SUPPLEMENTARY MATERIAL

Discovery of novel West Nile Virus protease inhibitor based on isobenzonafuranone and triazolic derivatives of eugenol and indan-1,3-dione scaffolds

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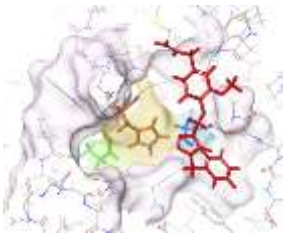
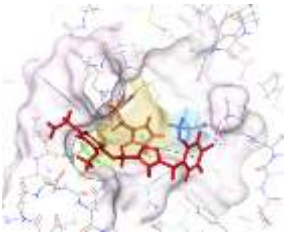
Table A: Docking of the compounds 23 to 49 with WNV protease					
	Ligation				
Comp.	Ligation type	Description	Interaction distance (Å)	aa	Docking/Ligation Energy
23	Hydrogen Bond	OH of the amino acid with the oxygen of the carbonic chain of the molecule	2,45	Thr^{132}	 EnergyEnergy: -2,318
24		No chemical interaction predicted			 Energy: -1,081
25	Hydrogen Bond	NH_2 of the amino acid with the oxygen of the carbonic chain of the molecule	1,92	Asn^{84}	 Energy: +2,058
25	Halogen Bond	OH of the amino acid with the chlorine of the molecule	3,26	Thr^{134}	
25	Halogen Bond	NH^+ of the amino acid with the iodine of the molecule	2,62	Gly^{133}	
25	Halogen Bond	NH^+ of the amino acid with the iodine of the molecule	3,42	Thr^{134}	
25	cation-π	NH^+ of the amino acid ring with the phenyl ring of the molecule	6,39	**His^{51}**	
25	π-π stacking	Amino acid ringwith the triazole ring of the molecule	4,11	**His^{51}**	

Table A: Docking of the compounds 23 to 49 with WNV protease

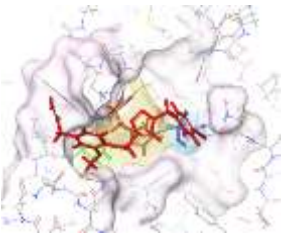
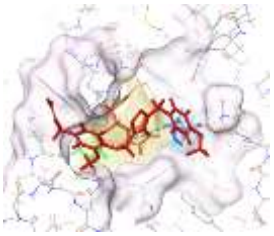
Comp.	Ligation				Docking/Ligation Energy
	Ligation type	Description	Interaction distance (Å)	aa	
26		No chemical interaction predicted			 Energy: -0,429
27	cation-π	NH^+ of the amino acid ring with the triazole ring of the molecule	5,43	**His^{51}**	 Energy: -0,055
27	cation-π	NH^+ of the amino acid ring with the phenyl ring of the molecule	6,20	**His^{51}**	
27	π-π stacking	Amino acid ringwith the phenyl ring of the molecule	5,15	**His^{51}**	
27	Halogen Bond	NH^+ of the amino acid with the iodine of the molecule	2,43	**Ser^{135}**	
27	Halogen Bond	NH^+ of the amino acid with the iodine of the molecule	2,82	Thr^{134}	
28	Hydrogen Bond	OH of the amino acid with the oxygen of the carbonic chain of the molecule	2,24	Thr^{132}	 Energy: -2,732
28	Hydrogen Bond	O^- of the amino acid with the NO_2H_2 of the molecule	1,89	Asp^{129}	
28	Hydrogen Bond	O^- of the amino acid with the NO_2H_2 of the molecule	2,07	Asp^{129}	
28	Hydrogen Bond	NH^+ of the amino acid with the nitrogen of triazole ring of the molecule	2,46	**Ser^{135}**	
28	π-π stacking	Amino acid ring with the phenyl ring of the molecule	4,39	Tyr^{161}	
29	Hydrogen Bond	NH^+ of the amino acid wit the OCH_3 of the phenyl ring in the molecule	1,98	Gly^{133}	

Table A: Docking of the compounds 23 to 49 with WNV protease

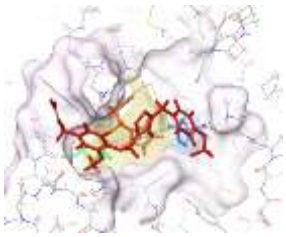
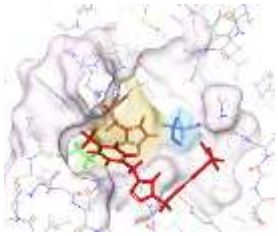
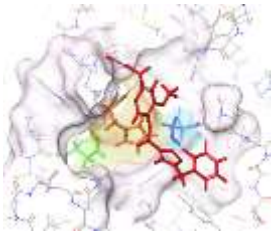
Comp.	Ligation				Docking/Ligation Energy
	Ligation type	Description	Interaction distance (Å)	aa	
29	cation-π	NH^+ of the amino acid ring with the triazole ring of the molecule	6,13	**His^{51}**	Energy: -3,991
29	cation-π	NH^+ of the amino acid ring with the triazole ring of the molecule	3,81	**His^{51}**	
29	π-π stacking	Amino acid ring with the phenyl ring of the molecule	5,04	**His^{51}**	
29	π-π stacking	Amino acid ring with the eugenol ring of the molecule	3,96	**His^{51}**	
30	Hydrogen Bond	NH^+ of the amino acid with the OF_3 of the phenyl ring of the molecule	1,96	Gly^{133}	 Energy: -1,459
30	Hydrogen Bond	NH_2 of the amino acid with the OCH_3 of the molecule	2,08	Asn^{84}	
30	cation-π	NH^+ of the amino acid ring with the phenyl ring of the molecule	6,01	**His^{51}**	
30	π-π stacking	Amino acid ringwith the phenyl ring of the molecule	4,93	**His^{51}**	
31	π-π stacking	Ring of the amino acid with the eugenol ring of the molecule	5,08	Tyr^{161}	 Energy: +1,993
32	No chemical interaction predicted				 Energy: +2,136

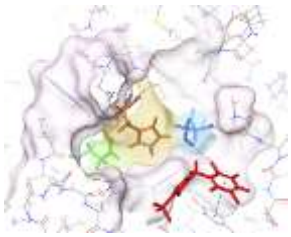
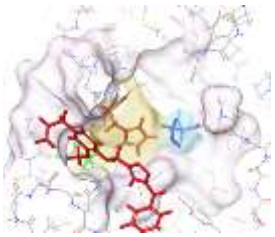
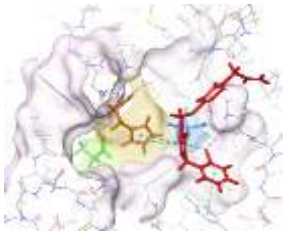
Table A: Docking of the compounds 23 to 49 with WNV protease					
	Ligation				
Comp.	**Ligation type**	**Description**	**Interaction distance (Å)**	**aa**	**Docking/Ligation Energy**
33	Hydrogen Bond	NH^+ of the amino acid with the OCH_3 of the eugenol of the molecule	1,80	Ile^{155}	 Energy: -1,473
33	Halogen Bond	OH of the amino acid with the iodine of the molecule	2,68	Ser^{135}	
33	π-π stacking	Ring of the amino acid with the phenyl ring of the molecule	3,80	Tyr^{161}	
34	Hydrogen Bond	NH_2 of the amino acid with the oxygen of the carbonic chain of the molecule	1,84	Asn^{84}	 Energy: +1,863
35	cation-π	NH^+ of the amino acid ring with the triazole ring of the molecule	5,88	His^{51}	 Energy: -2,343
35	π-π stacking	Amino acid ring with the triazole ring of the molecule	5,04	His^{51}	
35	π-π stacking	Amino acid ring with the phenyl ring of the molecule	4,22	Tyr^{161}	
35	Halogen Bond	OH of the amino acid with Bromo of the molecule	2,10	Ser^{135}	
35	Halogen Bond	NH^+ do of the amino acid with Bromo of the molecule	3,25	Thr^{134}	
36	Hydrogen Bond	NH^+ of the amino acid with the nitrogen of triazole ring of the molecule	2,70	Gly^{153}	 Energy: +1,825
36	π-π stacking	Amino acid ringwith the phenyl ring of the molecule	4,30	Tyr^{161}	
36	Halogen Bond	NH^+ of the amino acid with Bromo of the molecule	3,19	Gly^{133}	
36	Halogen Bond	NH^+ of the amino acid with Bromo of the molecule	3,01	Thr^{134}	
36	Halogen Bond	OH of the amino acid with Bromo of the molecule	2,56	Ser^{135}	

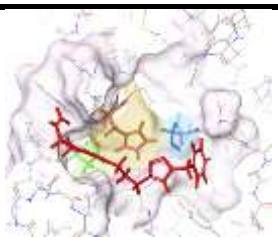
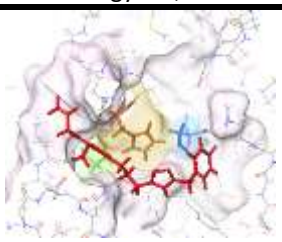
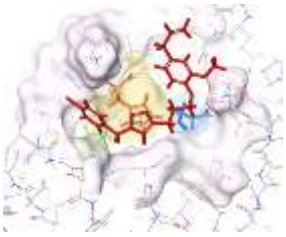
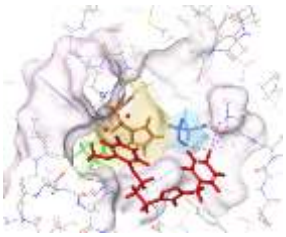
Table A: Docking of the compounds 23 to 49 with WNV protease					
Comp.	Ligation				Docking/Ligation Energy
	Ligation type	Description	Interaction distance (Å)	aa	
37	cation-π	NH_3^+ do of the amino acid with the eugenol ring of the molecule	5,31	Lys^{54}	 Energy: +2,012
38	cation-π	NH_3^+ of the amino acid with the eugenol ring of the molecule	4,79	Lys^{54}	 Energy: +1,608
39	Hydrogen Bond	OH of the amino acid with the OCH_3 of the eugenol of the molecule	2,32	Thr^{132}	 Energy: -2,863
39	cation-π	NH^+ of the amino acid ring with the triazole ring of the molecule	3,82	**His^{51}**	
39	π-π stacking	Amino acid ring with the triazole ring of the molecule	3,51	**His^{51}**	
40	Hydrogen Bond	NH^+ of the amino acid with the OCH_3 of the eugenol of the molecule	2,77	**His^{51}**	 Energy: +1,347
41	Hydrogen Bond	NH^+ of the amino acid with the oxigênio da cadeia carbônica of the molecule	2,48	Gly^{133}	 Energy: -2,436
41	Hydrogen Bond	OH of the amino acid with the OCH_3 of the eugenol of the molecule	2,48	Thr^{132}	
42	Hydrogen Bond	O^- of the amino acid with the NO_2H_2 of the molecule	2,00	Asp^{129}	

Table A: Docking of the compounds 23 to 49 with WNV protease

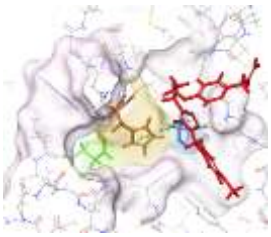
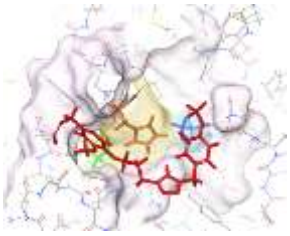
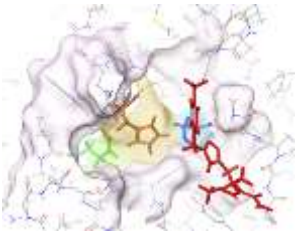
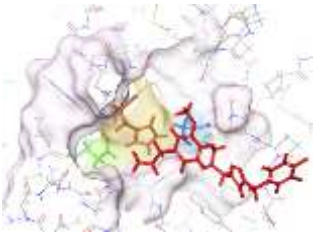
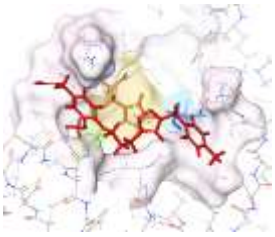
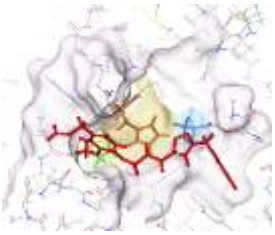
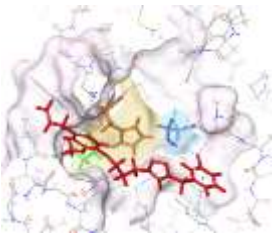
Comp.	Ligation				Docking/Ligation Energy
	Ligation type	Description	Interaction distance (Å)	aa	
42	Hydrogen Bond	O^- of the amino acid with the NO_2H_2 of the molecule	1,79	Asp^{129}	Energy: +0,463
42	cation-π	NH^+ of the amino acid ring with the triazole ring of the molecule	4,49	**His^{51}**	
42	π-π stacking	Amino acid ringwith the triazole ring of the molecule	3,96	**His^{51}**	
43	Hydrogen Bond	NH^+ of the amino acid with the nitrogen of triazole ring of the molecule	2,26	Gly^{133}	 Energy: +0,304
43	cation-π	NH^+ of the amino acid ring with the triazole ring of the molecule	6,25	**His^{51}**	
43	π-π stacking	Amino acid ringwith the triazole ring of the molecule	5,15	**His^{51}**	
44	Hydrogen Bond	NH^+ of the amino acid with the OF_3 of the molecule	2,07	Gly^{133}	 Energy: +0,877
44	Hydrogen Bond	NH_2 of the amino acid with thexigênio da cadeia carbônica of the molecule	1,73	Asn^{84}	
45	Hydrogen Bond	NH^+ of the amino acid with the nitrogênio da anel triazólico of the molecule	2,62	Gly^{133}	 Energy: +0,392
46	Hydrogen Bond	NH^+ of the amino acid with the oxygen of the carbonic chain of the molecule	2,63	Gly^{133}	 Energy: +2,811

Table A: Docking of the compounds 23 to 49 with WNV protease					
	Ligation				
Comp.	**Ligation type**	**Description**	**Interaction distance (Å)**	**aa**	**Docking/Ligation Energy**
47	Hydrogen Bond	NH_2 of the amino acid with the oxygen of the carbonic chain of the molecule	2,03	Asn^{84}	 Energy: -3,613
47	π-π stacking	Amino acid ring with the triazole ring of the molecule	3,64	**His^{51}**	
48	cation-π	NH^+ of the amino acid ring with the triazole ring of the molecule	5,26	**His^{51}**	 Energy: +0,947
48	Halogen Bond	OH of the amino acid with Bromo of the molecule	2,13	**Ser^{135}**	
49	π-π stacking	Amino acid ring with the phenyl ring of the molecule	4,11	Tyr^{161}	 Energy: +0,969
49	Halogen Bond	OH of the amino acid with Bromo of the molecule	2,49	**Ser^{135}**	
49	Halogen Bond	NH^+ of the amino acid with Bromo of the molecule	3,41	**Ser^{135}**	

SELECTED IR AND NMR SPECTRA

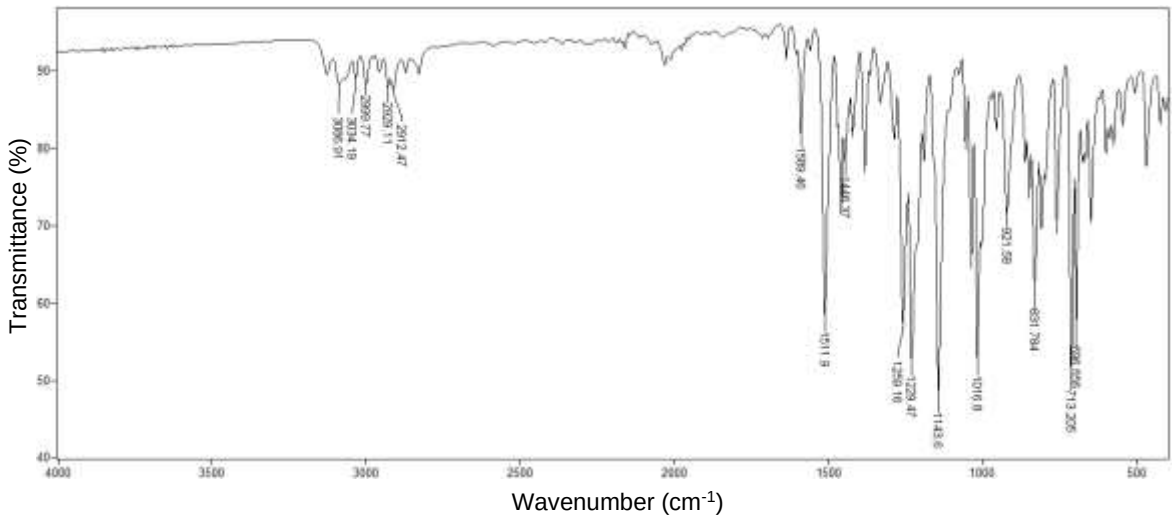


Fig. A. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-benzyl-*1H*-1,2,3-triazole (**23**).

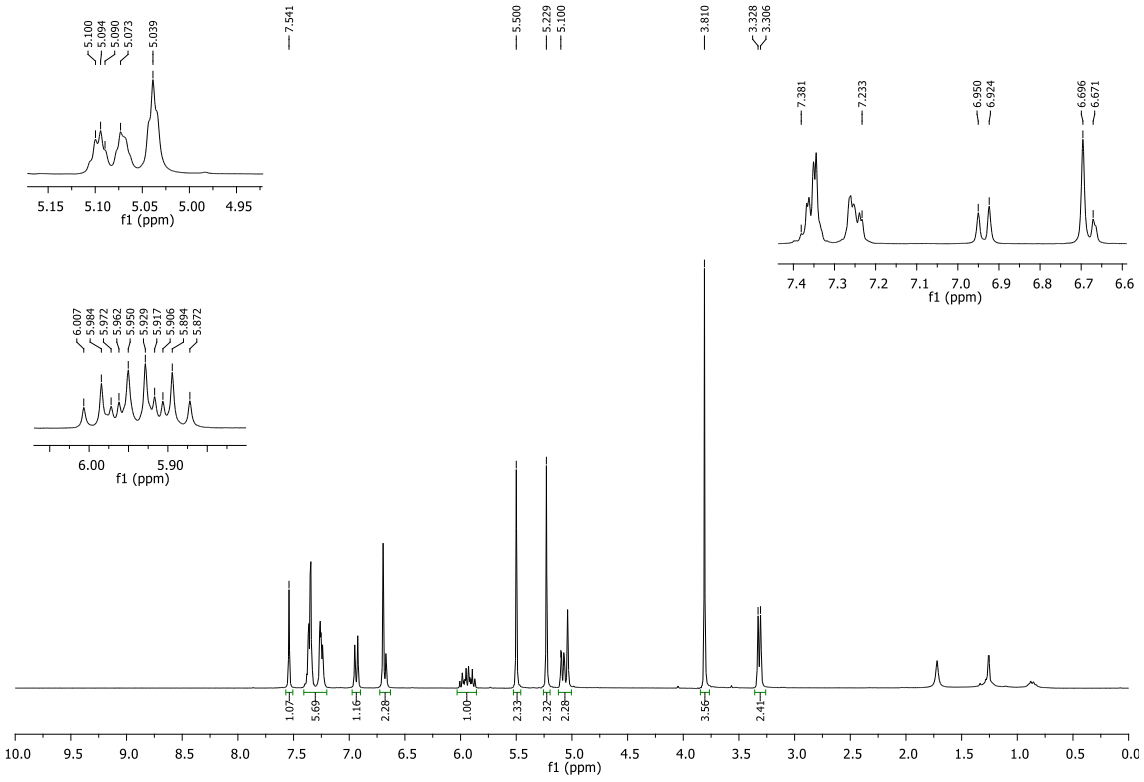


Fig. B. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-benzyl-*1H*-1,2,3-triazole (**23**).

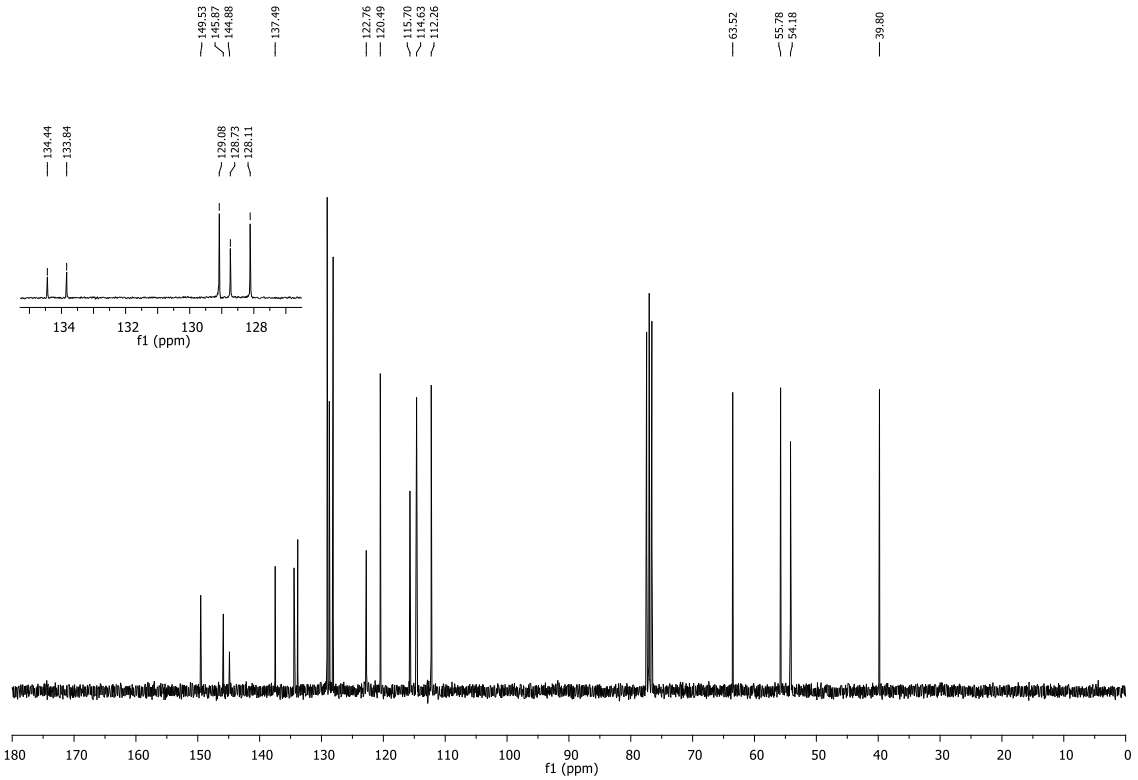


Fig. C. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-benzyl-*1H*-1,2,3-triazole (**23**).

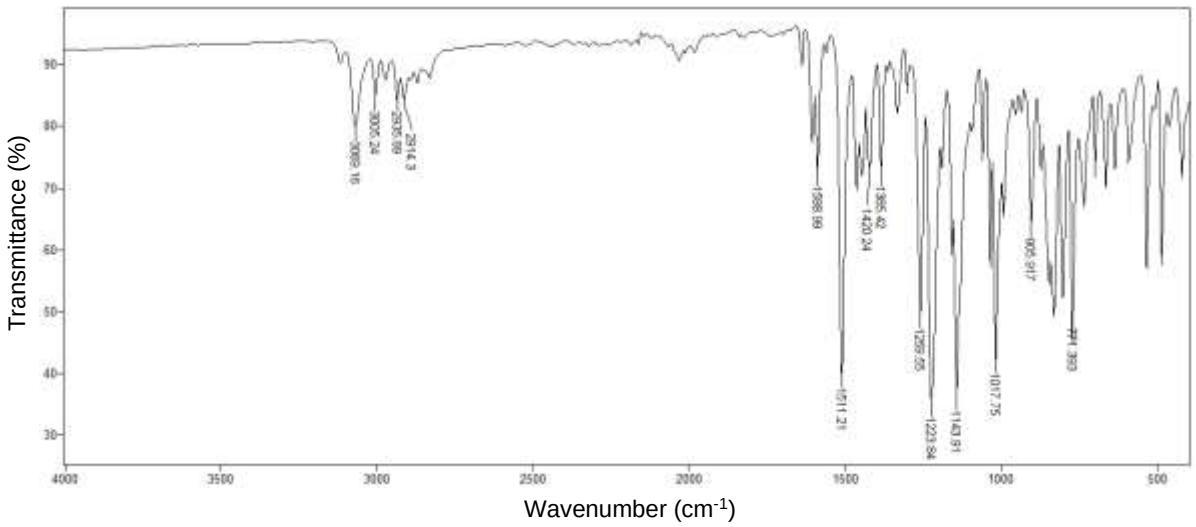


Fig. D. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-fluorobenzyl)-*1H*-1,2,3-triazole (**24**).

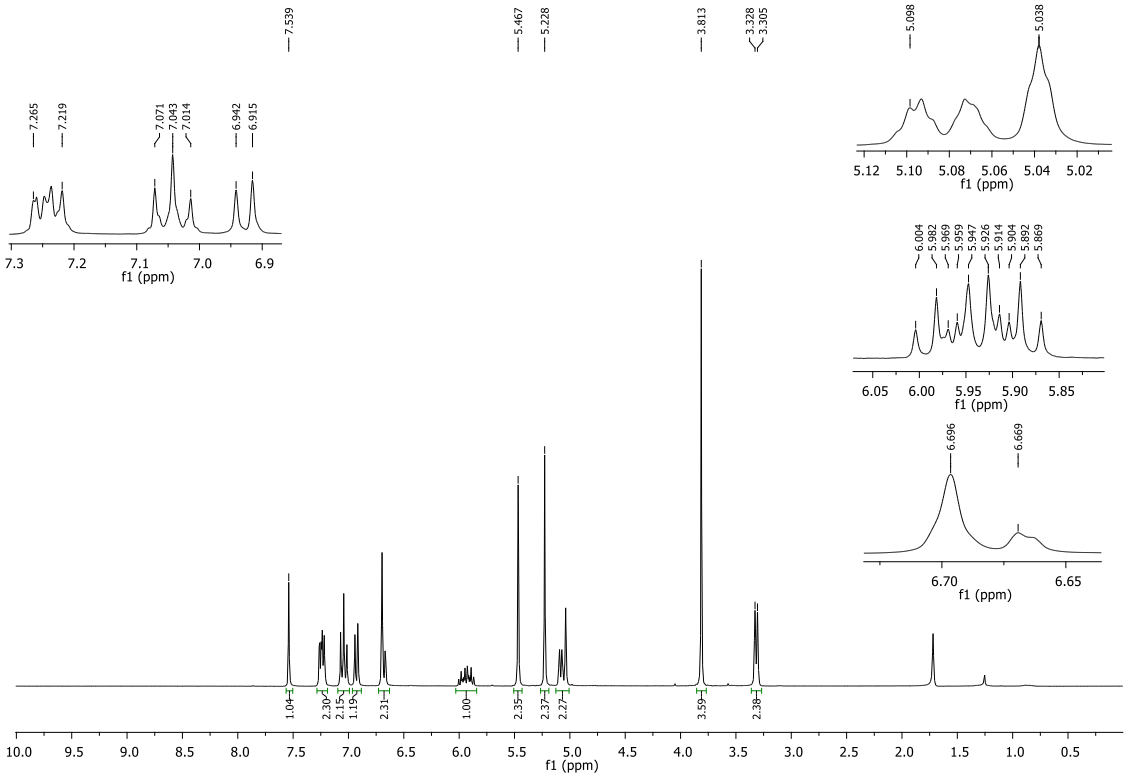


Fig. E. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-fluorobenzyl)-*1H*-1,2,3-triazole (**24**).

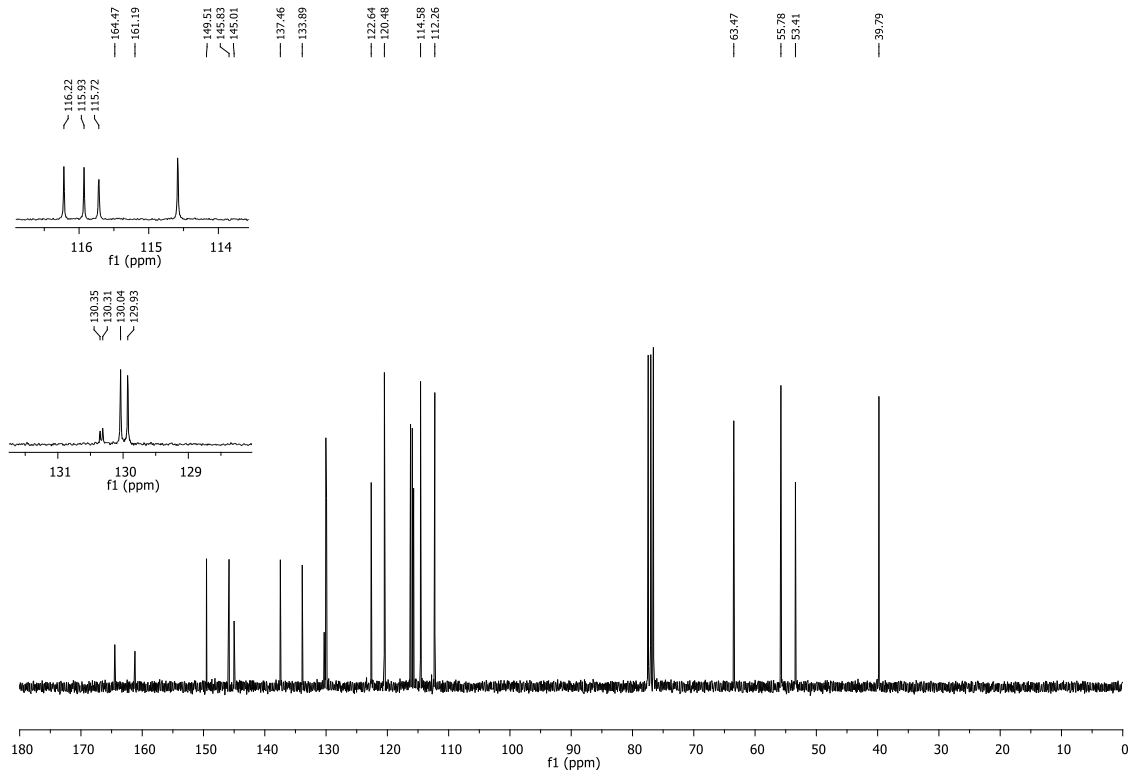


Fig. F. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-fluorobenzyl)-*1H*-1,2,3-triazole (**24**).

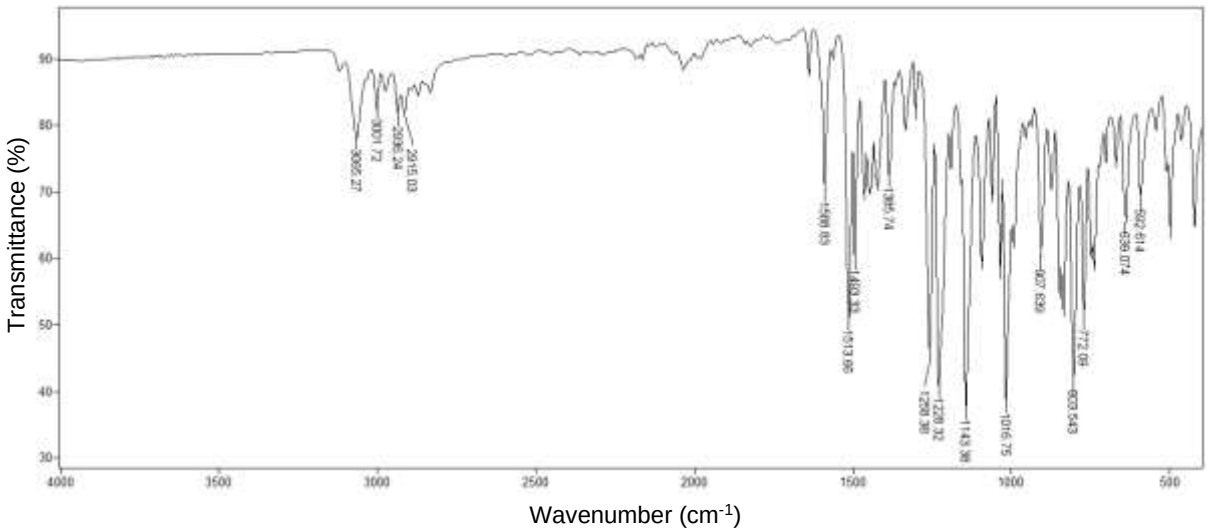


Fig. G. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-chlorobenzyl)-*1H*-1,2,3-triazole (**25**).

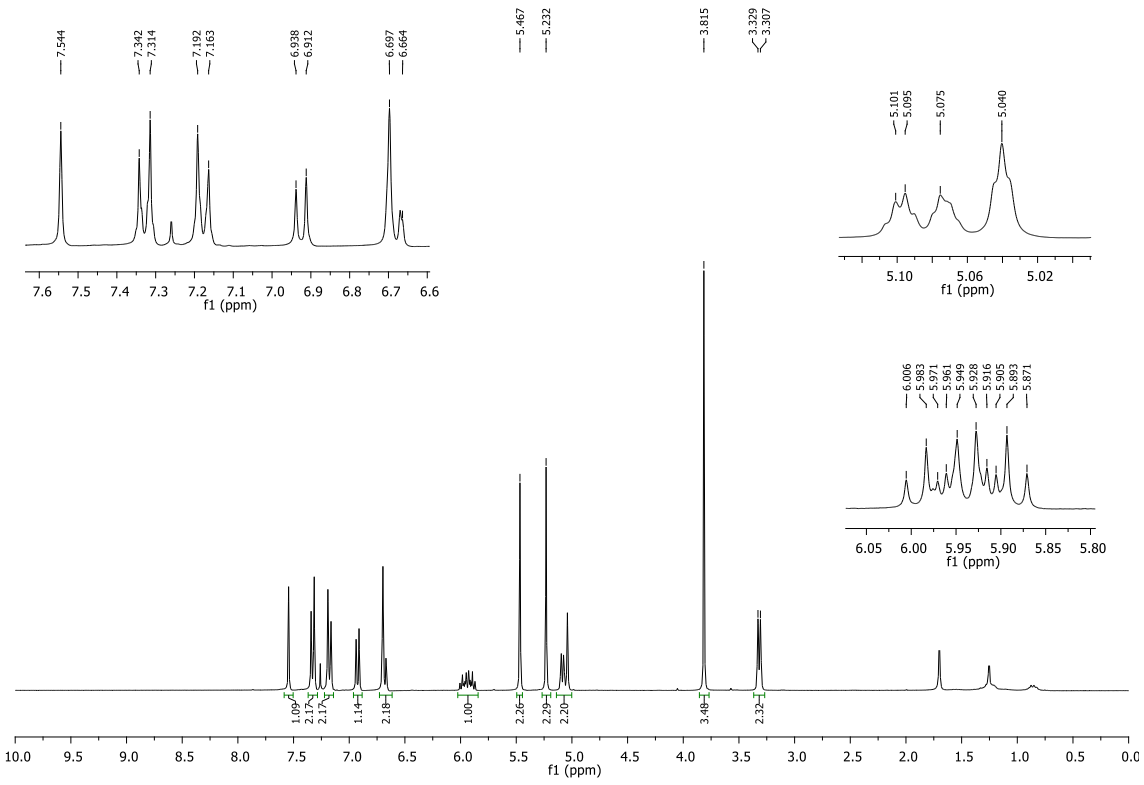


Fig. H. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-chlorobenzyl)-*1H*-1,2,3-triazole (**25**).

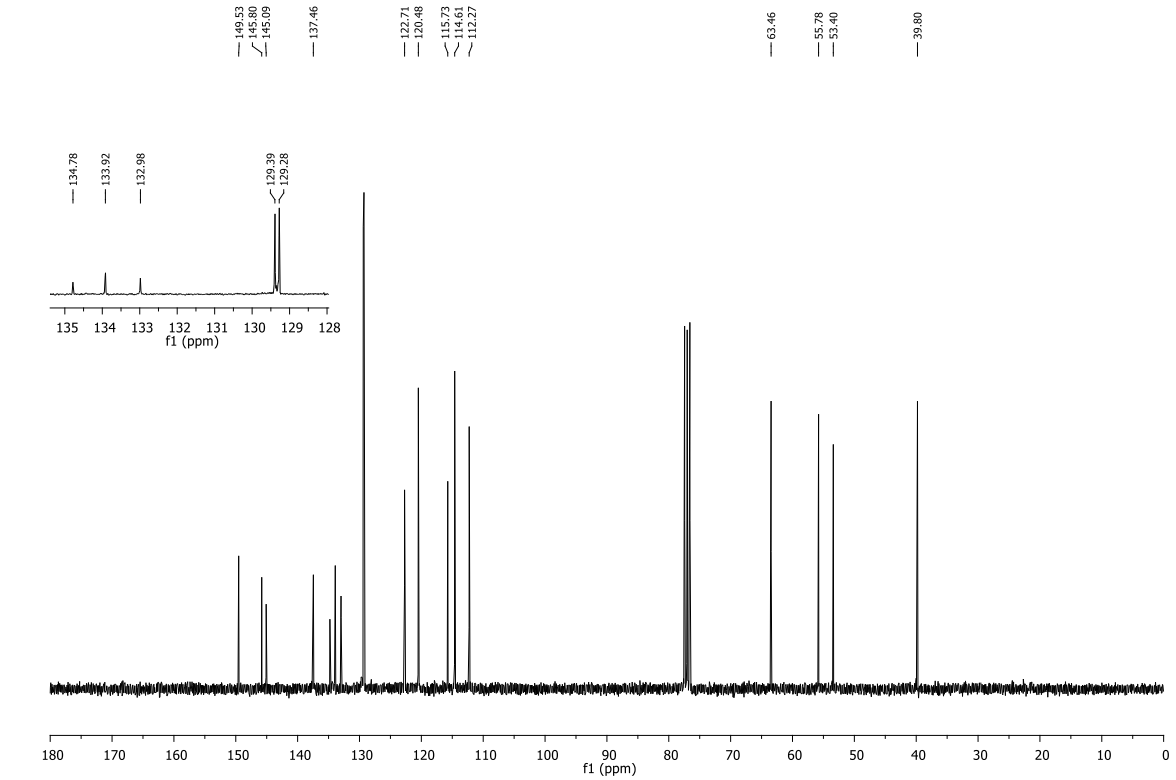


Fig. I. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-chlorobenzyl)-*1H*-1,2,3-triazole (**25**).

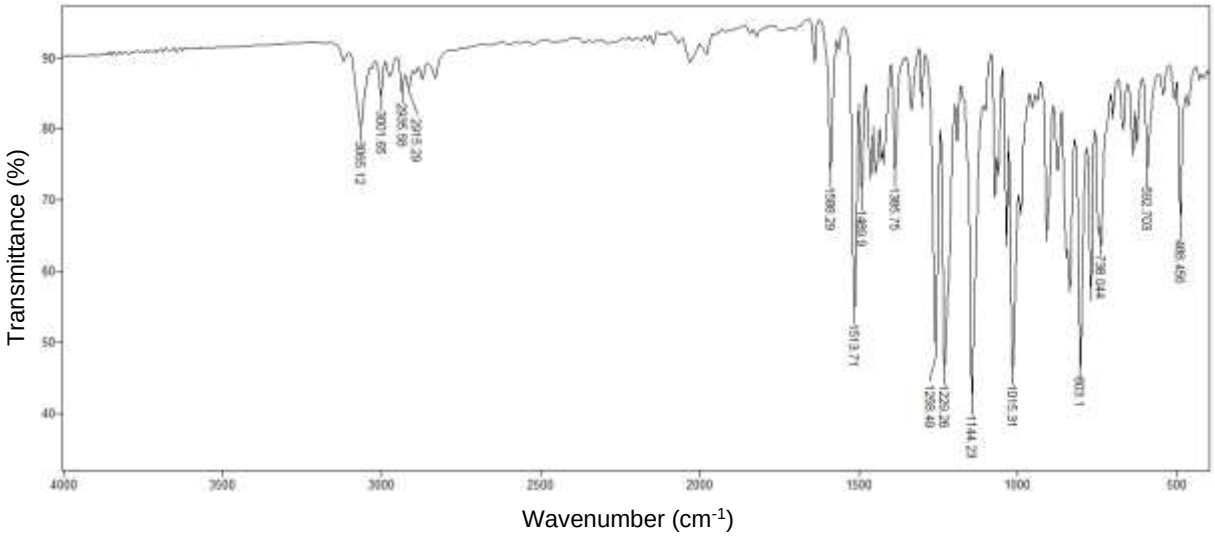


Fig. J. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-bromobenzyl)-*1H*-1,2,3-triazole (**26**).

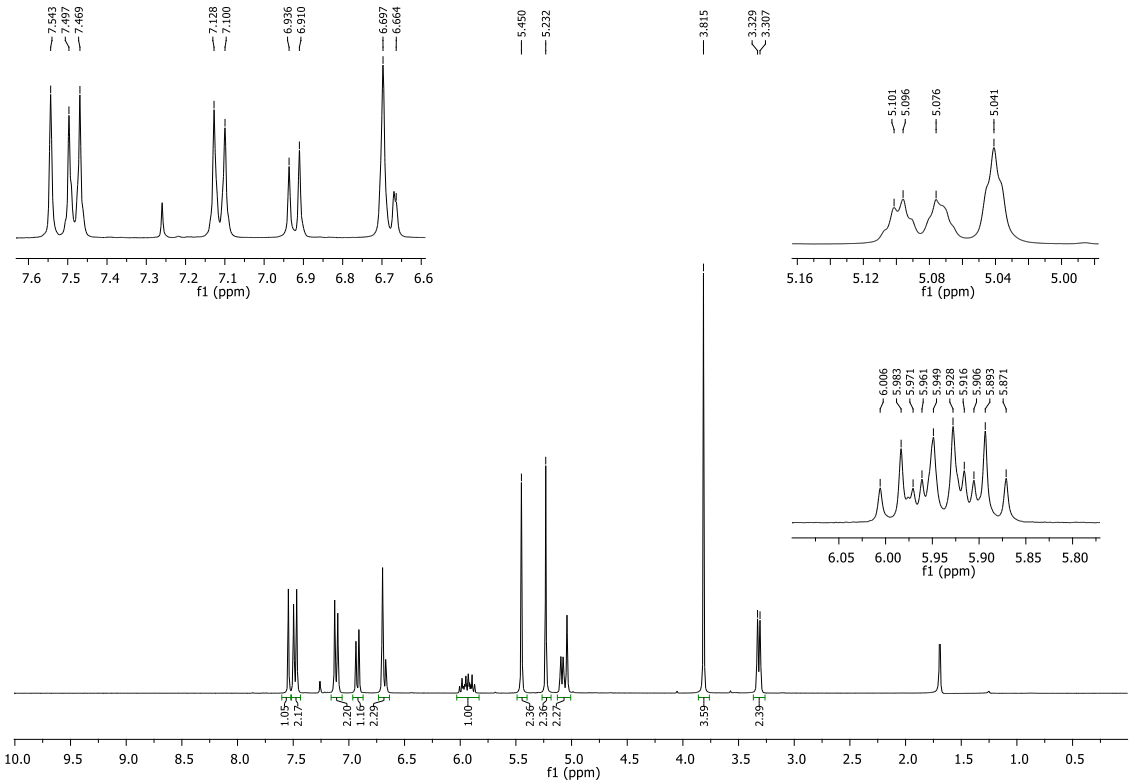


Fig. K. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-bromobenzyl)-*1H*-1,2,3-triazole (**26**).

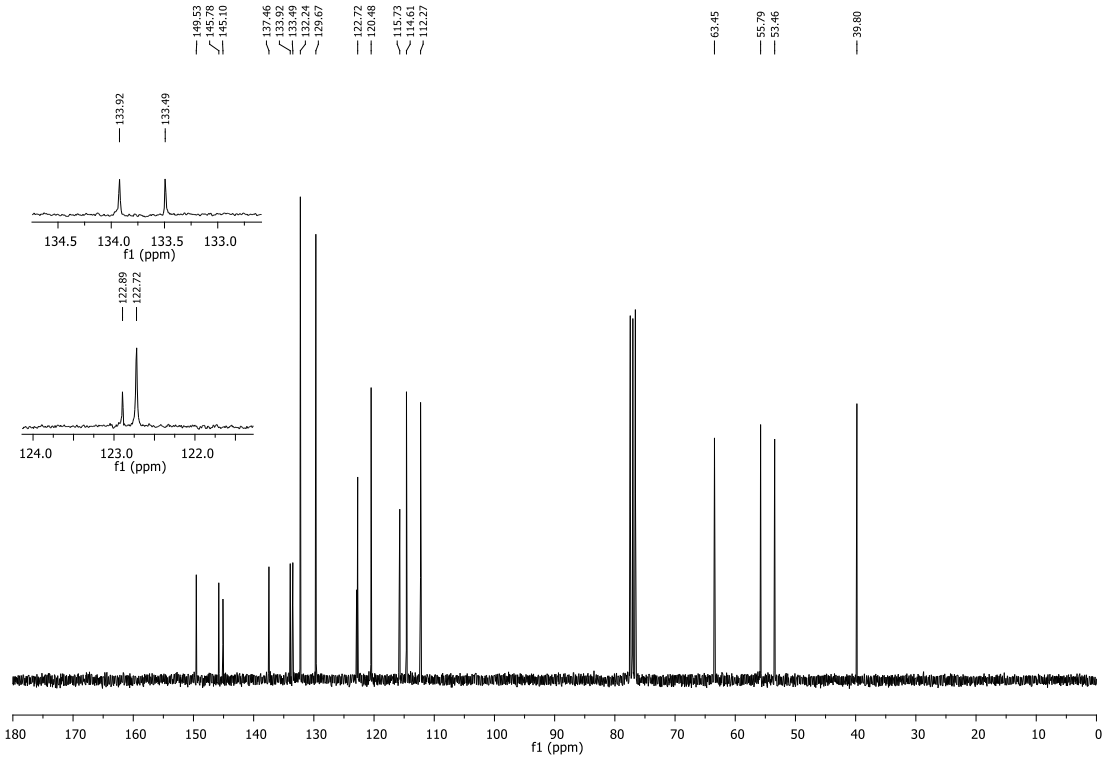


Fig. L. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-bromobenzyl)-*1H*-1,2,3-triazole (**26**).

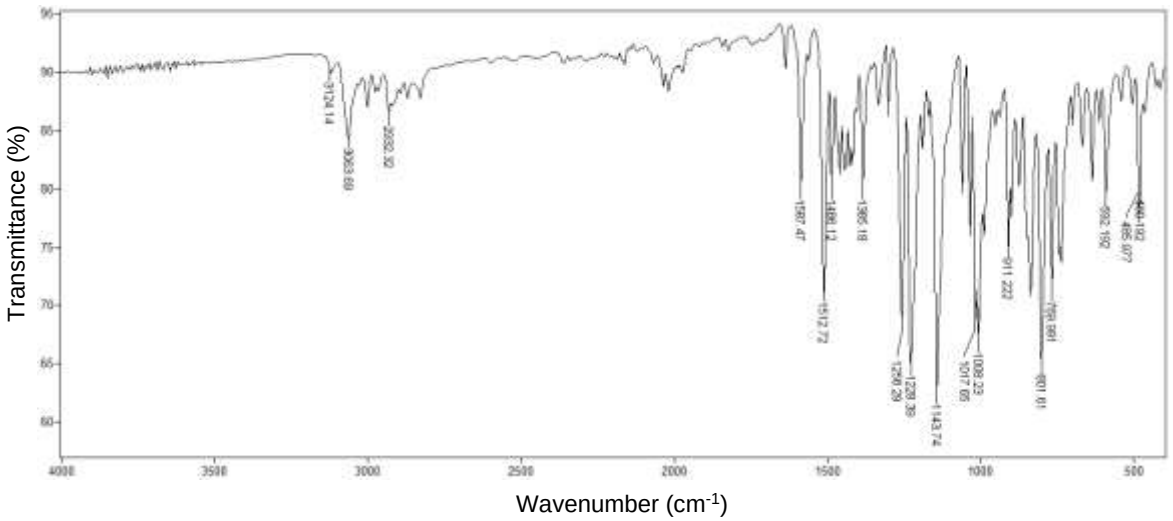


Fig. M. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-iodobenzyl)-*1H*-1,2,3-triazole (**27**).

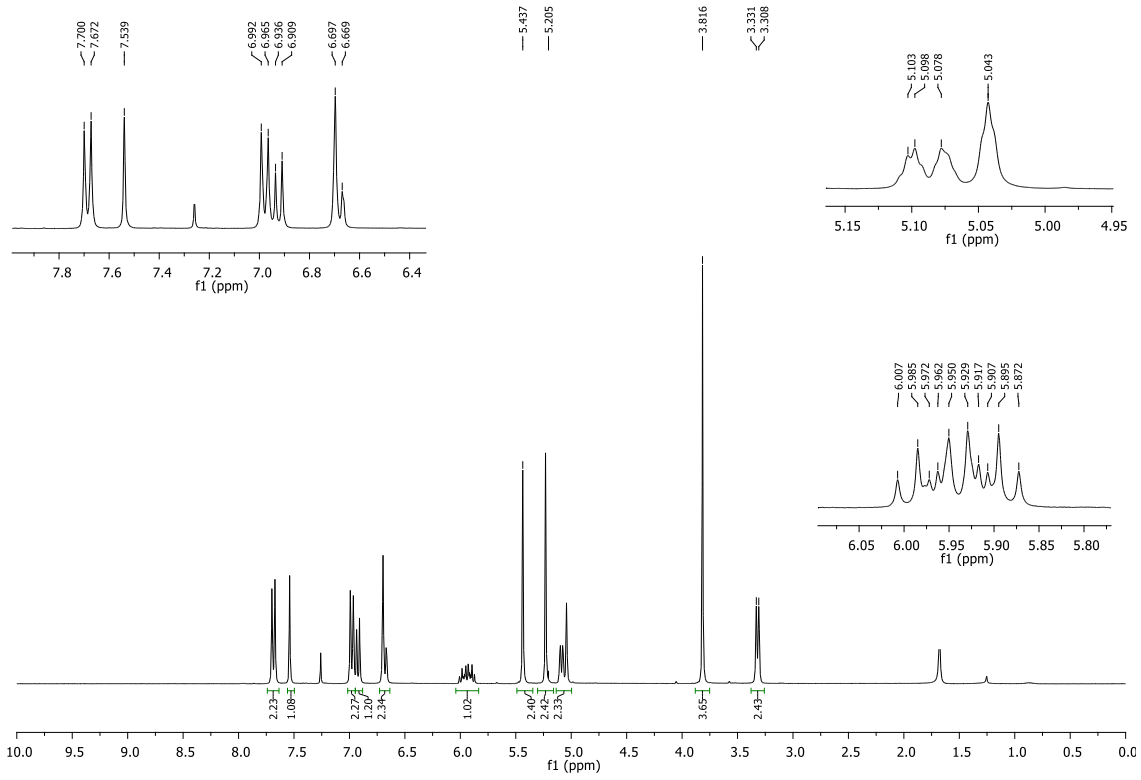


Fig. N. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-iodobenzyl)-*1H*-1,2,3-triazole (**27**).

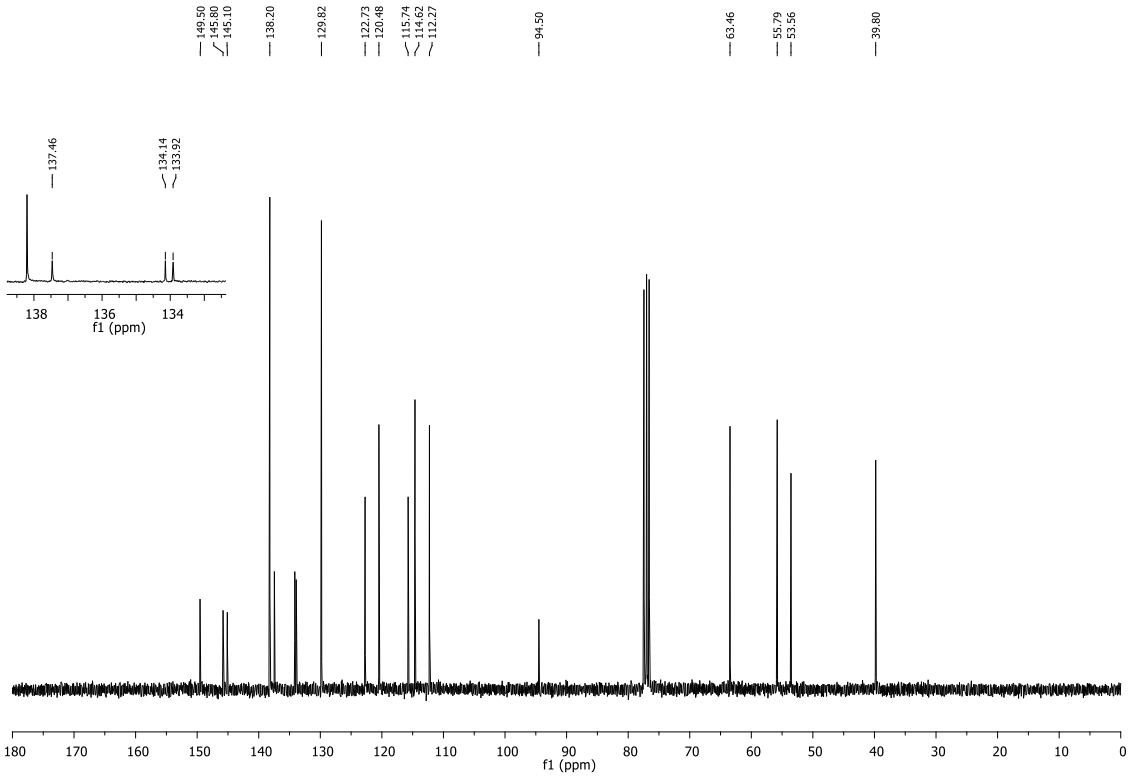


Fig. O. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-iodobenzyl)-*1H*-1,2,3-triazole (**27**).

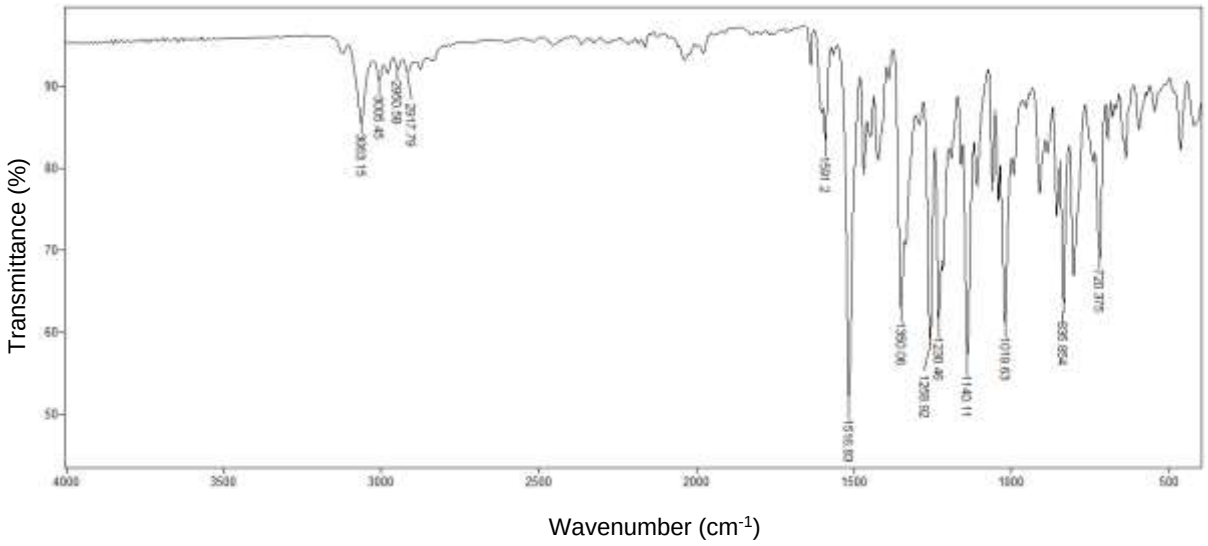


Fig. P. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-nitrobenzyl)-*1H*-1,2,3-triazole (**28**).

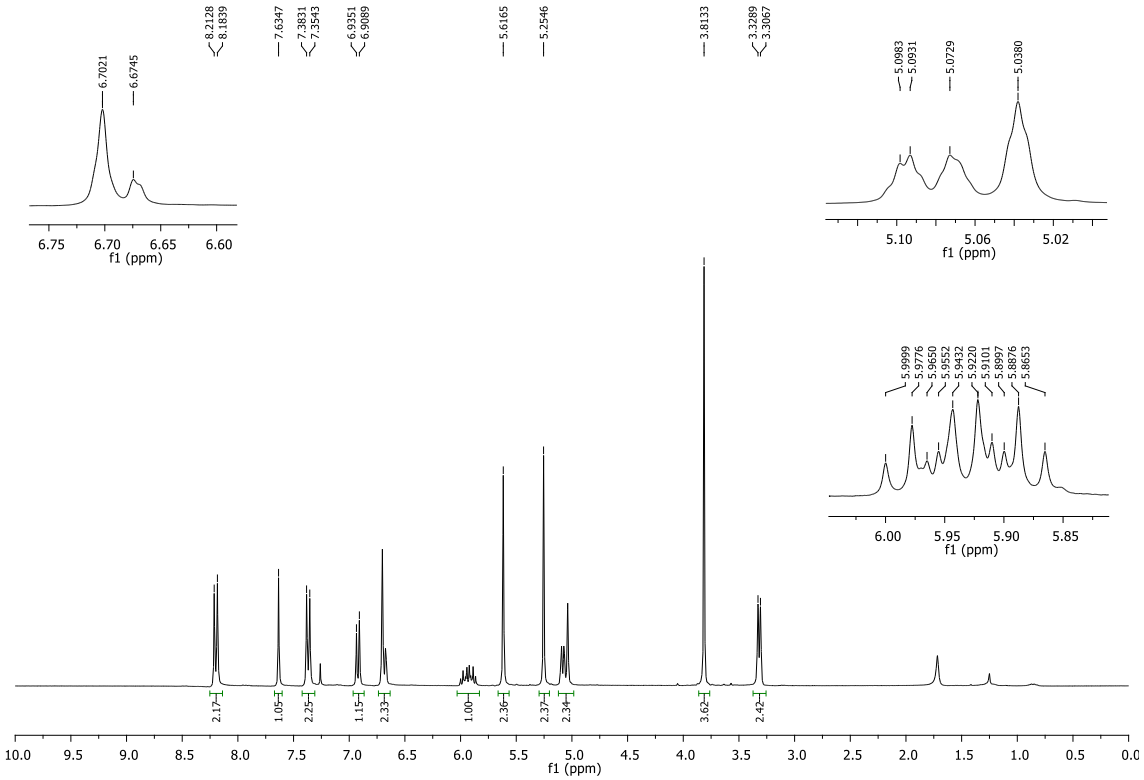


Fig. Q. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-nitrobenzyl)-*1H*-1,2,3-triazole (**28**).

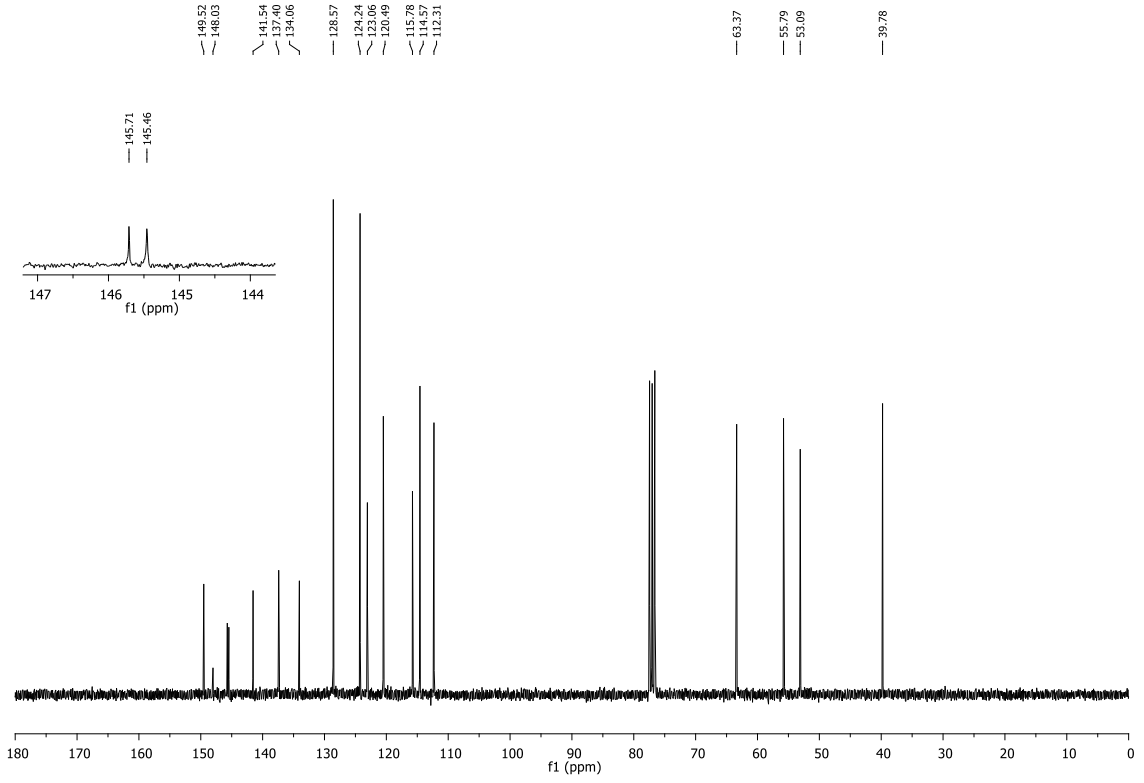


Fig. R. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-nitrobenzyl)-*1H*-1,2,3-triazole (**28**).

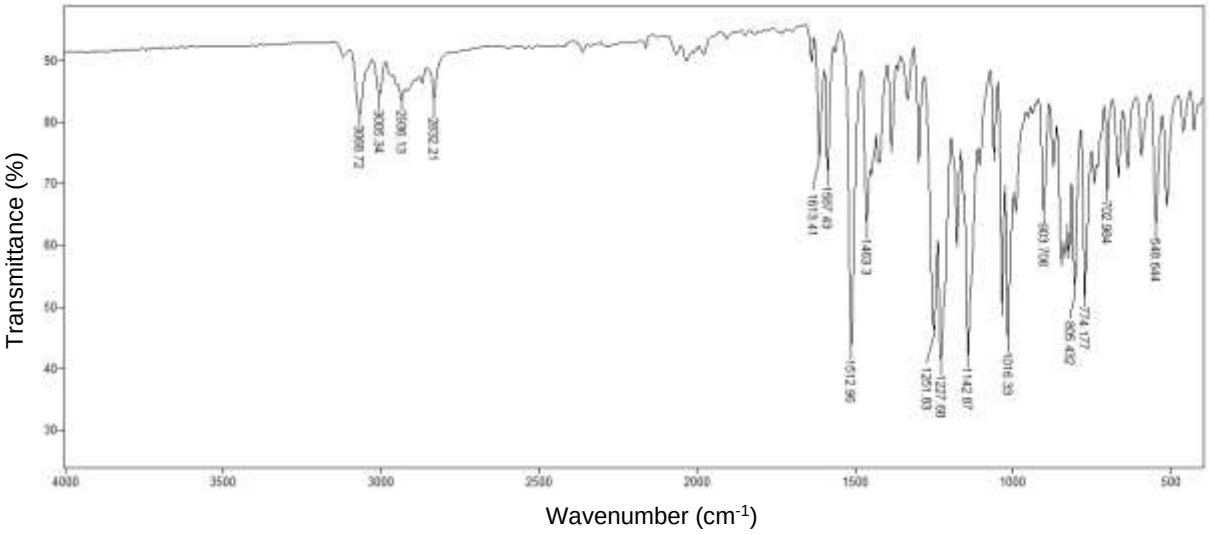


Fig. S. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-methoxybenzyl)-*1H*-1,2,3-triazole (**29**).

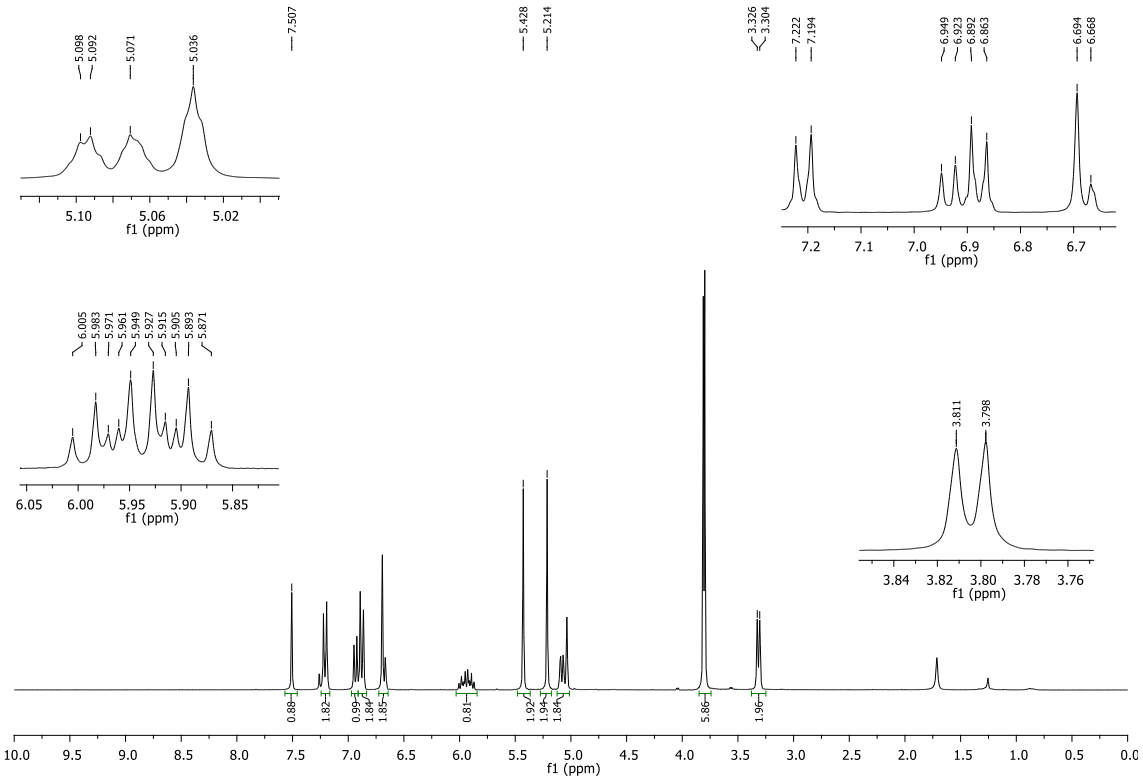


Fig. T. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-methoxybenzyl)-*1H*-1,2,3-triazole (**29**).

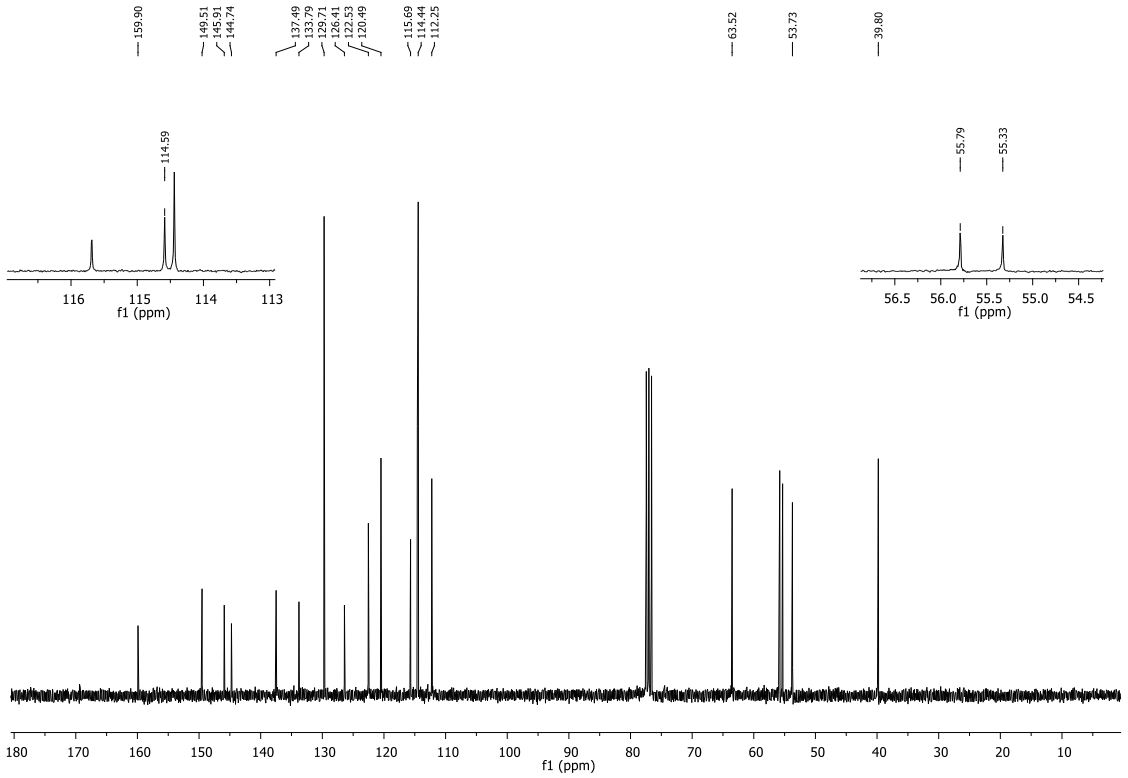


Fig. U. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-methoxybenzyl)-*1H*-1,2,3-triazole (**29**).

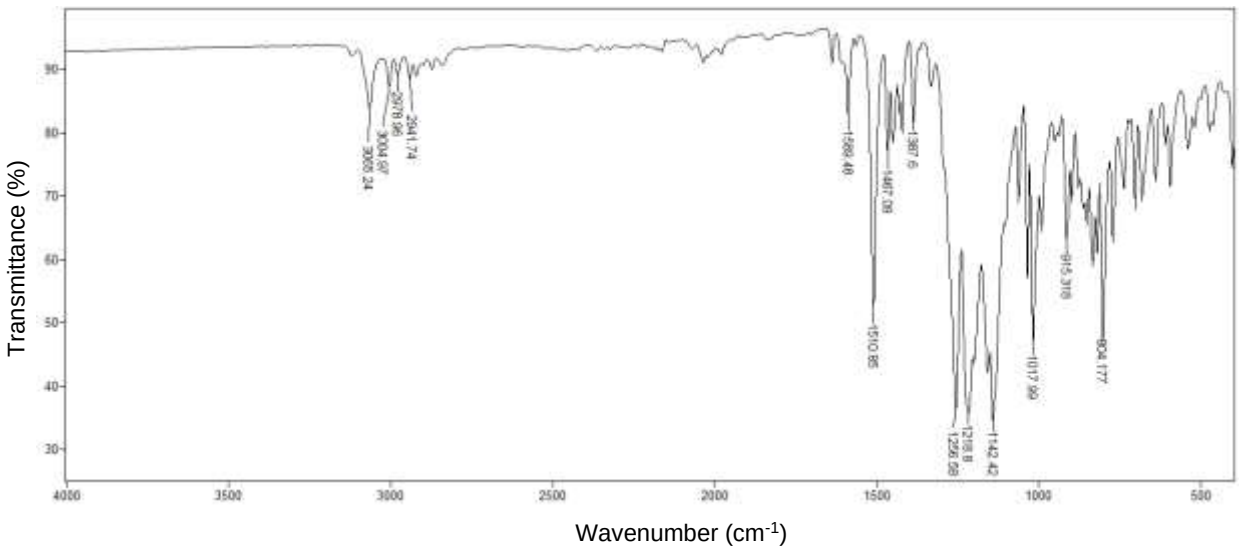


Fig. V. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-(trifluoromethoxy)benzyl)-*1H*-1,2,3-triazole (**30**).

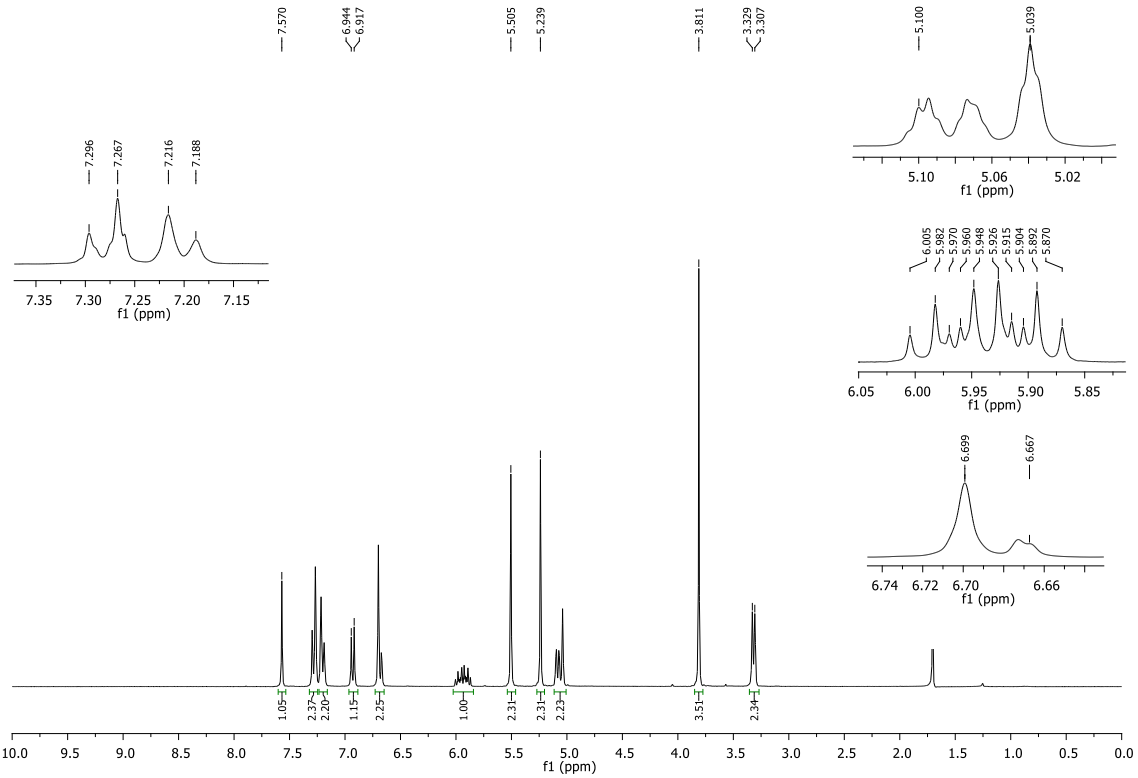


Fig. X. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-(trifluoromethoxy)benzyl)-*1H*-1,2,3-triazole (**30**).

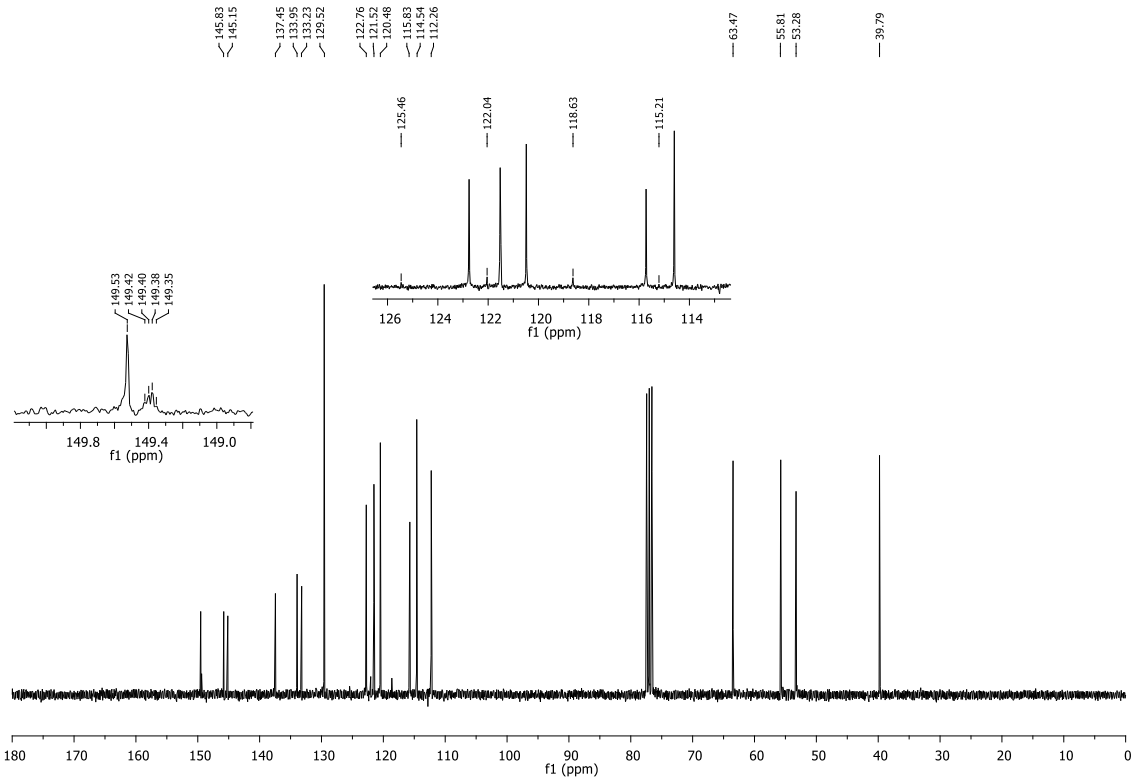


Fig. W. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-(trifluoromethoxy)benzyl)-*1H*-1,2,3-triazole (**30**).

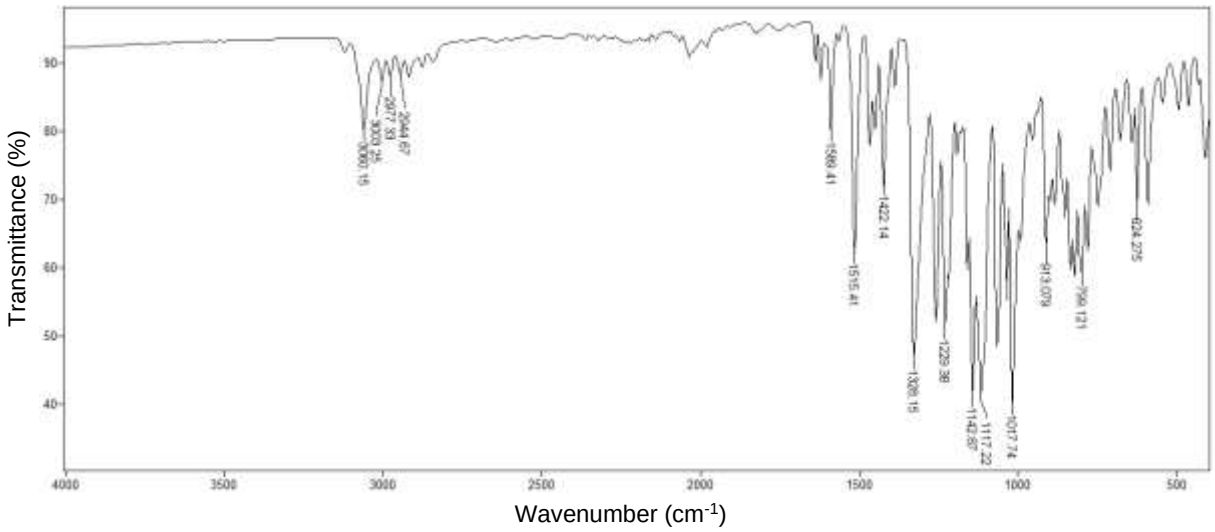


Fig. Y. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-(trifluoromethyl)benzyl)-*1H*-1,2,3-triazole (**31**).

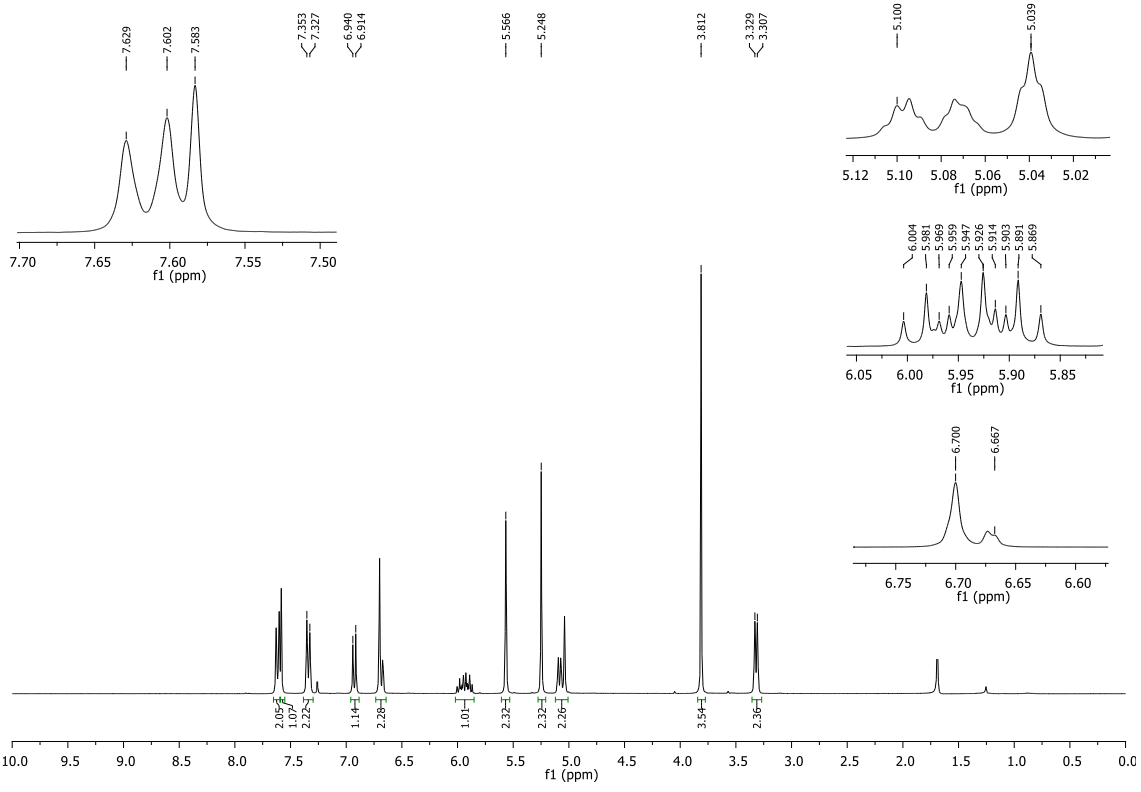


Fig. Z. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-(trifluoromethyl)benzyl)-*1H*-1,2,3-triazole (**31**).

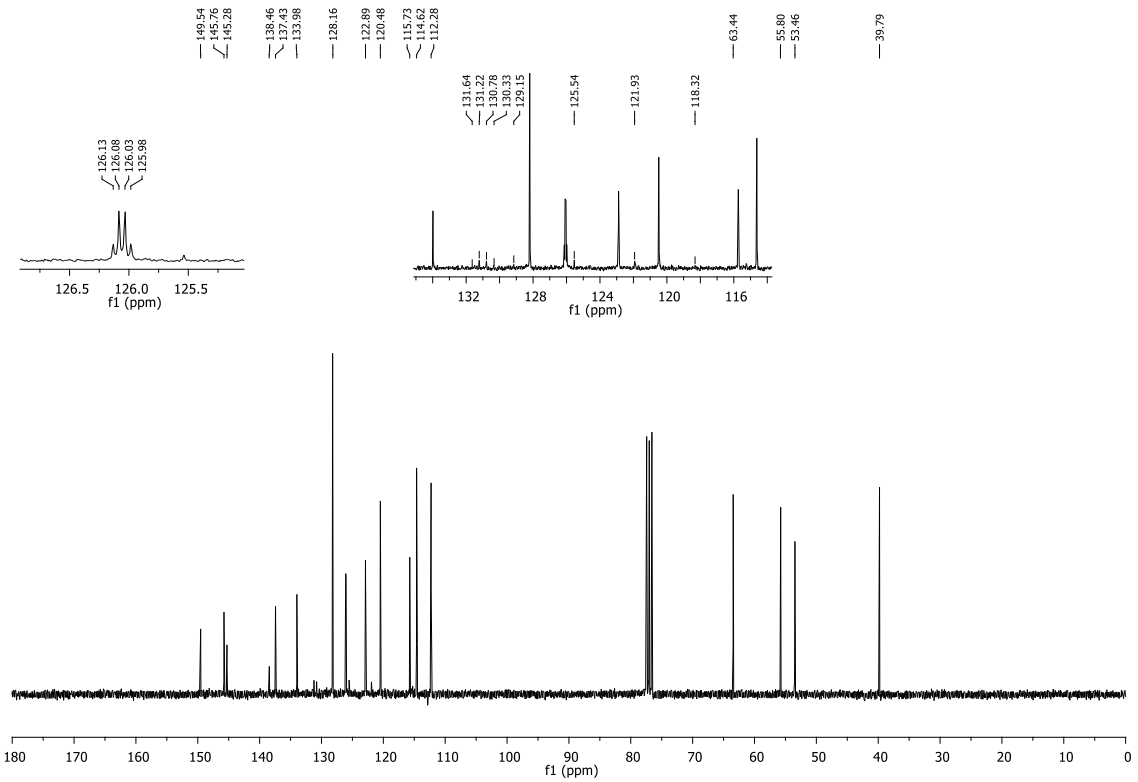


Fig. AA. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-(trifluoromethyl)benzyl)-*1H*-1,2,3-triazole (**31**).

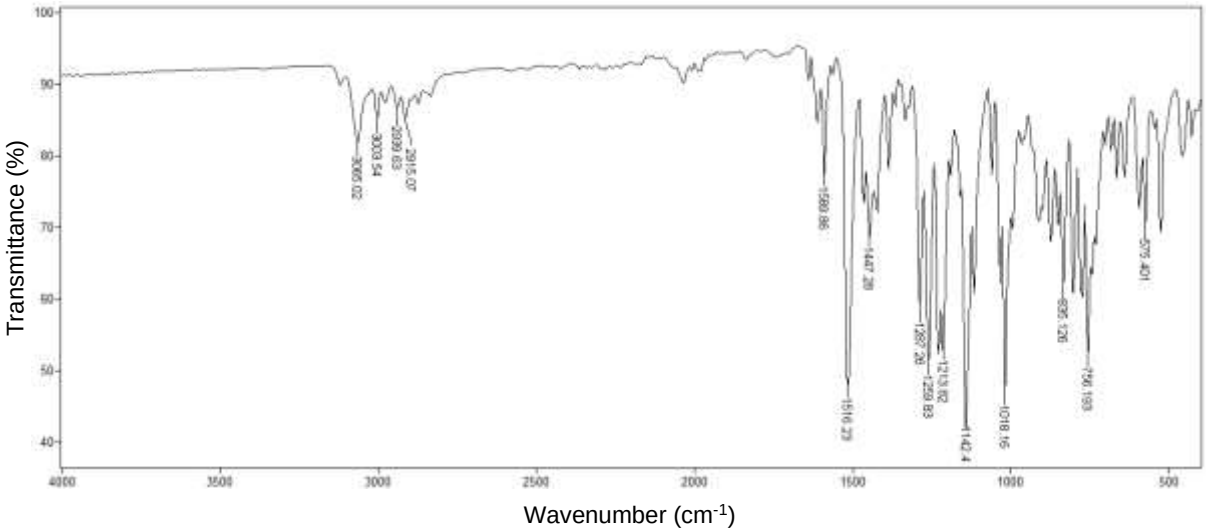


Fig. AB. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(3,4-difluorobenzyl)-*1H*-1,2,3-triazole (**32**).

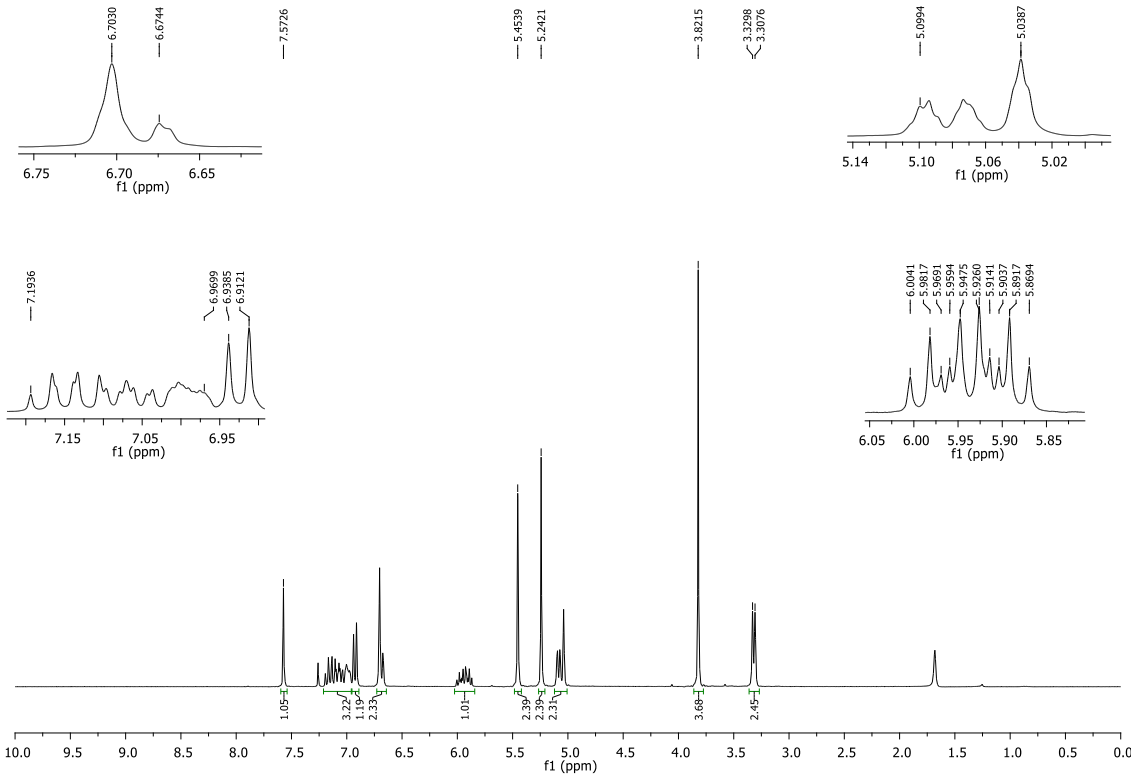


Fig. AC. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(3,4-difluorobenzyl)-*1H*-1,2,3-triazole (**32**).

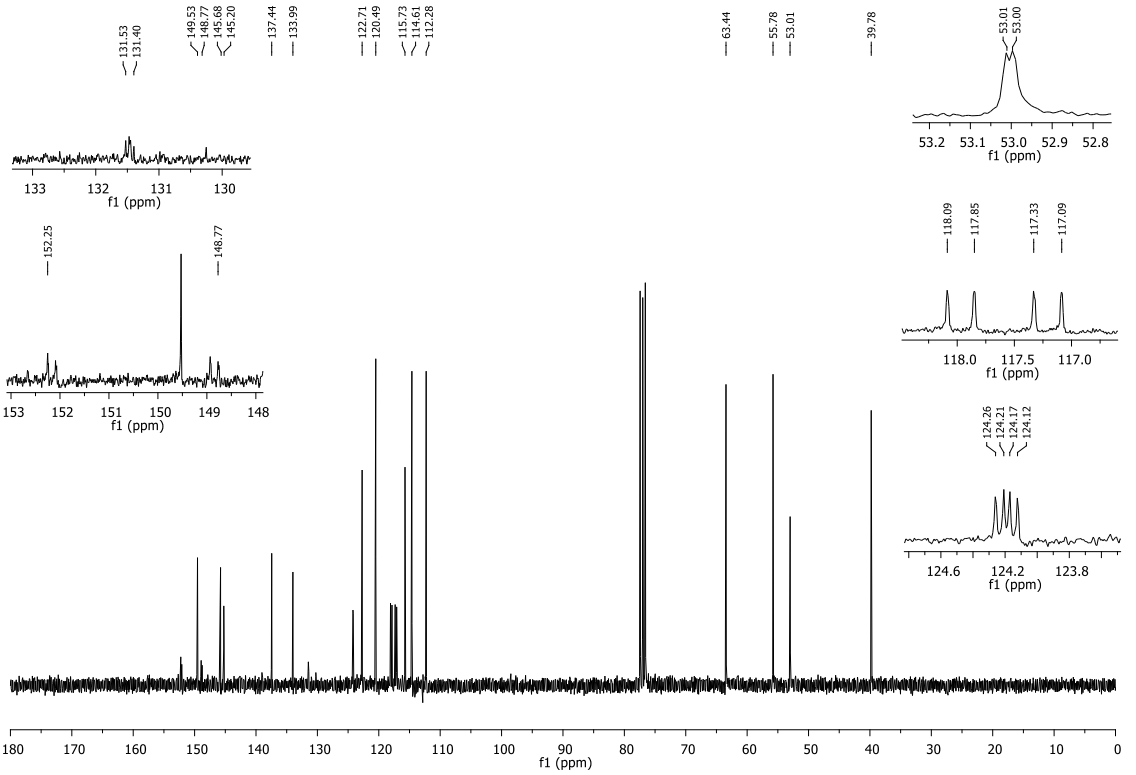


Fig. AD. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(3,4-difluorobenzyl)-*1H*-1,2,3-triazole (**32**).

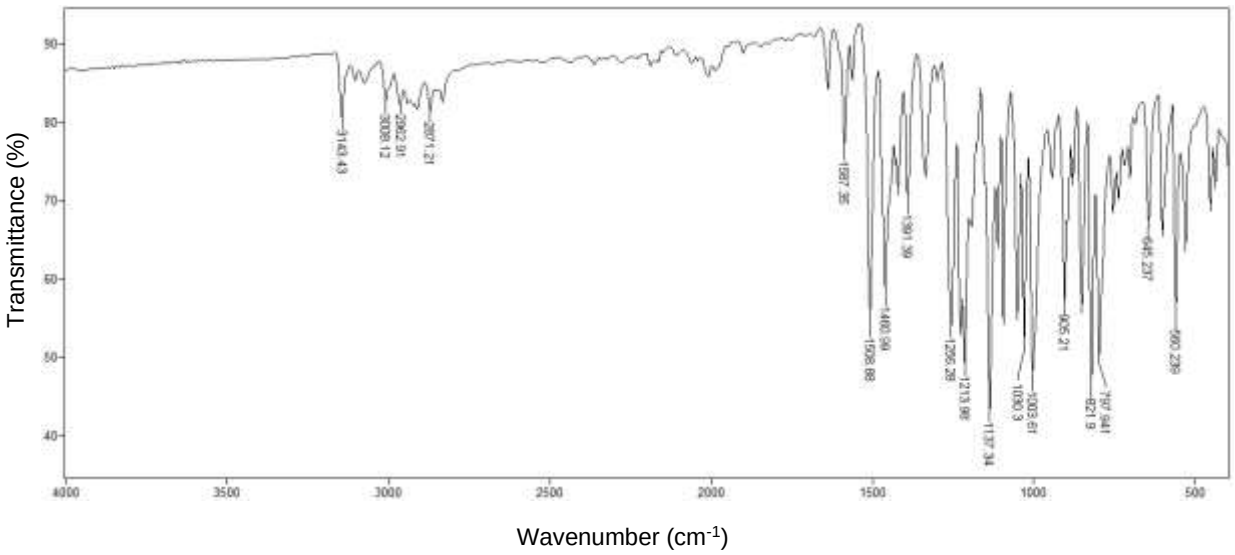


Fig. AE. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(2,5-dichlorobenzyl)-*1H*-1,2,3-triazole (**33**).

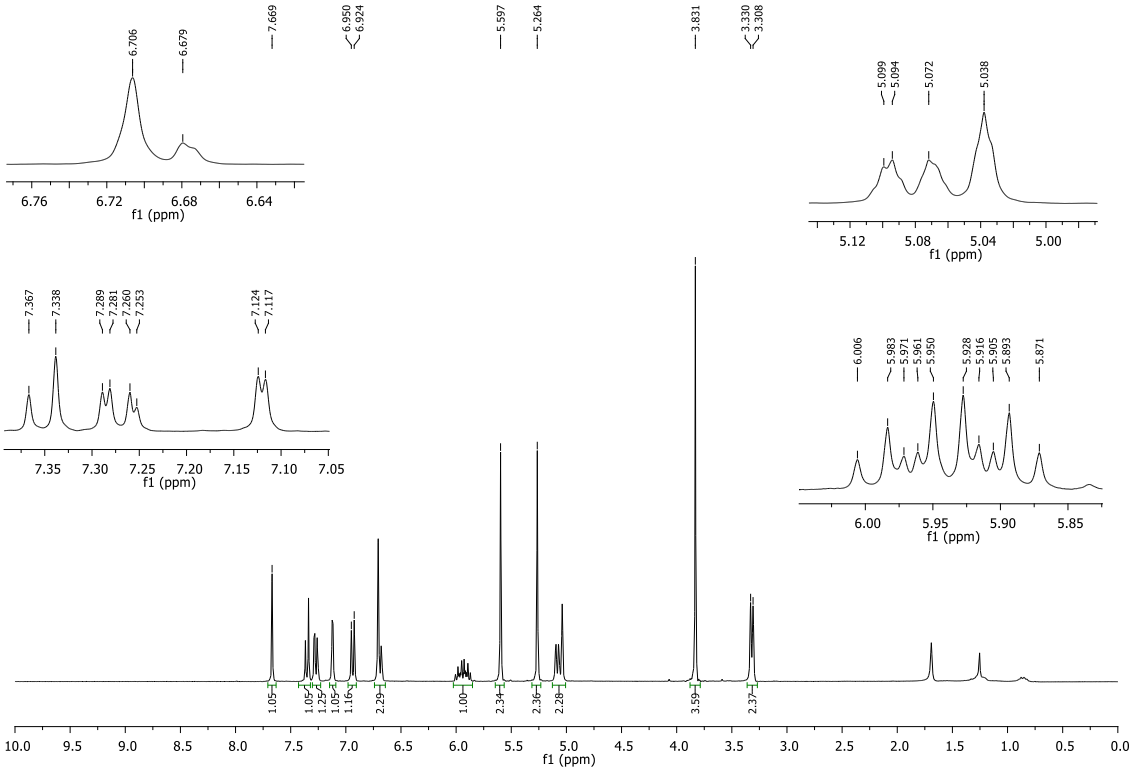


Fig. AF. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(2,5-dichlorobenzyl)-*1H*-1,2,3-triazole (**33**).

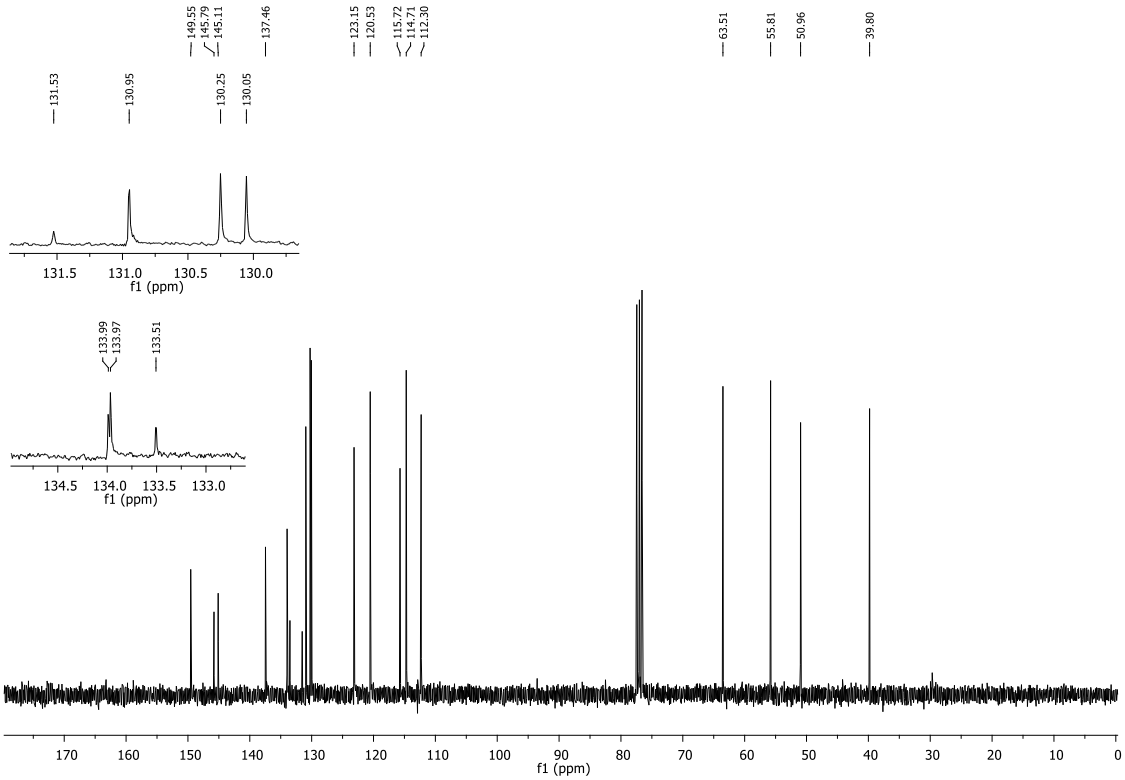


Fig. AG. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(2,5-dichlorobenzyl)-*1H*-1,2,3-triazole (**33**).

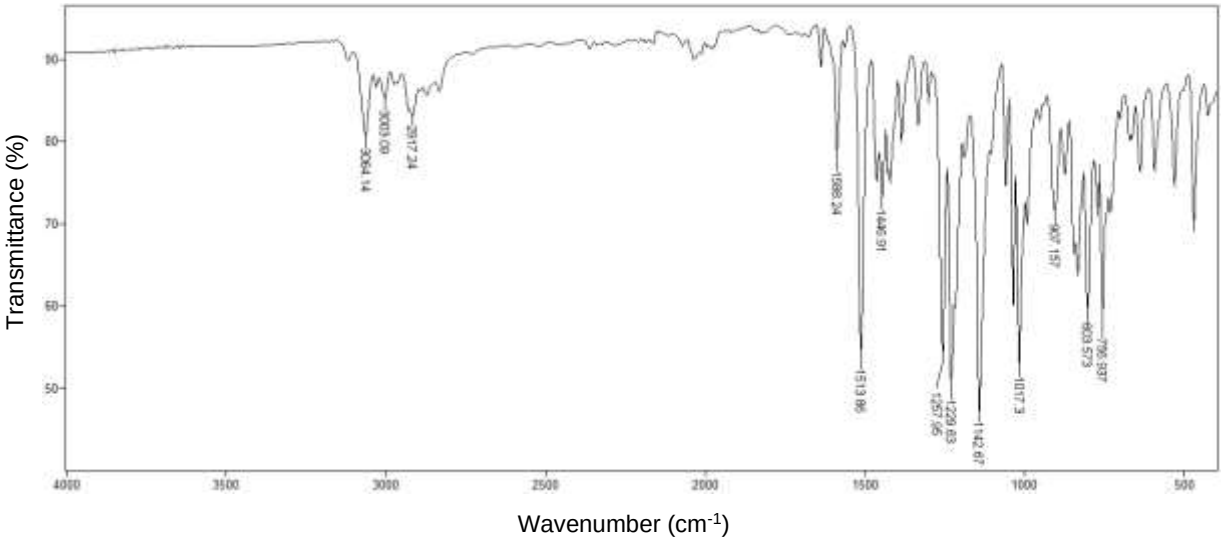


Fig. AH. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-methylbenzyl)-*1H*-1,2,3-triazole (**34**).

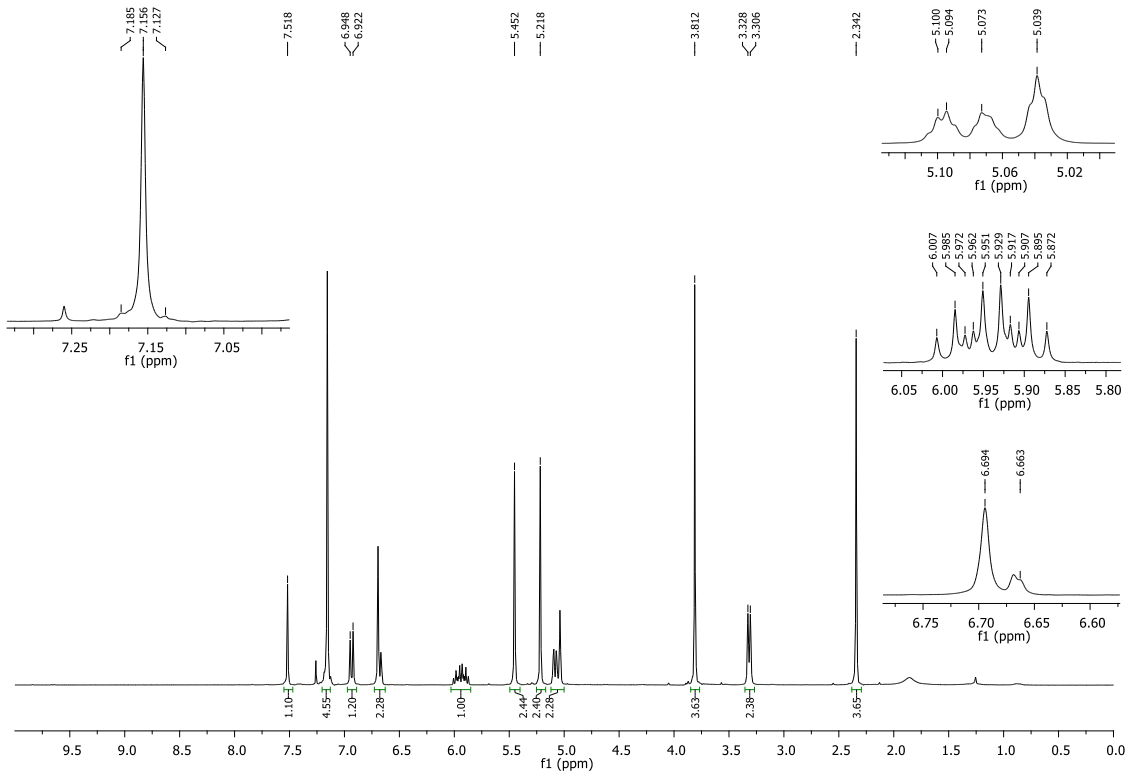


Fig. AI. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-methylbenzyl)-*1H*-1,2,3-triazole (**34**).

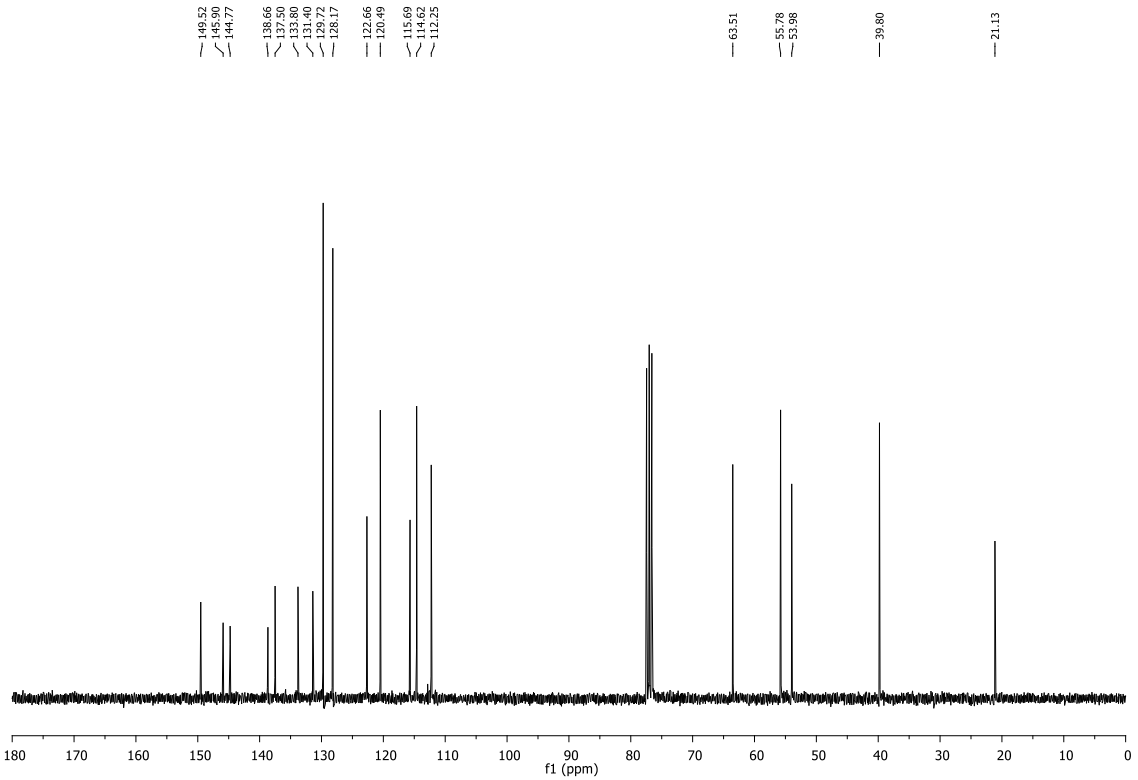


Fig. AJ. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(4-methylbenzyl)-*1H*-1,2,3-triazole (**34**).

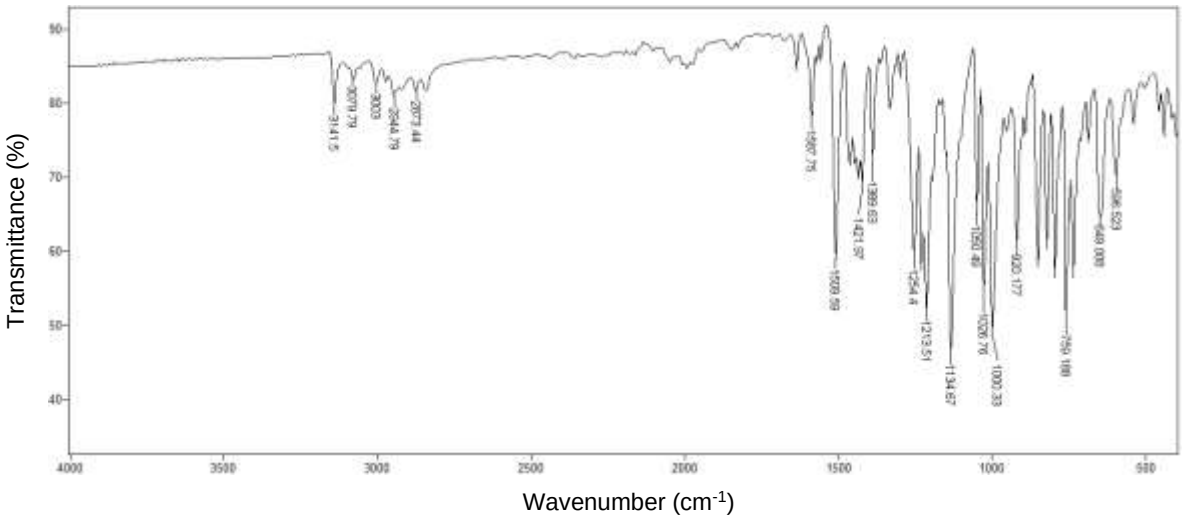


Fig. AK. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(2-bromobenzyl)-*1H*-1,2,3-triazole (**35**).

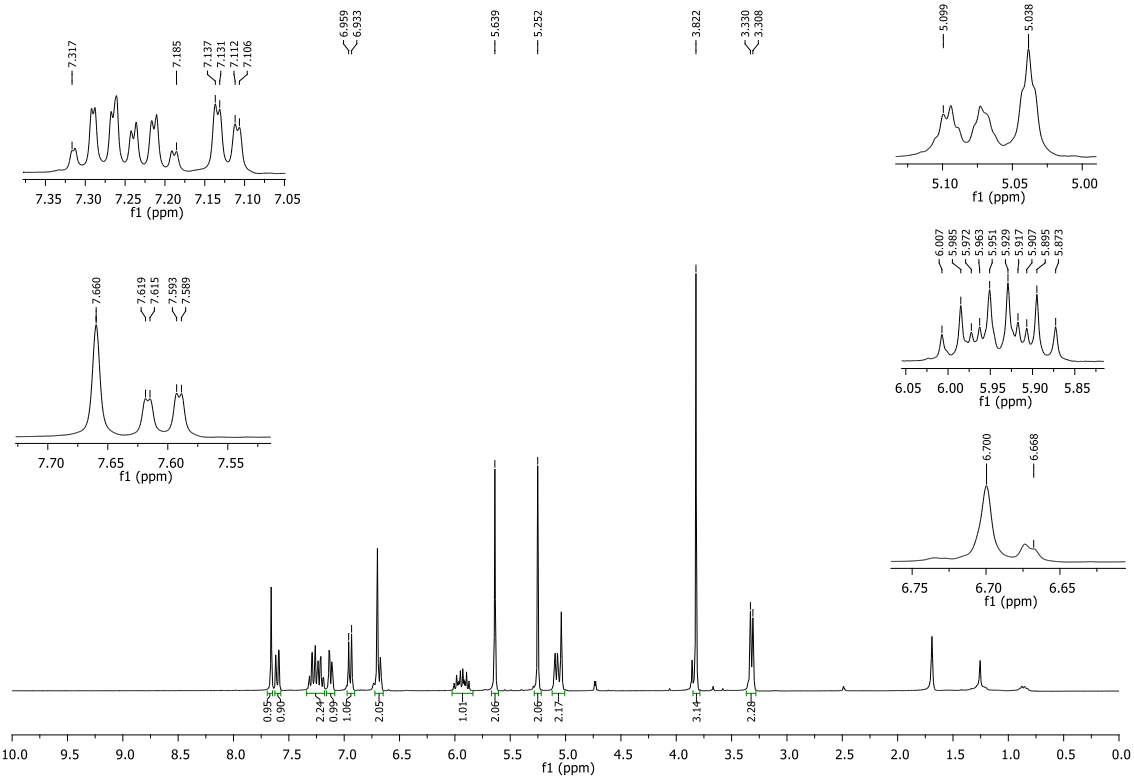


Fig. AL. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(2-bromobenzyl)-*1H*-1,2,3-triazole (**35**).

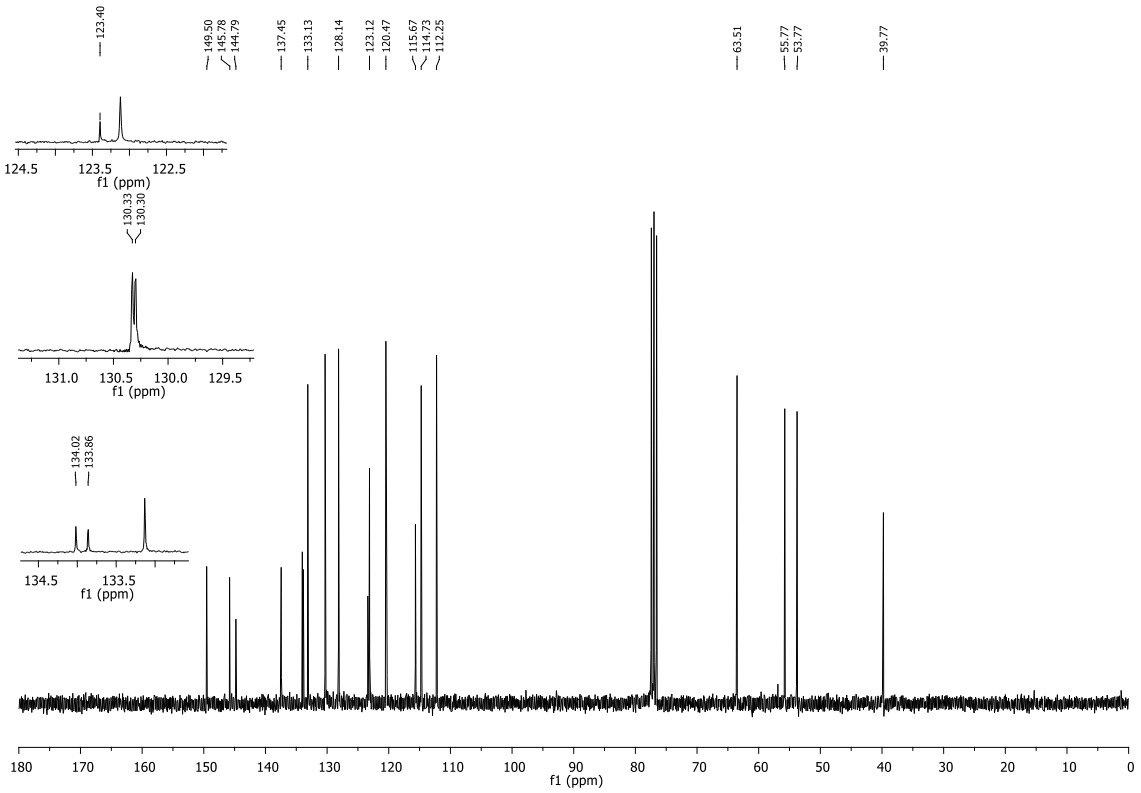


Fig. AM. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(2-bromobenzyl)-*1H*-1,2,3-triazole (**35**).

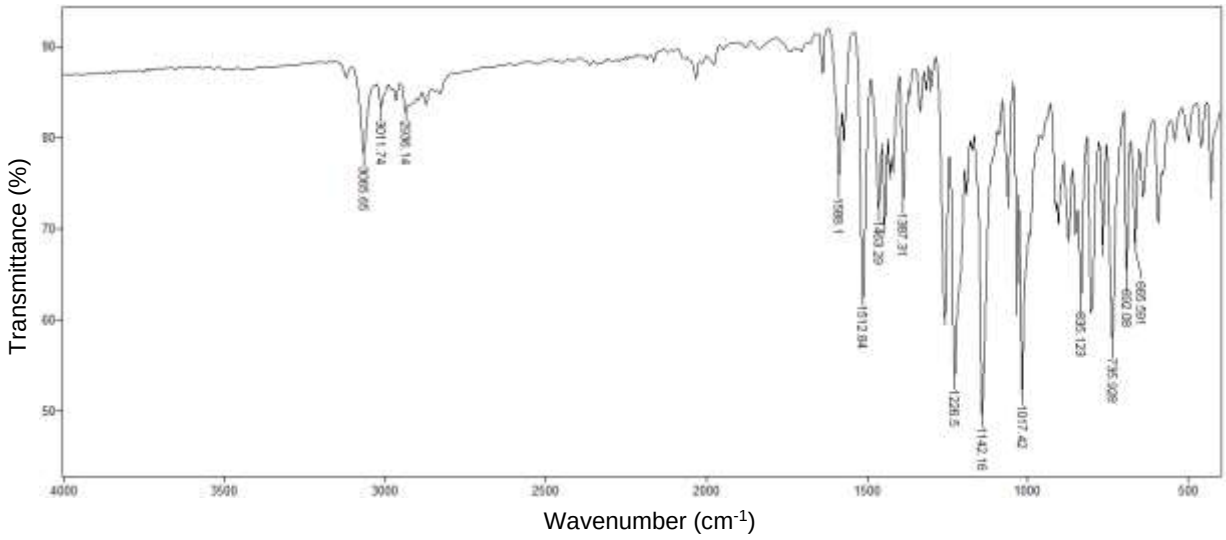


Fig. AN. IR spectrum (ATR) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(3-bromobenzyl)-*1H*-1,2,3-triazole (**36**).

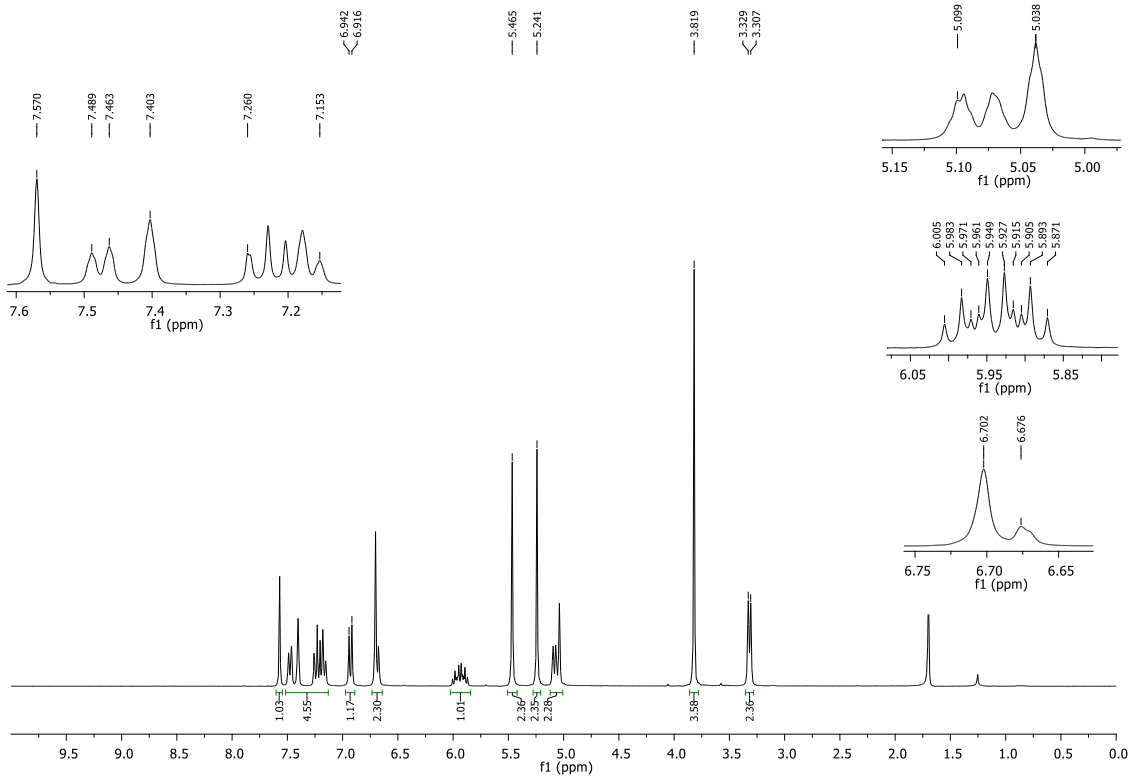


Fig. AO. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(3-bromobenzyl)-*1H*-1,2,3-triazole (**36**).

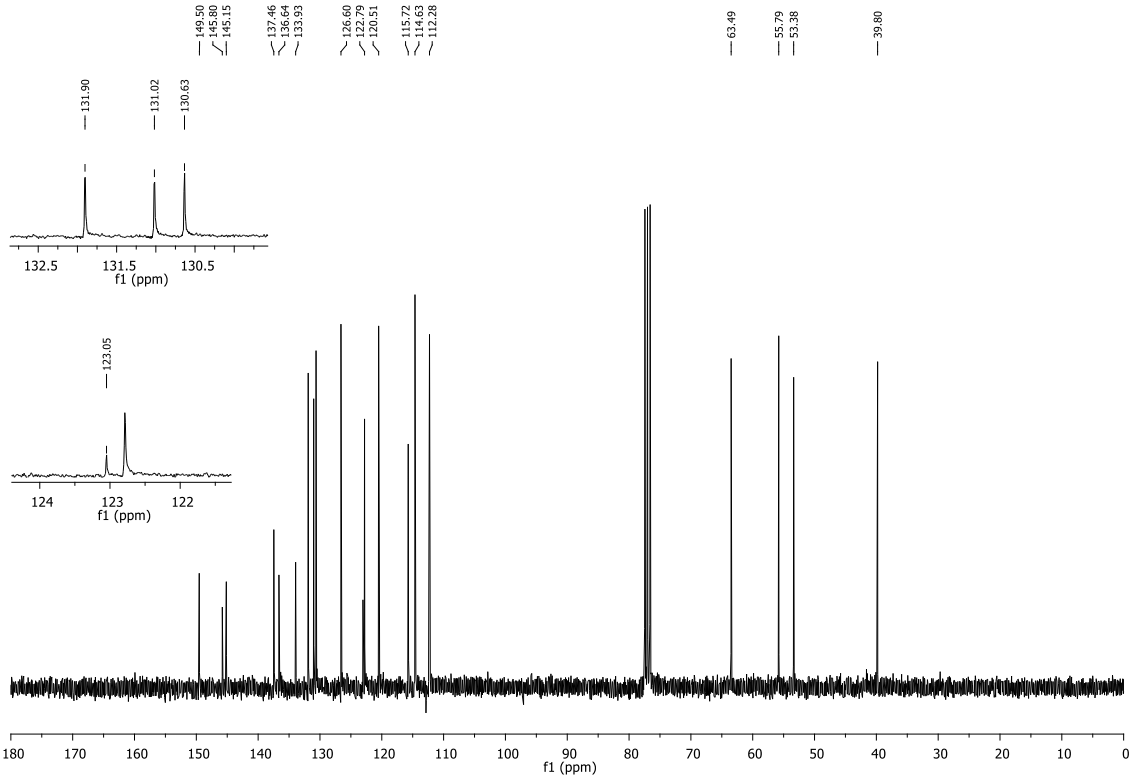


Fig. AP. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-((4-allyl-2-methoxyphenoxy)methyl)-1-(3-bromobenzyl)-*1H*-1,2,3-triazole (**36**).

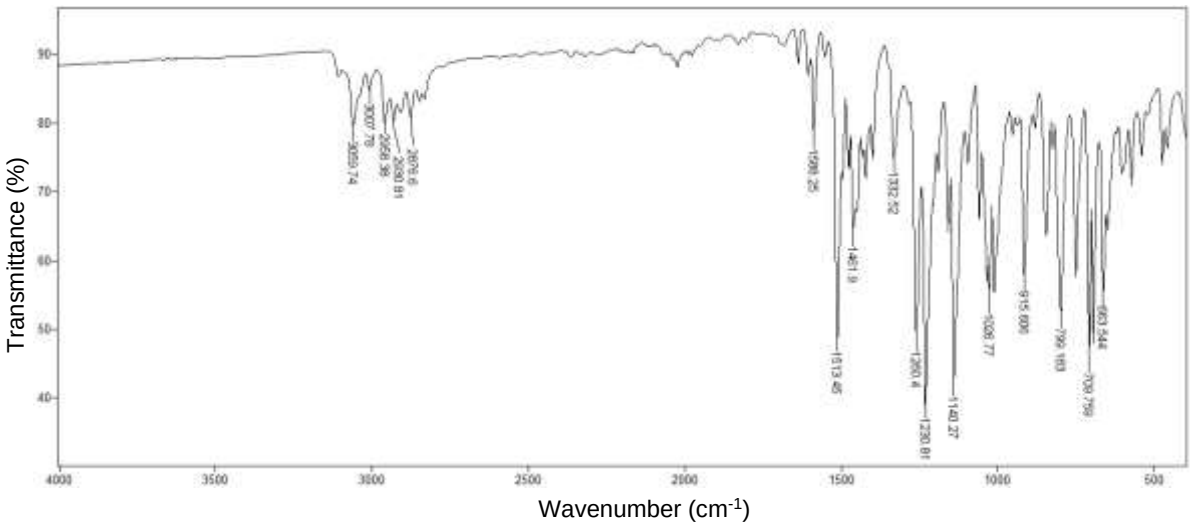


Fig. AQ. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-benzyl-*1H*-1,2,3-triazole (**37**).

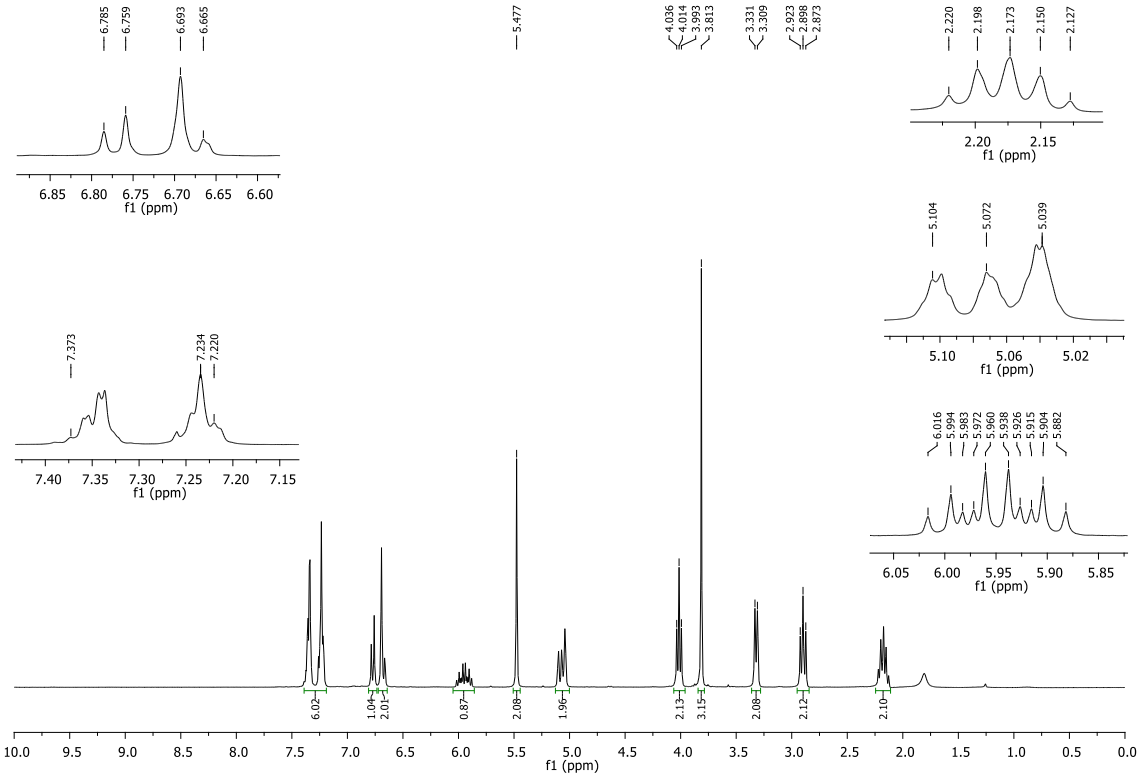


Fig. AR. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-benzyl-*1H*-1,2,3-triazole (**37**).

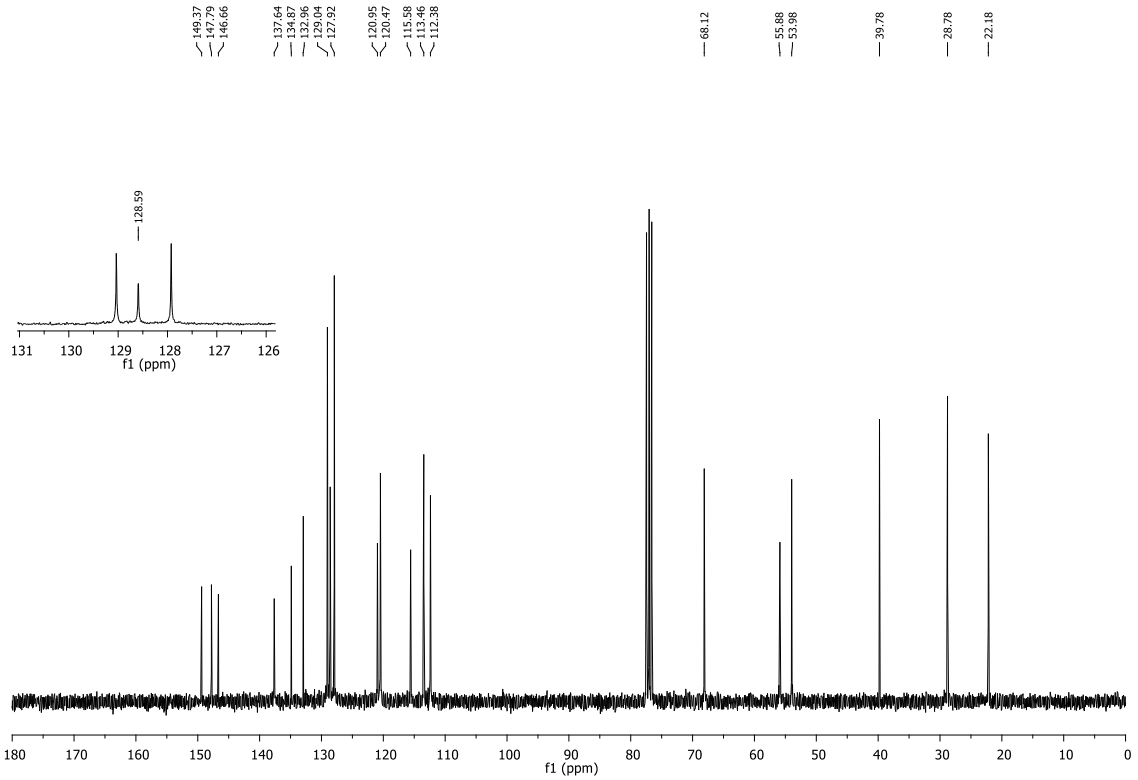


Fig. AS. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-benzyl-*1H*-1,2,3-triazole (**37**).

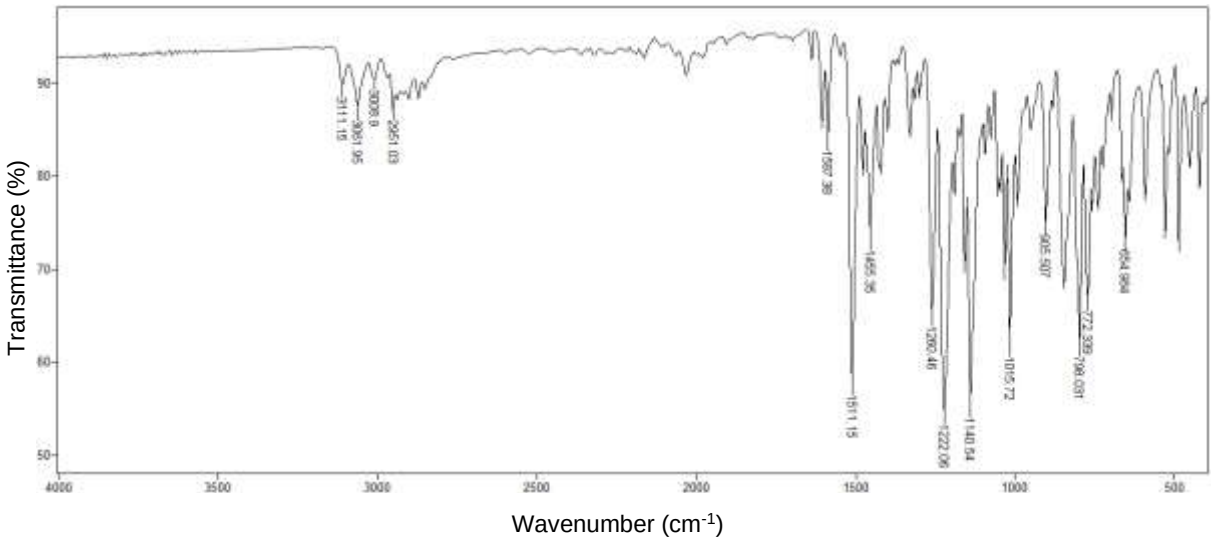


Fig. AT. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-fluorobenzyl)-*1H*-1,2,3-triazole (**38**).

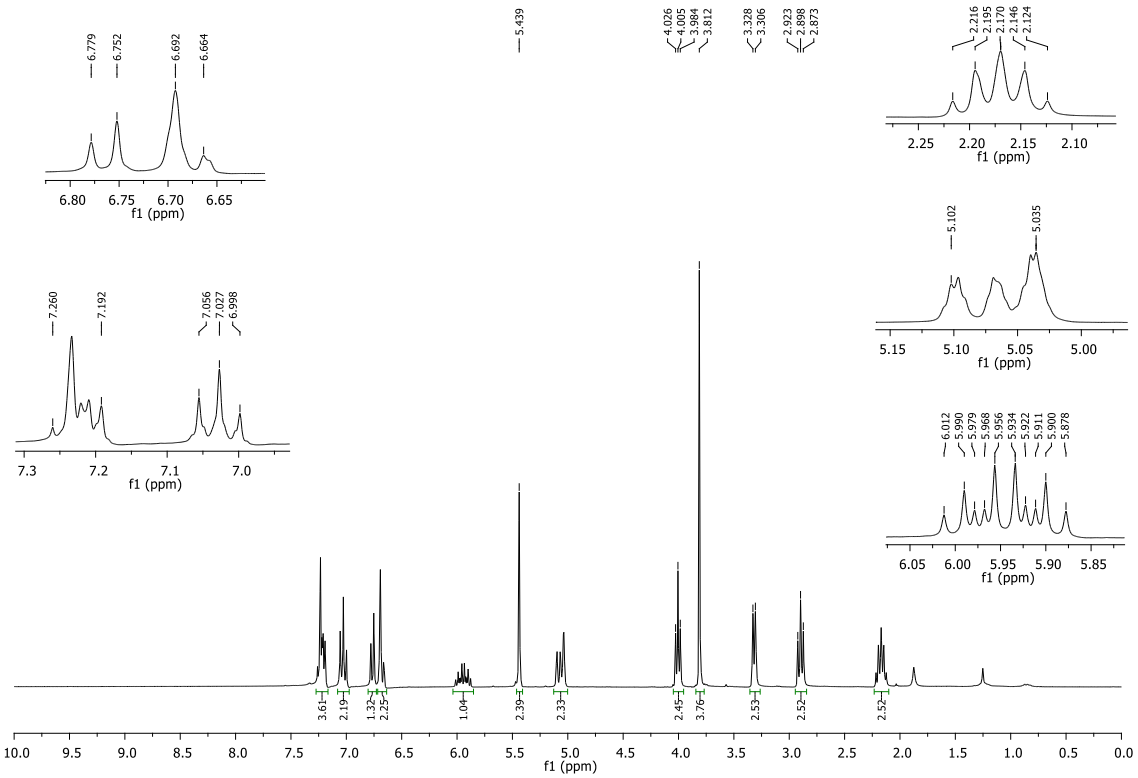


Fig. AU. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-fluorobenzyl)-*1H*-1,2,3-triazole (**38**).

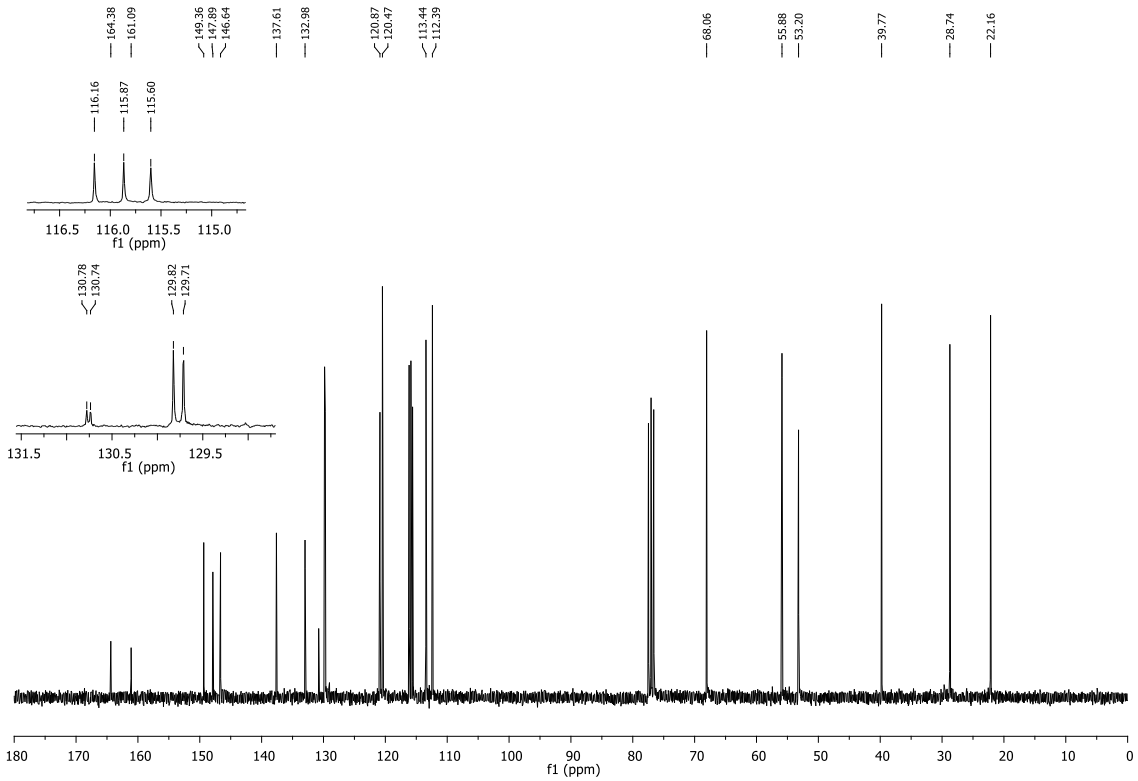


Fig. AV. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-fluorobenzyl)-*1H*-1,2,3-triazole (**38**).

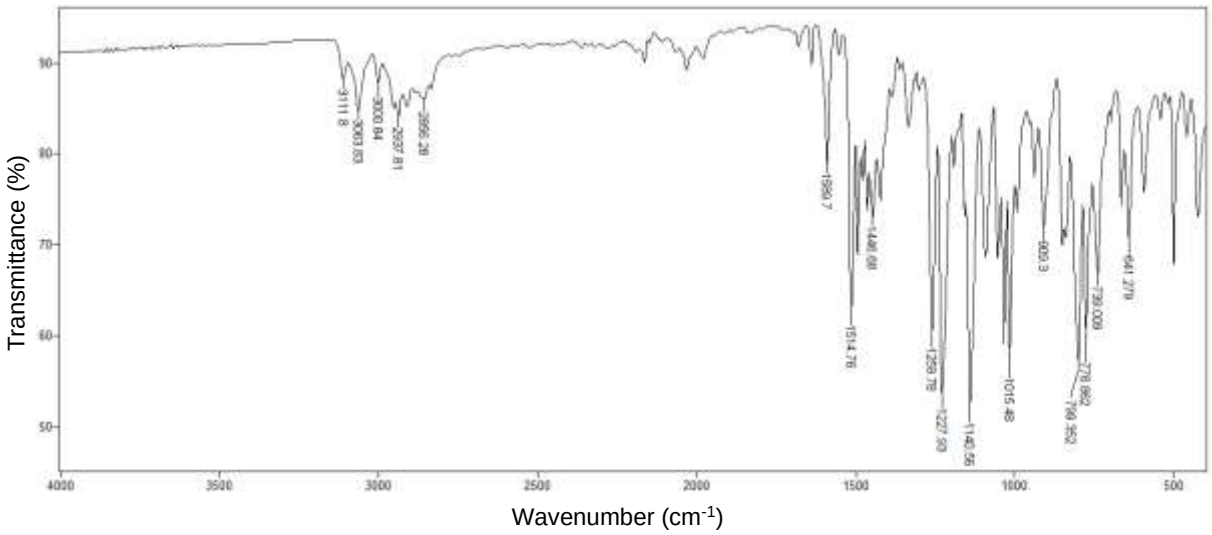


Fig. AX. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-chlorobenzyl)-*1H*-1,2,3-triazole (**39**).

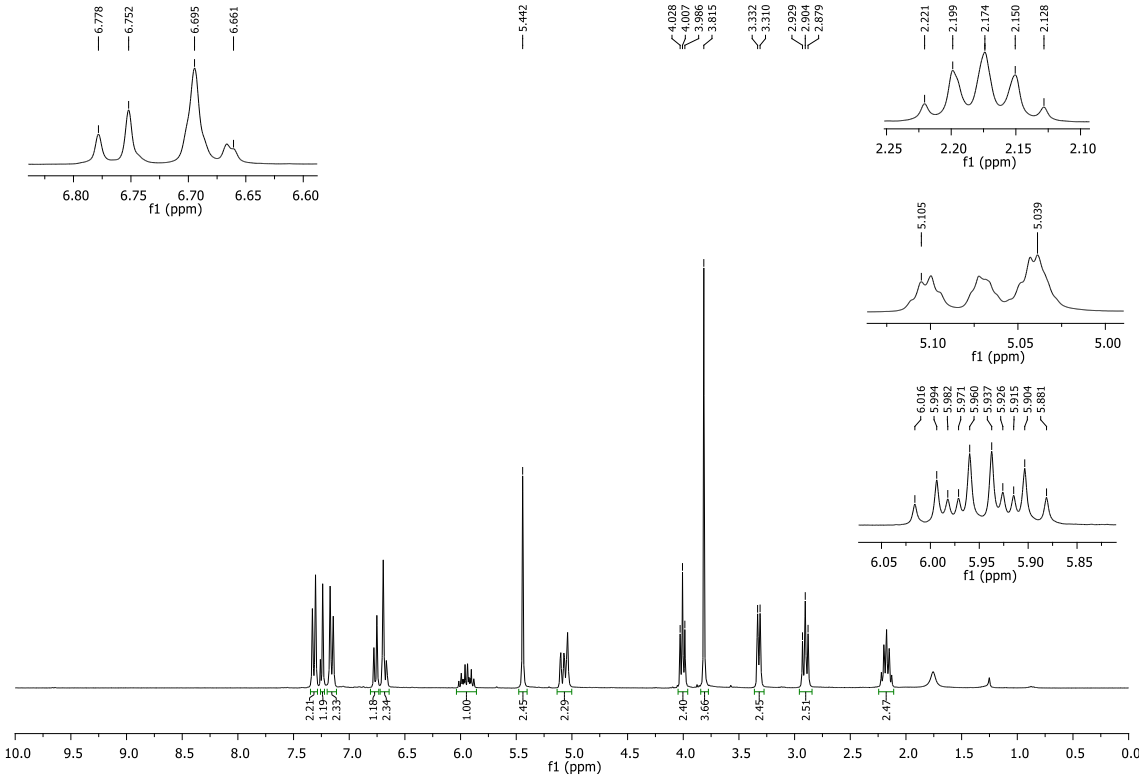


Fig. AW. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-chlorobenzyl)-*1H*-1,2,3-triazole (**39**).

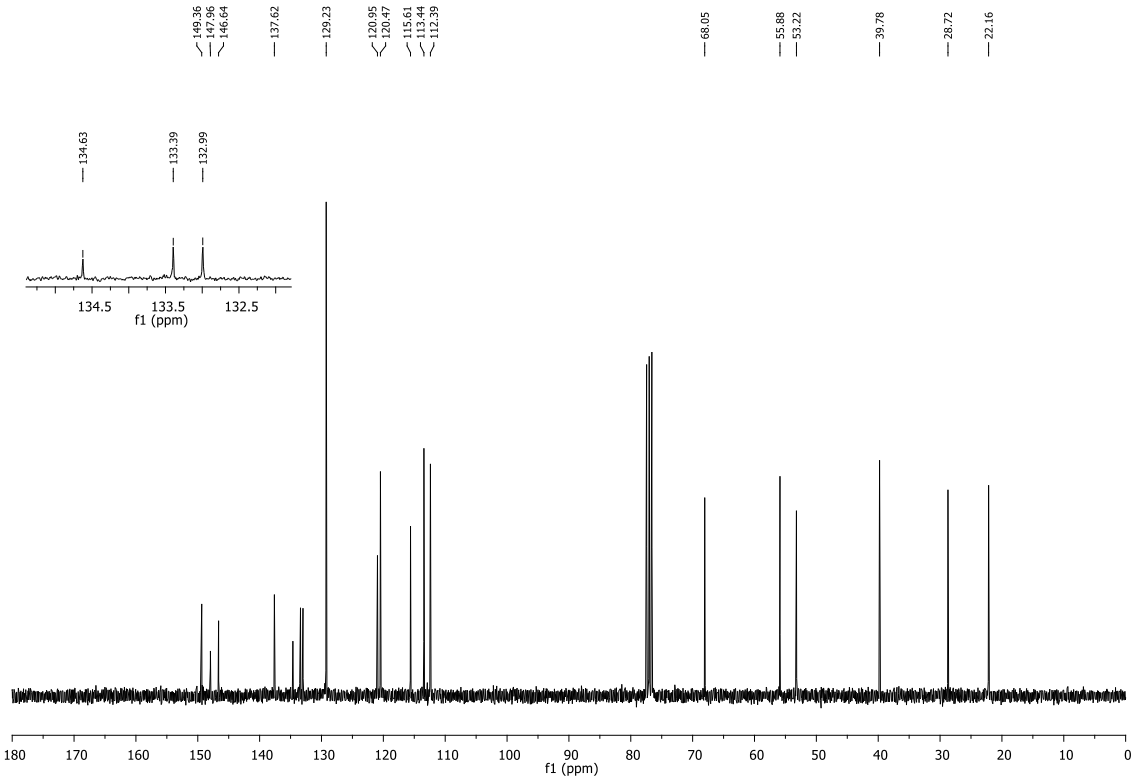


Fig. AY. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-chlorobenzyl)-*1H*-1,2,3-triazole (**39**).

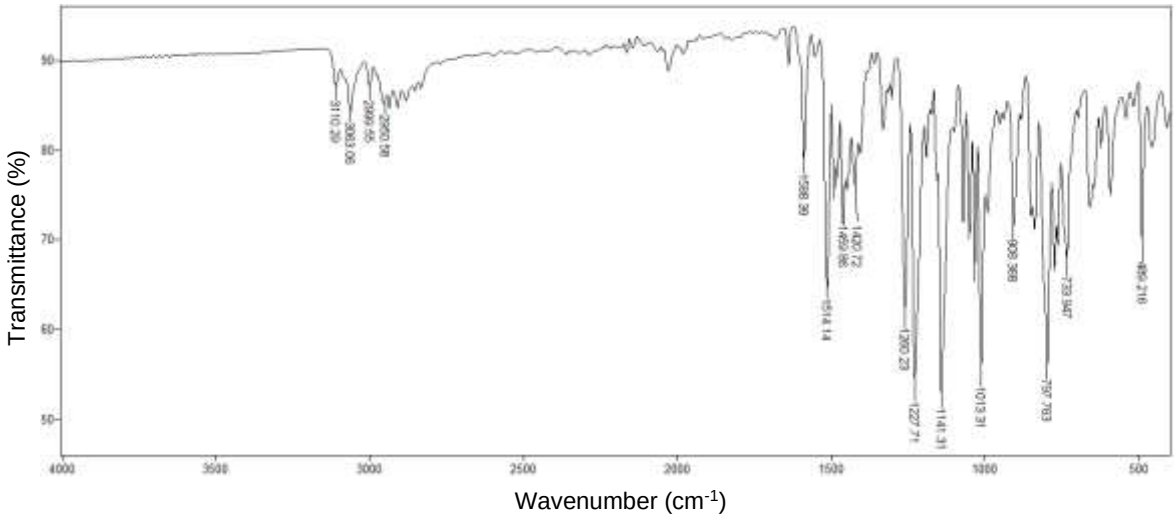


Fig. AZ. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-bromobenzyl)-*1H*-1,2,3-triazole (**40**).

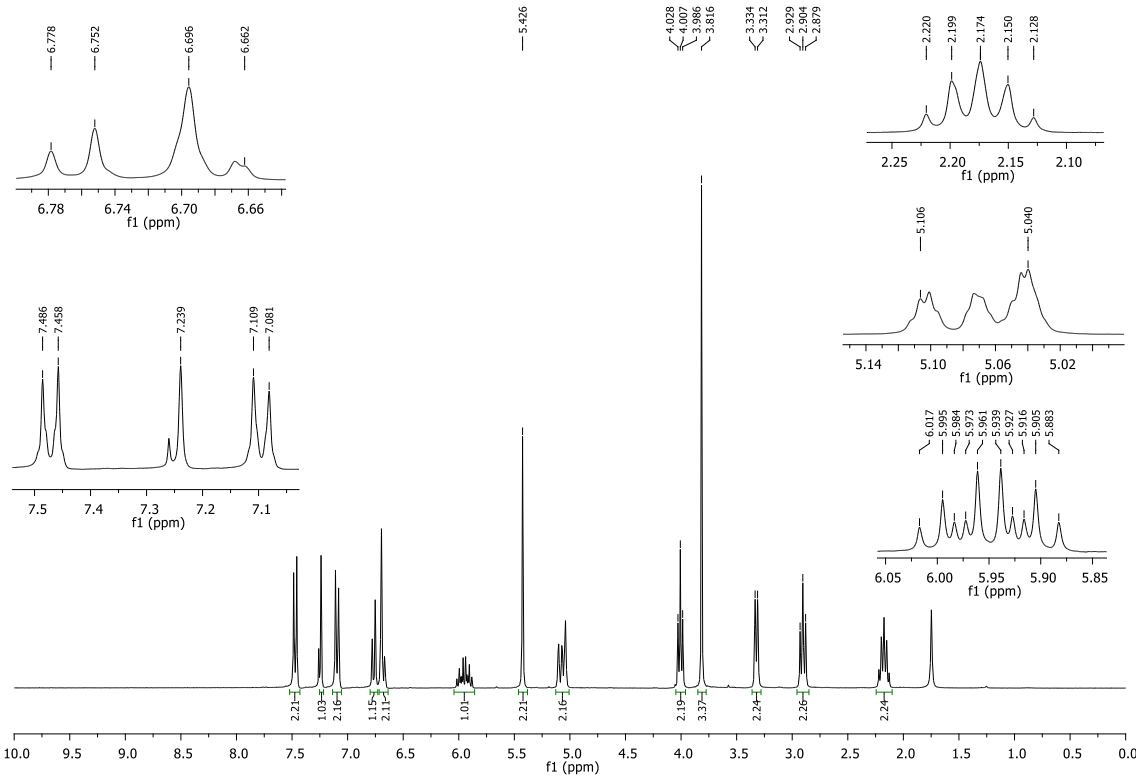


Fig. BA. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-bromobenzyl)-*1H*-1,2,3-triazole (**40**).

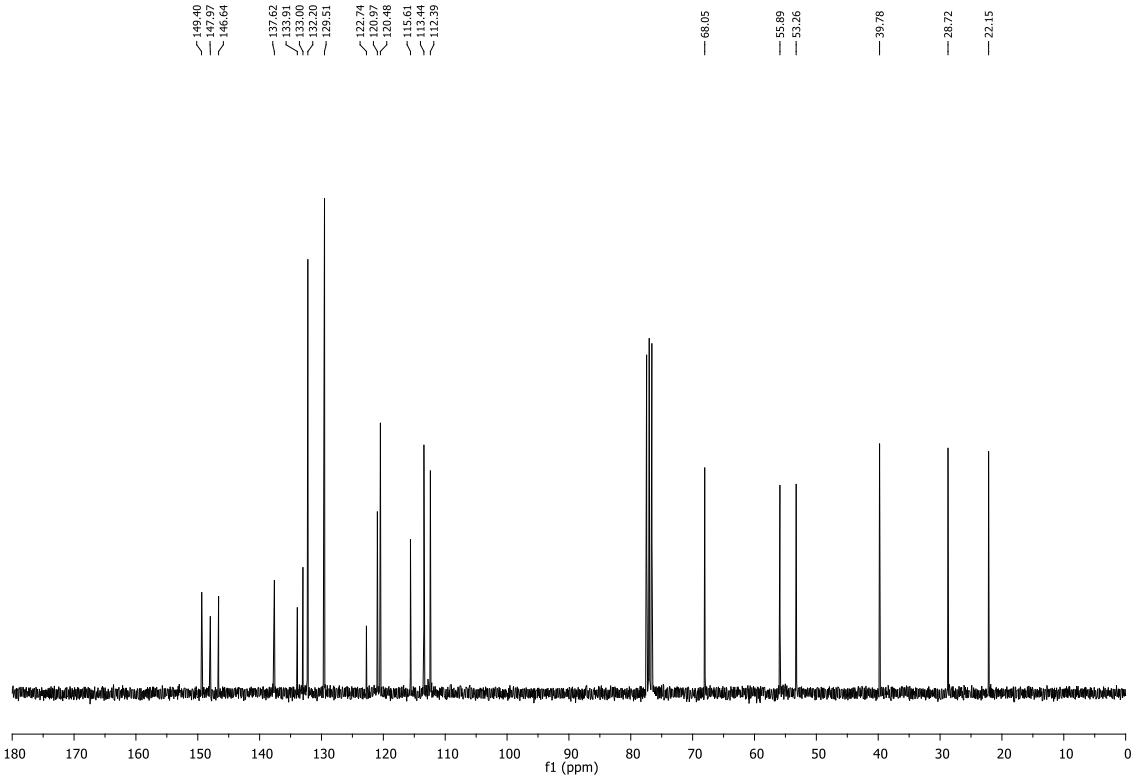


Fig. BB. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-bromobenzyl)-*1H*-1,2,3-triazole (**40**).

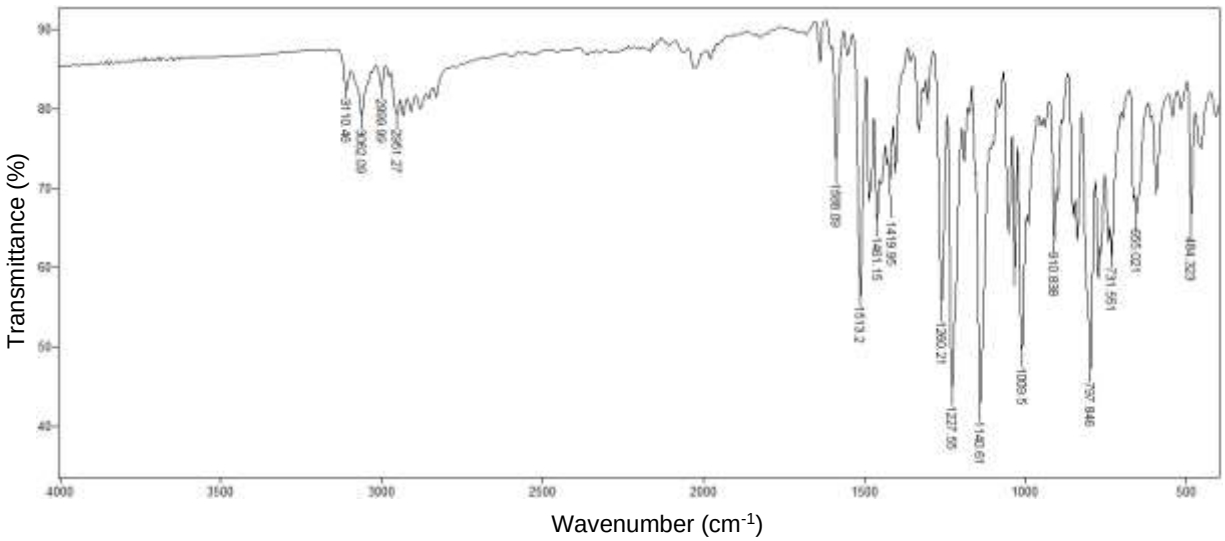


Fig. BC. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-iodobenzyl)-*1H*-1,2,3-triazole (**41**).

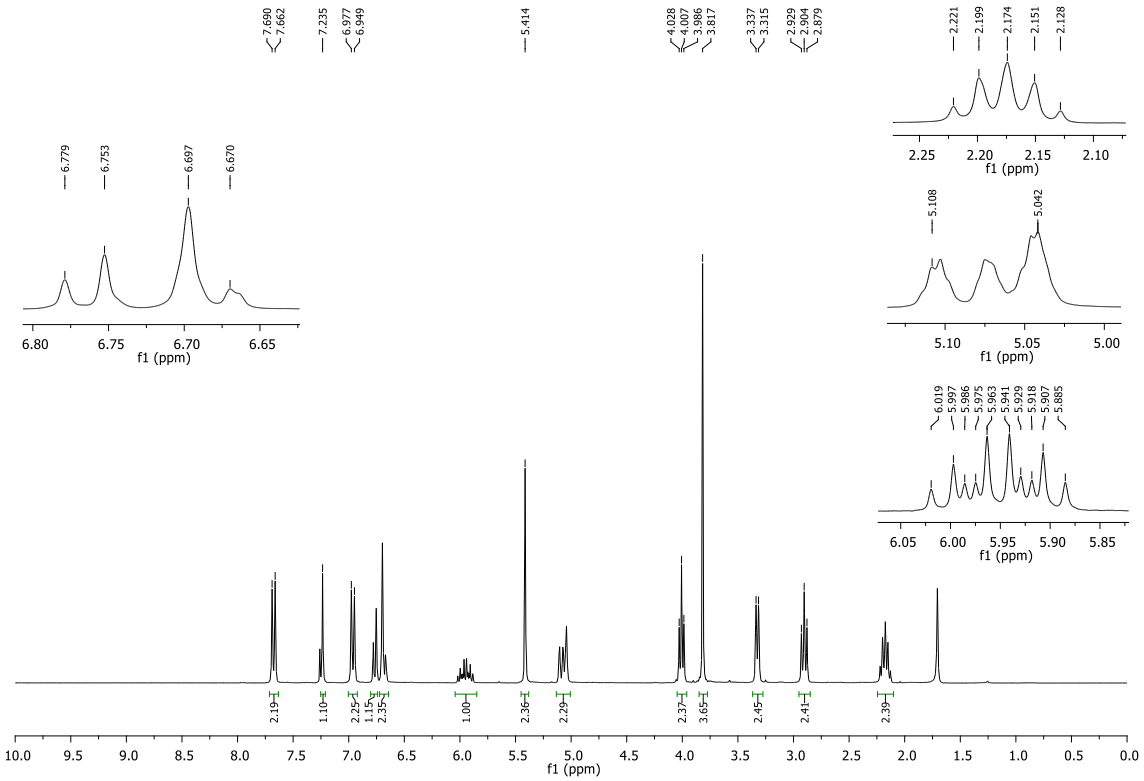


Fig. BD. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-iodobenzyl)-*1H*-1,2,3-triazole (**41**).

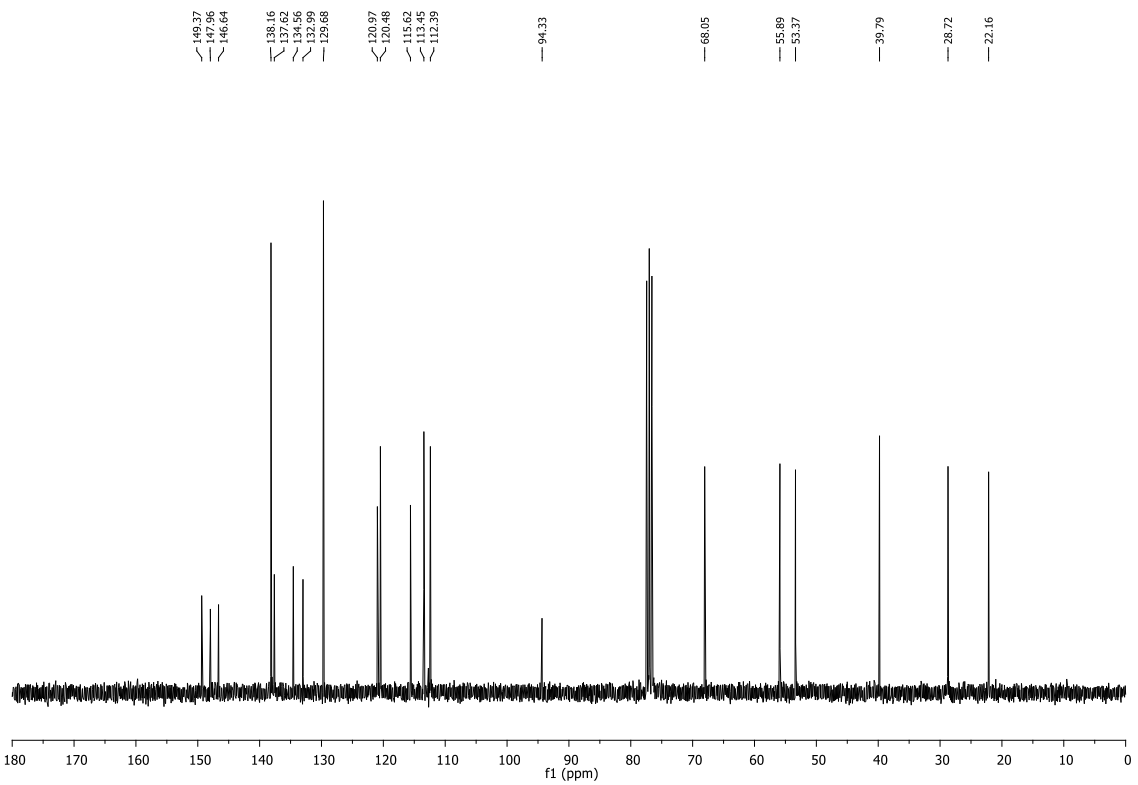


Fig. BE. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-iodobenzyl)-*1H*-1,2,3-triazole (**41**).

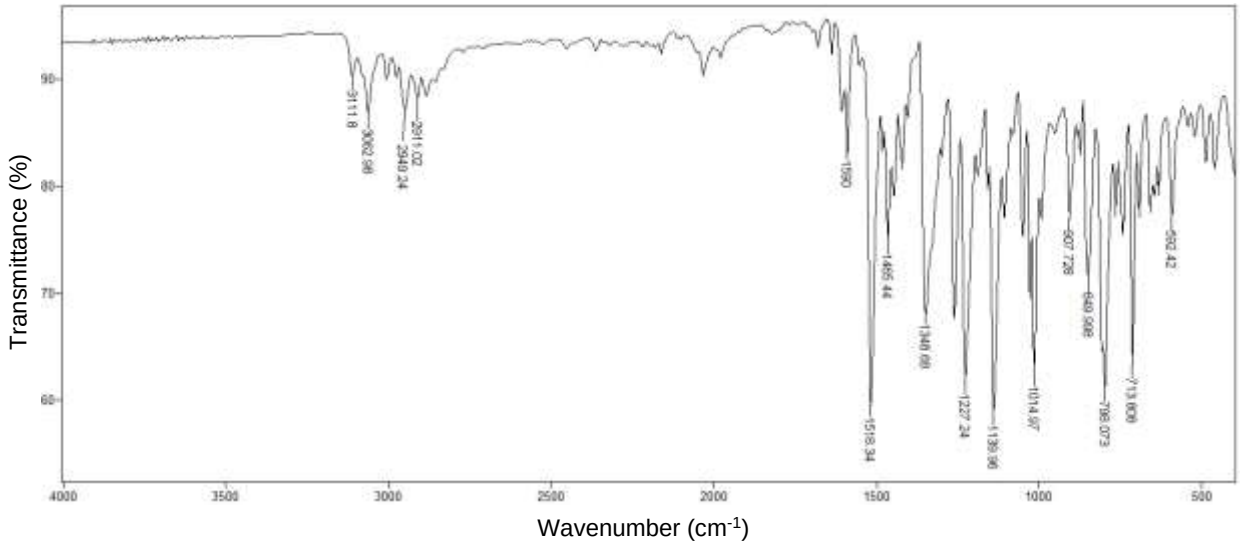


Fig. BF. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-nitrobenzyl)-*1H*-1,2,3-triazole (**42**).

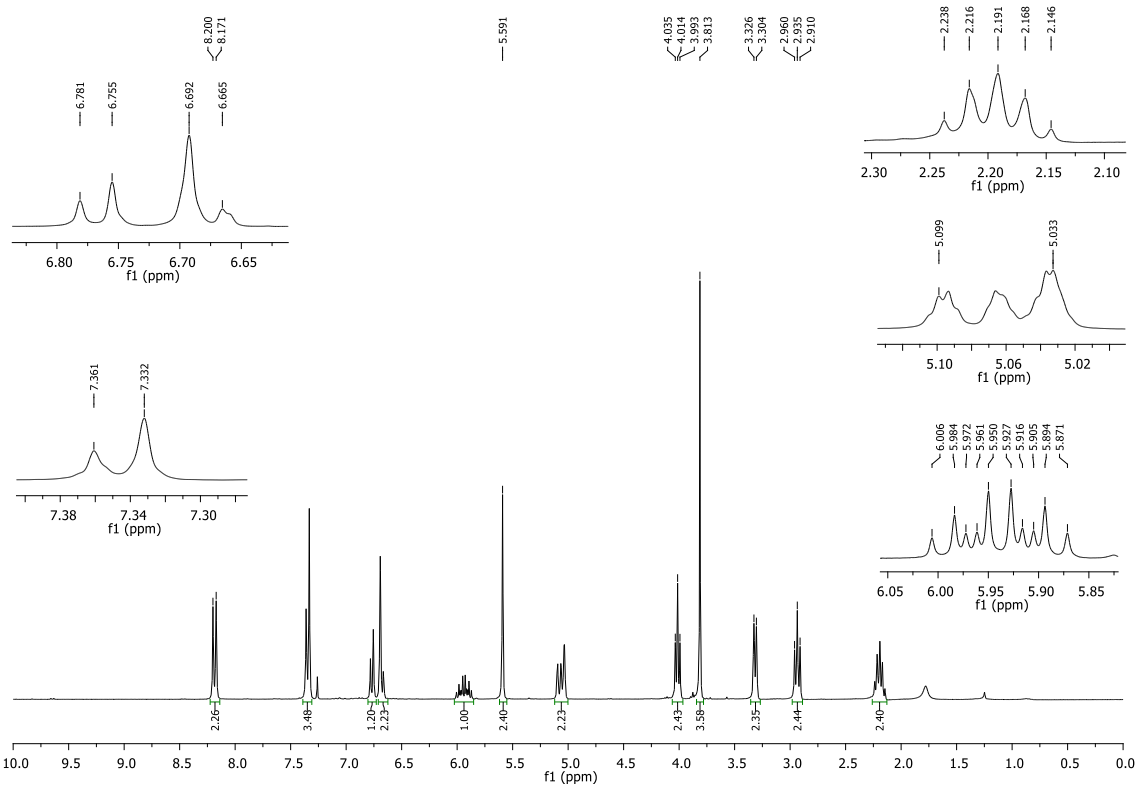


Fig. BG. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-nitrobenzyl)-*1H*-1,2,3-triazole (**42**).

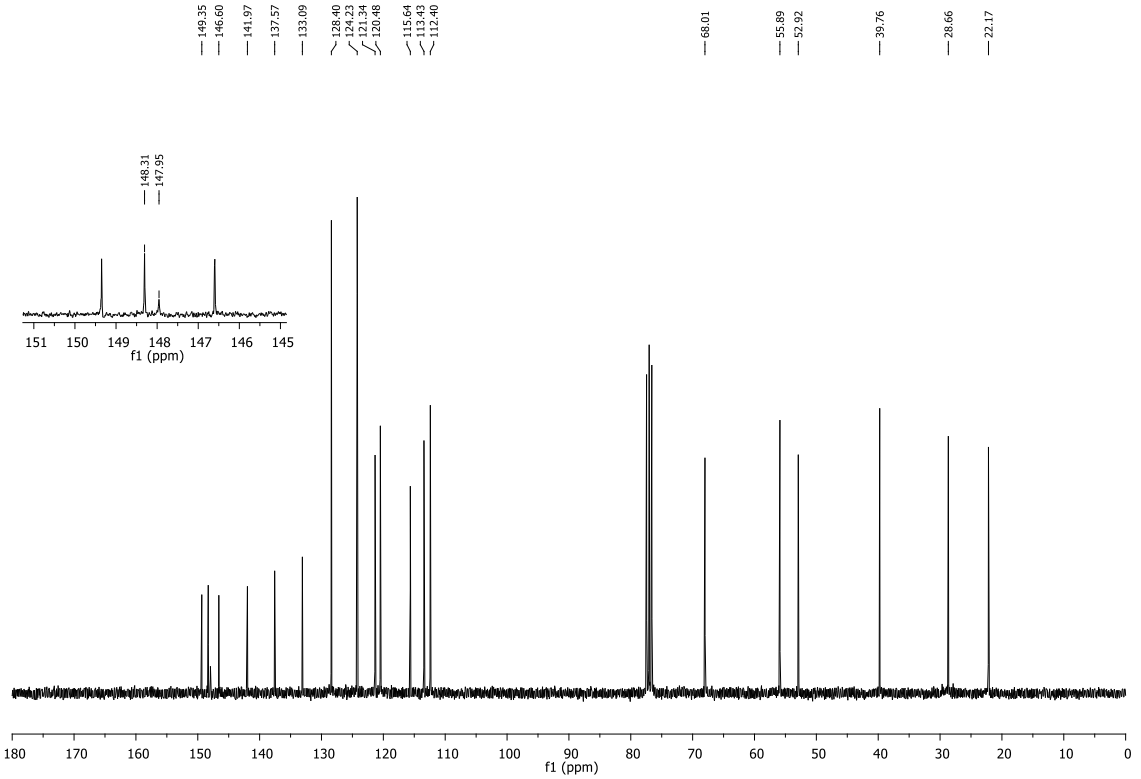


Fig. BH. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-nitrobenzyl)-*1H*-1,2,3-triazole (**42**).

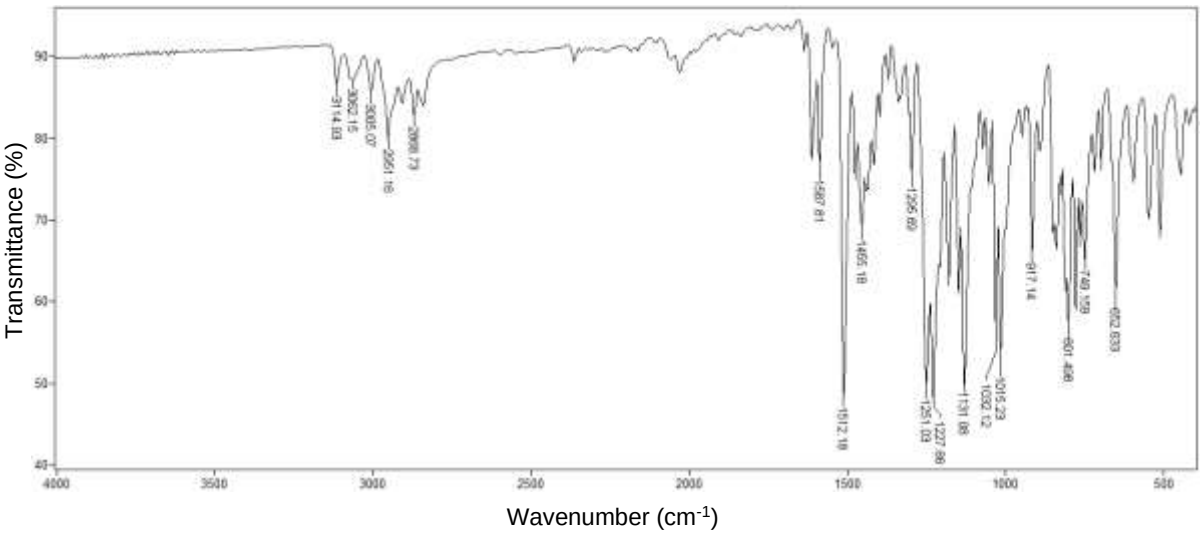


Fig. BI. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-methoxybenzyl)-*1H*-1,2,3-triazole (**43**).

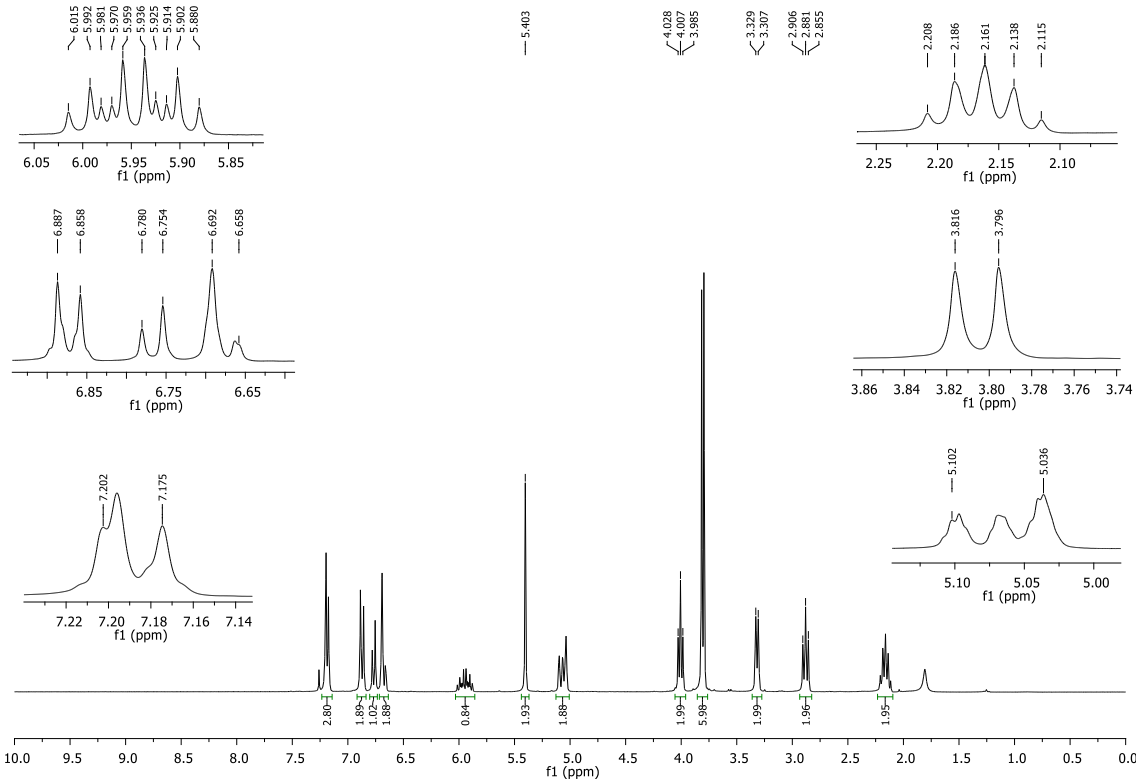


Fig. BJ. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-methoxybenzyl)-*1H*-1,2,3-triazole (**43**).

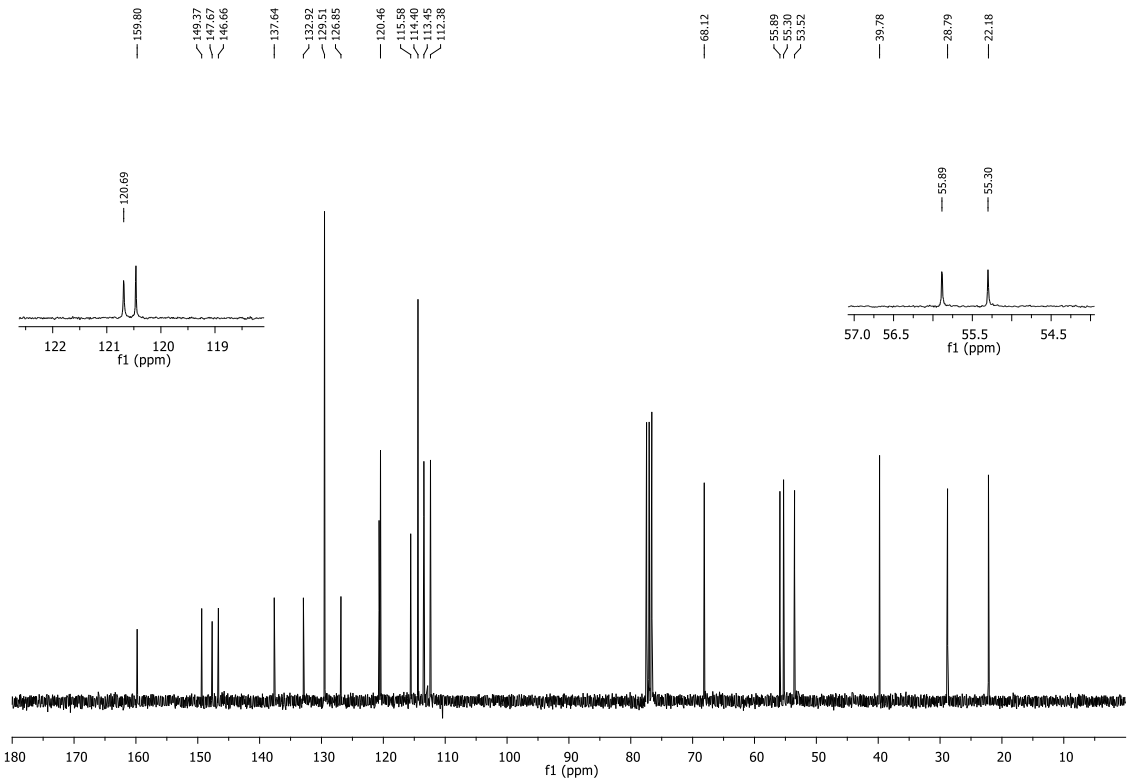


Fig. BK. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-methoxybenzyl)-*1H*-1,2,3-triazole (**43**).

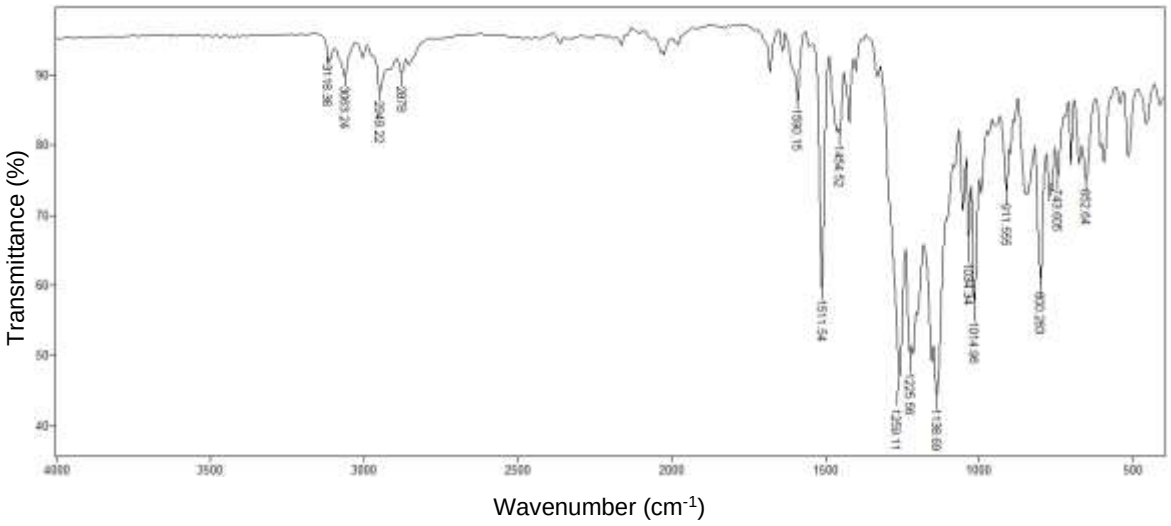


Fig. BL. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-(trifluoromethoxy)benzyl)-*1H*-1,2,3-triazole (**44**).

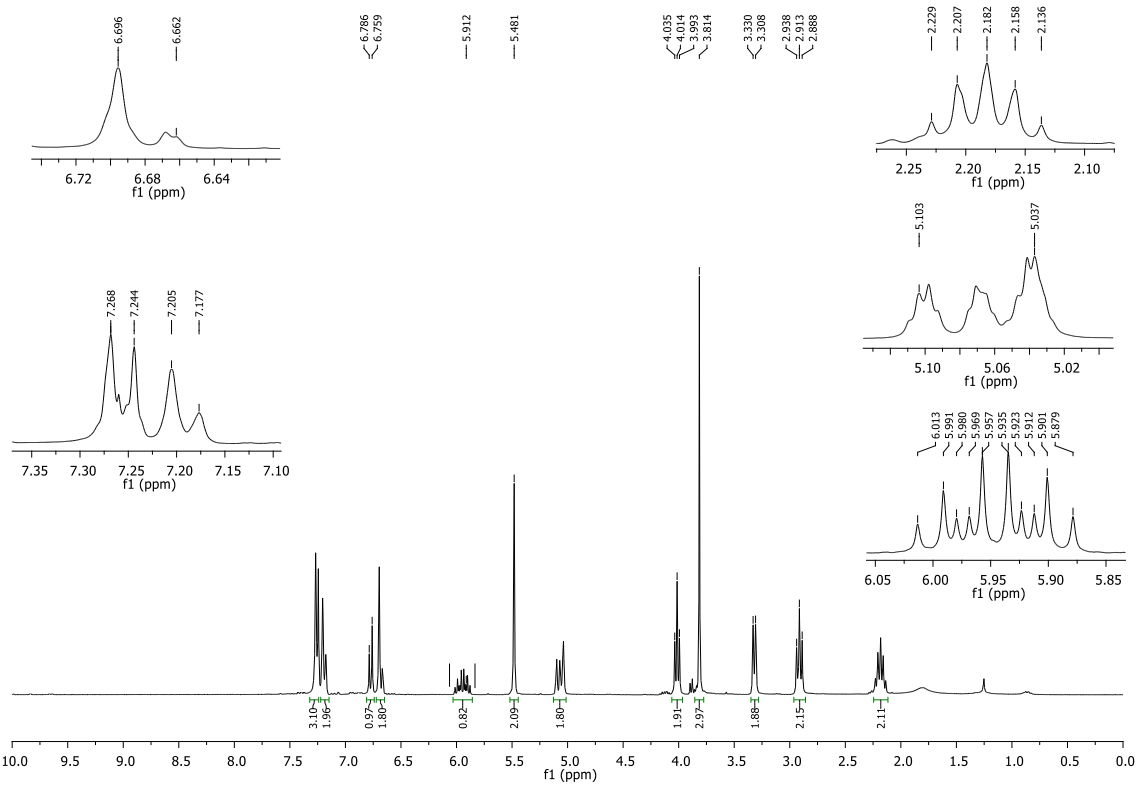


Fig. BM. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-(trifluoromethoxy)benzyl)-*1H*-1,2,3-triazole (**44**).

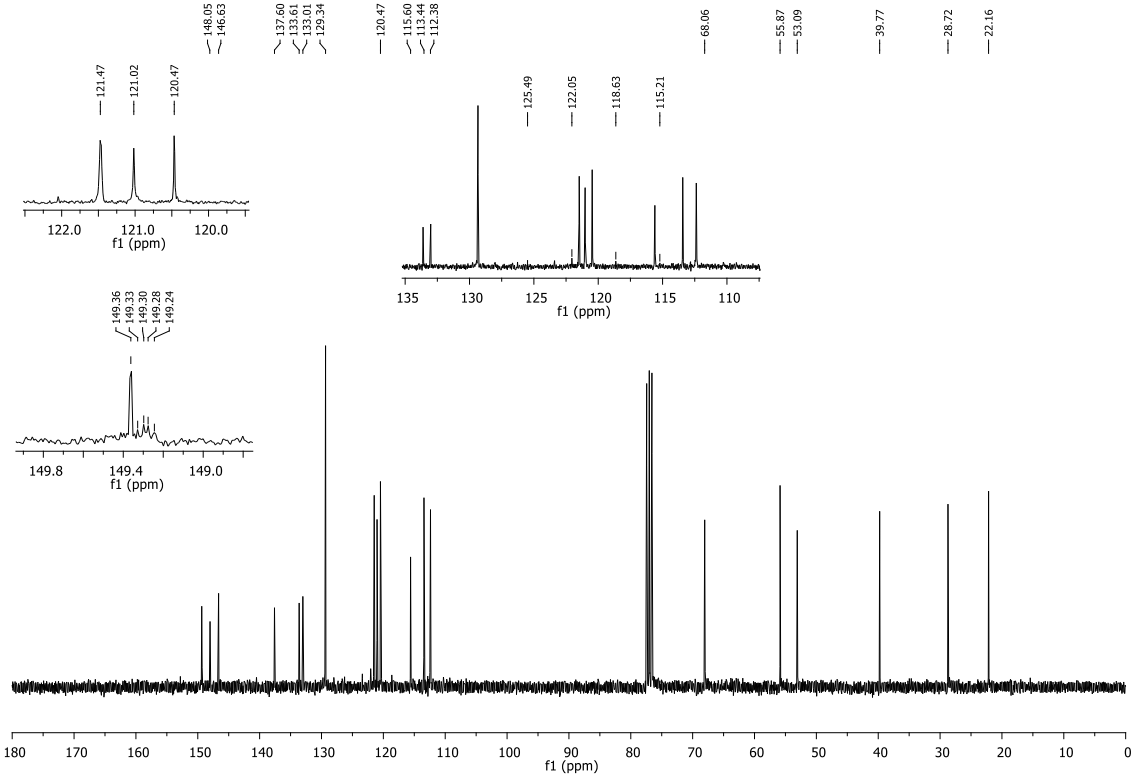


Fig. BN. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-(trifluoromethoxy)benzyl)-*1H*-1,2,3-triazole (**44**).

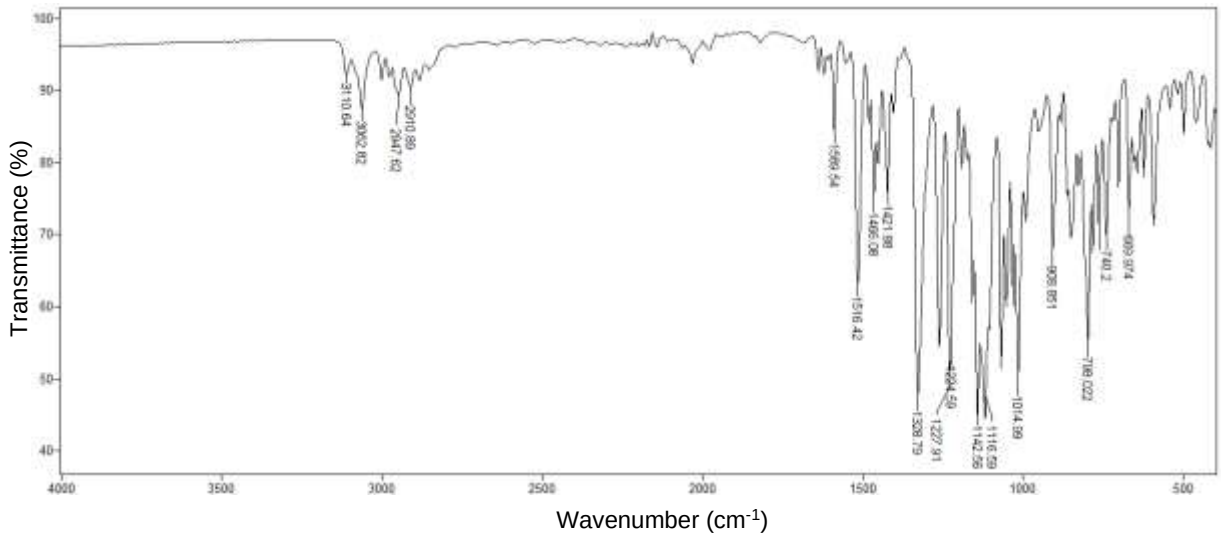


Fig. BO. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-(trifluoromethyl)benzyl)-*1H*-1,2,3-triazole (**45**).

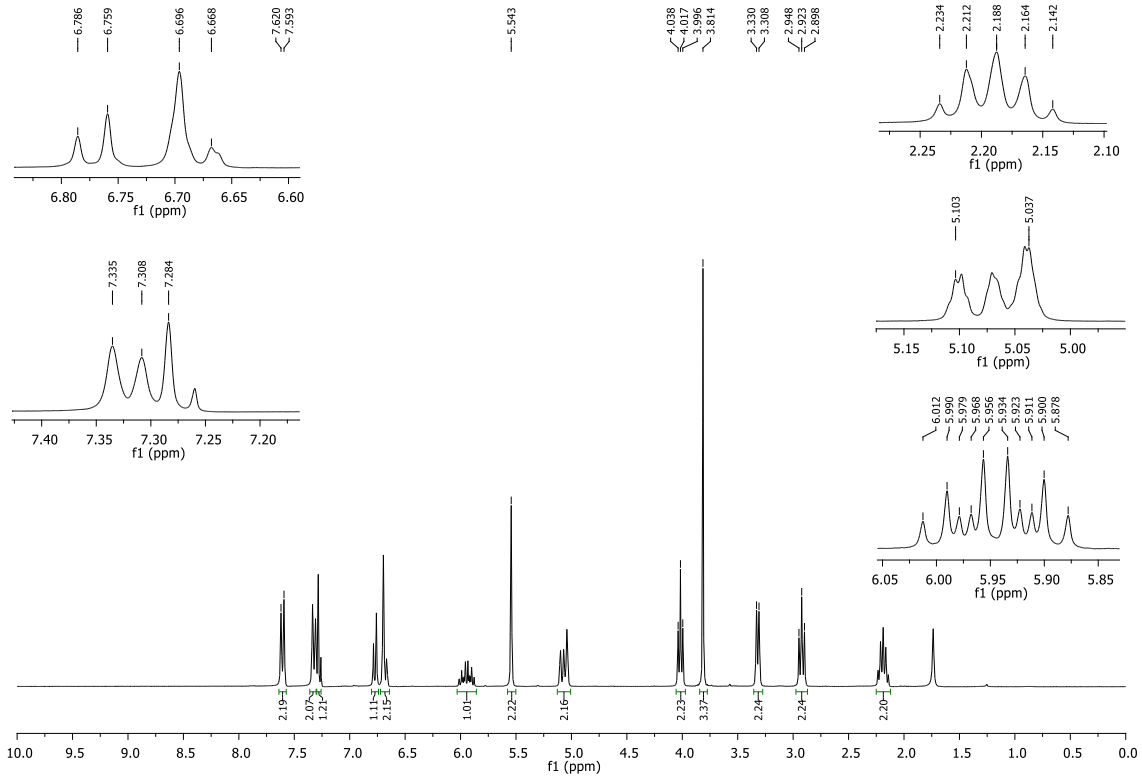


Fig. BP. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-(trifluoromethyl)benzyl)-*1H*-1,2,3-triazole (**45**).

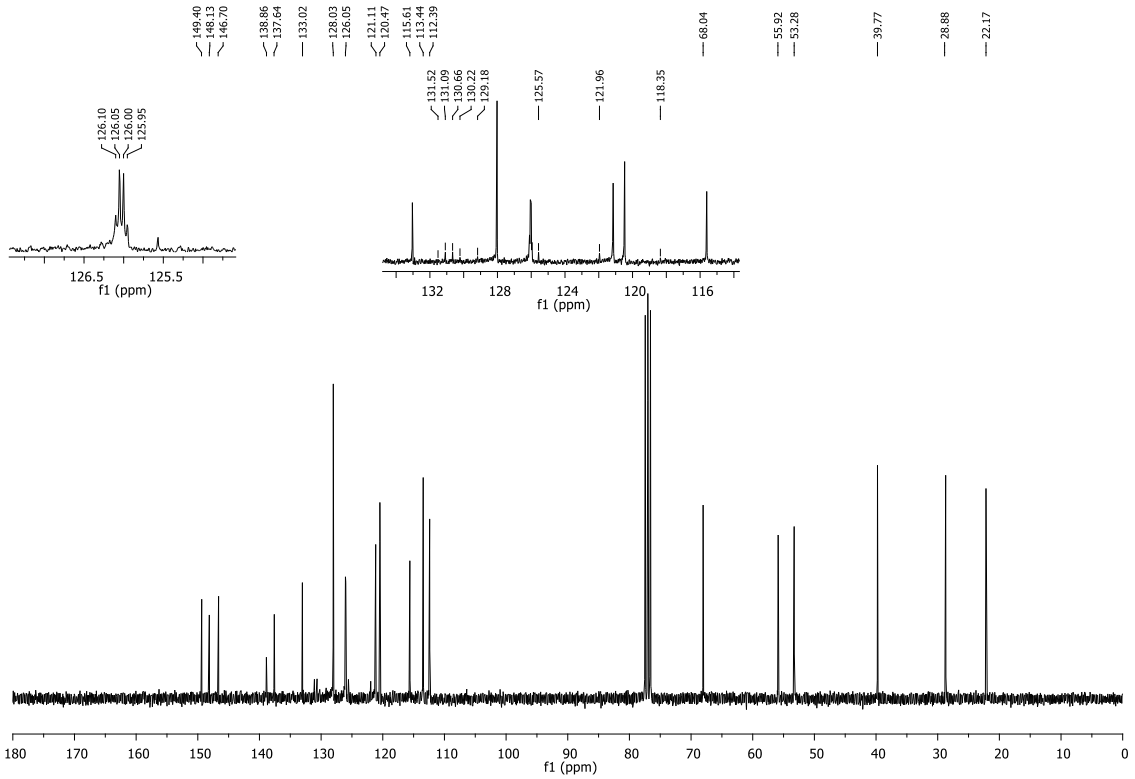


Fig. BQ. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-(trifluoromethyl)benzyl)-*1H*-1,2,3-triazole (**45**).

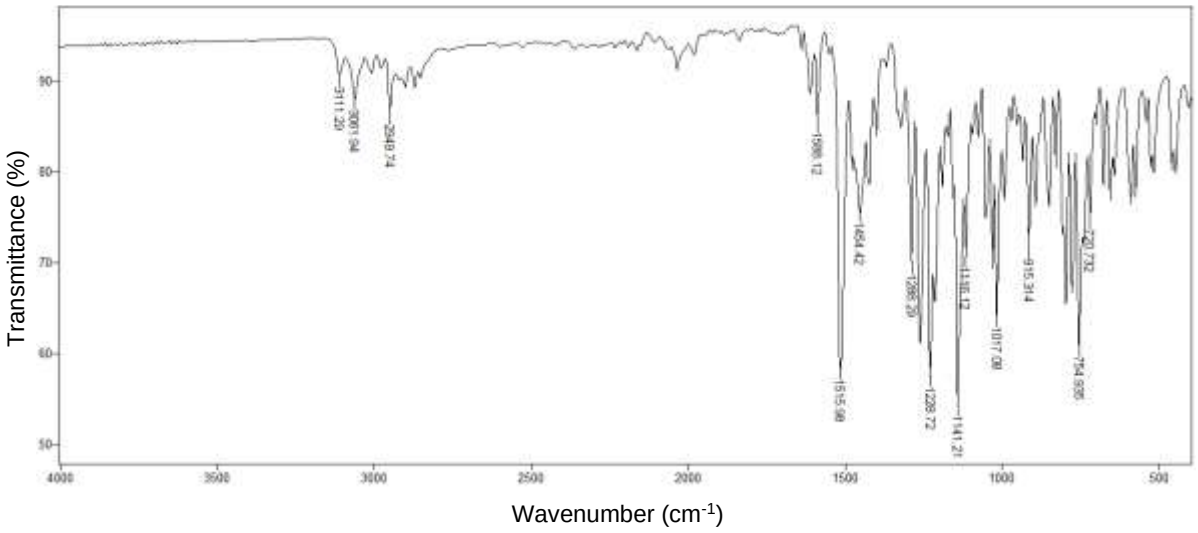


Fig. BR. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(3,4-difluorobenzyl)-*1H*-1,2,3-triazole (**46**).

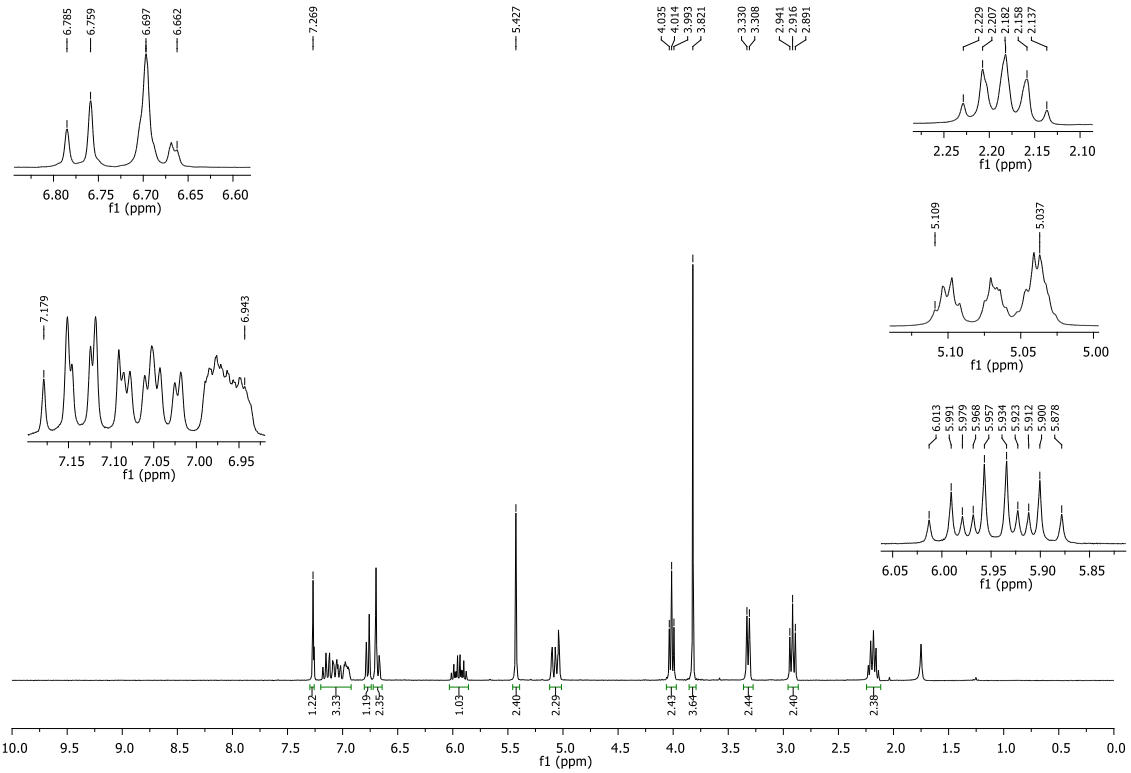


Fig. BS. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(3,4-difluorobenzyl)-*1H*-1,2,3-triazole (**46**).

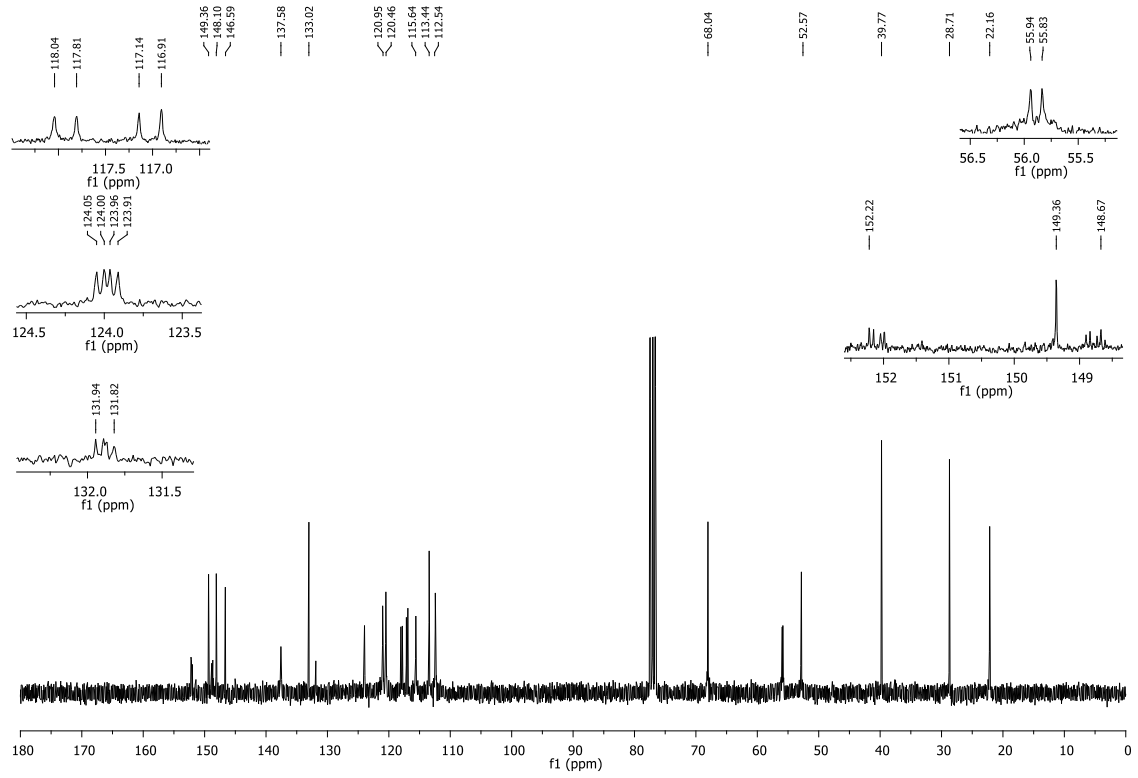


Fig. BT. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(3,4-difluorobenzyl)-*1H*-1,2,3-triazole (**46**).

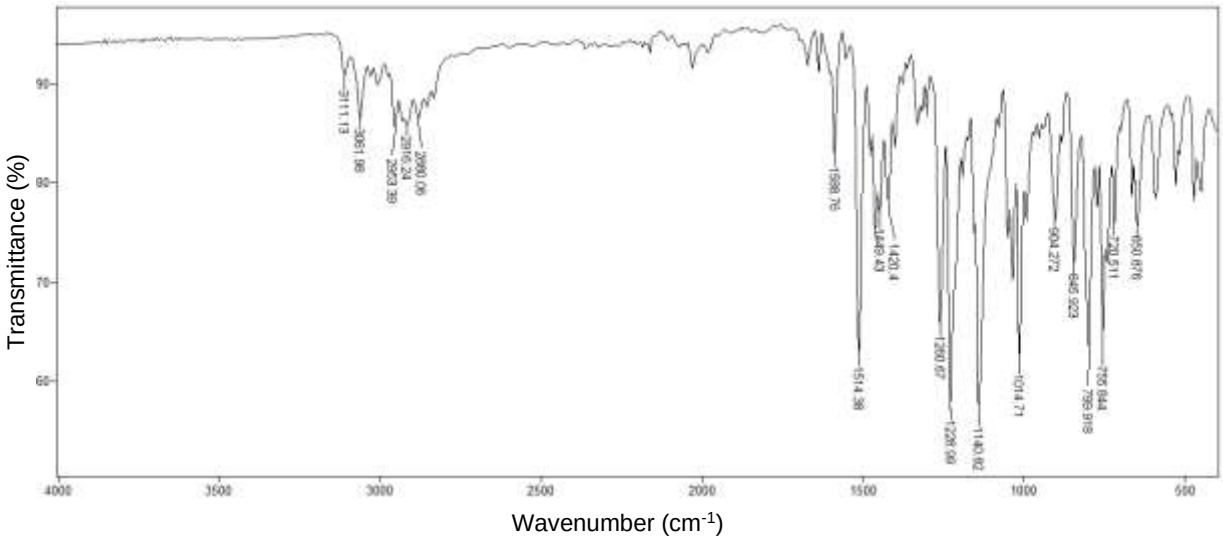


Fig. BU. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-methylbenzyl)-*1H*-1,2,3-triazole (**47**).

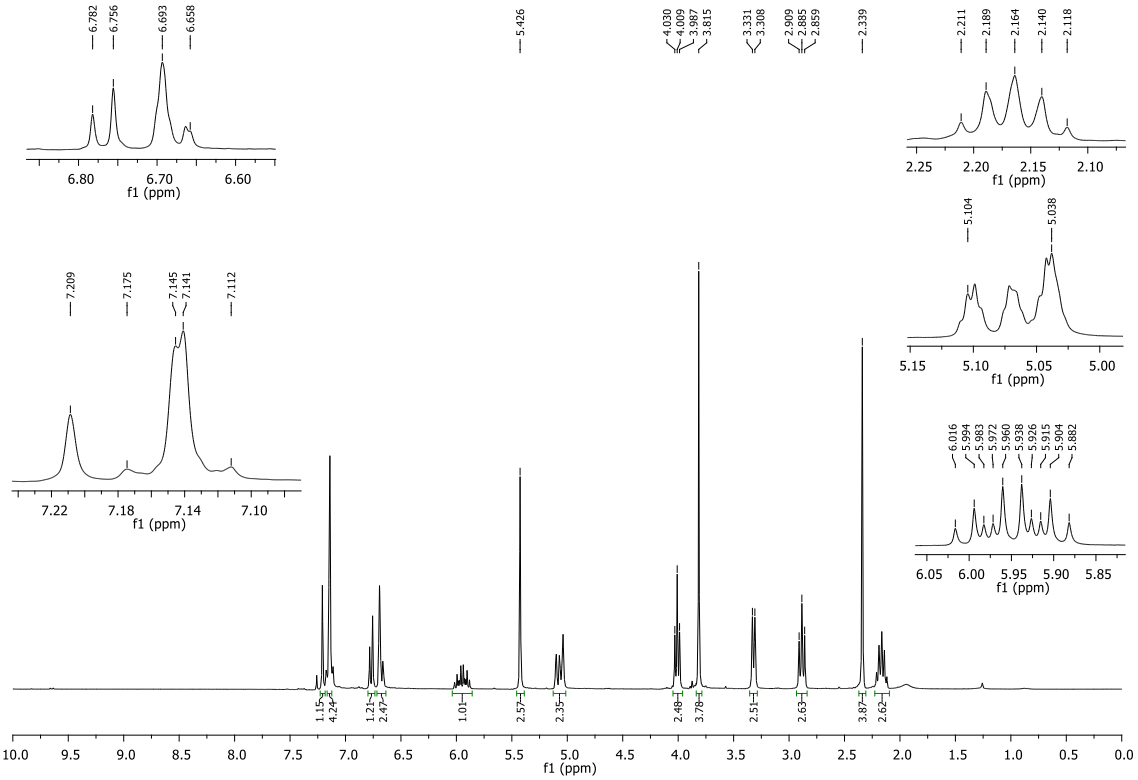


Fig. BV. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-methylbenzyl)-*1H*-1,2,3-triazole (**47**).

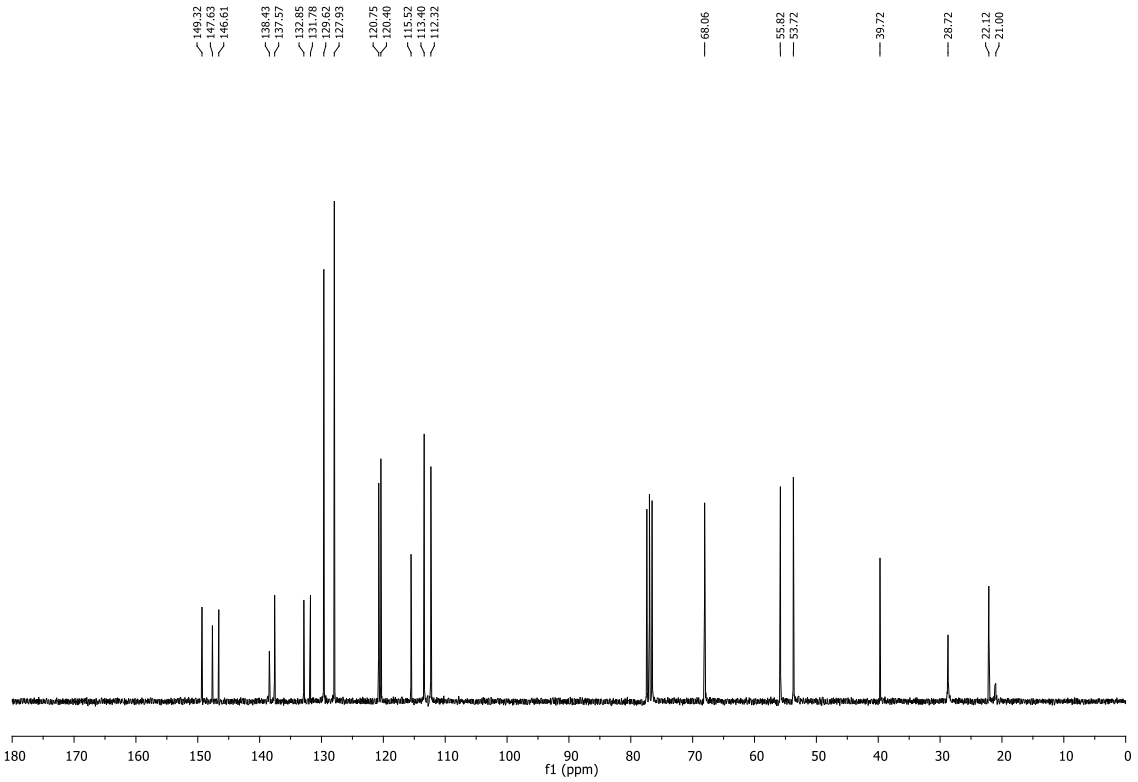


Fig. BX. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(4-methylbenzyl)-*1H*-1,2,3-triazole (**47**).

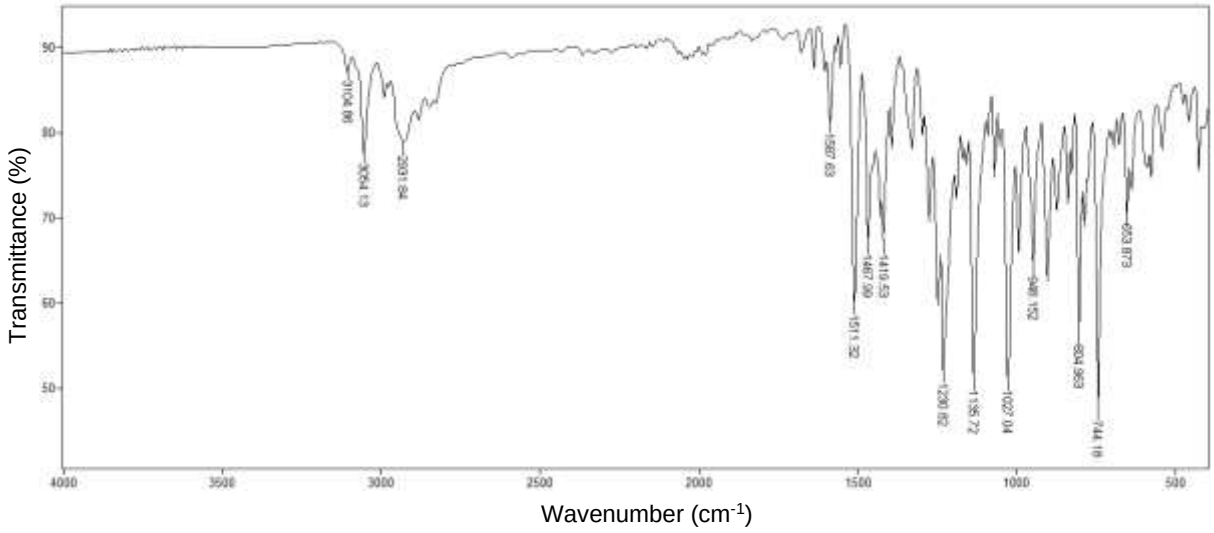


Fig. BW. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(2-bromobenzyl)-*1H*-1,2,3-triazole (**48**).

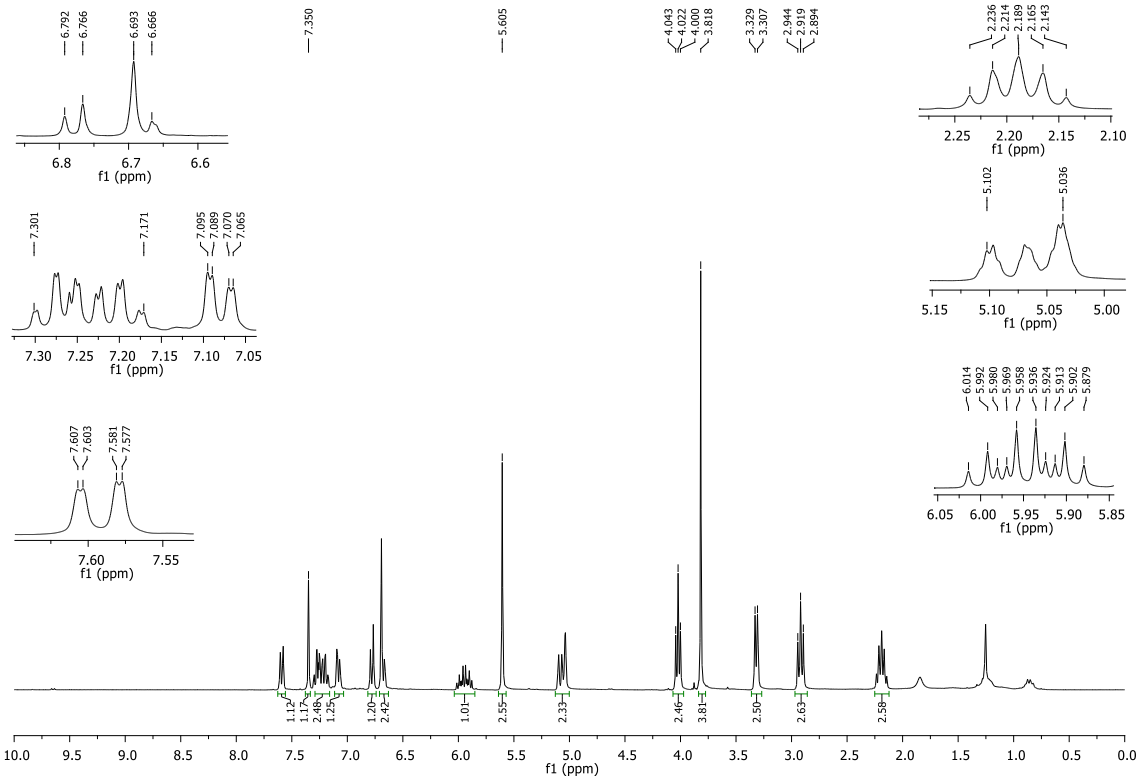


Fig. BY. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(2-bromobenzyl)-*1H*-1,2,3-triazole (**48**).

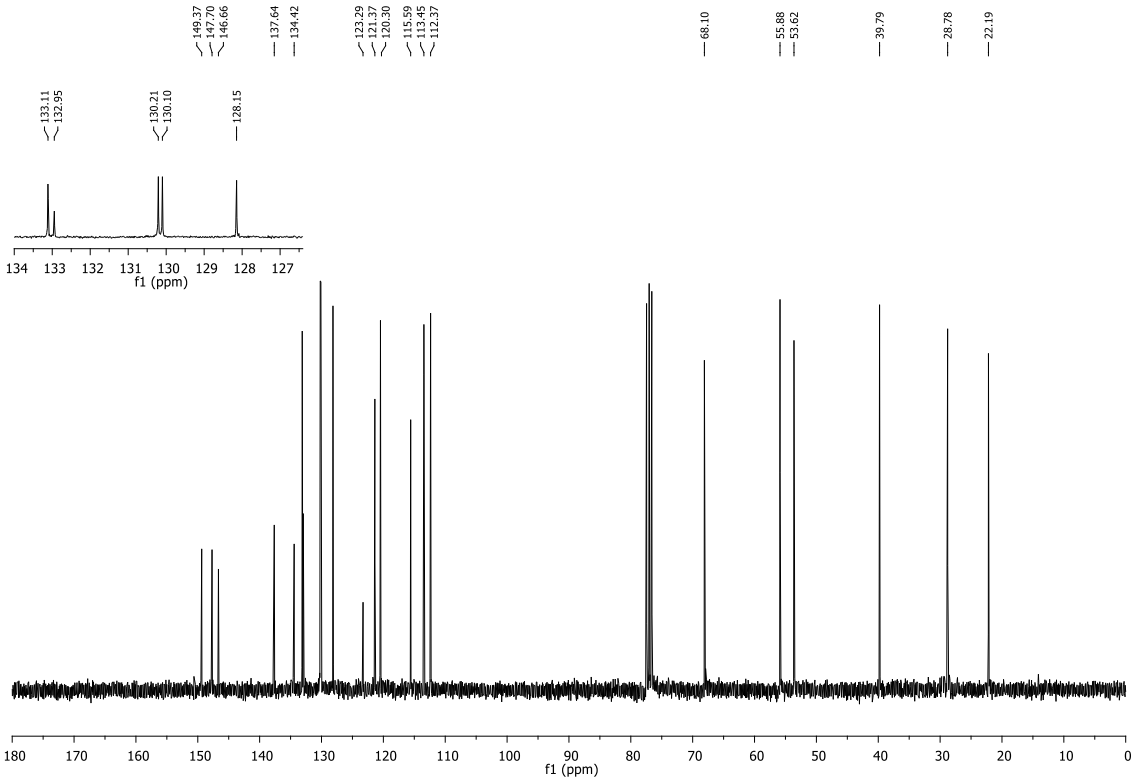


Fig. BZ. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(2-bromobenzyl)-*1H*-1,2,3-triazole (**48**).

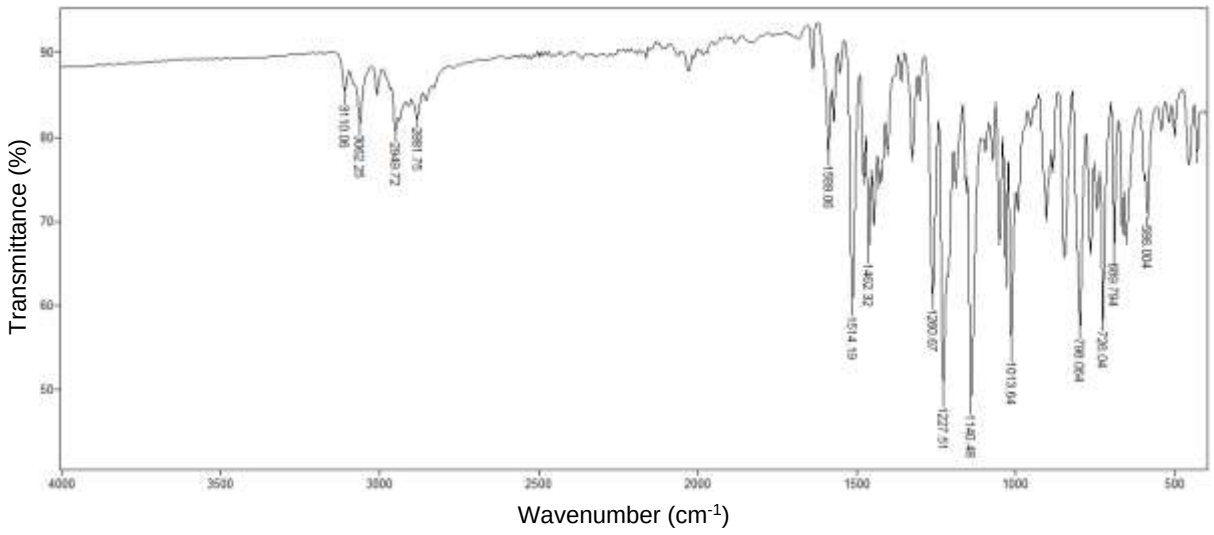


Fig. CA. IR spectrum (ATR) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(3-bromobenzyl)-*1H*-1,2,3-triazole (**49**).

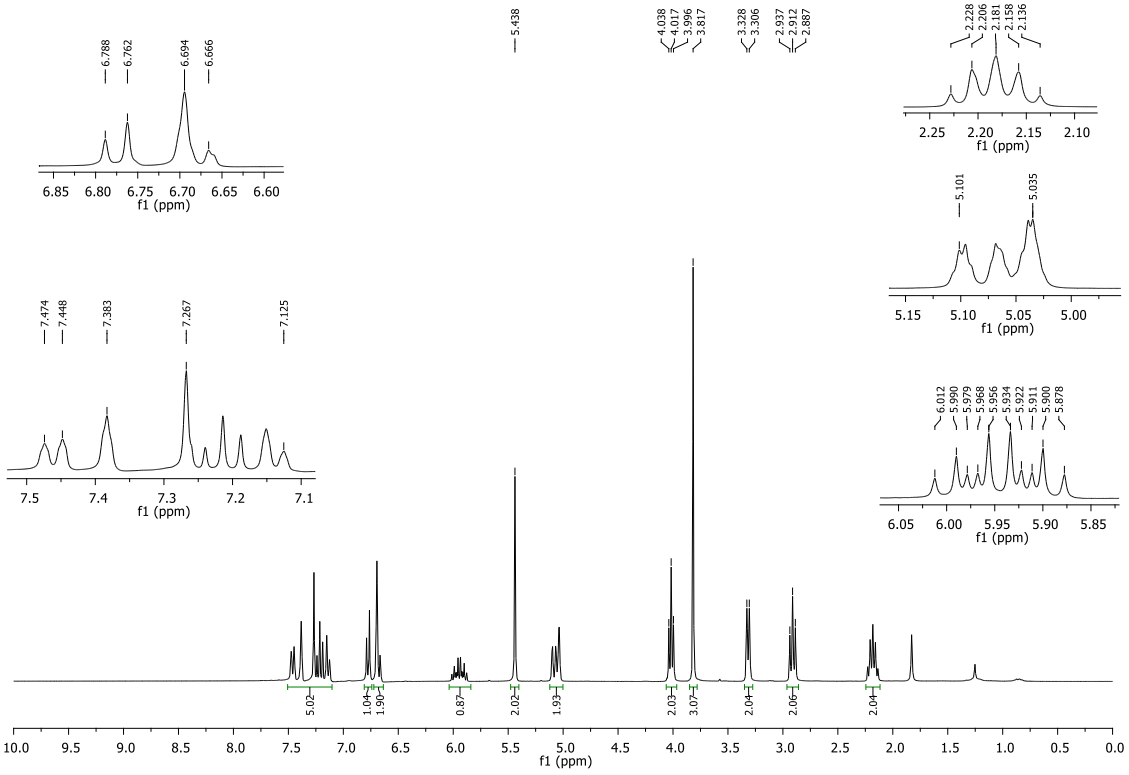


Fig. CB. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(3-bromobenzyl)-*1H*-1,2,3-triazole (**49**).

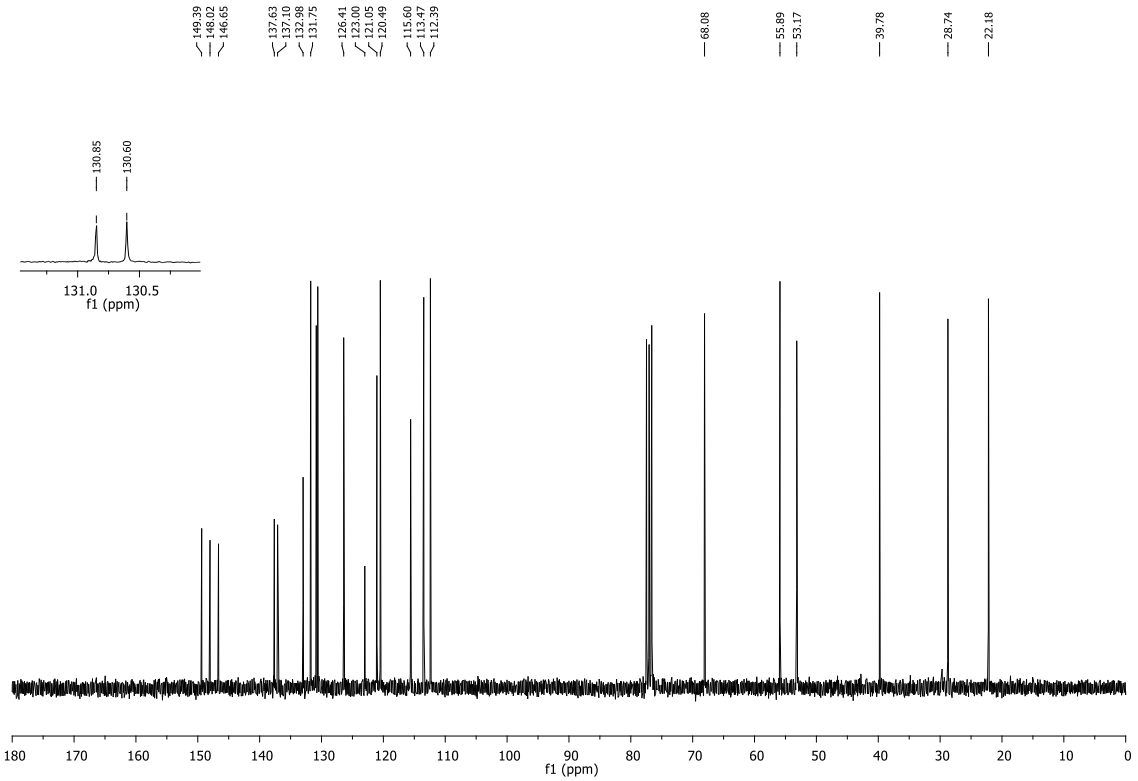


Fig. CC. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of of 4-(3-(4-allyl-2-methoxyphenoxy)propyl)-1-(3-bromobenzyl)-*1H*-1,2,3-triazole (**49**).

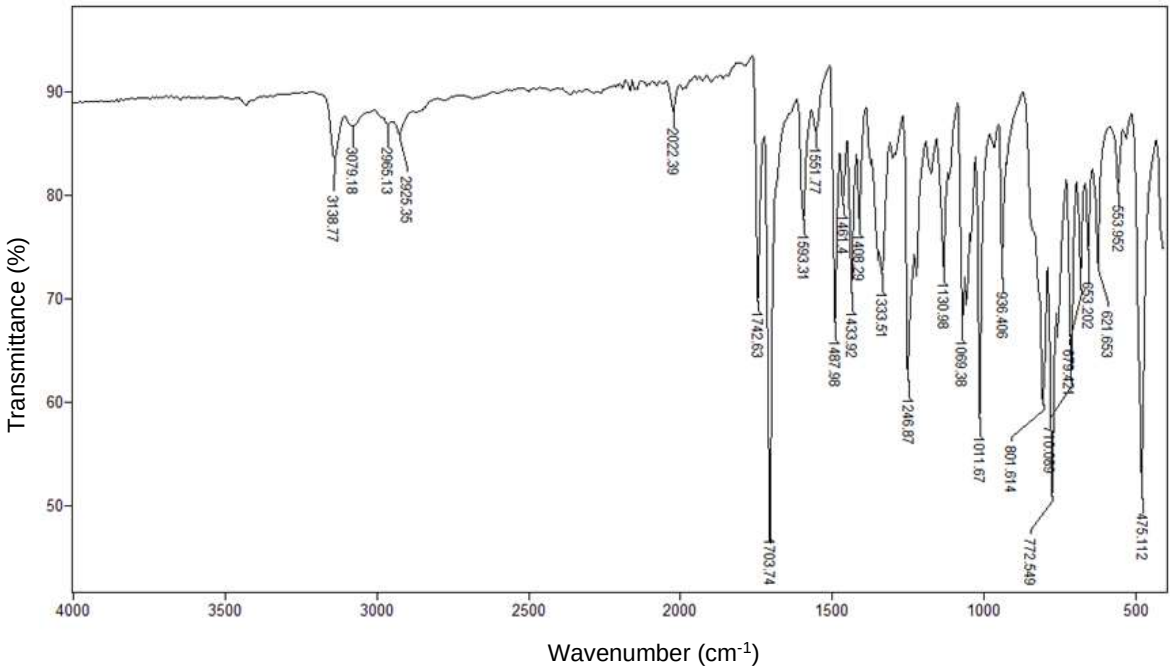


Fig. CD. IR spectrum (ATR) of 2,2-*bis*((1-(4-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**51**).

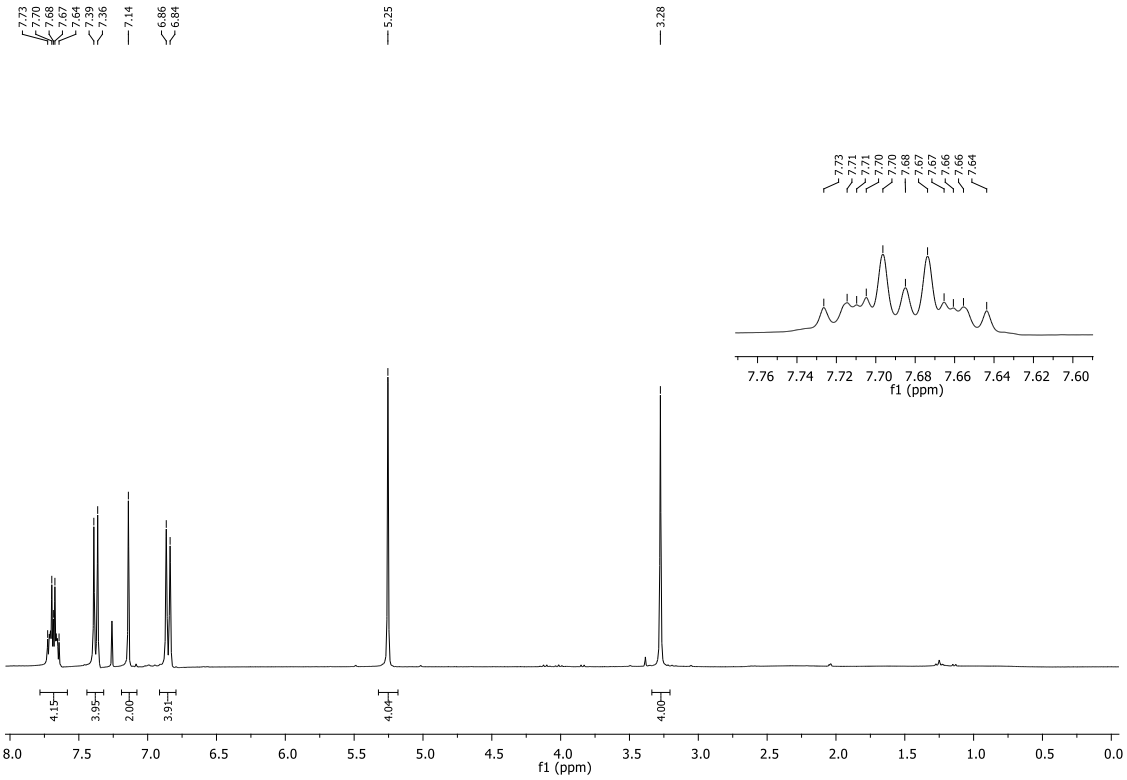


Fig. CE. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**51**).

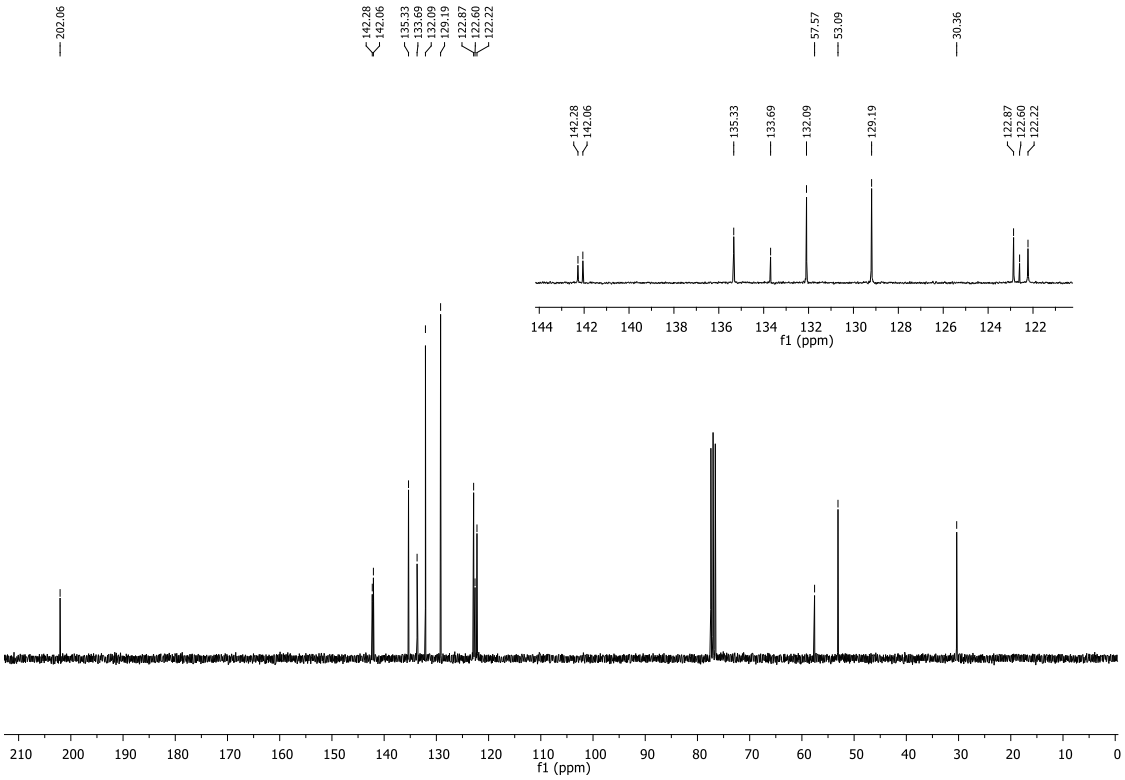


Fig. CF. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**51**).

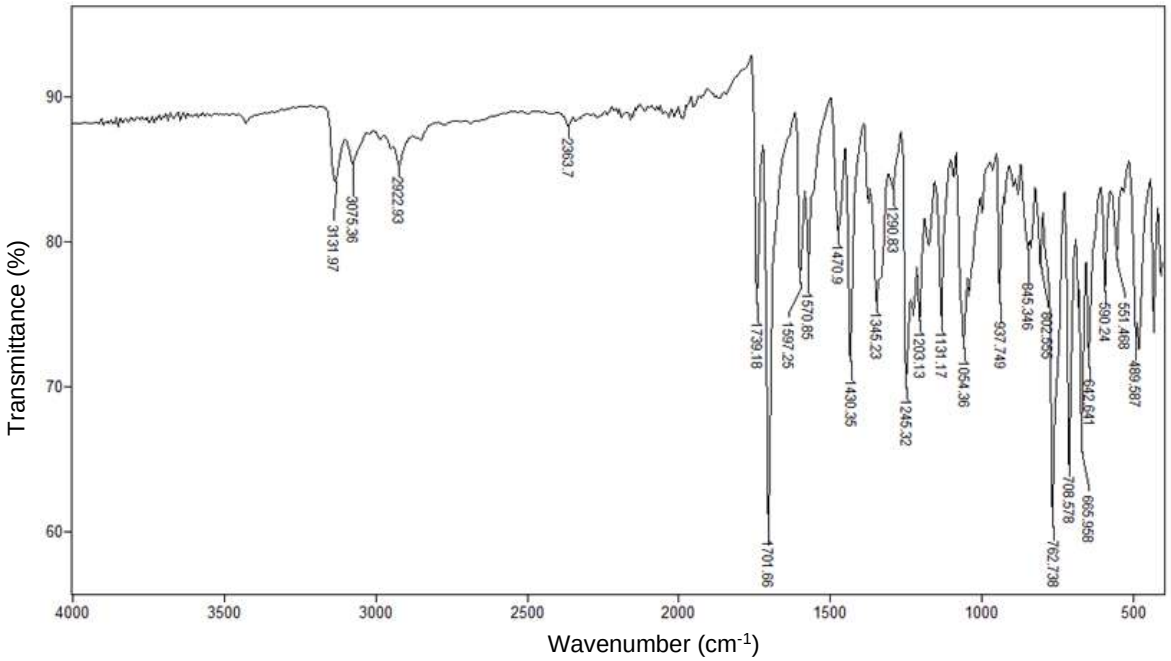


Fig. CG. IR spectrum (ATR) of 2,2-*bis*((1-(3-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**52**).

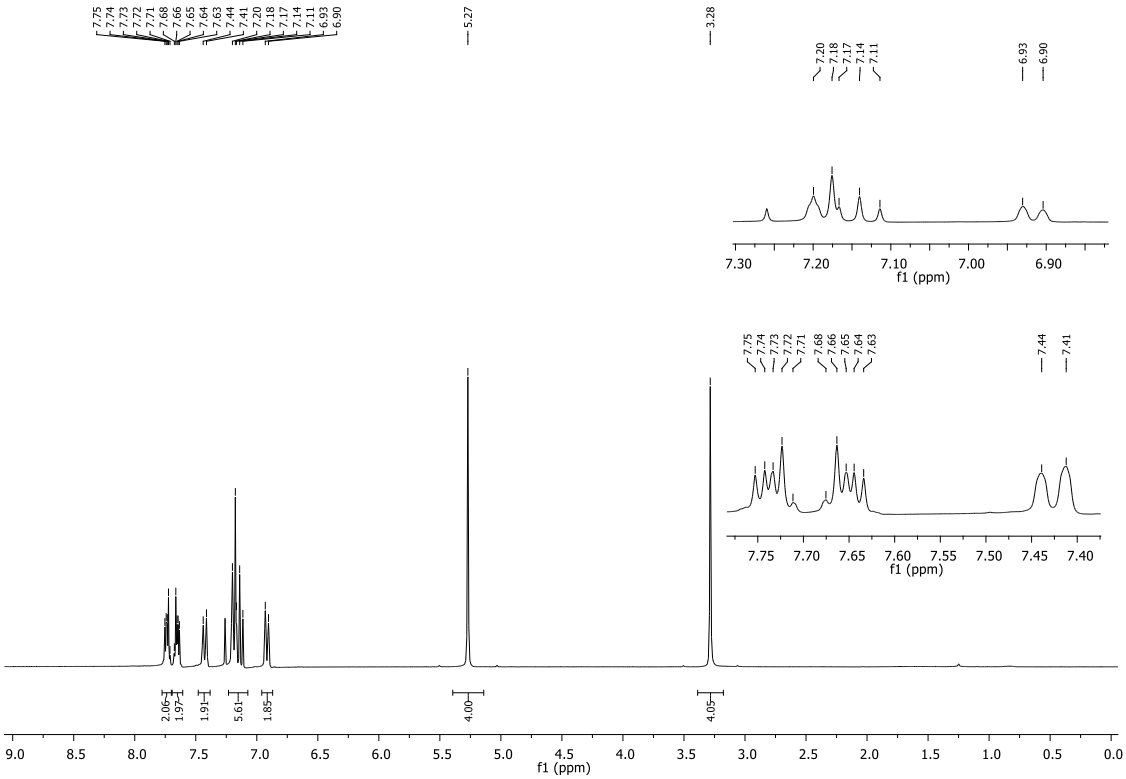


Fig. CH. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(3-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**52**).

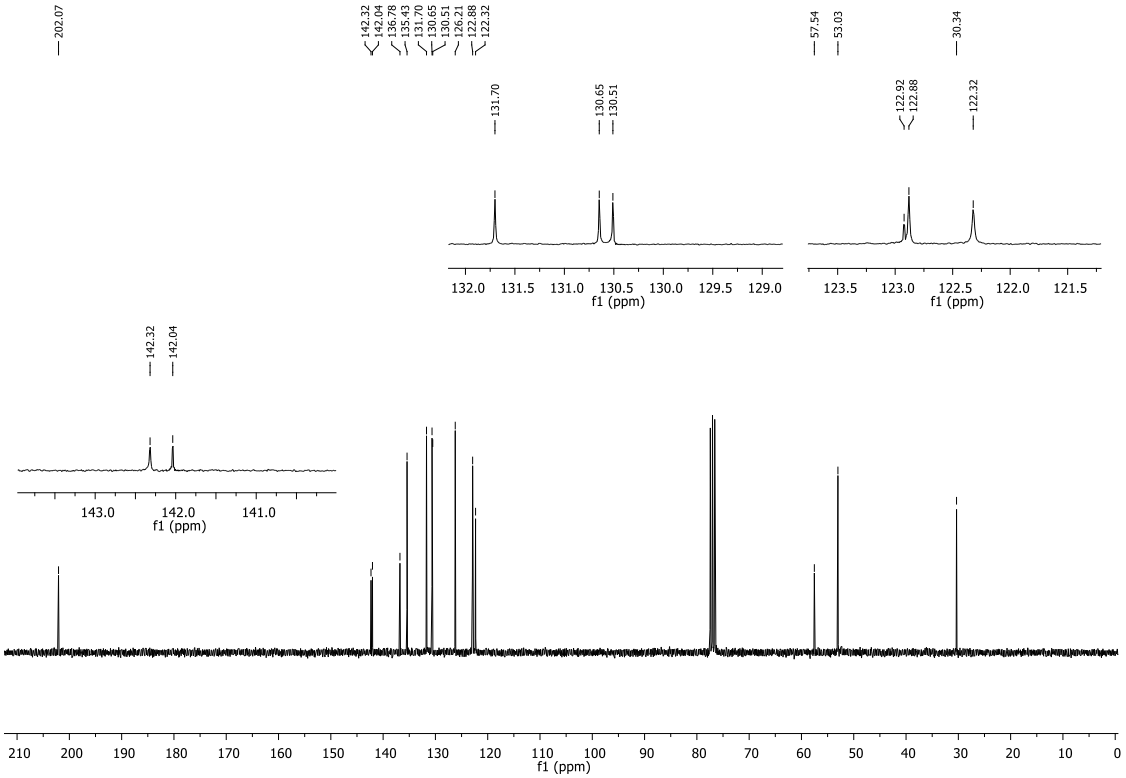


Fig. CI. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(3-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**52**).

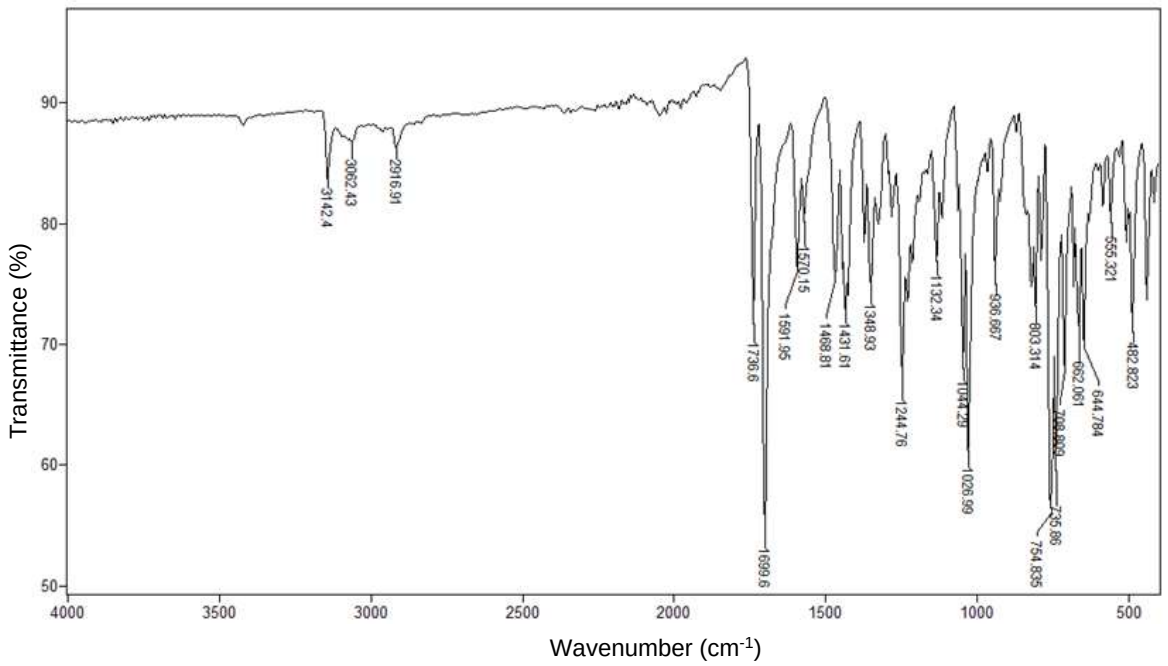


Fig. CJ. IR spectrum (ATR) of 2,2-*bis*((1-(2-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**53**).

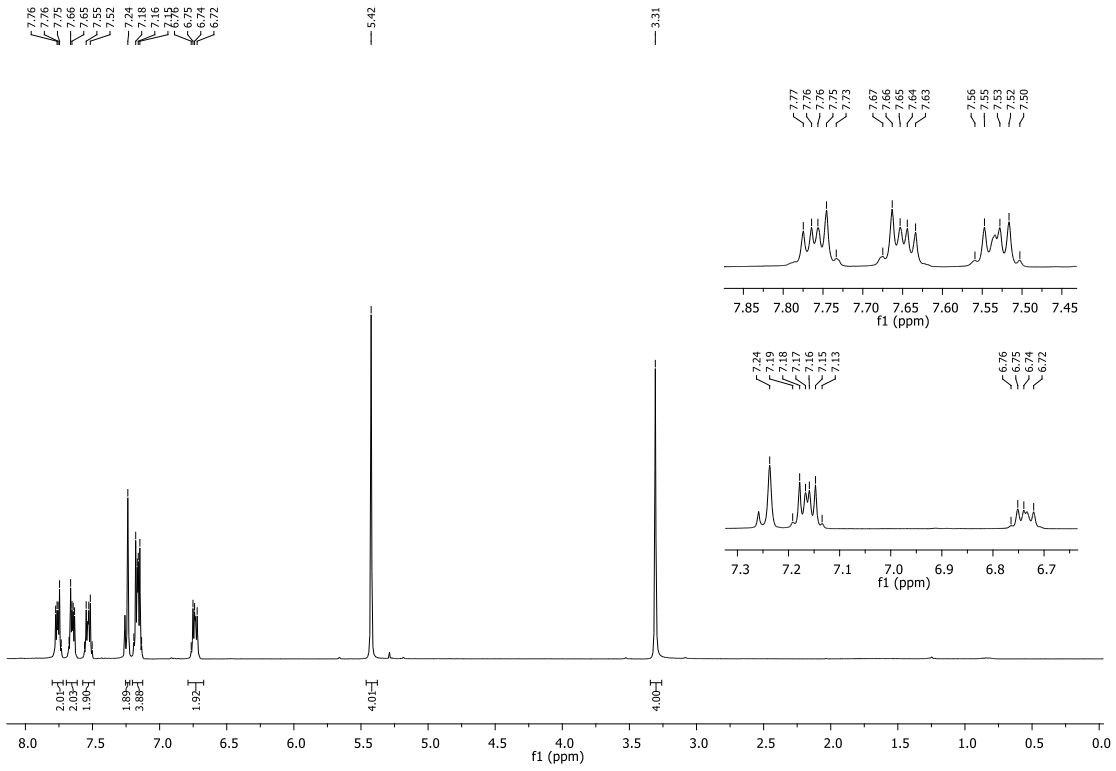


Fig. CK. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(2-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**53**).

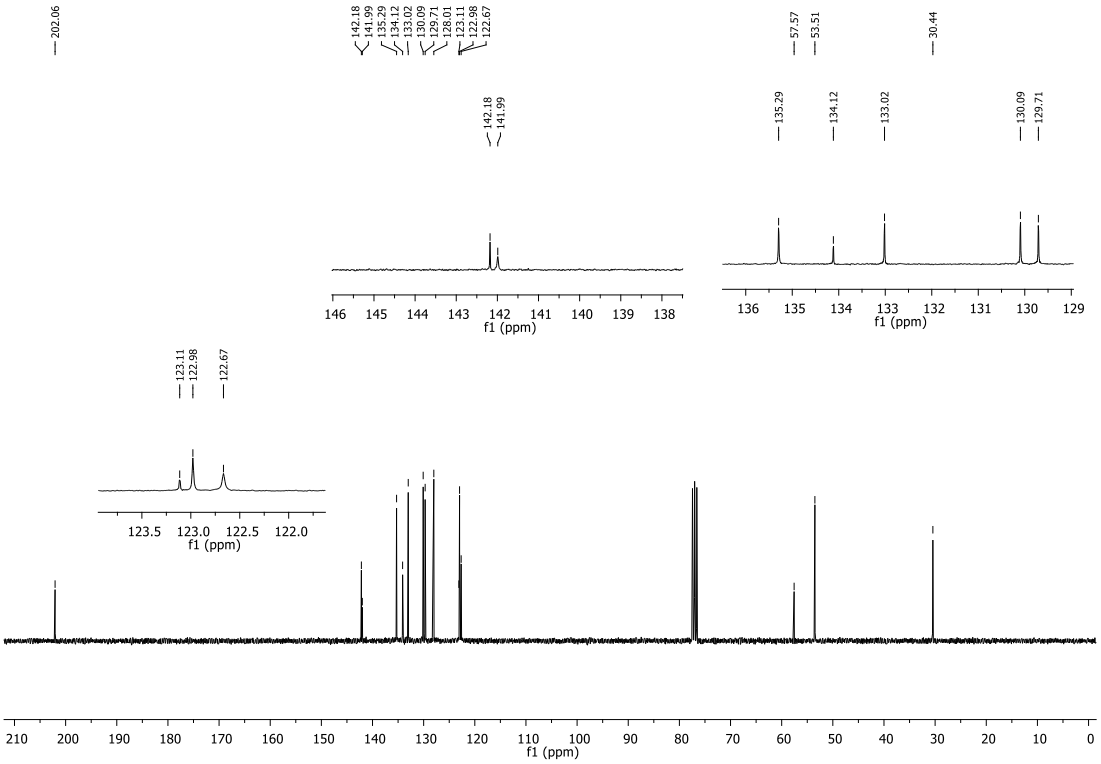


Fig. CL. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(2-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**53**).

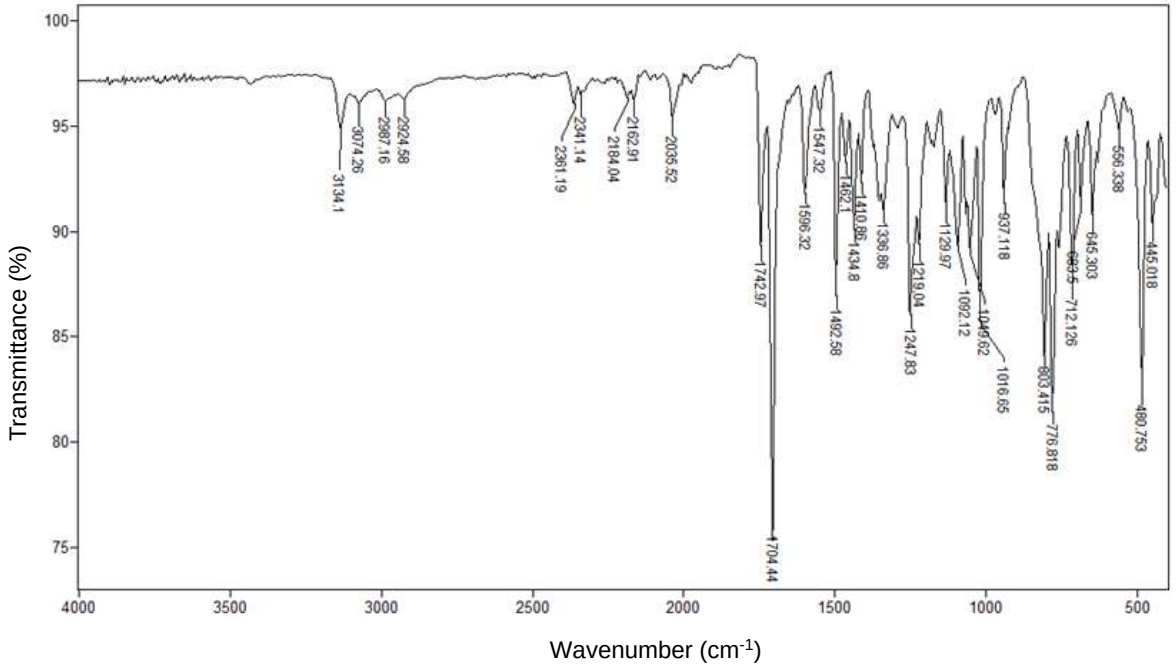


Fig. CM. IR spectrum (ATR) of 2,2-*bis*((1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**54**).

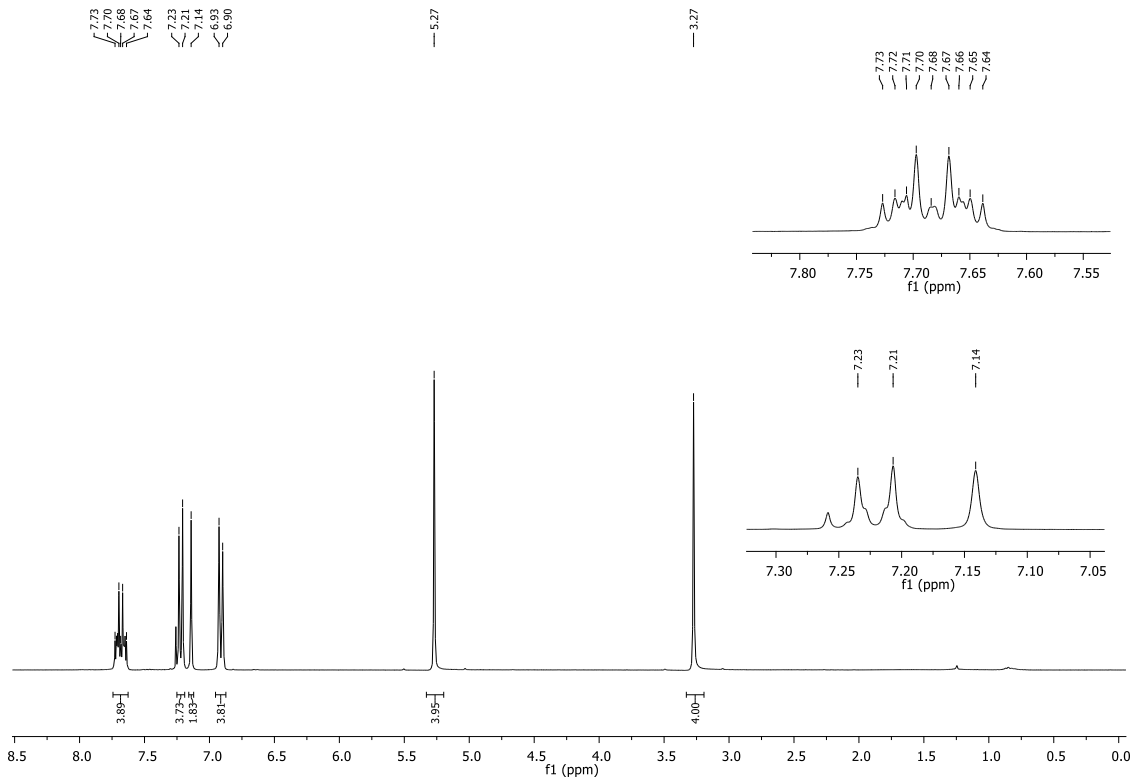


Fig. CN. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**54**).

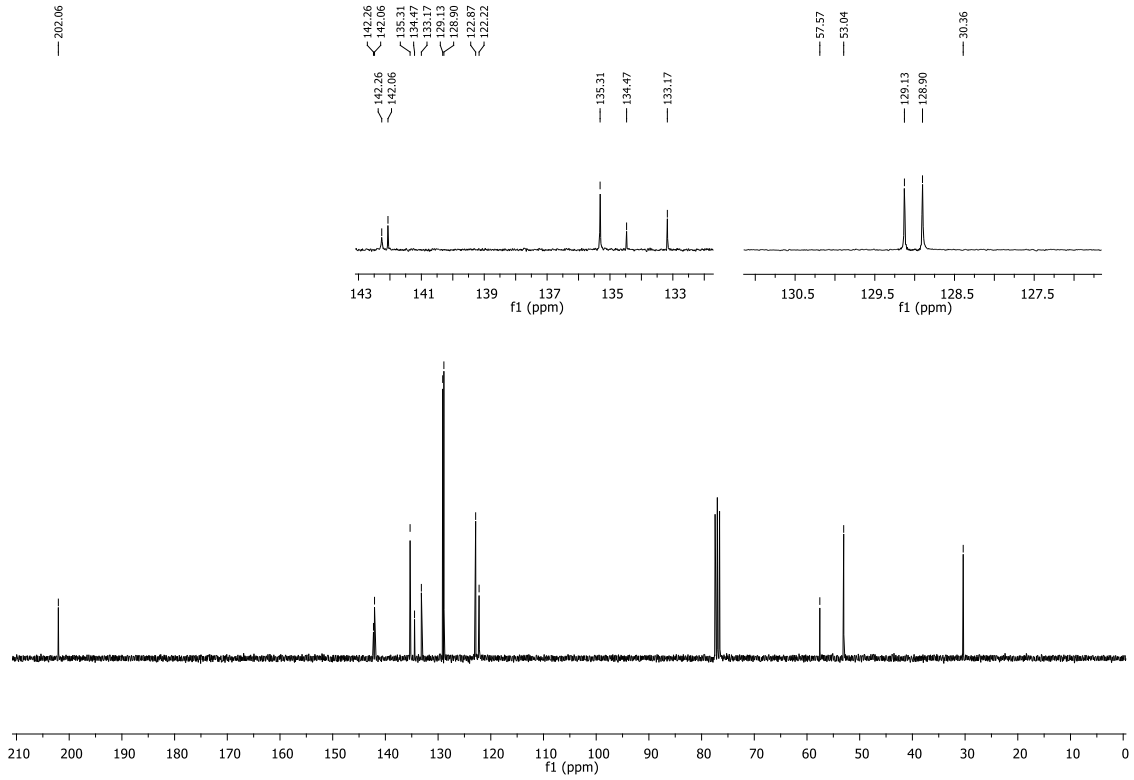


Fig. CO. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**54**).

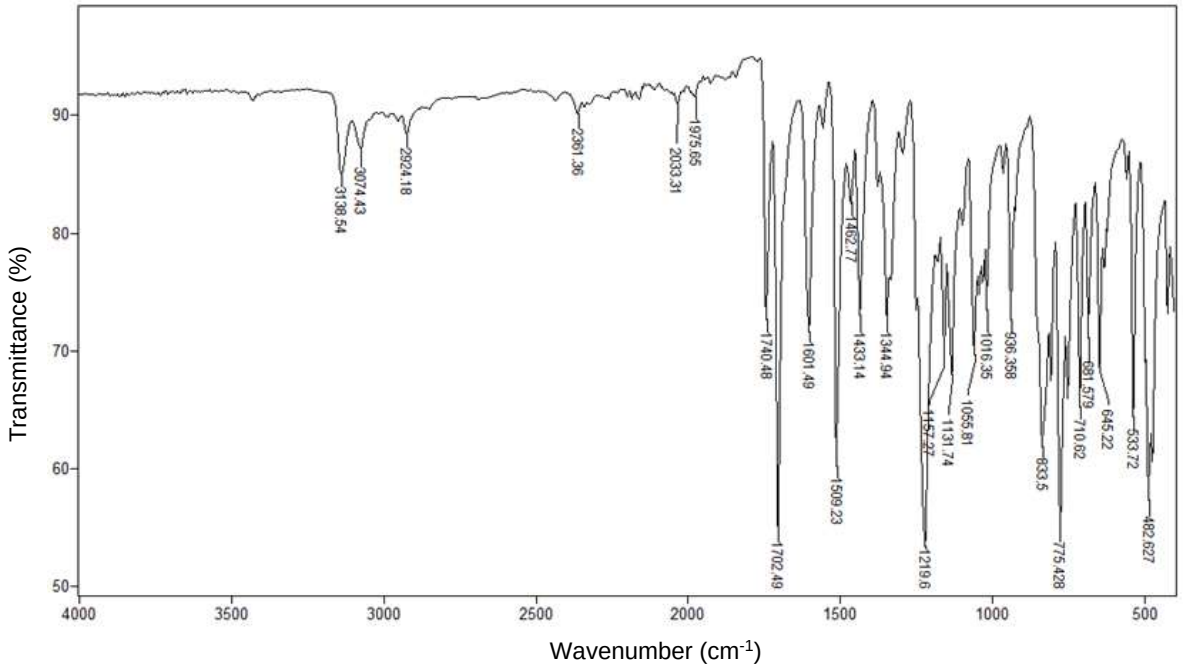


Fig. CP. IR spectrum (ATR) of 2,2-*bis*((1-(4-fluorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**55**).

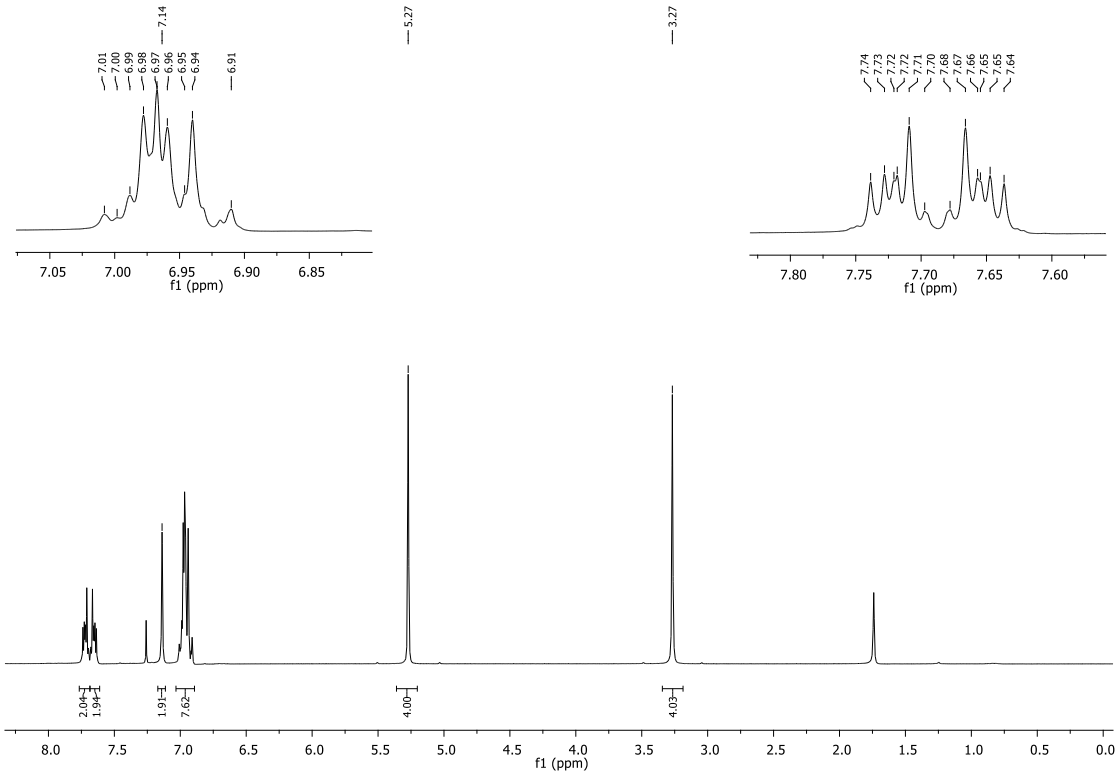


Fig. CQ. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-fluorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**55**).

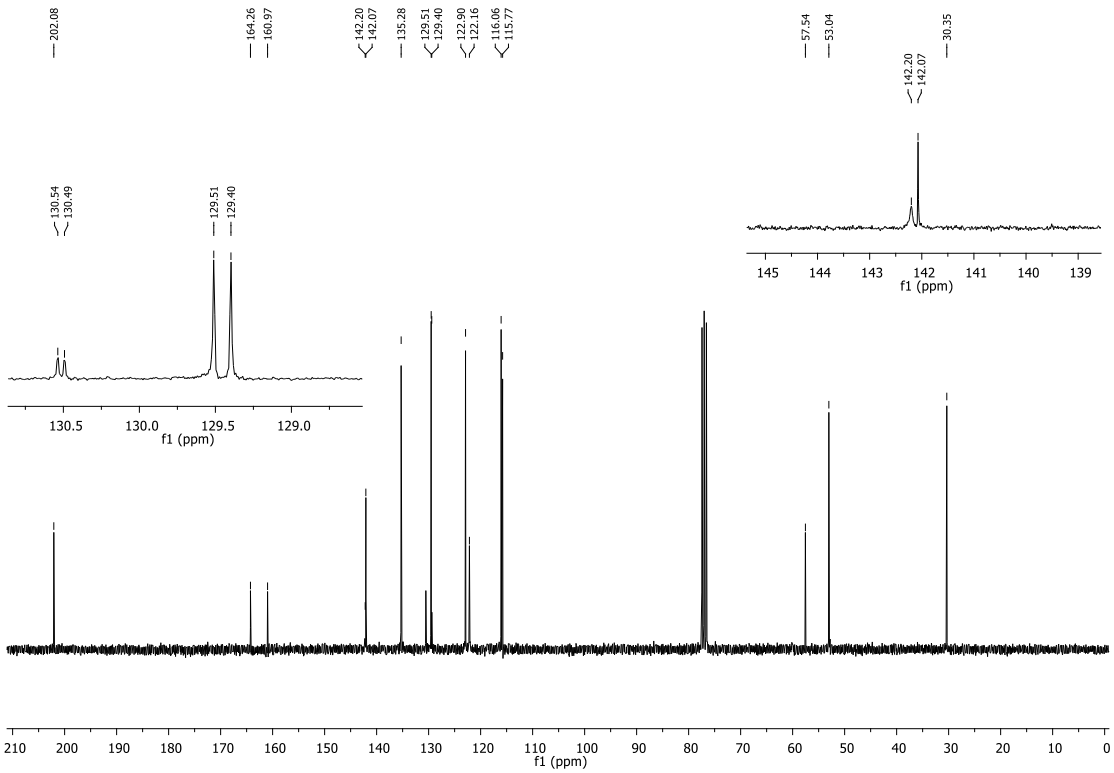


Fig. CR. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-fluorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**55**).

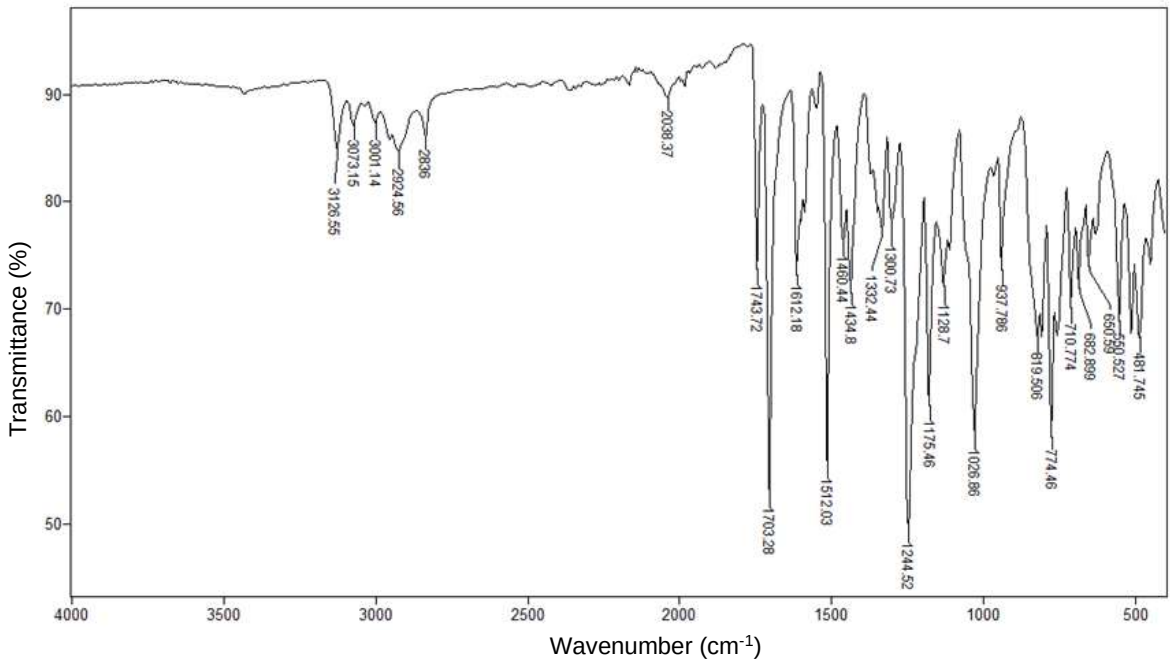


Fig. CS. IR spectrum (ATR) of 2,2-*bis*((1-(4-methoxybenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**56**).

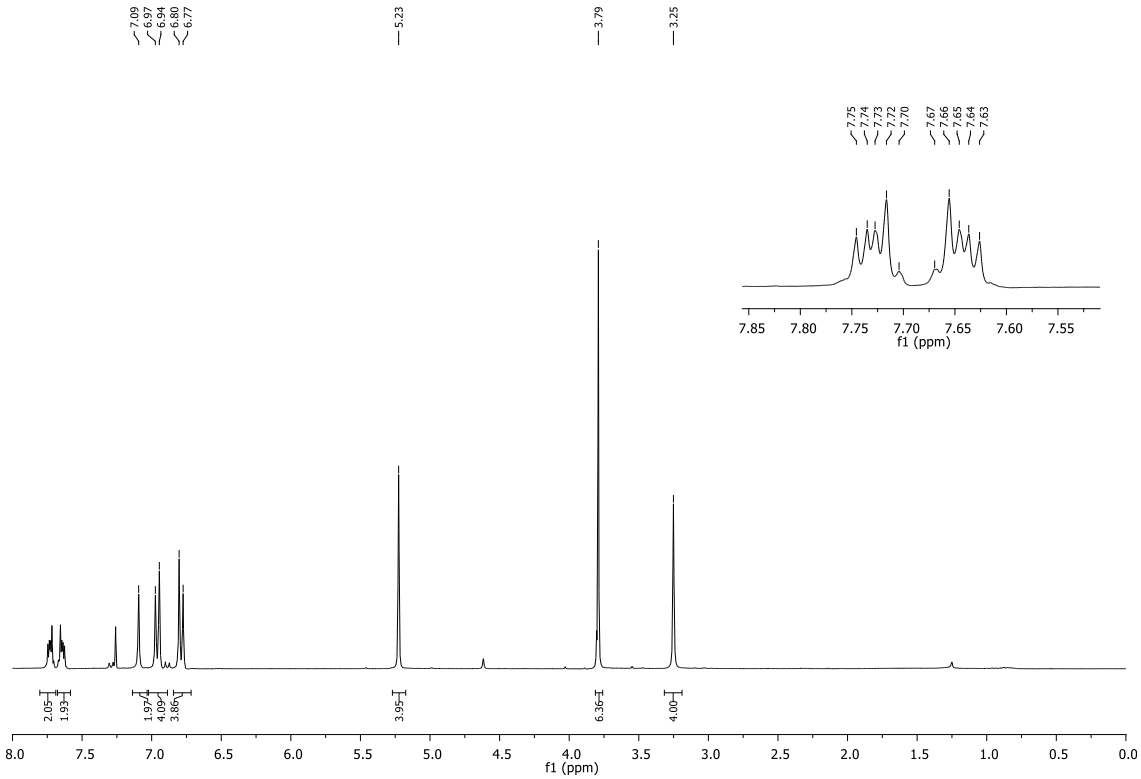


Fig. CT. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-methoxybenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**56**).

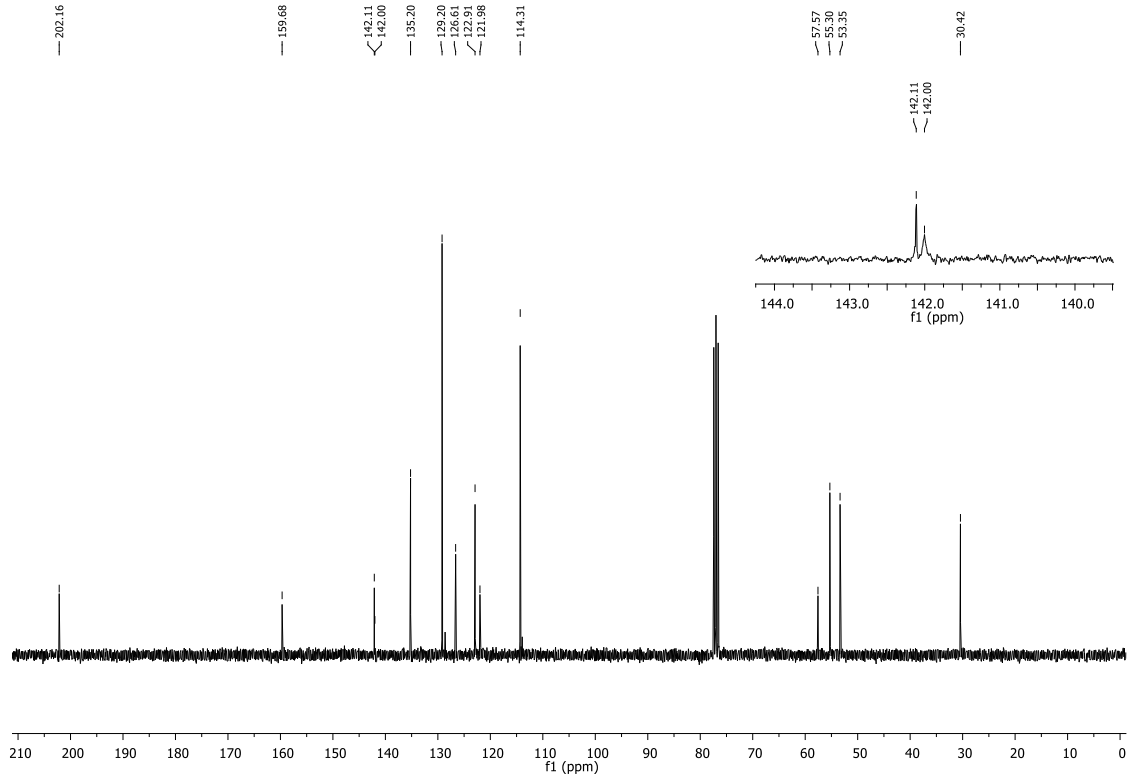


Fig. CU. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-methoxybenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**56**).

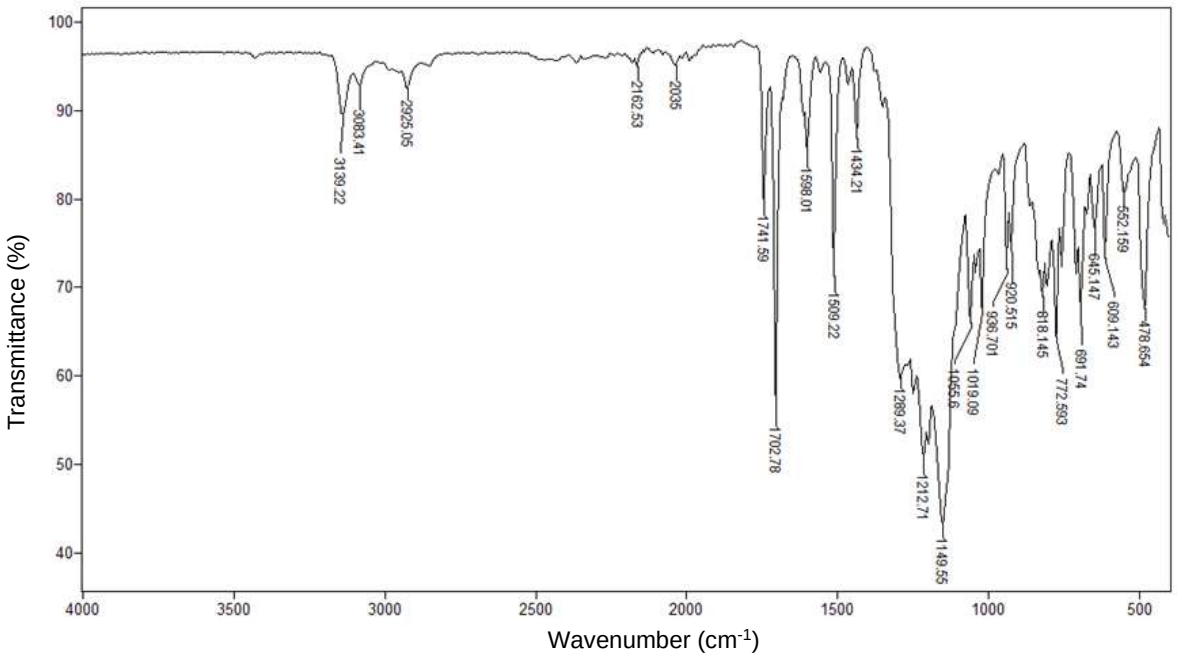


Fig. CV. IR spectrum (ATR) of 2,2-*bis*((1-(4-(trifluoromethoxy)benzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**57**).

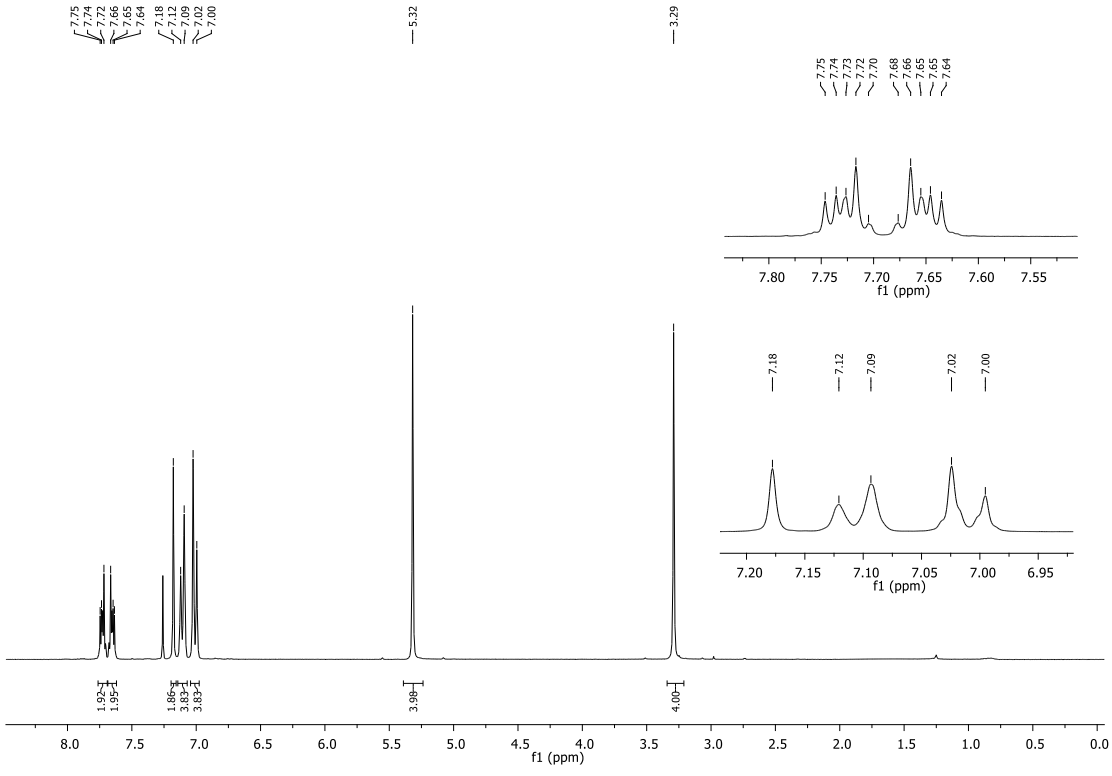


Fig. CX. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-(trifluoromethoxy)benzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**57**).

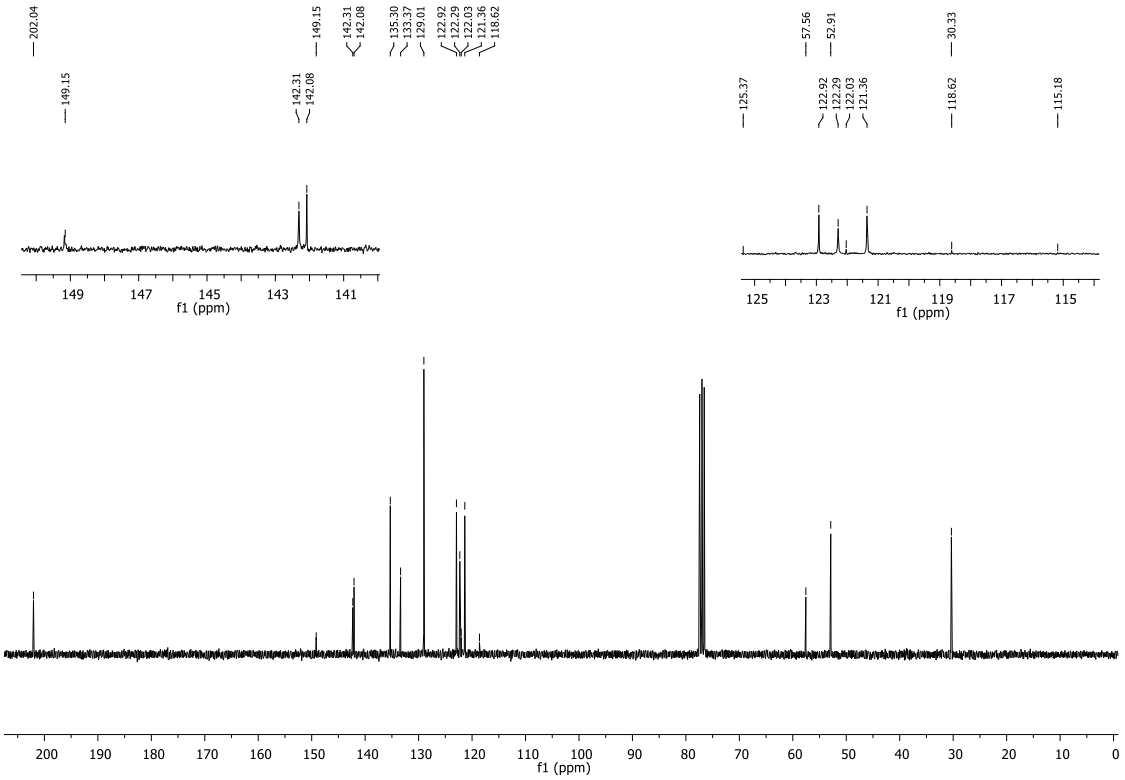


Fig. CW. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-(trifluoromethoxy)benzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**57**).

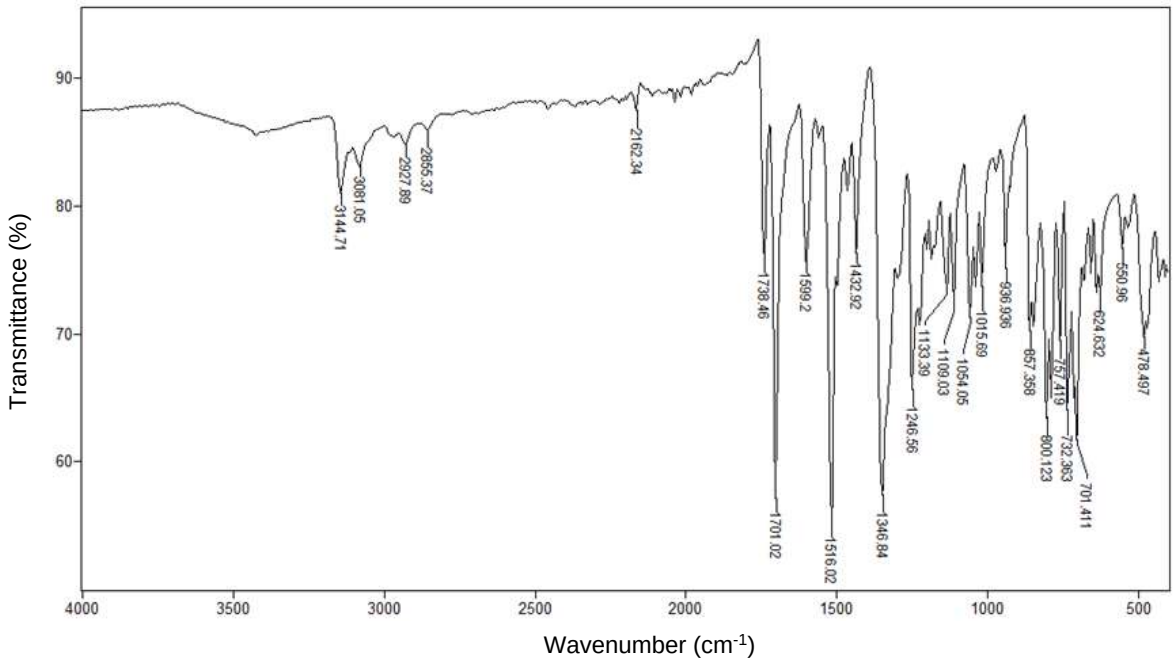


Fig. CY. IR spectrum (ATR) of 2,2-*bis*((1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**58**).

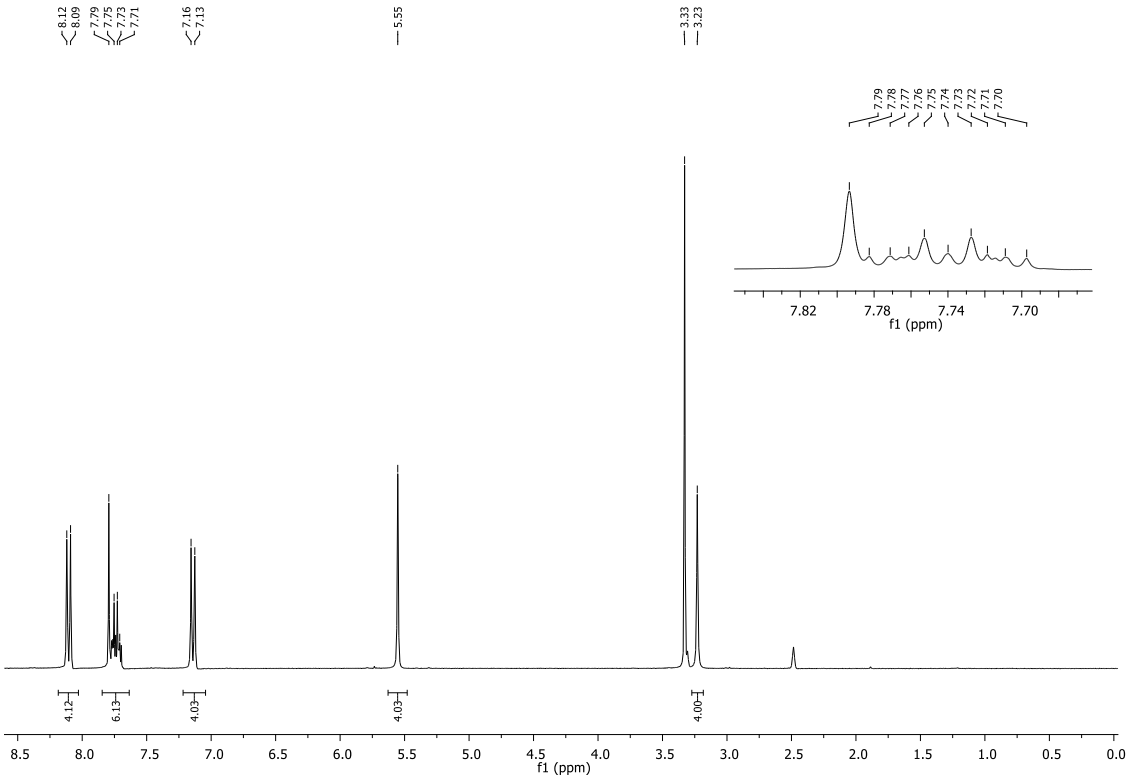


Fig. CZ. ^{1}H NMR spectrum (300 MHz, DMSO-d_6) of 2,2-*bis*((1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**58**).

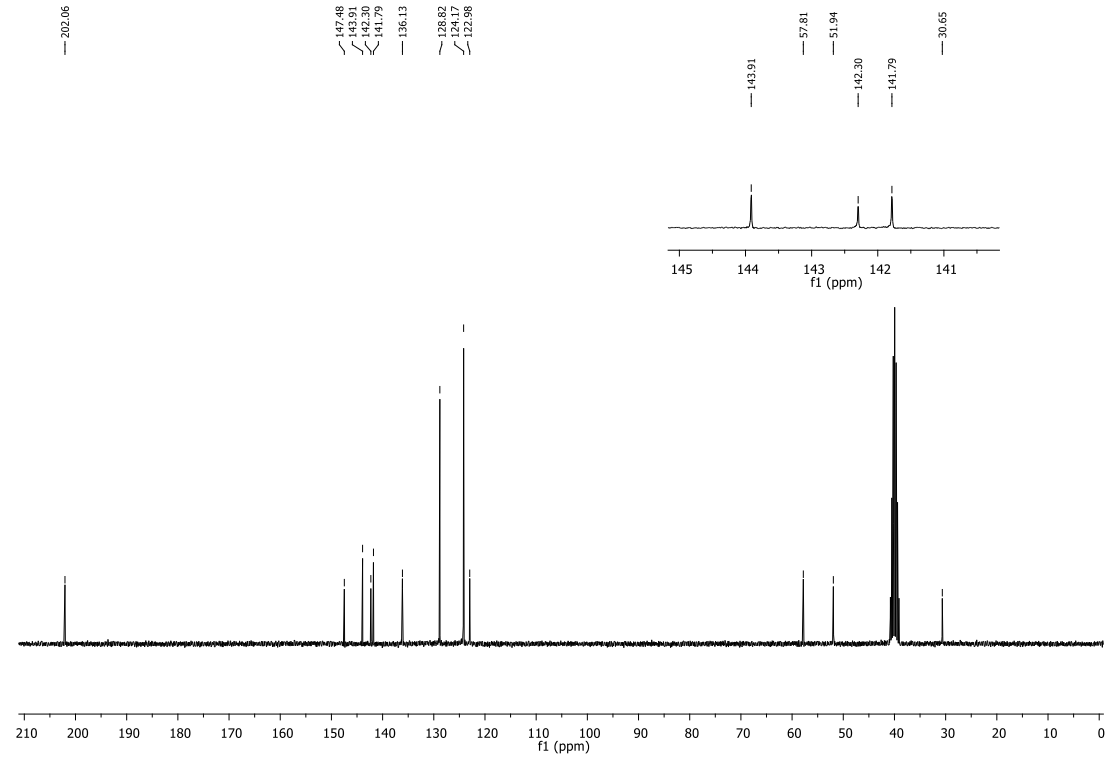


Fig. DA. ^{13}C NMR spectrum (75 MHz, DMSO-d_6) of 2,2-*bis*((1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**58**).

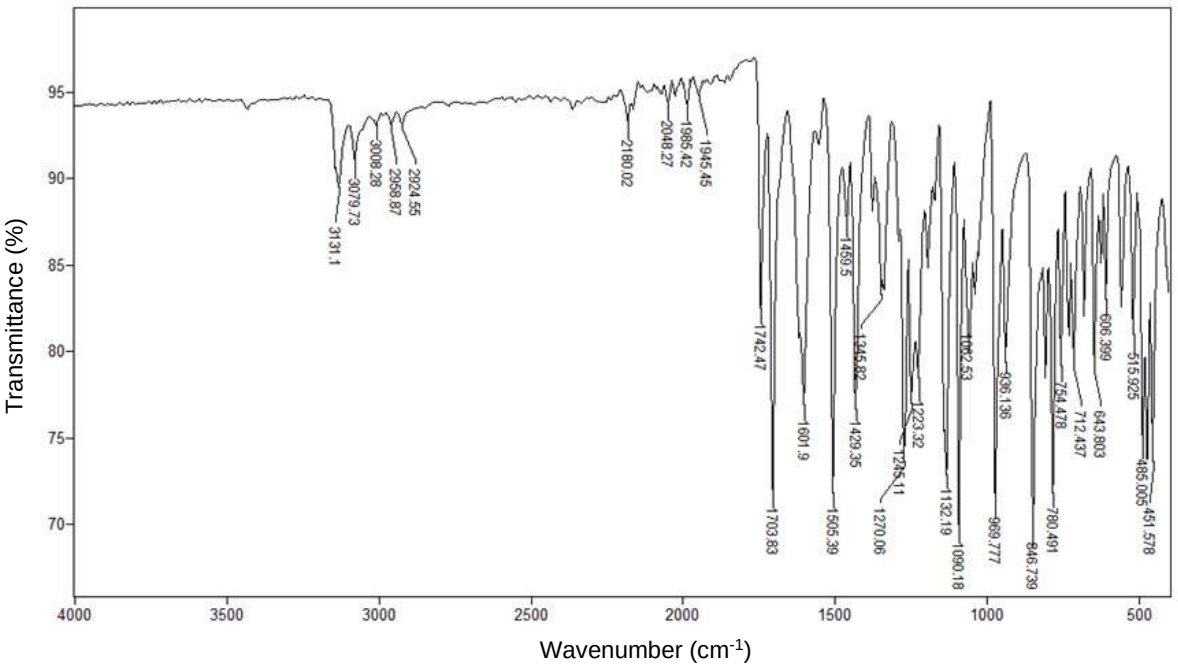


Fig. DB. IR spectrum (ATR) of 2,2-*bis*((1-(2,4-difluorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**59**).

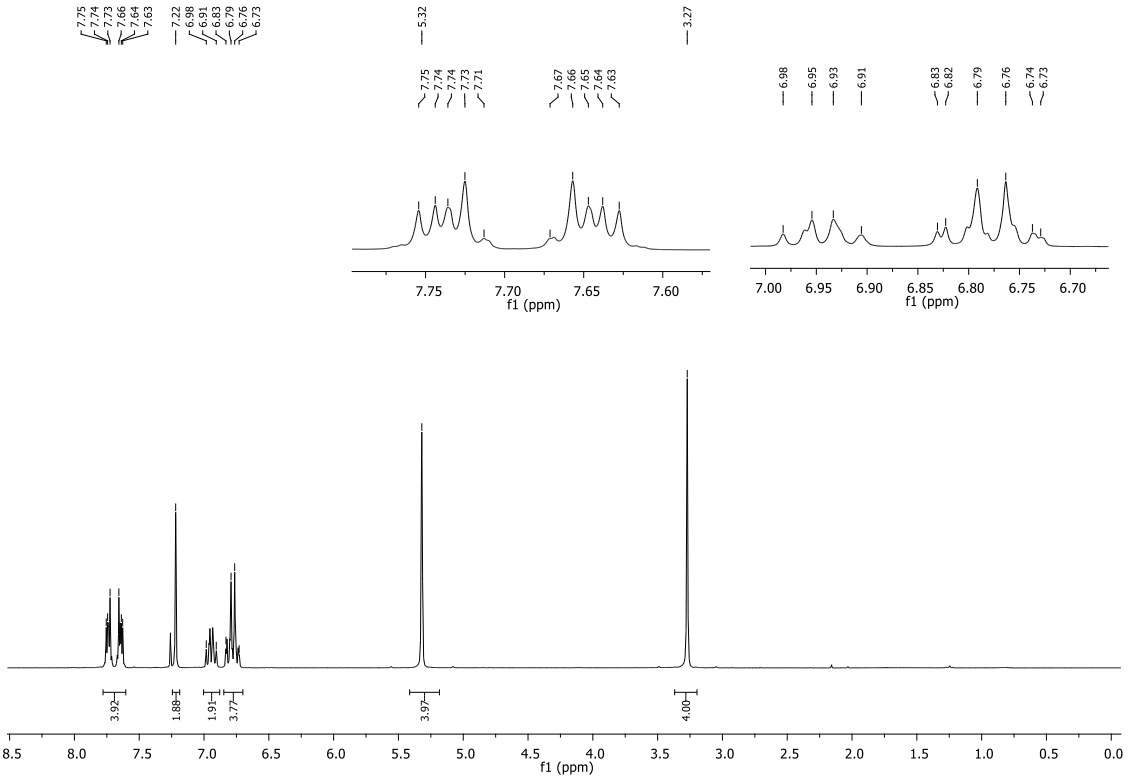


Fig. DC. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(2,4-difluorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**59**).

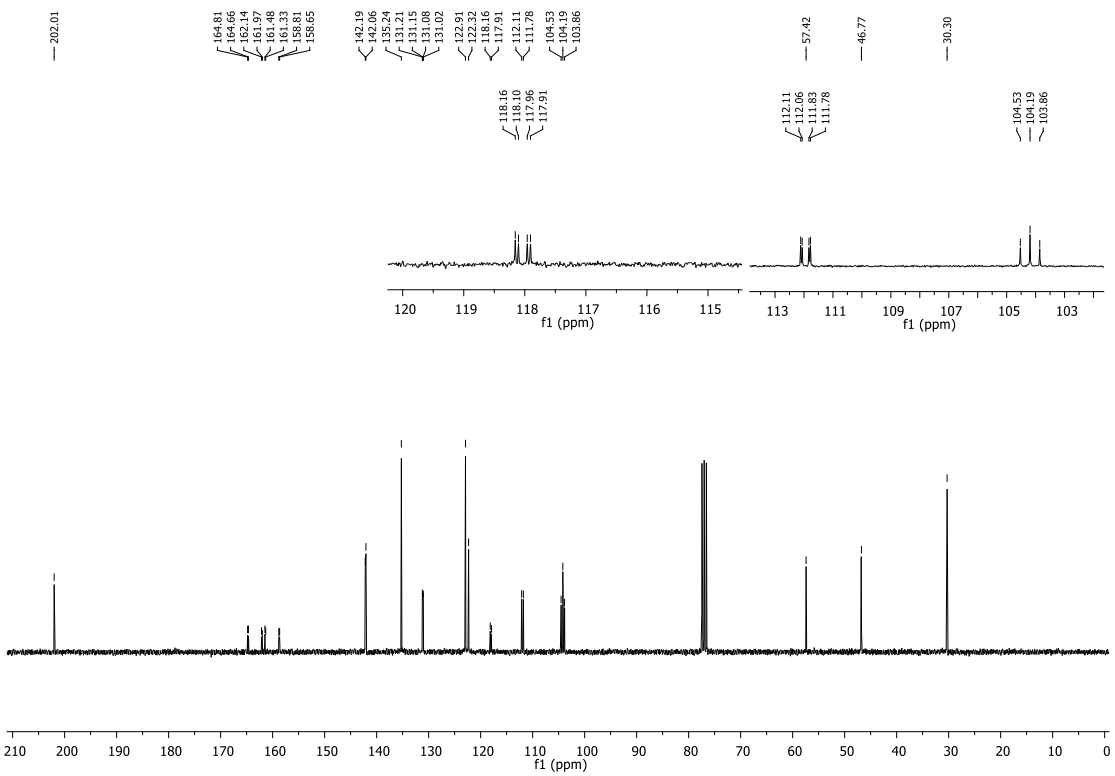


Fig. DD. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(2,4-difluorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**59**).

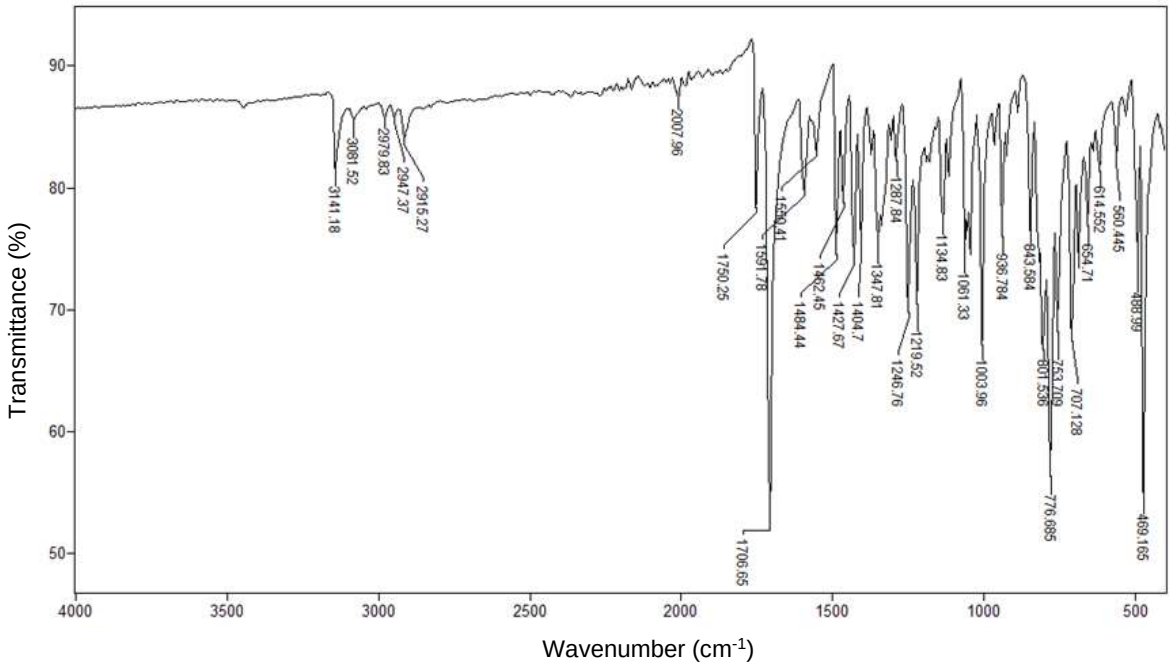


Fig. DE. IR spectrum (ATR) of 2,2-*bis*((1-(4-iodobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**60**).

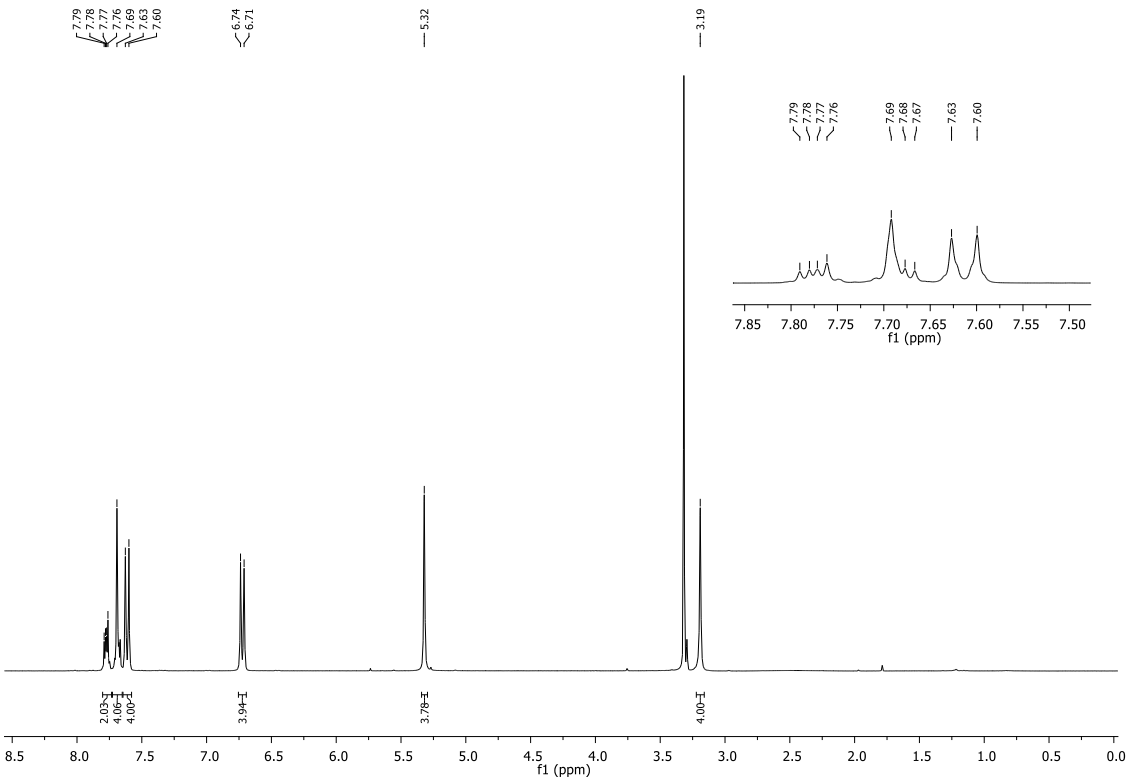


Fig. DF. ^{1}H NMR spectrum (300 MHz, DMSO-d_6) of 2,2-*bis*((1-(4-iodobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**60**).

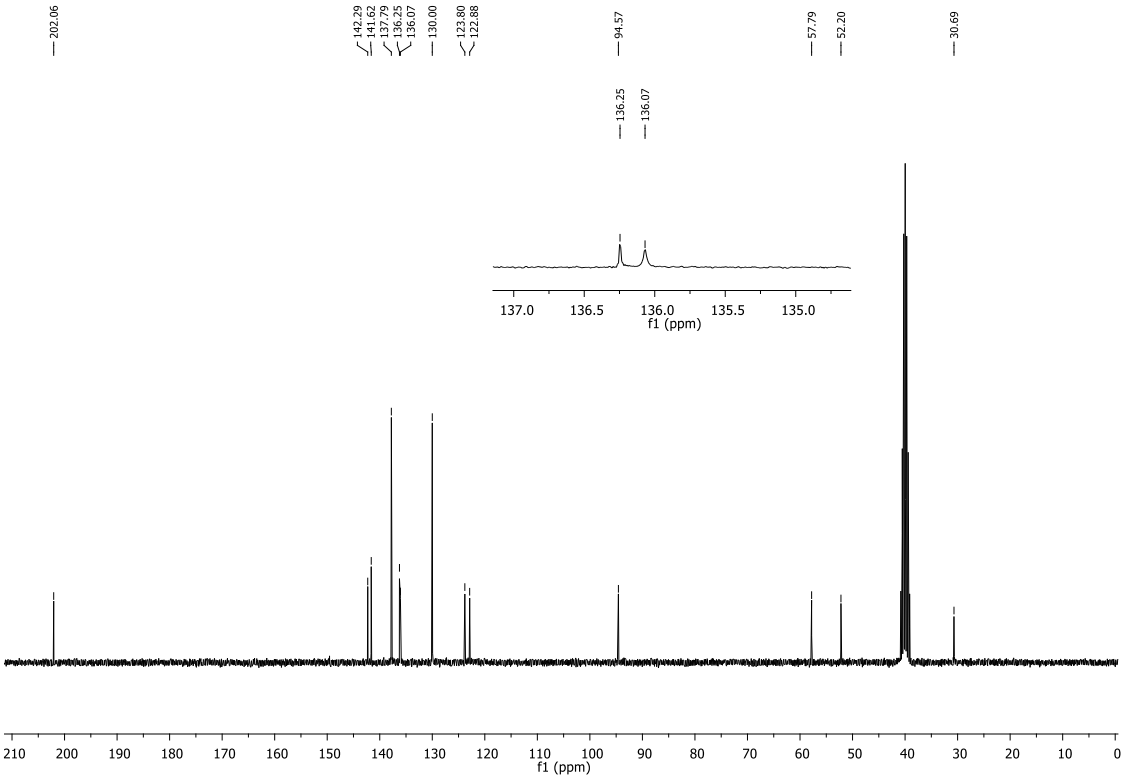


Fig. DG. ^{13}C NMR spectrum (75 MHz, DMSO-d_6) of 2,2-*bis*((1-(4-iodobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**60**).

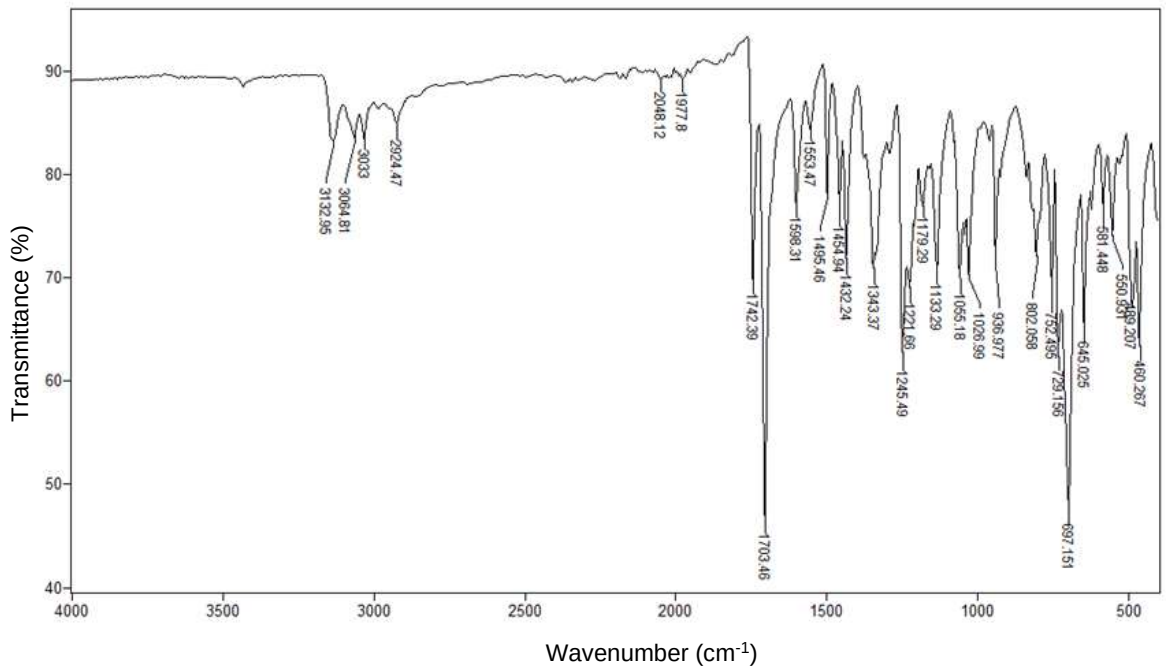


Fig. DH. IR spectrum (ATR) of 2,2-*bis*((1-(2-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**61**).

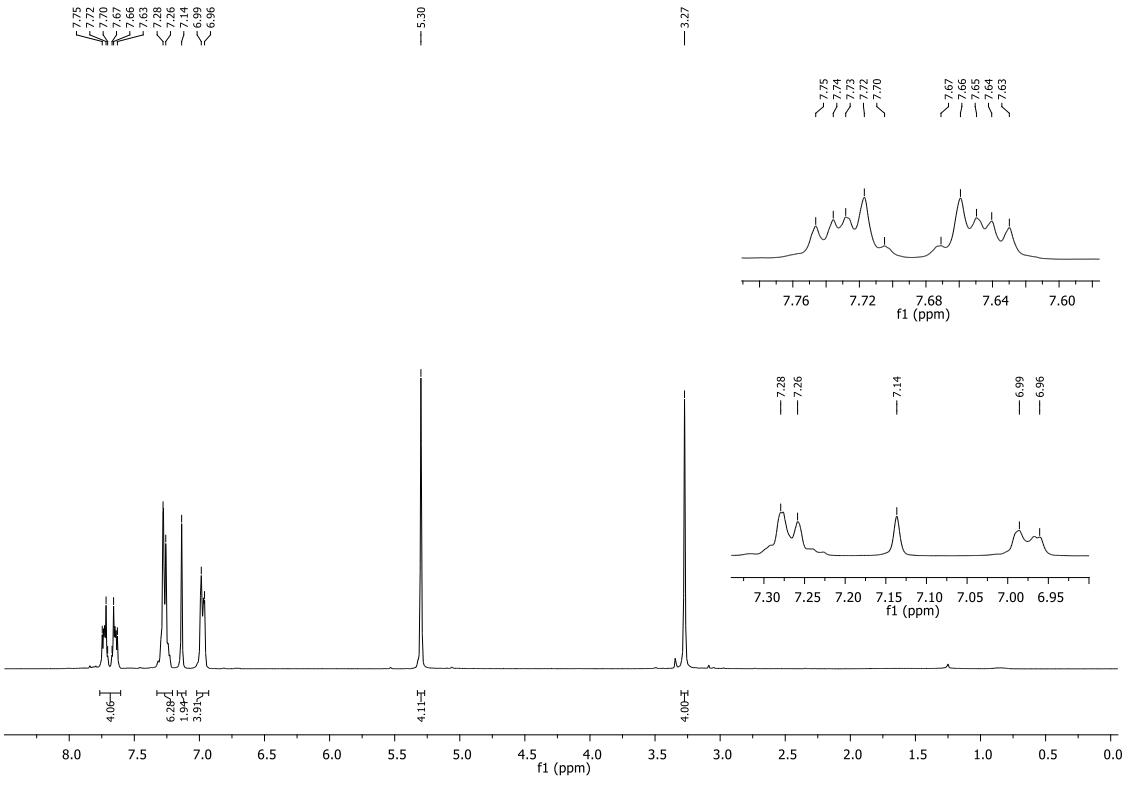


Fig. DI. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(2-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**61**).

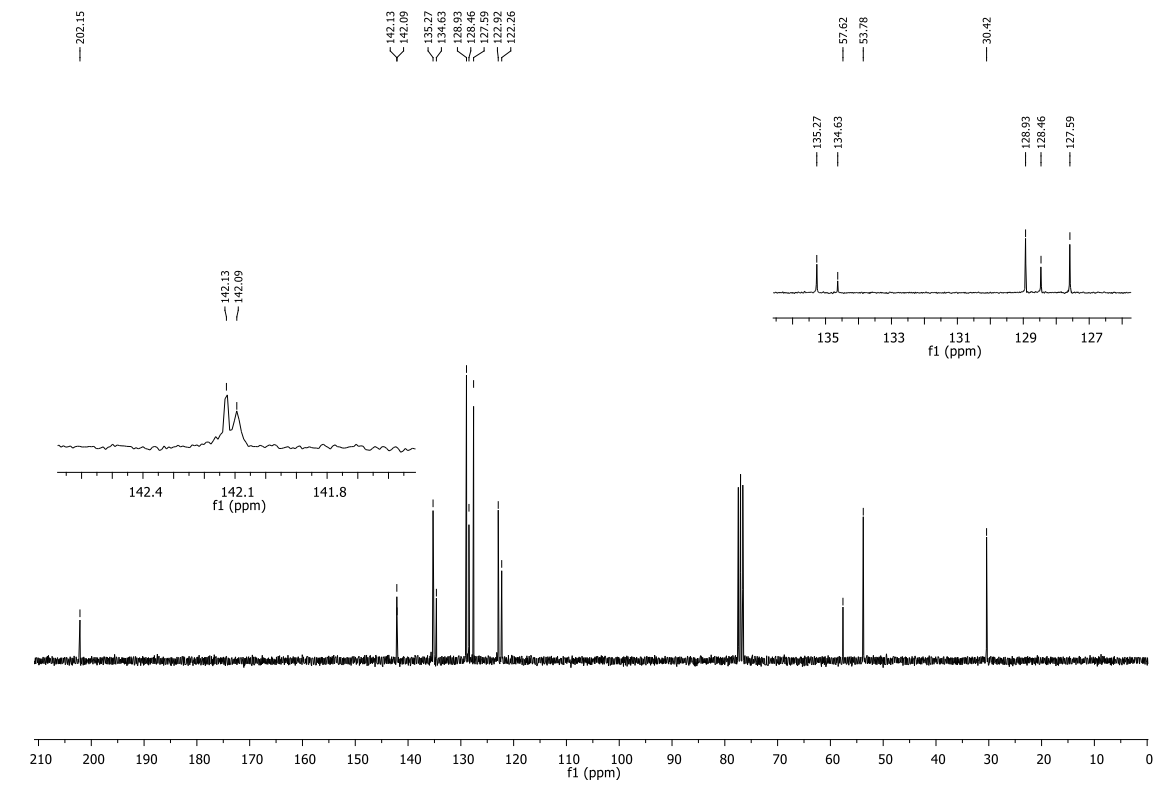


Fig. DJ. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(2-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**61**).

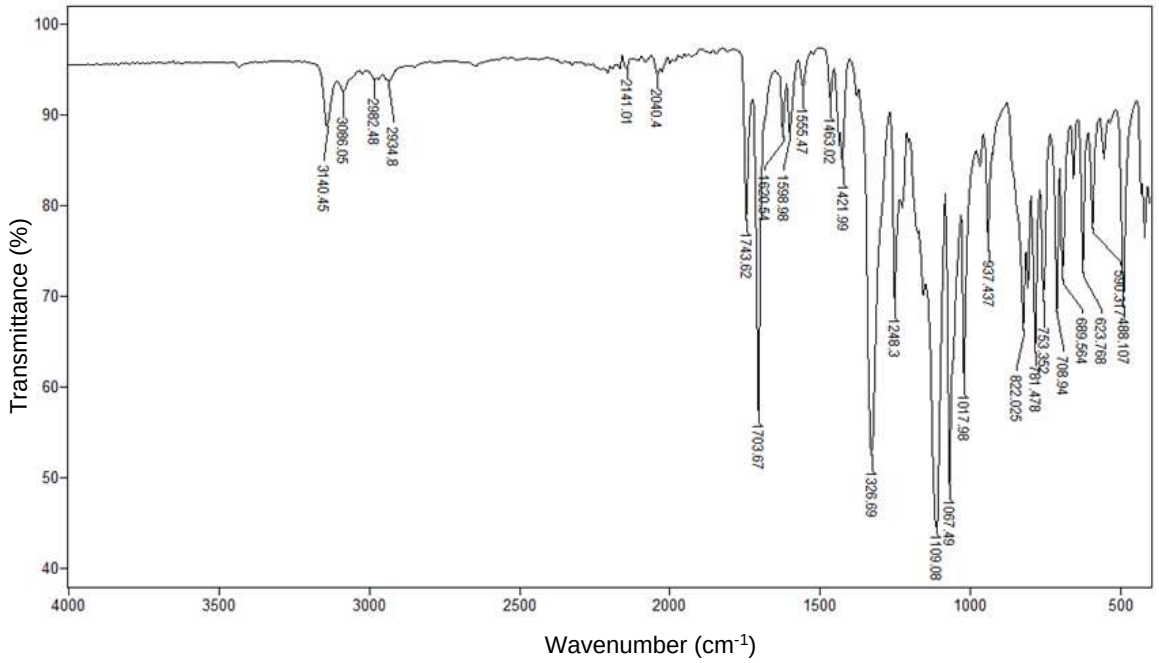


Fig. DK. IR spectrum (ATR) of 2,2-*bis*((1-(4-(trifluoromethyl)benzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**62**).

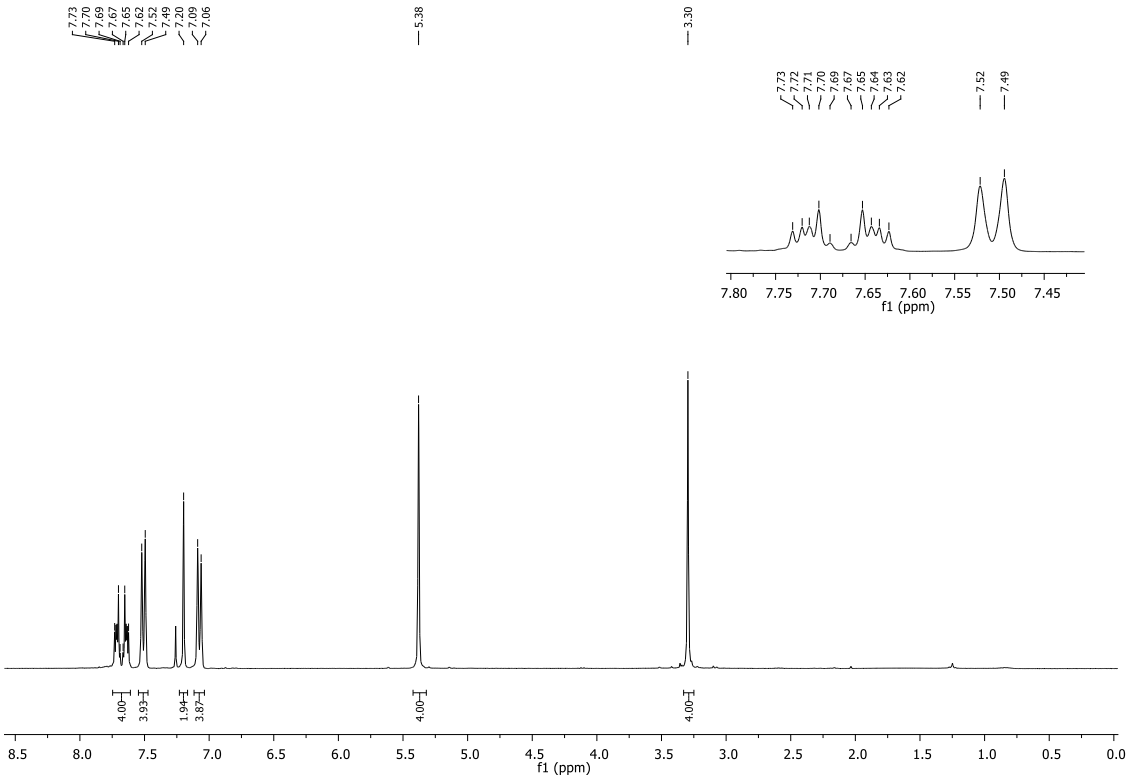


Fig. DL. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-(trifluoromethyl)benzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**62**).

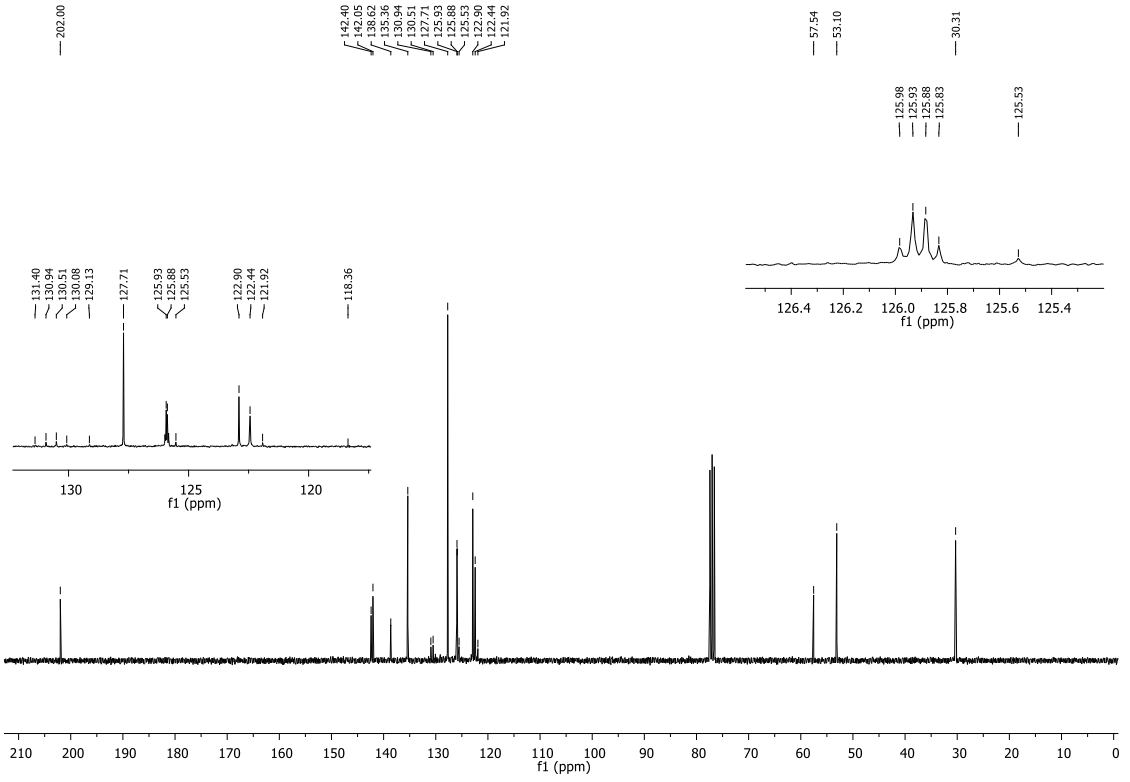


Fig. DM. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-(trifluoromethyl)benzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**62**).

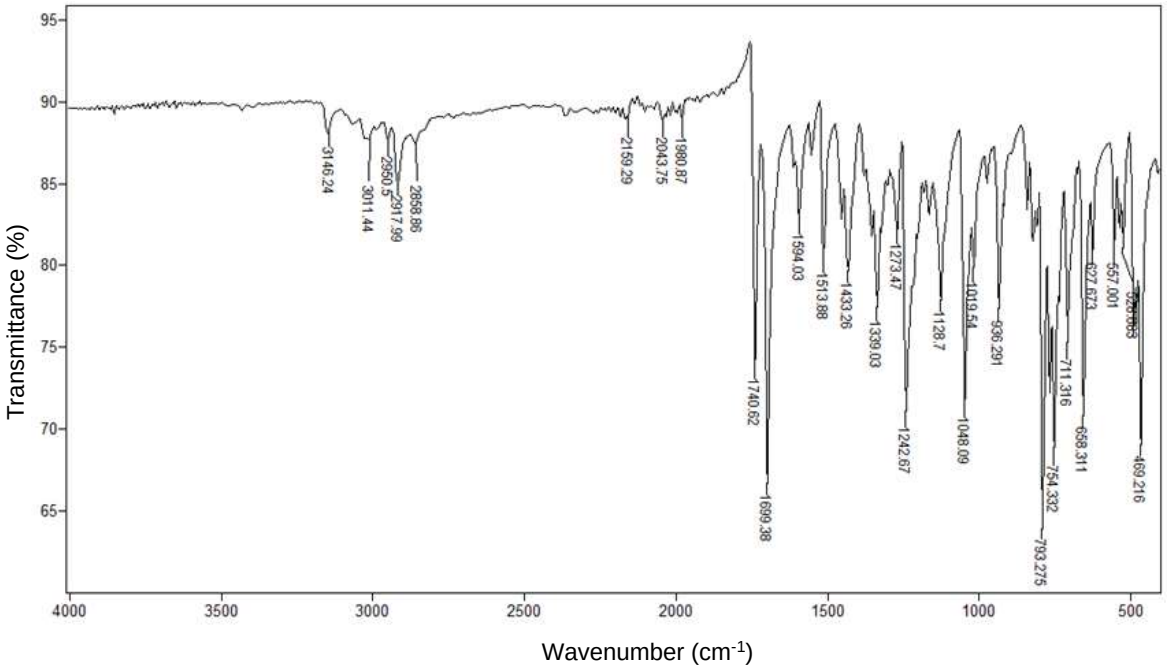


Fig. DN. IR spectrum (ATR) of 2,2-*bis*((1-(4-methylbenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**63**).

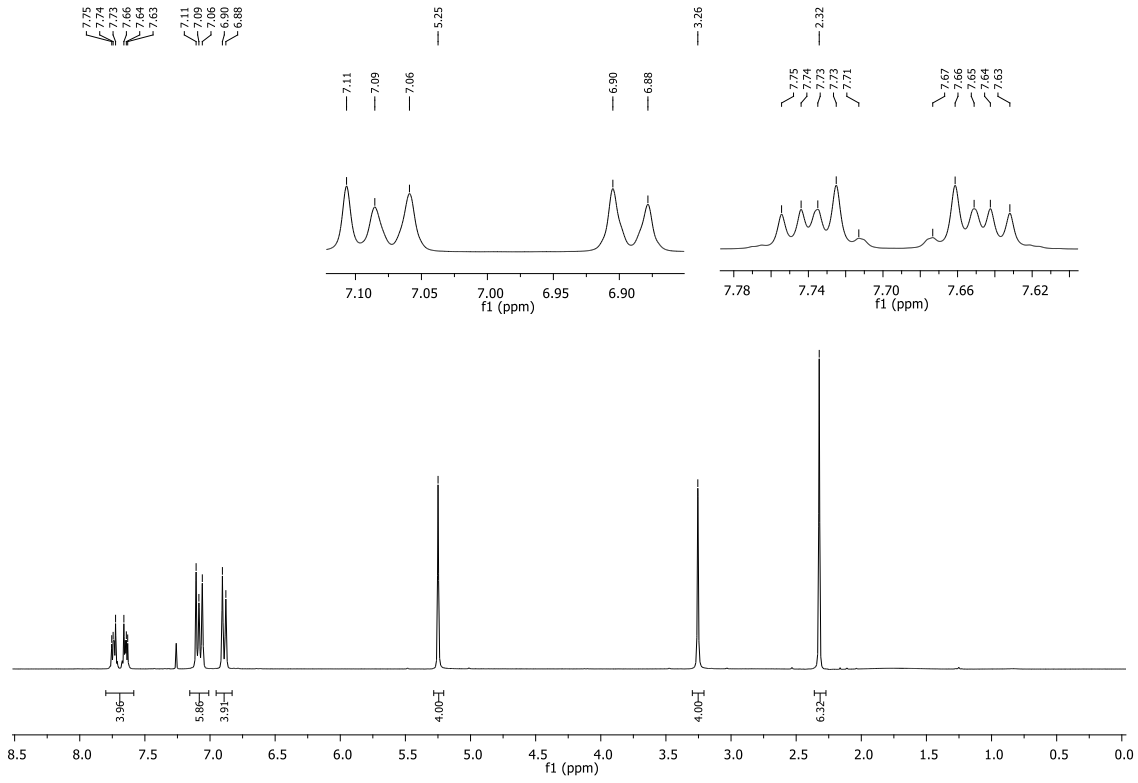


Fig. DO. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-methylbenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**63**).

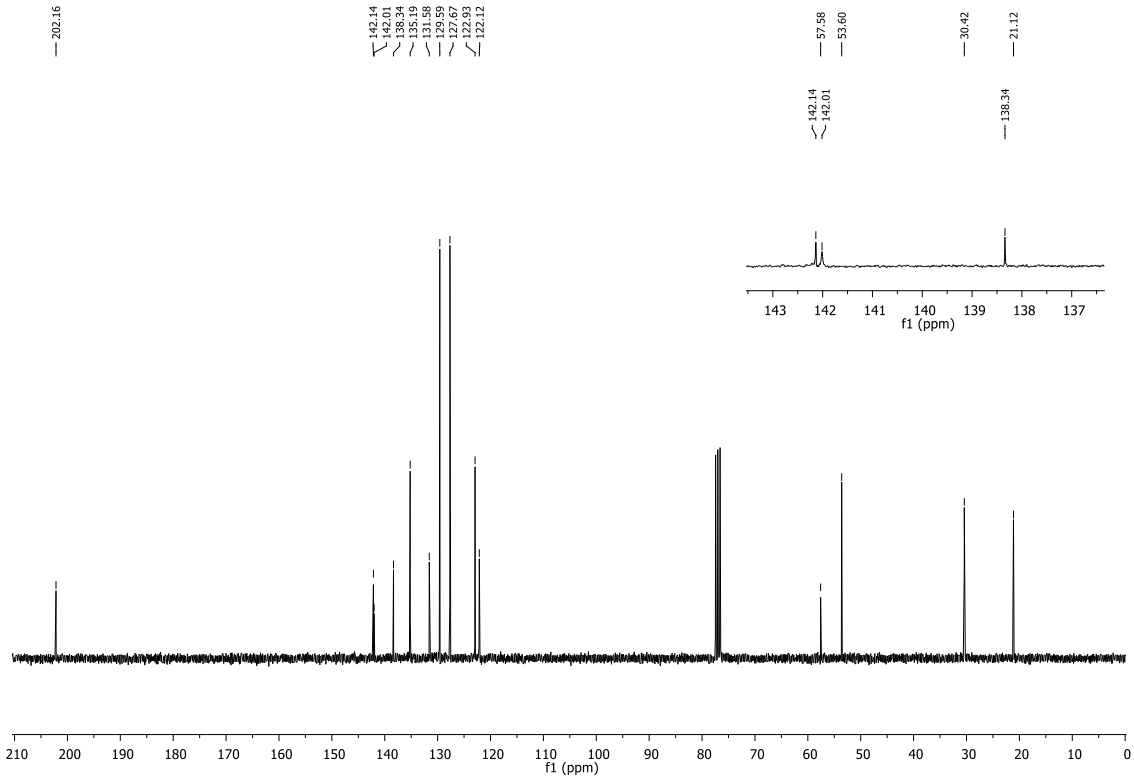


Fig. DP. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of 2,2-*bis*((1-(4-methylbenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-indene-1,3(2*H*)-dione (**63**).