

Synthesis of 1,5-Substituted Pyrrolidin-2-ones from Donor-Acceptor Cyclopropanes and Anilines/Benzylamines

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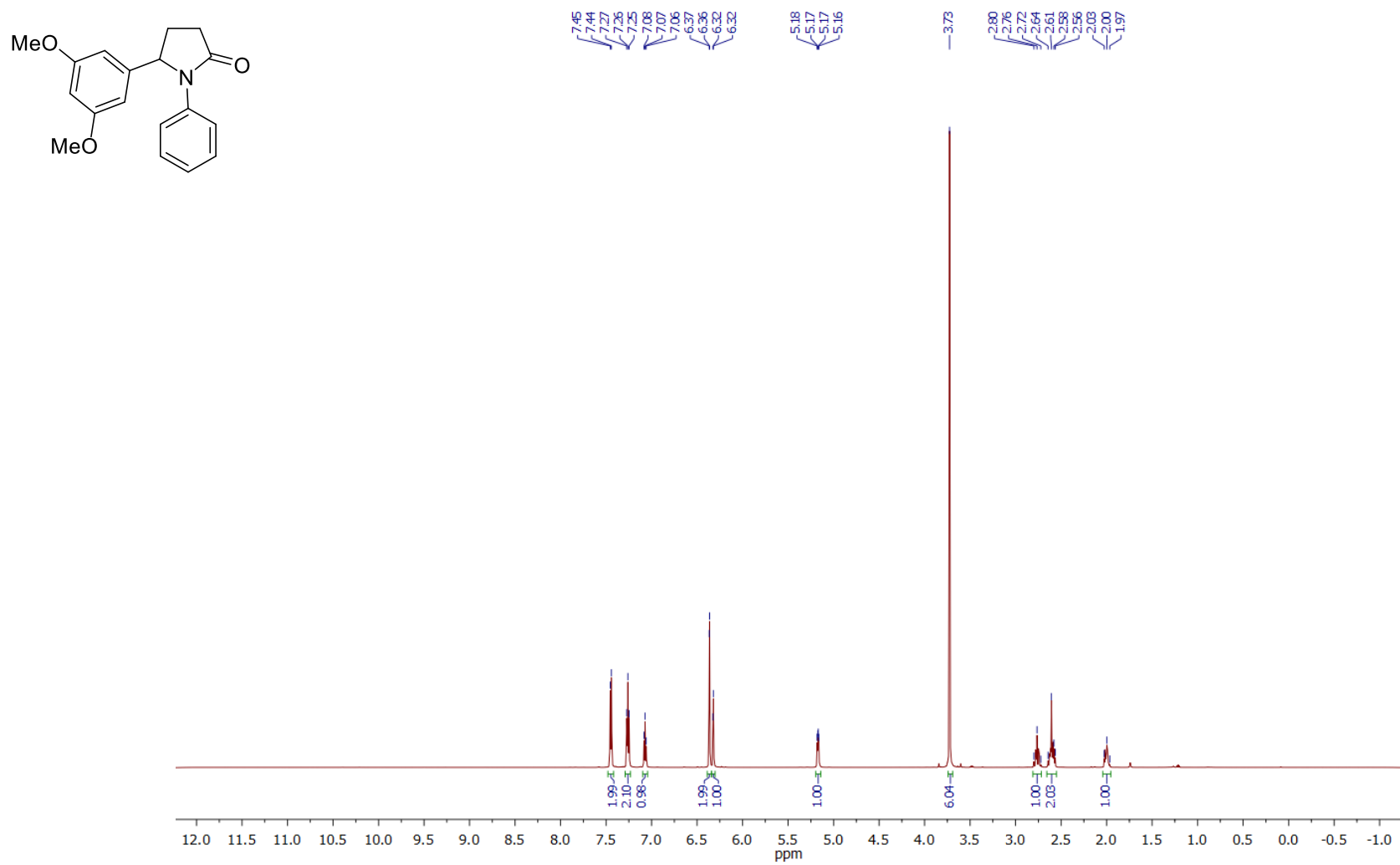
SUPPORTING INFORMATION

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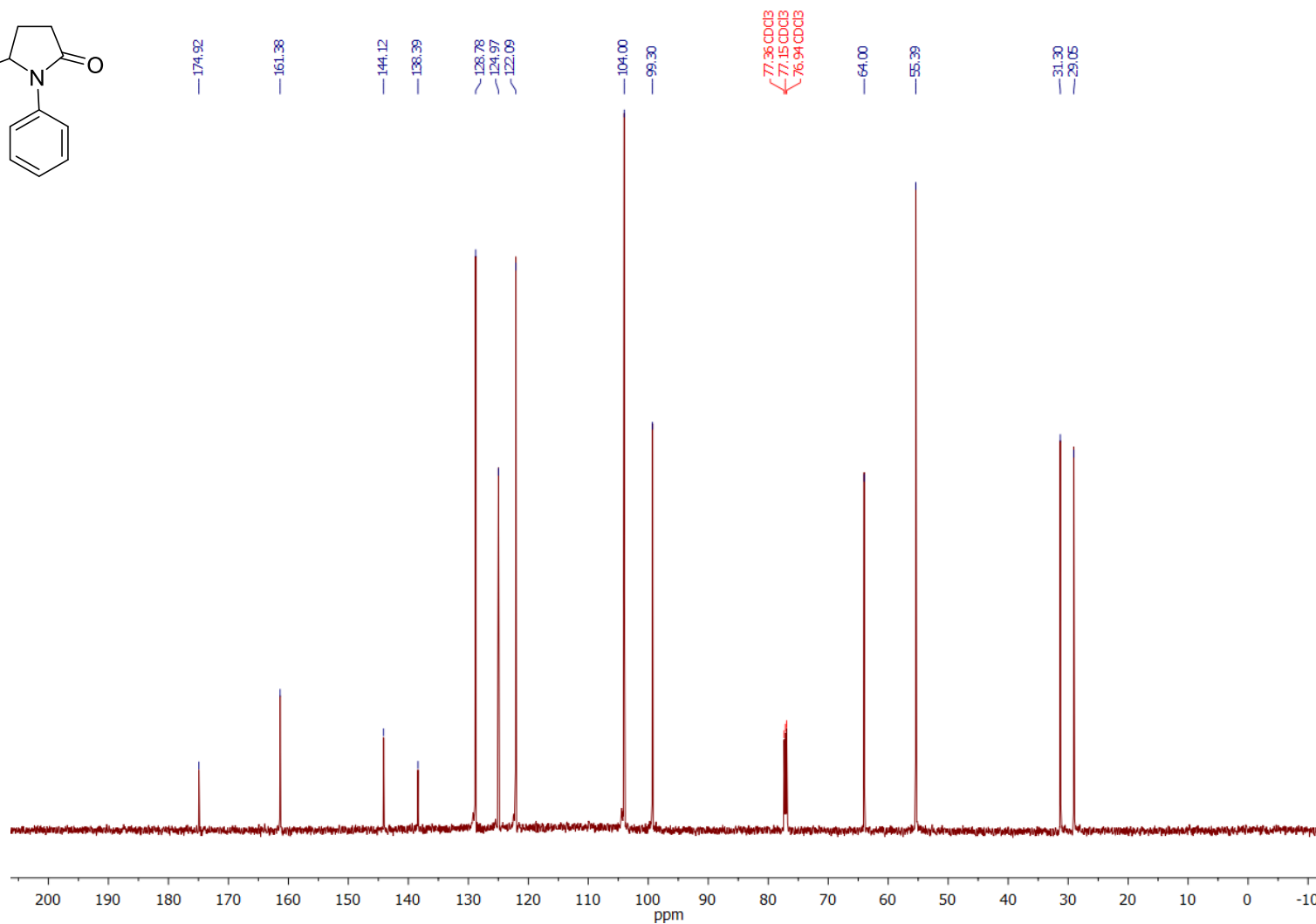
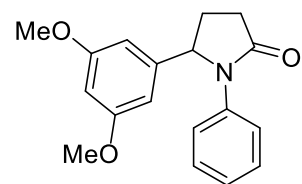
5-(3,5-Dimethoxyphenyl)-1-phenylpyrrolidin-2-one (2a)

^1H NMR (CDCl_3 , 600 MHz)



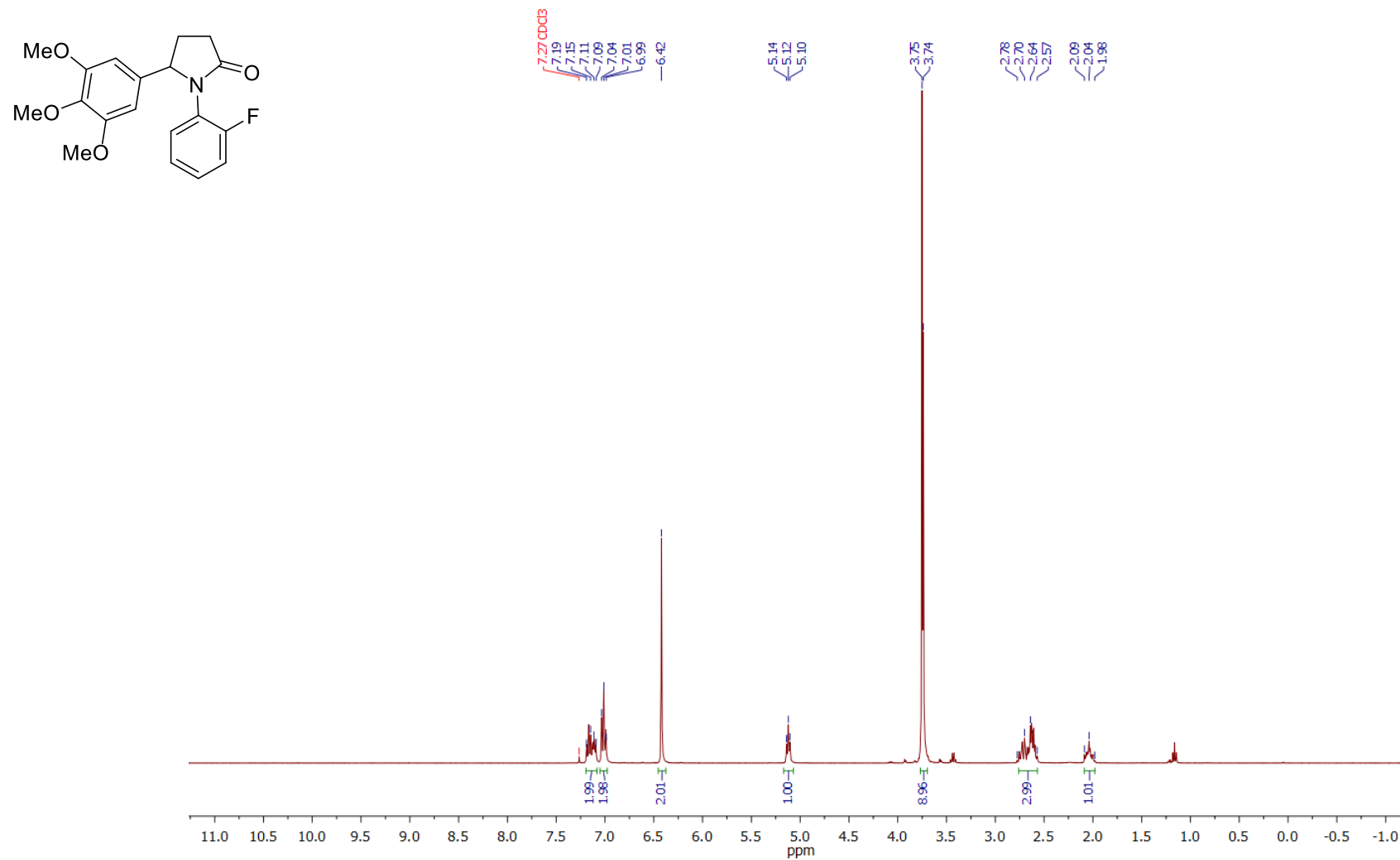
5-(3,5-Dimethoxyphenyl)-1-phenylpyrrolidin-2-one (2a)

^{13}C NMR (CDCl_3 , 150 MHz)



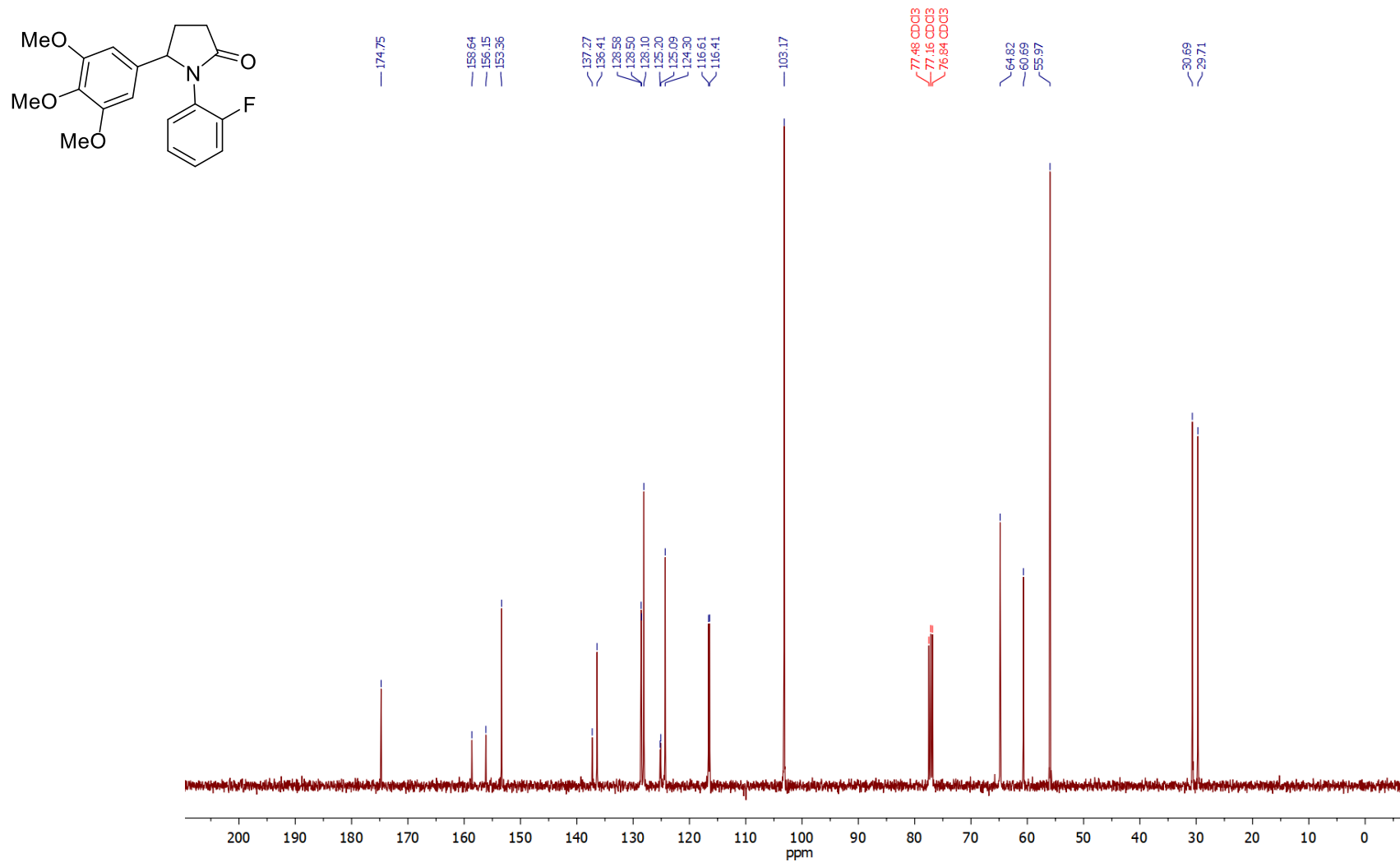
5-(3,4,5-Trimethoxyphenyl)-1-(2-fluorophenyl)pyrrolidin-2-one (2b)

^1H NMR (CDCl_3 , 400 MHz)



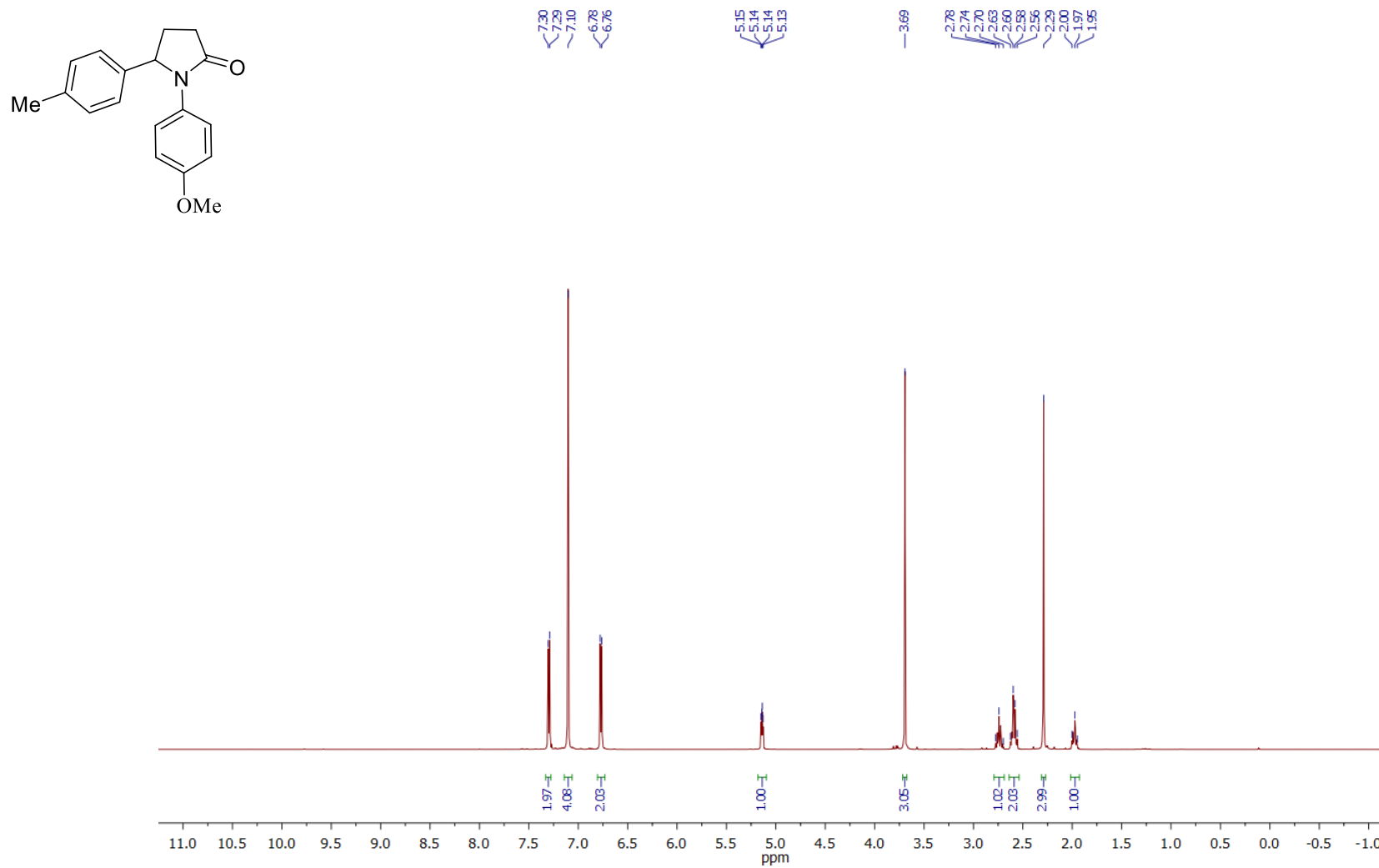
5-(3,4,5-Trimethoxyphenyl)-1-(2-fluorophenyl)pyrrolidin-2-one (2b)

^{13}C NMR (CDCl_3 , 100 MHz)



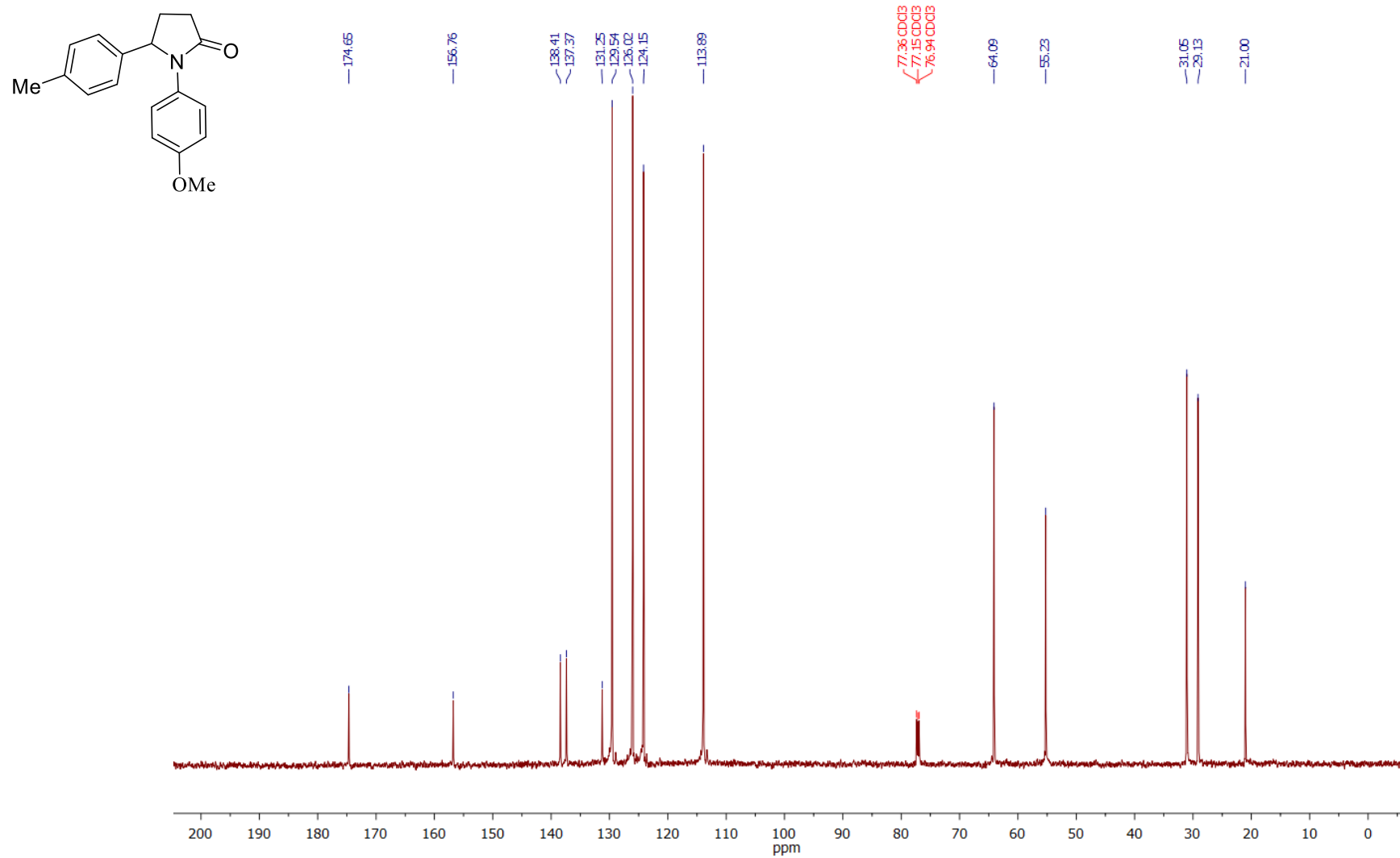
1-(4-Methoxyphenyl)-5-(*p*-tolyl)pyrrolidin-2-one (2d)

¹H NMR (CDCl₃, 600 MHz)



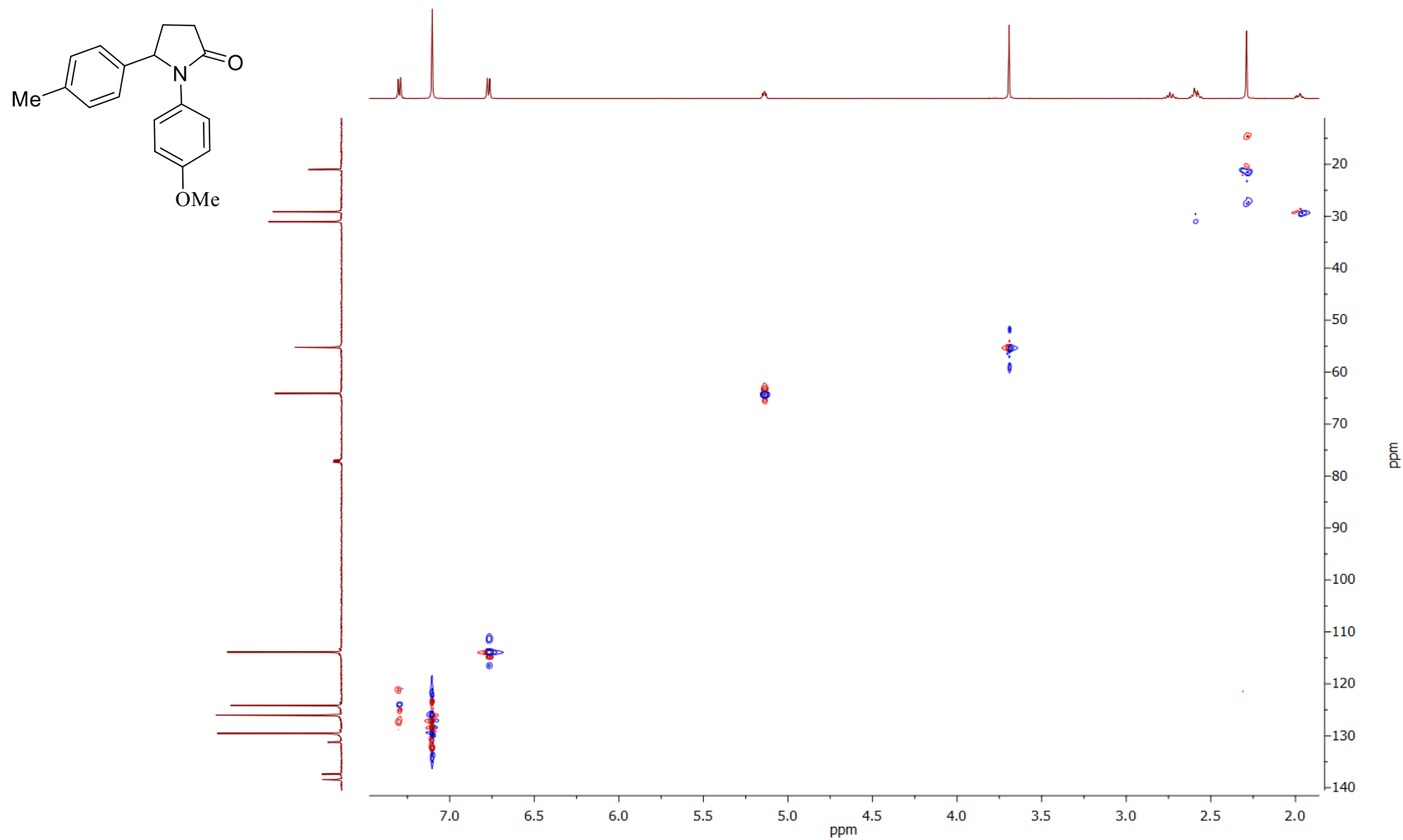
1-(4-Methoxyphenyl)-5-(*p*-tolyl)pyrrolidin-2-one (2d)

^{13}C NMR (CDCl_3 , 150 MHz)



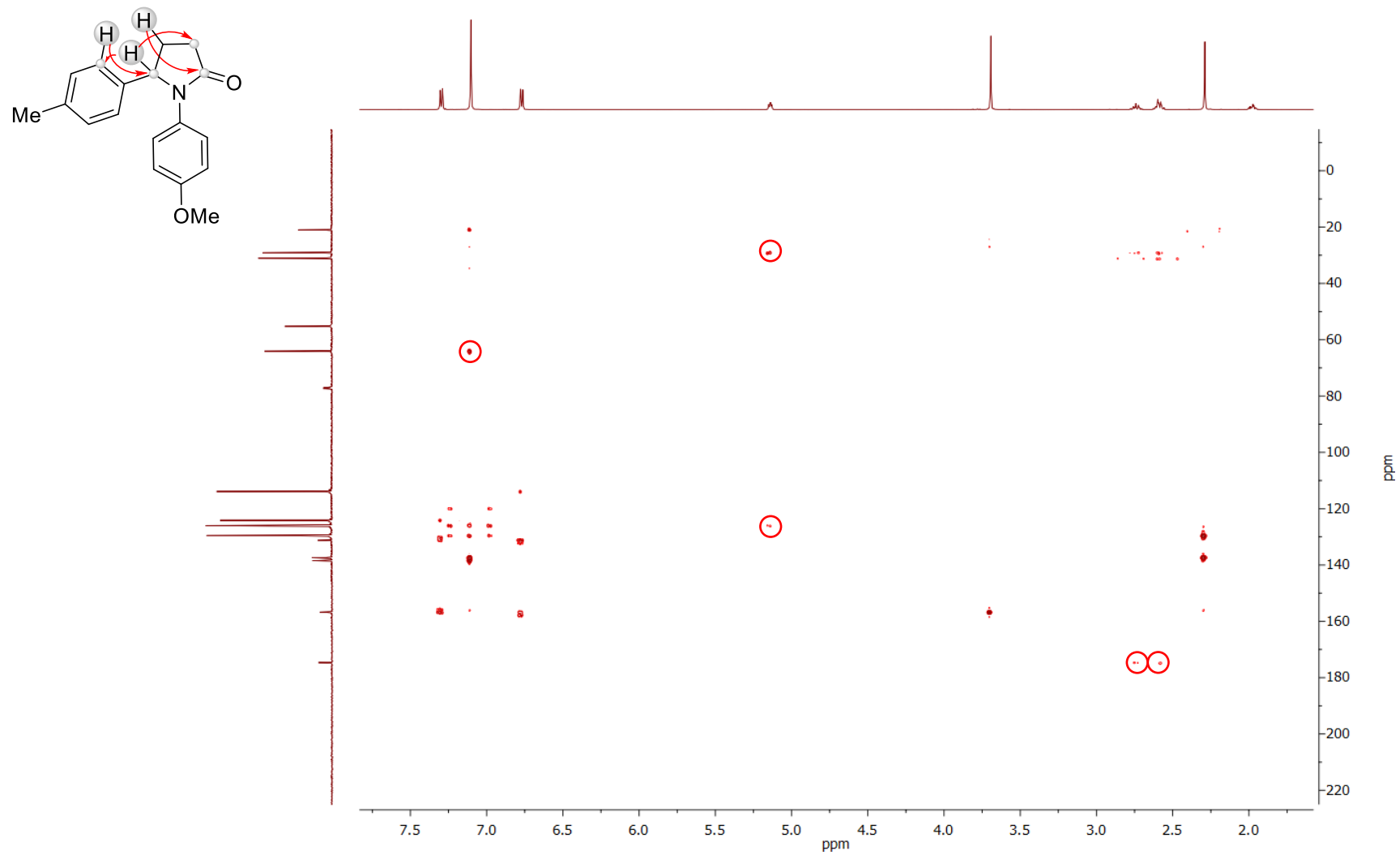
1-(4-Methoxyphenyl)-5-(p-tolyl)pyrrolidin-2-one (2d)

HSQC ^1H - ^{13}C (CDCl_3)



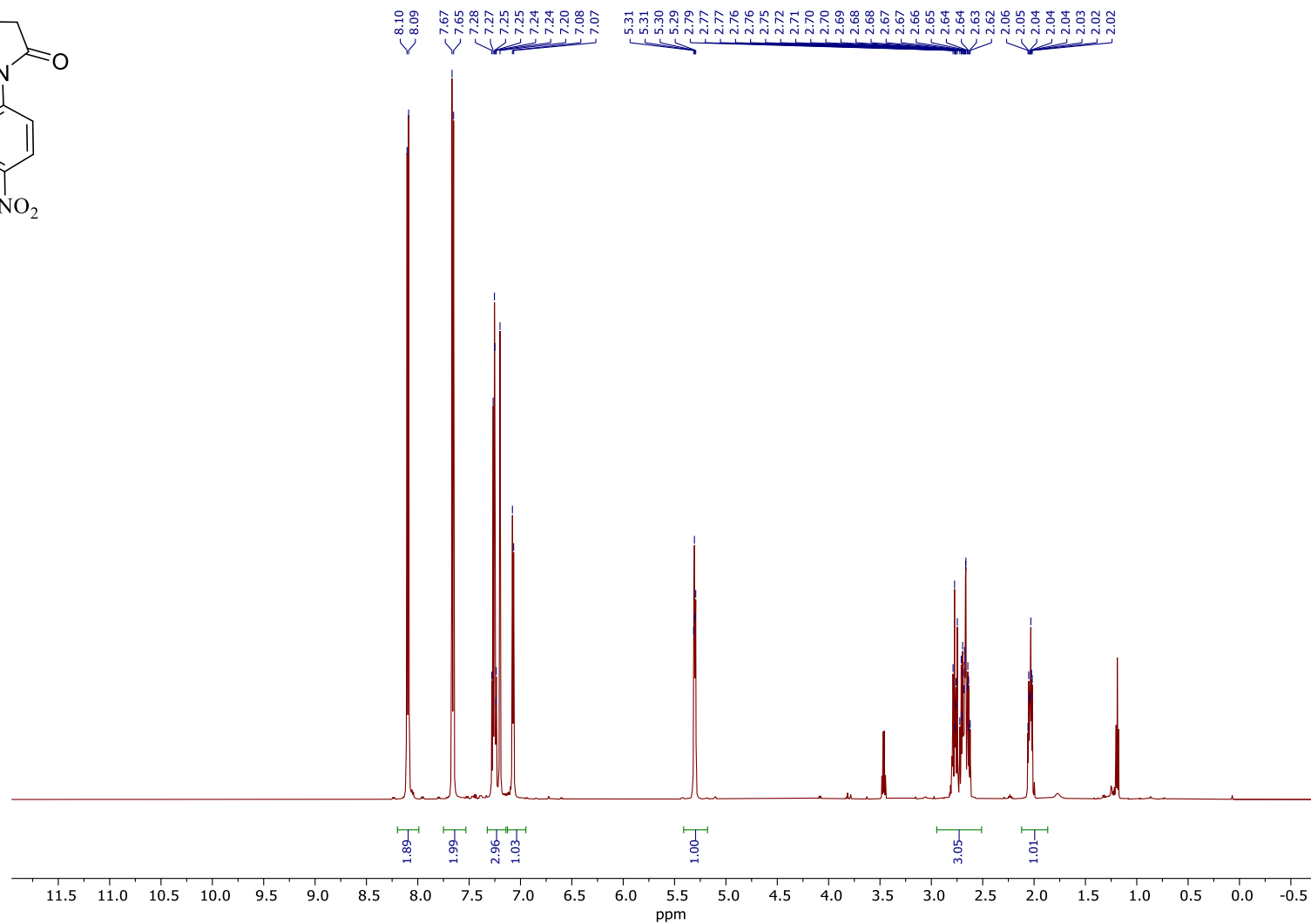
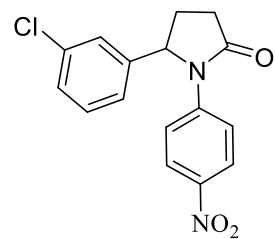
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HMBC ^1H - ^{13}C (CDCl_3)



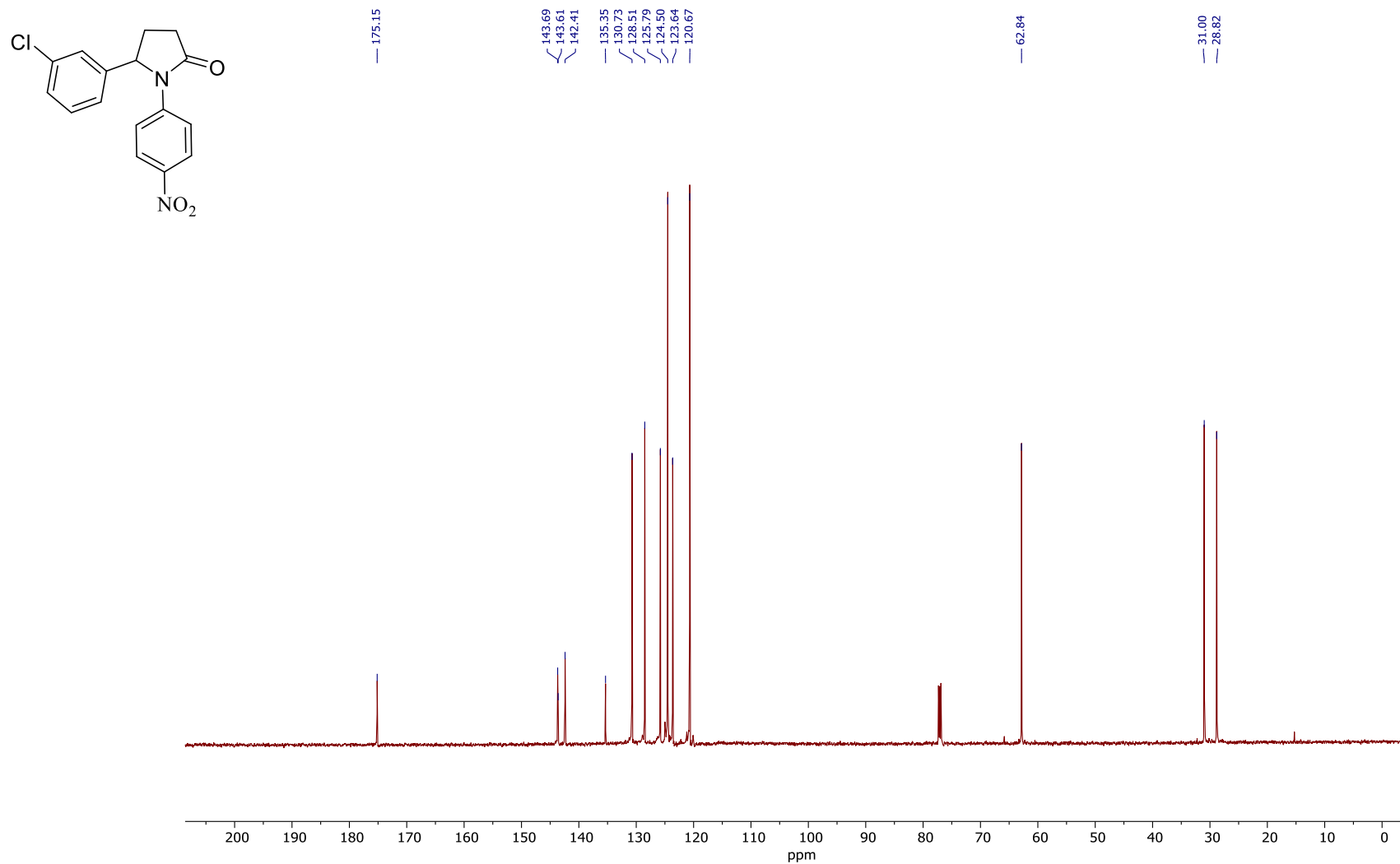
5-(3-Chlorophenyl)-1-(4-nitrophenyl)pyrrolidin-2-one (2e)

¹H NMR (CDCl₃, 600 MHz)



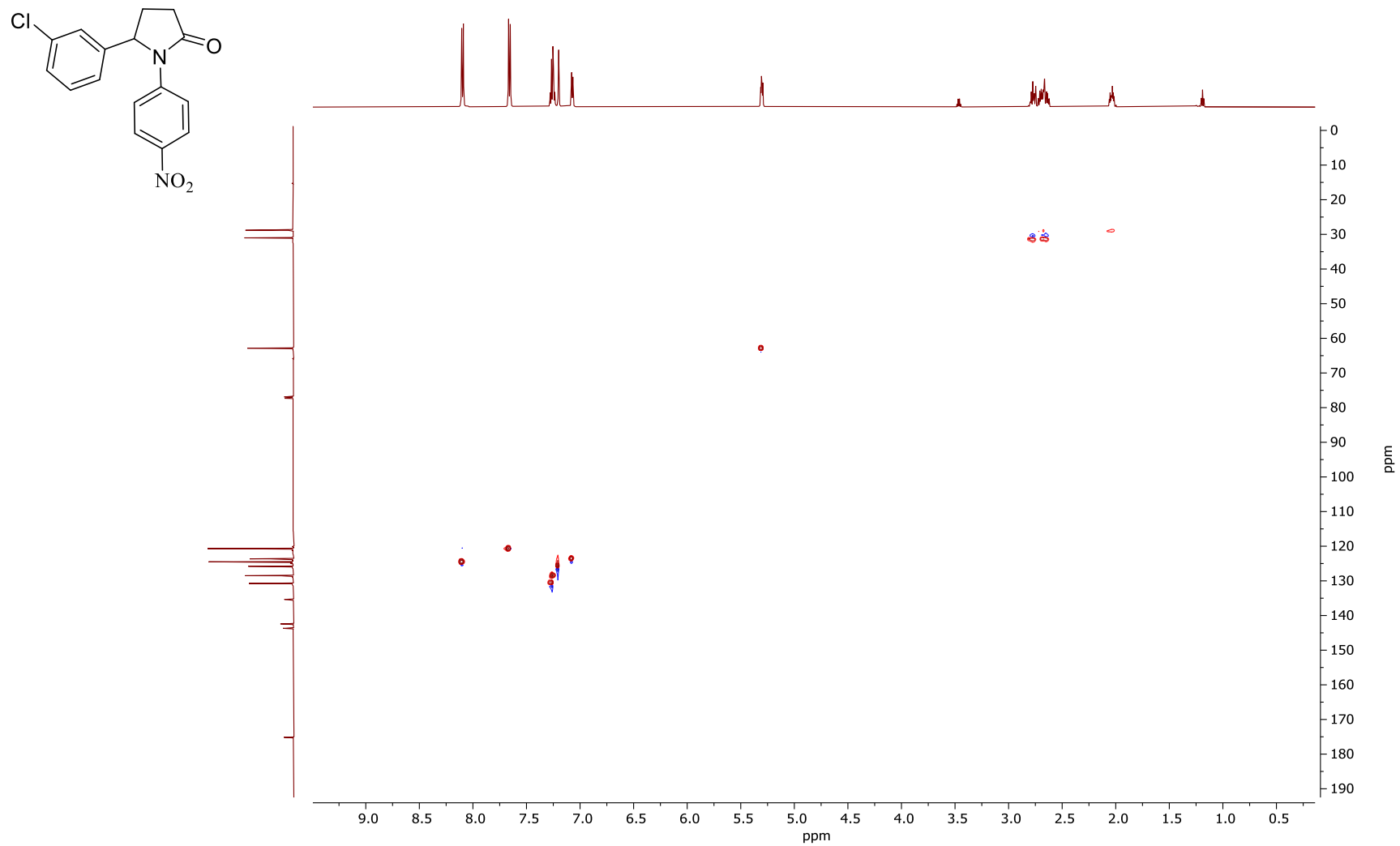
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^{13}C NMR (CDCl_3 , 150 MHz)



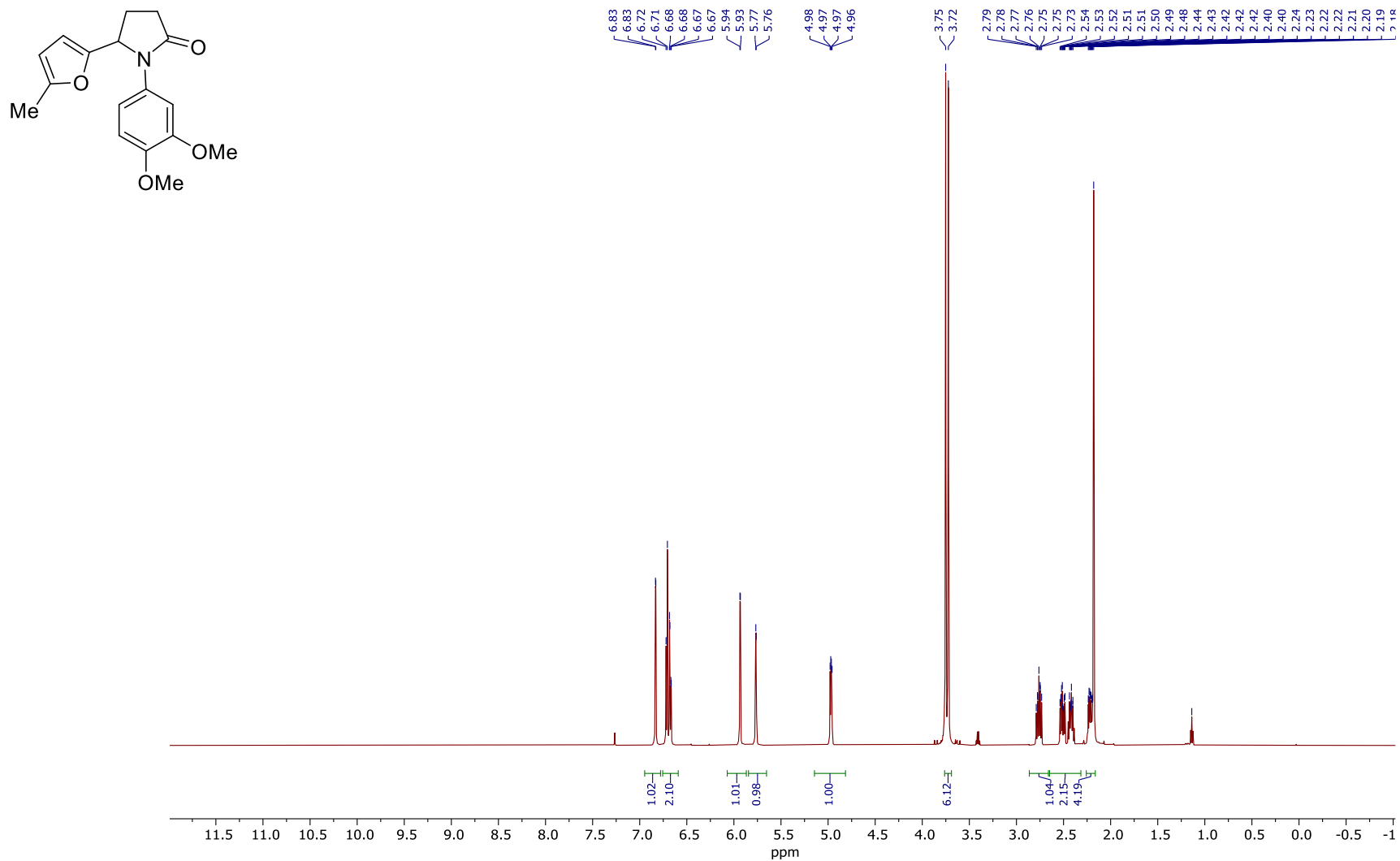
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HSQC ^1H - ^{13}C (CDCl_3)



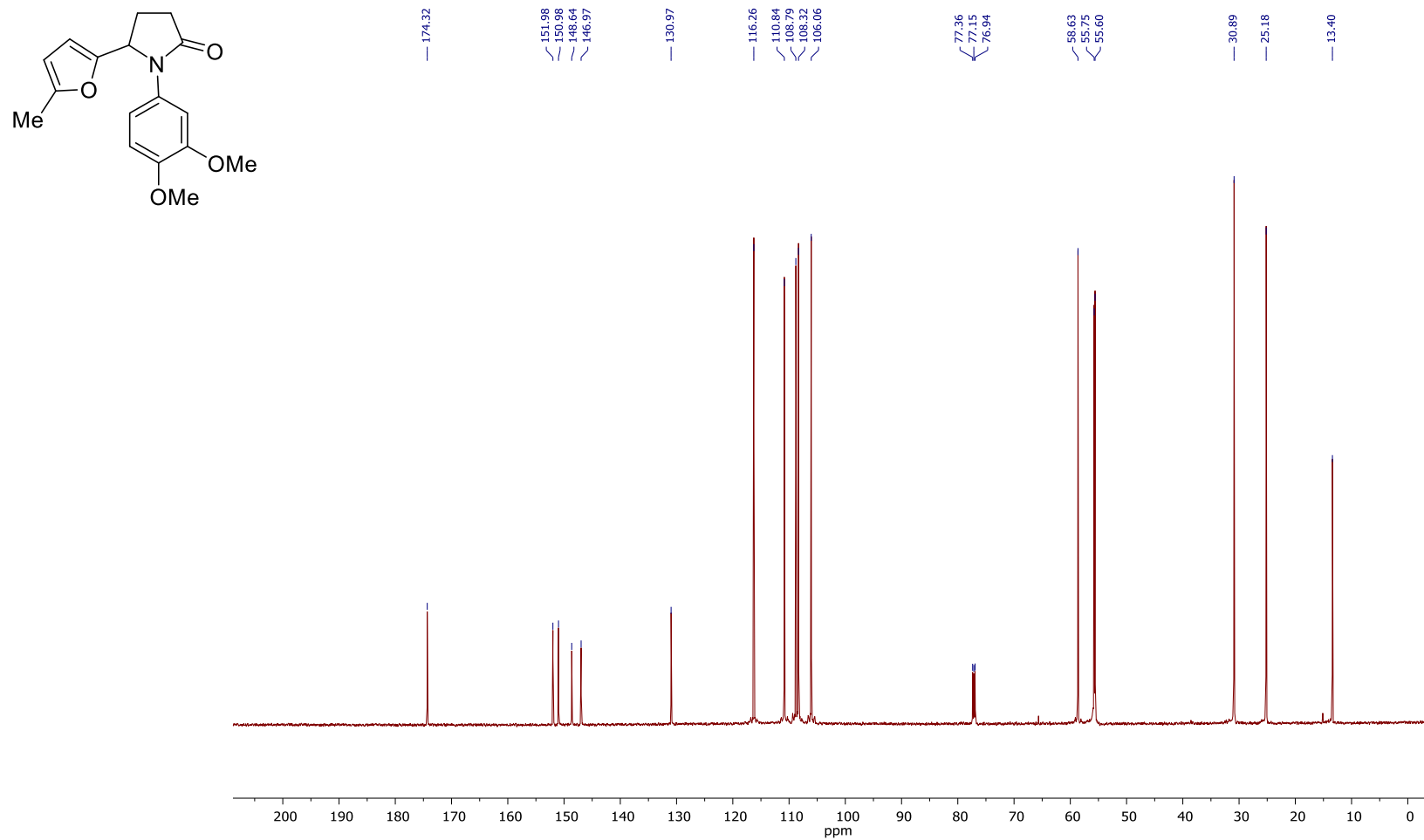
1-(3,4-Dimethoxyphenyl)-5-(5-methylfuran-2-yl)pyrrolidin-2-one (2f)

¹H NMR (CDCl₃, 600 MHz)



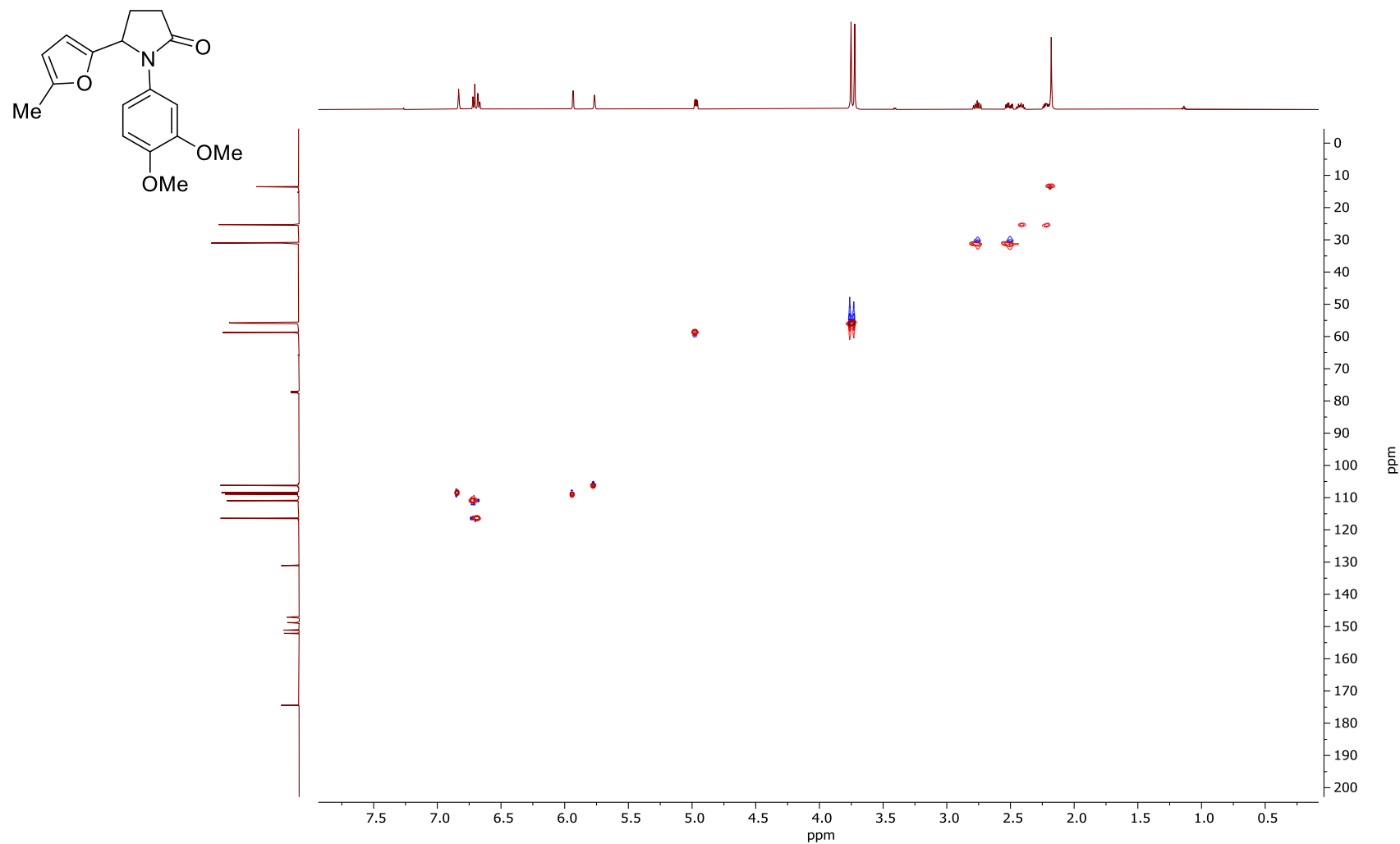
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^{13}C NMR (CDCl_3 , 150 MHz)



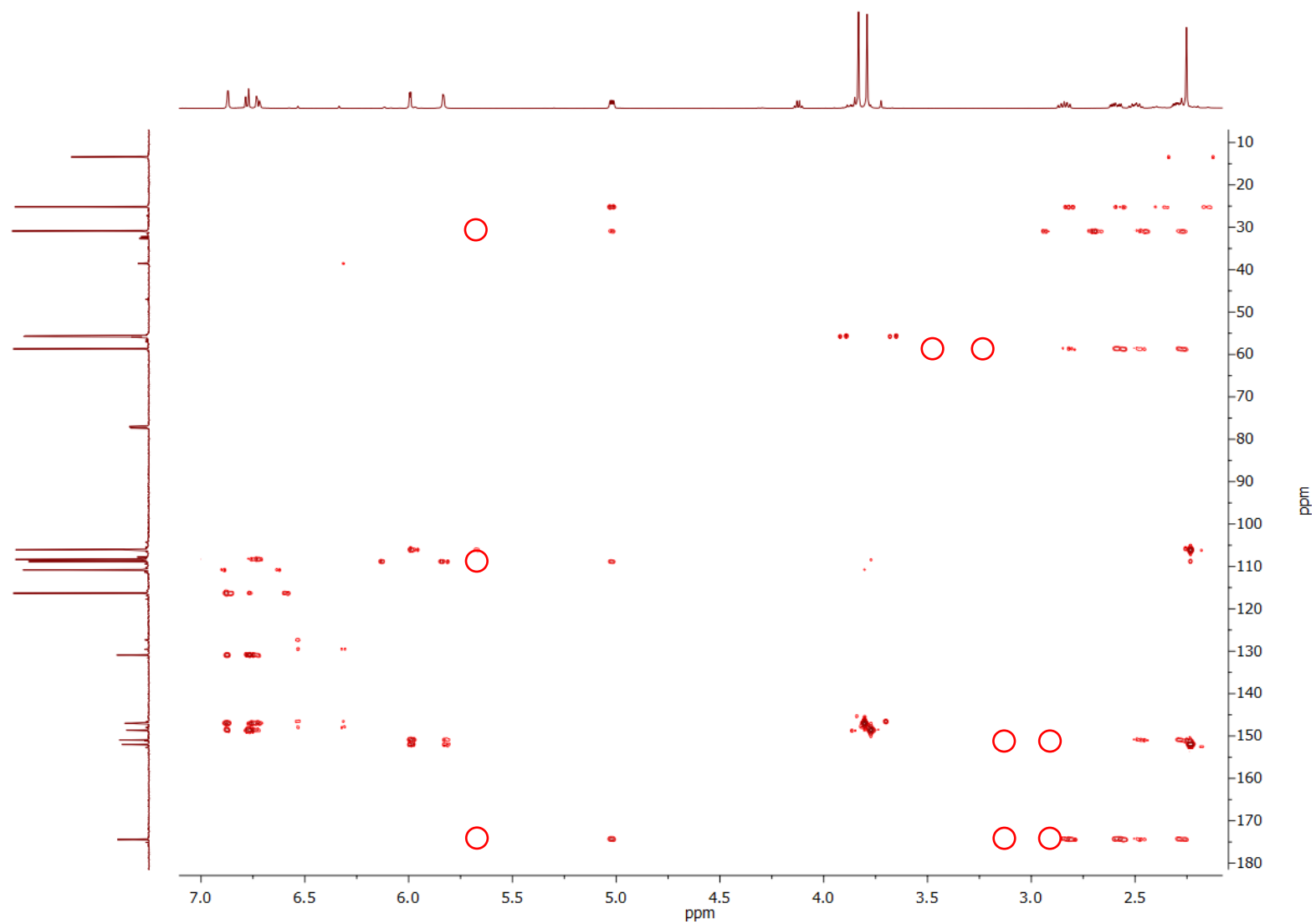
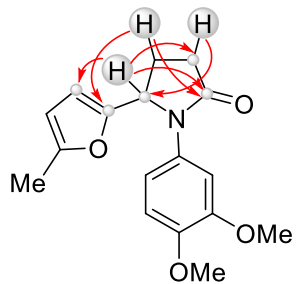
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HSQC ^1H - ^{13}C (CDCl_3)



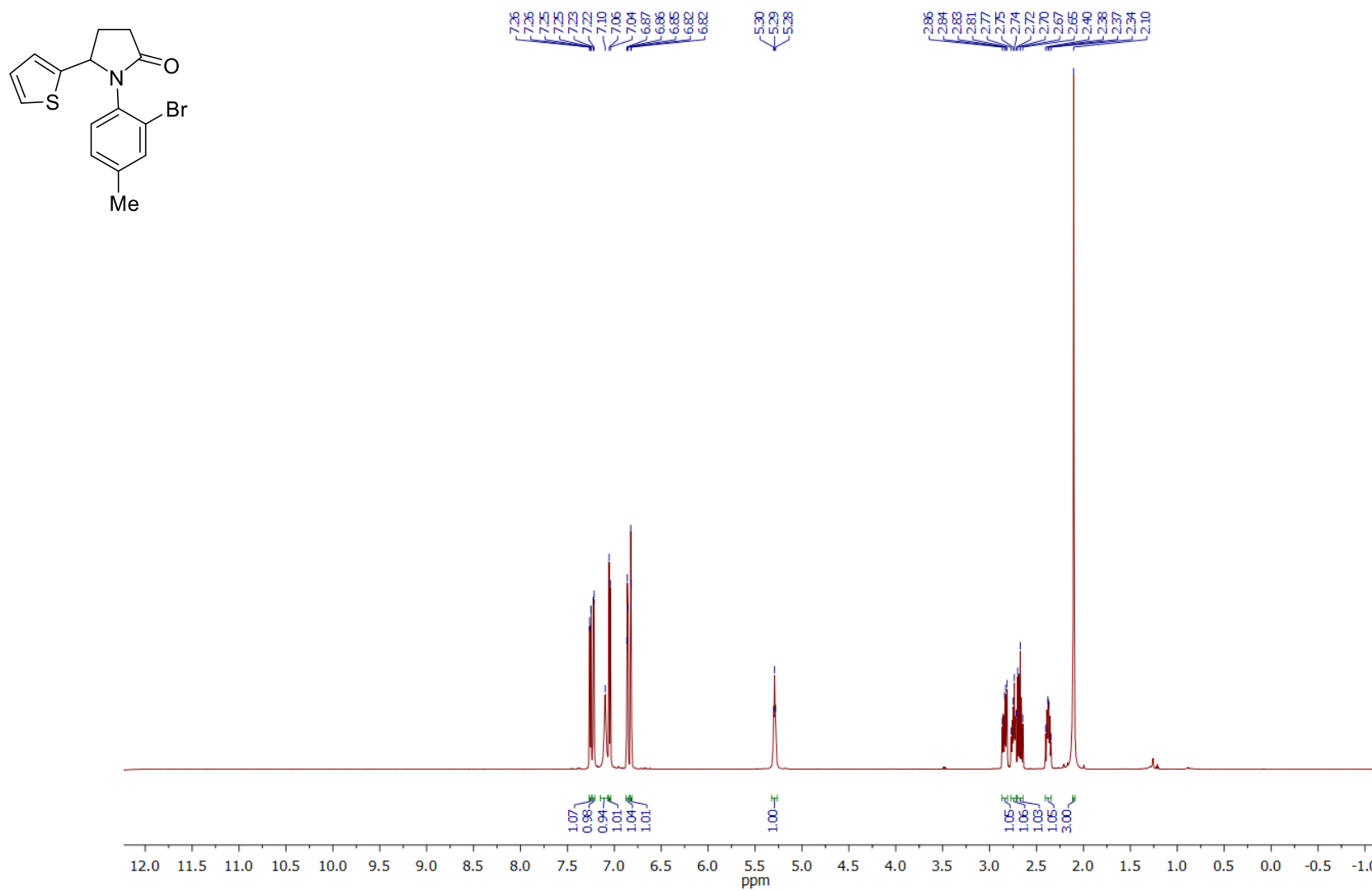
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HMBC ^1H - ^{13}C (CDCl_3)



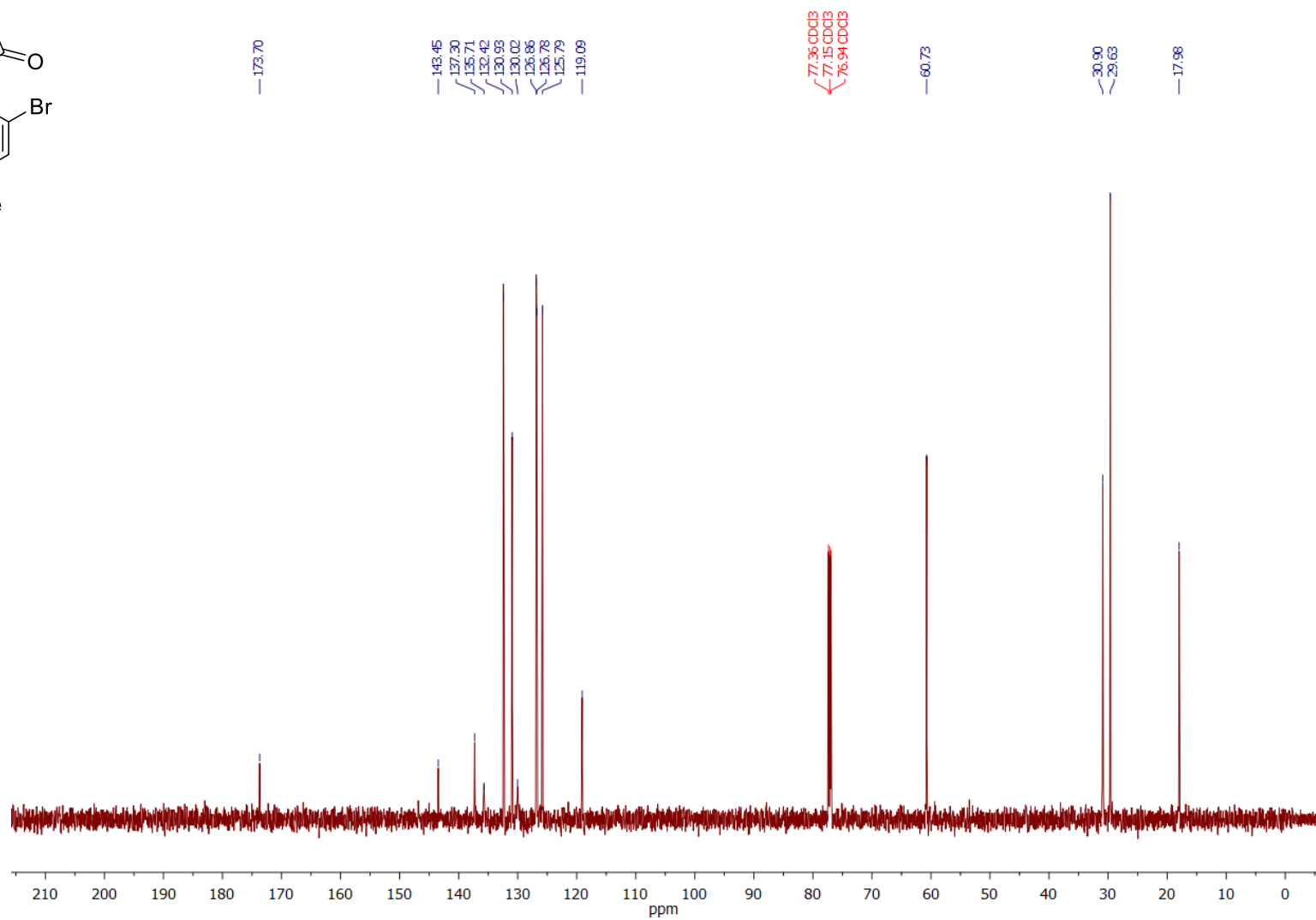
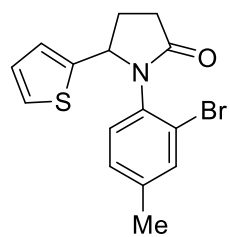
1-(2-Bromo-4-methylphenyl)-5-(thiophen-2-yl)pyrrolidin-2-one (2g)

^1H NMR (CDCl_3 , 600 MHz)



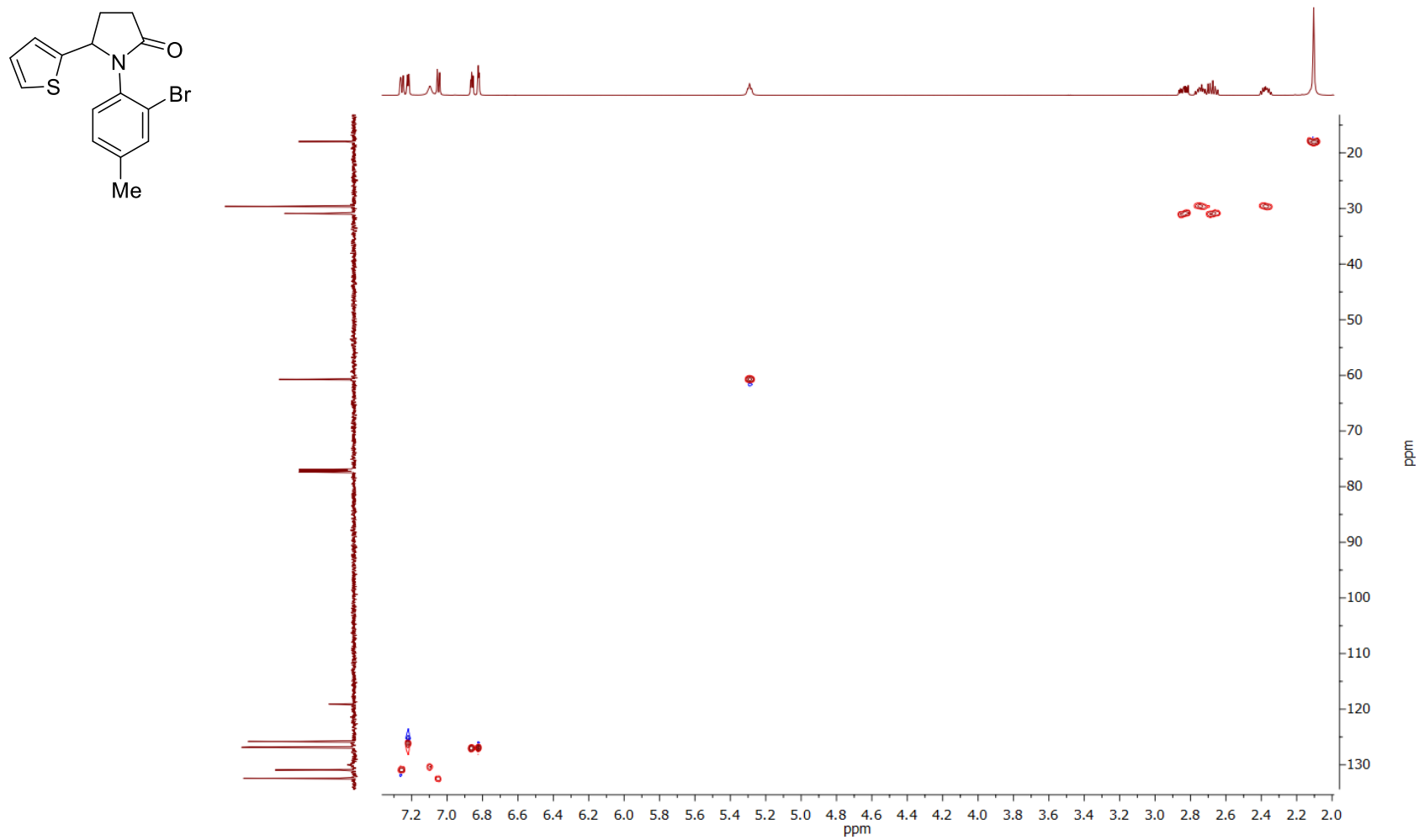
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^{13}C NMR (CDCl_3 , 150 MHz)



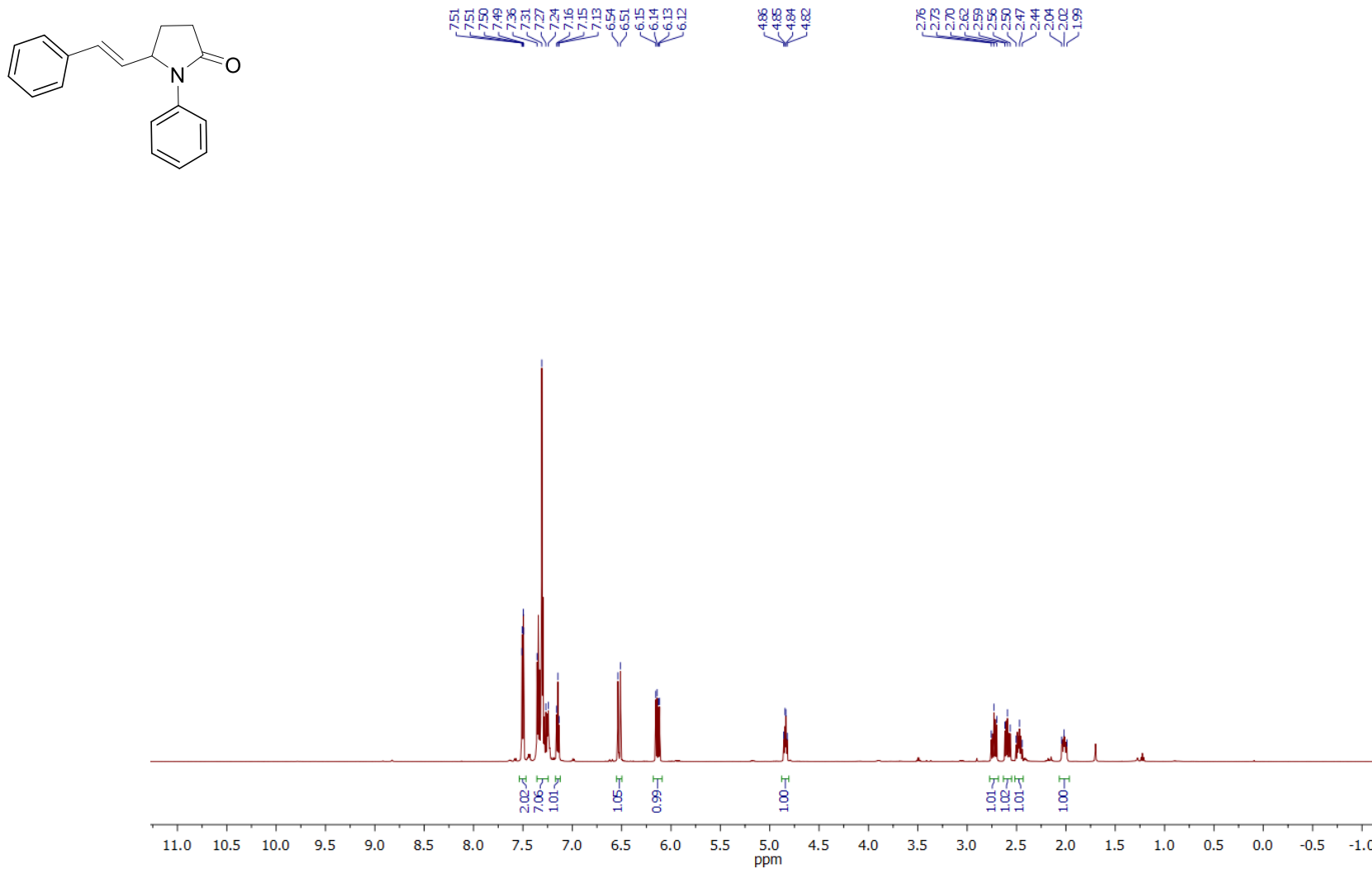
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HSQC ^1H - ^{13}C (CDCl_3)



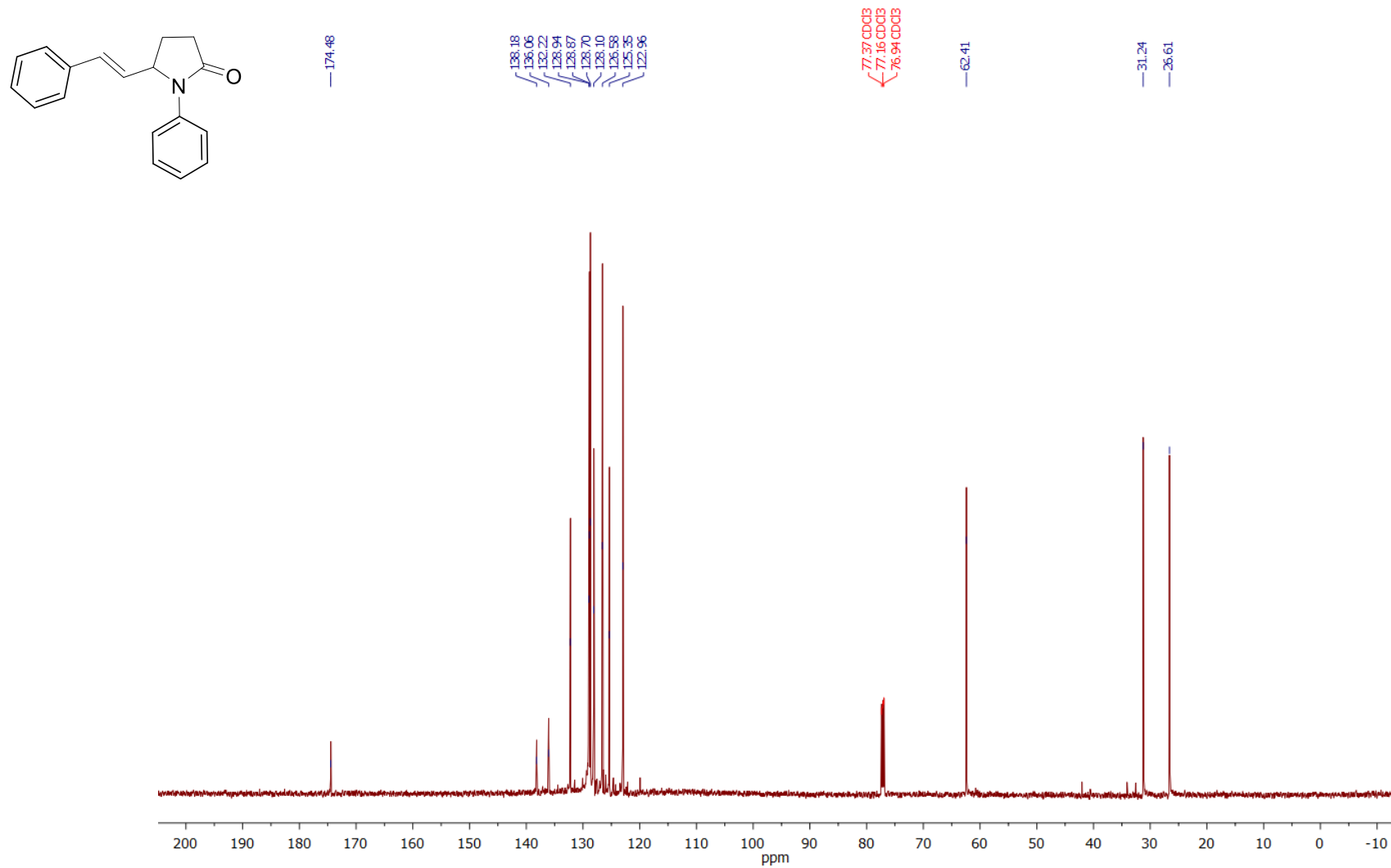
(*E*)-1-Phenyl-5-styrylpyrrolidin-2-one (2h)

¹H NMR (CDCl₃, 600 MHz)



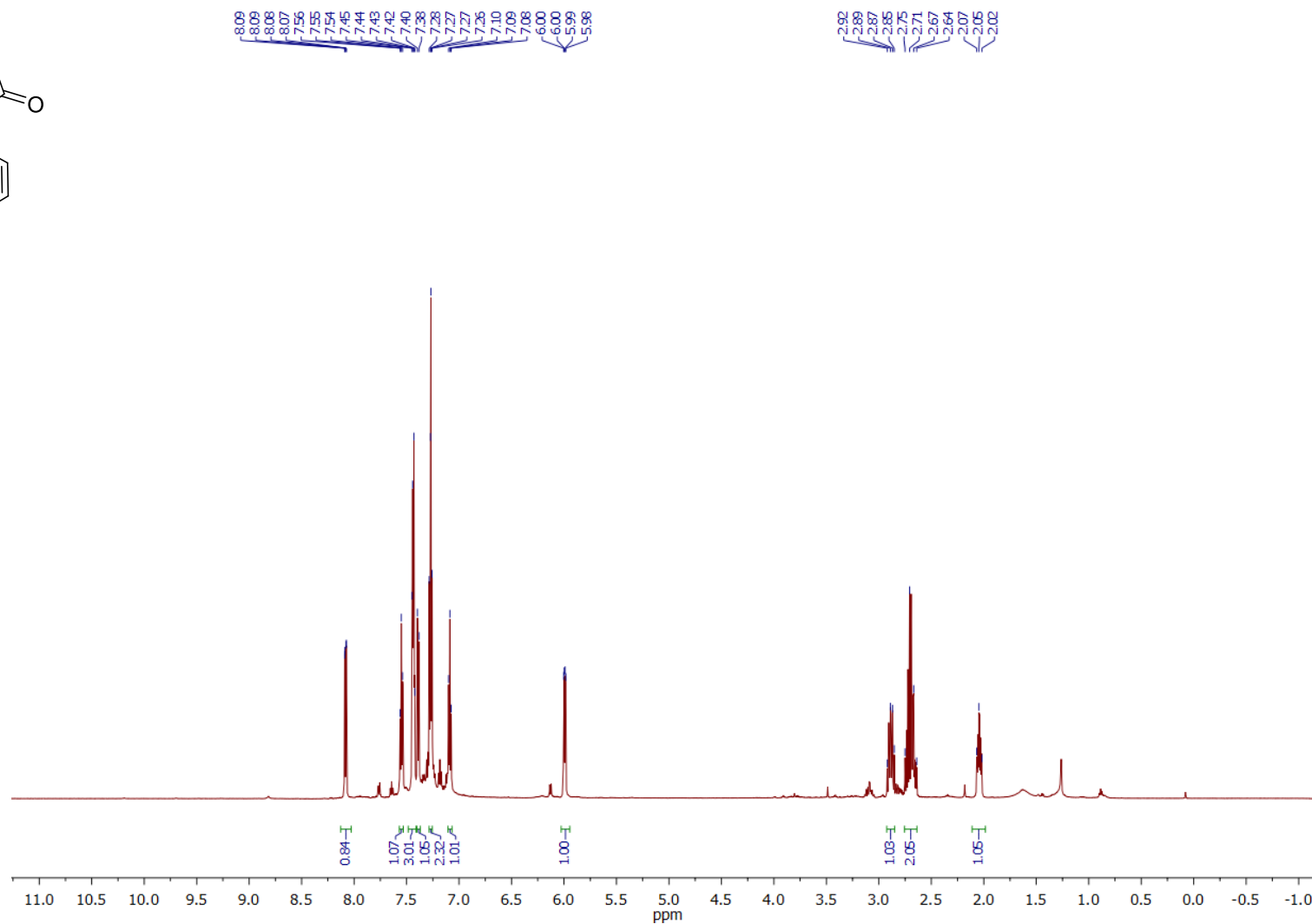
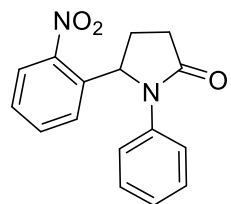
(E)-1-Phenyl-5-styrylpyrrolidin-2-one (2h)

^{13}C NMR (CDCl_3 , 150 MHz)



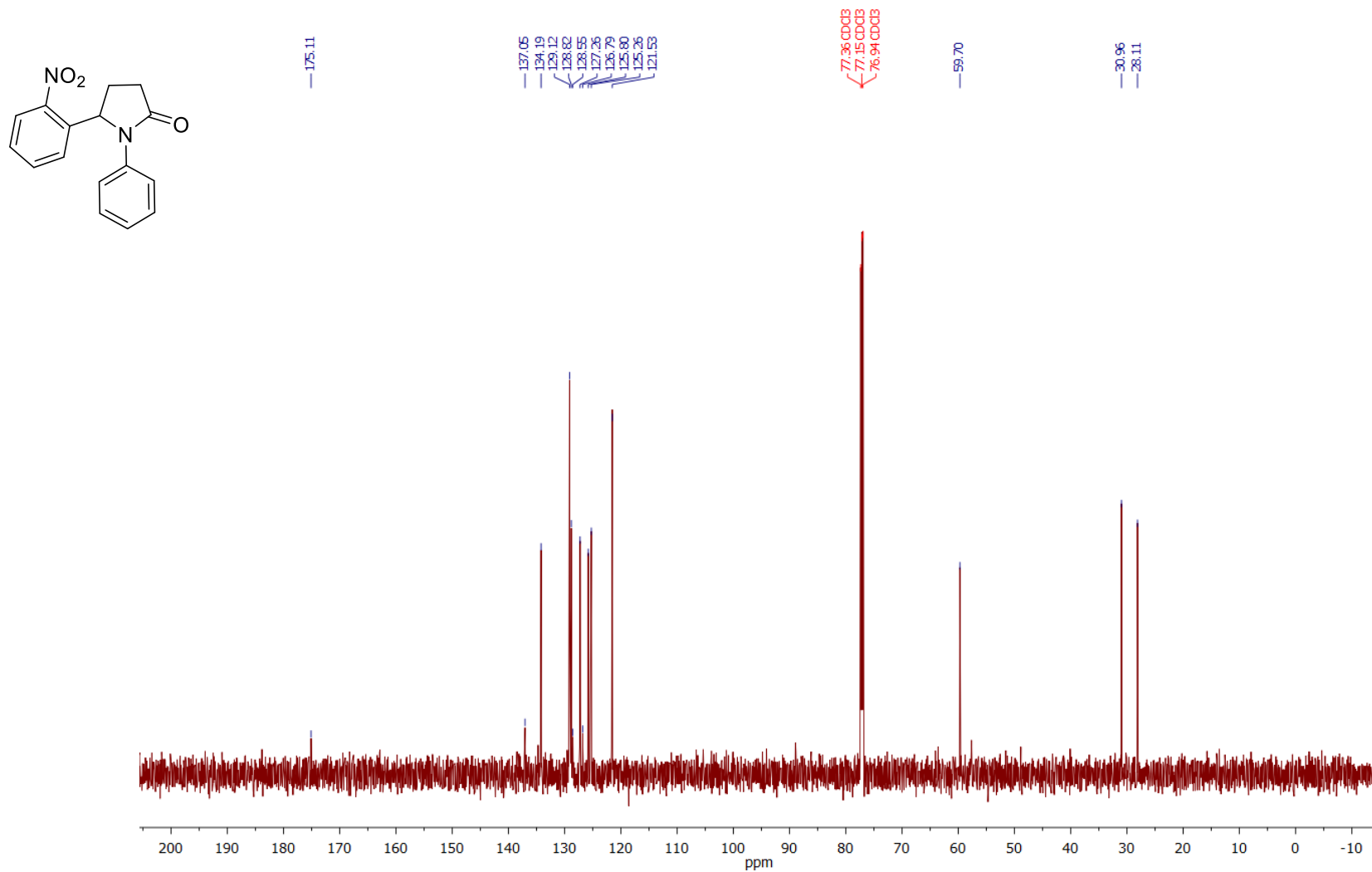
5-(2-Nitrophenyl)-1-phenylpyrrolidin-2-one (2i)

^1H NMR (CDCl_3 , 600 MHz)



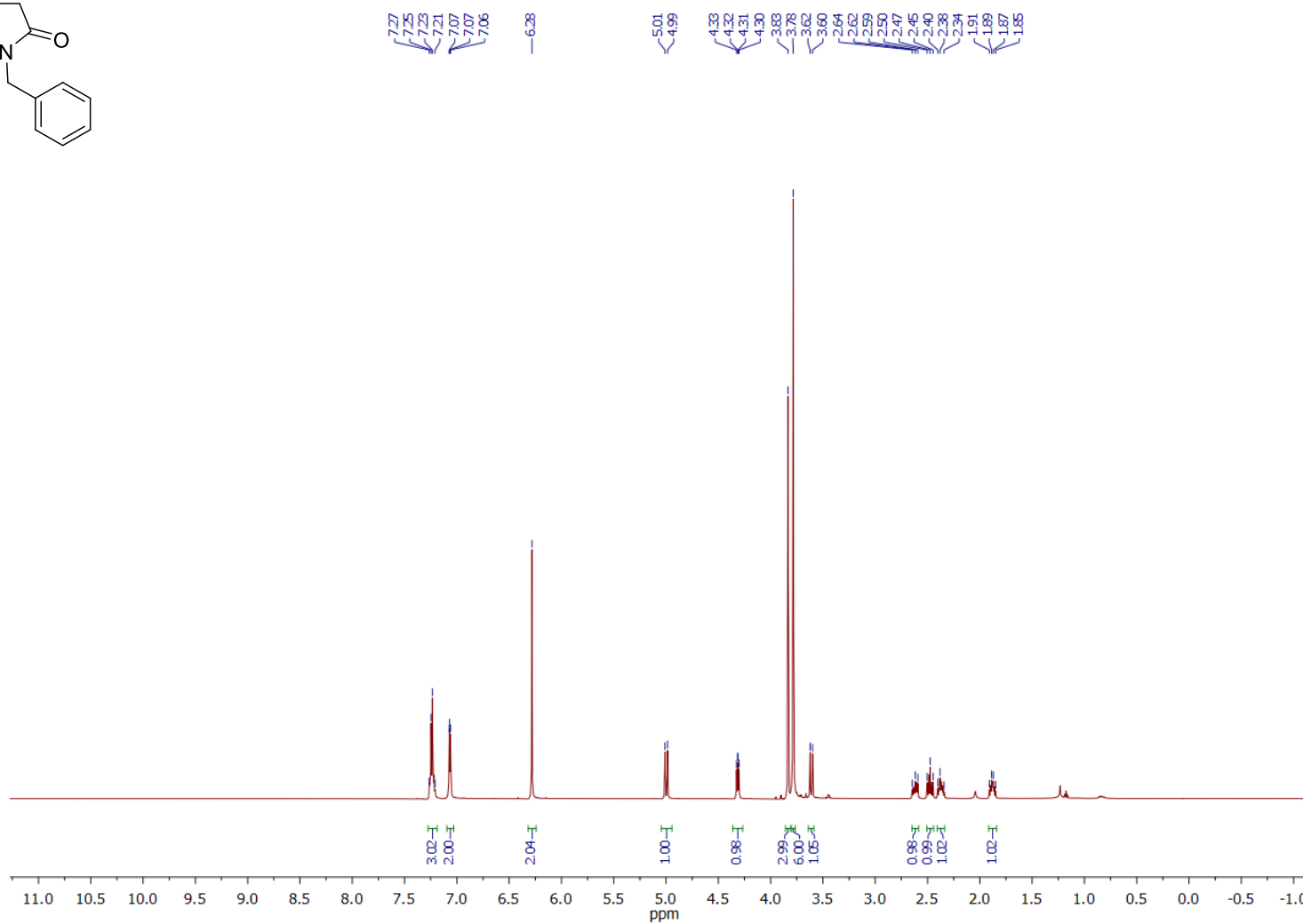
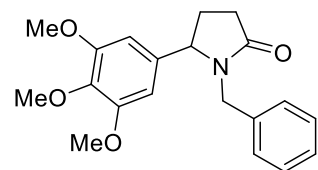
5-(2-Nitrophenyl)-1-phenylpyrrolidin-2-one (2i)

^{13}C NMR (CDCl_3 , 150 MHz)



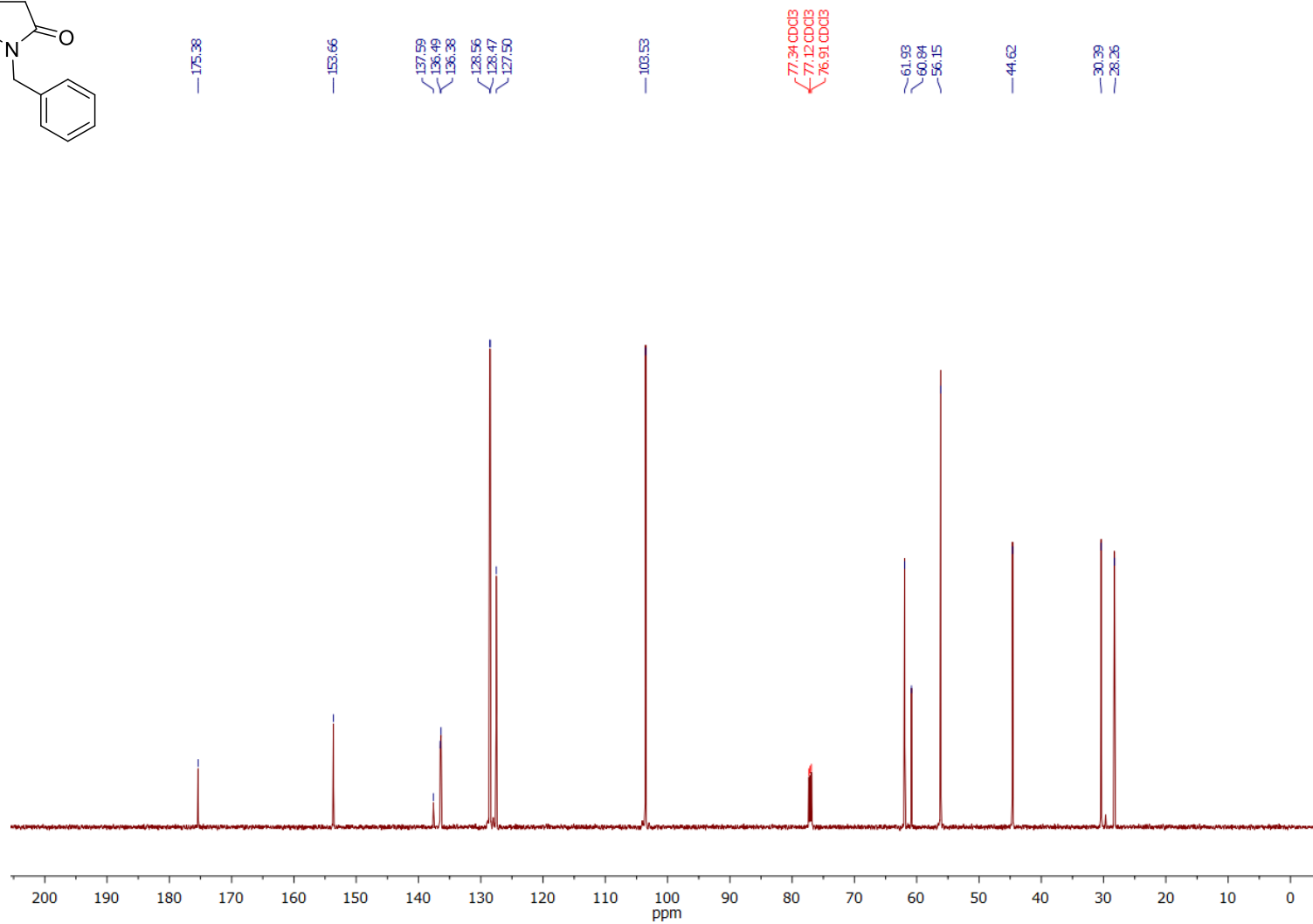
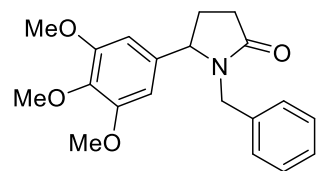
1-Benzyl-5-(3,4,5-trimethoxyphenyl)pyrrolidin-2-one (3a)

¹H NMR (CDCl₃, 600 MHz)



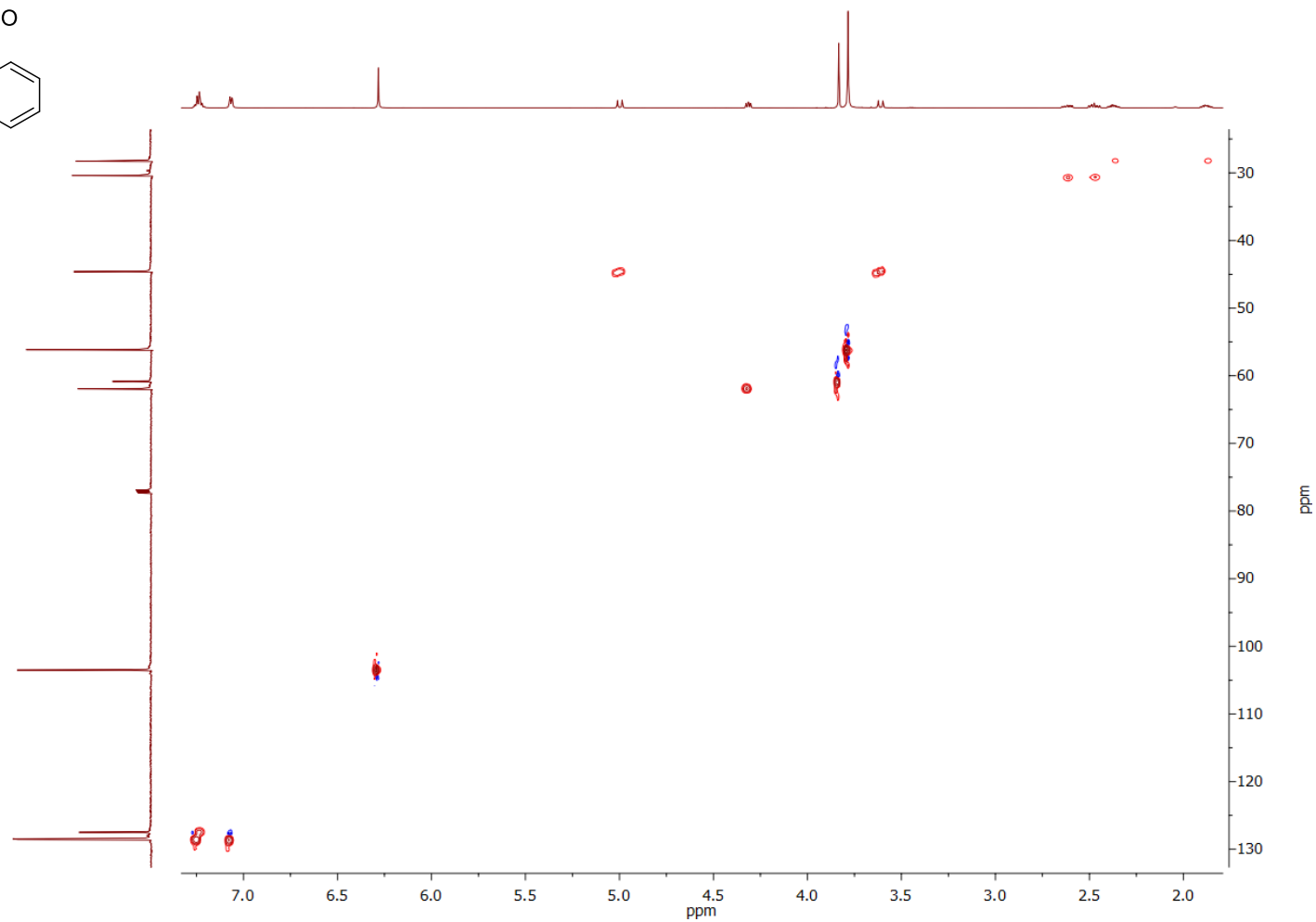
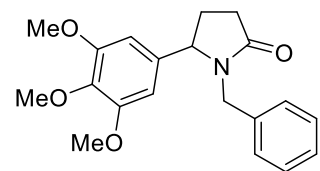
1-Benzyl-5-(3,4,5-trimethoxyphenyl)pyrrolidin-2-one (3a)

^{13}C NMR (CDCl_3 , 150 MHz)



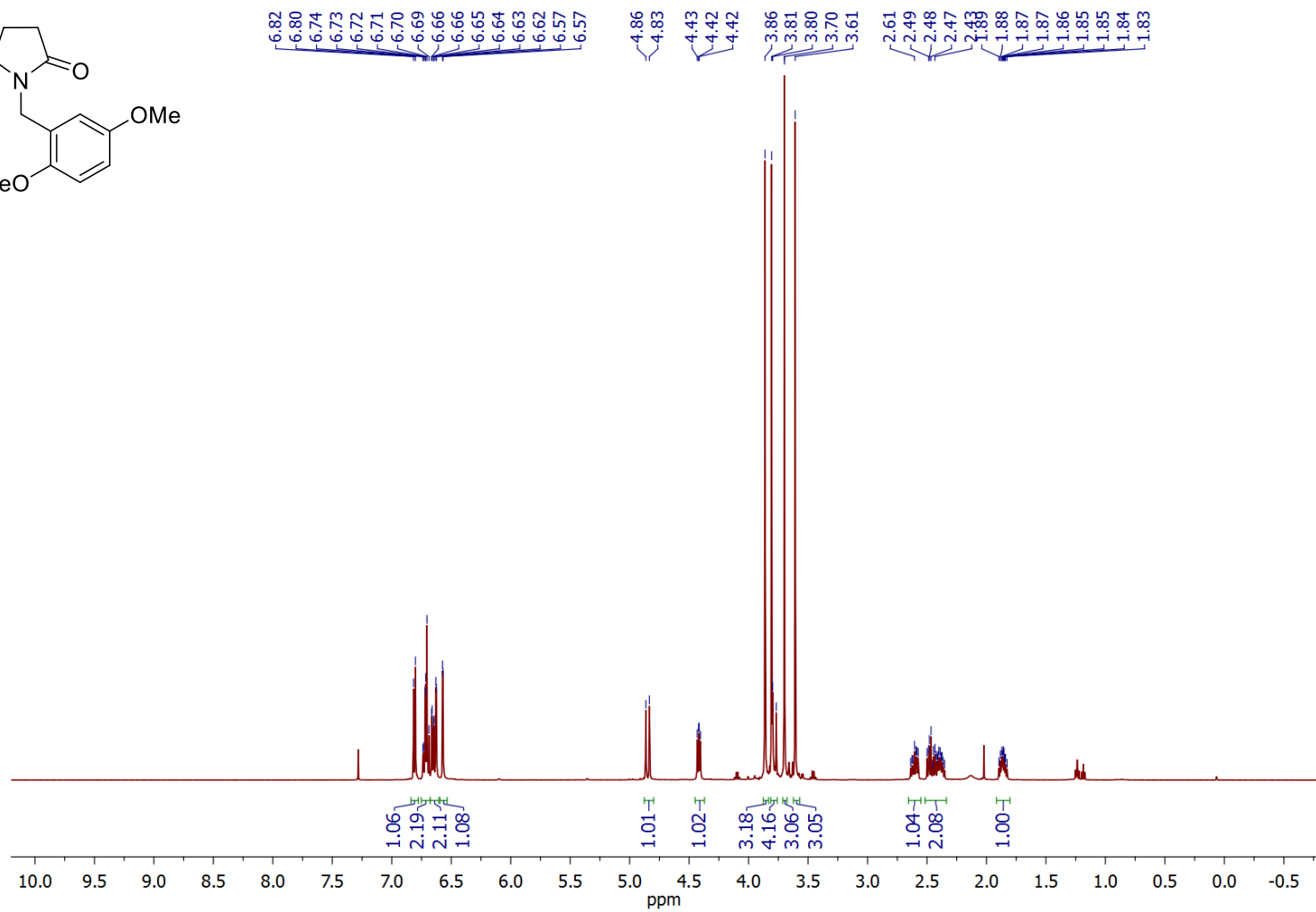
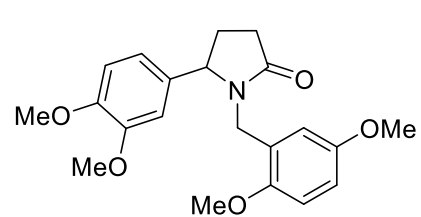
1-Benzyl-5-(3,4,5-trimethoxyphenyl)pyrrolidin-2-one (3a)

HSQC ^1H - ^{13}C (CDCl_3)



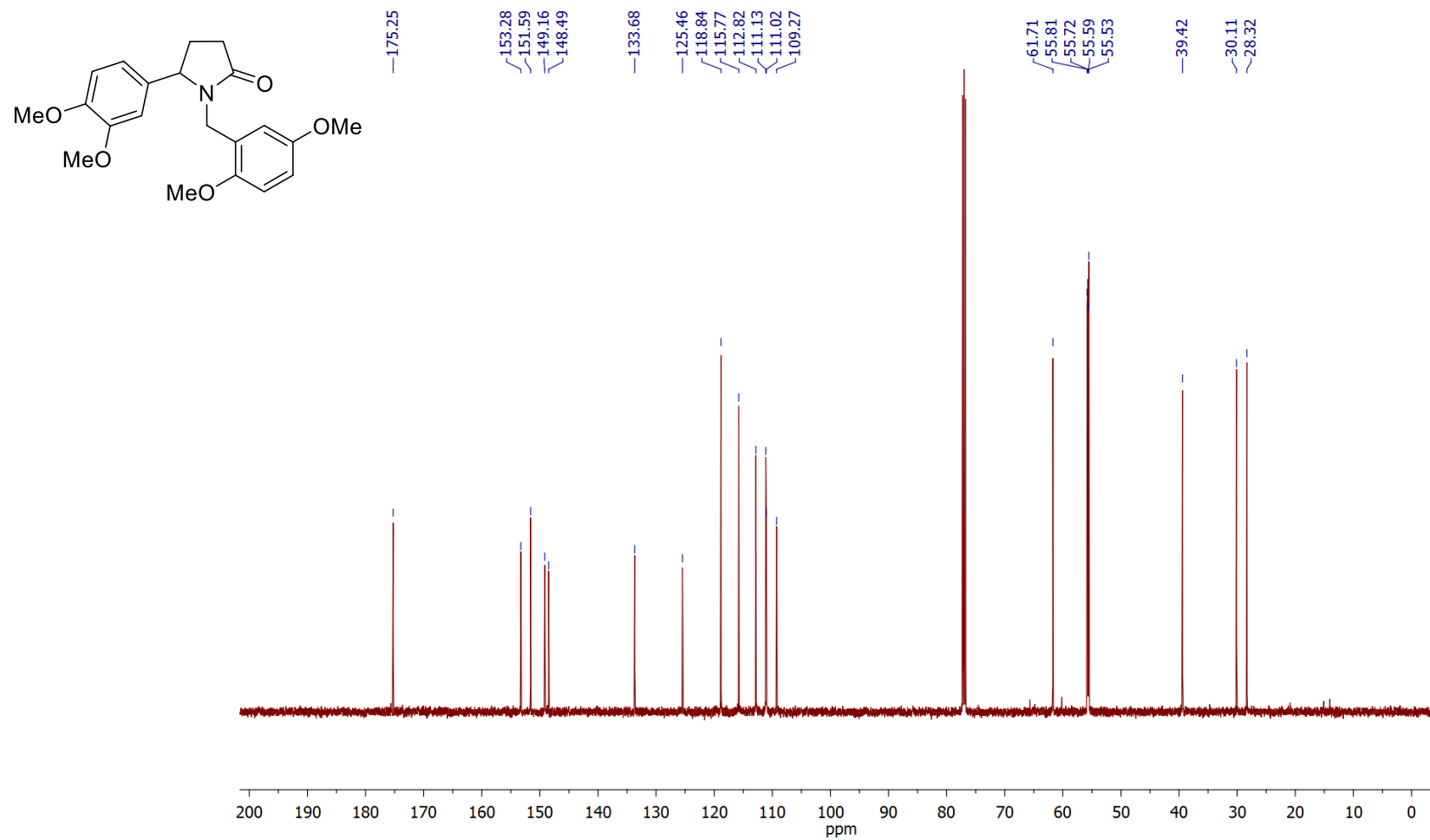
1-(2,5-Dimethoxybenzyl)-5-(3,4-dimethoxyphenyl)pyrrolidin-2-on (3d)

^1H NMR (CDCl_3 , 500 MHz)



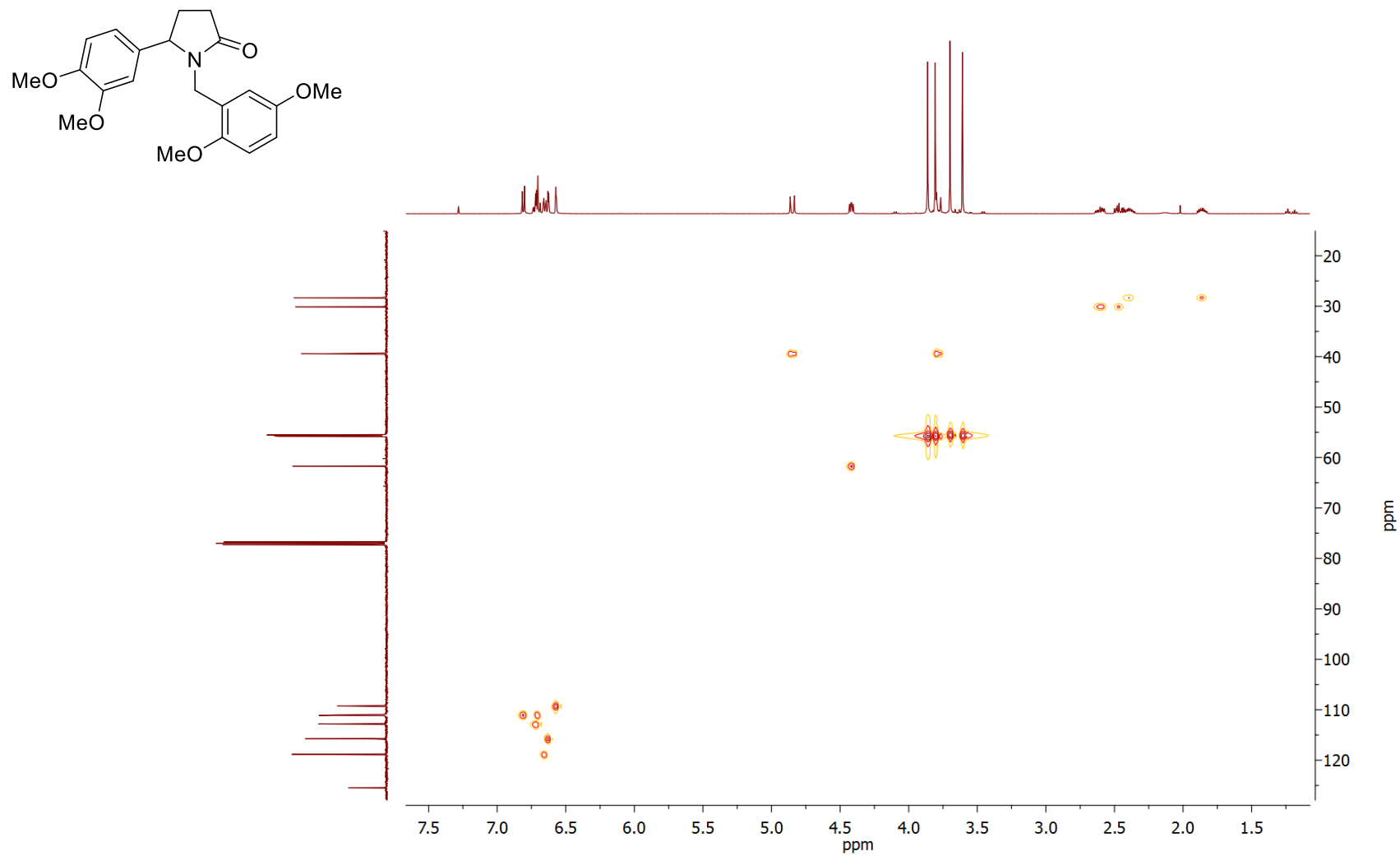
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^{13}C NMR (CDCl_3 , 125 MHz)



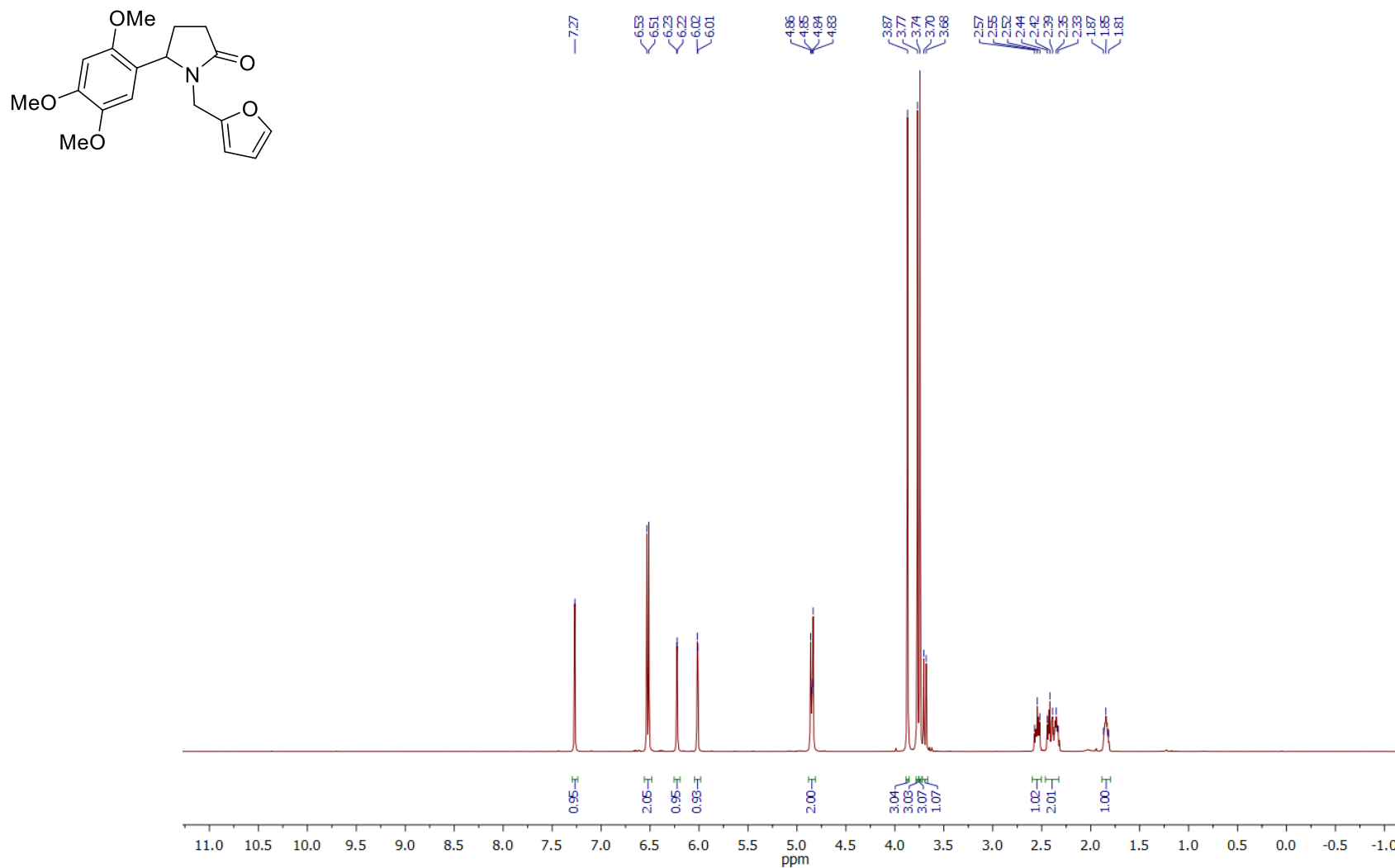
1-(2,5-Dimethoxybenzyl)-5-(3,4-dimethoxyphenyl)pyrrolidin-2-on (3d)

HSQC ^1H - ^{13}C (CDCl_3)



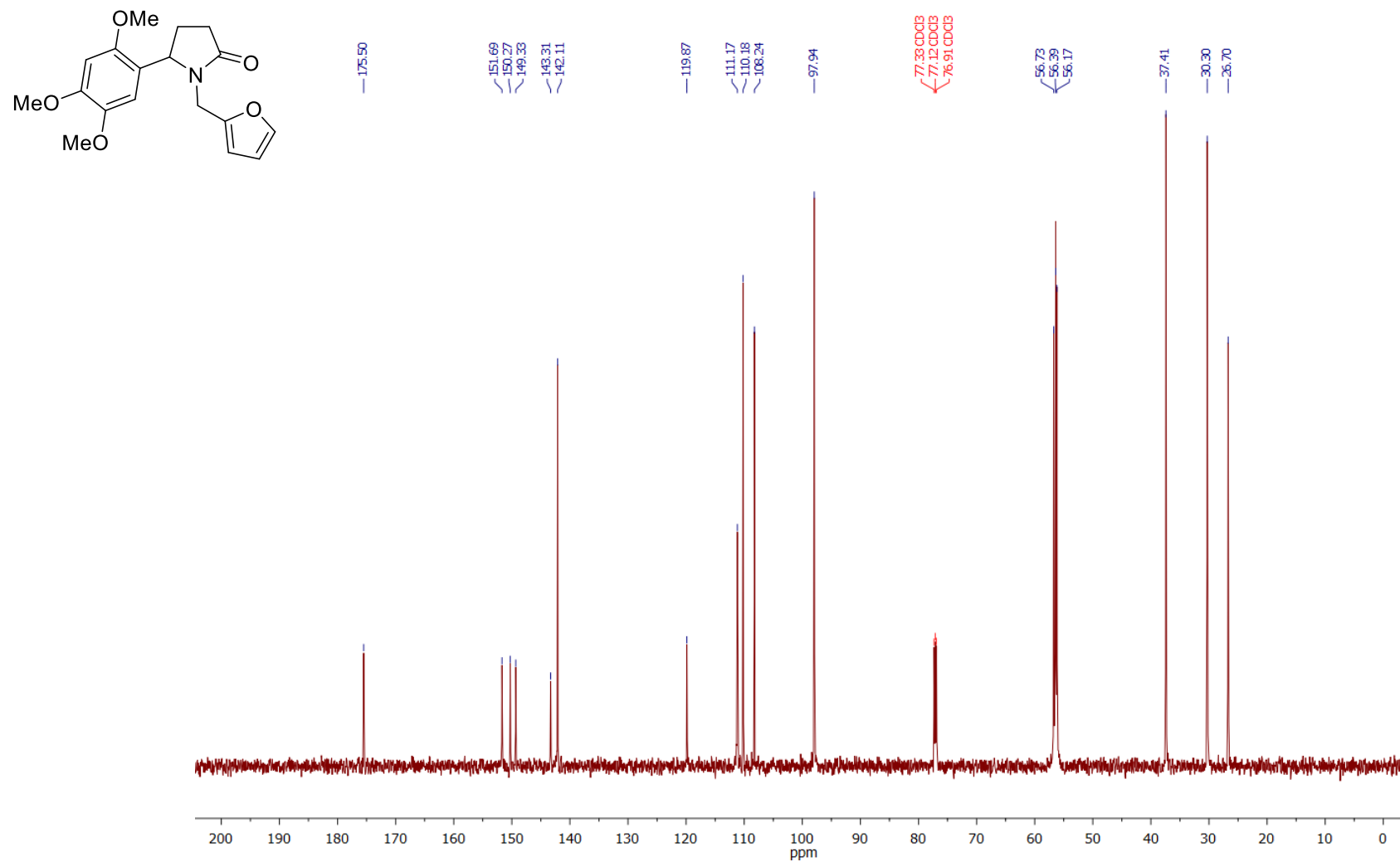
1-Furfuryl-5-(2,4,5-trimethoxyphenyl)pyrrolidin-2-one (3e)

^1H NMR (CDCl_3 , 600 MHz)



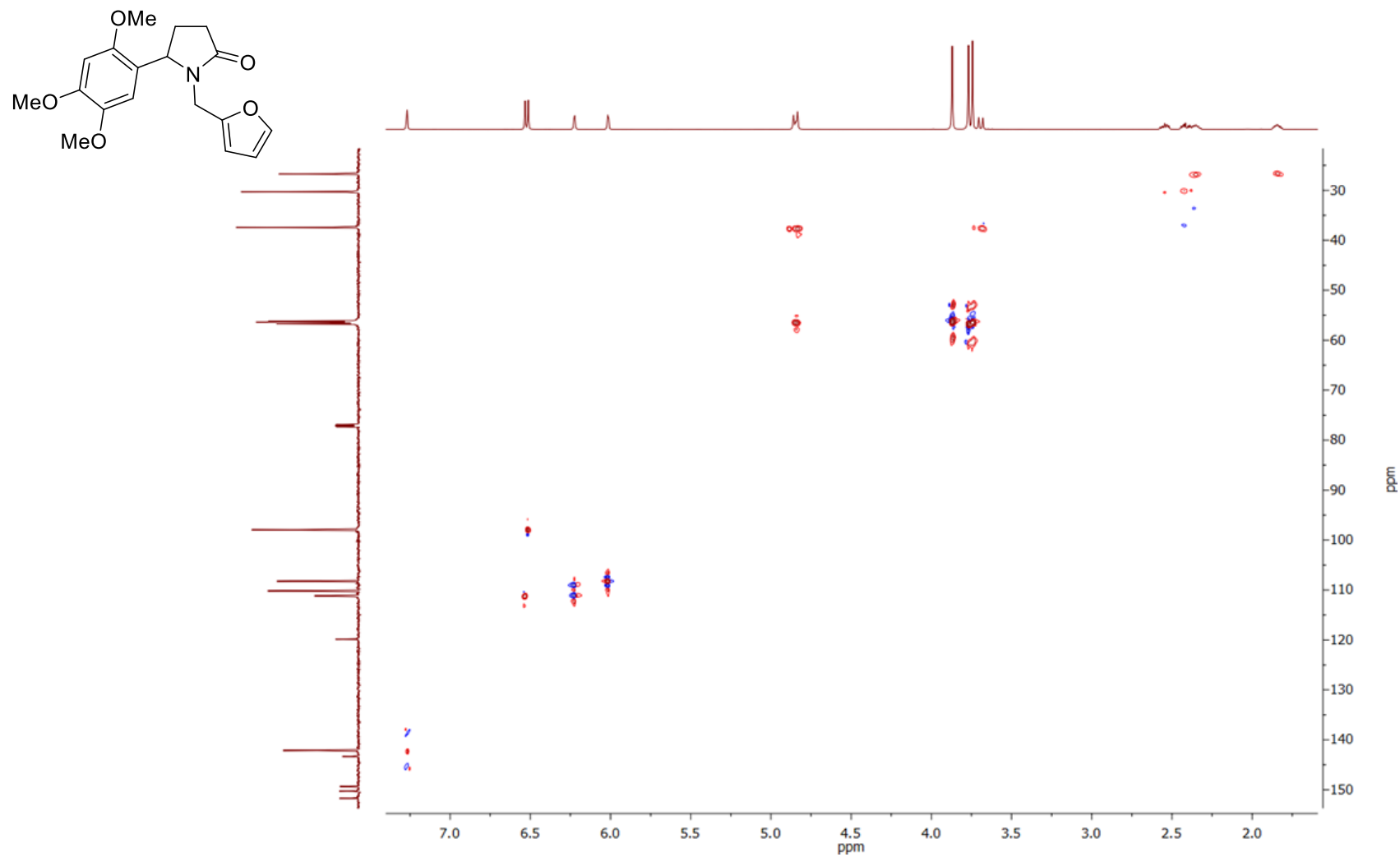
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^{13}C NMR (CDCl_3 , 150 MHz)



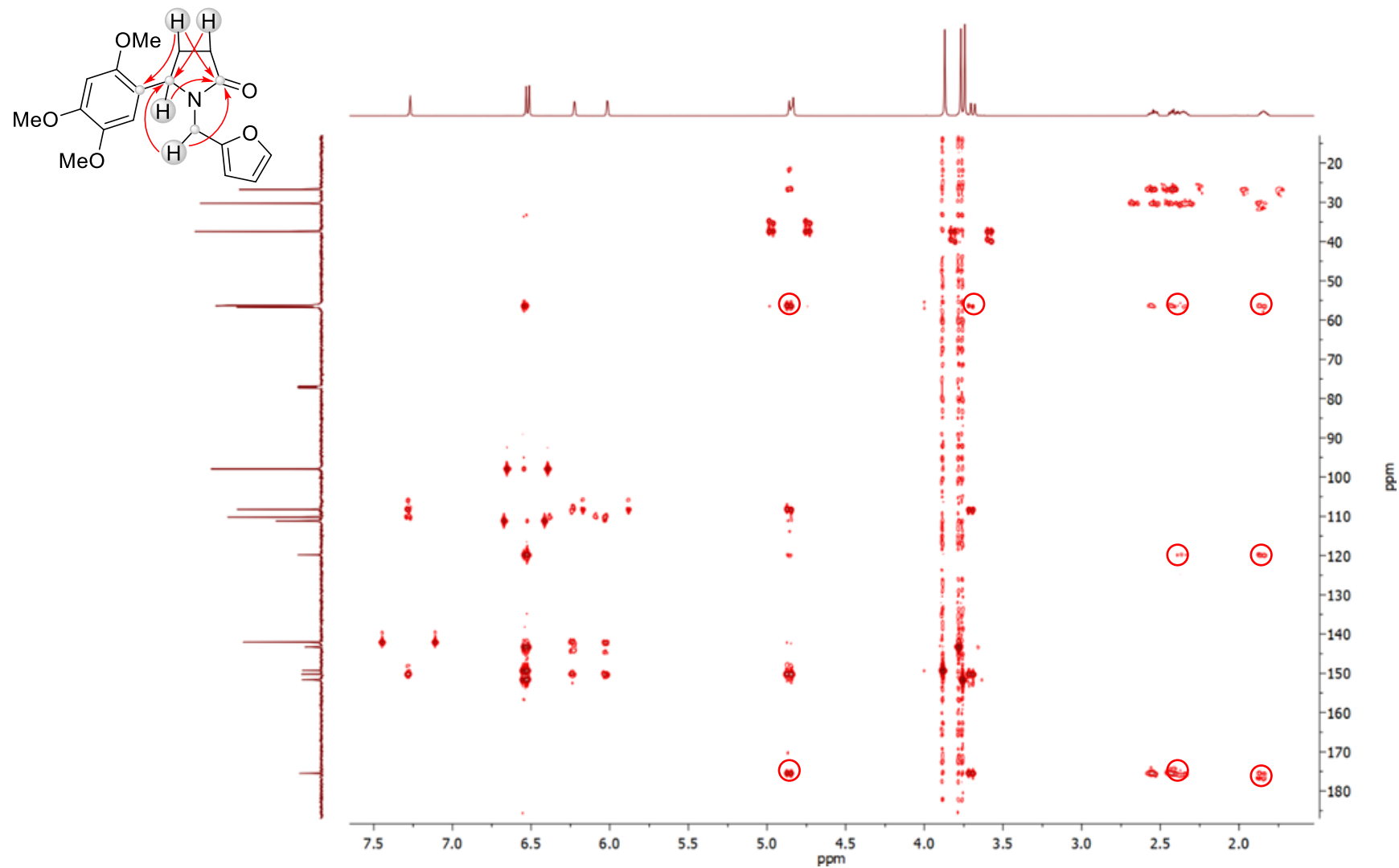
1-Furfuryl-5-(2,4,5-trimethoxyphenyl)pyrrolidin-2-one (3e)

HSQC ^1H - ^{13}C (CDCl_3)



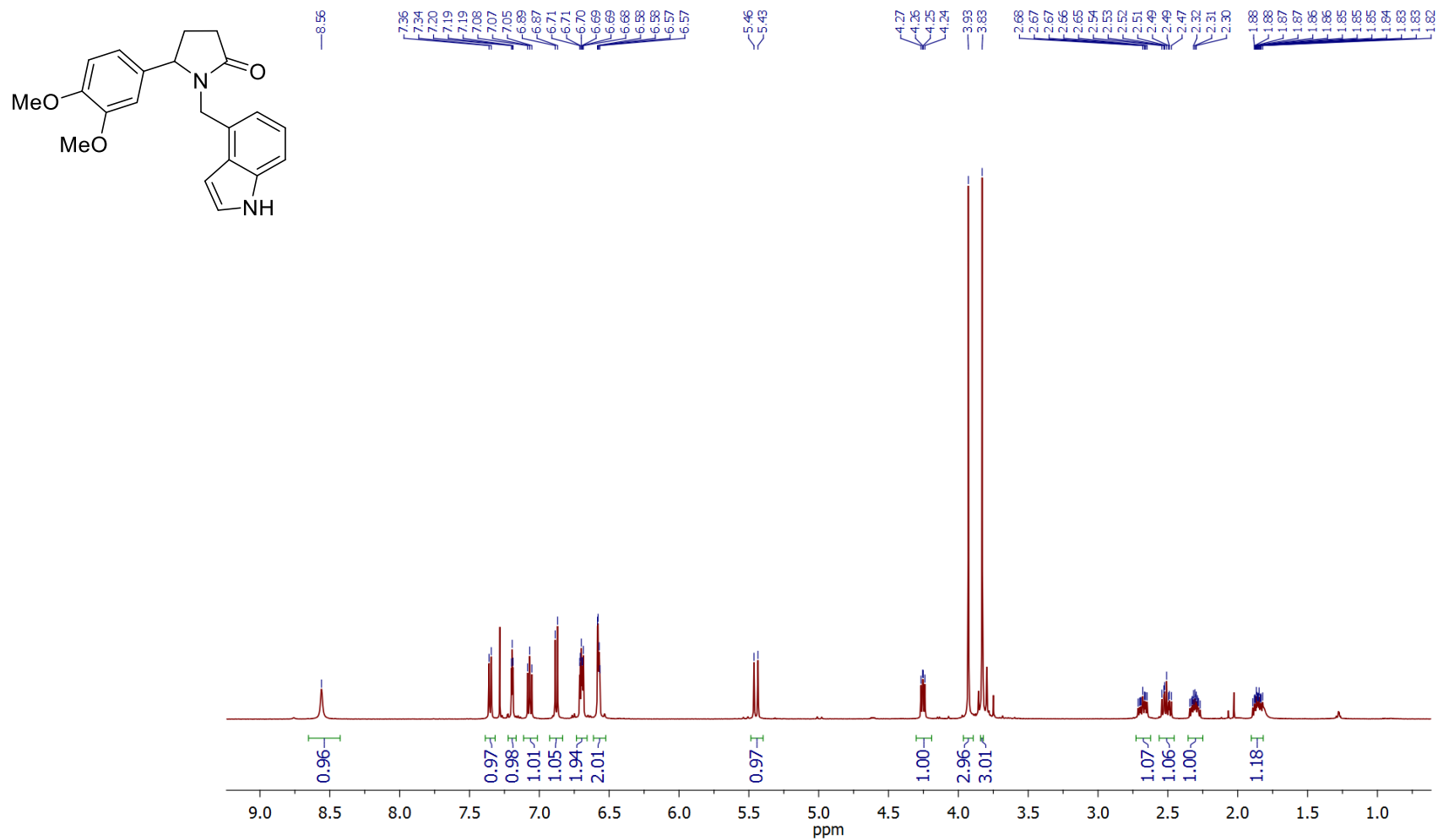
1-Furfuryl-5-(2,4,5-trimethoxyphenyl)pyrrolidin-2-one (3e)

HMBC ^1H - ^{13}C (CDCl_3)



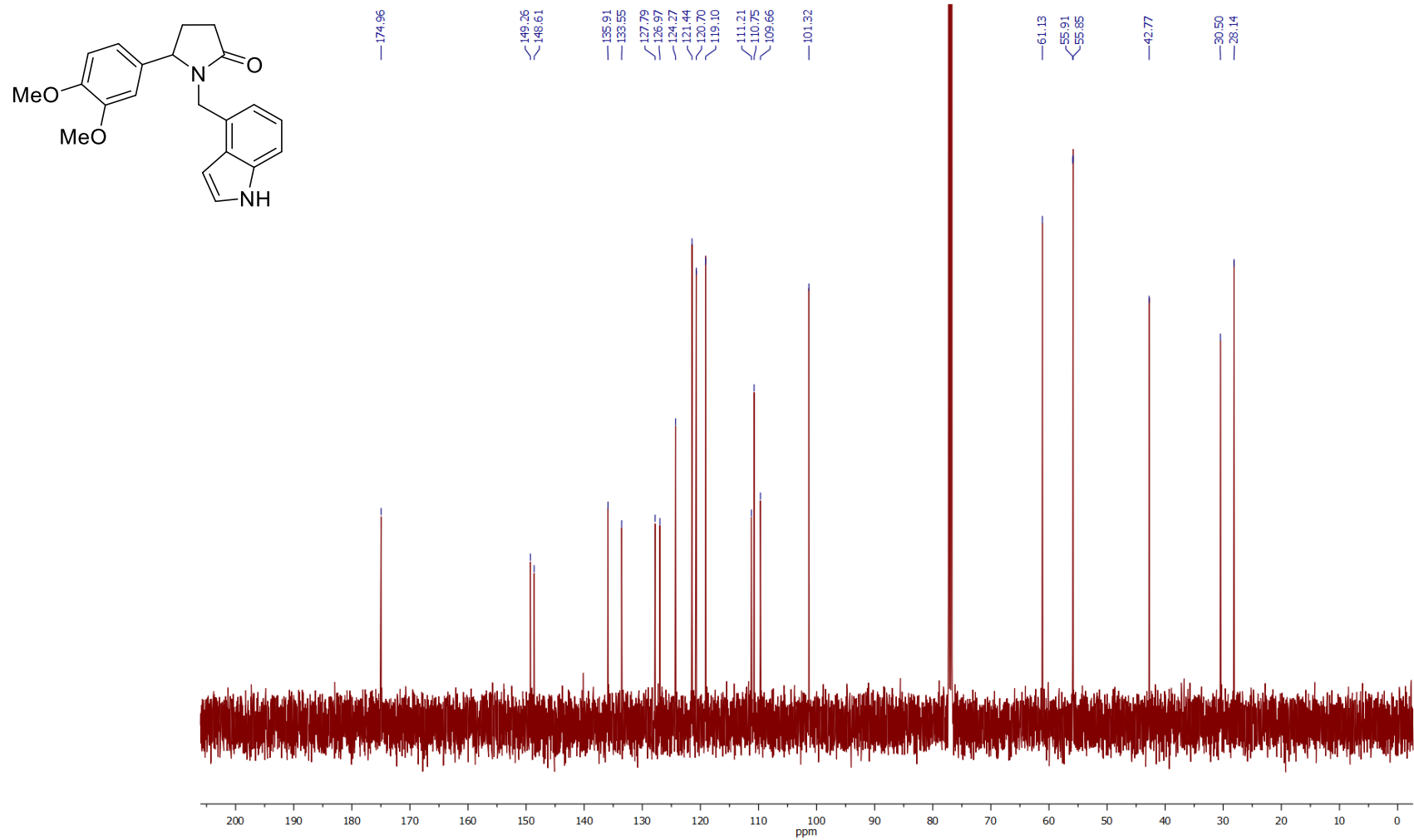
1-[(1*H*-Indol-4-yl)methyl]-5-(3,4-dimethoxyphenyl)pyrrolidin-2-one (3f)

¹H NMR (CDCl₃, 500 MHz)



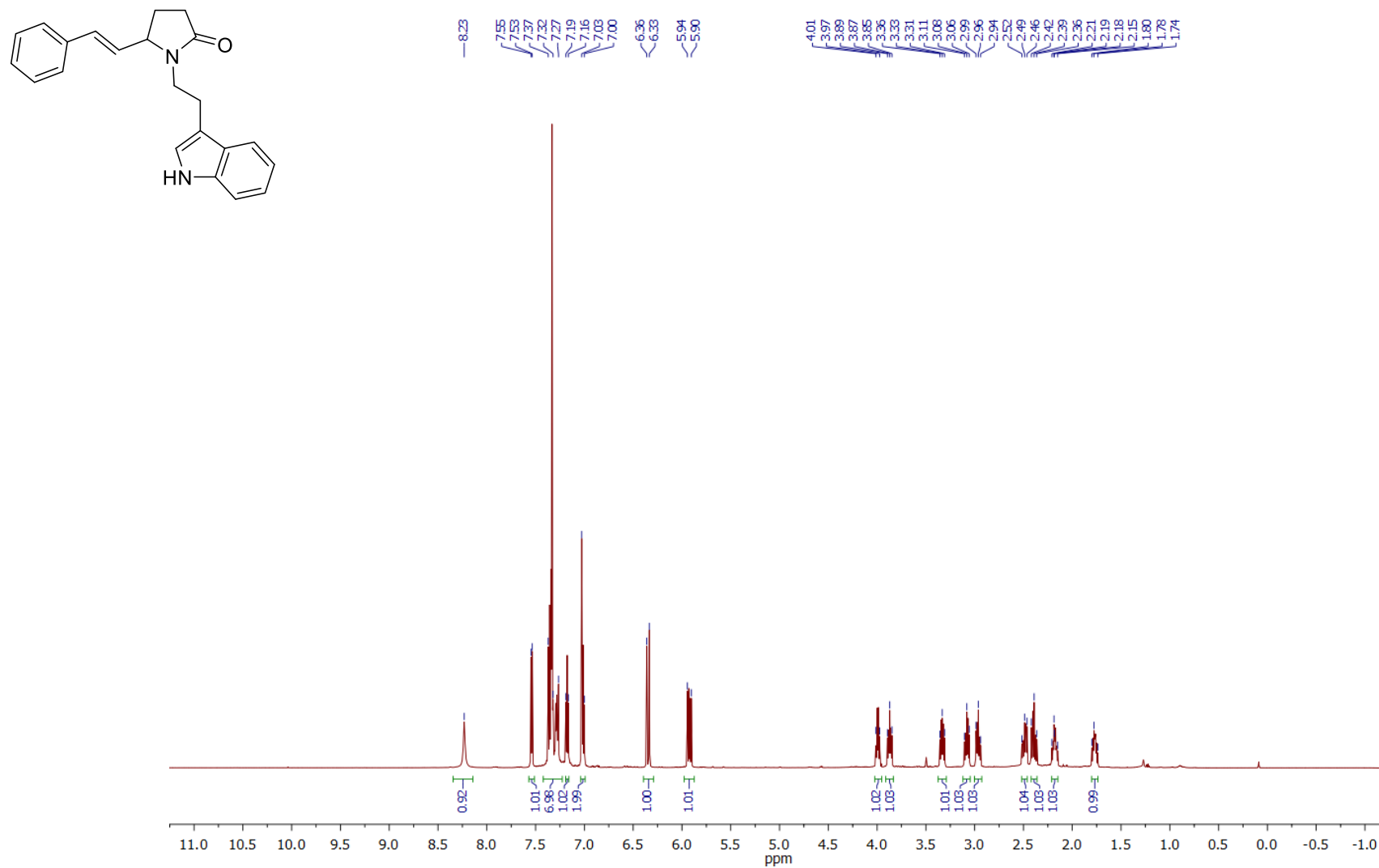
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¹³C NMR (CDCl₃, 125 MHz)



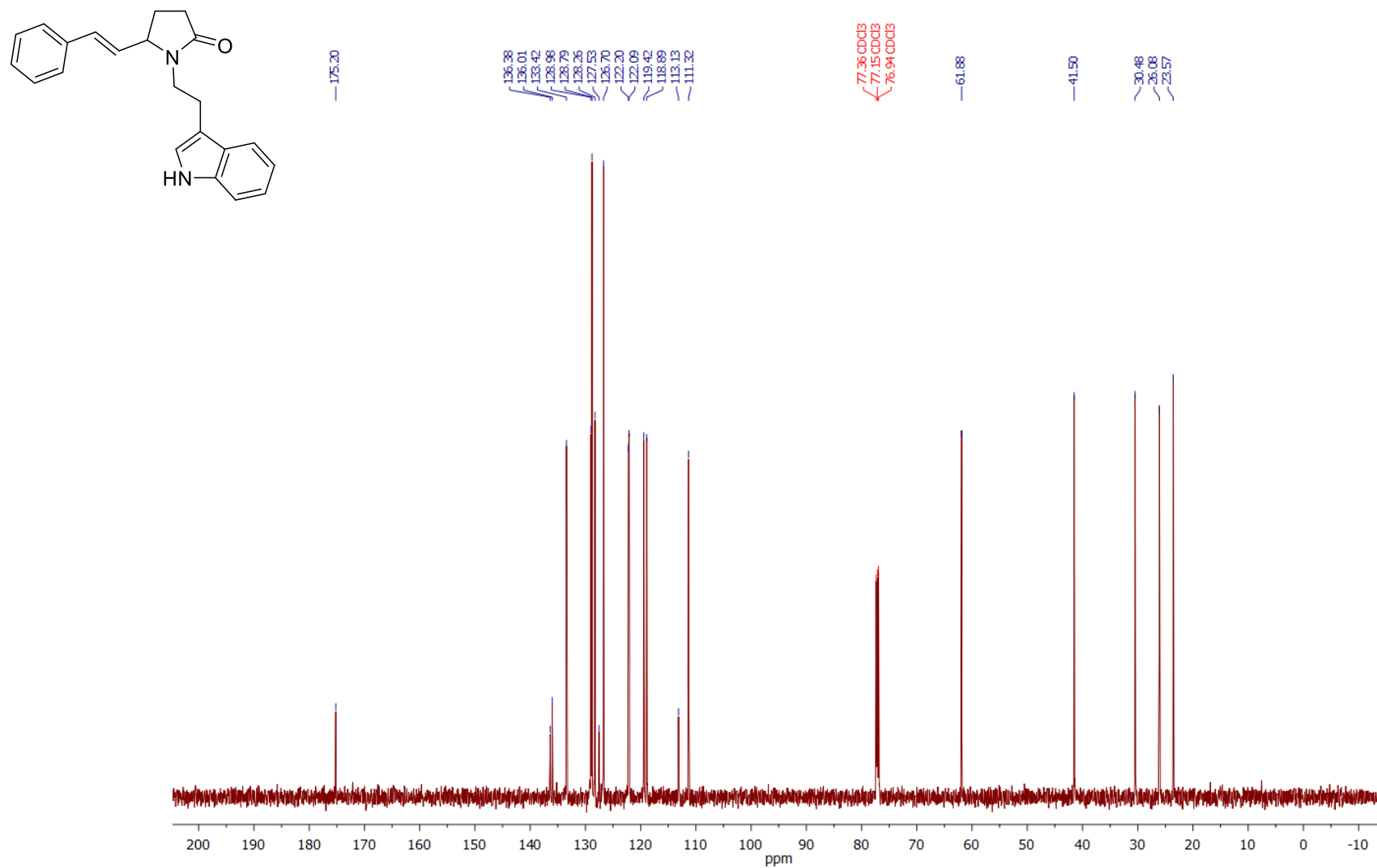
(E)-1-[2-(1H-Indol-3-yl)ethyl]-5-styrylpyrrolidin-2-one (3g)

¹H NMR (CDCl₃, 600 MHz)



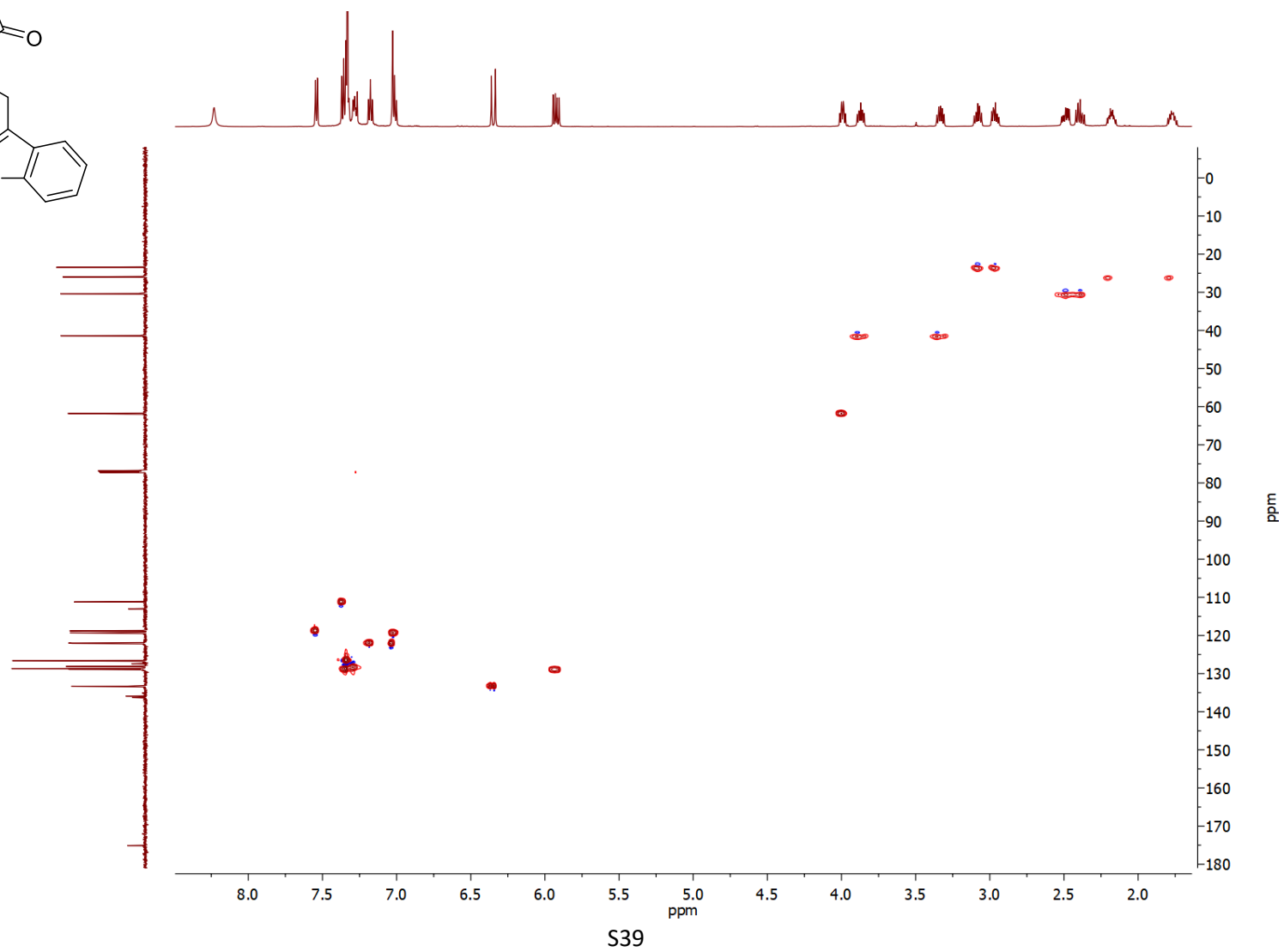
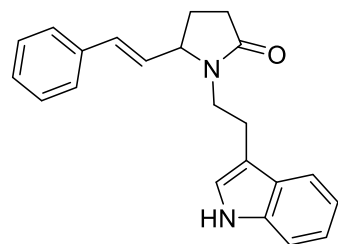
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¹³C NMR (CDCl₃, 150 MHz)



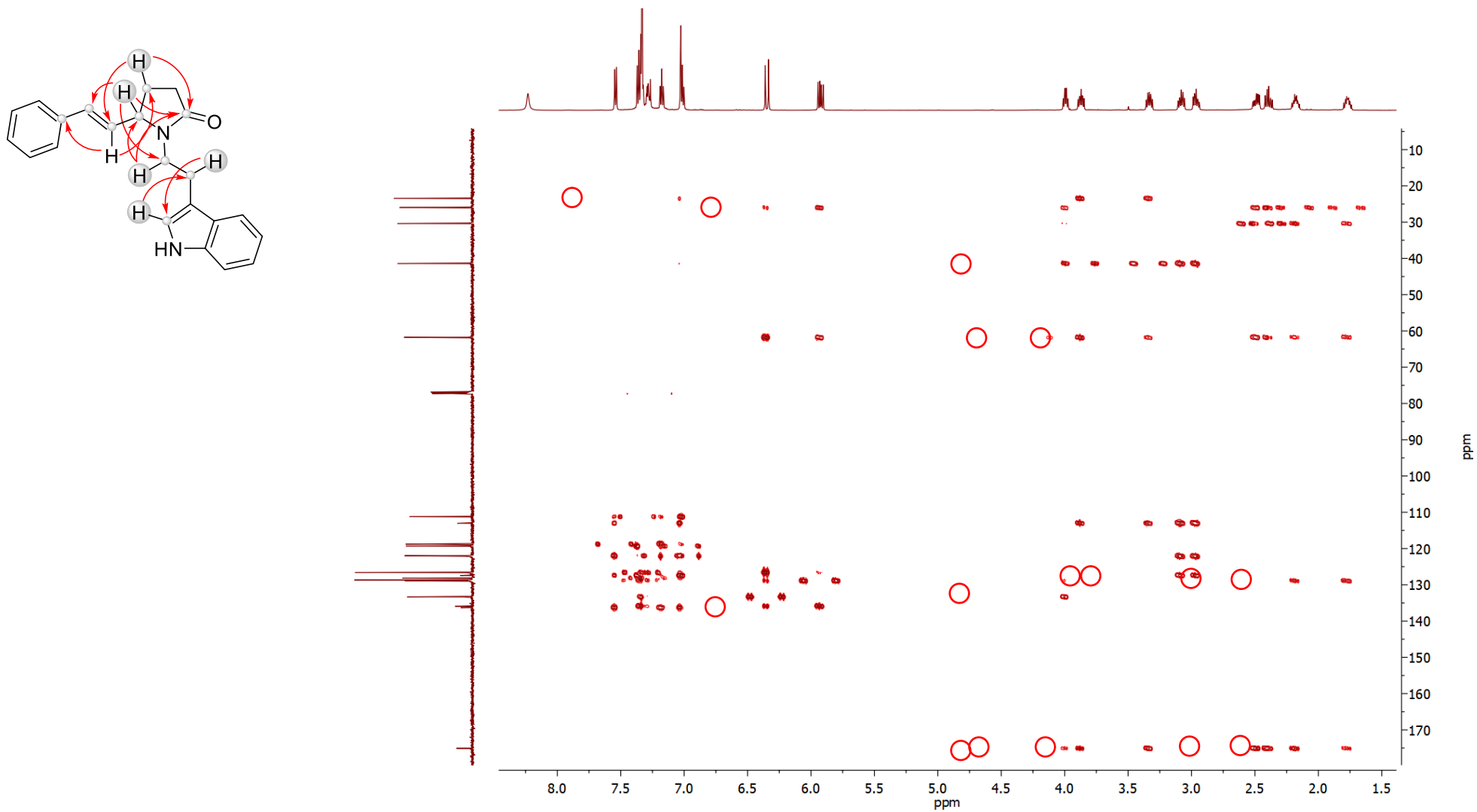
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HSQC ^1H - ^{13}C (CDCl_3)



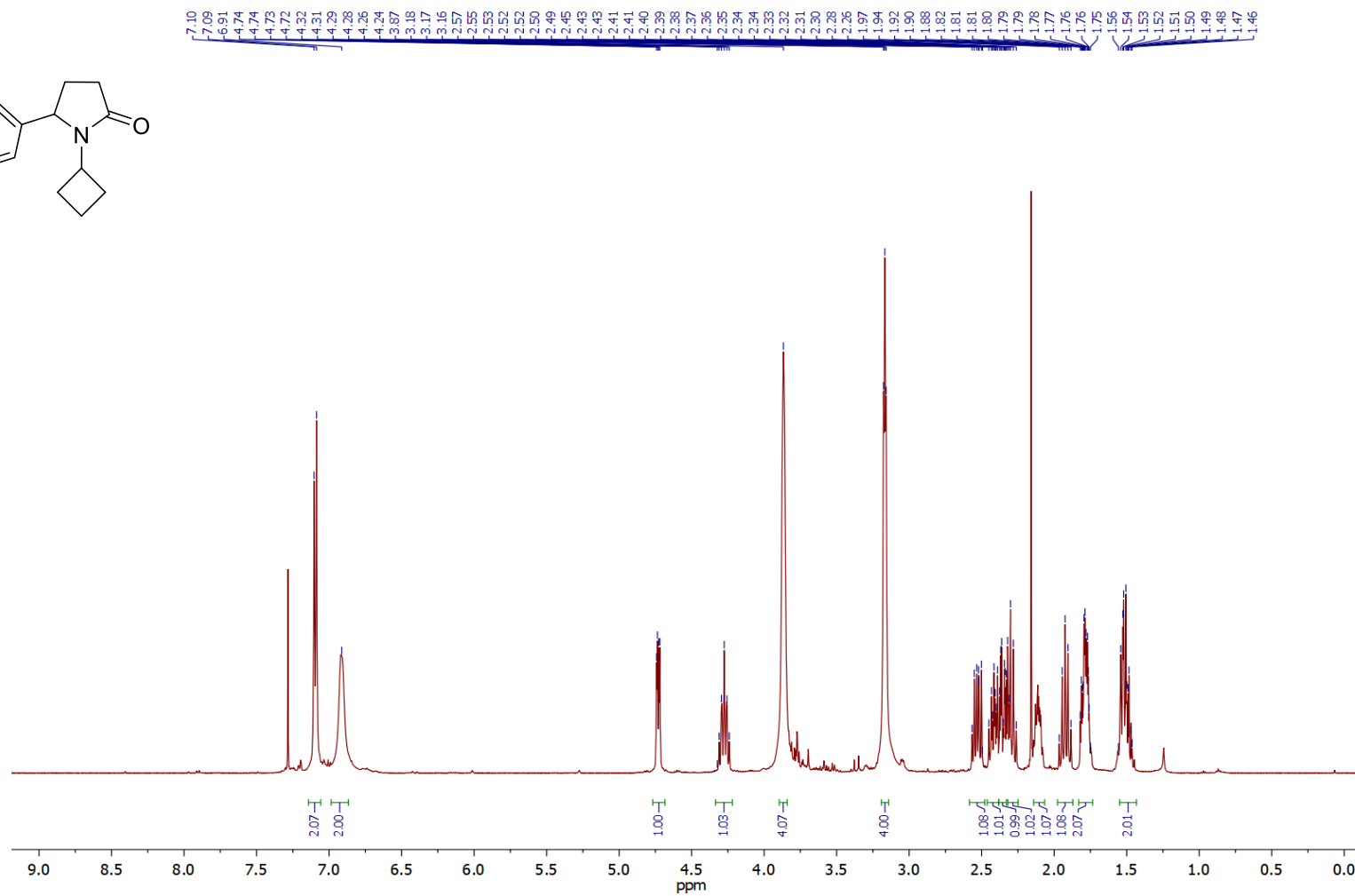
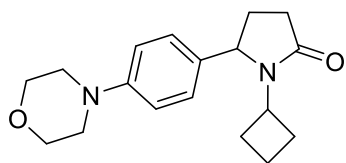
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HMBC ^1H - ^{13}C (CDCl_3)



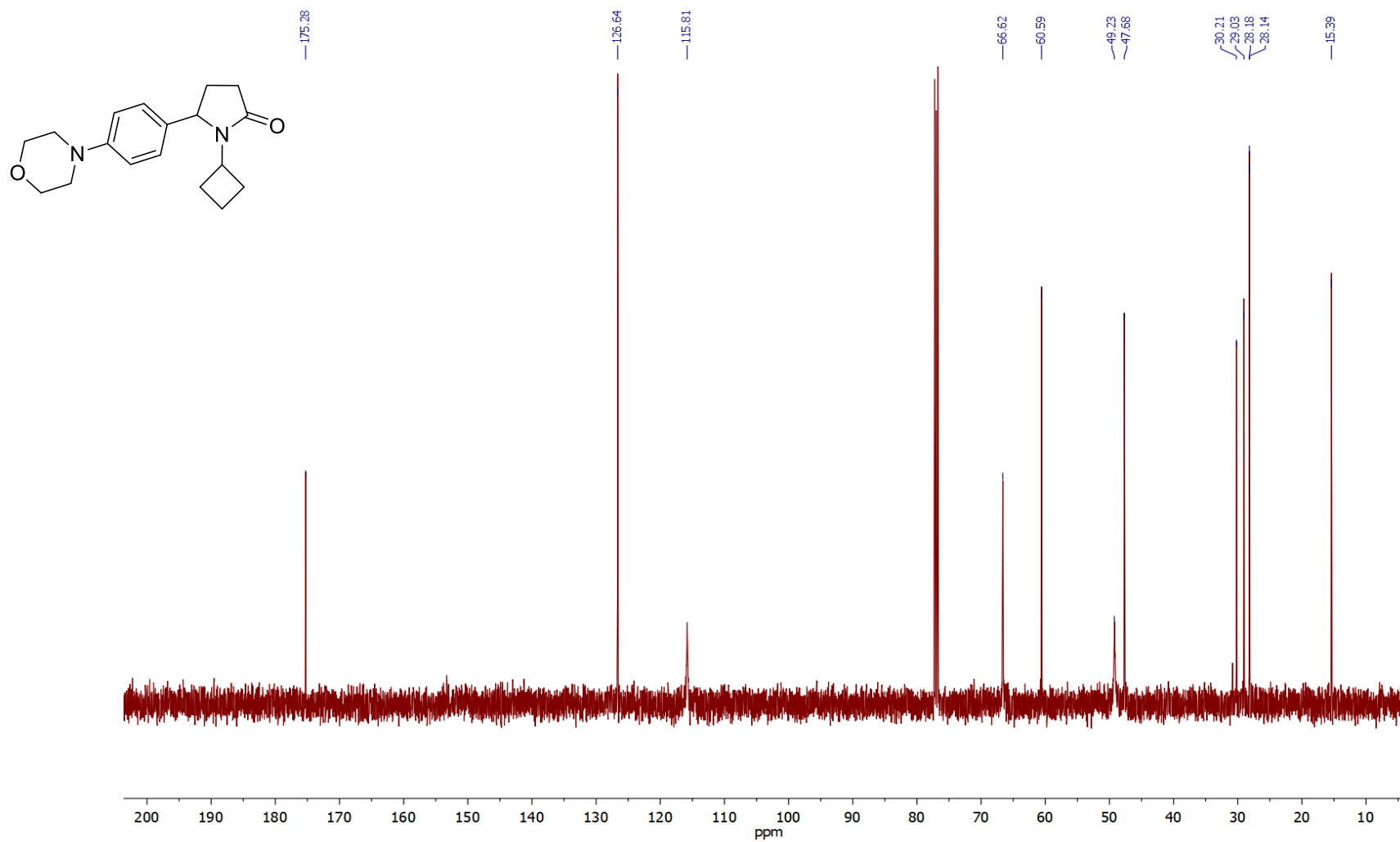
1-Cyclobutyl-5-(4-morpholinophenyl)pyrrolidin-2-one (3h)

^1H NMR (CDCl_3 , 500 MHz)



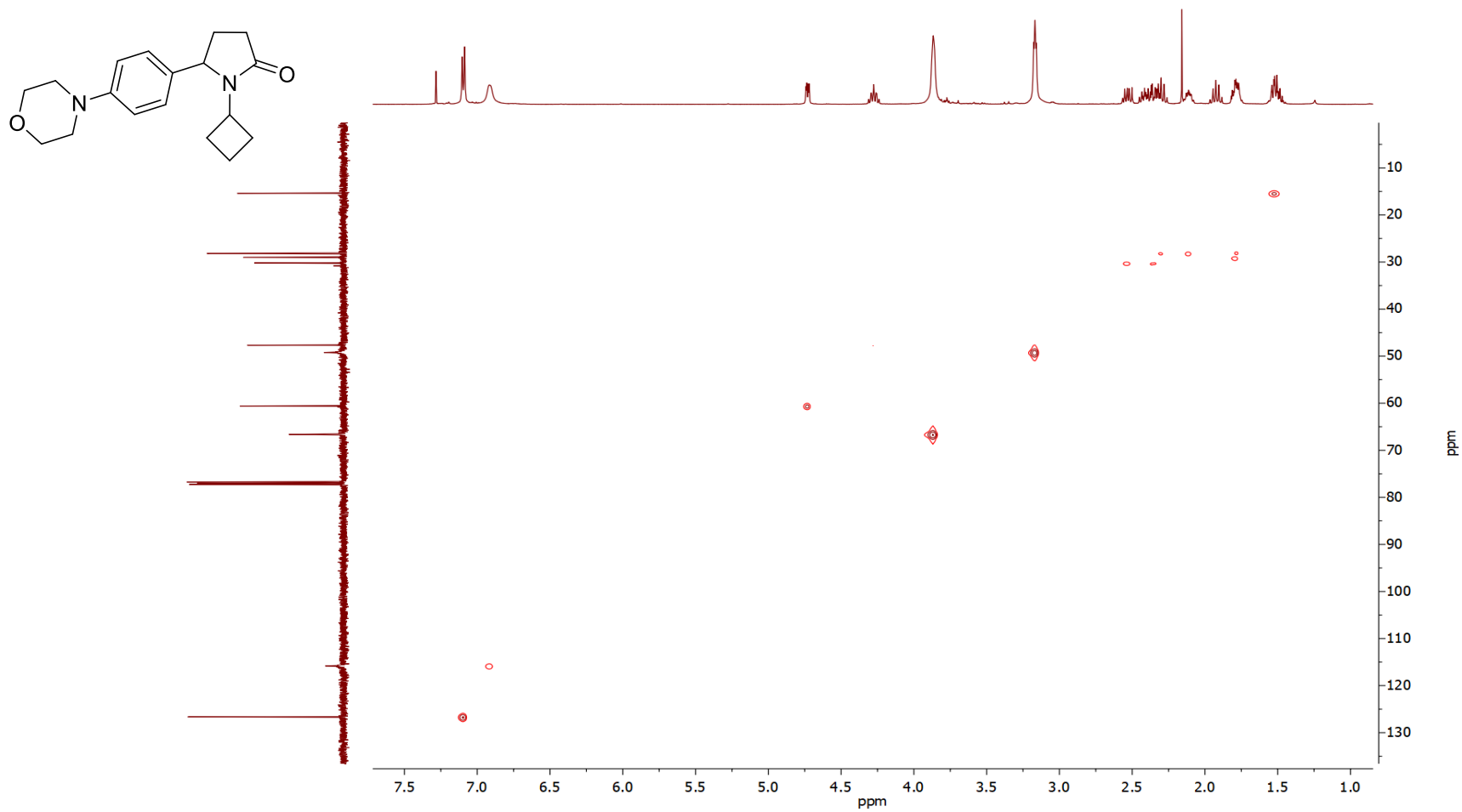
1-Cyclobutyl-5-(4-morpholinophenyl)pyrrolidin-2-one (3h)

^{13}C NMR (CDCl_3 , 125 MHz)



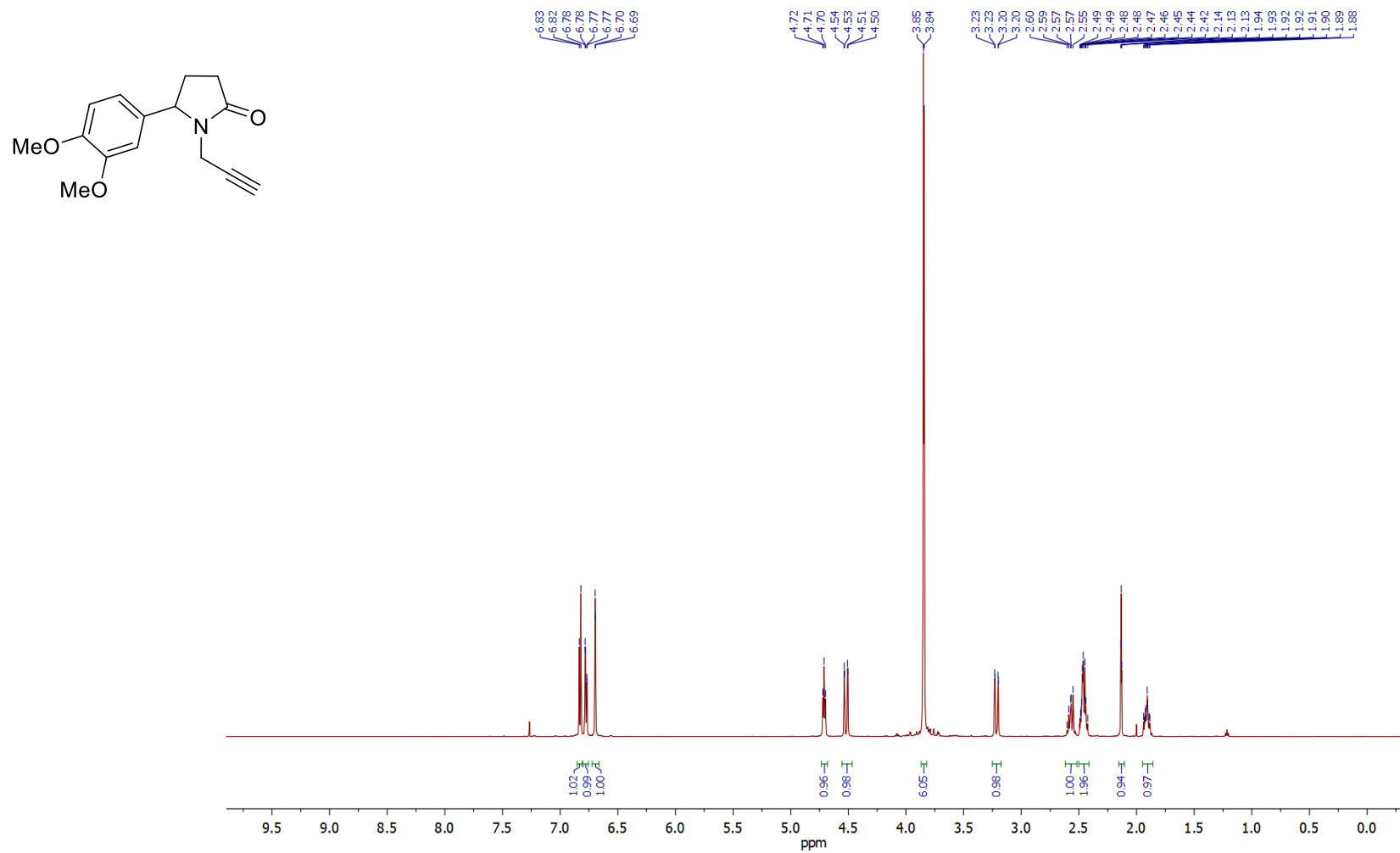
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HSQC ^1H - ^{13}C (CDCl_3)



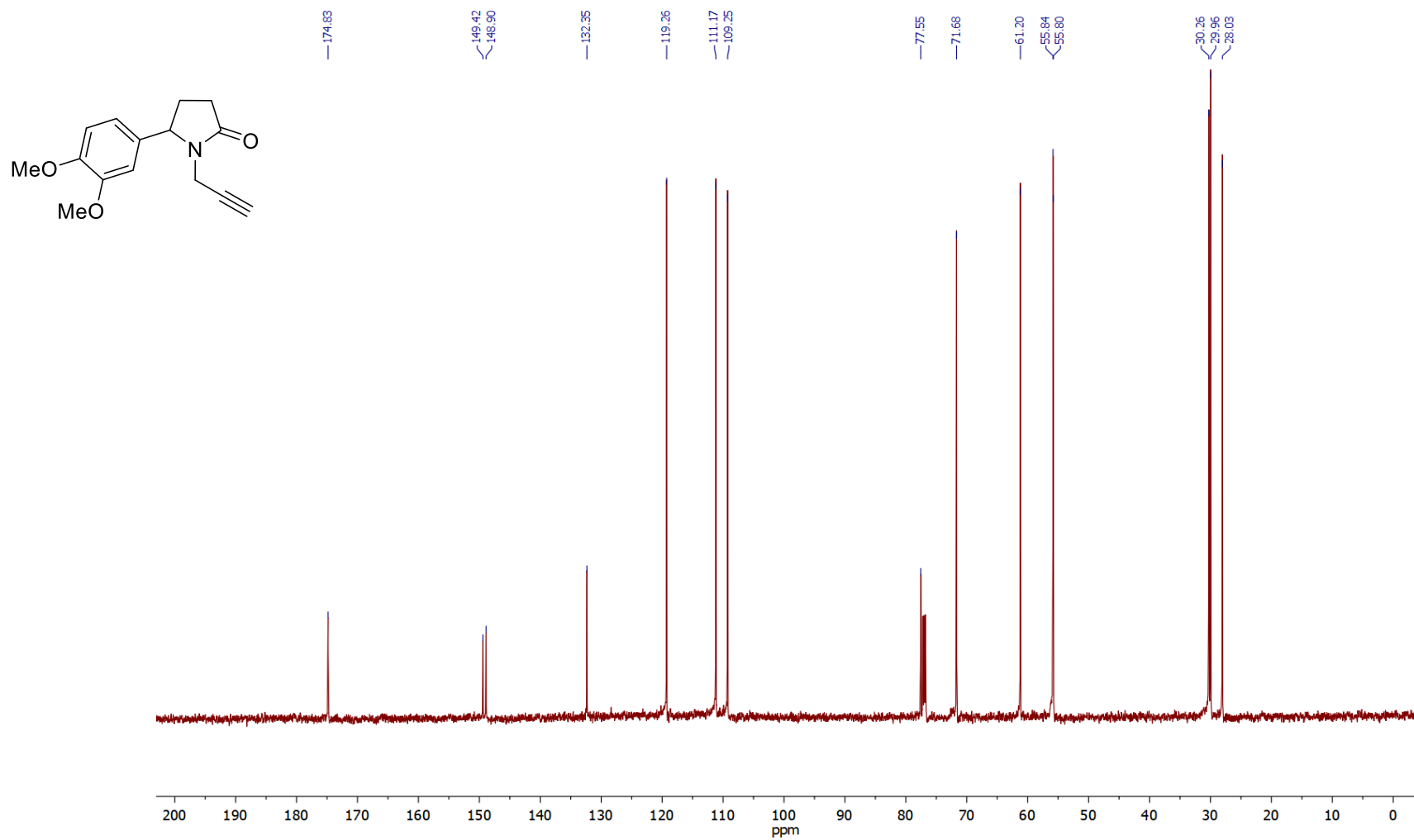
5-(3,4-Dimethoxyphenyl)-1-(prop-2-yn-1-yl)pyrrolidin-2-one (3i)

^1H NMR (CDCl_3 , 400 MHz)



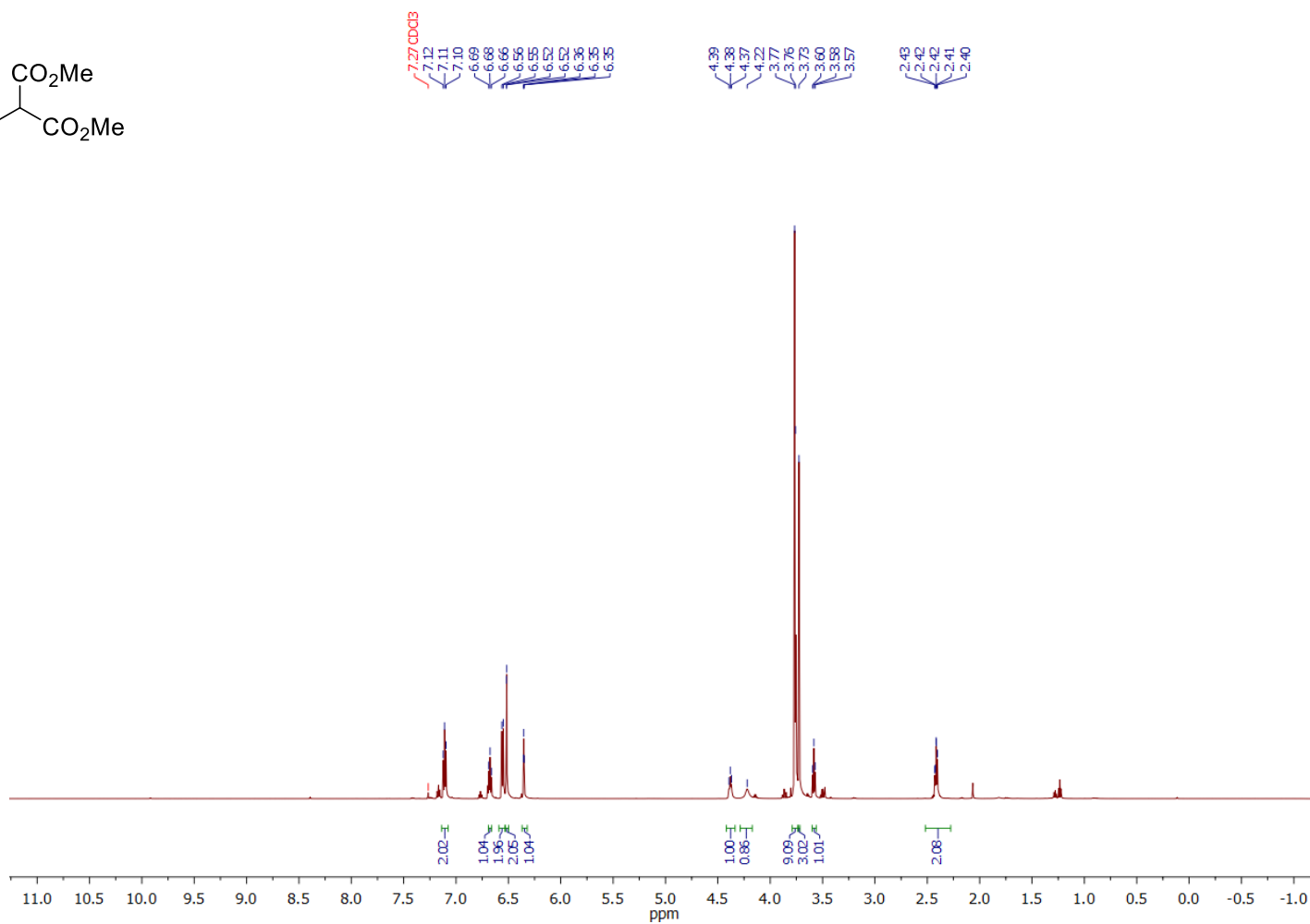
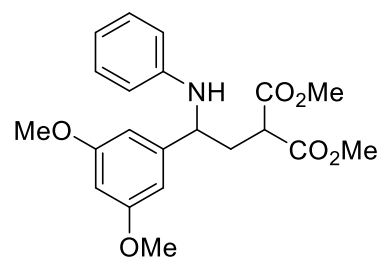
5-(3,4-Dimethoxyphenyl)-1-(prop-2-yn-1-yl)pyrrolidin-2-one (3i)

^{13}C NMR (CDCl_3 , 100 MHz)



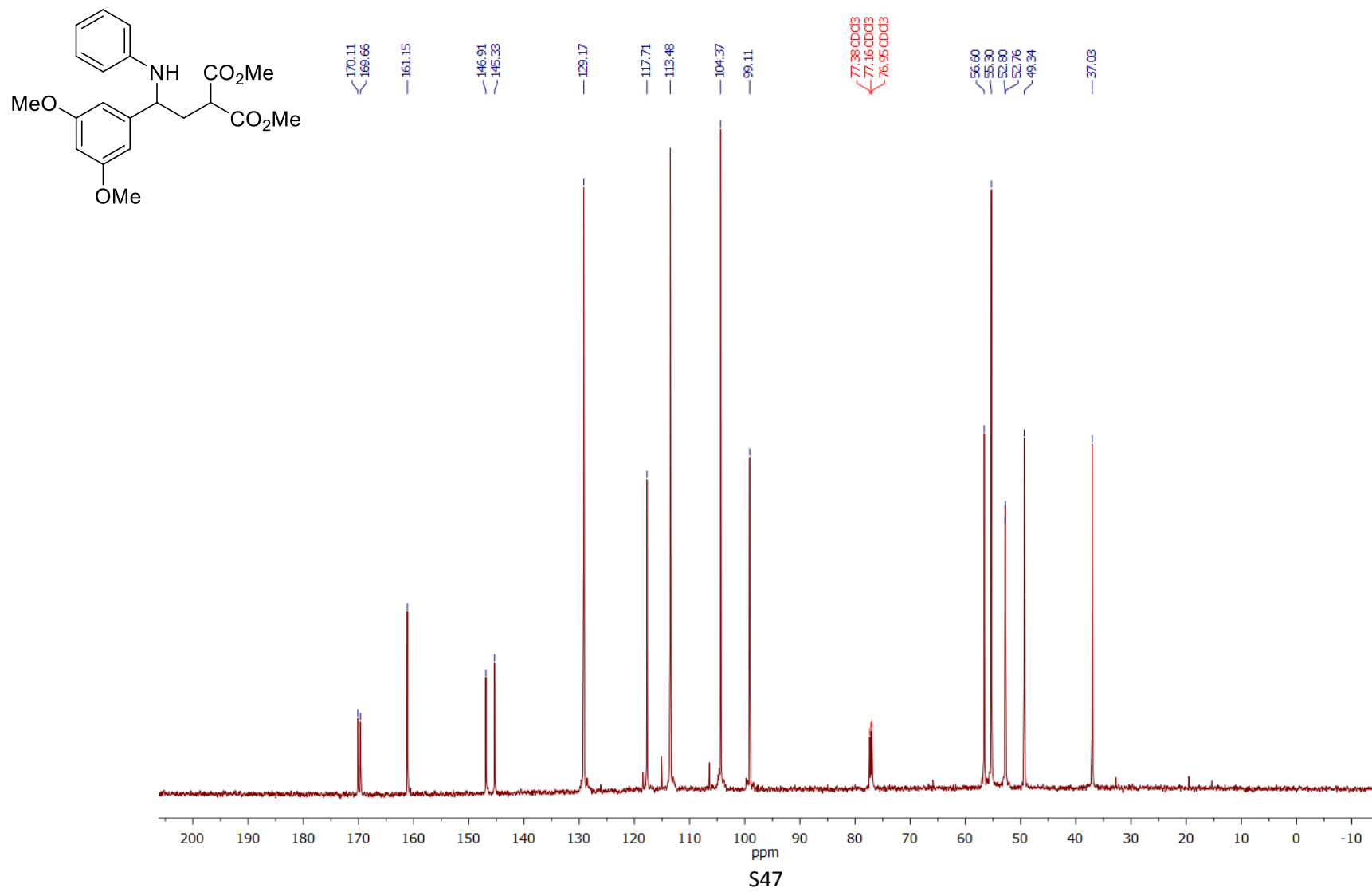
Dimethyl 2-[2-(3,5-dimethoxyphenyl)-2-(phenylamino)ethyl]malonate (4a)

^1H NMR (CDCl_3 , 600 MHz)



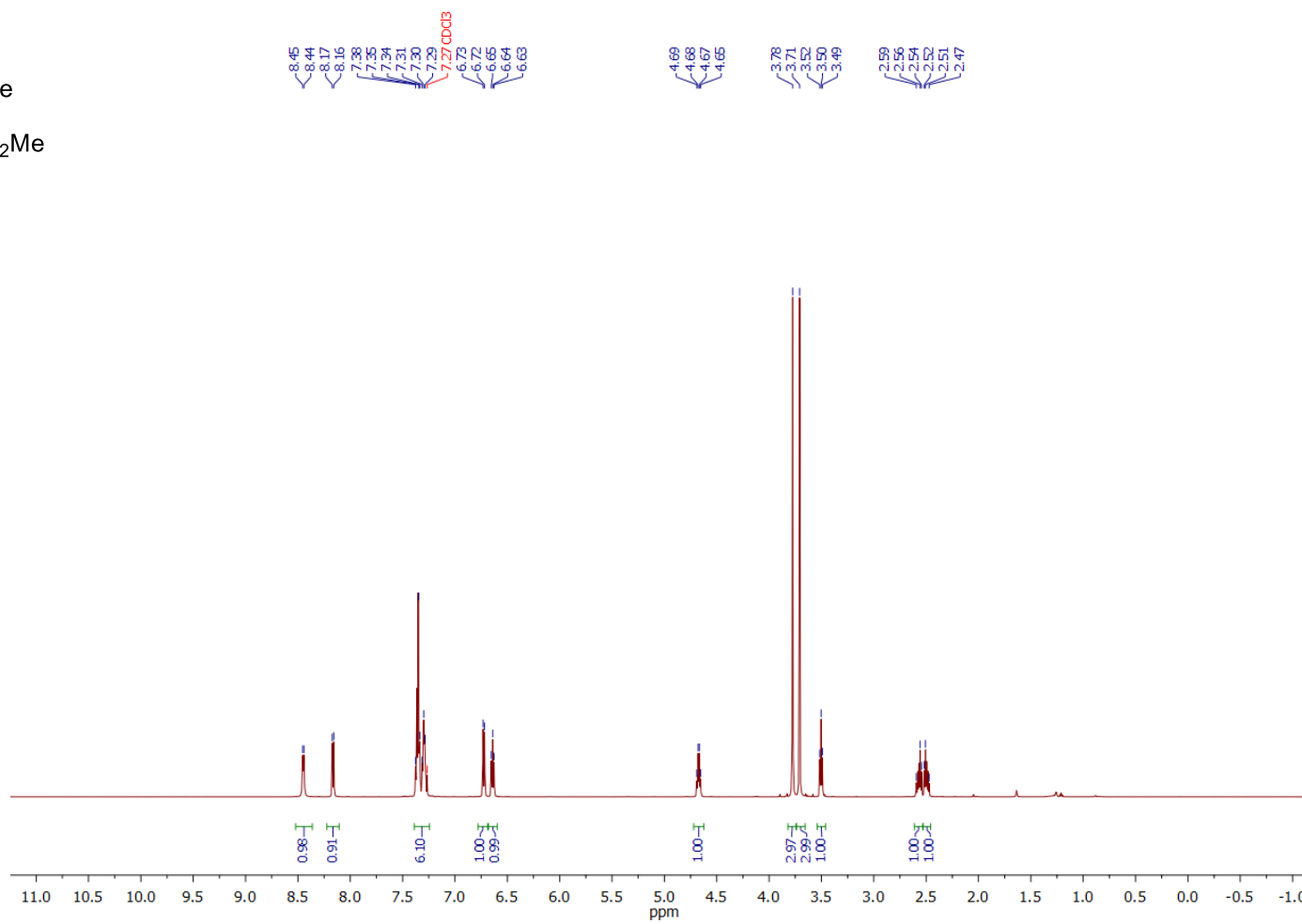
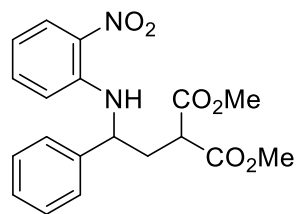
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^{13}C NMR (CDCl_3 , 150 MHz)



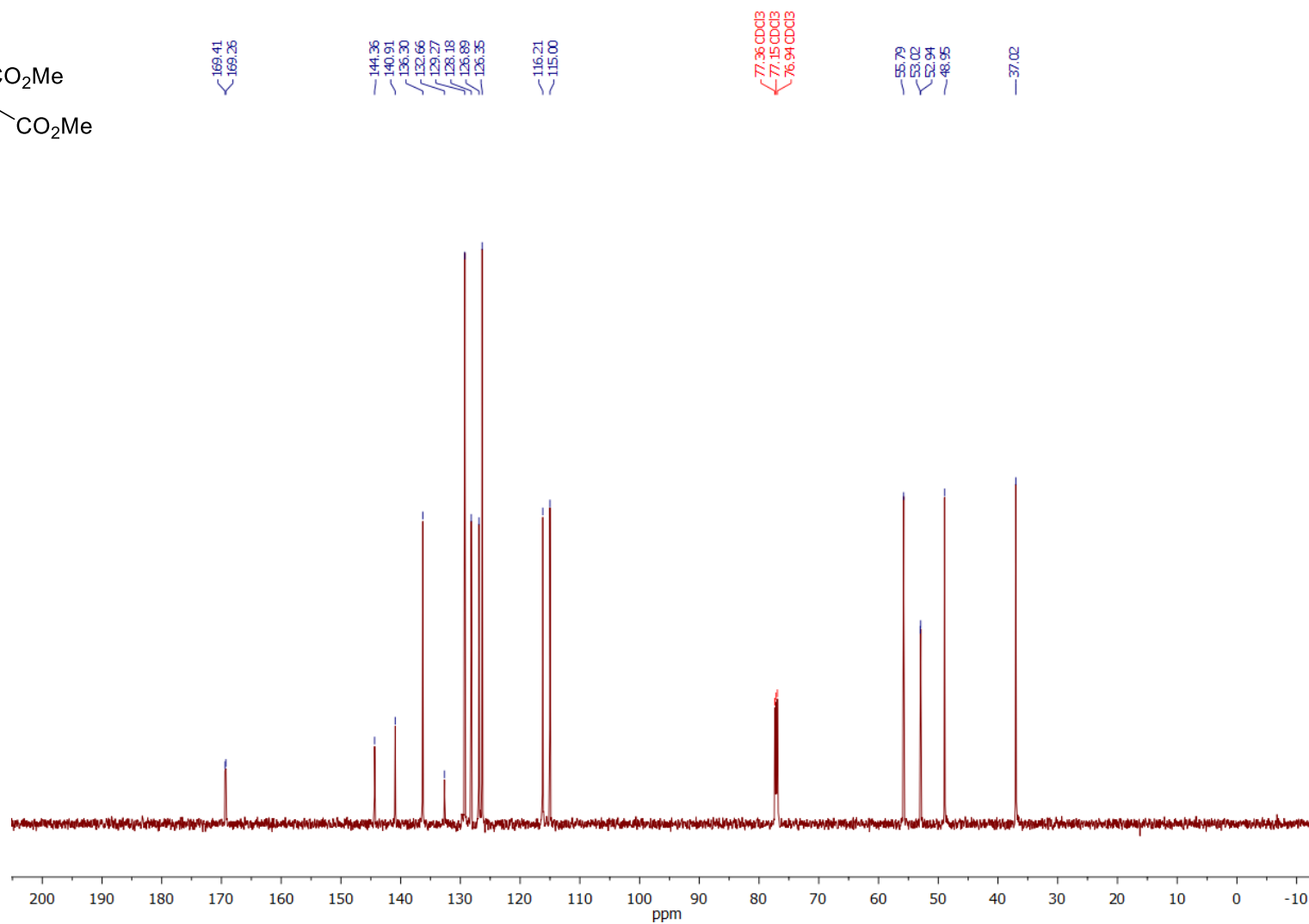
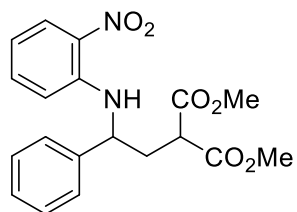
Dimethyl 2-{2-[(2-nitrophenyl)amino]-2-phenylethyl}malonate (4b)

^1H NMR (CDCl_3 , 600 MHz)



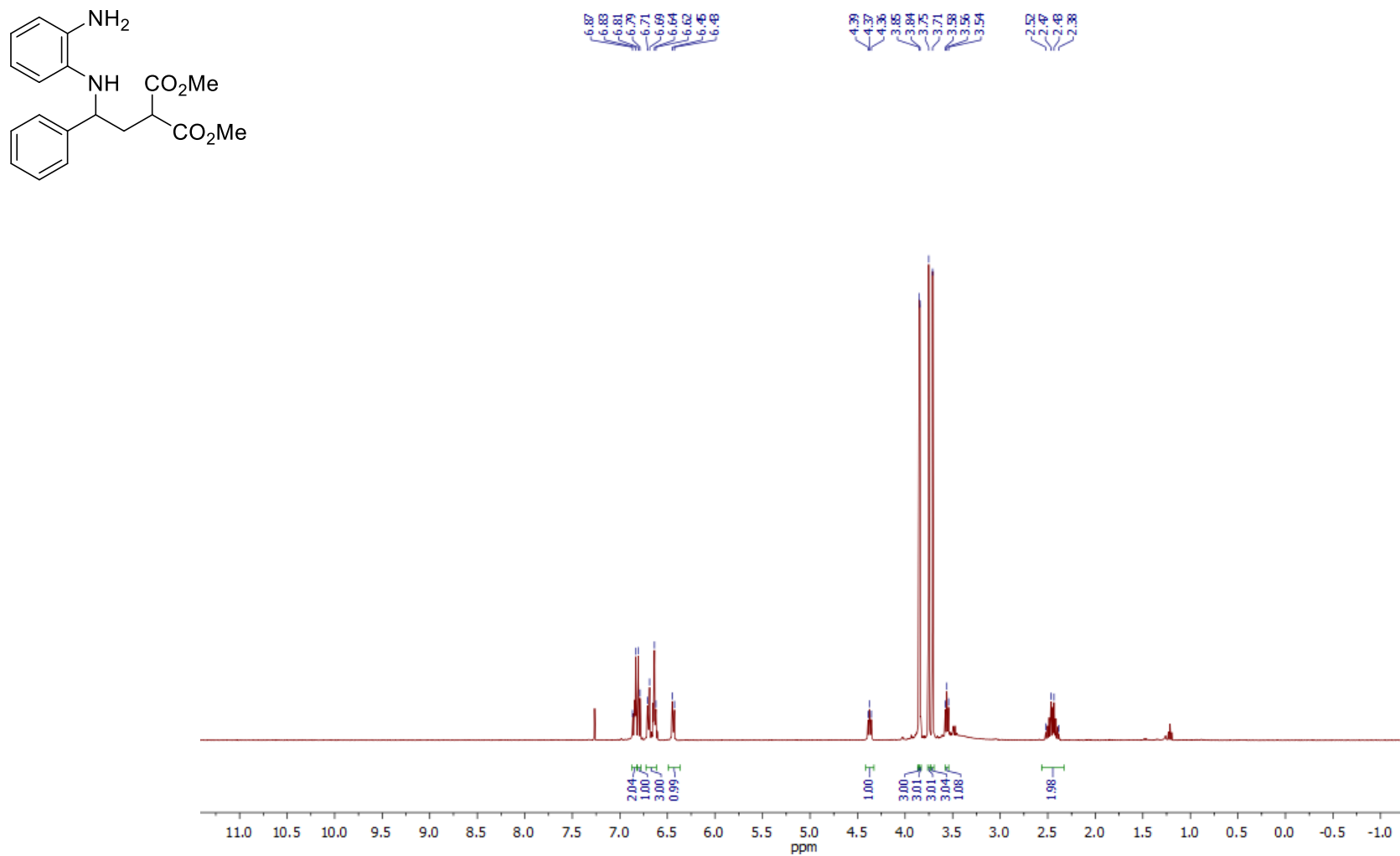
Dimethyl 2-{2-[(2-nitrophenyl)amino]-2-phenylethyl}malonate (4b)

^{13}C NMR (CDCl_3 , 150 MHz)



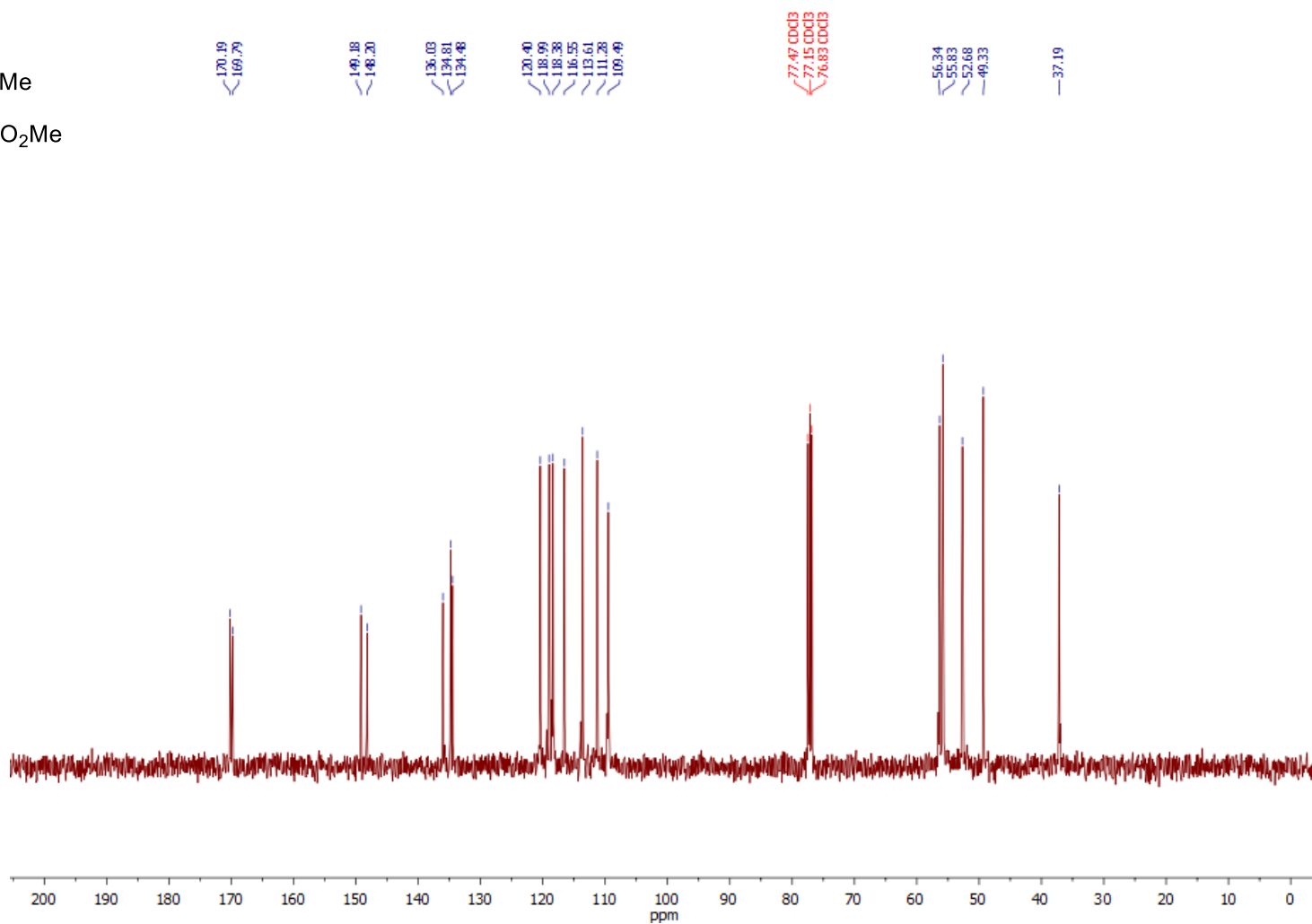
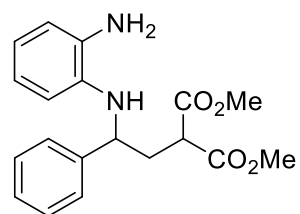
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^1H NMR (CDCl_3 , 400 MHz)



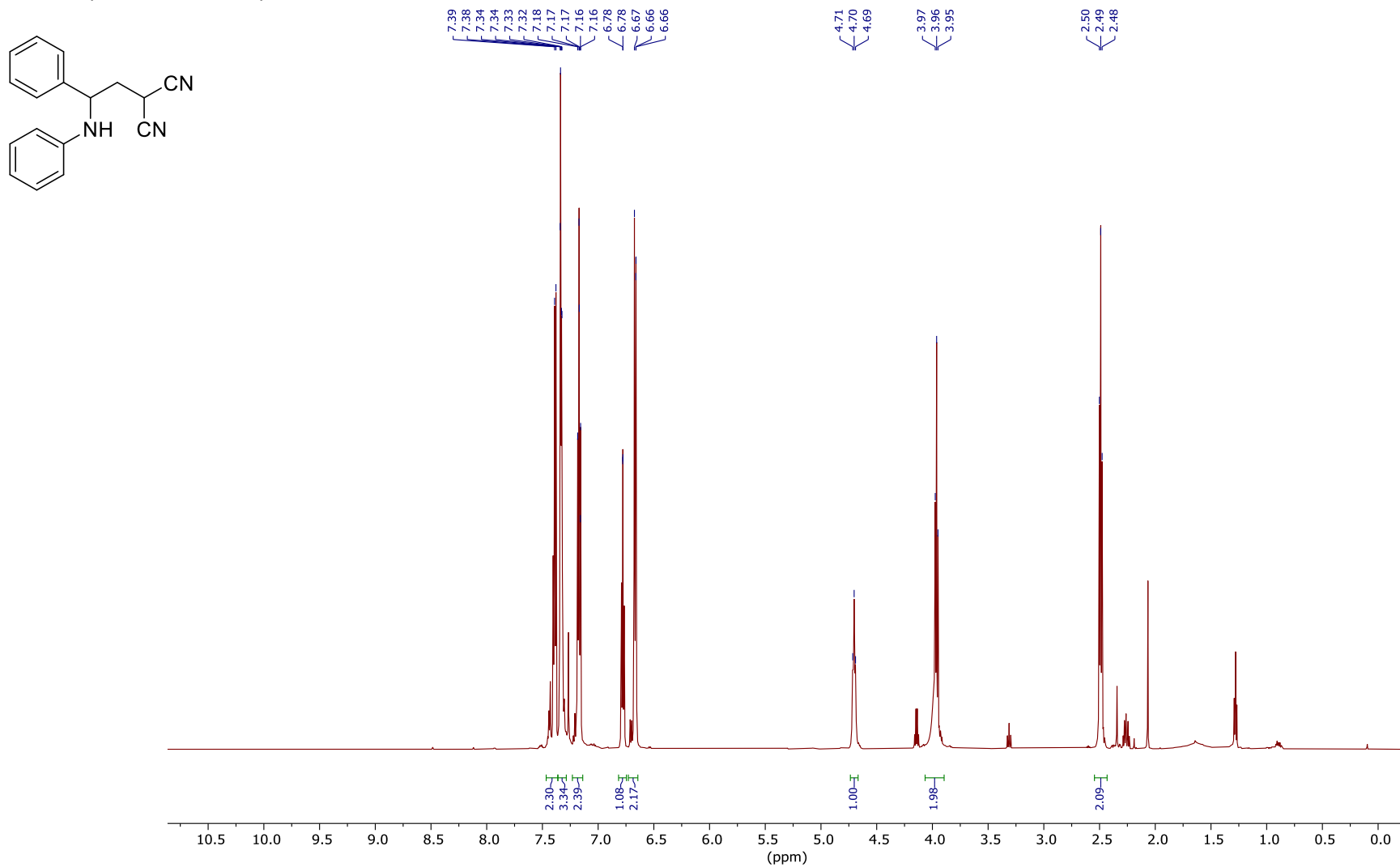
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^{13}C NMR (CDCl_3 , 100 MHz)



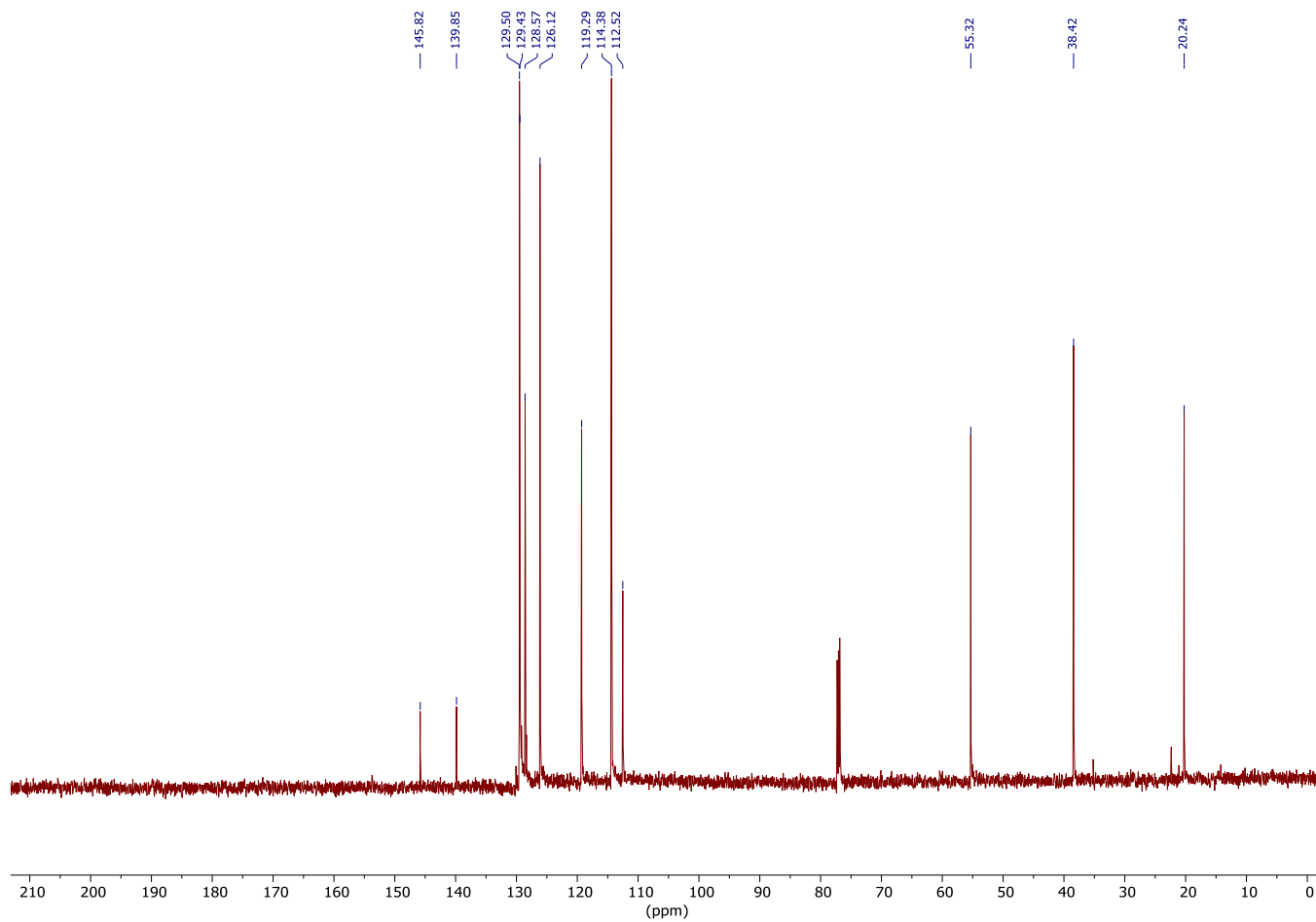
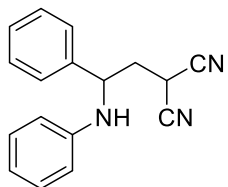
2-[2-Phenyl-2-(phenylamino)ethyl]malononitrile (4d)

¹H NMR (CDCl₃, 600 MHz)



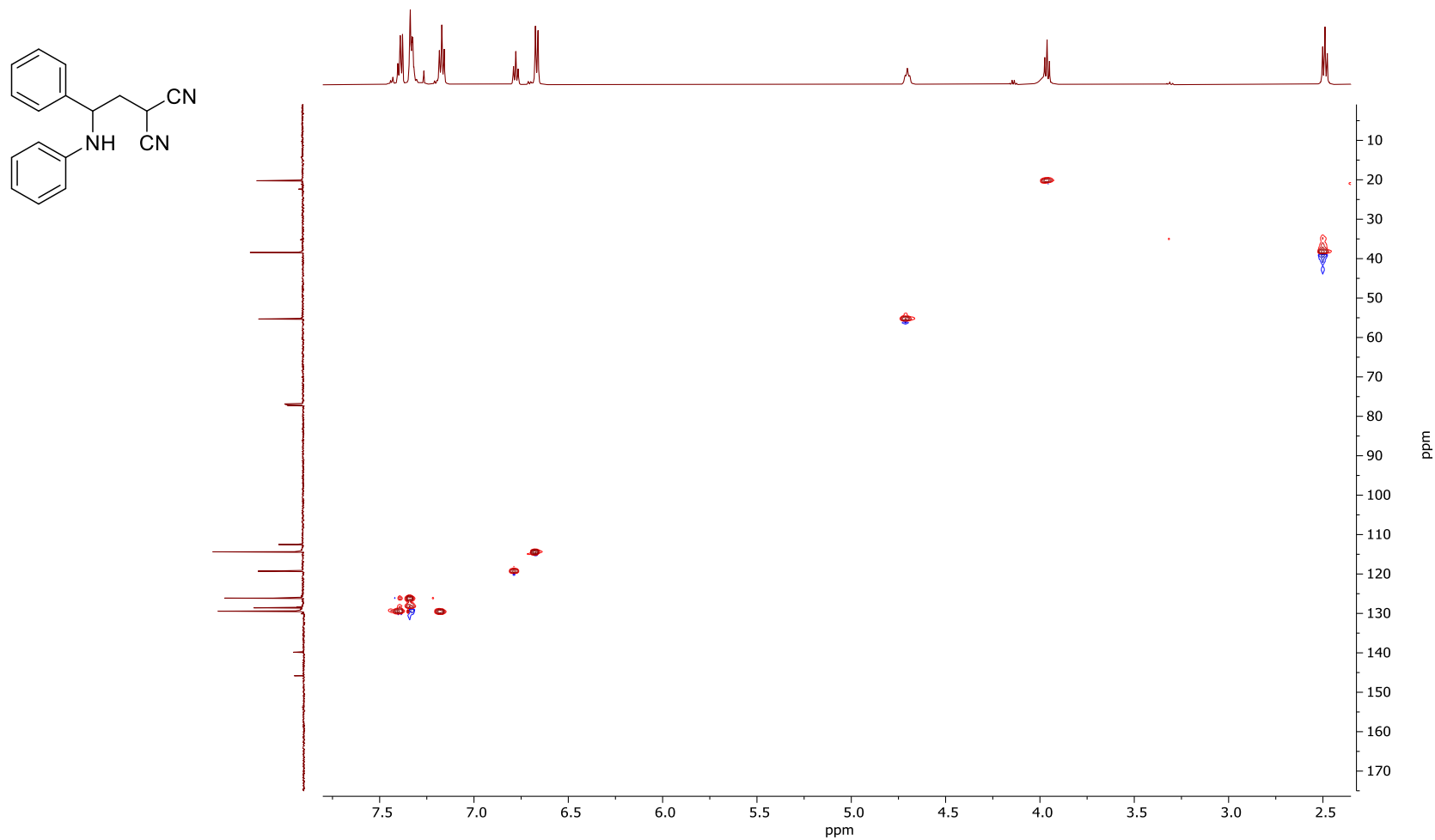
2-[2-Phenyl-2-(phenylamino)ethyl]malononitrile (4d)

^{13}C NMR (CDCl_3 , 150 MHz)



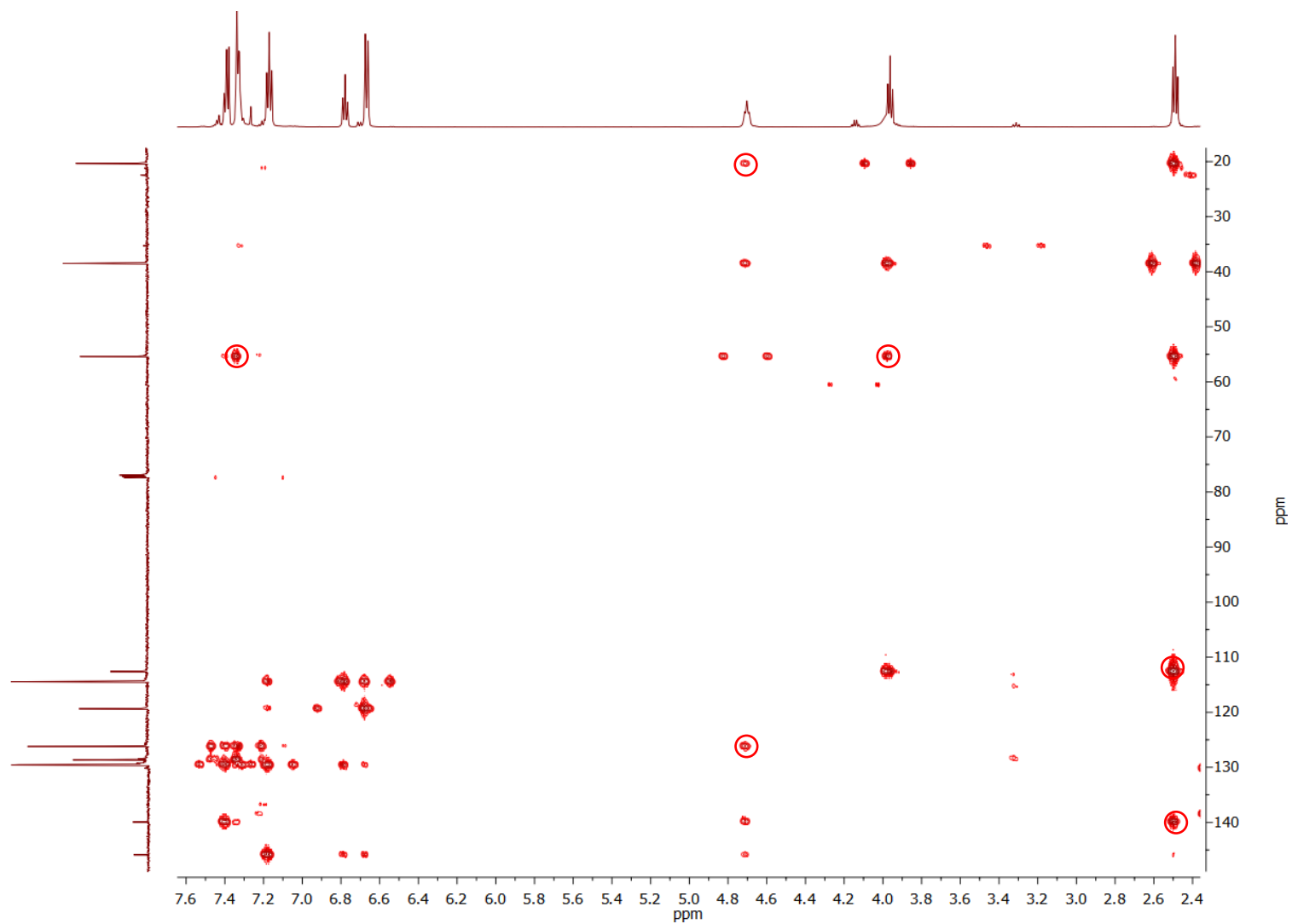
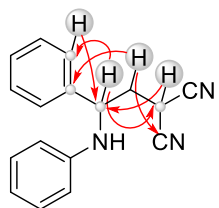
2-[2-Phenyl-2-(phenylamino)ethyl]malononitrile (4d)

HSQC ^1H - ^{13}C (CDCl_3)



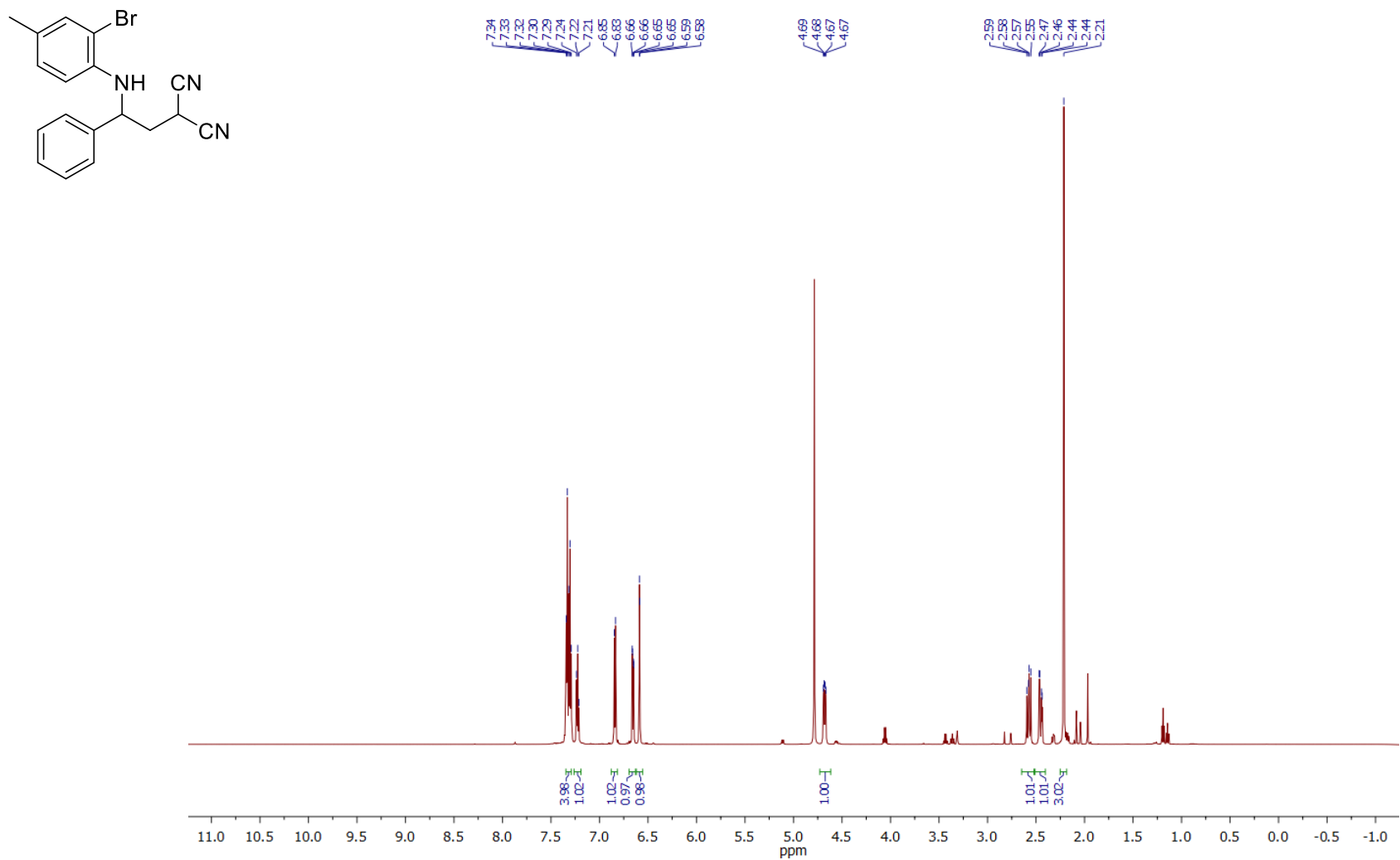
2-[2-Phenyl-2-(phenylamino)ethyl]malononitrile (4d)

HMBC ^1H - ^{13}C (CDCl_3)



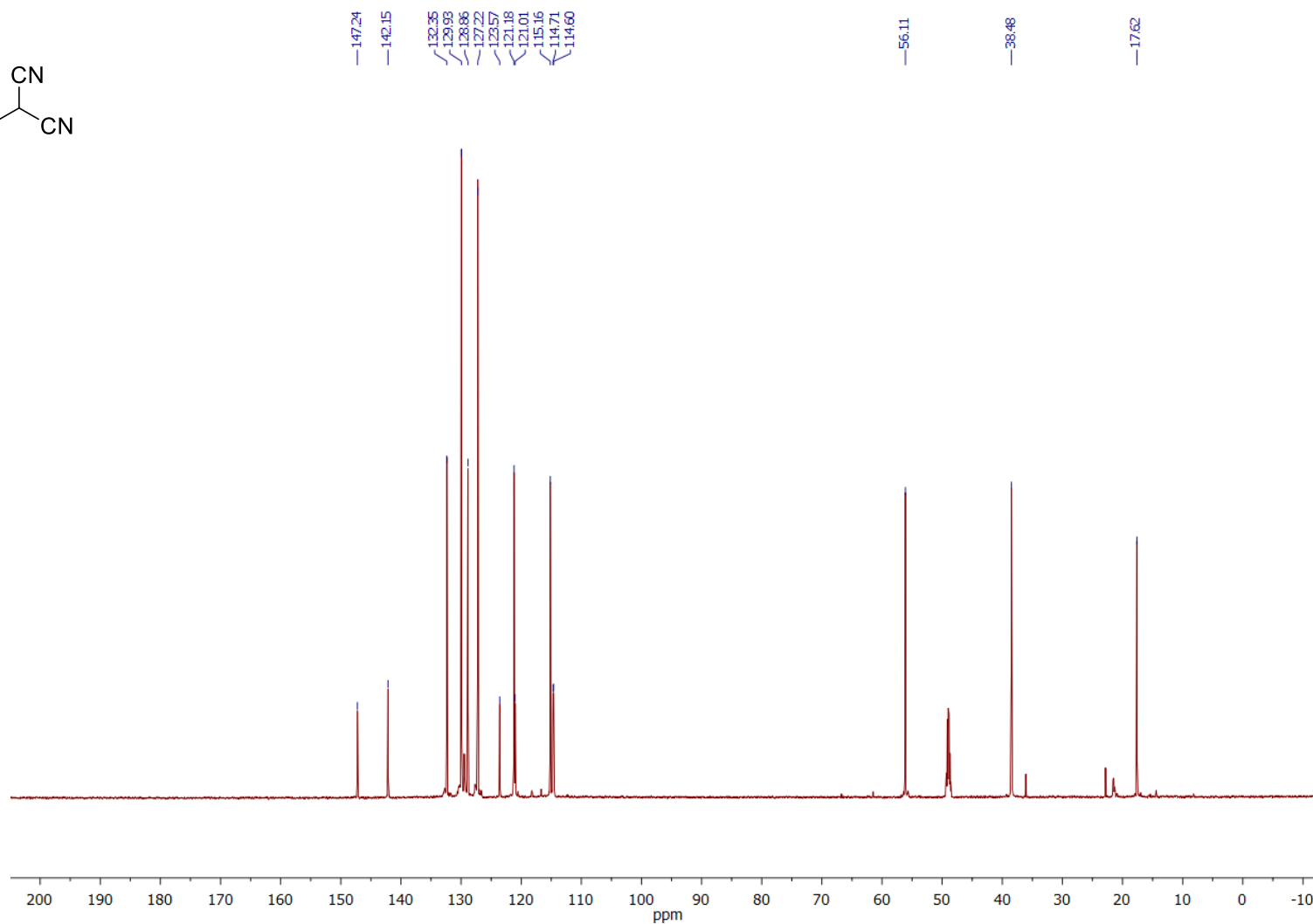
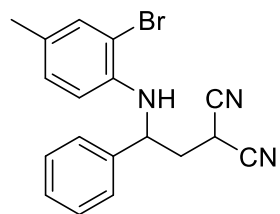
2-{2-[(2-Bromo-4-methylphenyl)amino]-2-phenylethyl}malononitrile (4e)

^1H NMR (CD_3OD , 600 MHz)



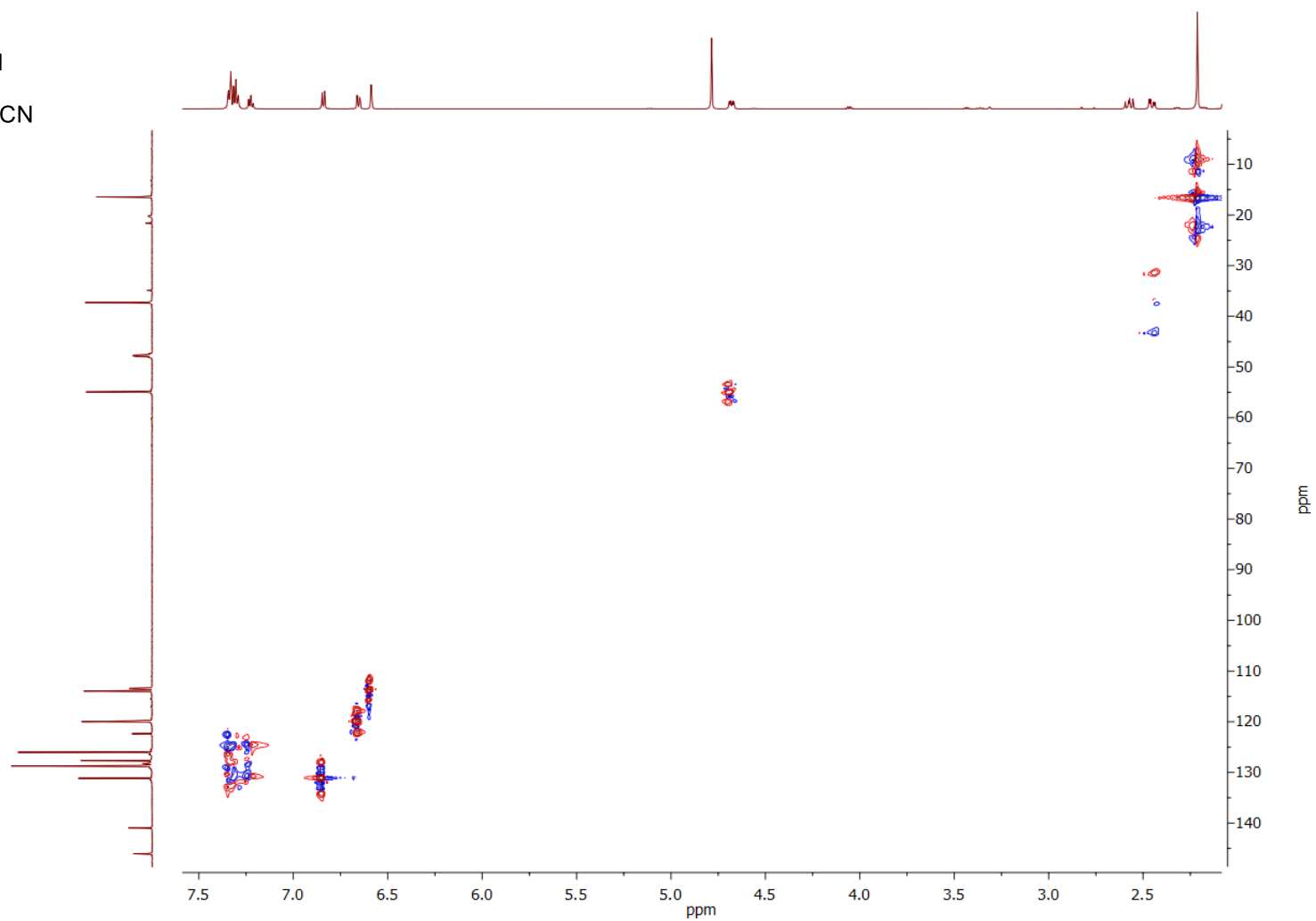
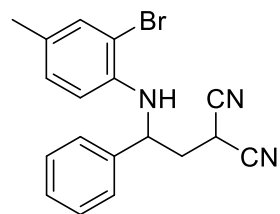
2-{2-[(2-Bromo-4-methylphenyl)amino]-2-phenylethyl}malononitrile (4e)

^{13}C NMR (CD_3OD , 150 MHz)



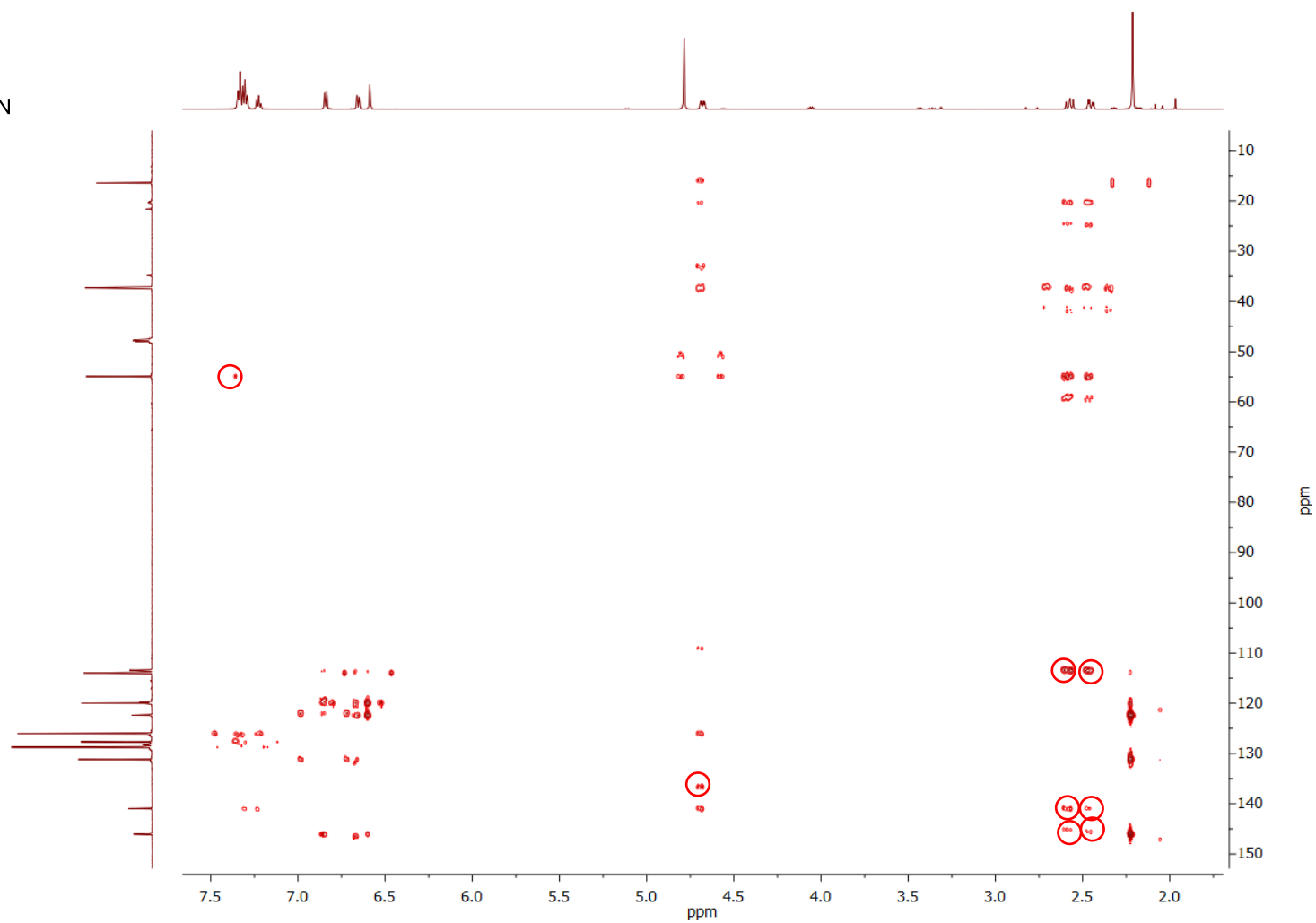
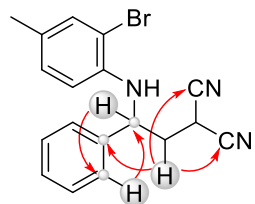
2-{2-[(2-Bromo-4-methylphenyl)amino]-2-phenylethyl}malononitrile (4e)

HSQC ^1H - ^{13}C (CD_3OD)



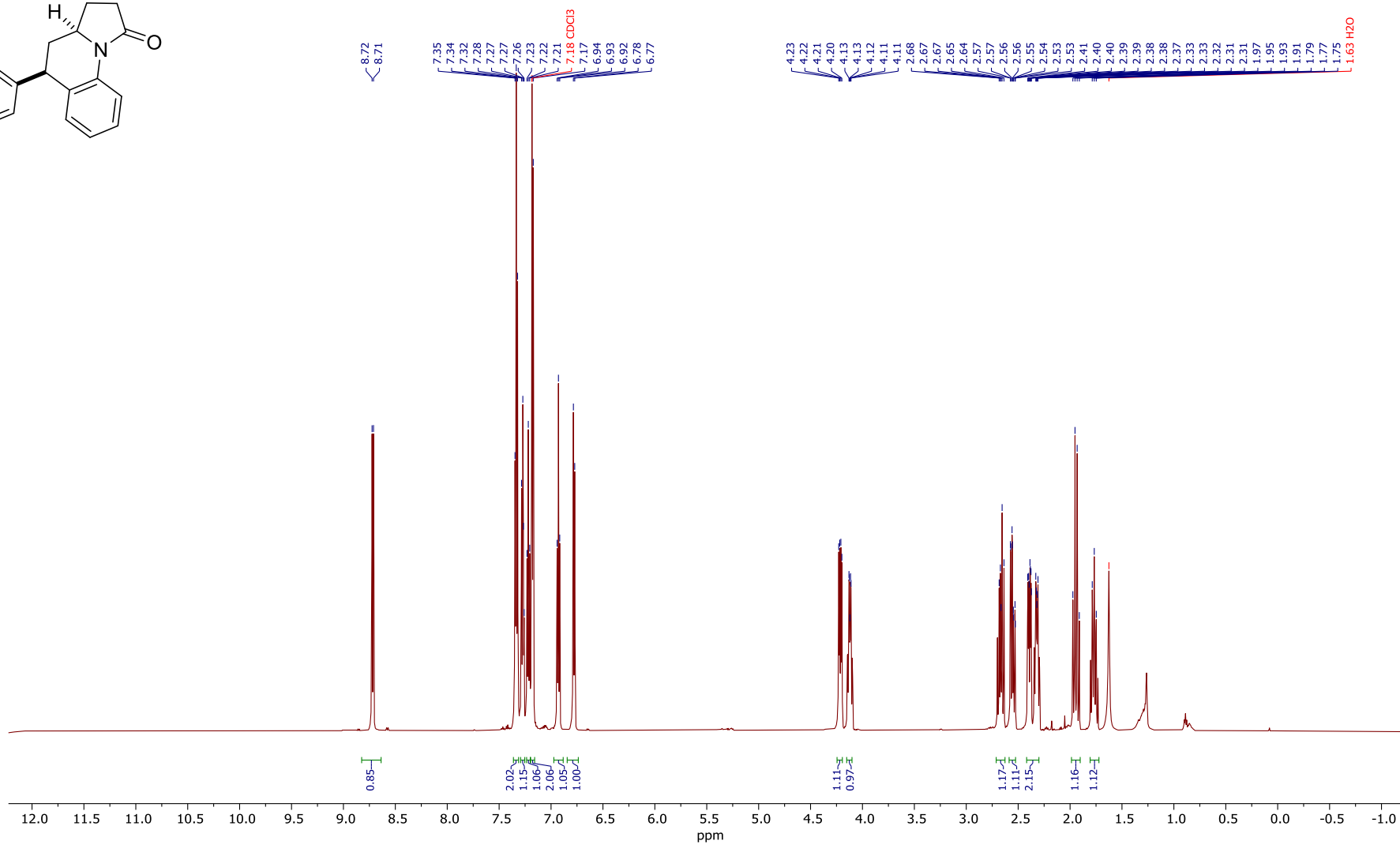
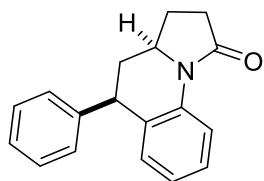
2-{2-[(2-Bromo-4-methylphenyl)amino]-2-phenylethyl}malononitrile (4e)

HMBC ^1H - ^{13}C (CD_3OD)



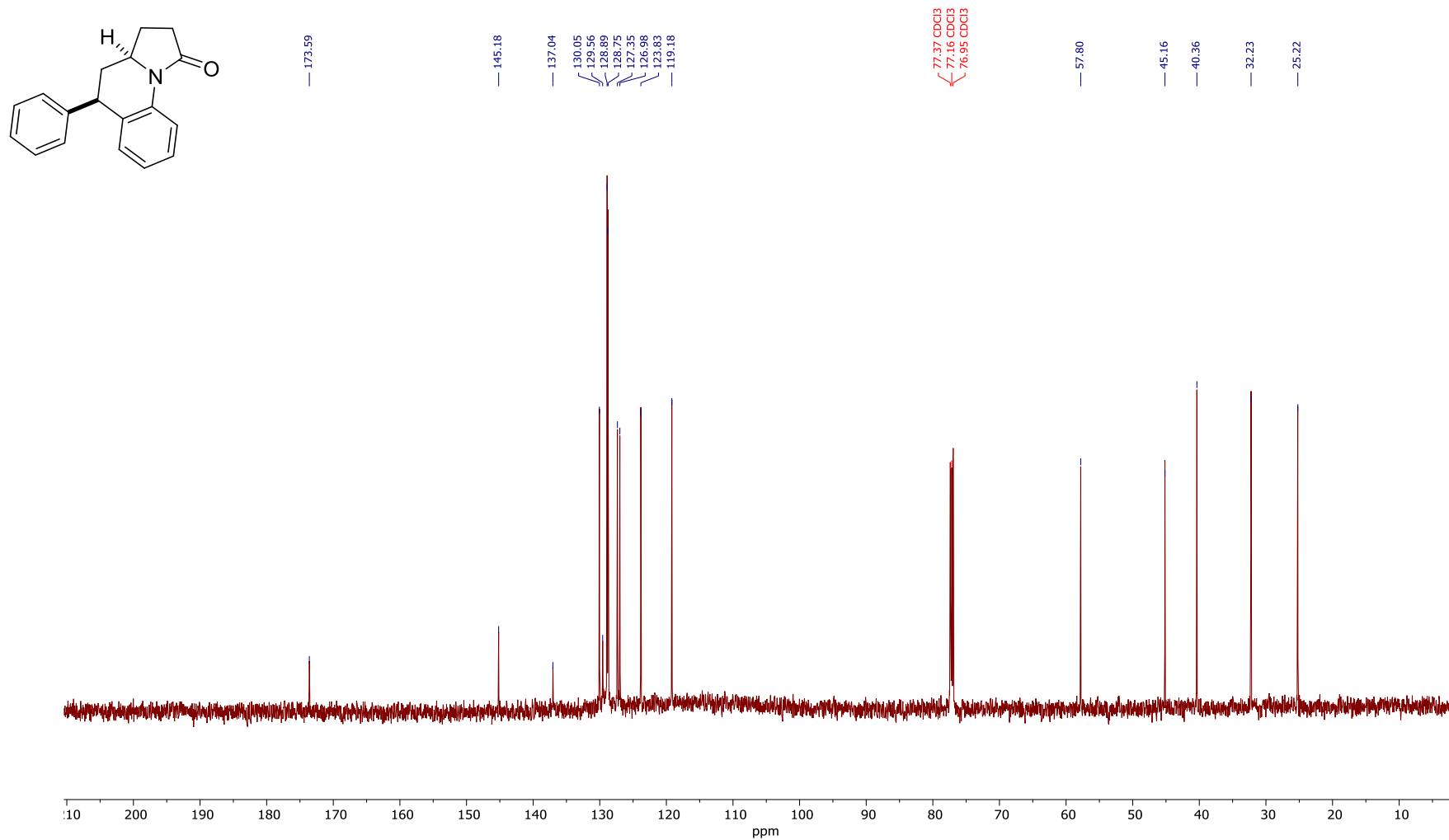
(3*aRS*,5*RS*)-5-Phenyl-3,3*a*,4,5-tetrahydropyrrolo[1,2-*a*]quinoline-1(2*H*)-one (5)

¹H NMR (CDCl₃, 600 MHz)



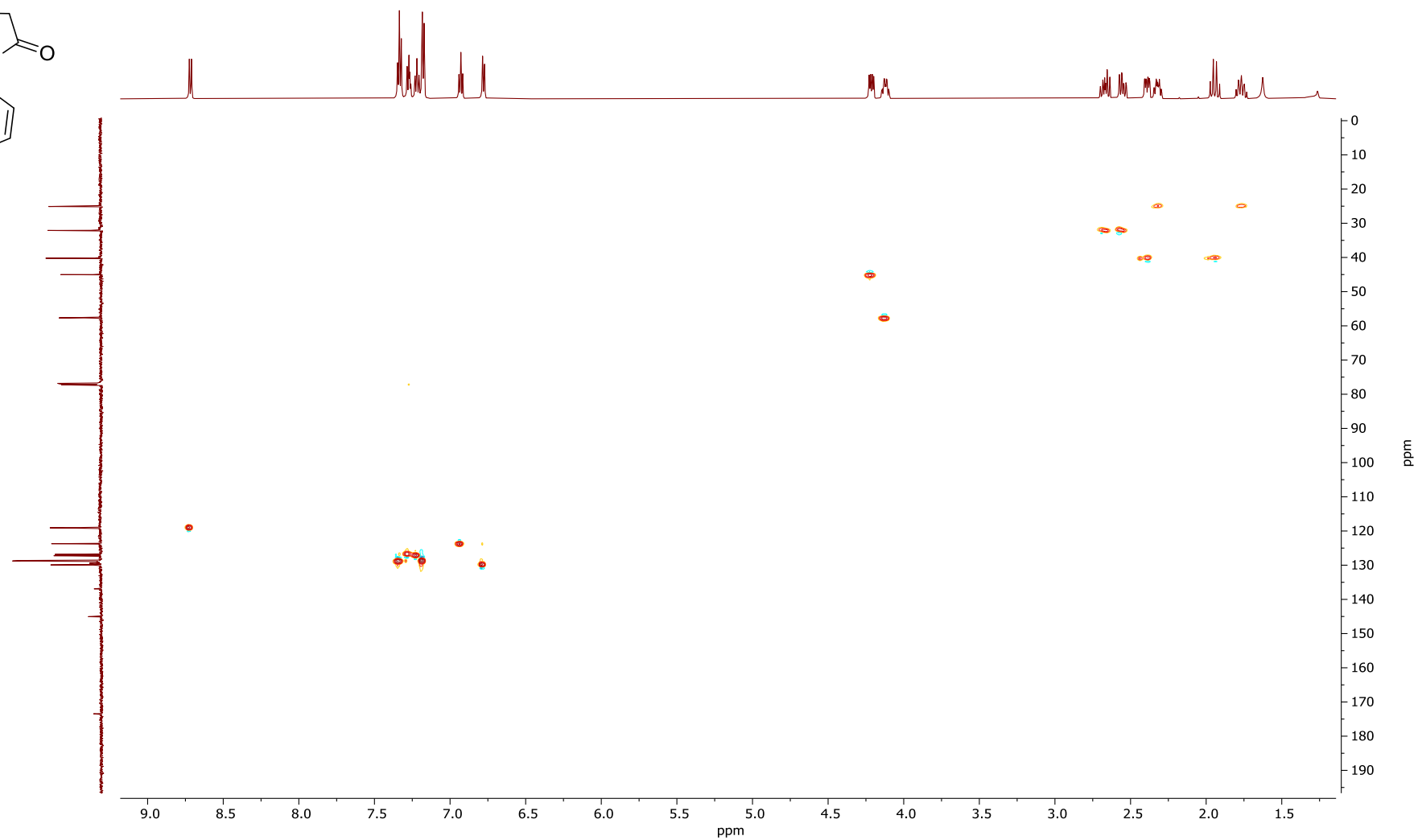
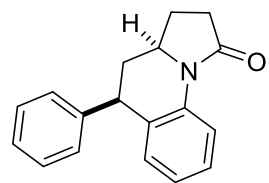
(3*aRS*,5*RS*)-5-Phenyl-3,3*a*,4,5-tetrahydropyrrolo[1,2-*a*]quinoline-1(2*H*)-one (5)

¹³C NMR (CDCl₃, 150 MHz)



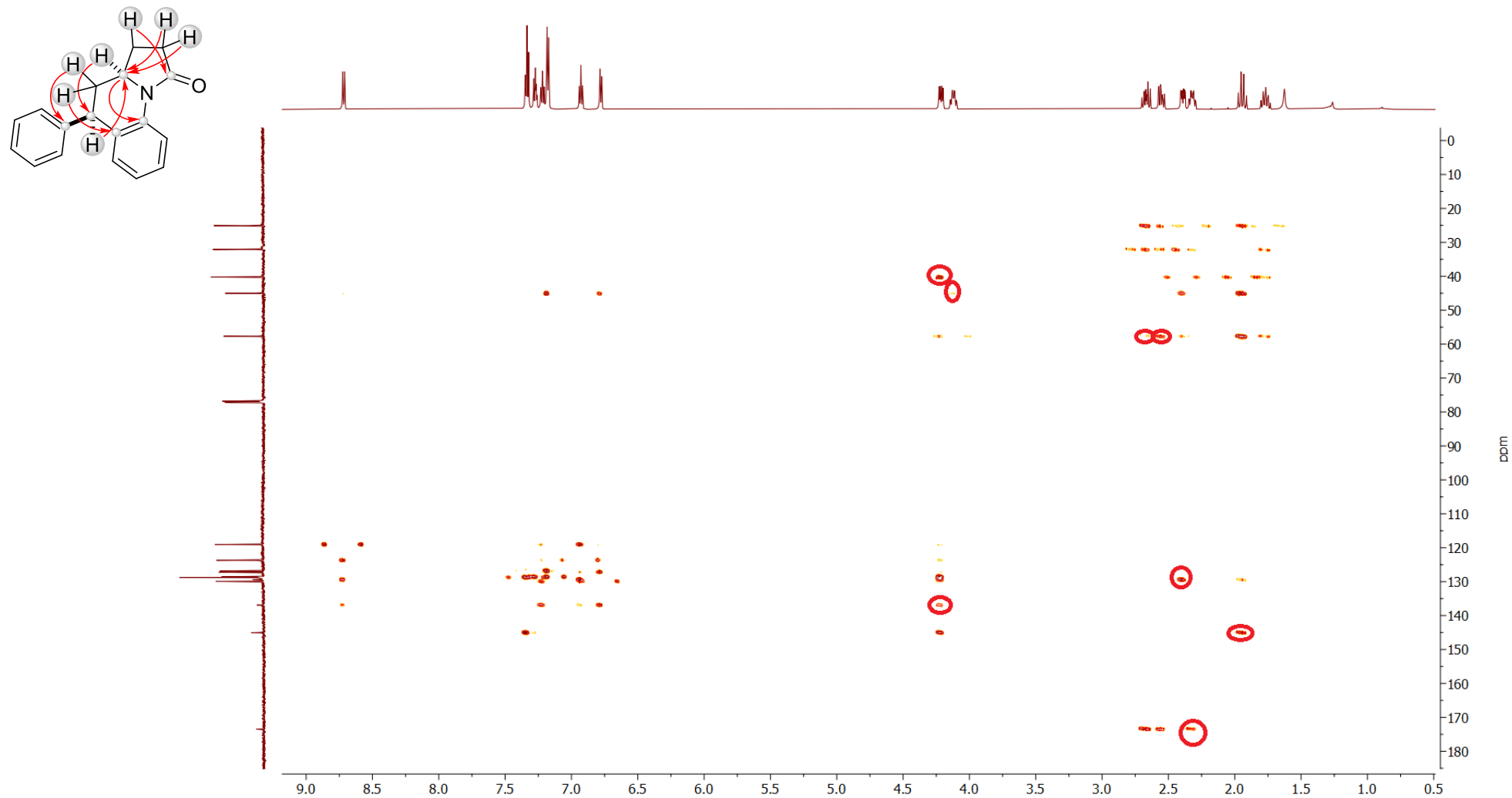
(3*aRS*,5*RS*)-5-Phenyl-3,3*a*,4,5-tetrahydropyrrolo[1,2-*a*]quinoline-1(2*H*)-one (5)

HSQC ^1H - ^{13}C (CDCl_3)



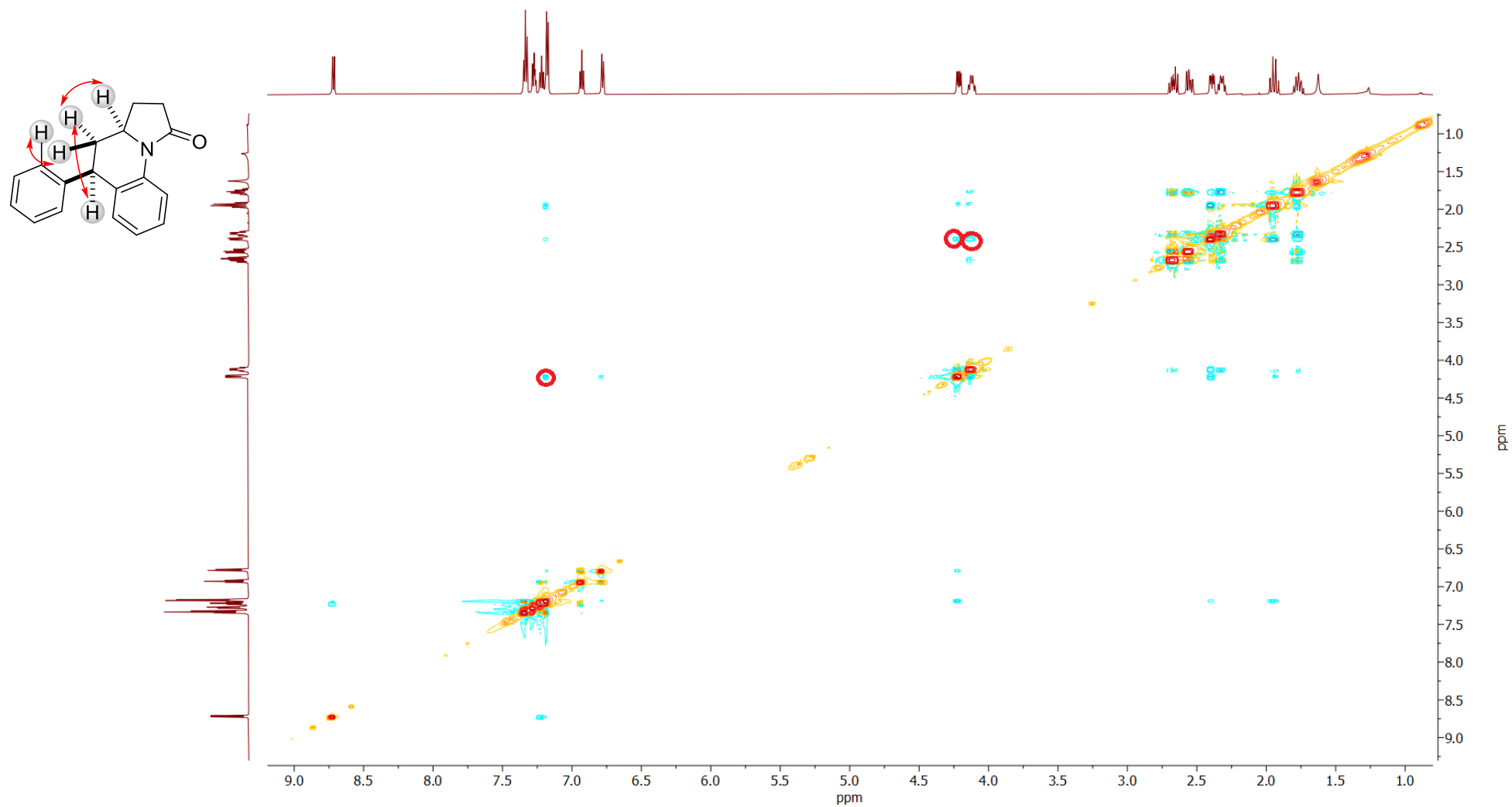
(3*aRS*,5*RS*)-5-Phenyl-3,3*a*,4,5-tetrahydropyrrolo[1,2-*a*]quinoline-1(2*H*)-one (5)

HMBC ^1H - ^{13}C (CDCl_3)

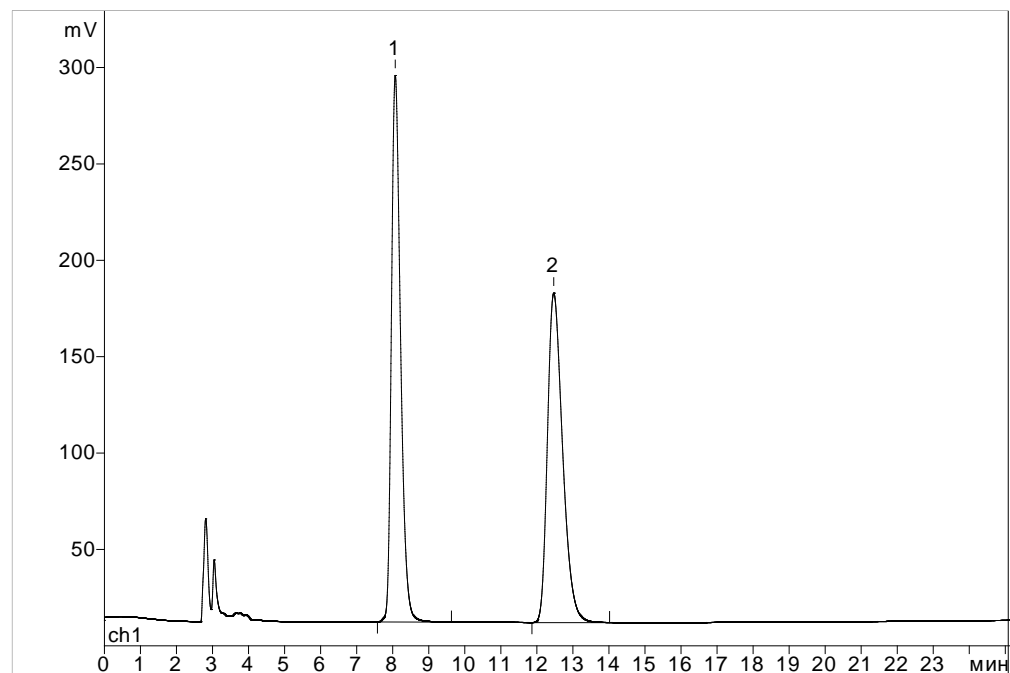


(3*aRS*,5*RS*)-5-Phenyl-3,3*a*,4,5-tetrahydropyrrolo[1,2-*a*]quinoline-1(2*H*)-one (5)

NOESY (CDCl₃) (CDCl₃)

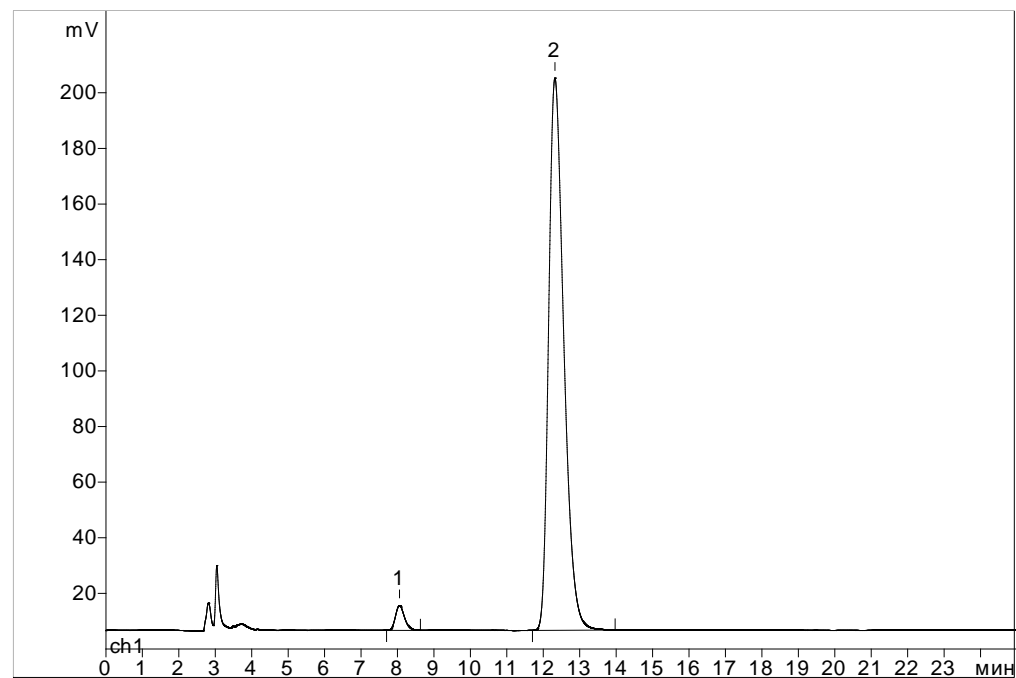


HPLC report for racemic 1-(4-methoxyphenyl)-5-(*p*-tolyl)pyrrolidin-2-one (2d)



No	Retention мин	Area mV*сек	Area %	Name
1	8.07	4999.208	50.04	
2	12.47	4990.657	49.96	
<hr/>				
2	25.15	9989.865	100.00	

HPLC report for enantioenriched 1-(4-methoxyphenyl)-5-(*p*-tolyl)pyrrolidin-2-one (*R*)-2d



No	Retention мин	Area mV*сек	Area %	Name
1	8.05	154.491	2.63	
2	12.32	5720.528	97.37	
<hr/>				
2	25.00	5875.020	100.00	