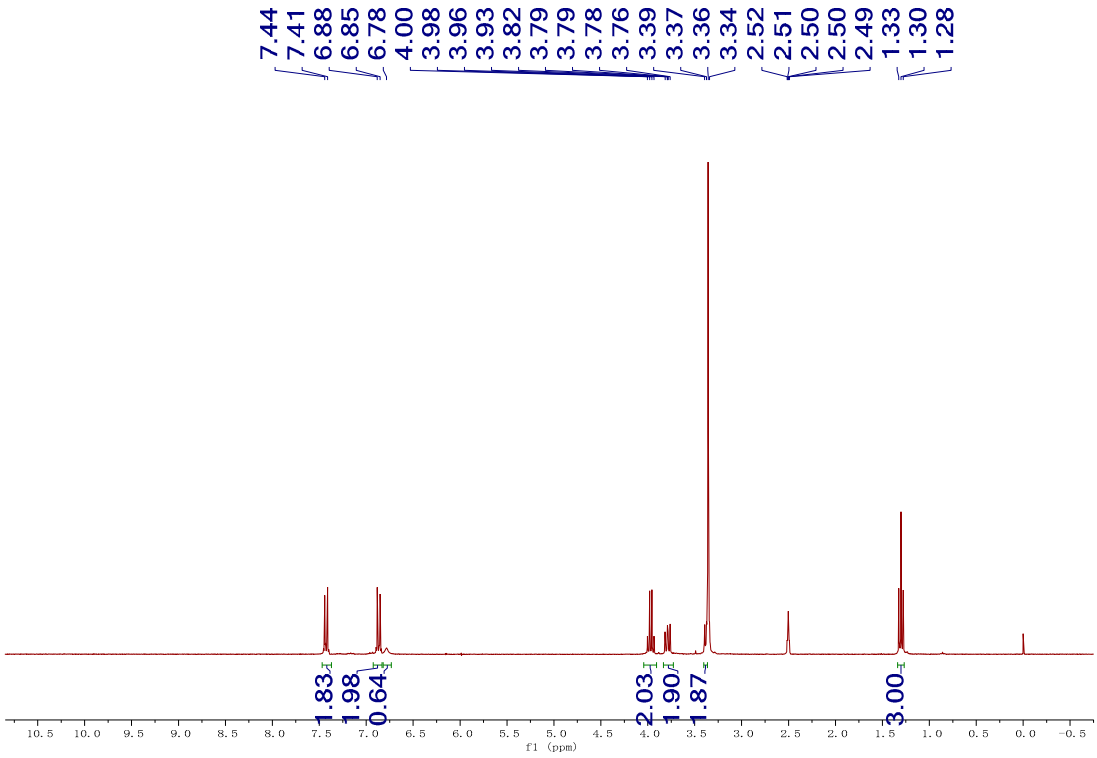


^{13}C NMR spectrum

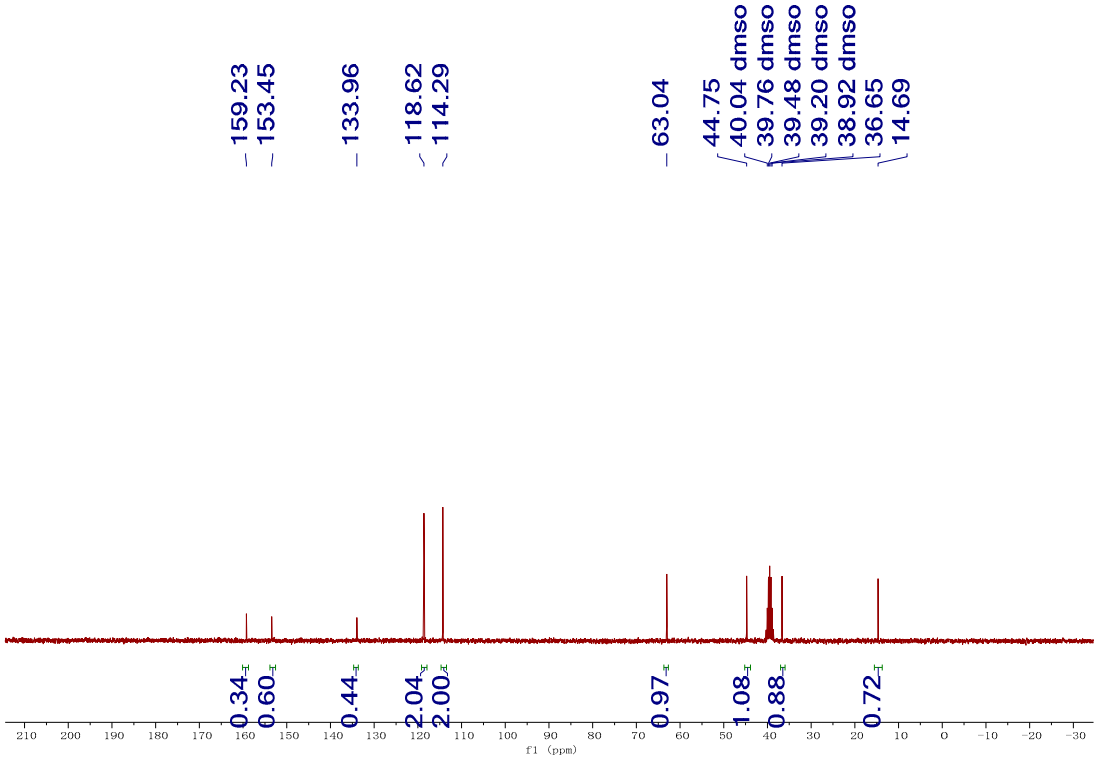


1-(4-ethoxyphenyl)imidazolidin-2-one (**3e**)

^{1}H NMR spectrum

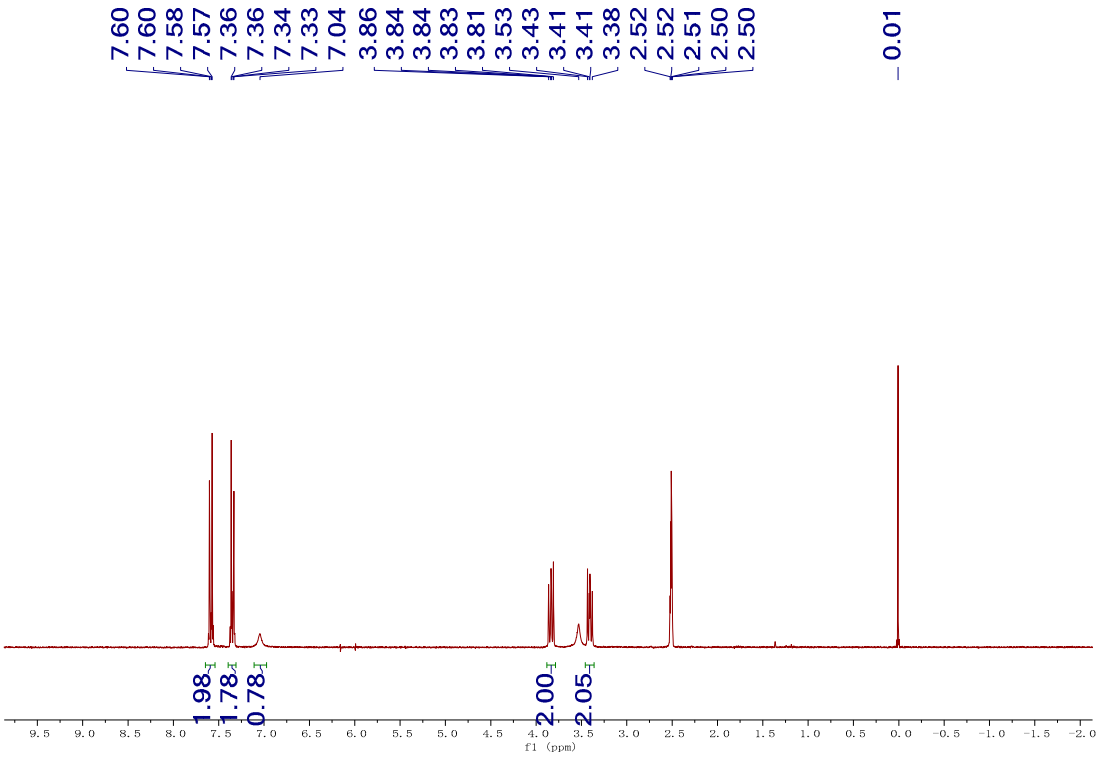


^{13}C NMR spectrum

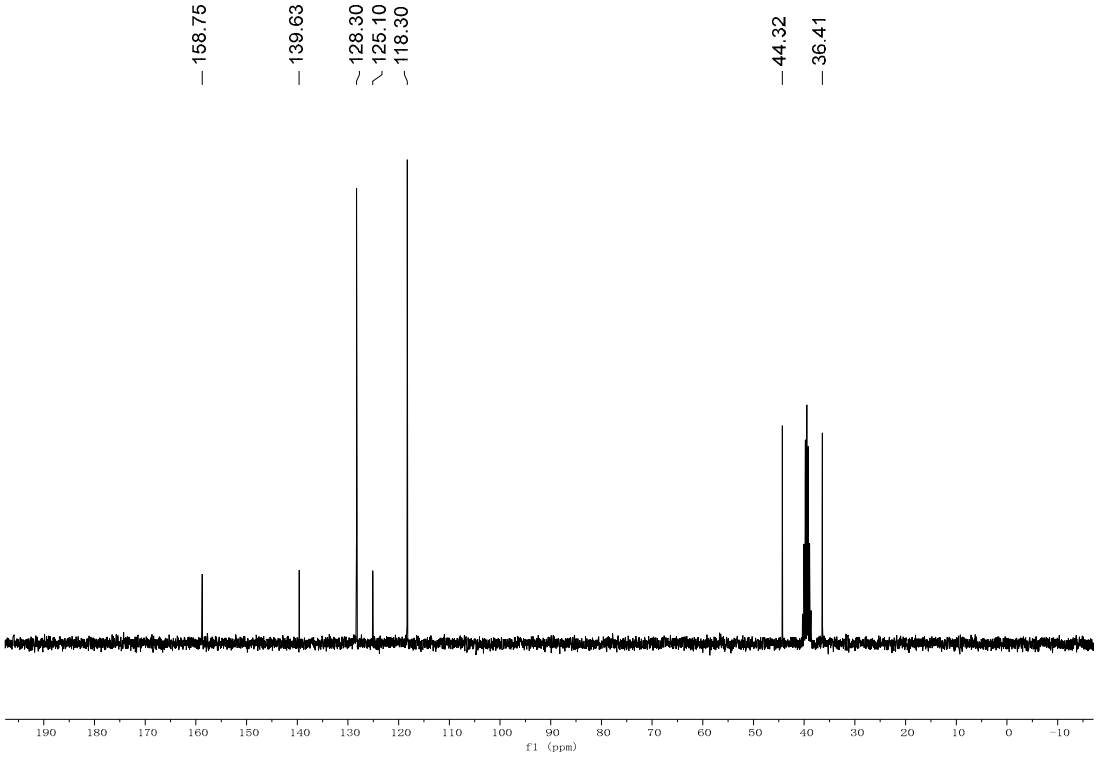


1-(4-chlorophenyl)imidazolidin-2-one (**3f**)

^{1}H NMR spectrum

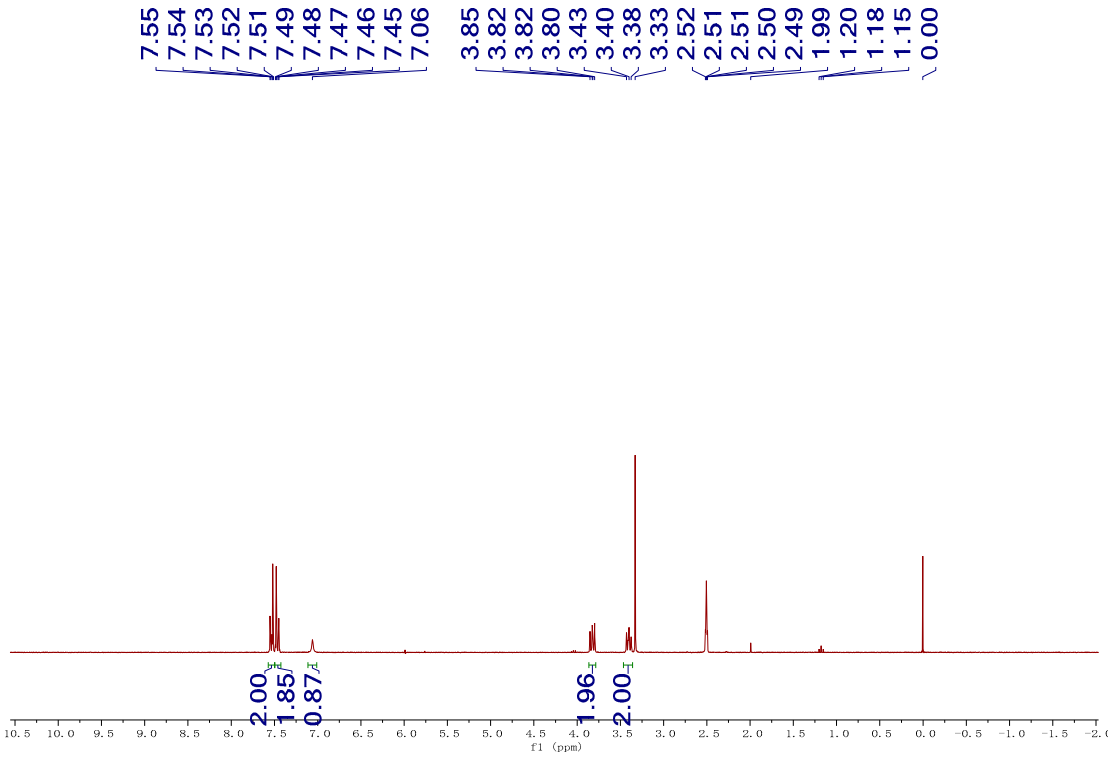


^{13}C NMR spectrum

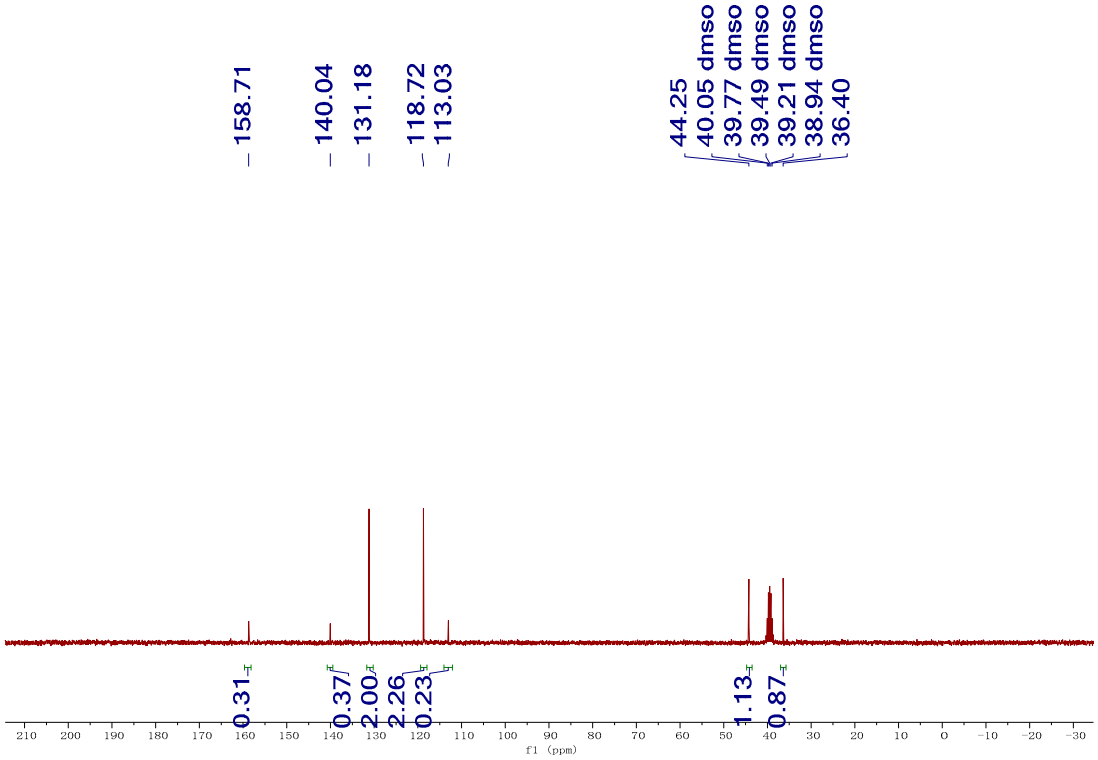


1-(4-bromophenyl)imidazolidin-2-one (**3g**)

^{1}H NMR spectrum

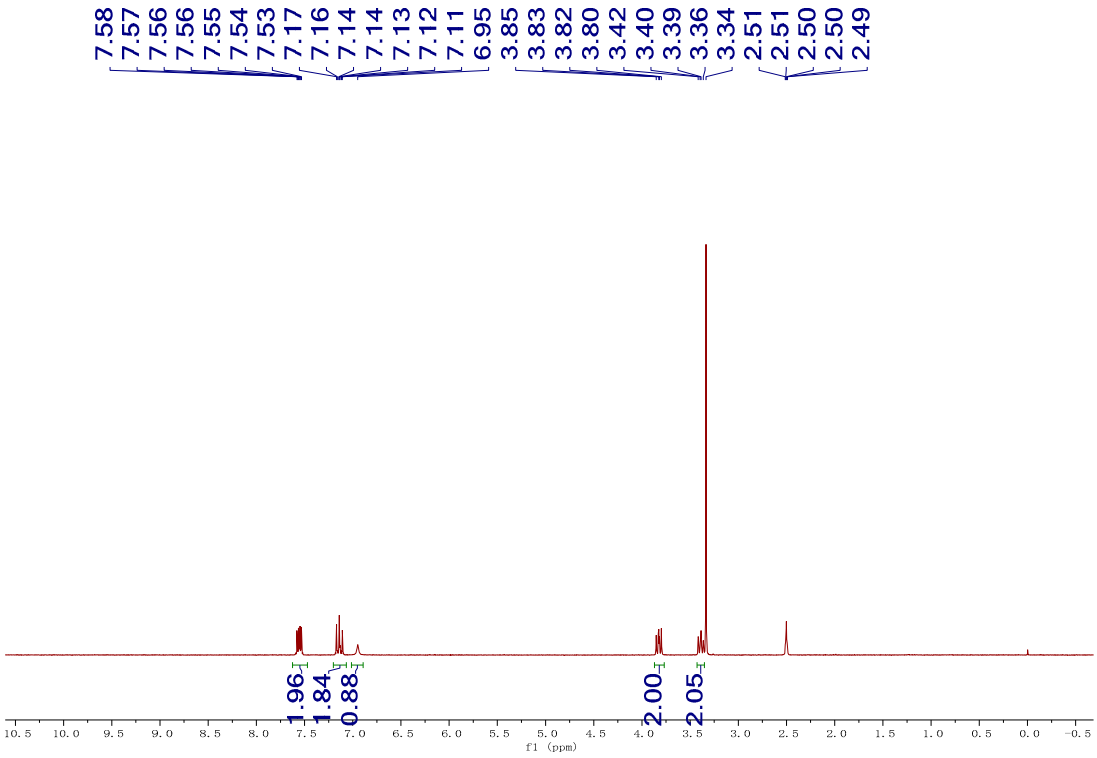


^{13}C NMR spectrum



1-(4-fluorophenyl)imidazolidin-2-one (**3h**)

^{1}H NMR spectrum



^{13}C NMR spectrum