

Expanding the isoflavone, pyrazole, and oxazole chemical space through 2'-carboxamido-2-hydroxydeoxybenzoin precursors

Kateryna V. Kukushkina¹, Viktoriia S. Moskvina^{1,2*}, Olga V. Shablykina^{1,2}, Volodymyr P. Khilya¹

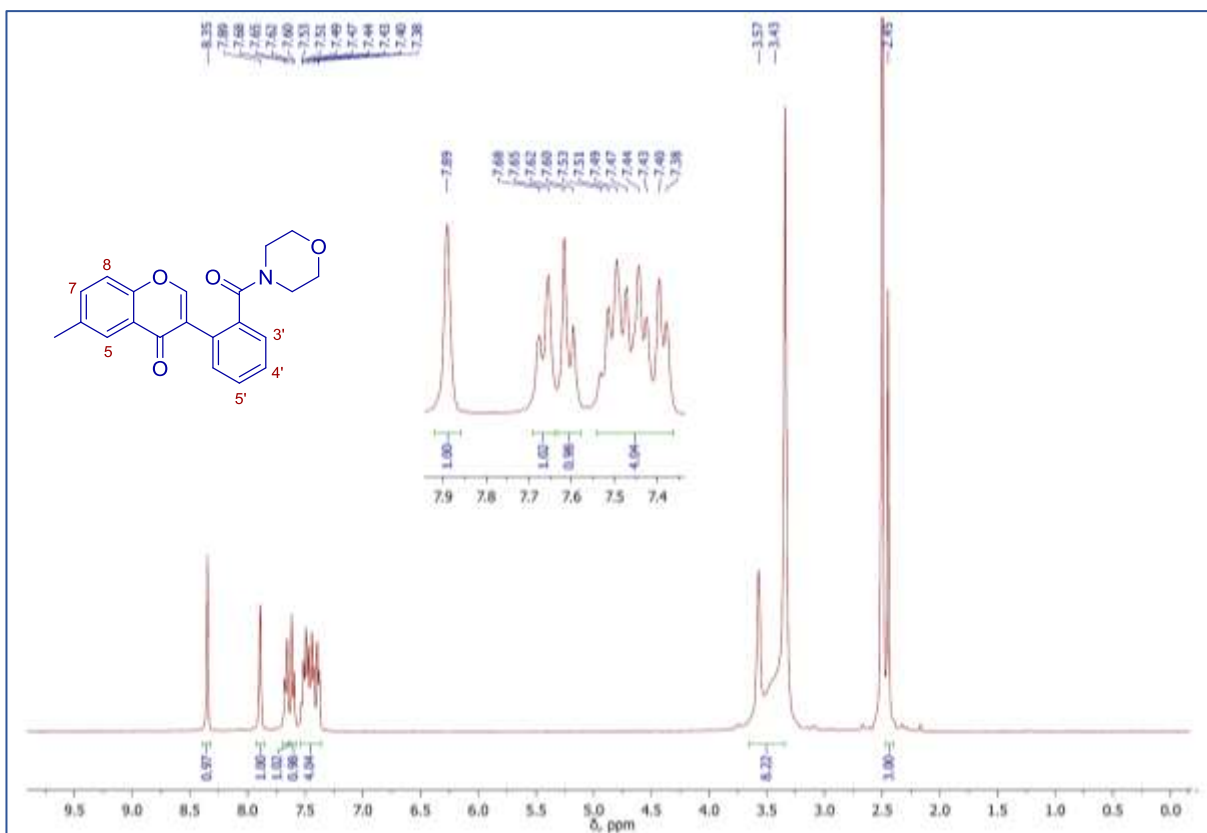
¹ Taras Shevchenko National University of Kyiv,
64/13 Volodymyrska St., Kyiv 01601, Ukraine

² V. P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry,
National Academy of Sciences of Ukraine,
1 Akademika Kukharya St., Kyiv 02094, Ukraine; e-mail: v.moskvina@gmail.com

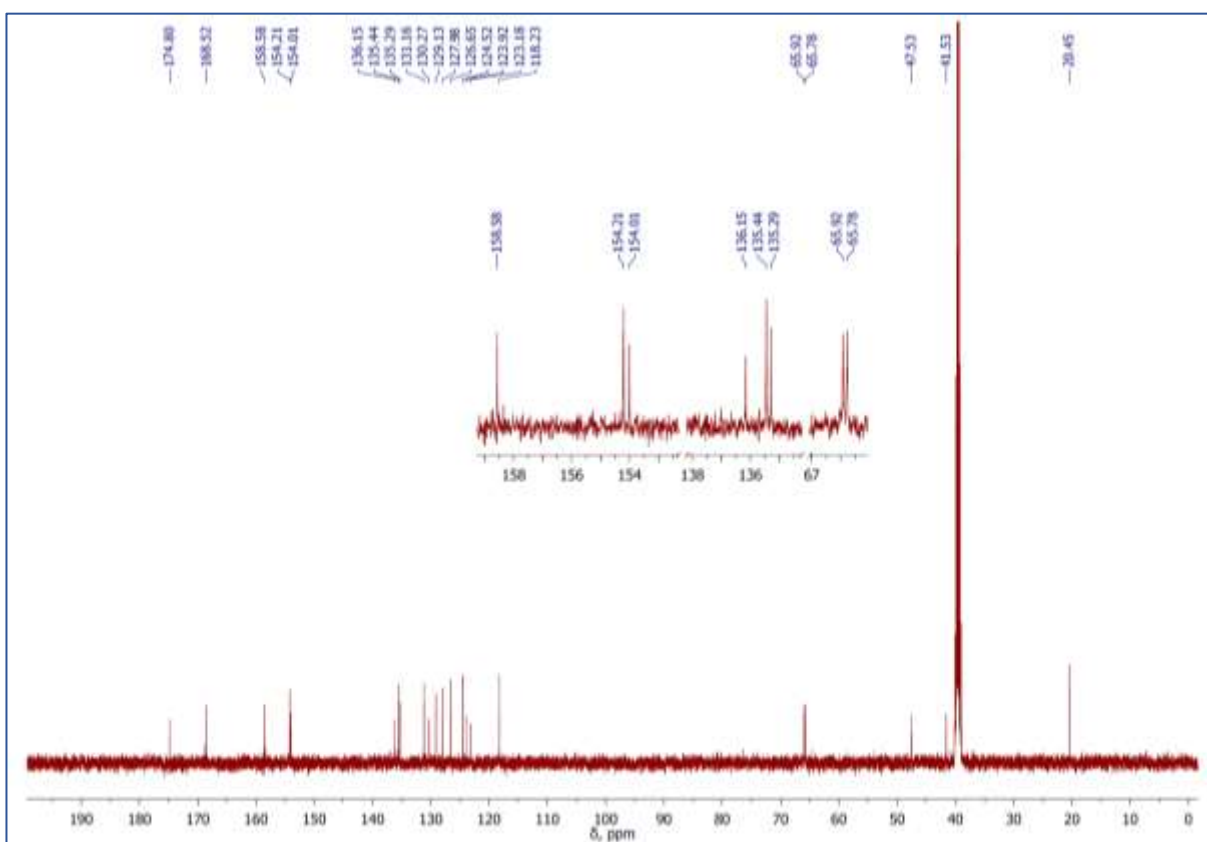
Supplementary Information

Table of Contents

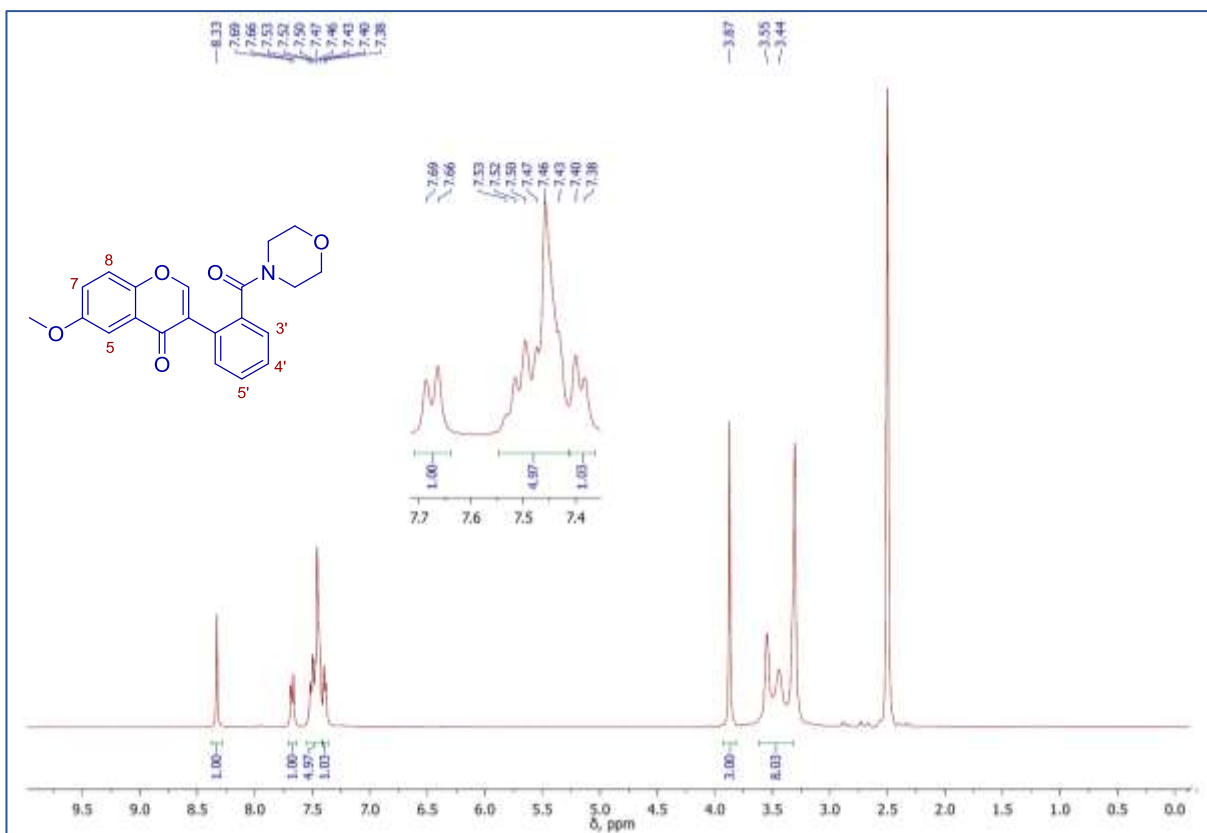
¹ H and ¹³ C NMR spectra of 6-methyl-3-[2-(morpholine-4-carbonyl)phenyl]-4 <i>H</i> -1-benzopyran-4-one (4a)	2
¹ H and ¹³ C NMR spectra of 6-methoxy-3-[2-(morpholine-4-carbonyl)phenyl]-4 <i>H</i> -1-benzopyran-4-one (4b)	3
¹ H and ¹³ C NMR spectra of 7-methoxy-3-[2-(morpholine-4-carbonyl)phenyl]-4 <i>H</i> -1-benzopyran-4-one (4c)	4
¹ H and ¹³ C NMR spectra of 7-methoxy-8-methyl-3-[2-(morpholine-4-carbonyl)phenyl]-4 <i>H</i> -1-benzopyran-4-one (4d)	5
¹ H and ¹³ C NMR spectra of {2-[3-(2-hydroxy-5-methylphenyl)-1 <i>H</i> -pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (5a)	6
¹ H and ¹³ C NMR spectra of {2-[3-(2-hydroxy-5-methoxyphenyl)-1 <i>H</i> -pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (5b)	7
¹ H and ¹³ C NMR spectra of {2-[3-(2-hydroxy-4-methoxyphenyl)-1 <i>H</i> -pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (5c)	8
¹ H and ¹³ C NMR spectra of {2-[3-(2-hydroxy-4-methoxy-3-methylphenyl)-1 <i>H</i> -pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (5d)	9
¹ H and ¹³ C NMR spectra of 2-[5-(2-hydroxy-5-methylphenyl)-1,2-oxazol-4-yl]benzoic acid (6a)	10
¹ H and ¹³ C NMR spectra of 2-[5-(2-hydroxy-5-methoxyphenyl)-1,2-oxazol-4-yl]benzoic acid (6b)	11
¹ H and ¹³ C NMR spectra of 2-[5-(2-hydroxy-4-methoxyphenyl)-1,2-oxazol-4-yl]benzoic acid (6c)	12
¹ H and ¹³ C NMR spectra of 2-[5-(2-hydroxy-4-methoxy-5-methylphenyl)-1,2-oxazol-4-yl]benzoic acid (6d)	13
¹ H and ¹³ C NMR spectra of <i>N</i> -hydroxy-2-[5-(2-hydroxy-5-methylphenyl)-1,2-oxazol-4-yl]benzamide (7a)	14



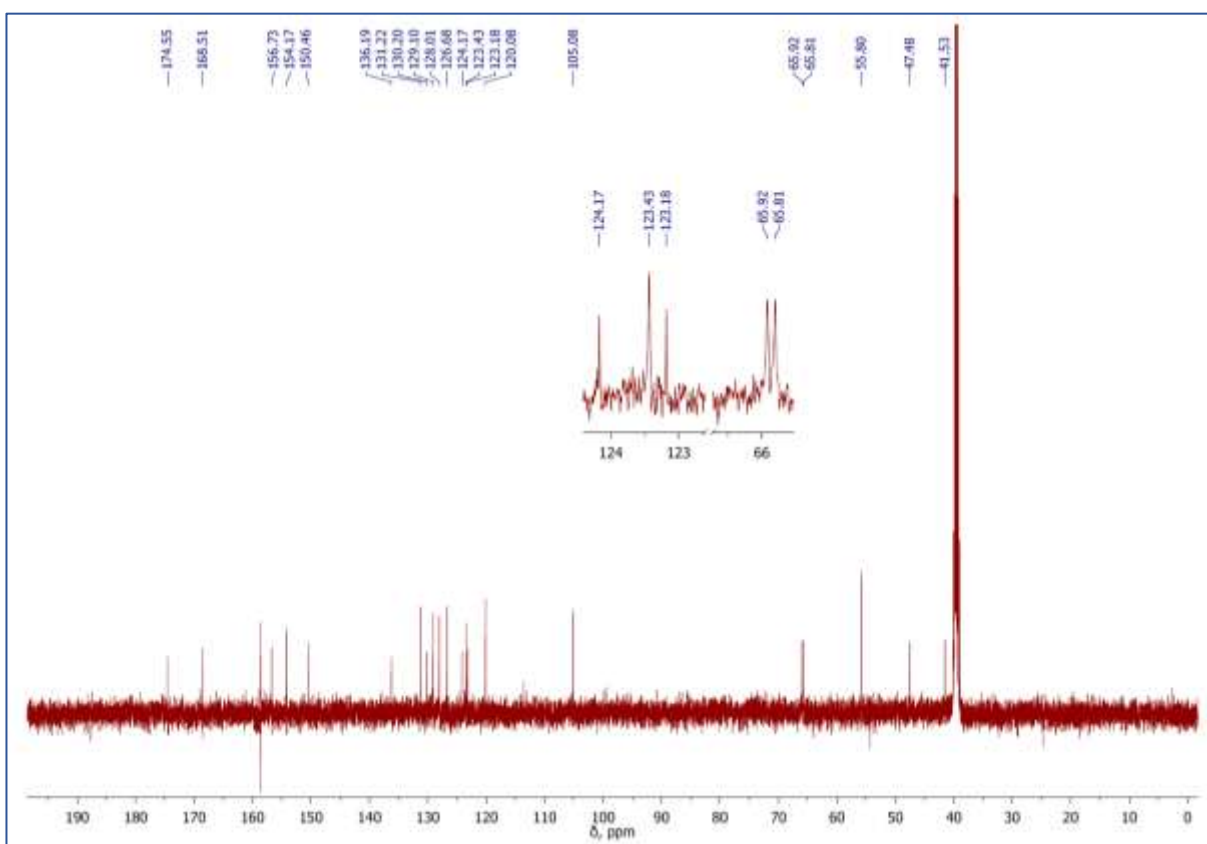
¹H NMR spectrum of 6-methyl-3-[2-(morpholine-4-carbonyl)phenyl]-4H-1-benzopyran-4-one (**4a**)



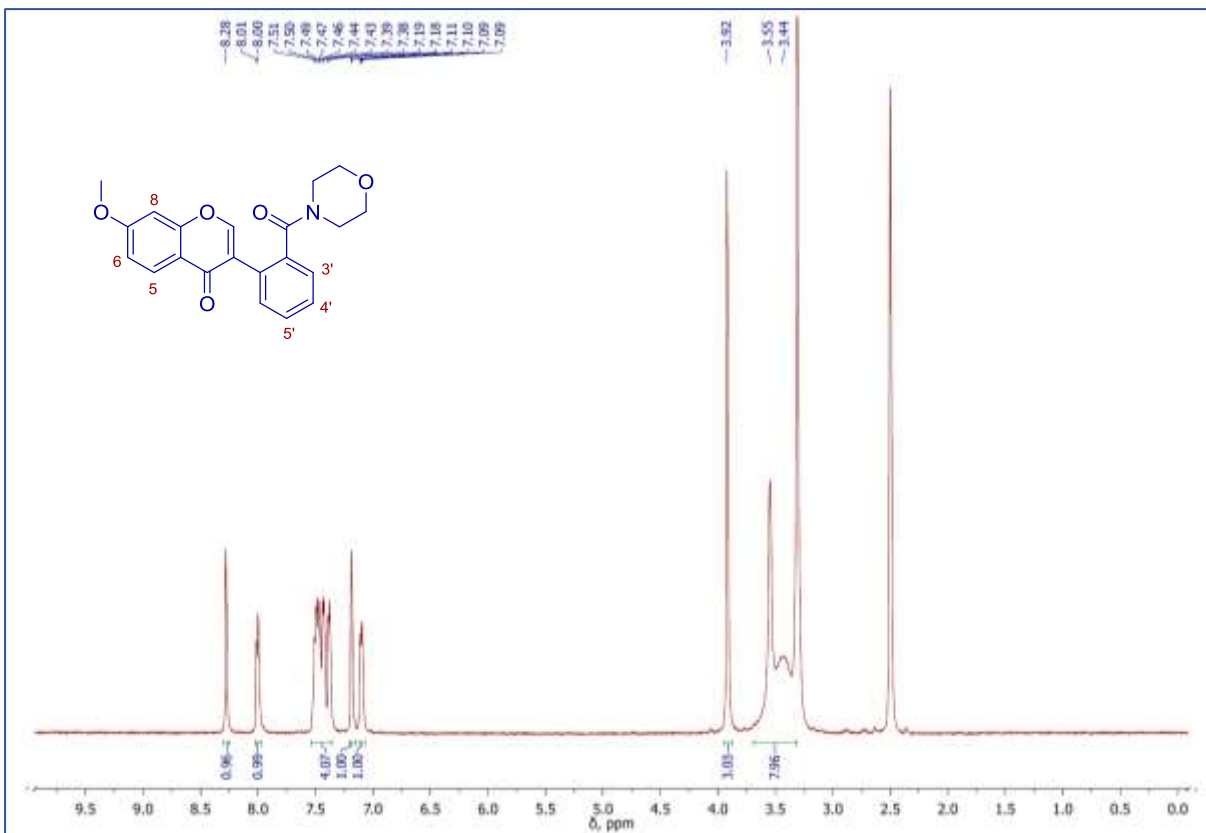
¹³C NMR spectrum of 6-methyl-3-[2-(morpholine-4-carbonyl)phenyl]-4H-1-benzopyran-4-one (**4a**)



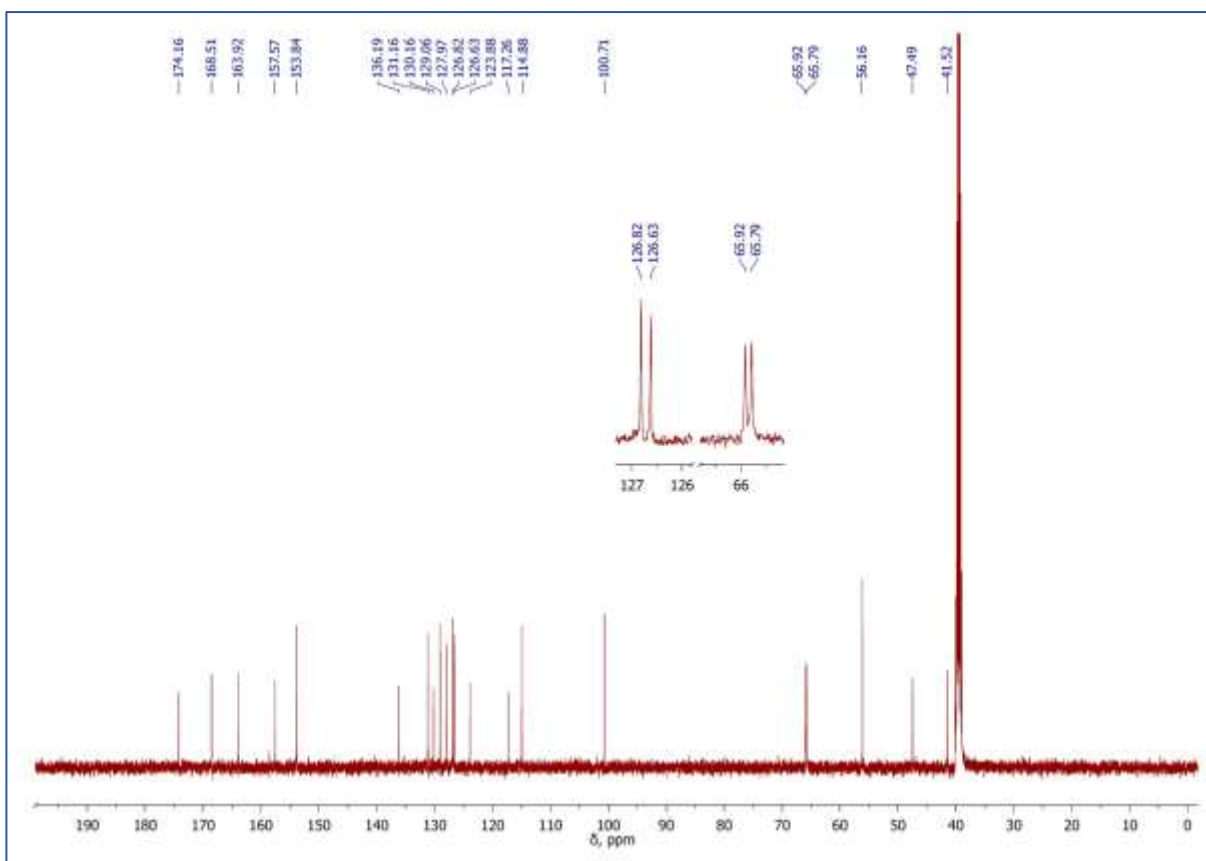
¹H NMR spectrum of 6-methoxy-3-[2-(morpholine-4-carbonyl)phenyl]-4H-1-benzopyran-4-one (**4b**)



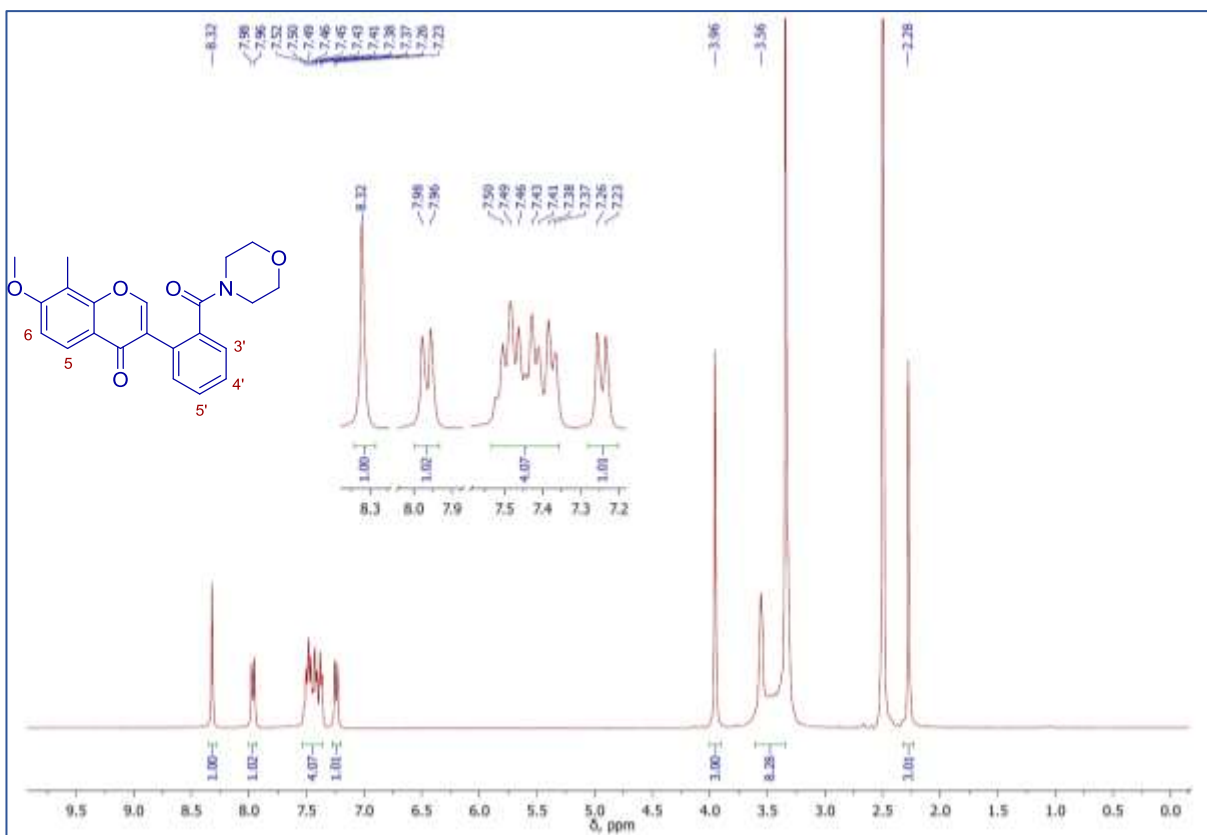
¹³C NMR spectrum of 6-methoxy-3-[2-(morpholine-4-carbonyl)phenyl]-4H-1-benzopyran-4-one (**4b**)



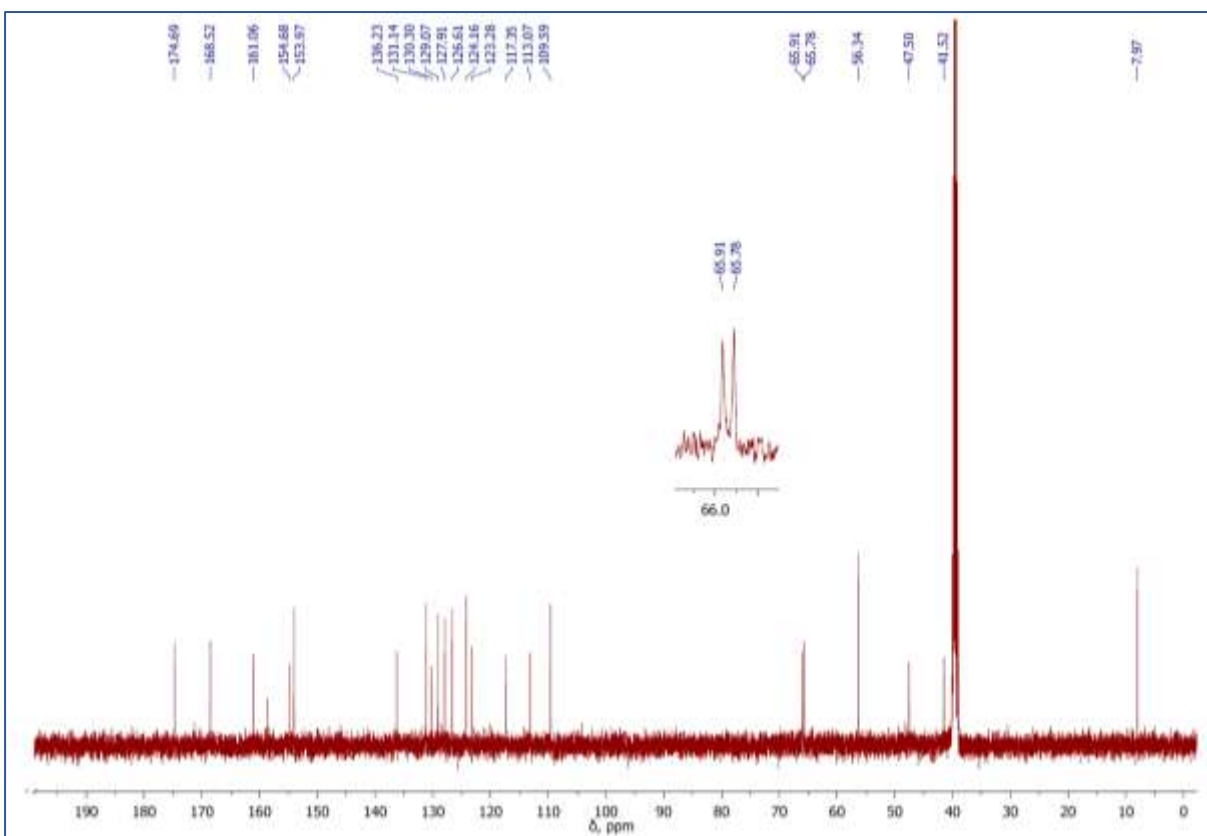
¹H NMR spectrum of 7-methoxy-3-[2-(morpholine-4-carbonyl)phenyl]-4H-1-benzopyran-4-one (**4c**)



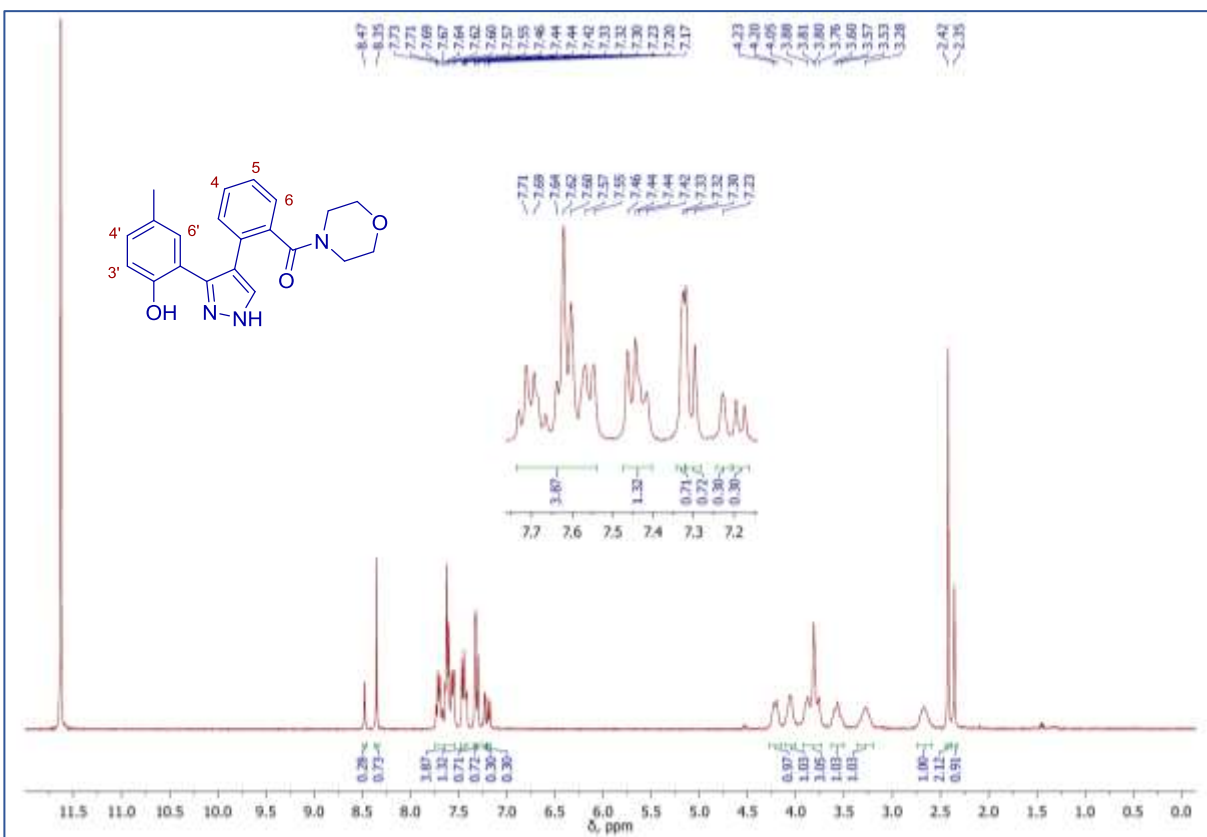
¹³C NMR spectrum of 7-methoxy-3-[2-(morpholine-4-carbonyl)phenyl]-4H-1-benzopyran-4-one (**4c**)



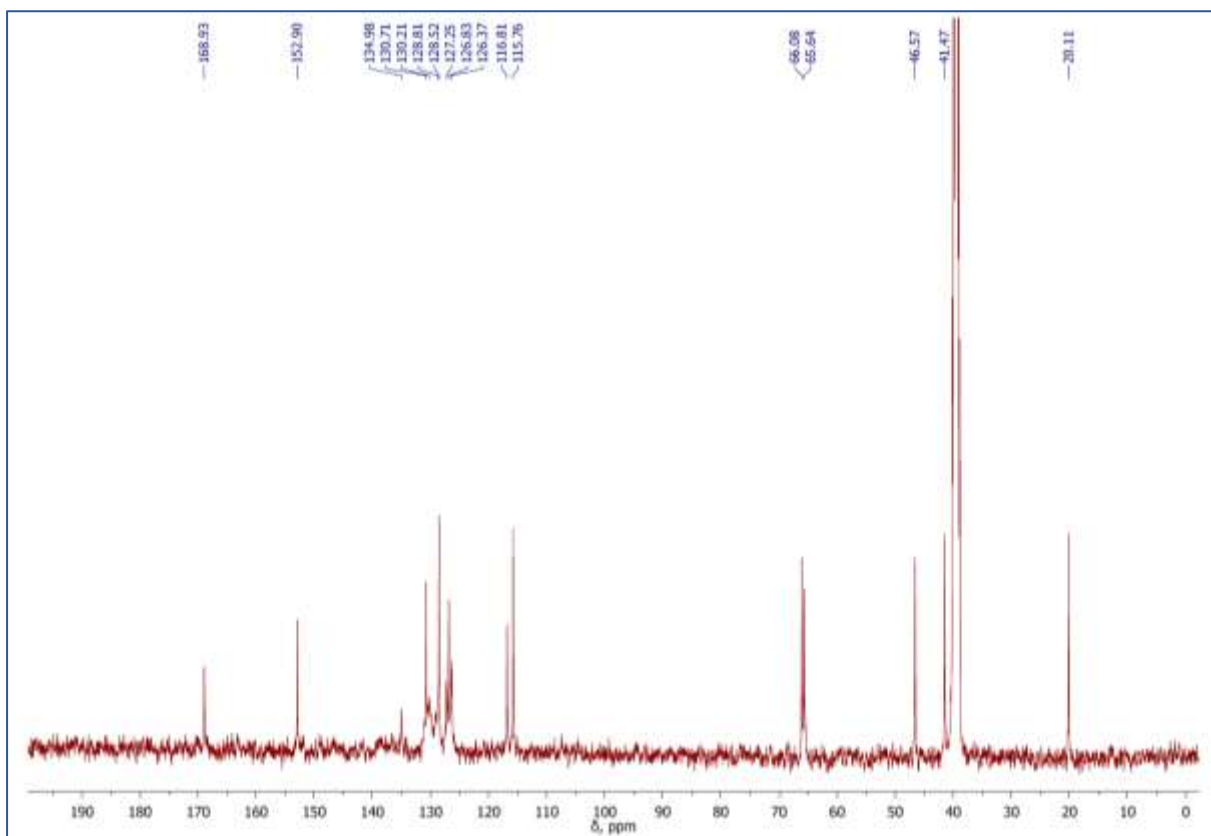
¹H NMR spectrum of 7-methoxy-8-methyl-3-[2-(morpholine-4-carbonyl)phenyl]-4H-1-benzopyran-4-one (**4d**)



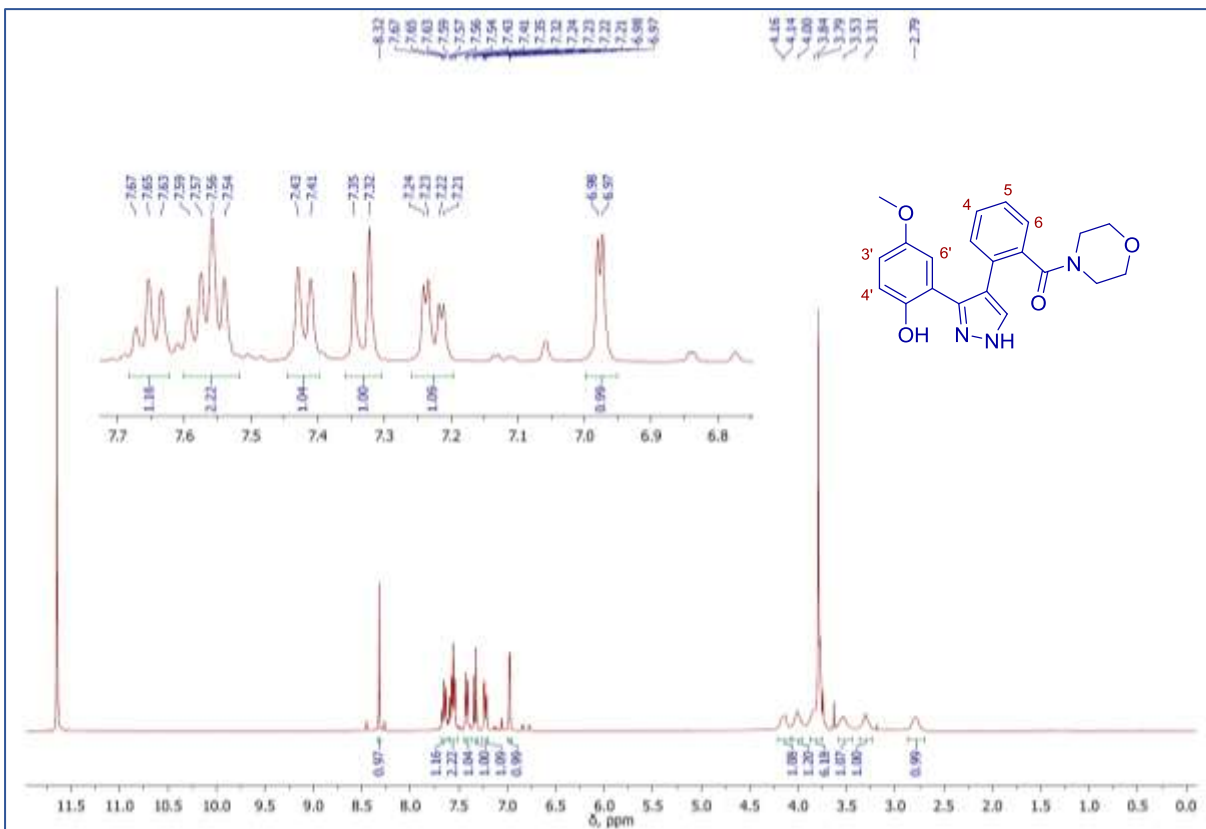
¹³C NMR spectrum of 7-methoxy-8-methyl-3-[2-(morpholine-4-carbonyl)phenyl]-4H-1-benzopyran-4-one (**4d**)



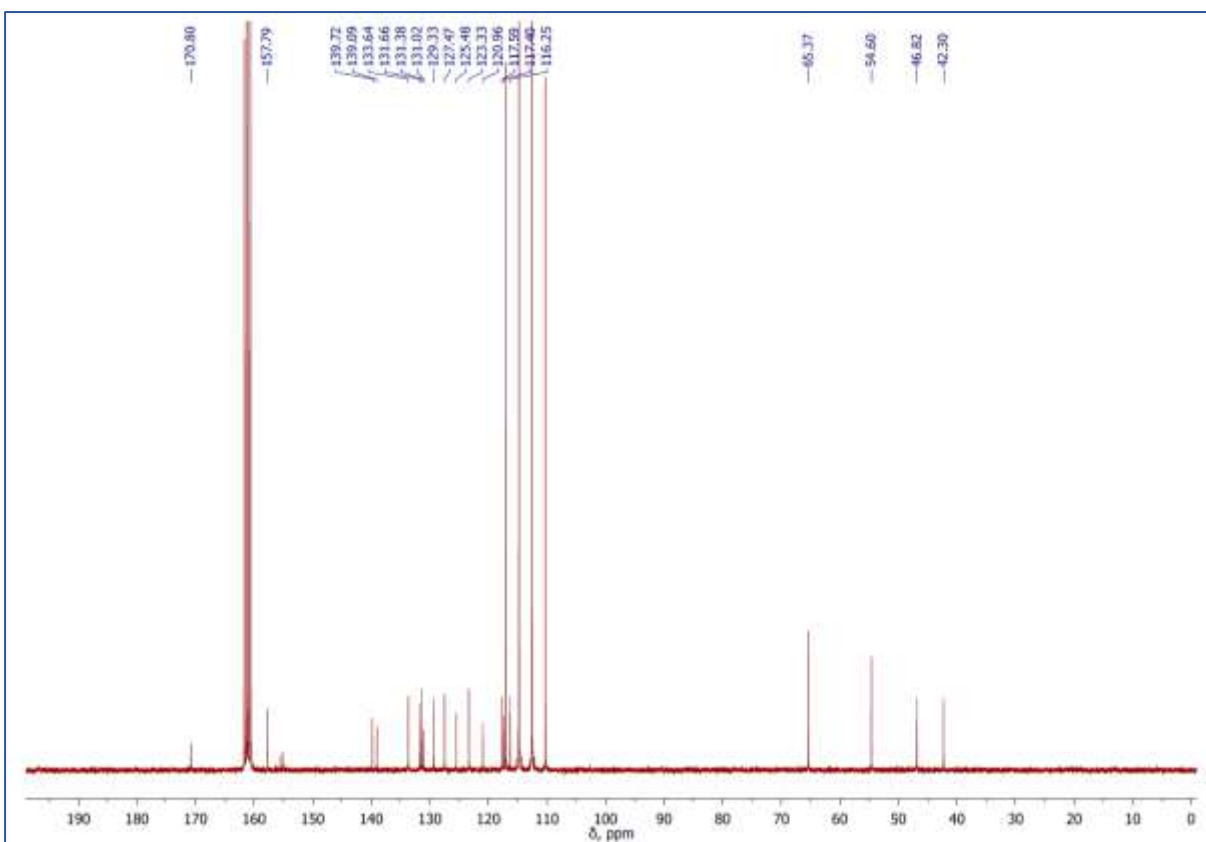
¹H NMR spectrum of {2-[3-(2-hydroxy-5-methylphenyl)-1H-pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (**5a**)



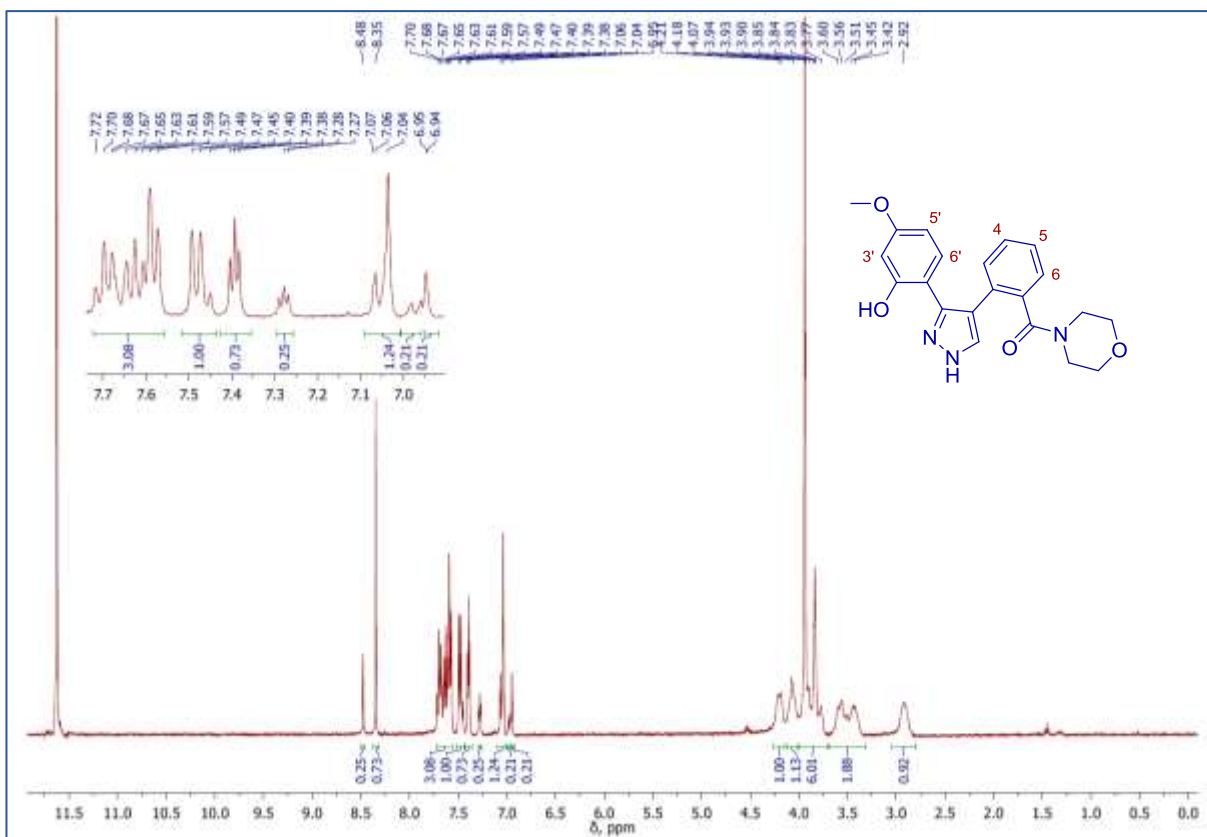
¹³C NMR spectrum of {2-[3-(2-hydroxy-5-methylphenyl)-1H-pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (**5a**)



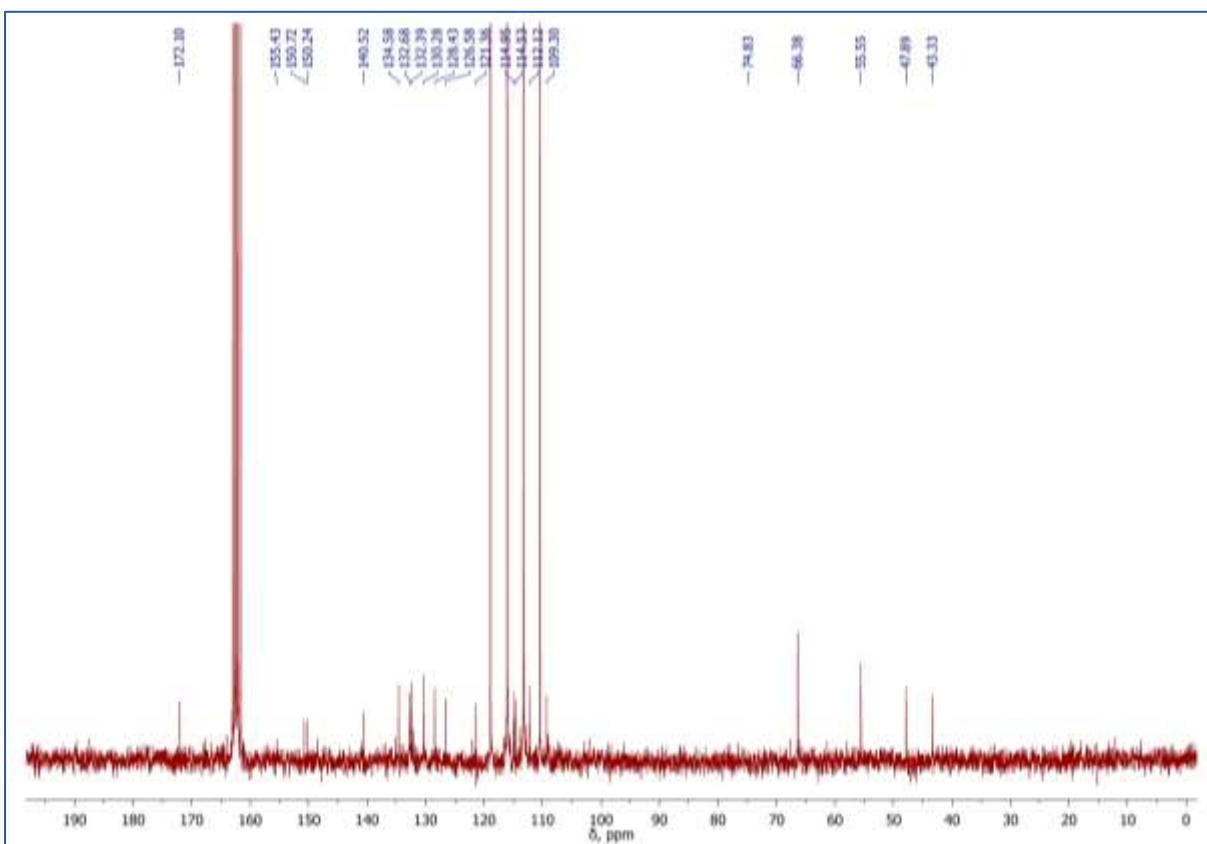
¹H NMR spectrum of {2-[3-(2-hydroxy-5-methoxyphenyl)-1*H*-pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (**5b**)



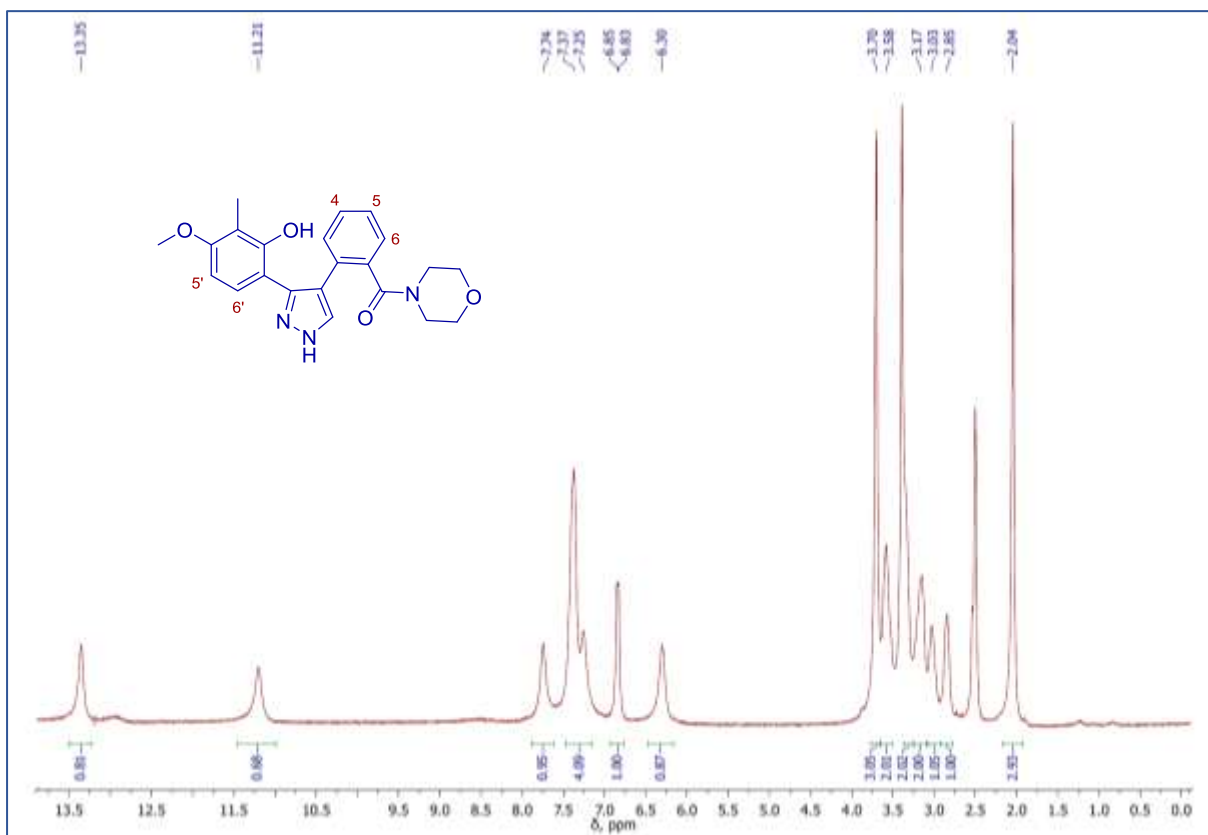
¹³C NMR spectrum of {2-[3-(2-hydroxy-5-methoxyphenyl)-1*H*-pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (**5b**)



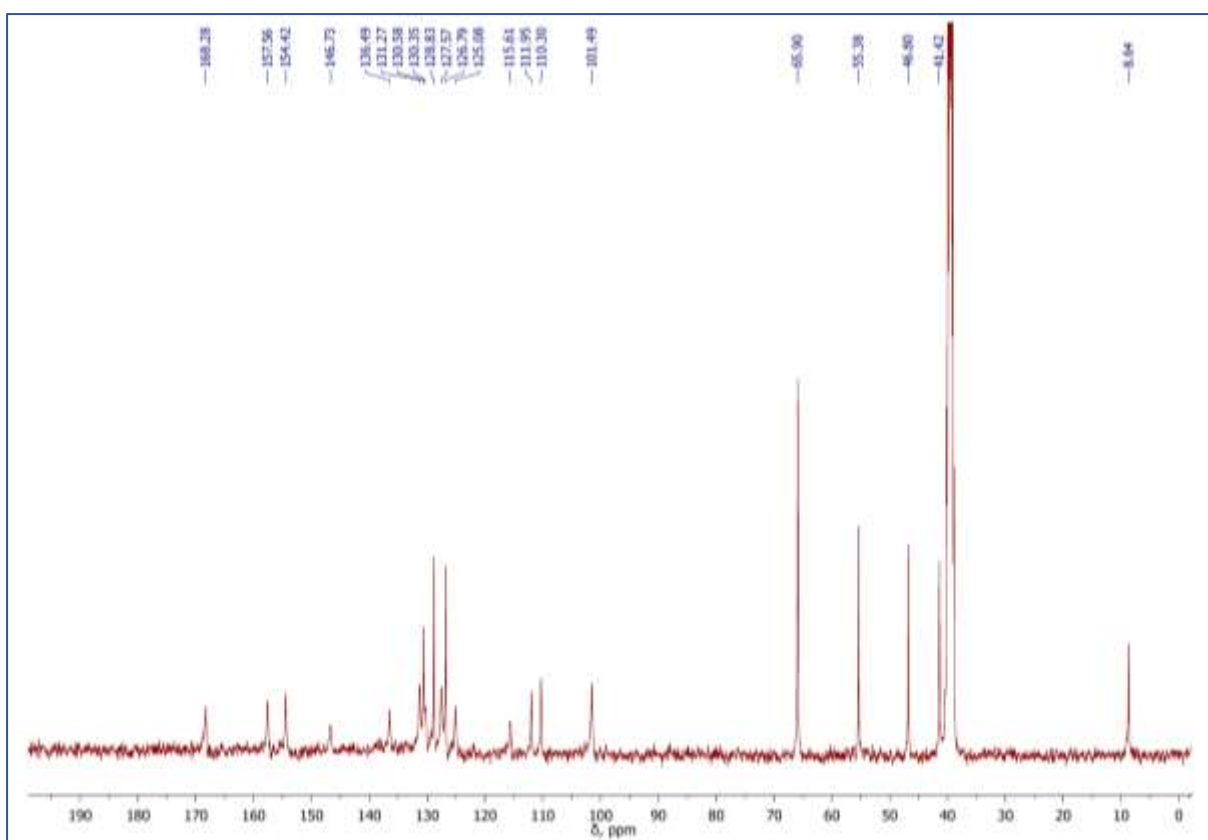
¹H NMR spectrum of {2-[3-(2-hydroxy-4-methoxyphenyl)-1*H*-pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (**5c**)



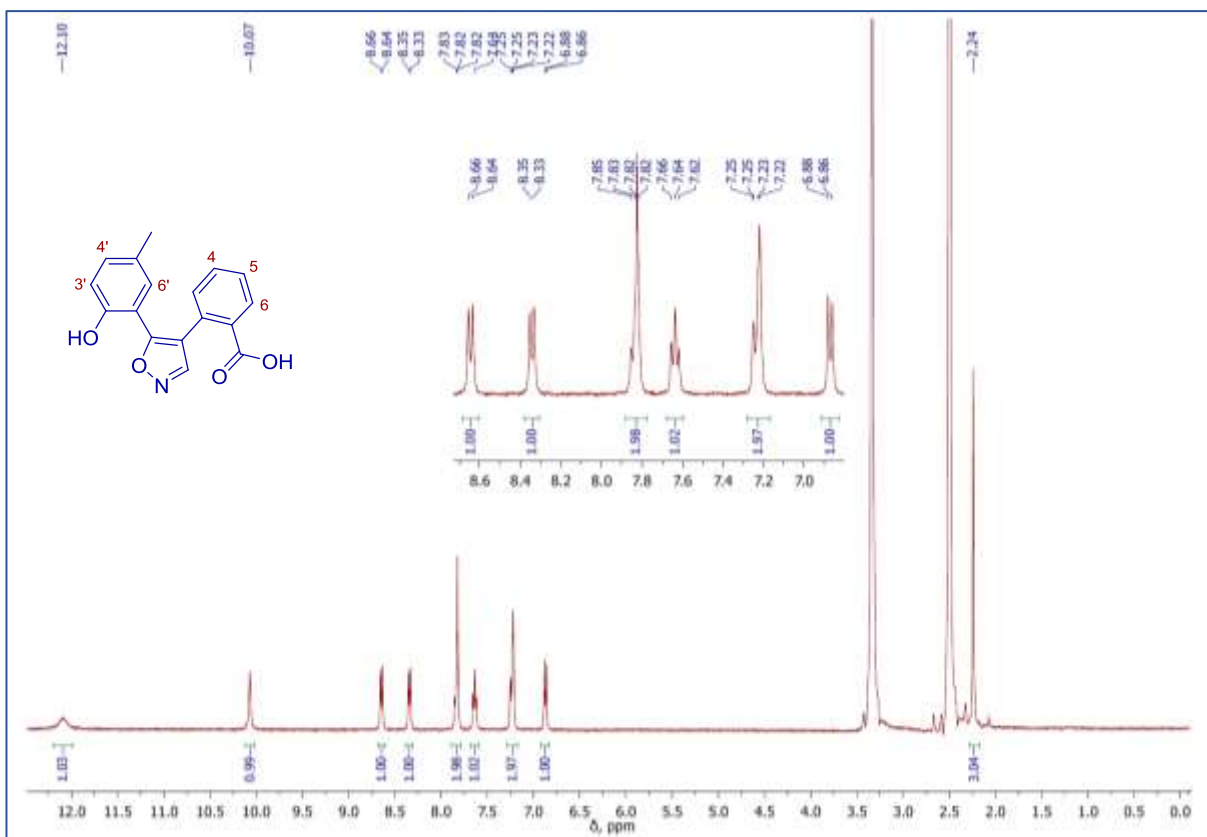
¹³C NMR spectrum of {2-[3-(2-hydroxy-4-methoxyphenyl)-1*H*-pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (**5c**)



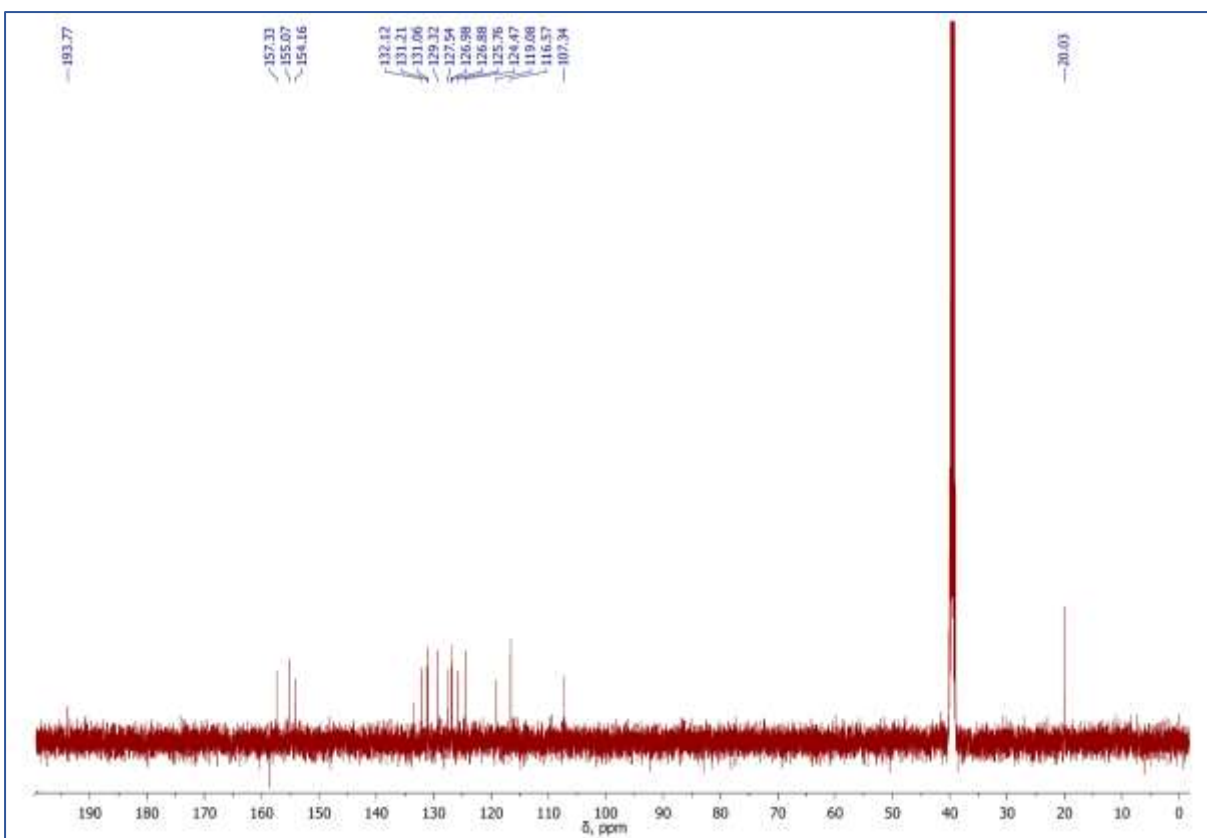
^1H NMR spectrum of {2-[3-(2-hydroxy-4-methoxy-3-methylphenyl)-1*H*-pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (**5d**)



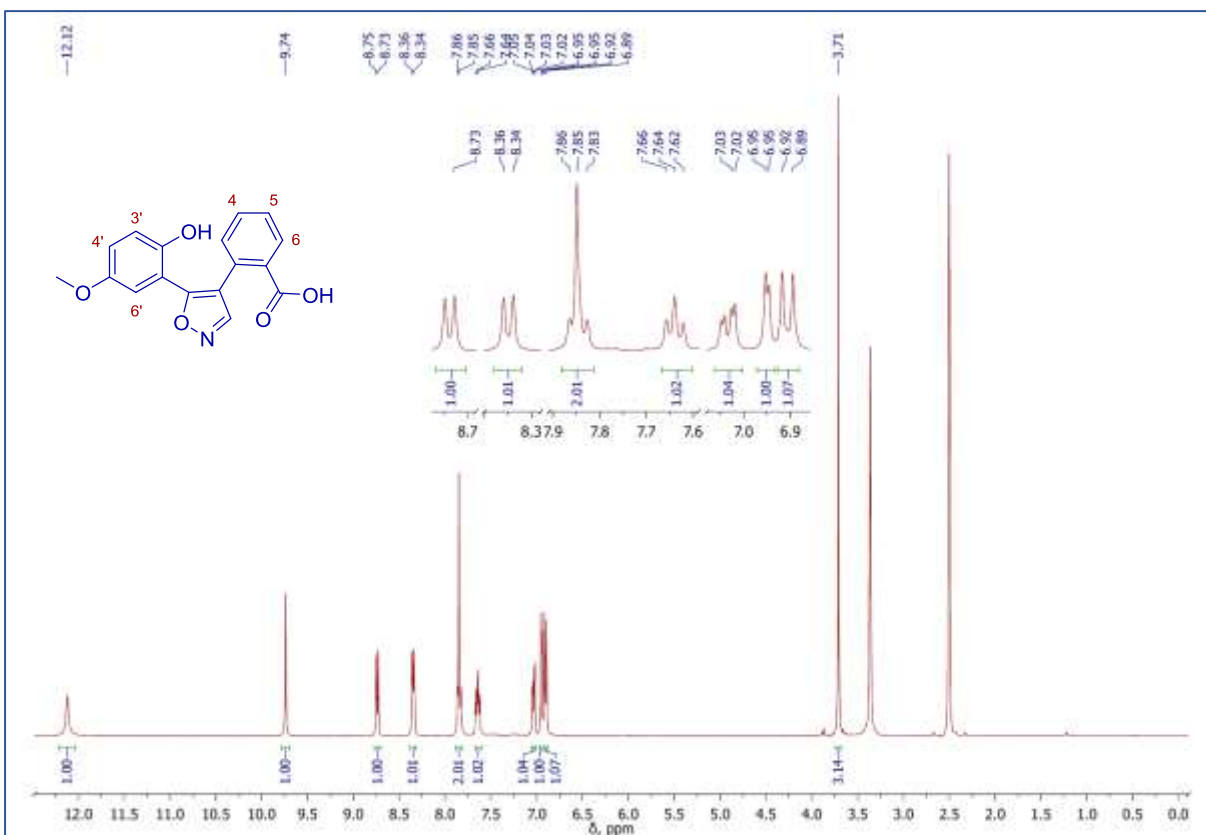
^{13}C NMR spectrum of {2-[3-(2-hydroxy-4-methoxy-3-methylphenyl)-1*H*-pyrazol-4-yl]phenyl}(morpholin-4-yl)methanone (**5d**)



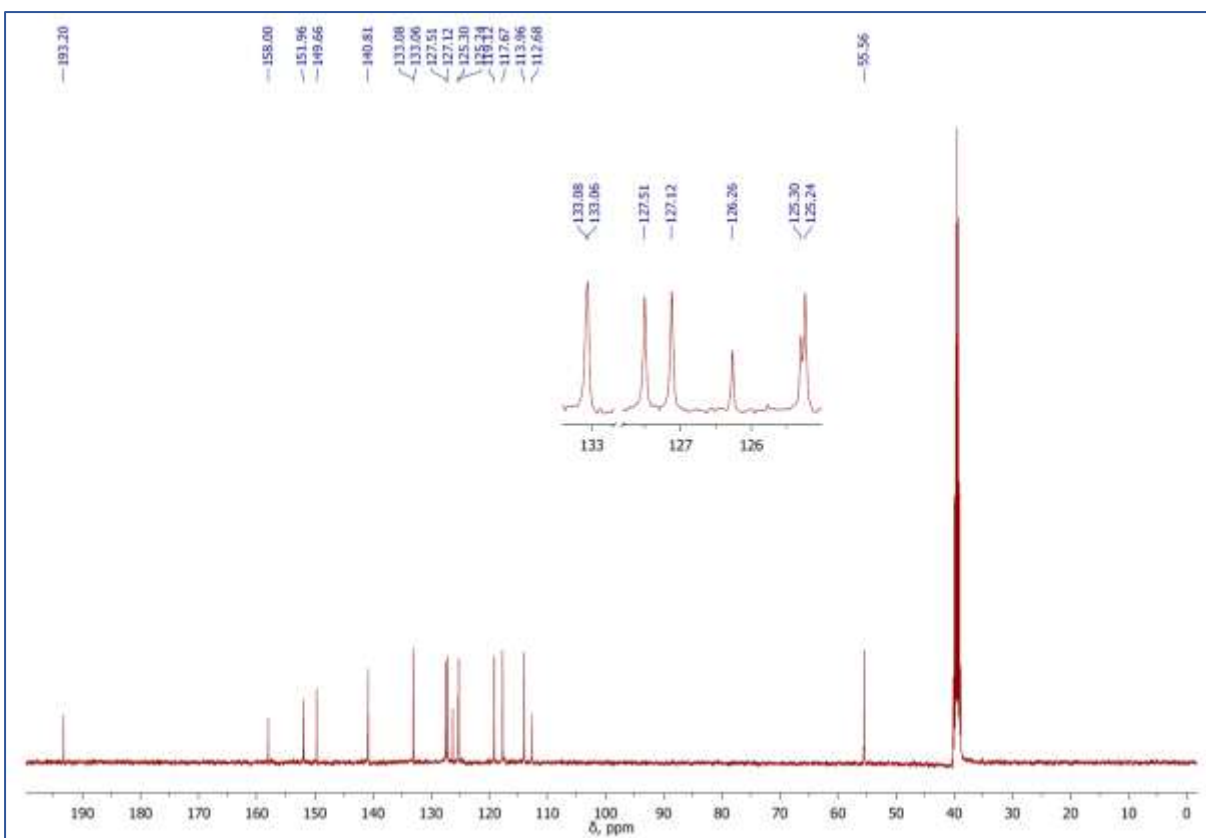
¹H NMR spectrum of 2-[5-(2-hydroxy-5-methylphenyl)-1,2-oxazol-4-yl]benzoic acid (**6a**)



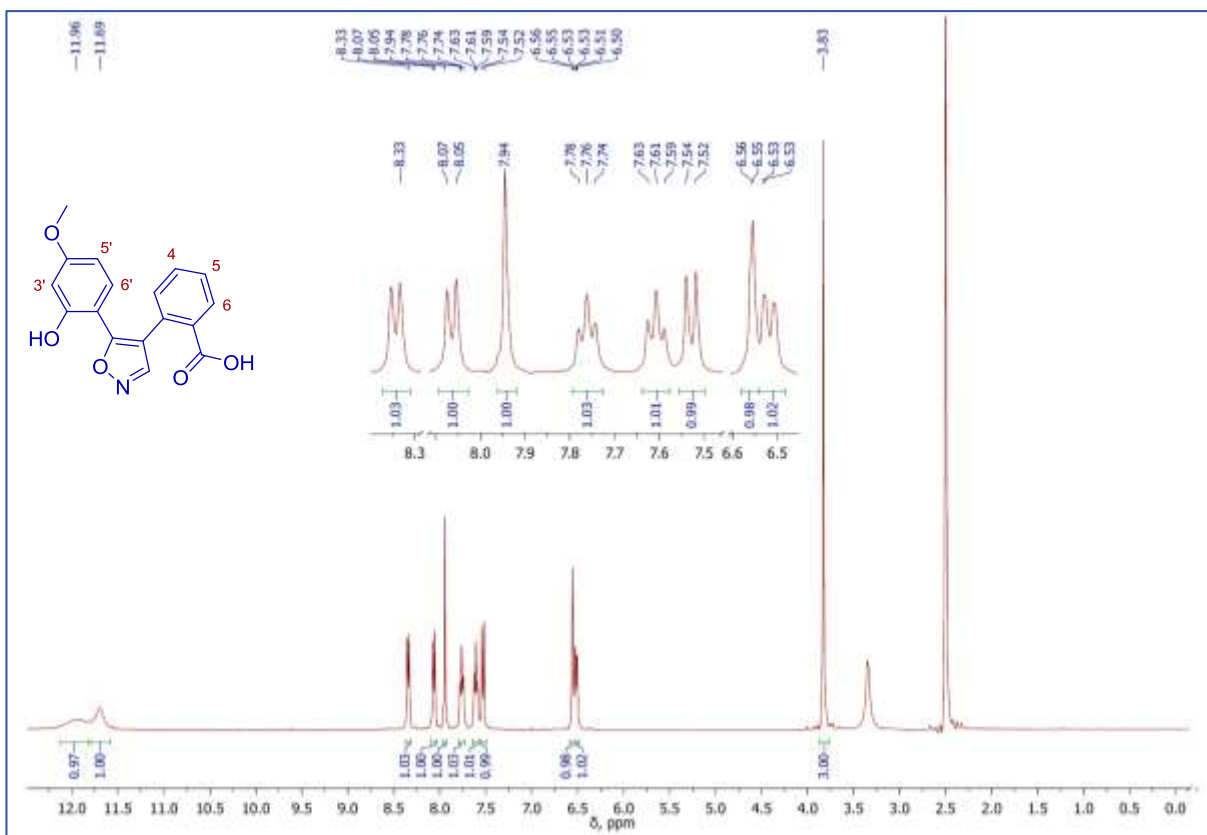
¹³C NMR spectrum of 2-[5-(2-hydroxy-5-methylphenyl)-1,2-oxazol-4-yl]benzoic acid (**6a**)



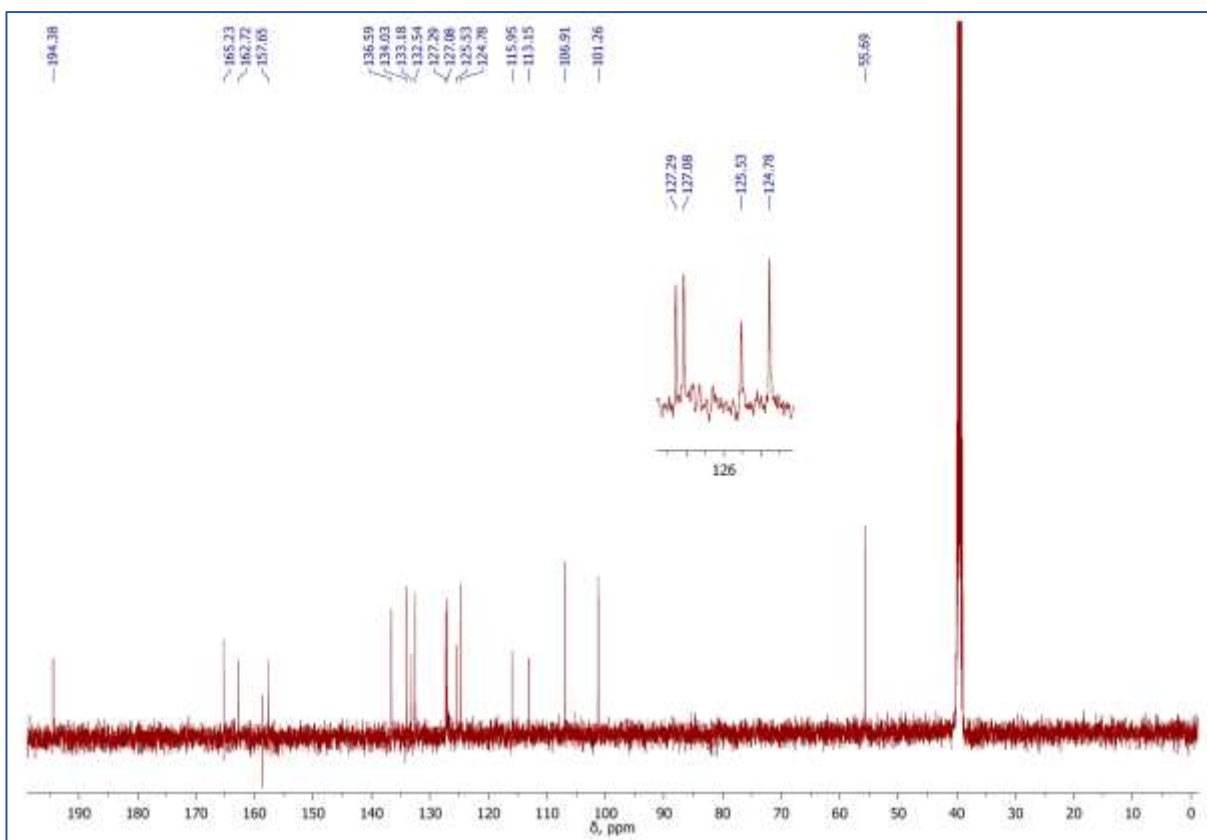
¹H NMR spectrum of 2-[5-(2-hydroxy-5-methoxyphenyl)-1,2-oxazol-4-yl]benzoic acid (**6b**)



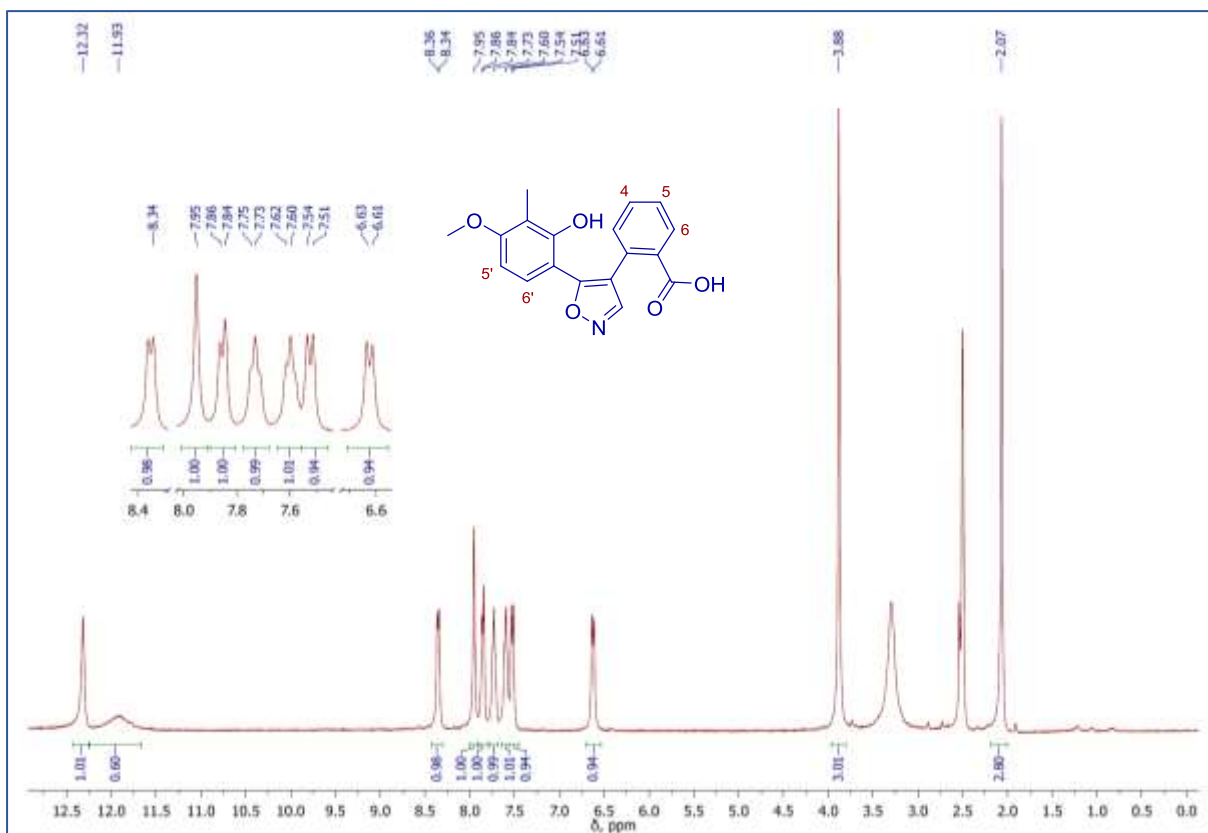
¹³C NMR spectrum of 2-[5-(2-hydroxy-5-methoxyphenyl)-1,2-oxazol-4-yl]benzoic acid (**6b**)



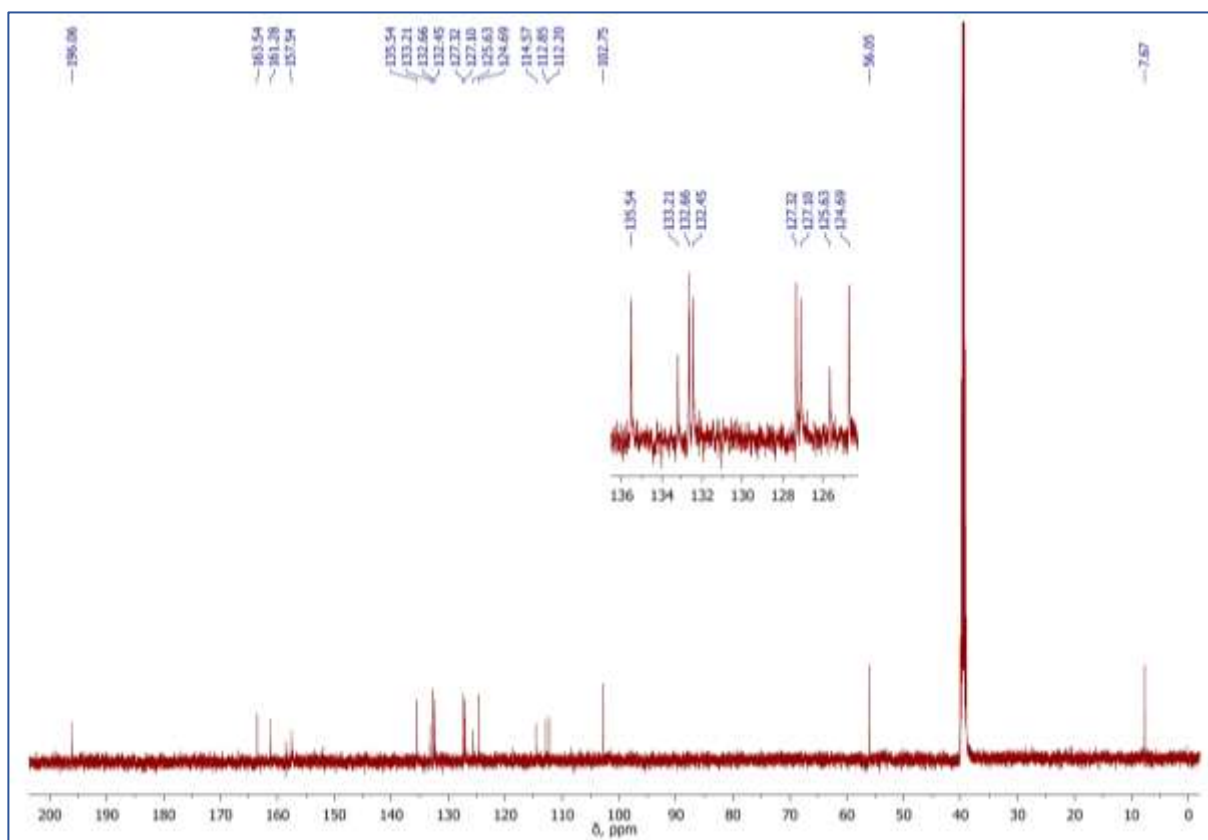
¹H NMR spectrum of 2-[5-(2-hydroxy-4-methoxyphenyl)-1,2-oxazol-4-yl]benzoic acid (**6c**)



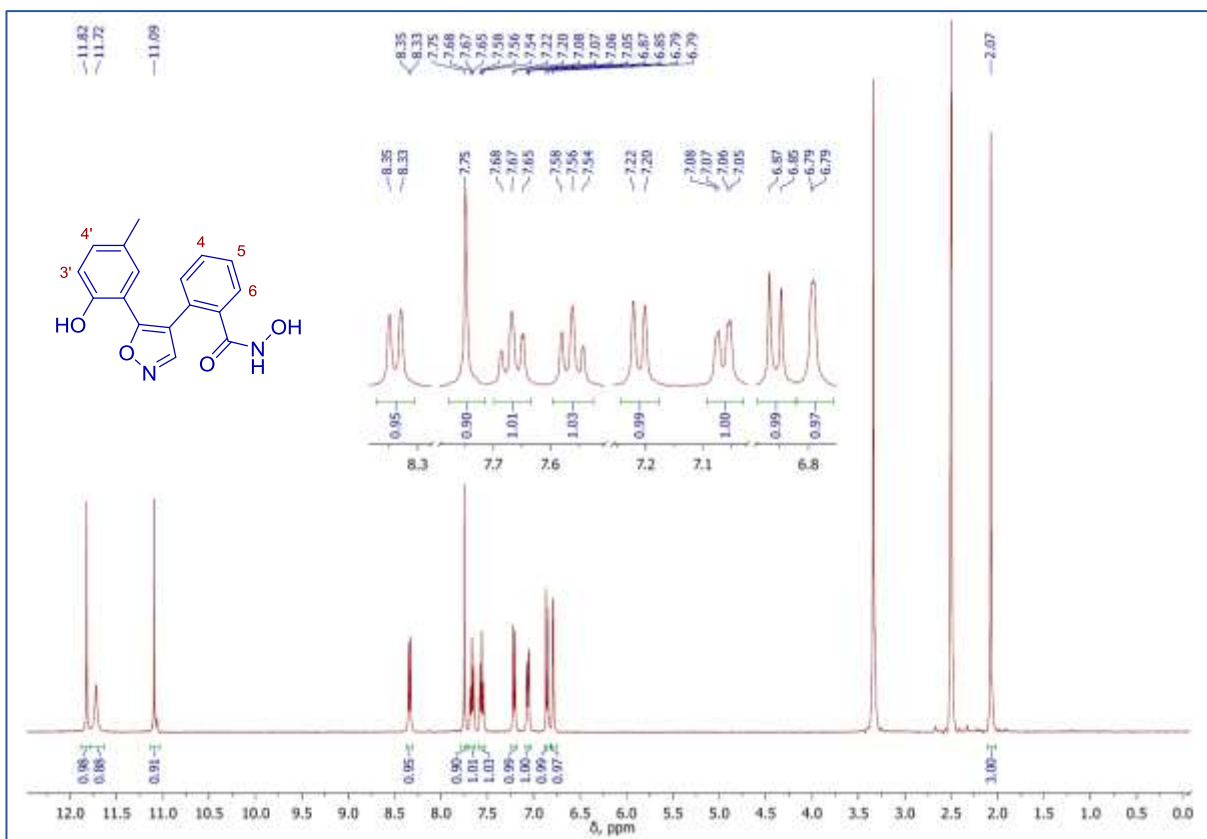
¹³C NMR spectrum of 2-[5-(2-hydroxy-4-methoxyphenyl)-1,2-oxazol-4-yl]benzoic acid (**6c**)



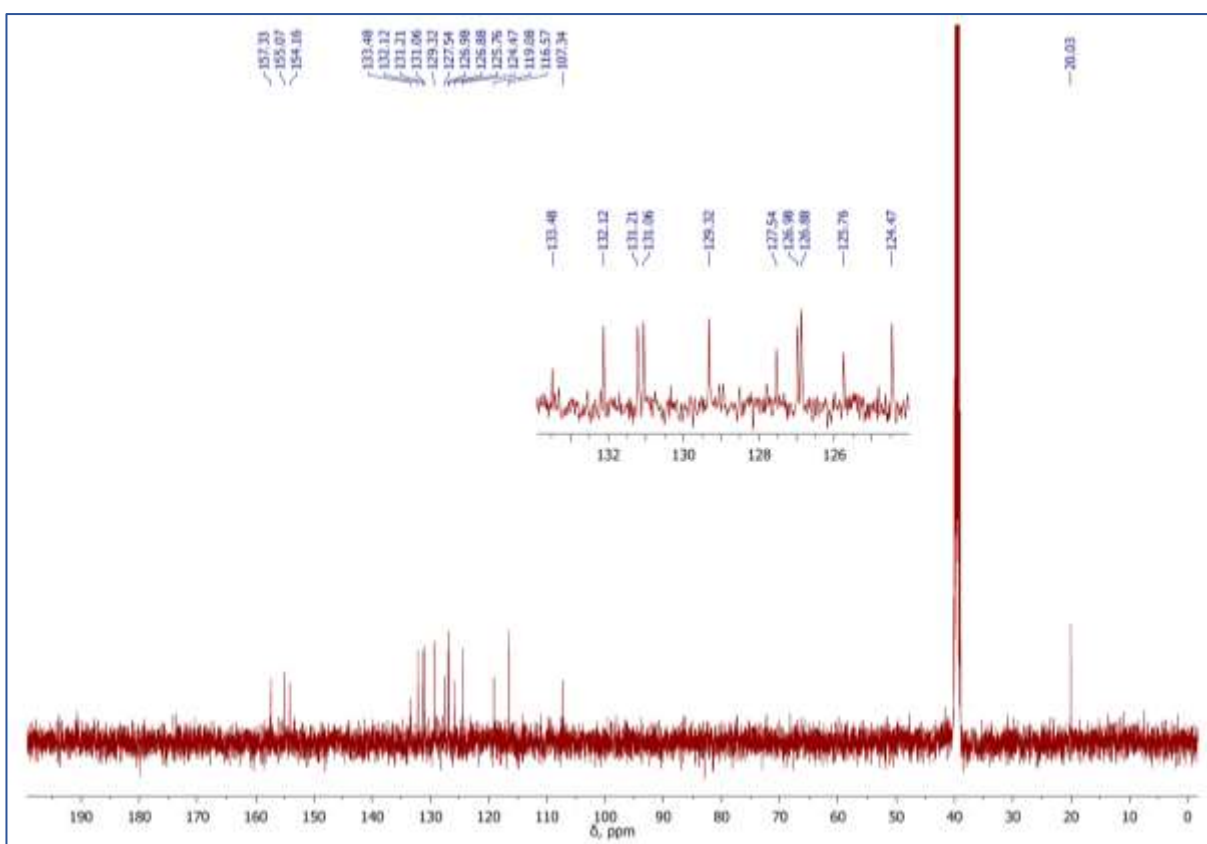
¹H NMR spectrum of 2-[5-(2-hydroxy-4-methoxy-5-methylphenyl)-1,2-oxazol-4-yl]benzoic acid (**6d**)



¹³C NMR spectrum of 2-[5-(2-hydroxy-4-methoxy-5-methylphenyl)-1,2-oxazol-4-yl]benzoic acid (**6d**)



¹H NMR spectrum of *N*-hydroxy-2-[5-(2-hydroxy-5-methylphenyl)-1,2-oxazol-4-yl]benzamide (**7a**)



¹³C NMR spectrum of *N*-hydroxy-2-[5-(2-hydroxy-5-methylphenyl)-1,2-oxazol-4-yl]benzamide (**7a**)