Supporting Information

Synthesis and SAR Studies of Novel Pyrazolopyridine Derivatives as Inhibitors of Enterovirus Replication

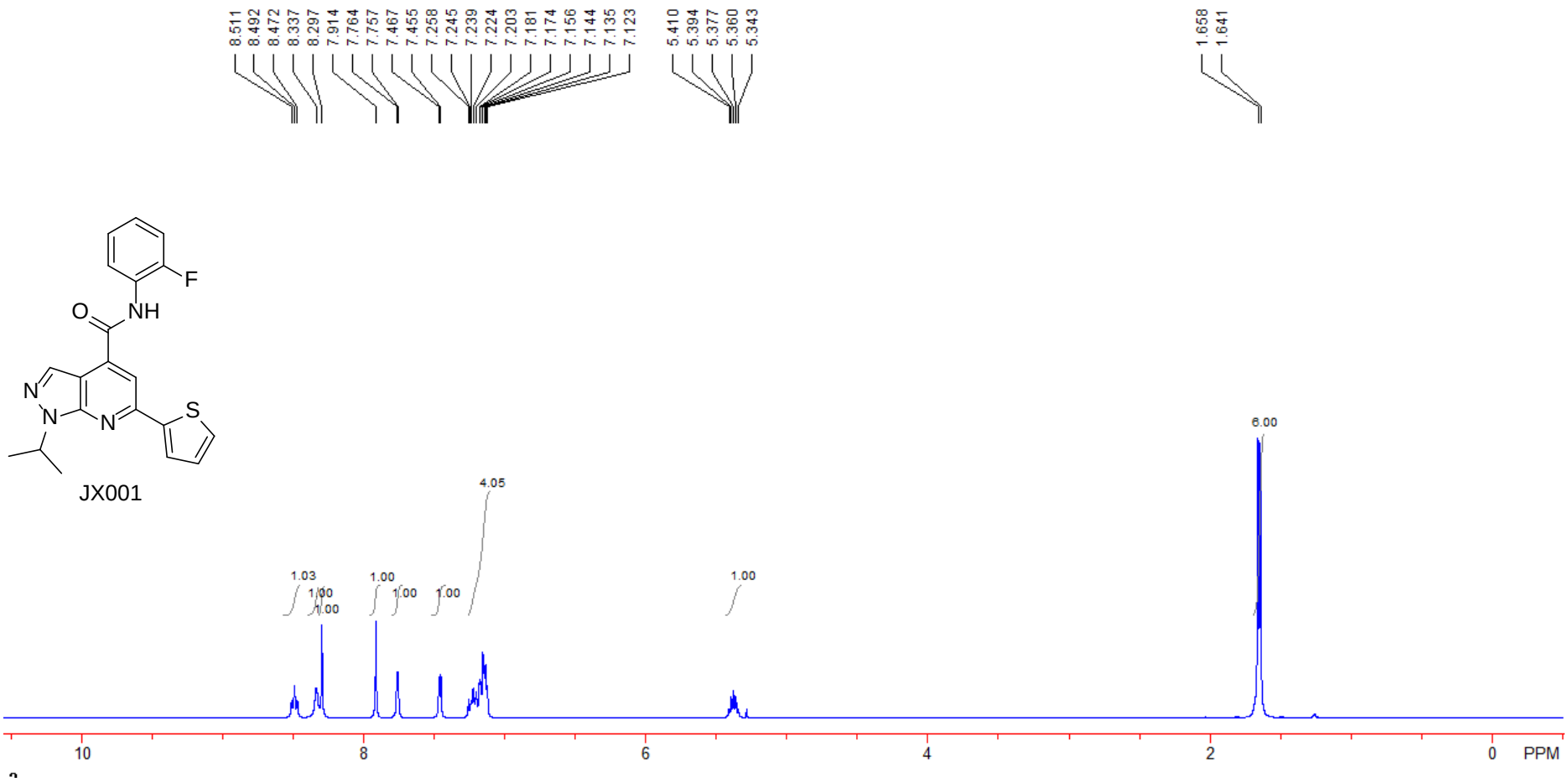
Yanpeng Xing,[#,¥] *Jun Zuo,*[‡,¥] *Paul Krogstad,* *[‡,§] *and Michael E. Jung** [#,§]

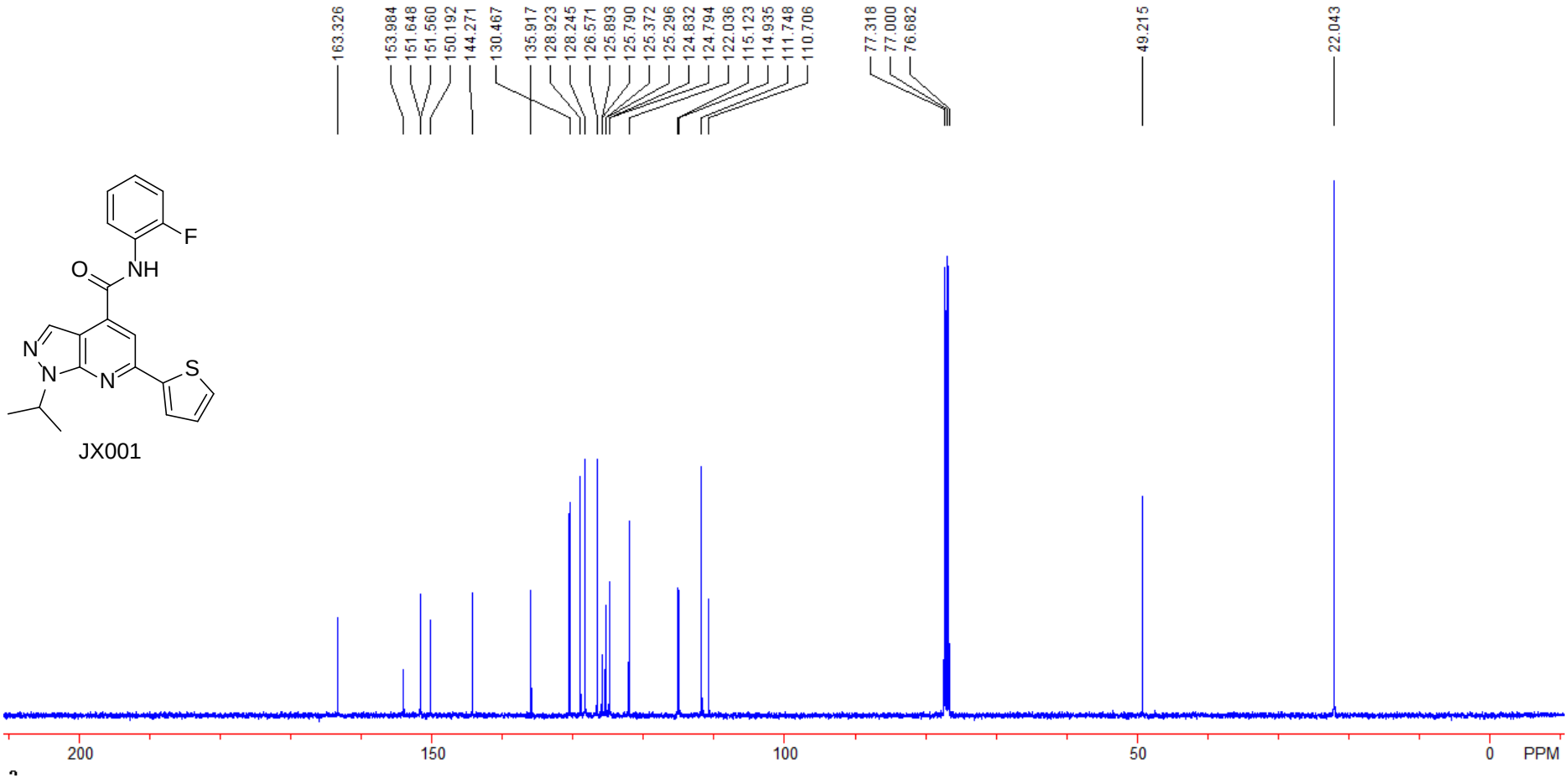
#Department of Chemistry and Biochemistry, ‡Department of Pediatrics, and §Department of Molecular and Medical Pharmacology, University of California, Los Angeles, CA 90095

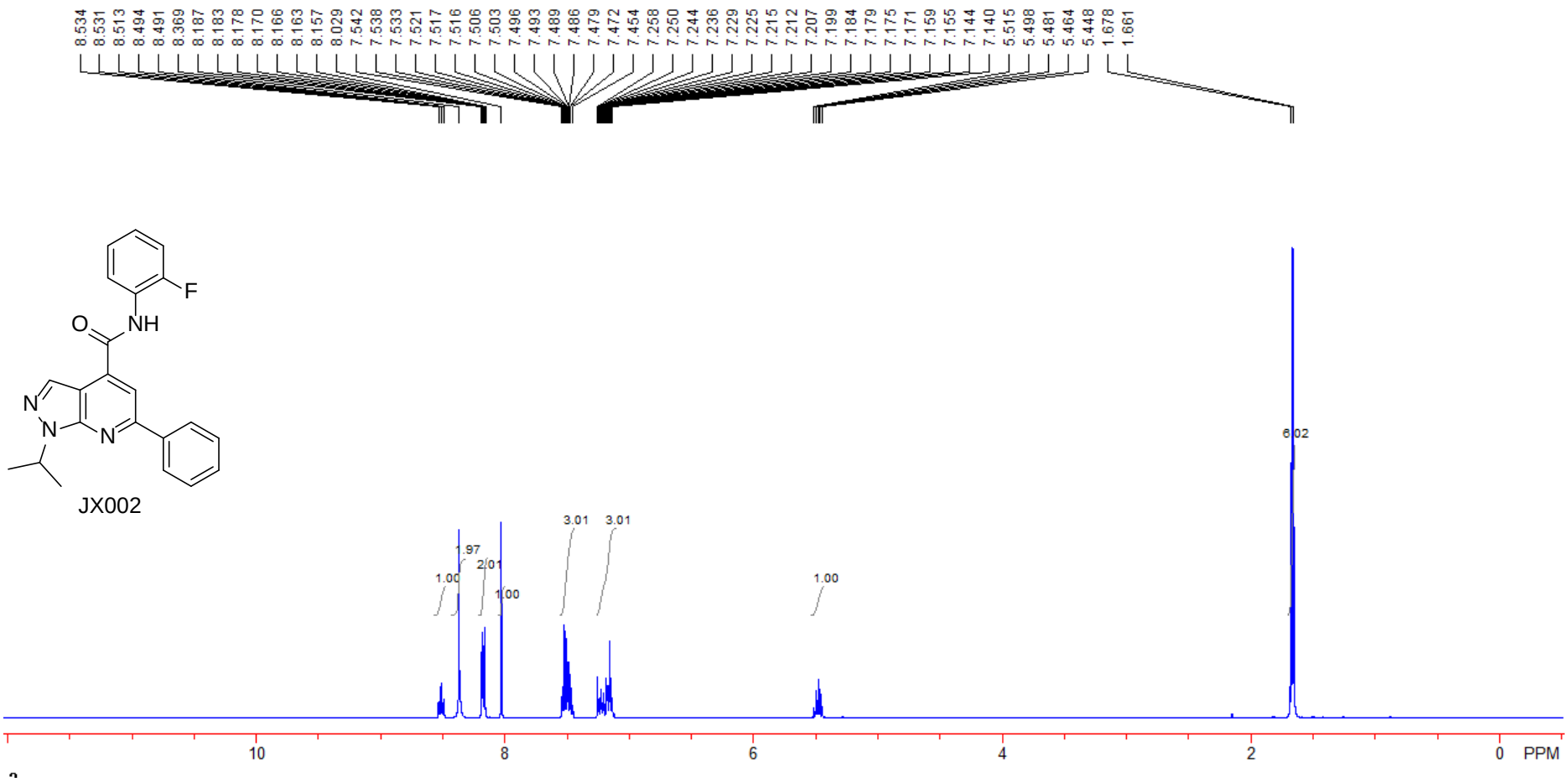
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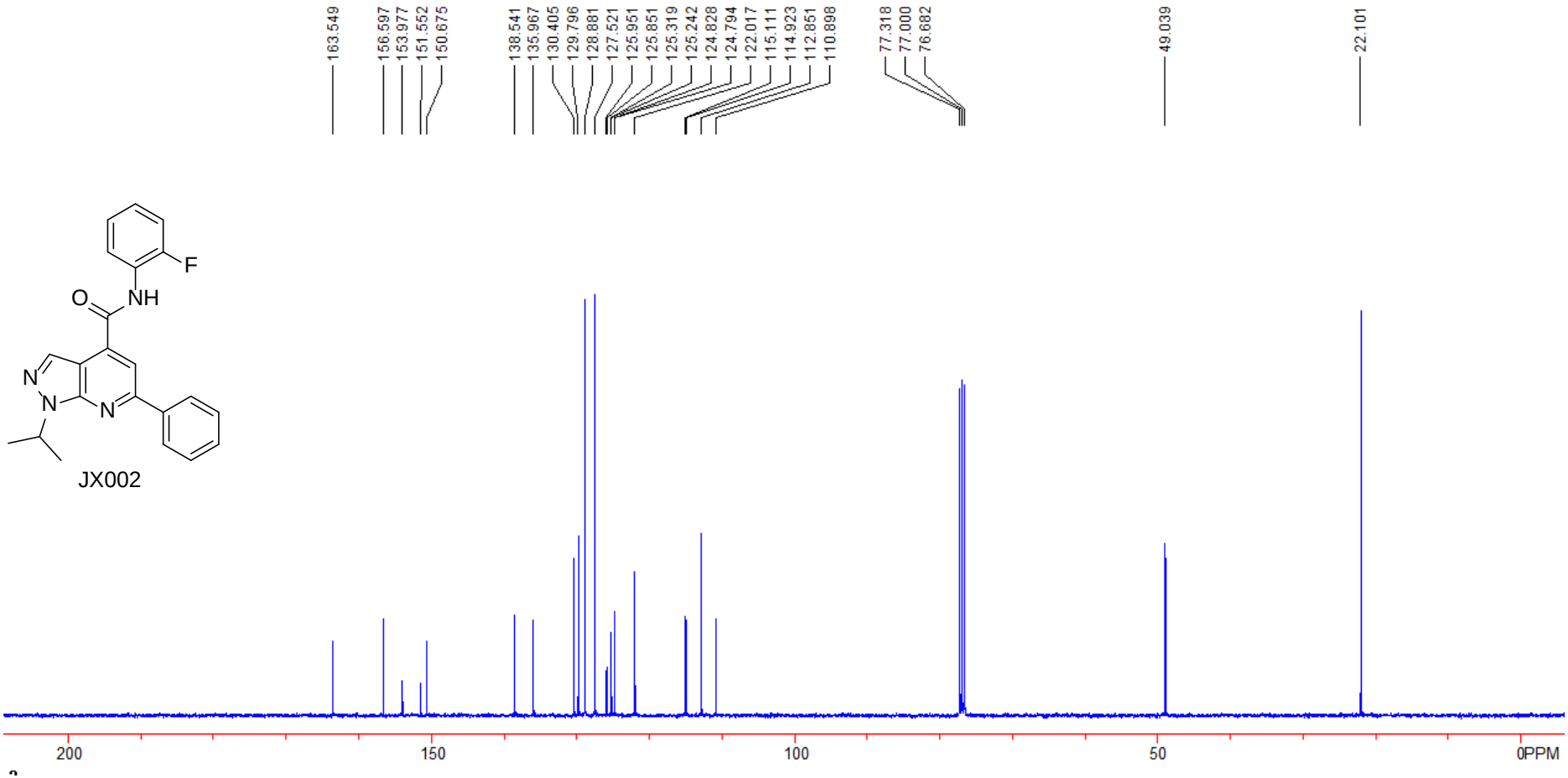
^{1}H and ^{13}C NMR Spectra of JX001 – JX076 .....S2

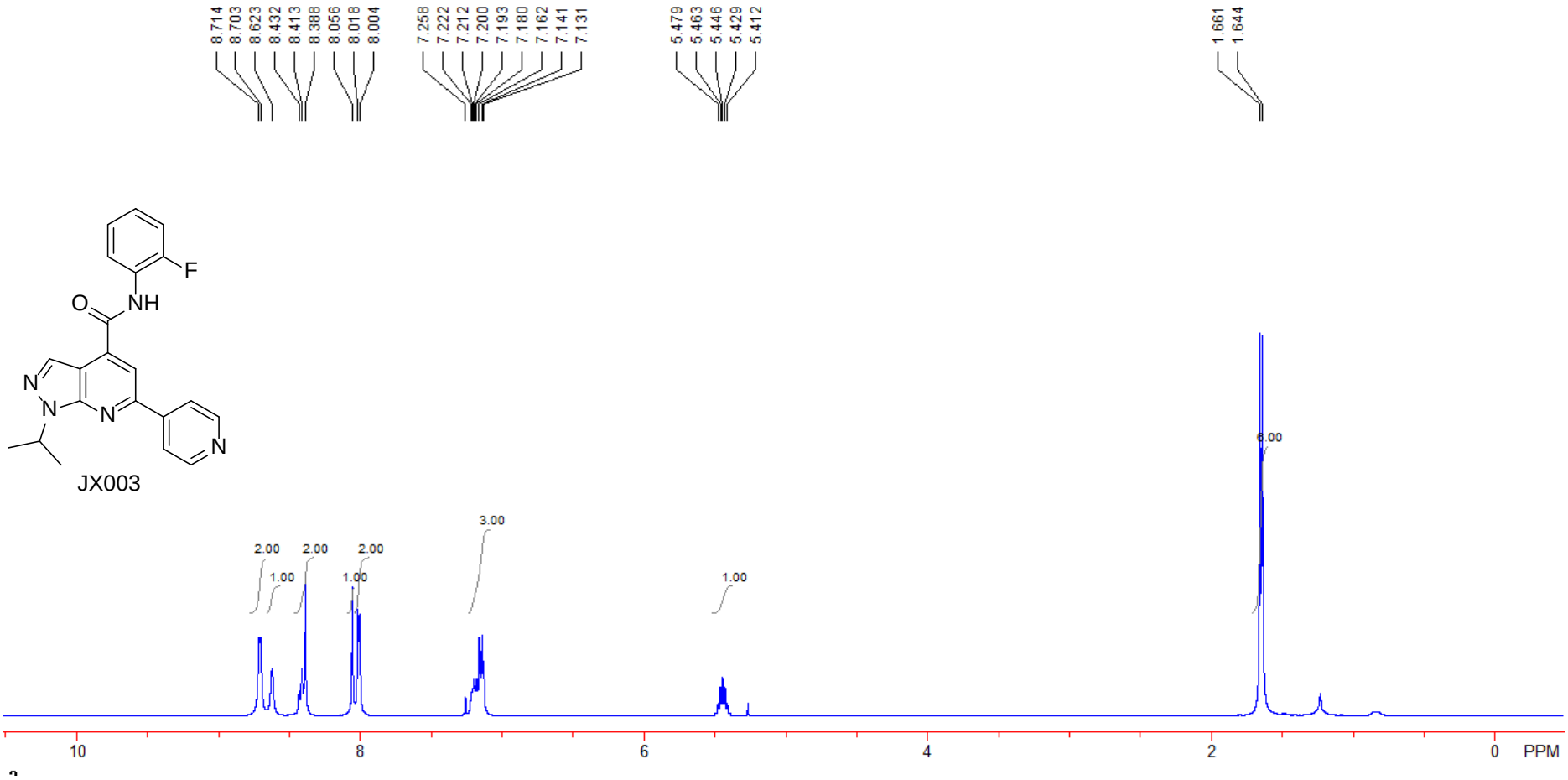
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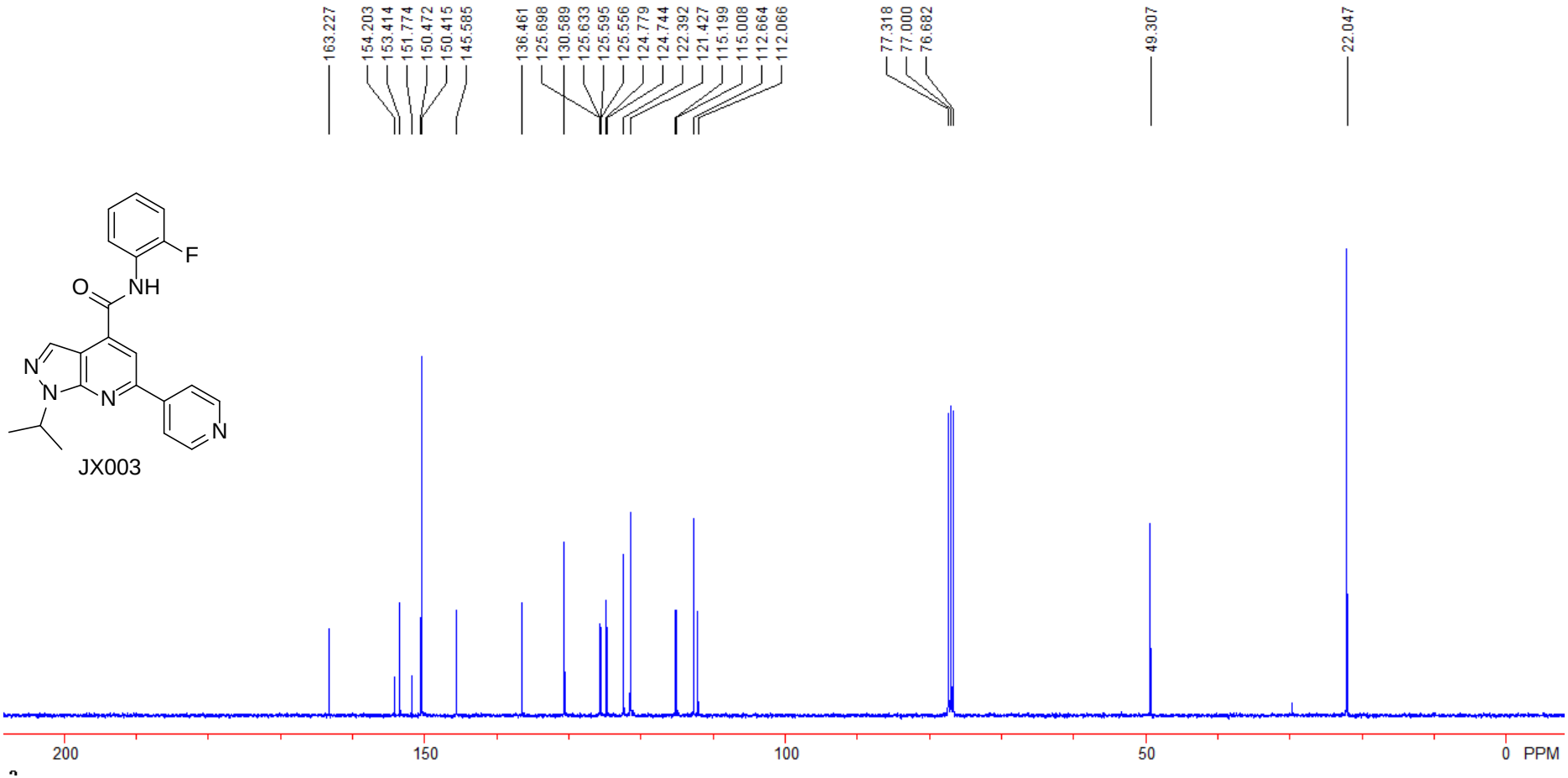

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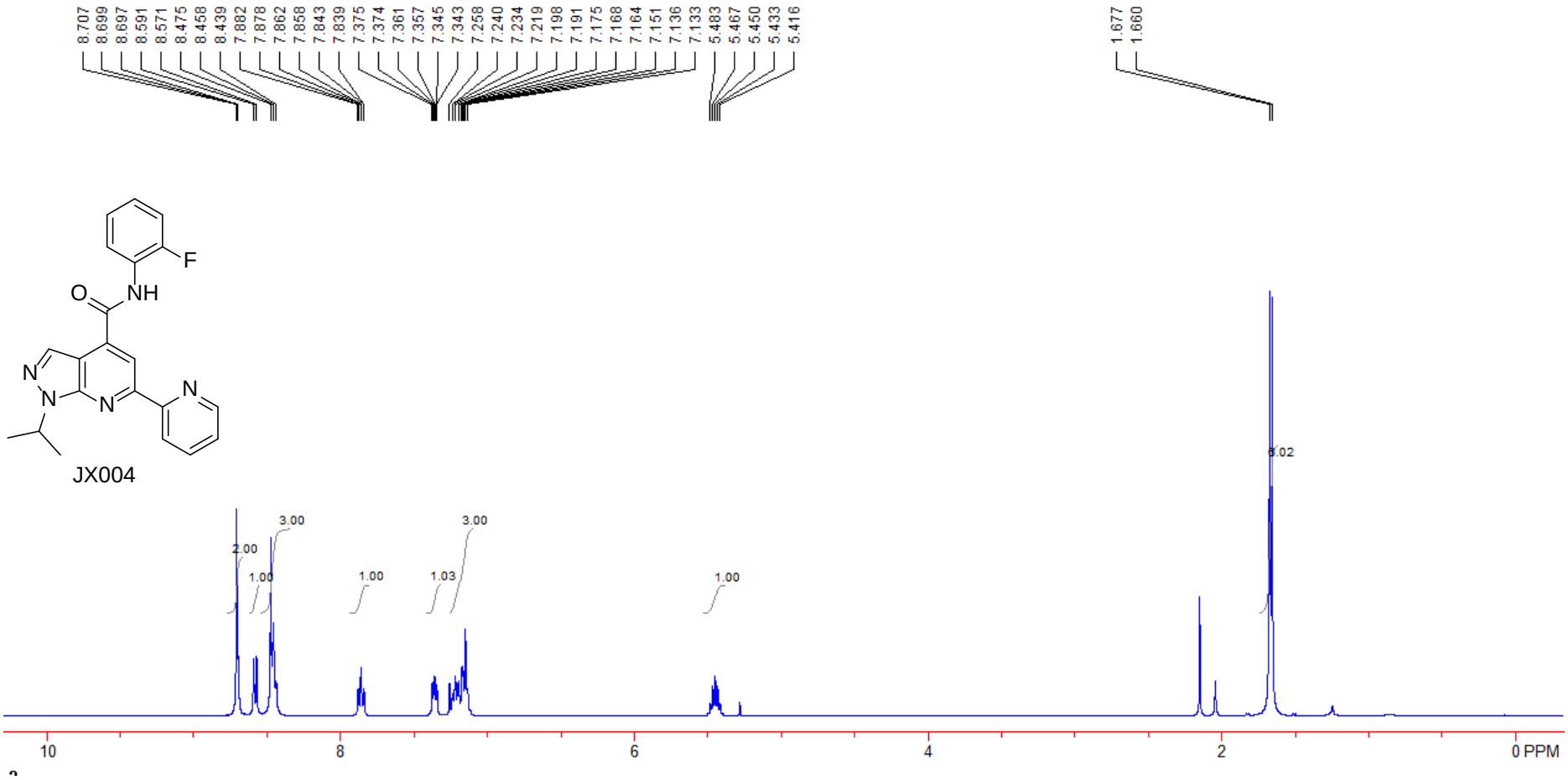

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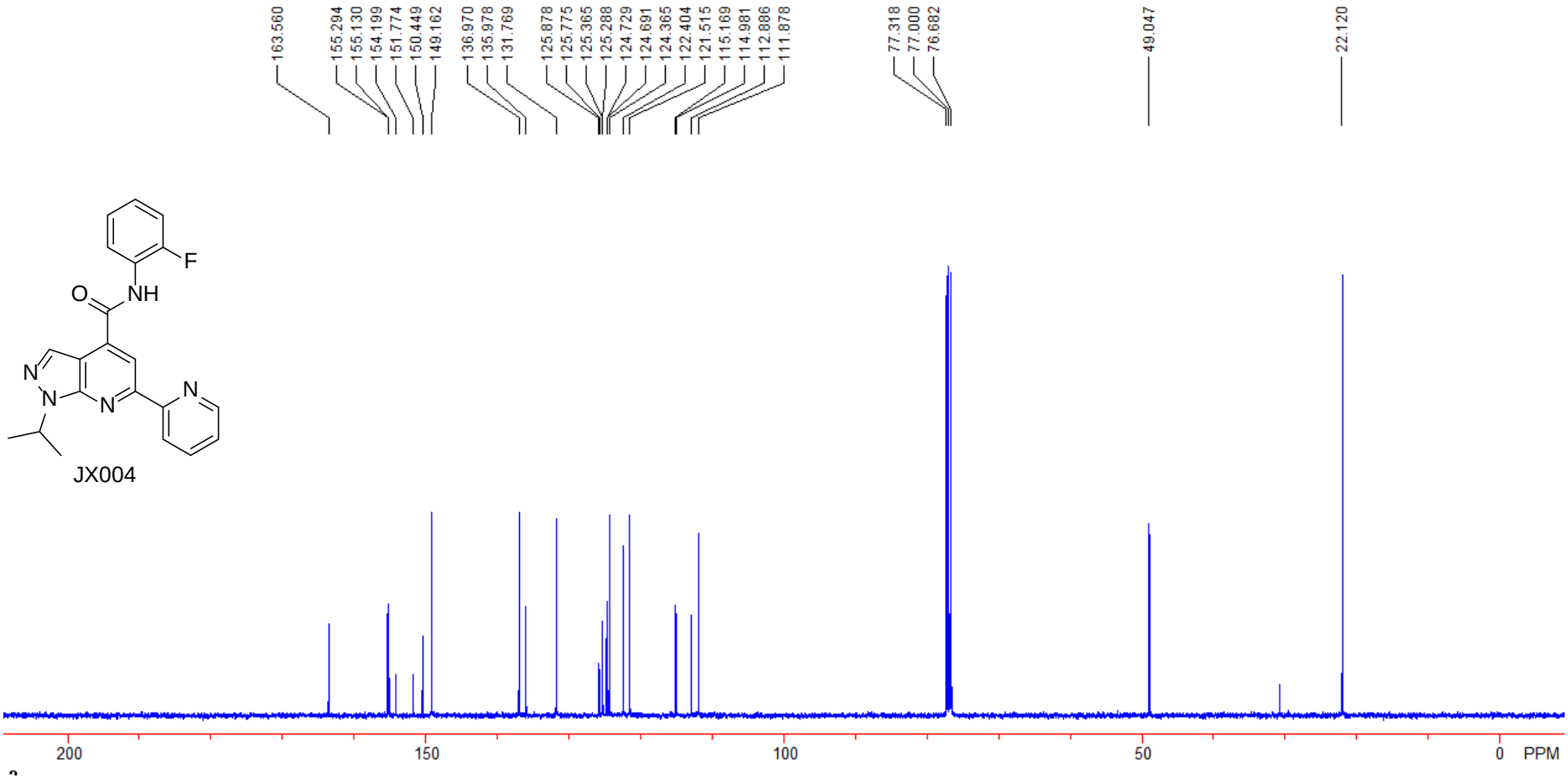

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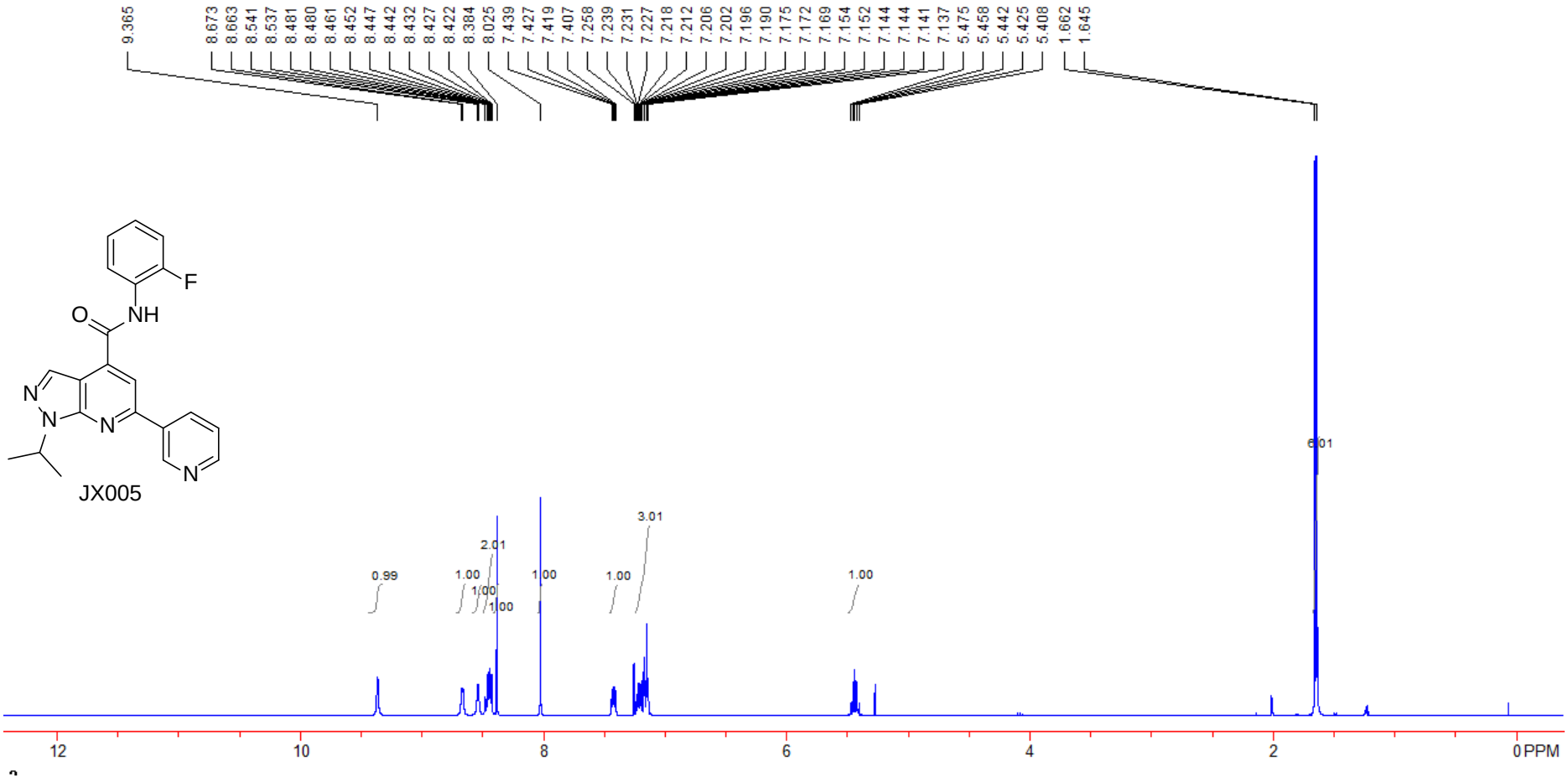

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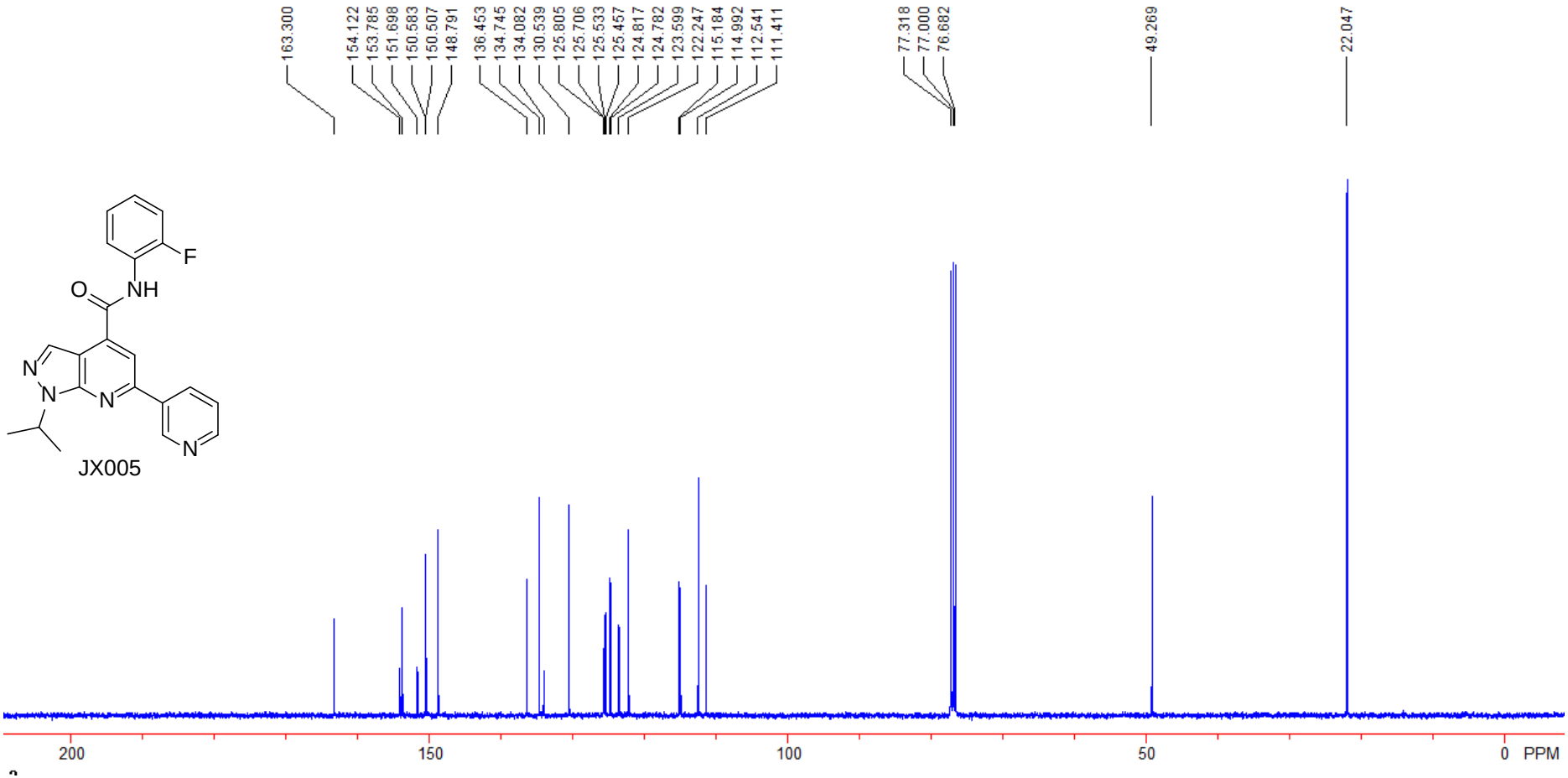

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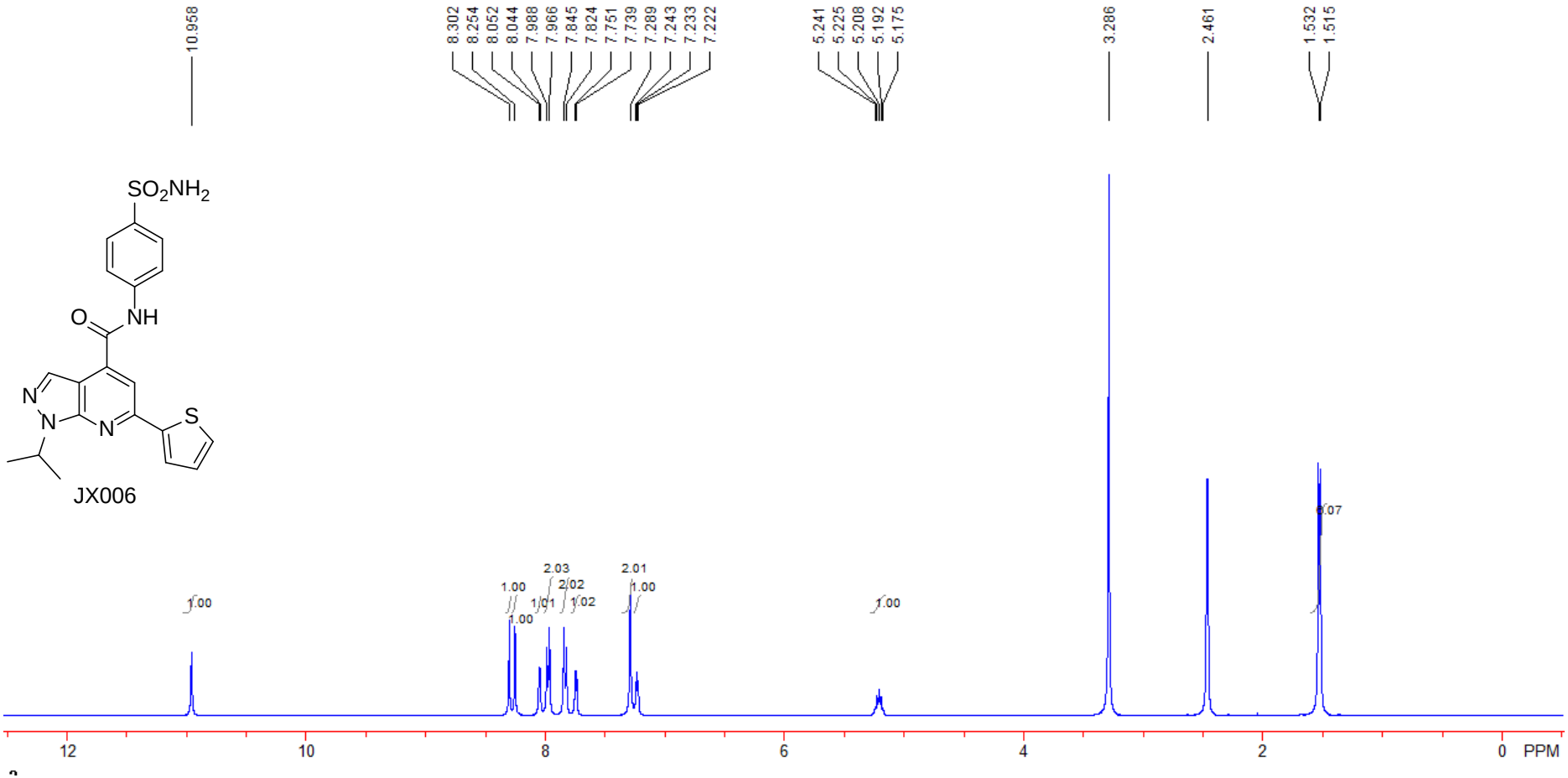

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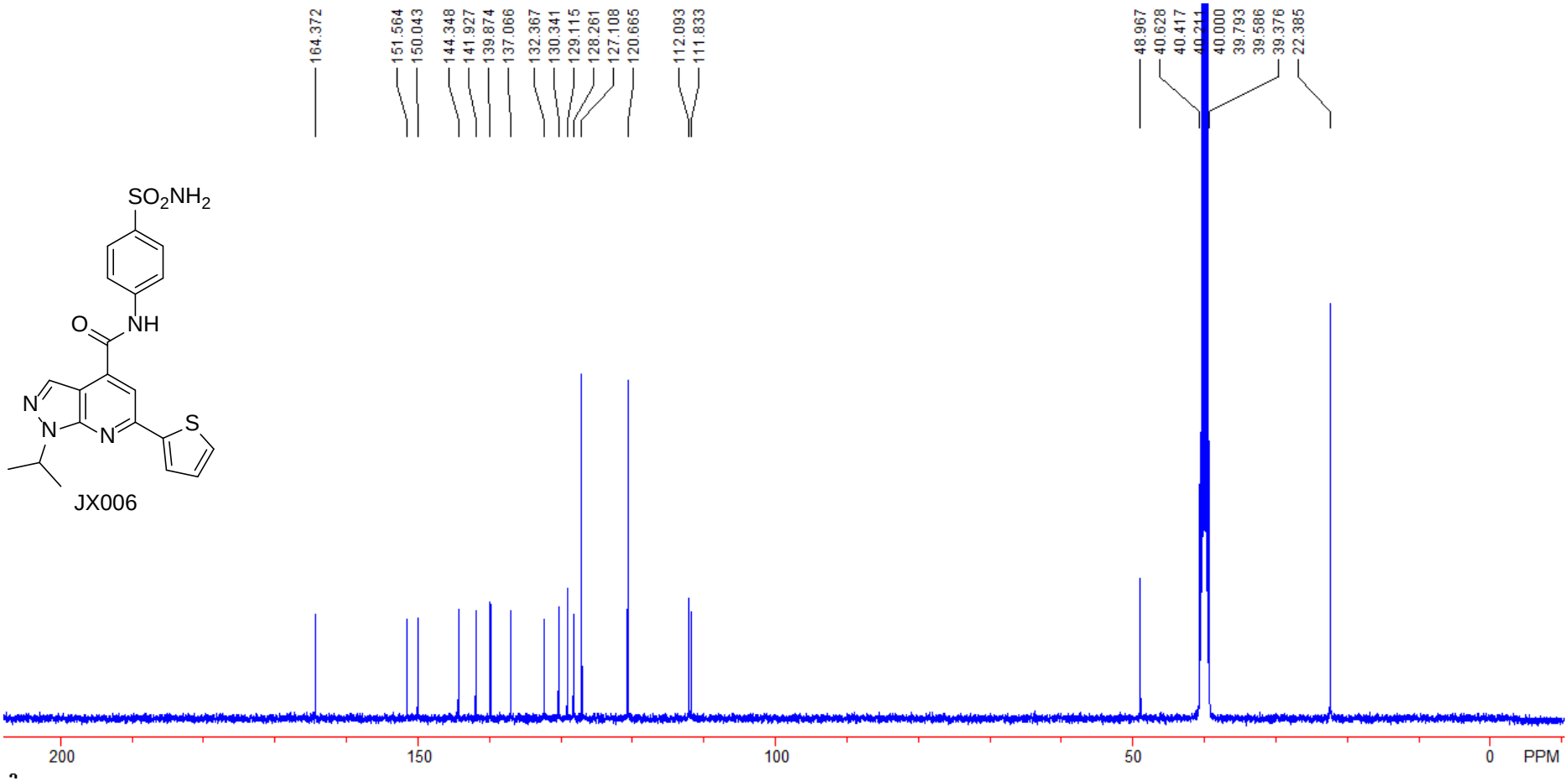

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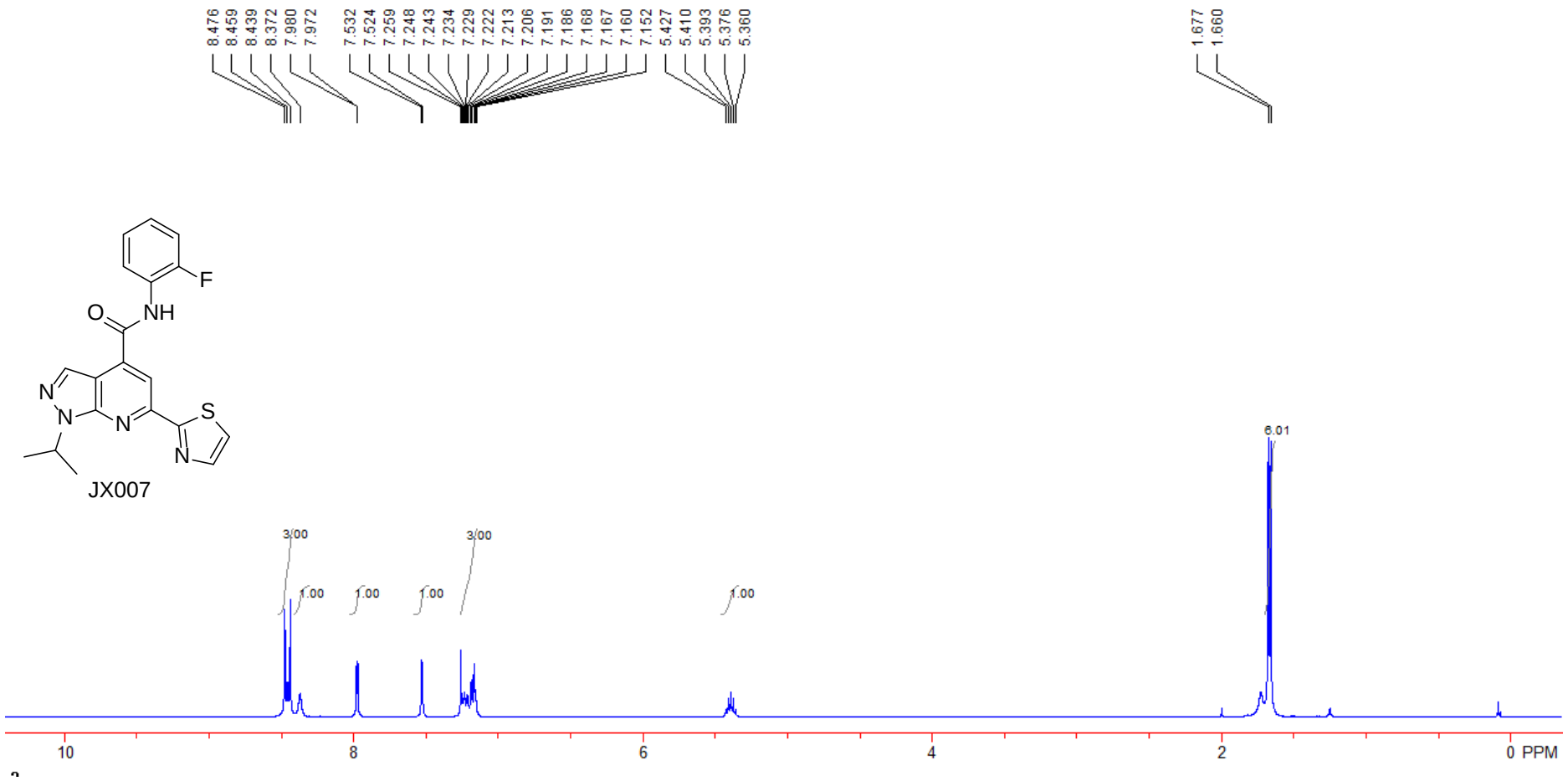

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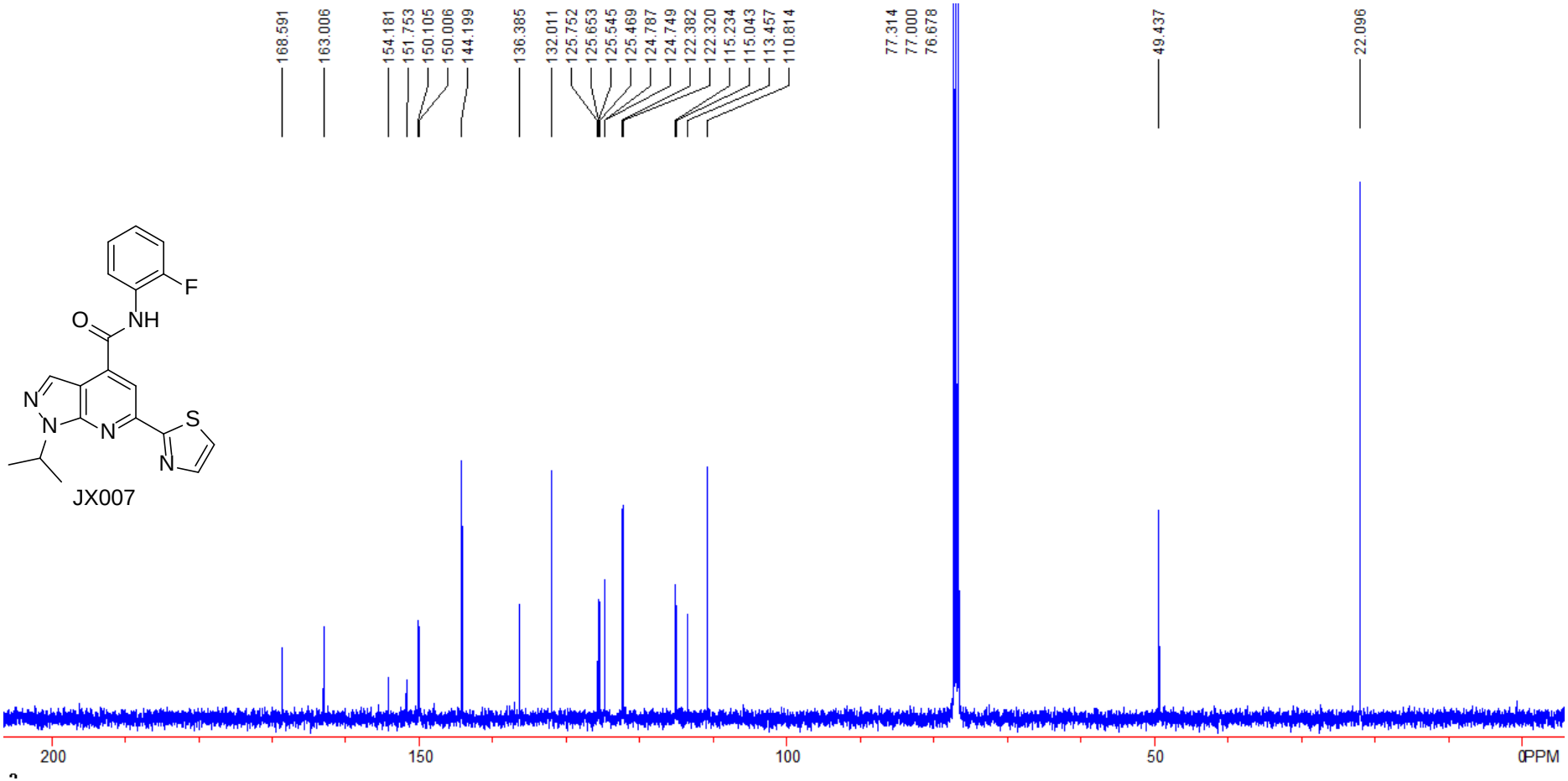

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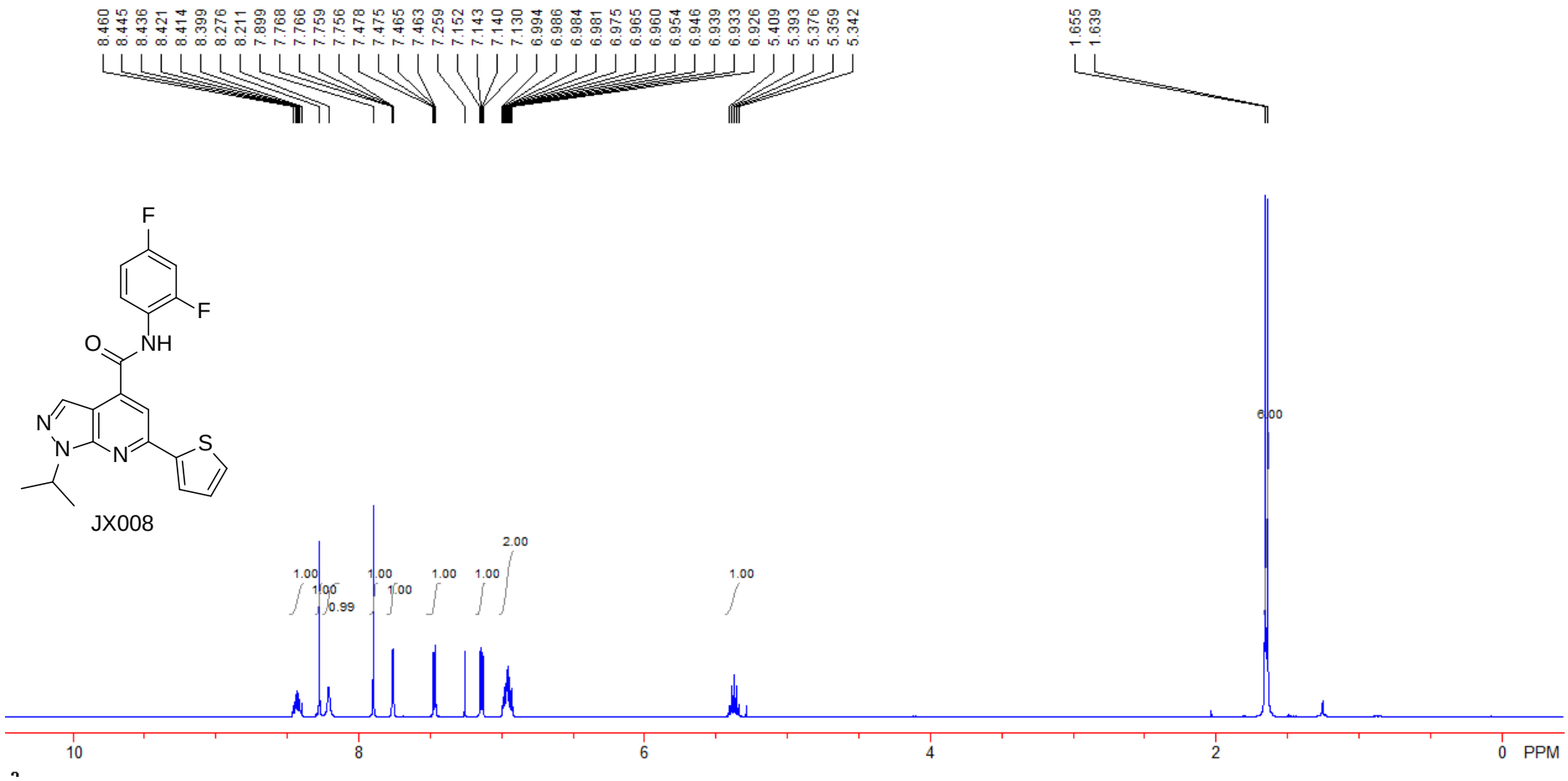

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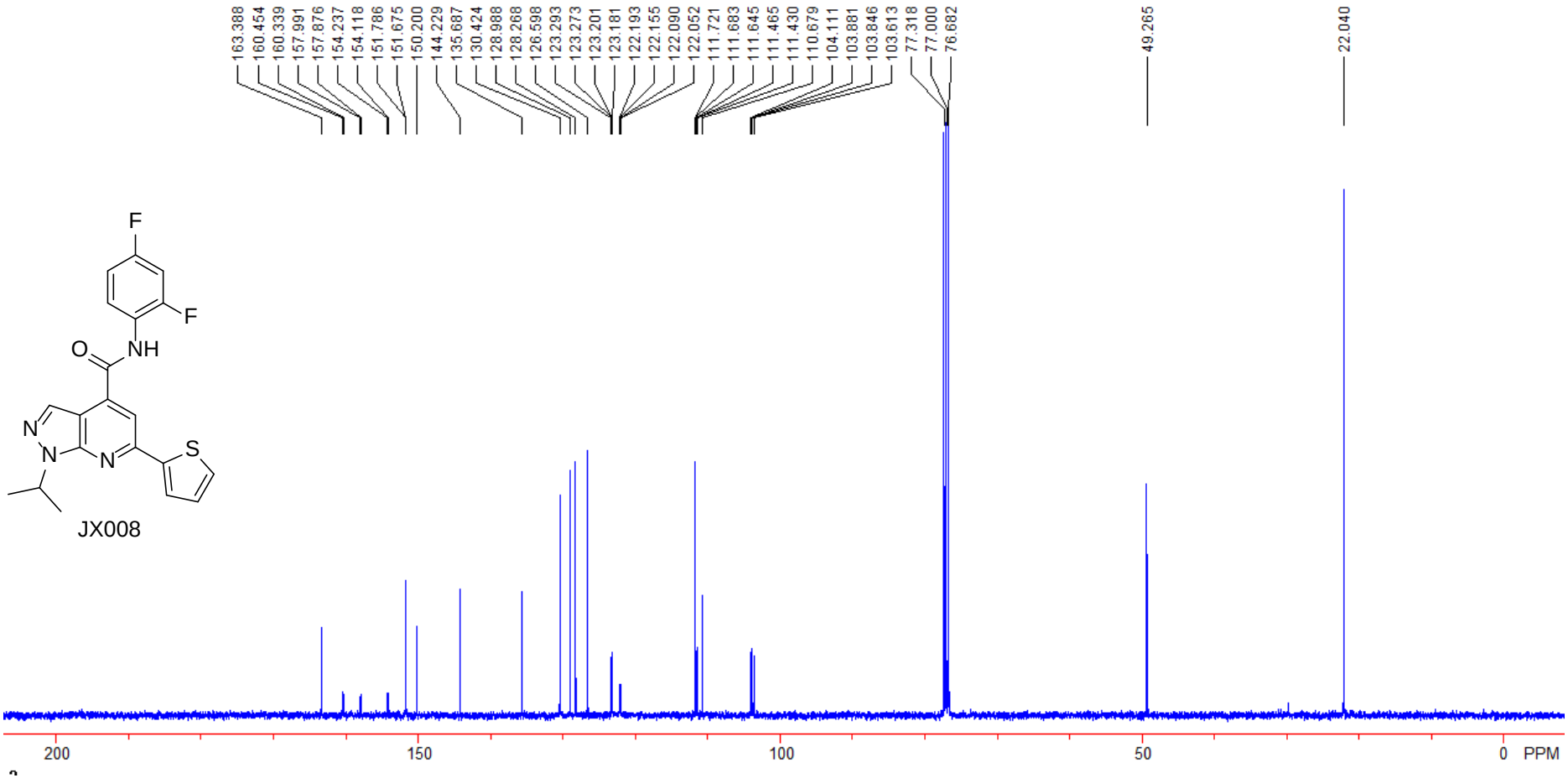

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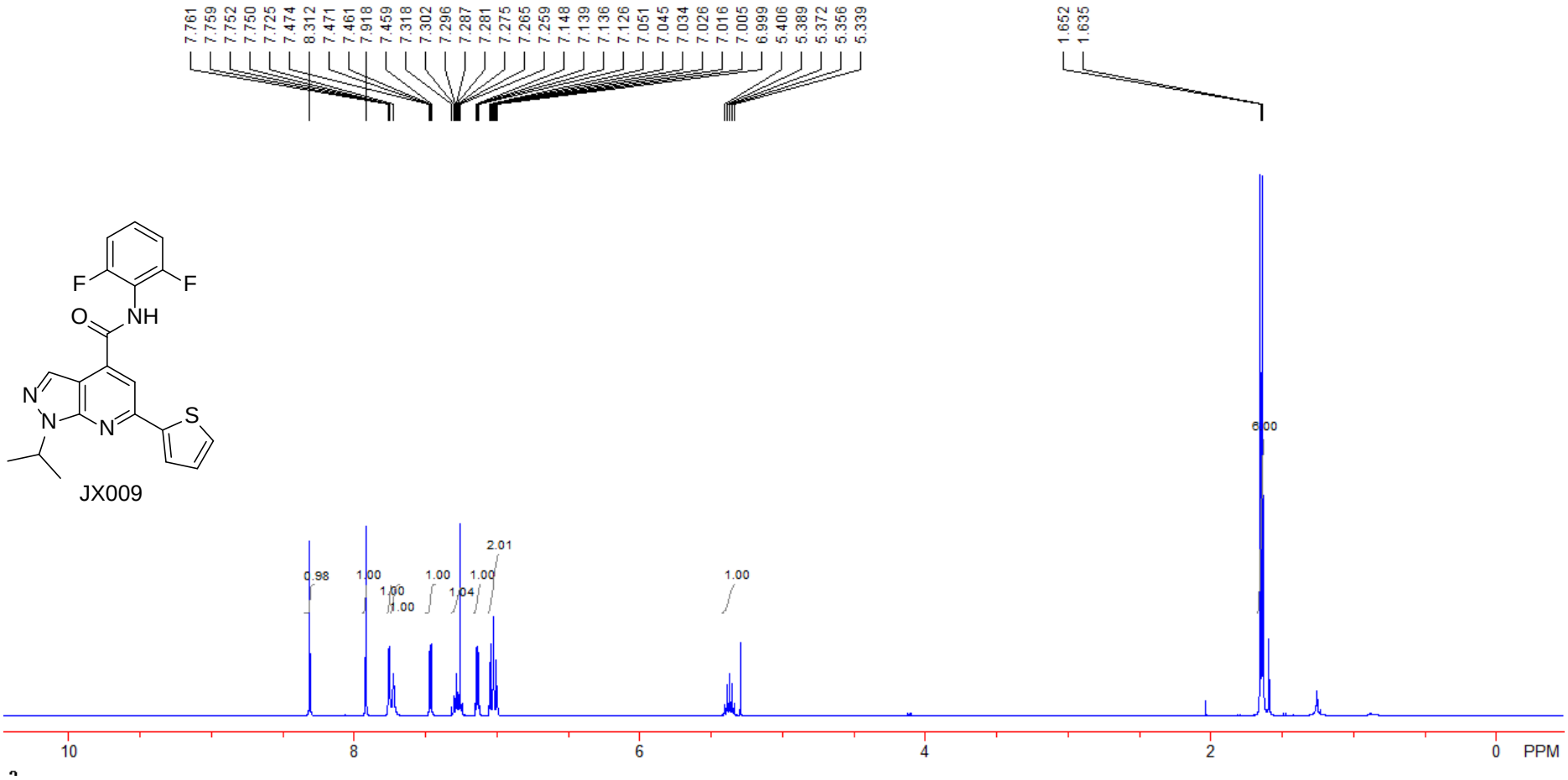

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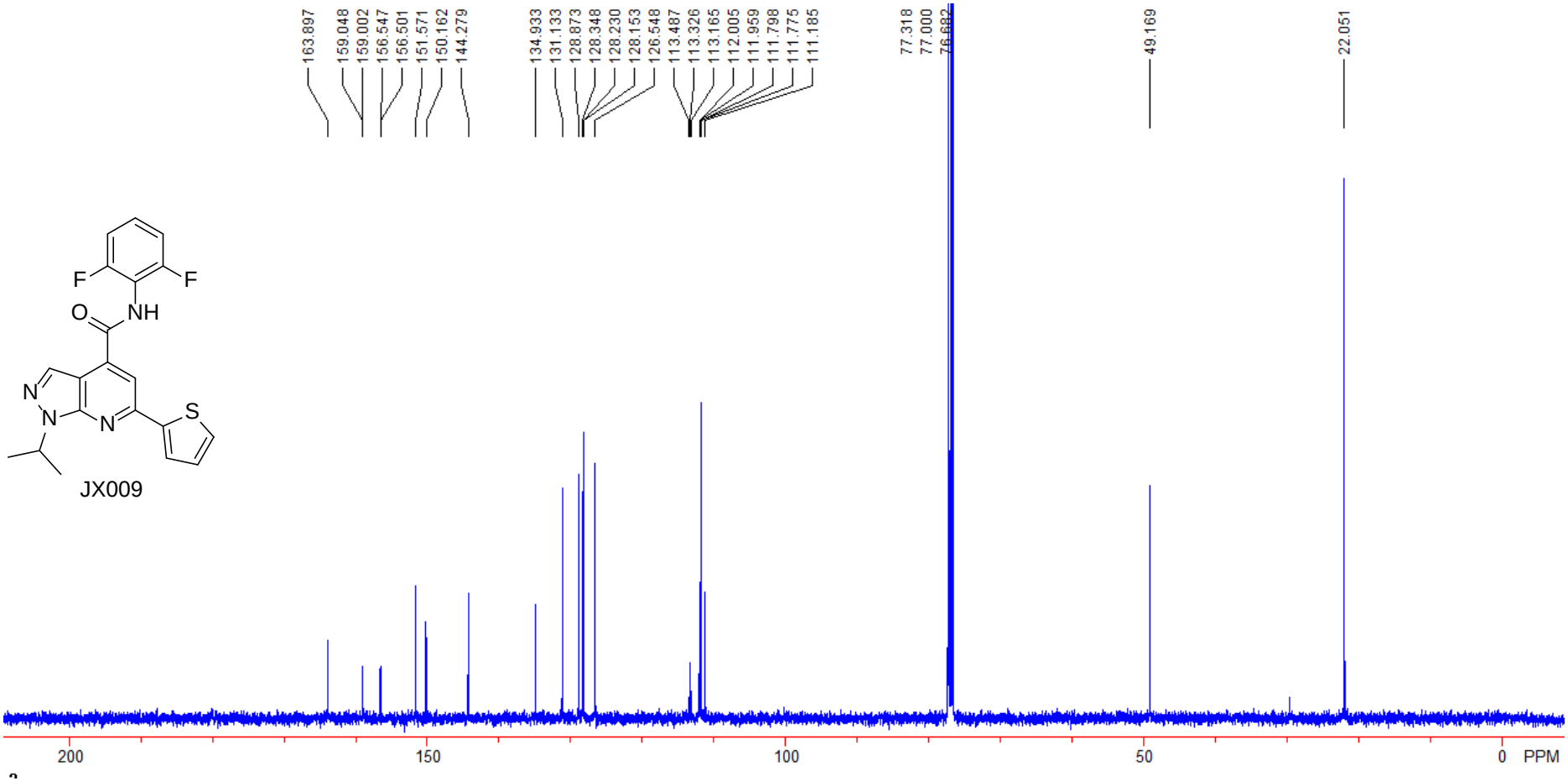

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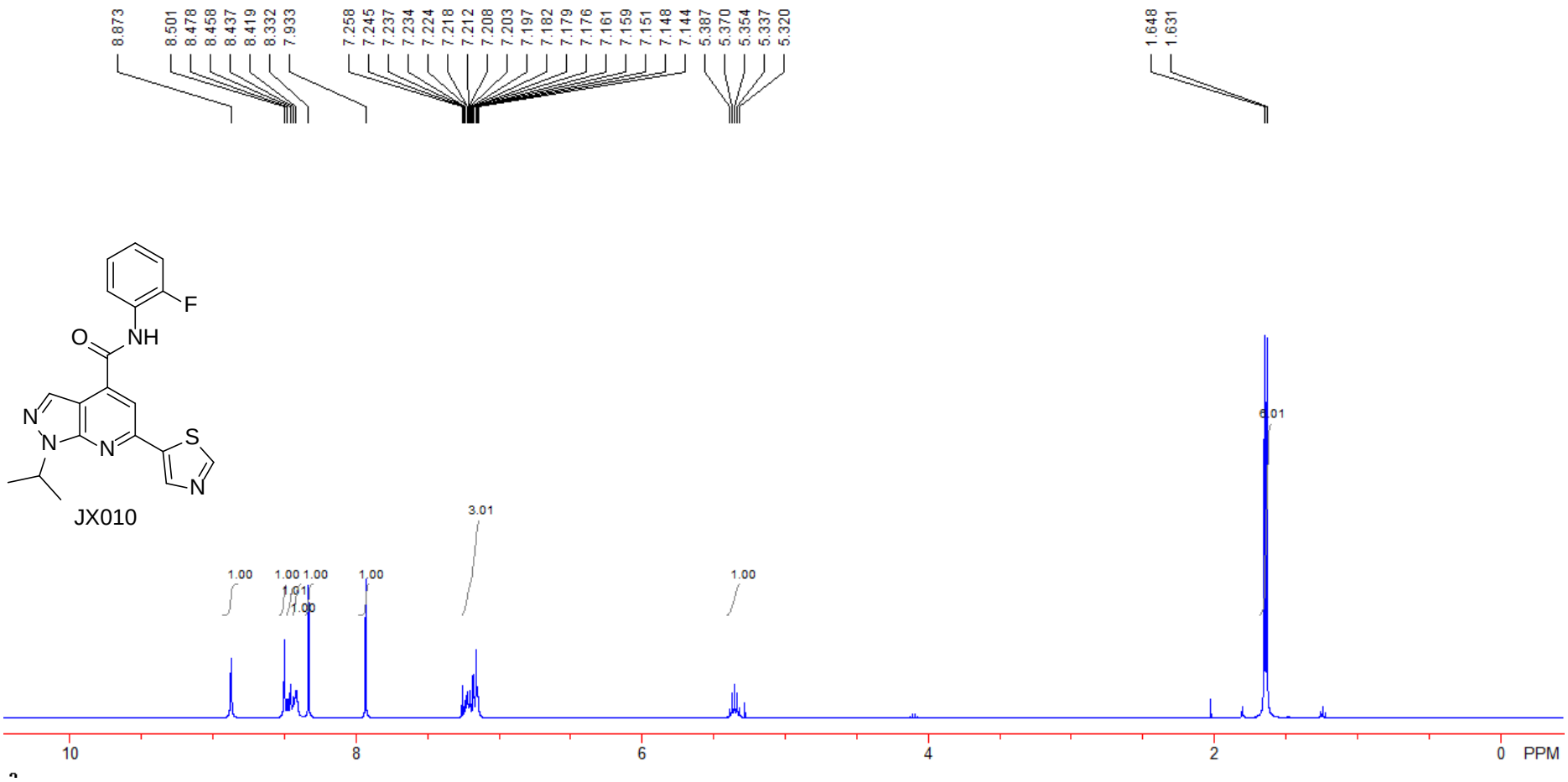

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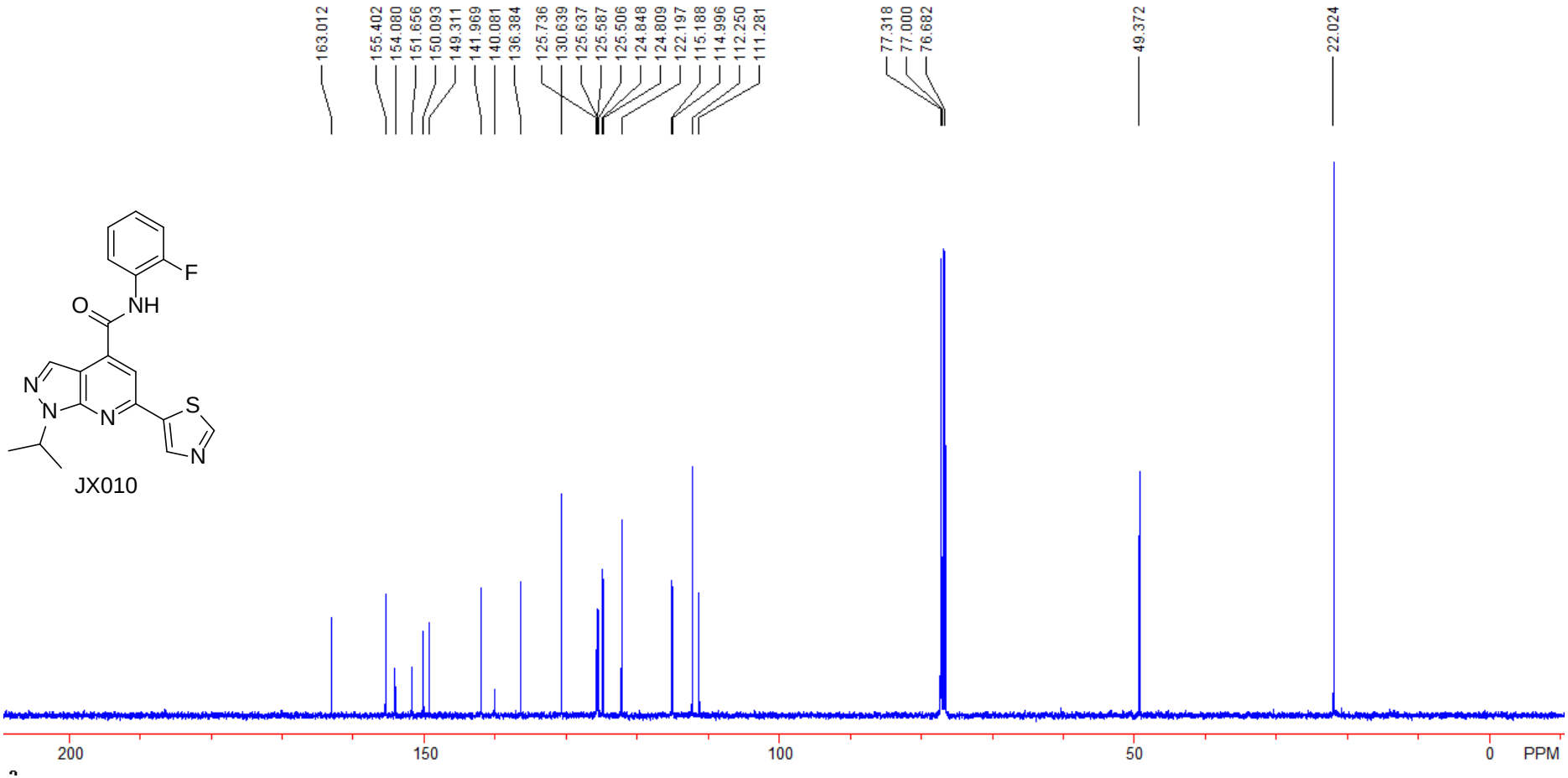

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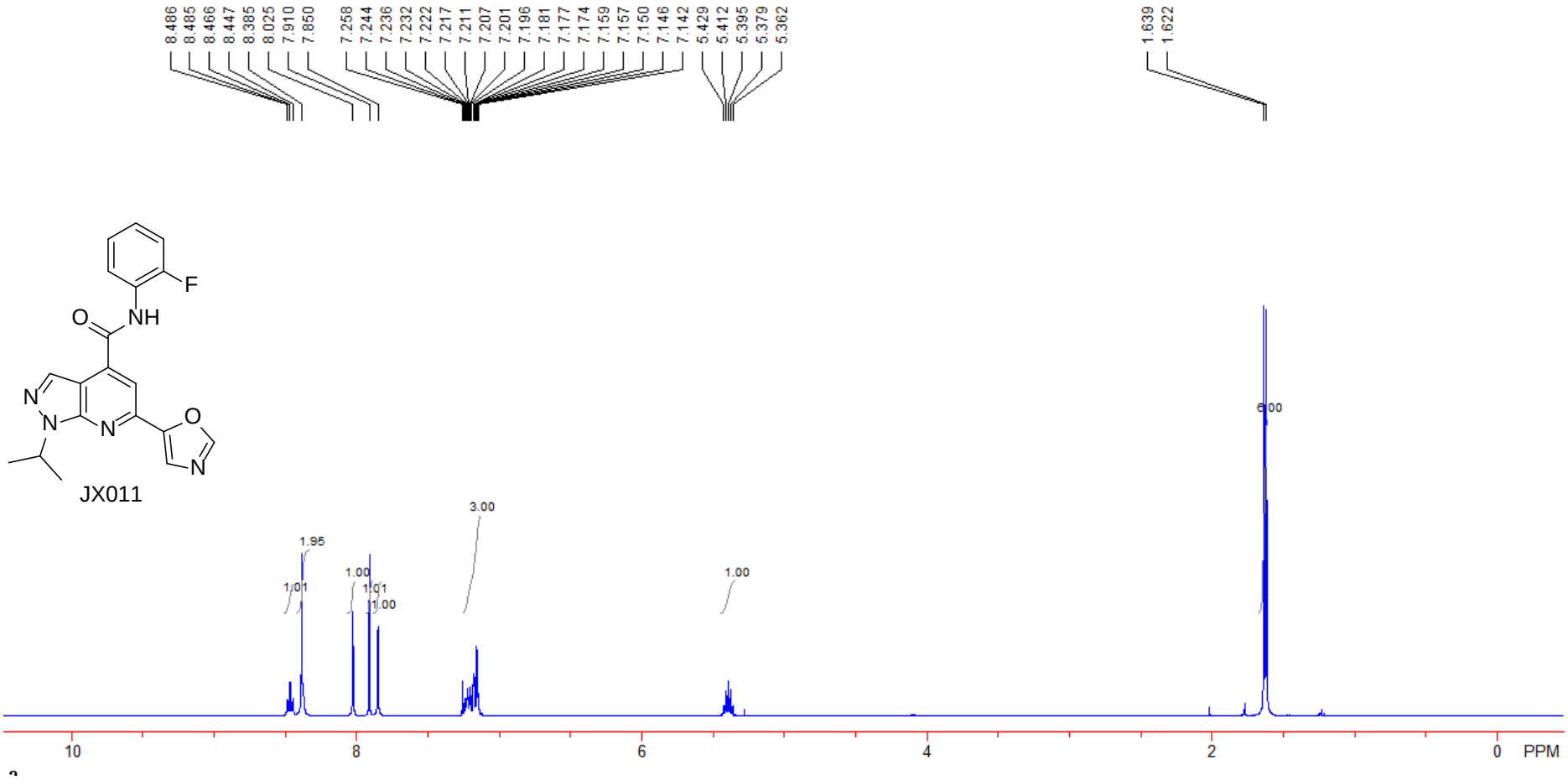

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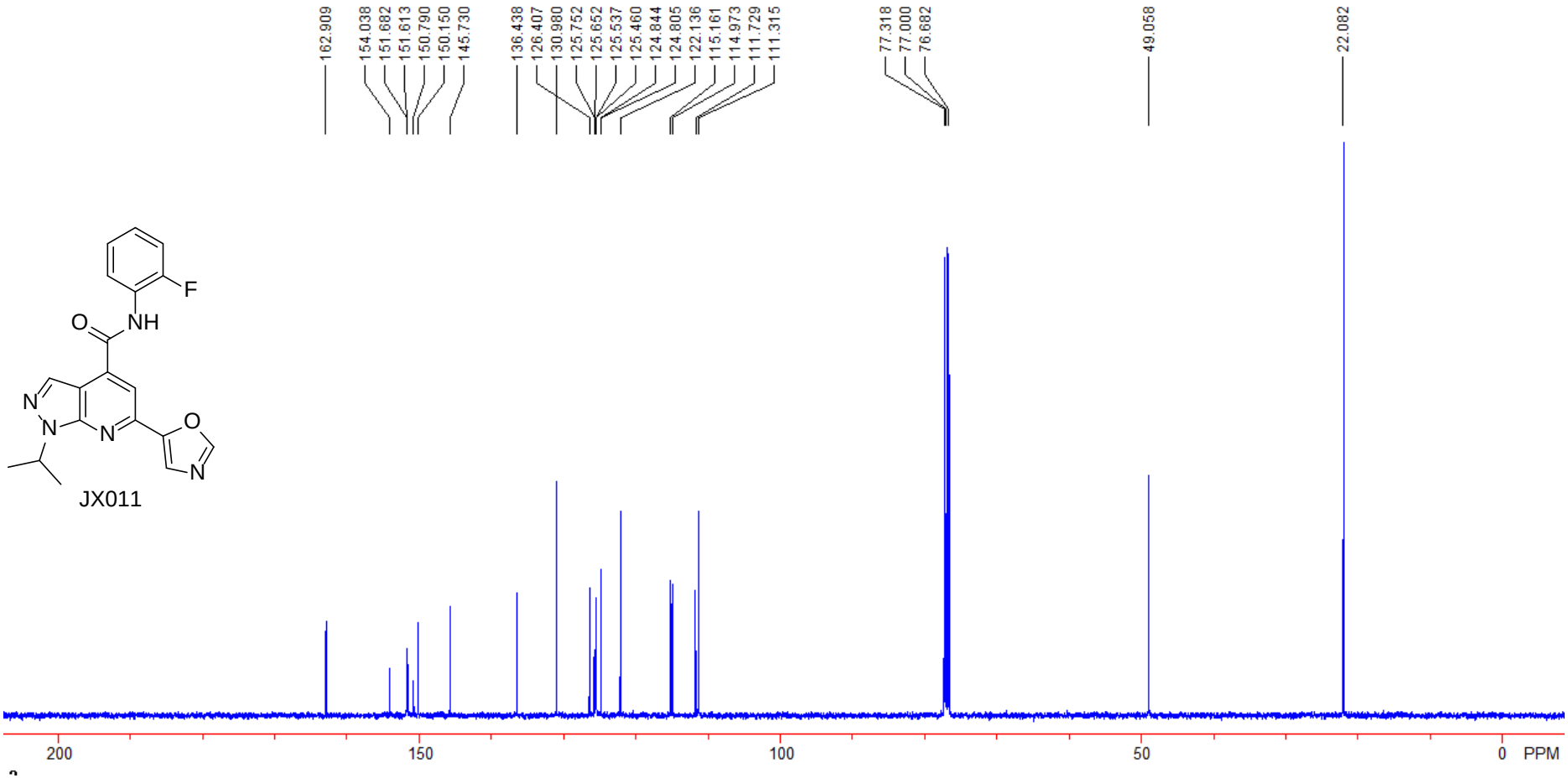

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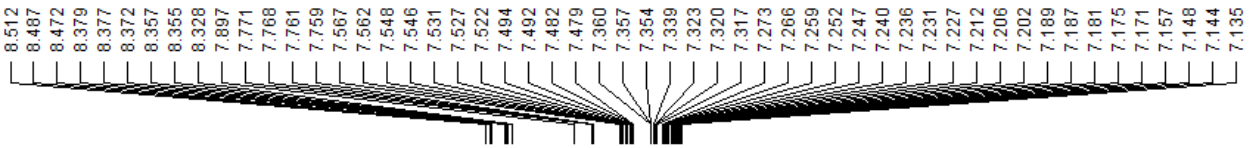

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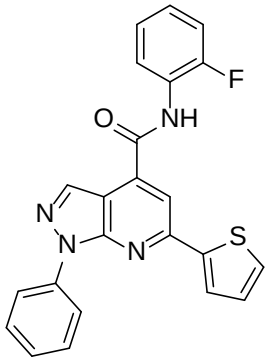

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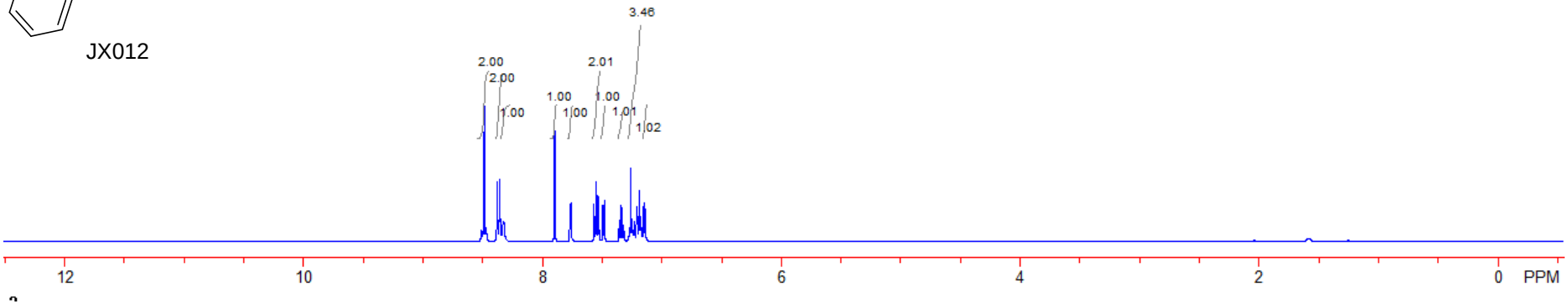

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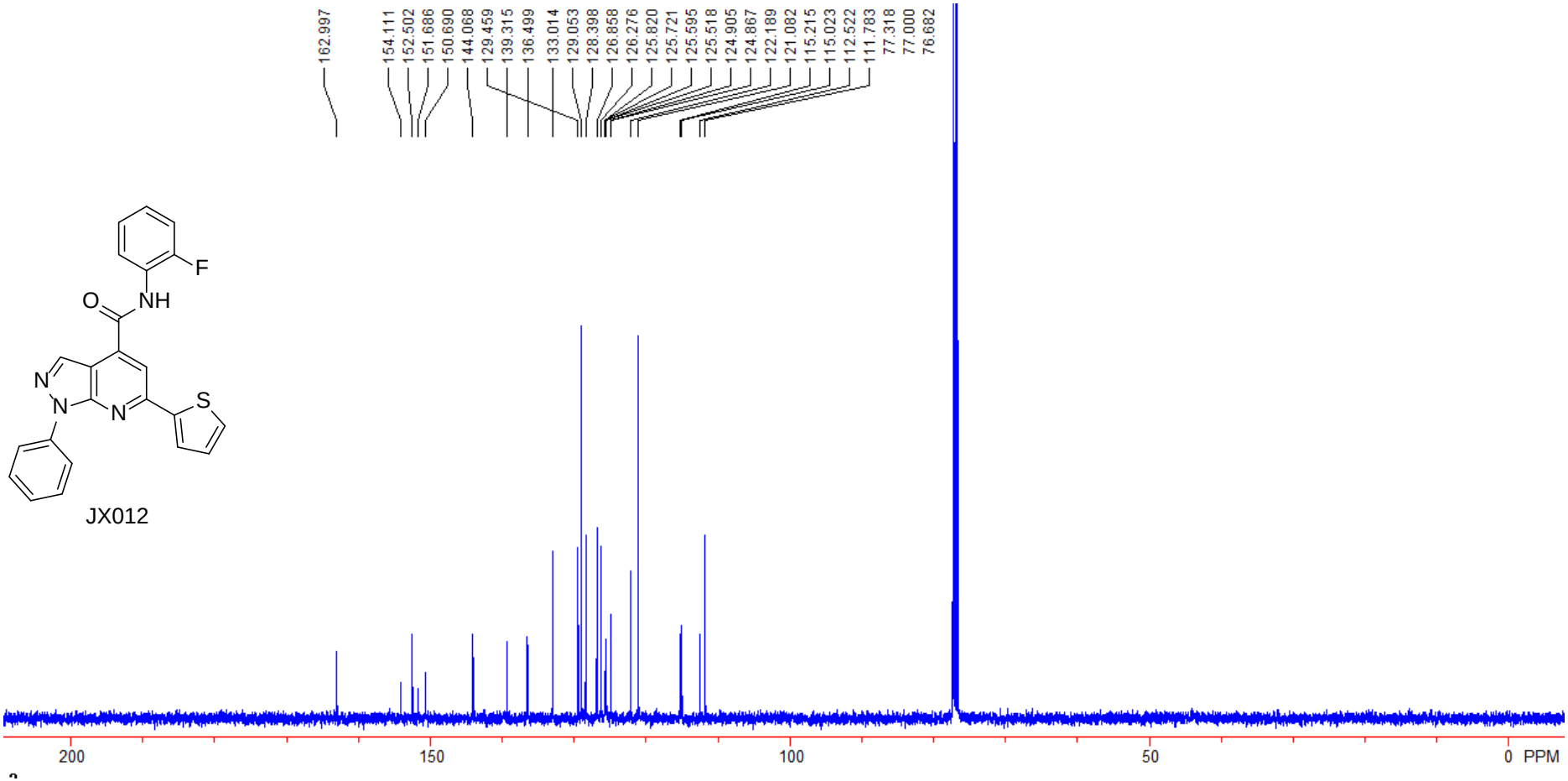

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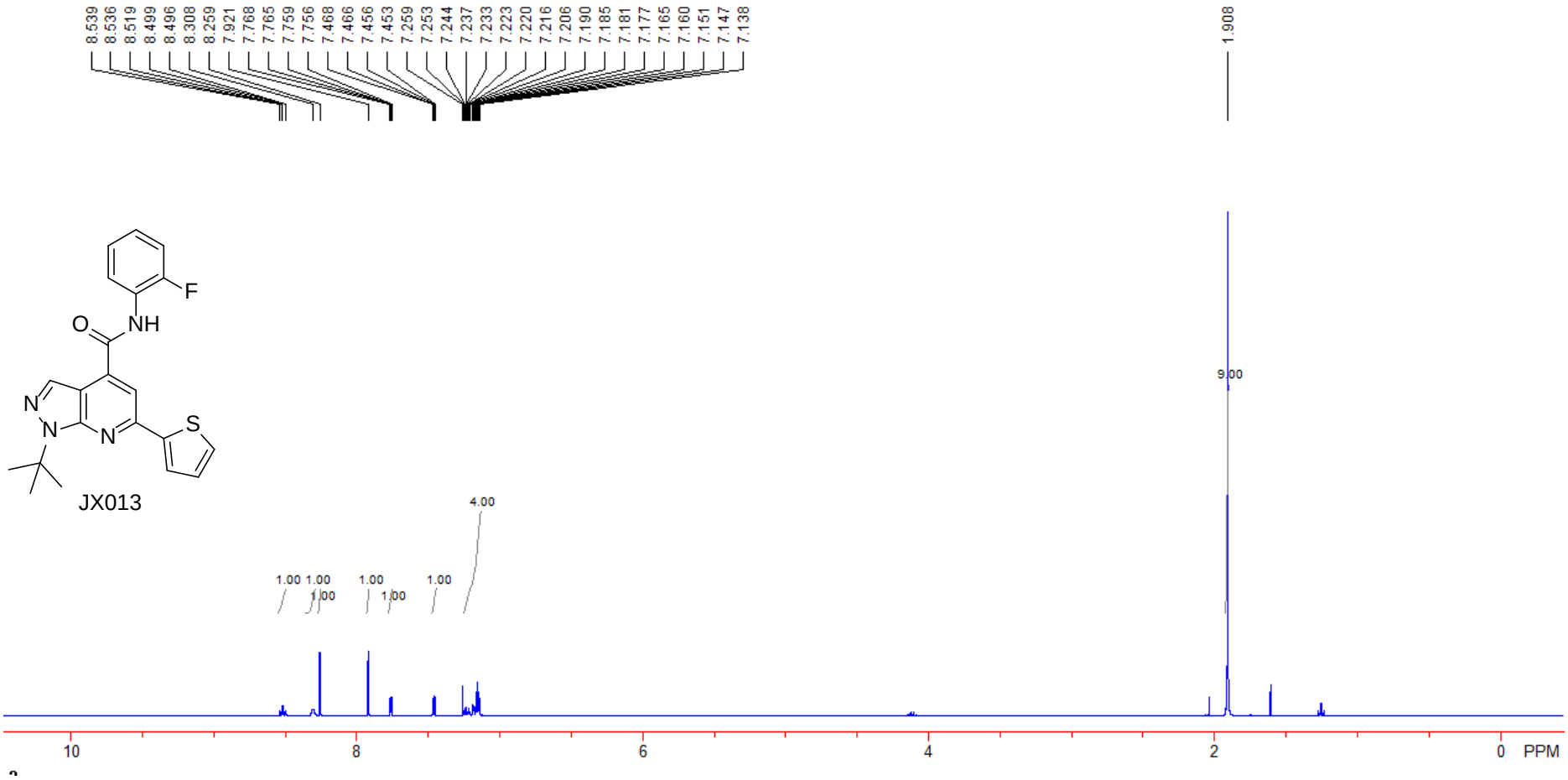

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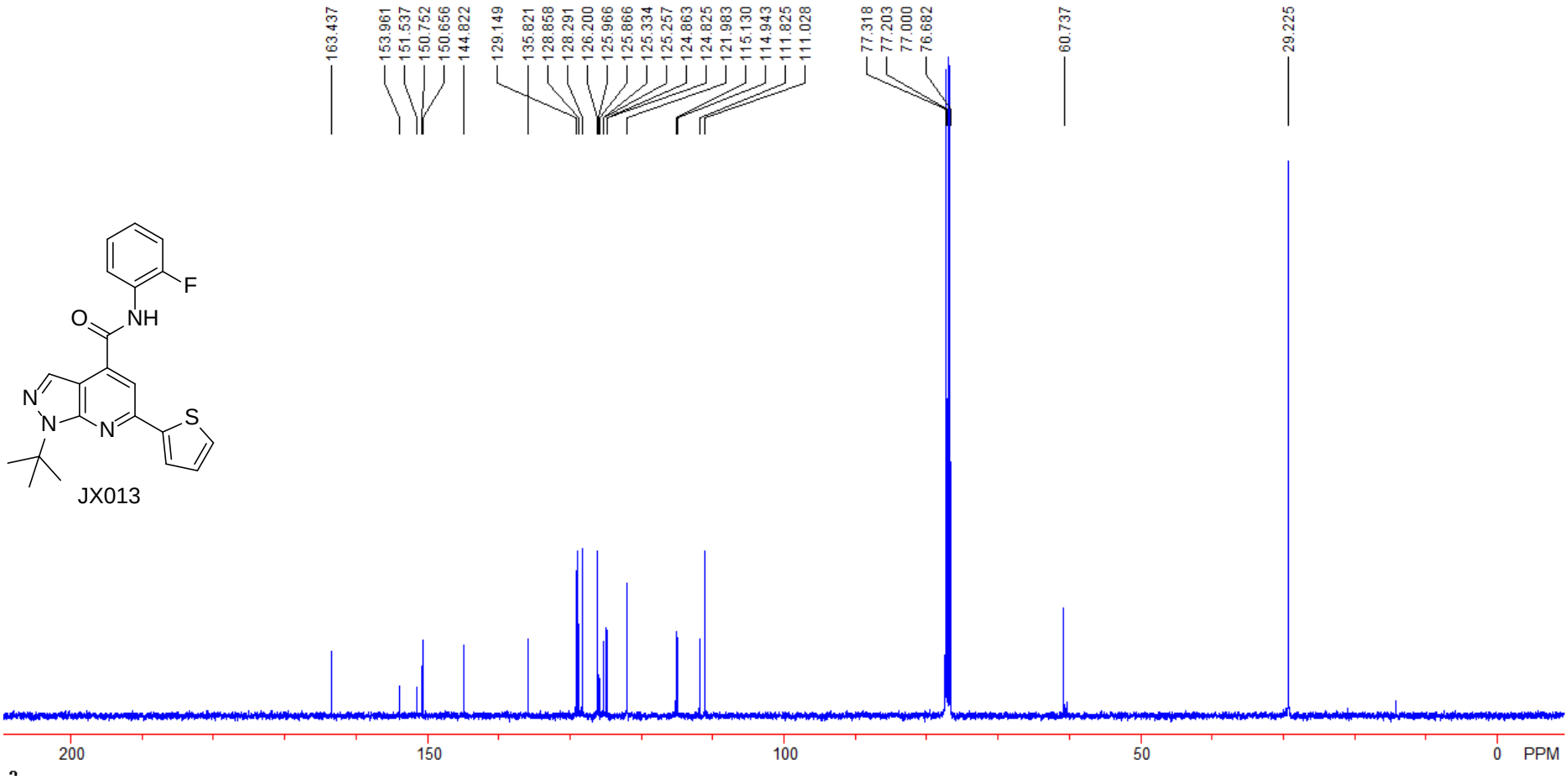

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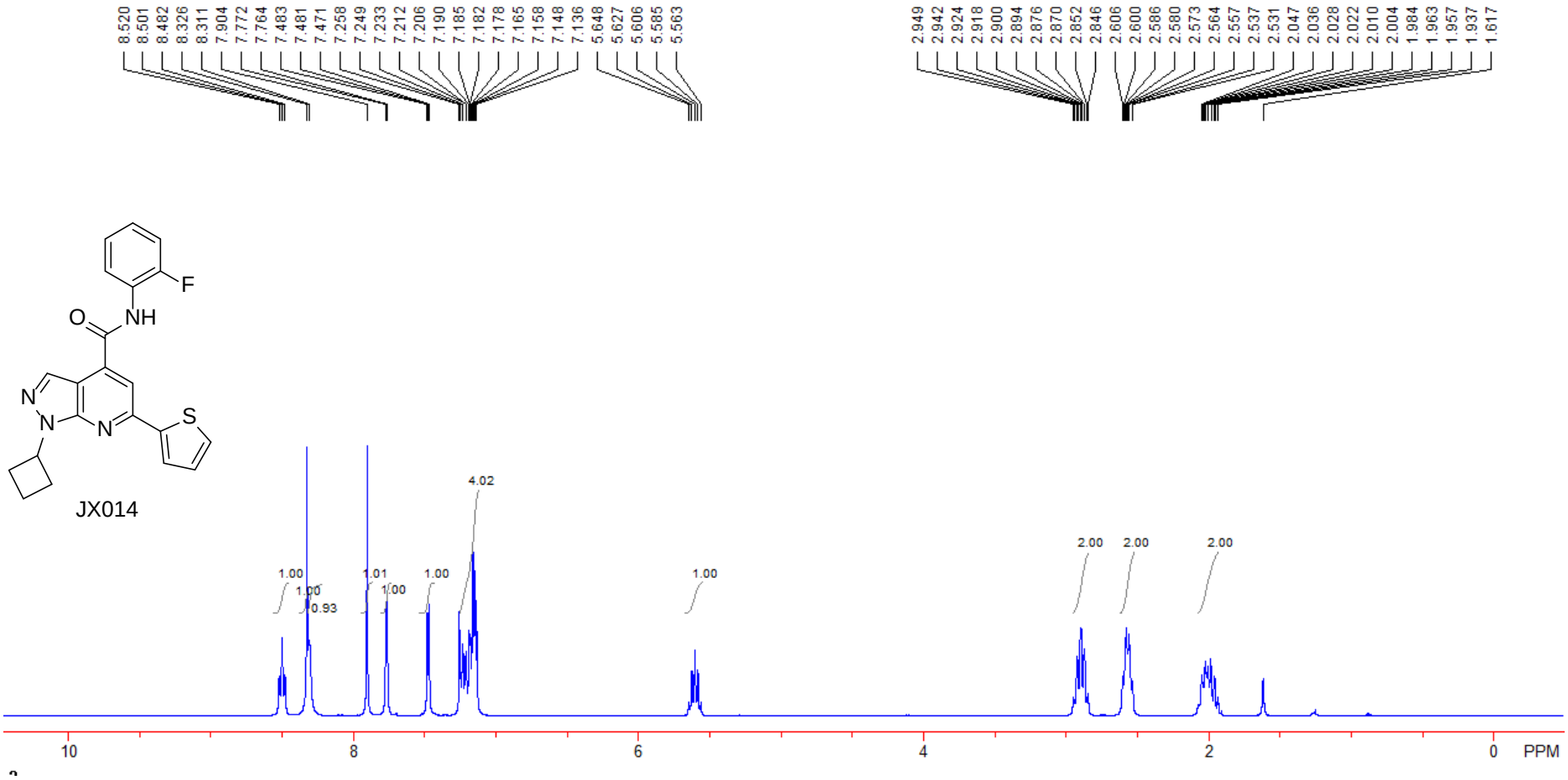
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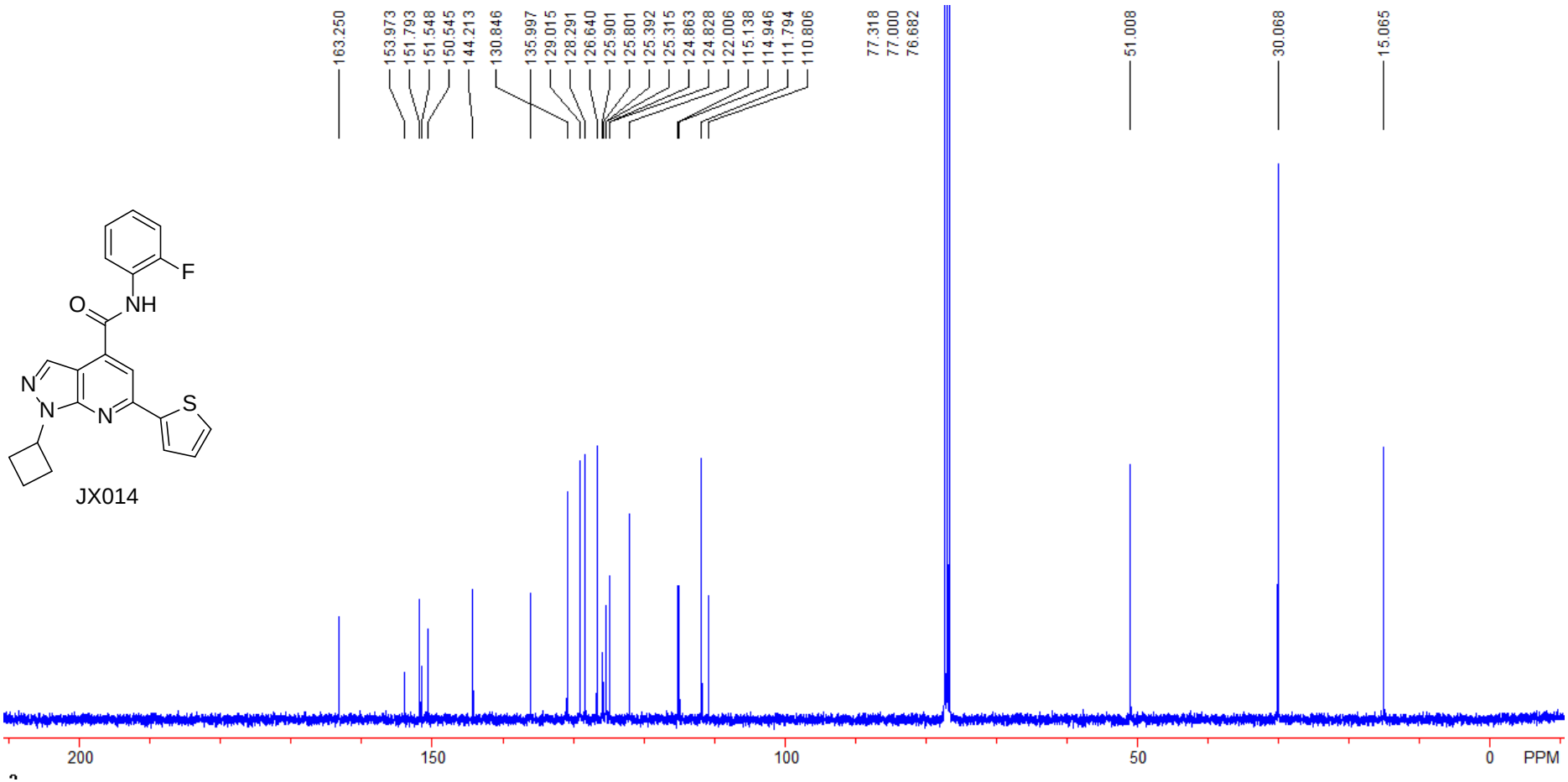

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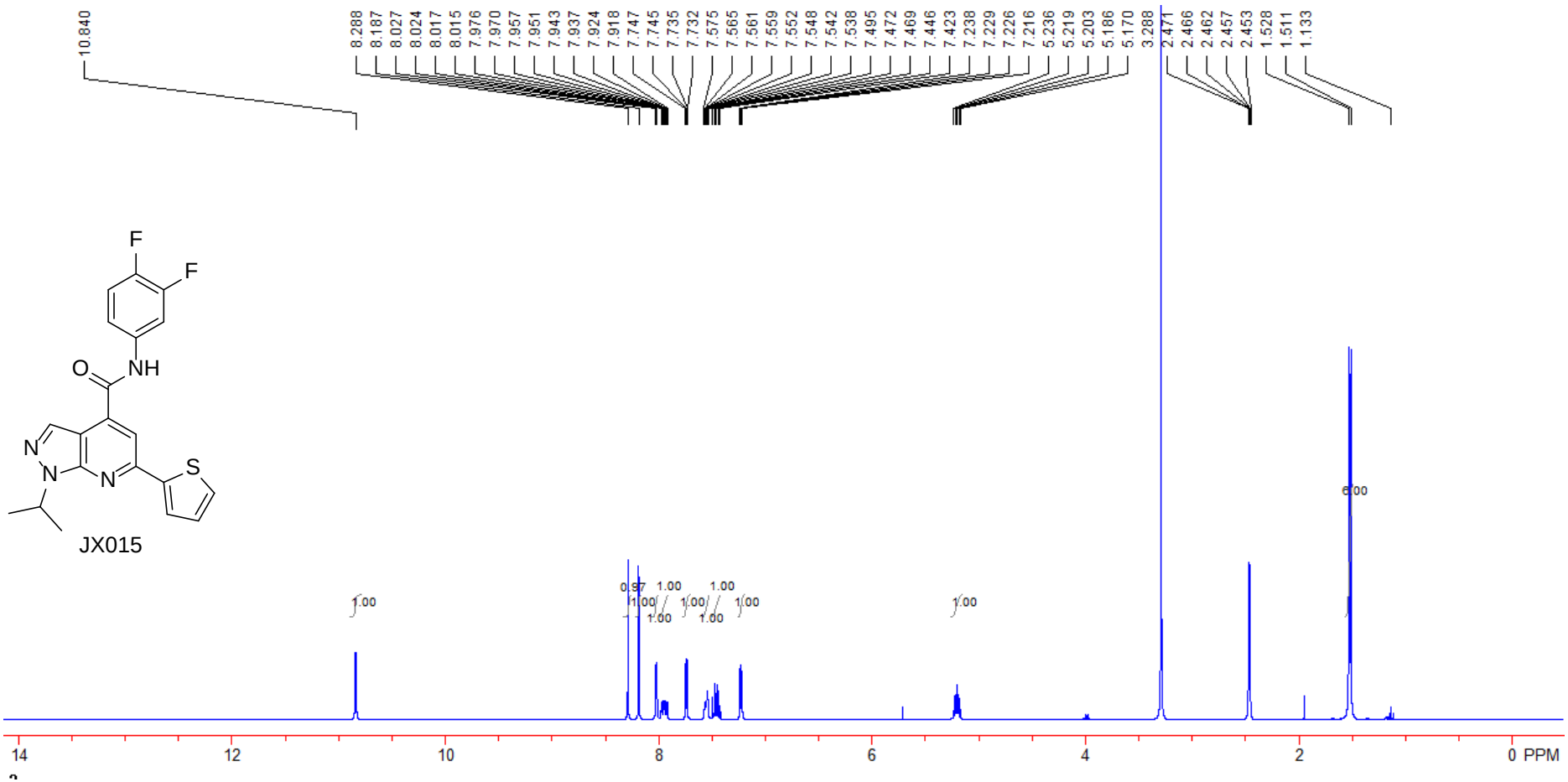

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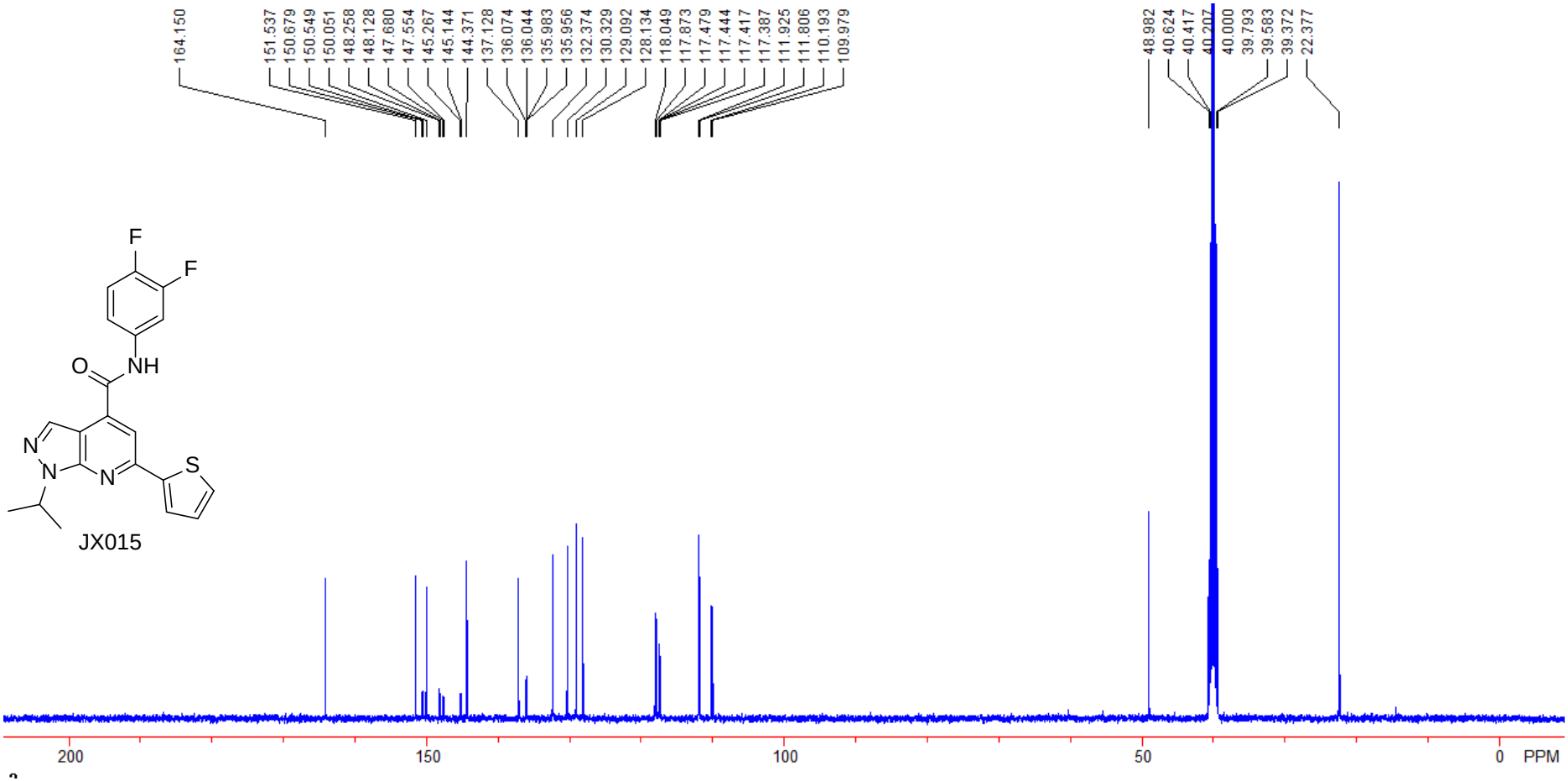

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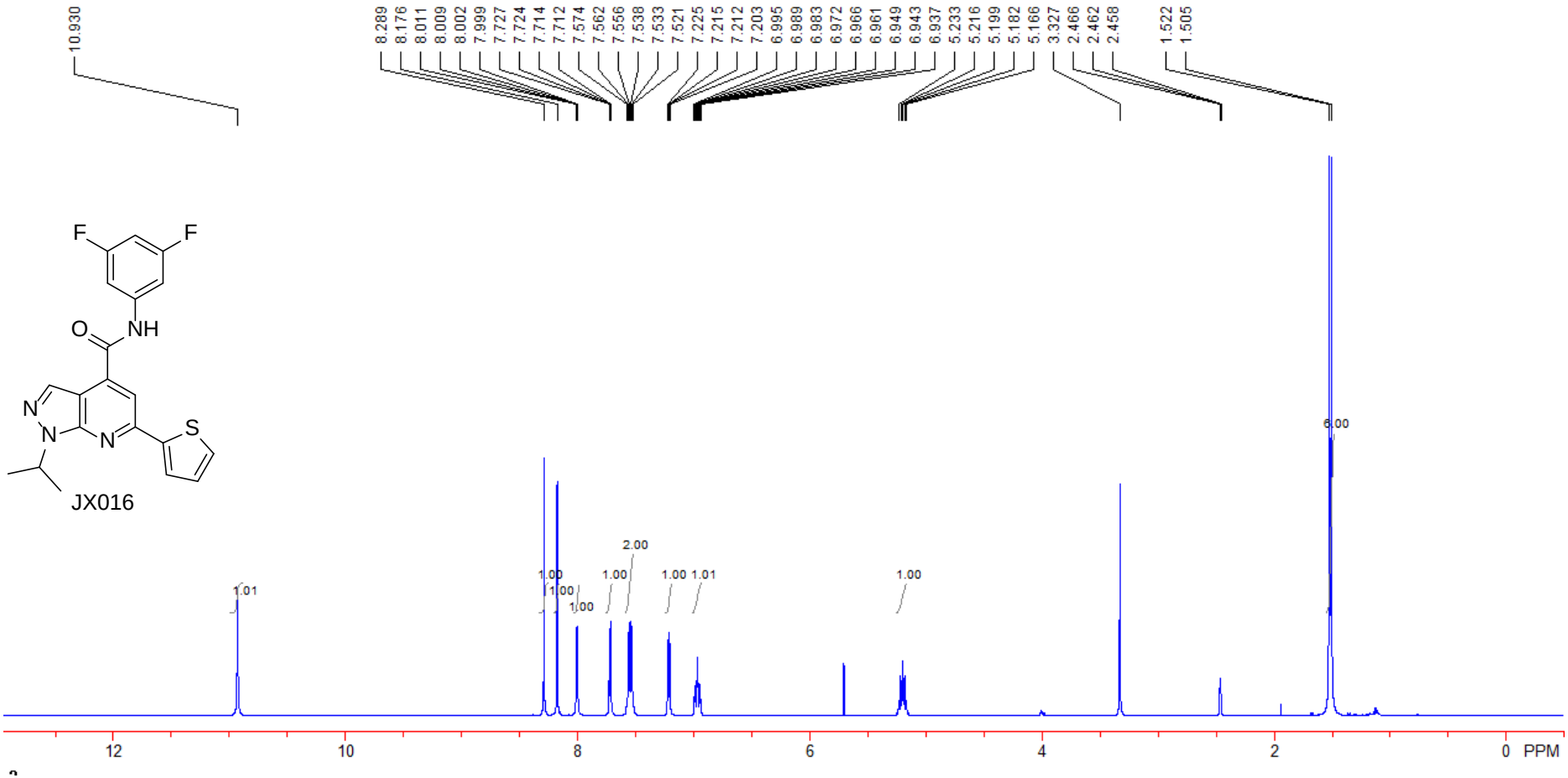

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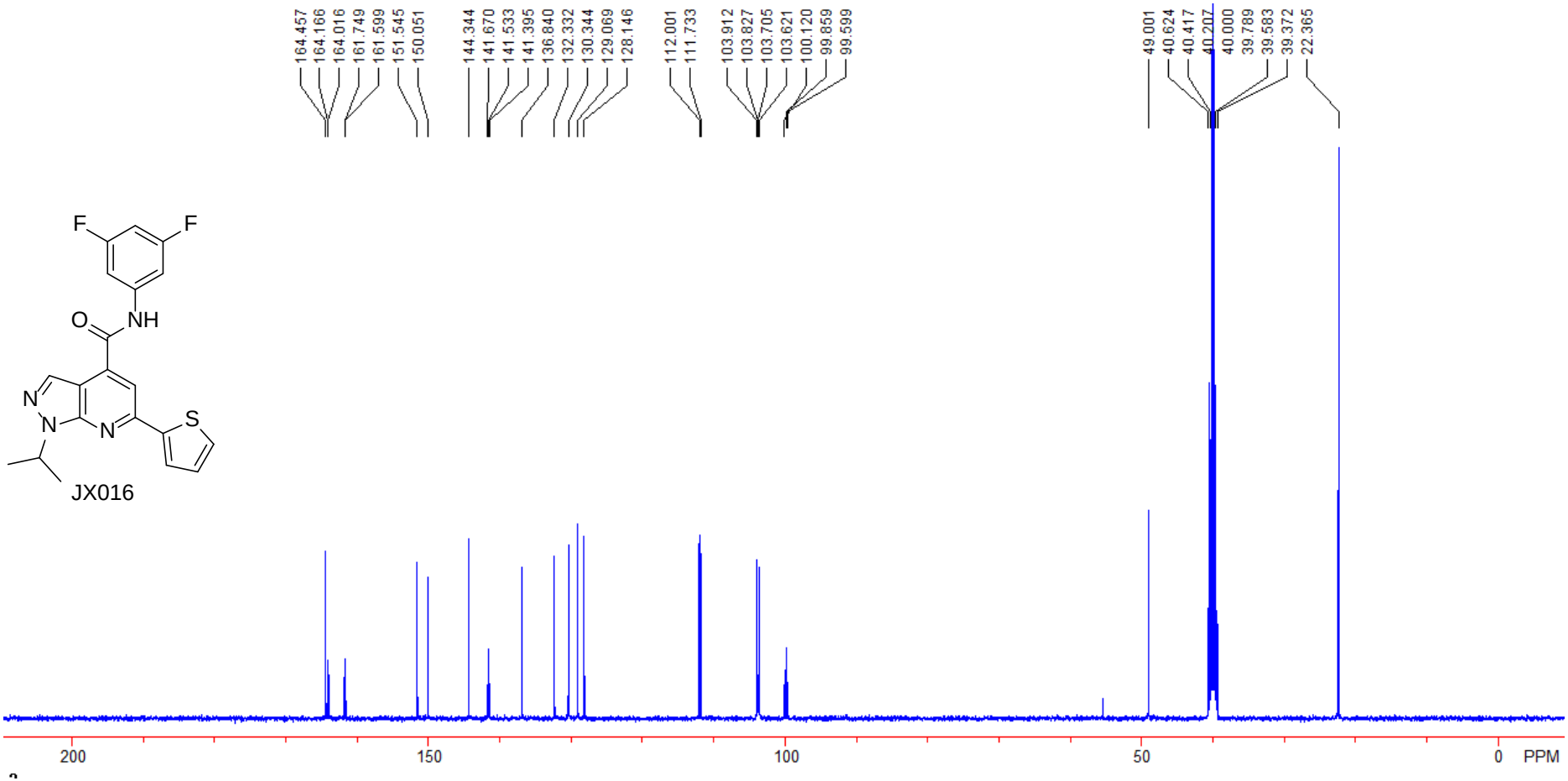

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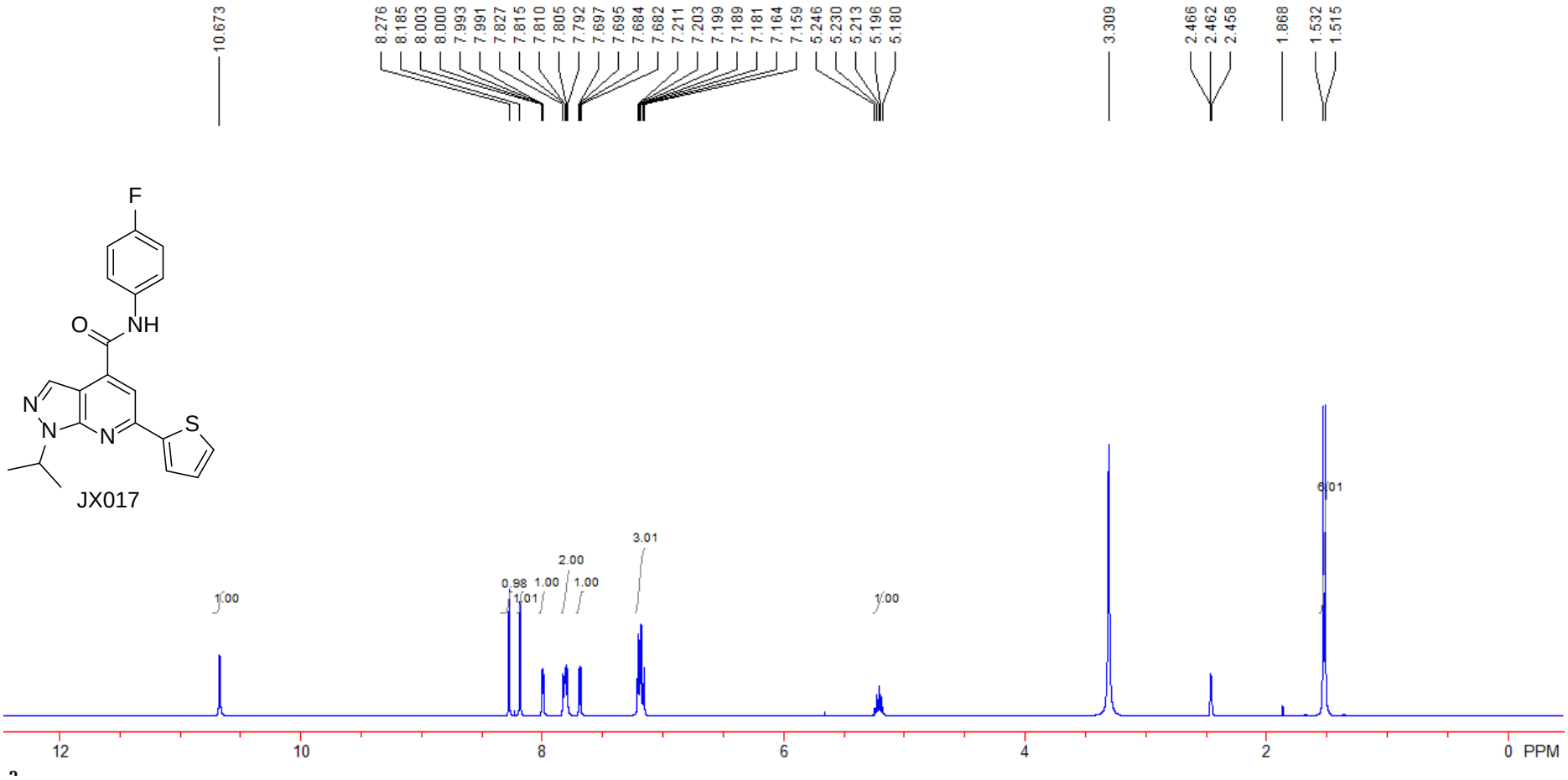

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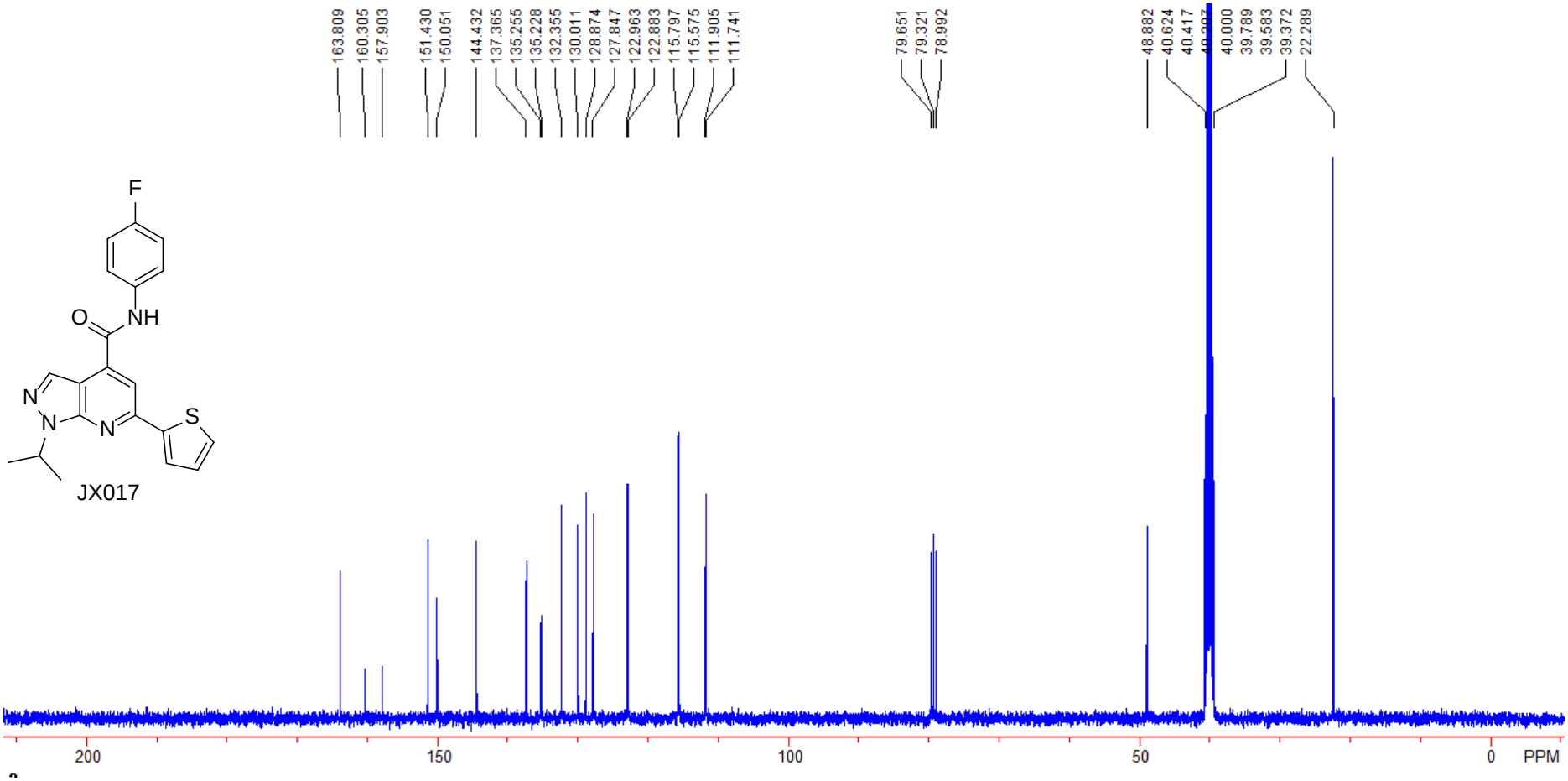

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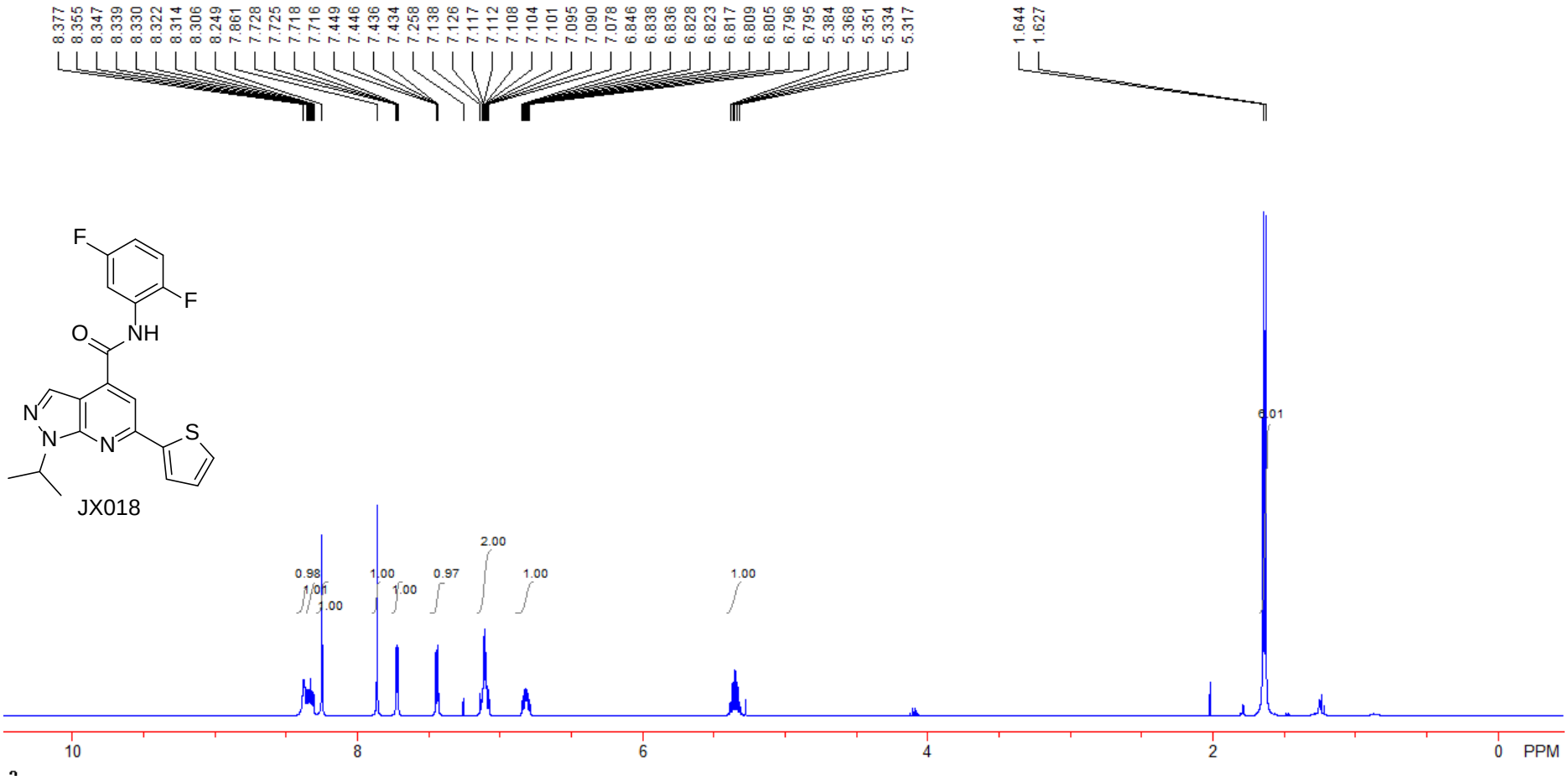

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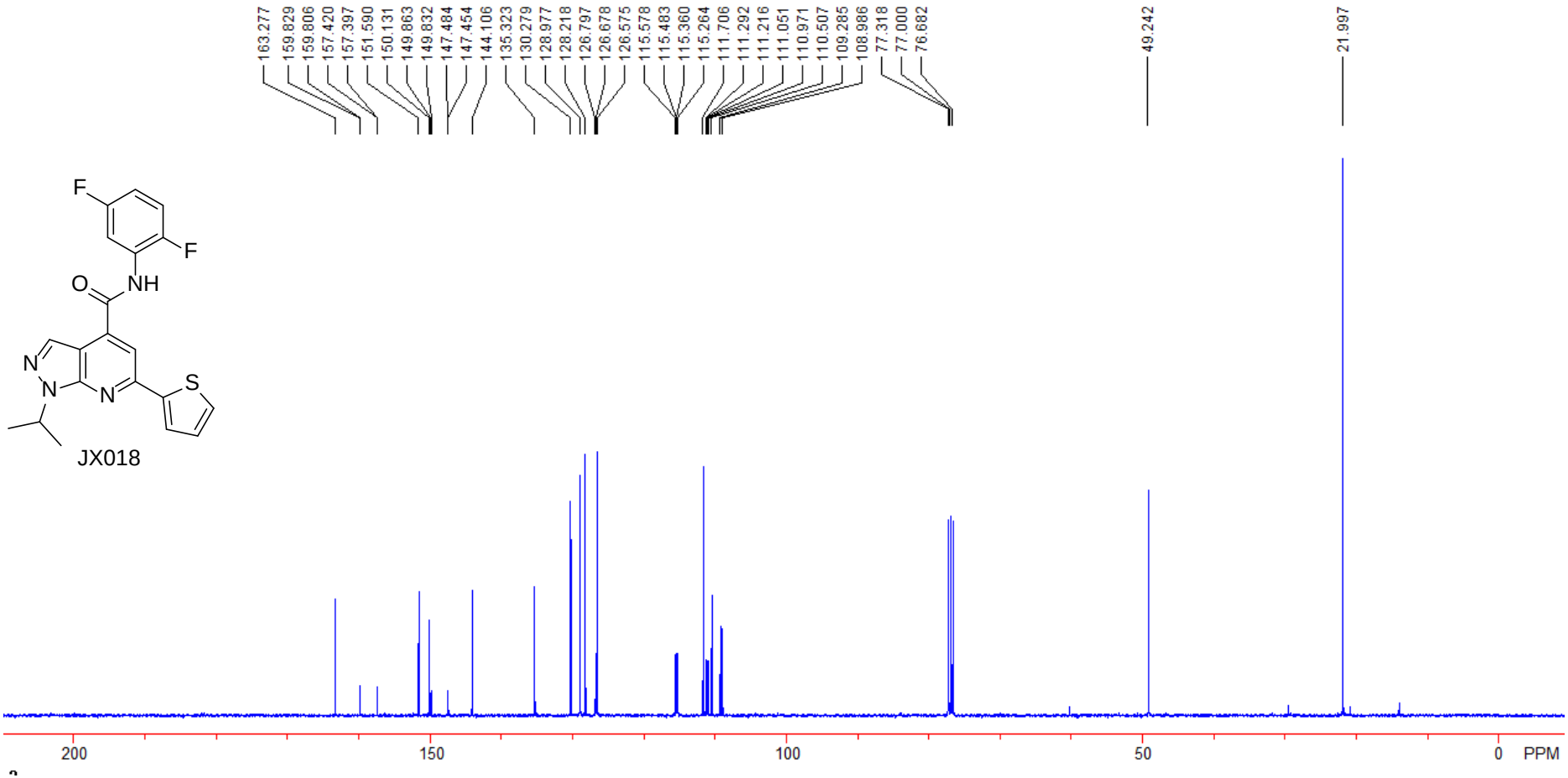

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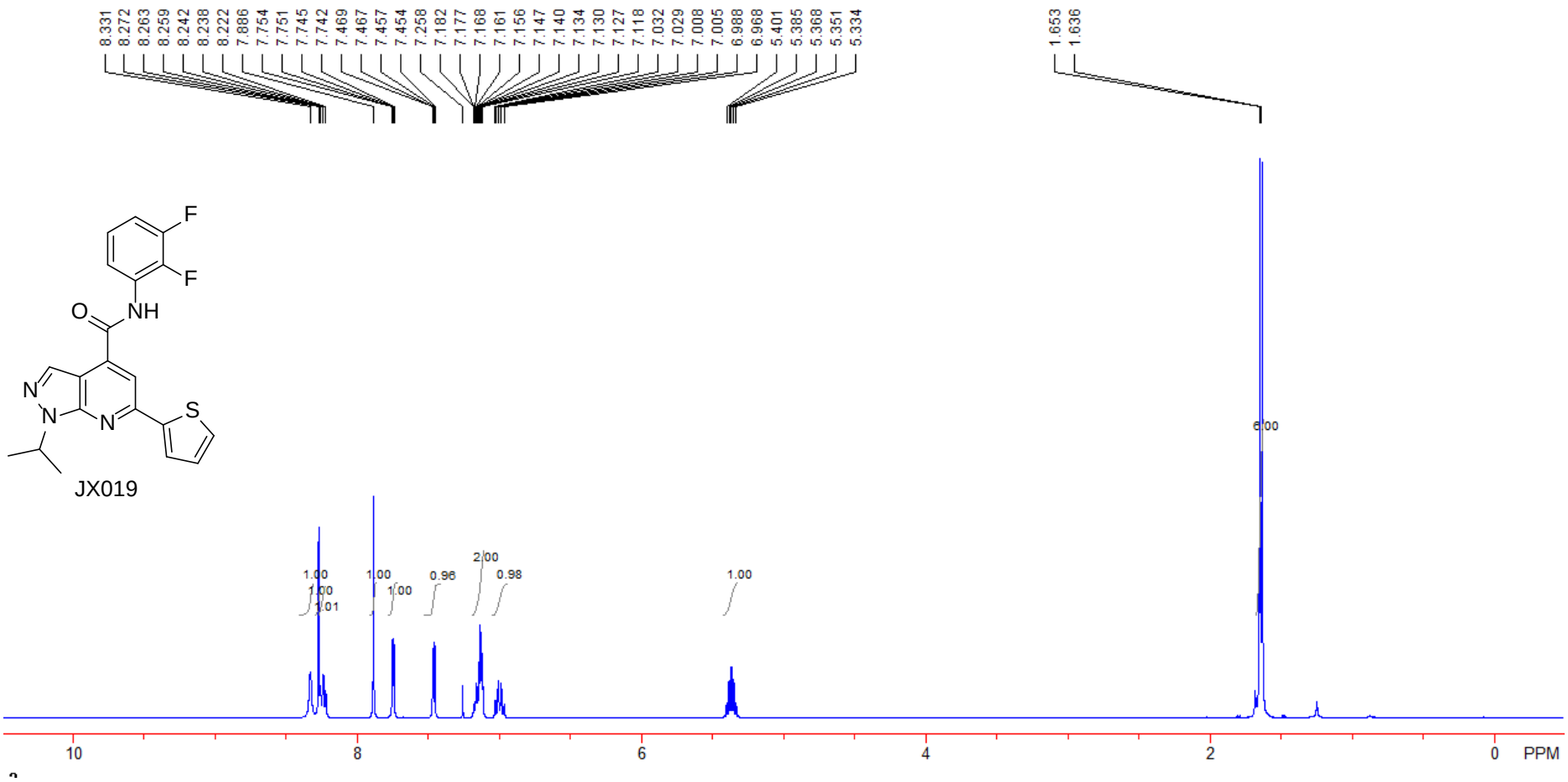

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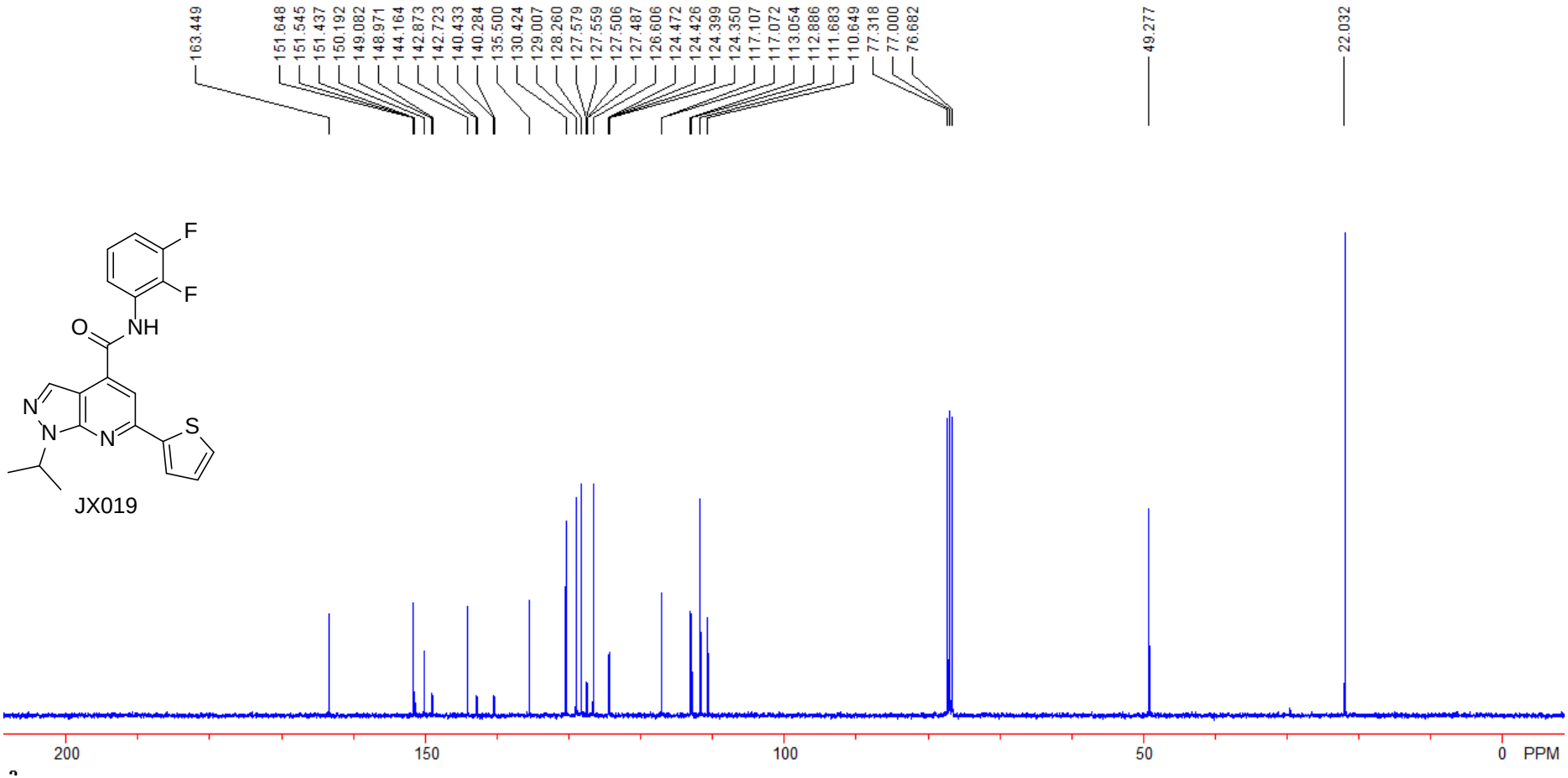

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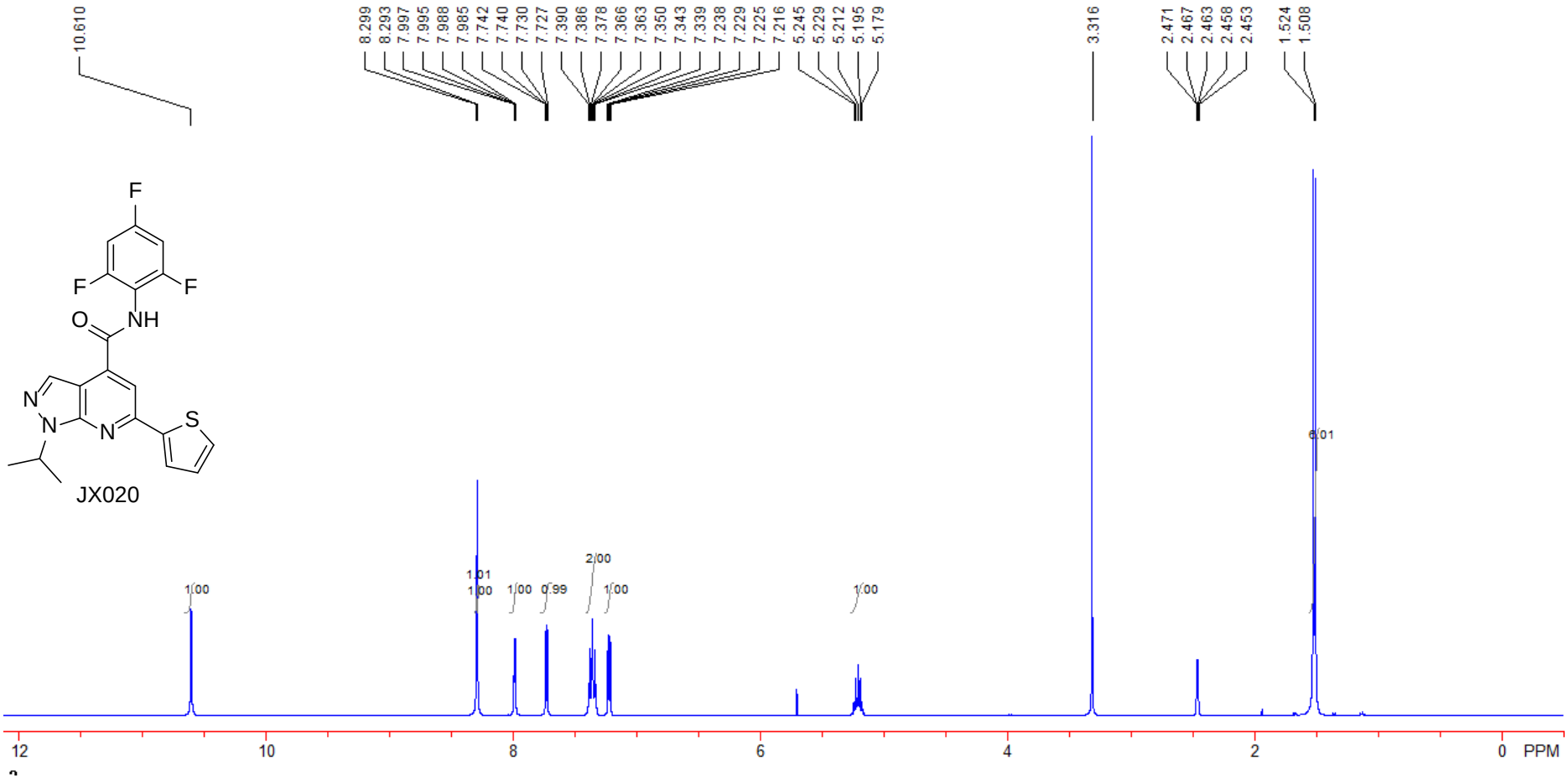

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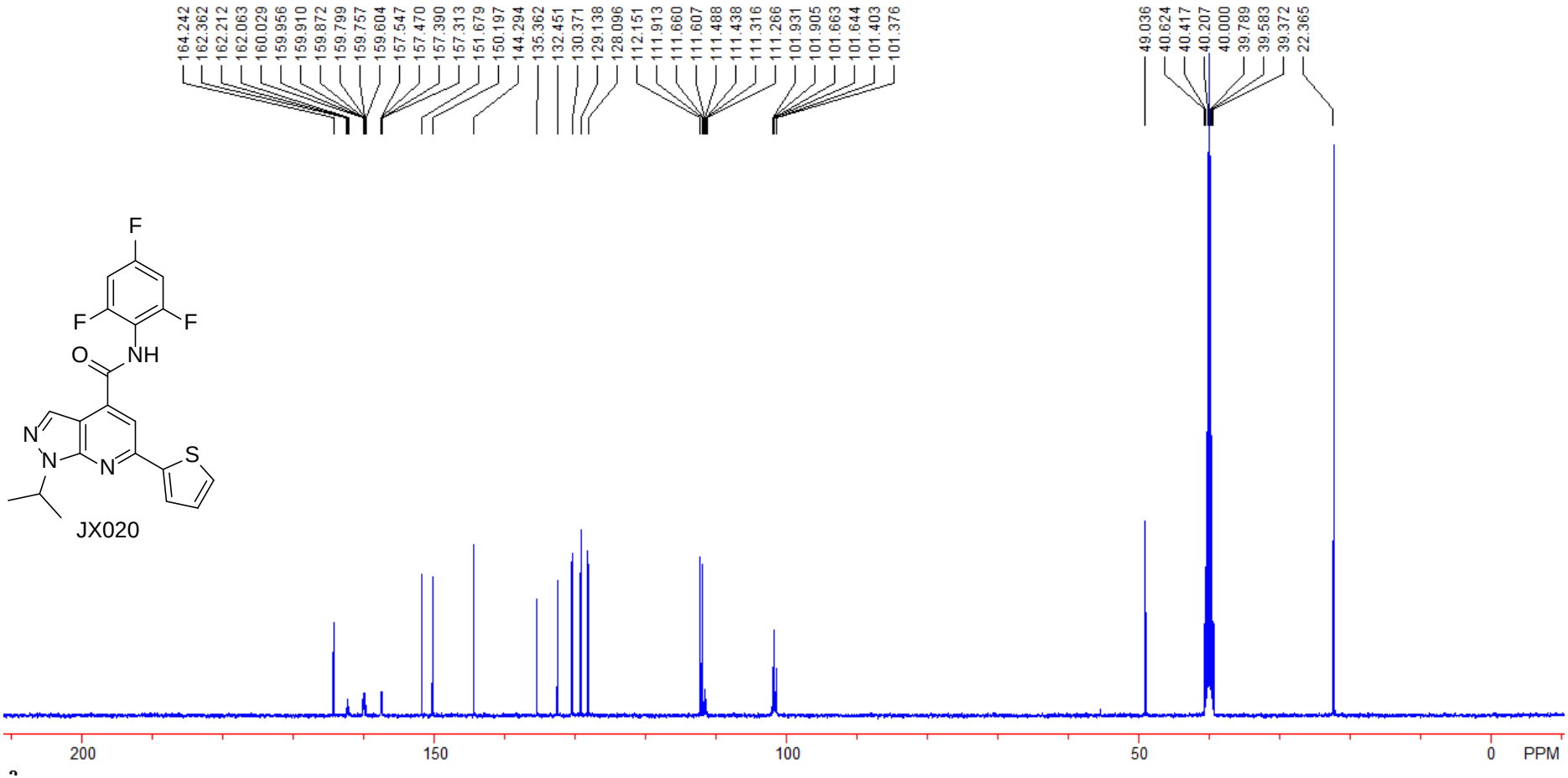

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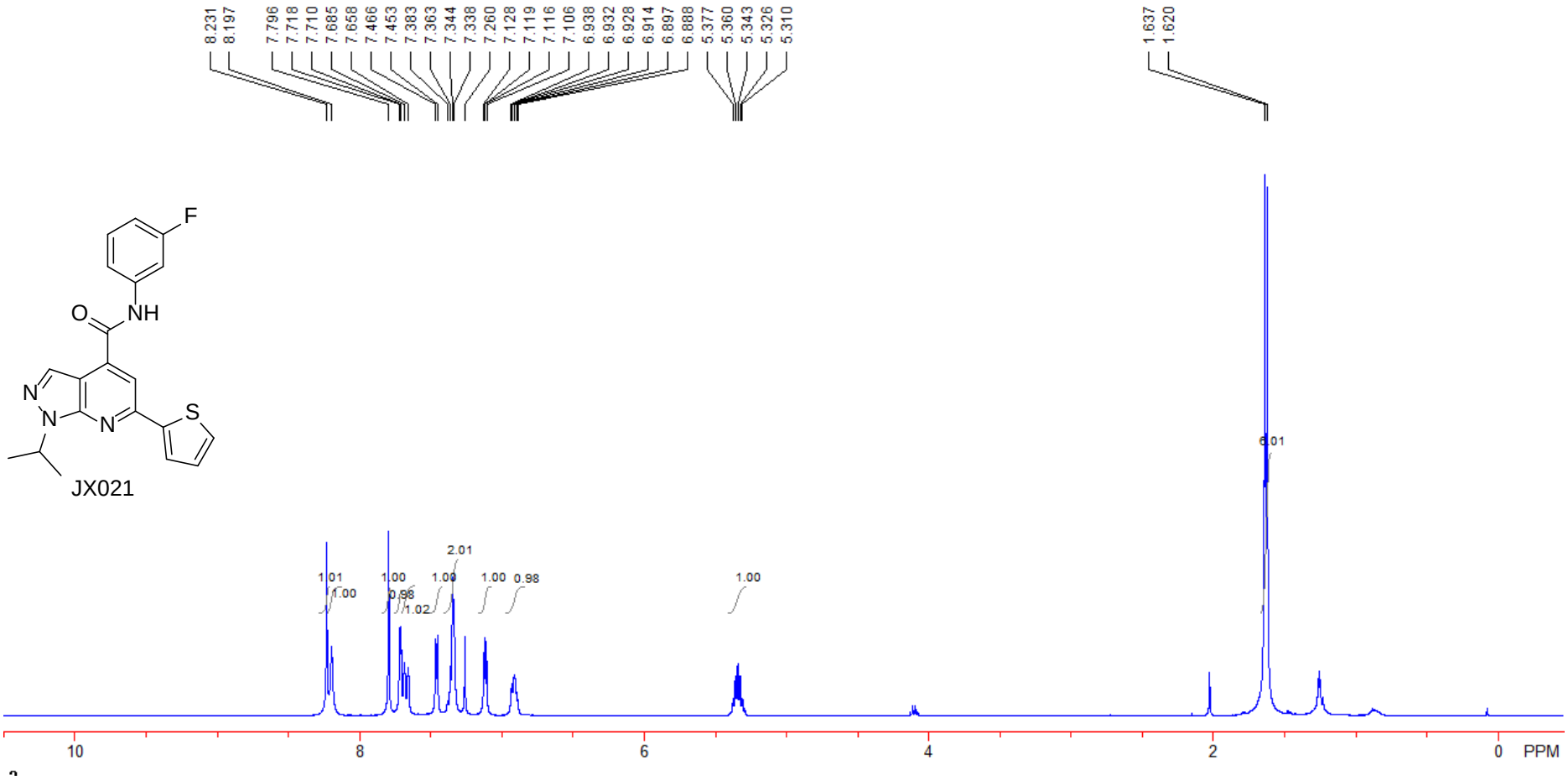

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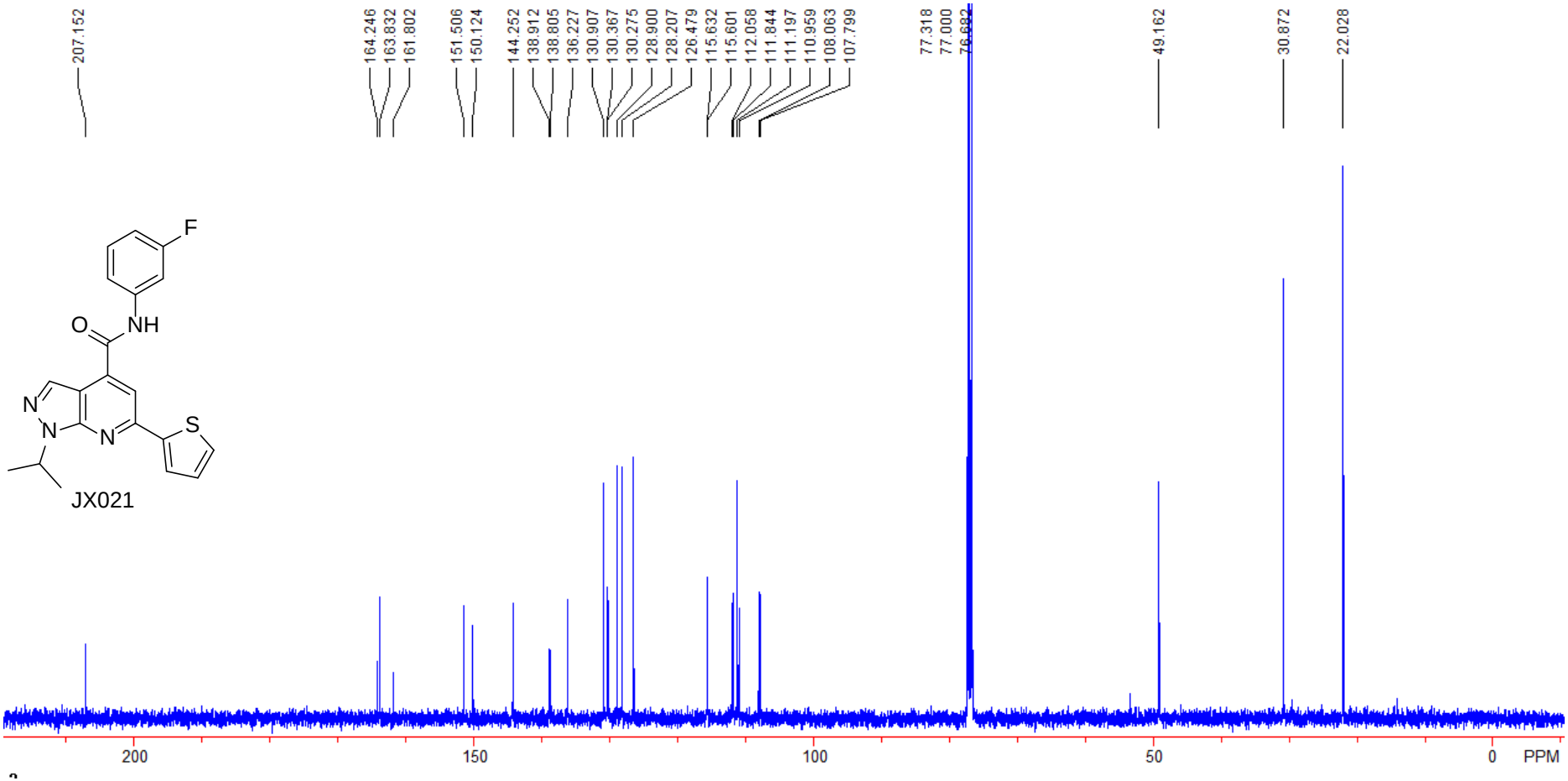

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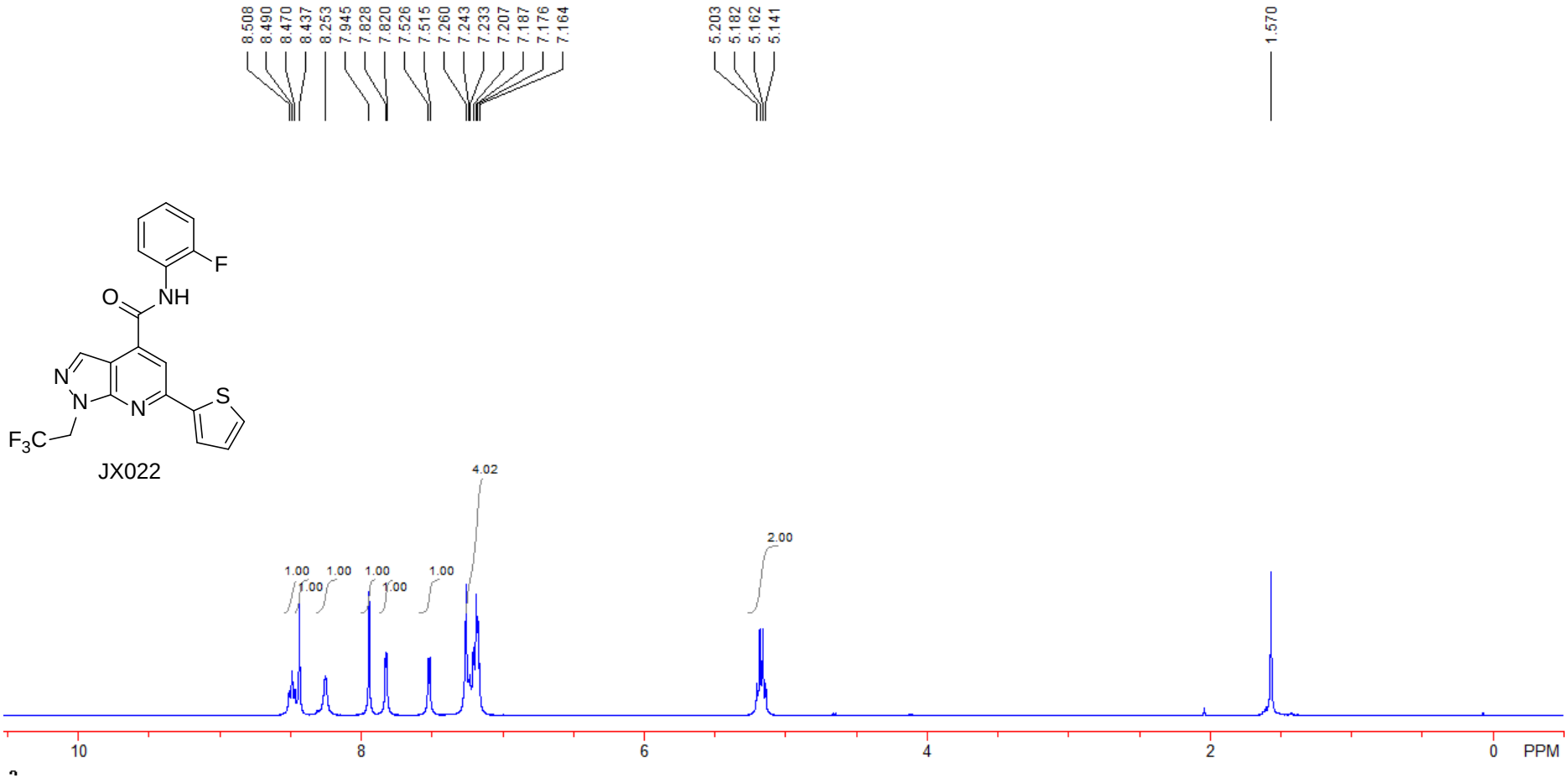

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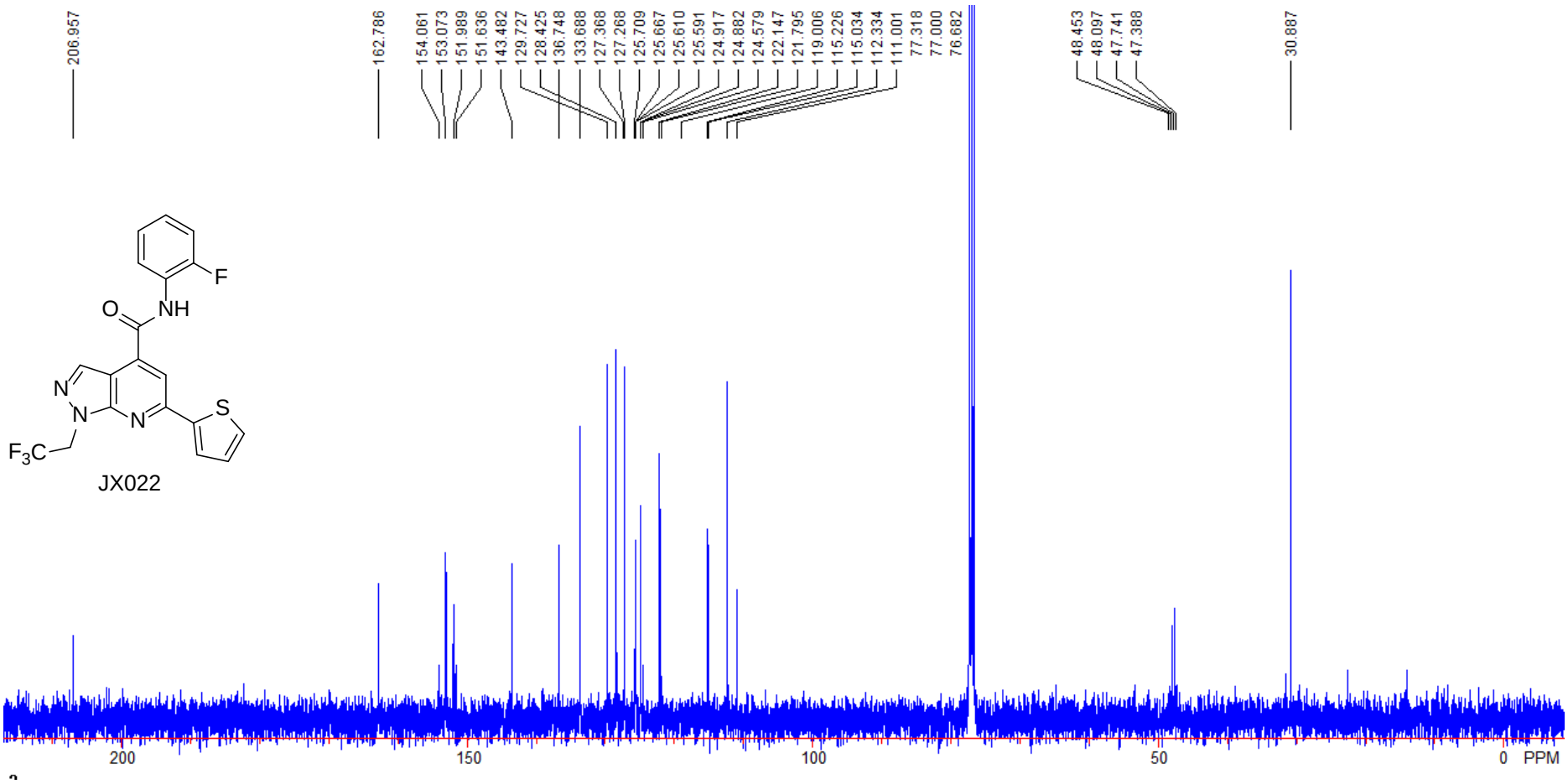

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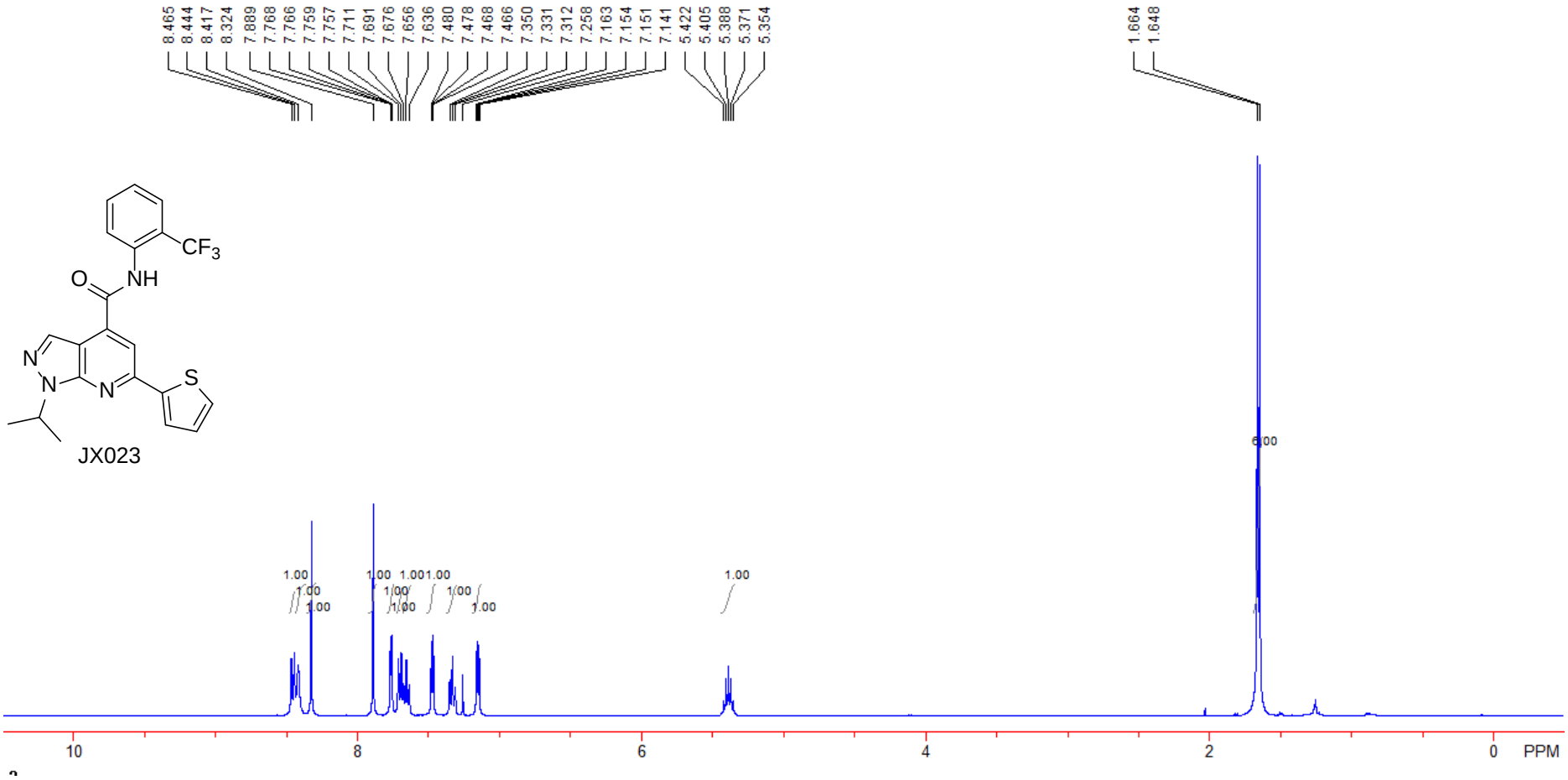

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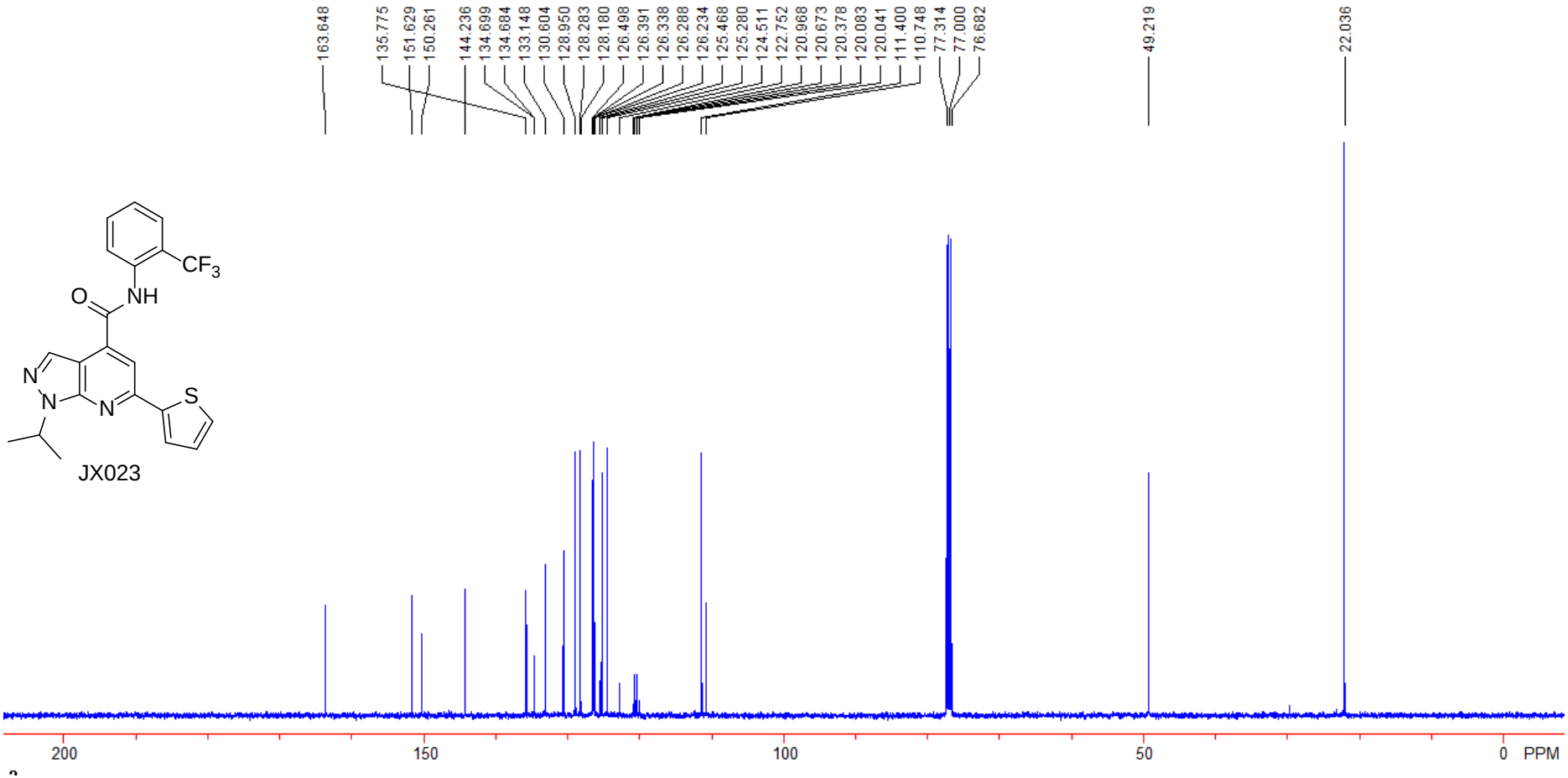

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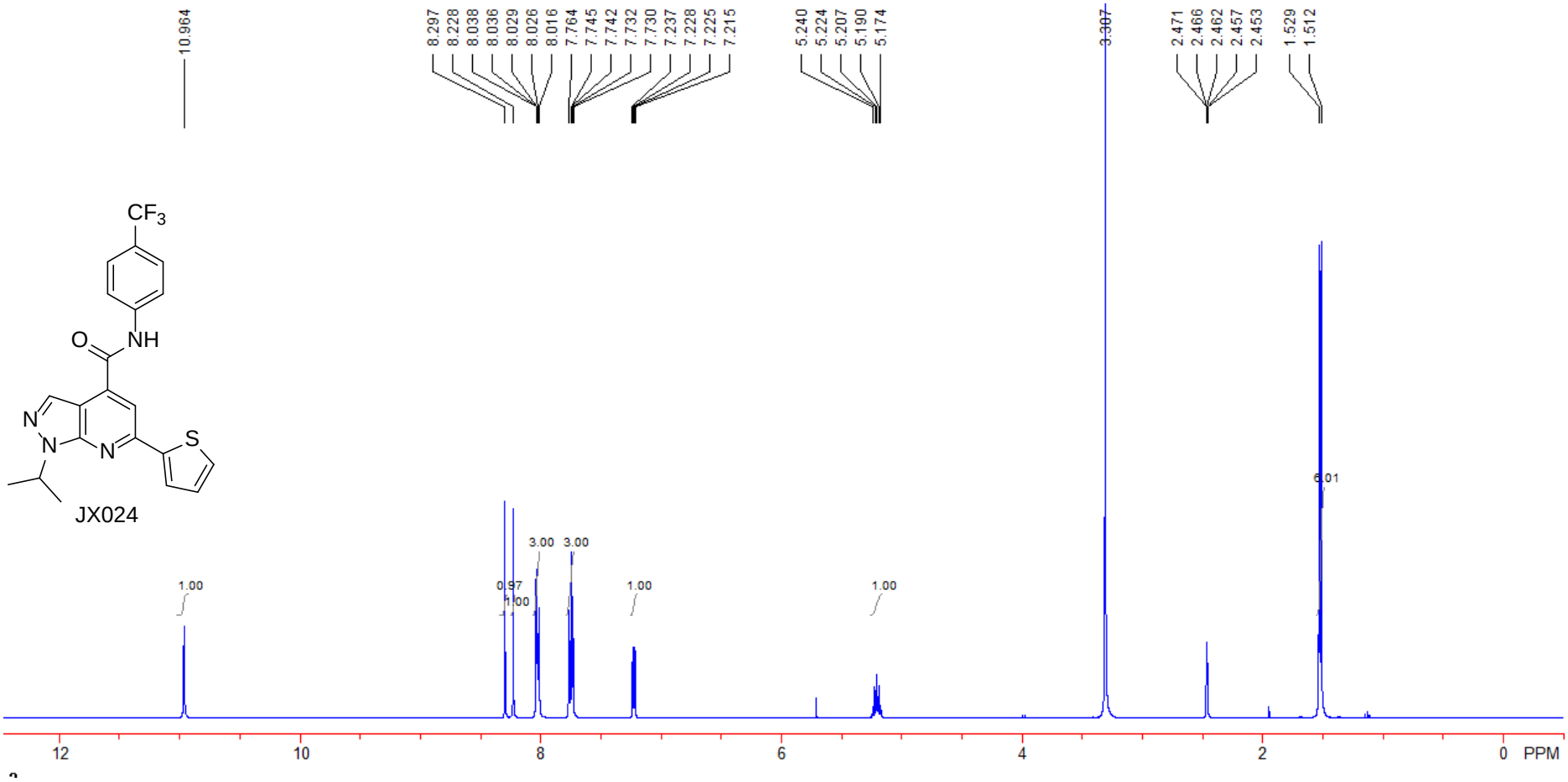

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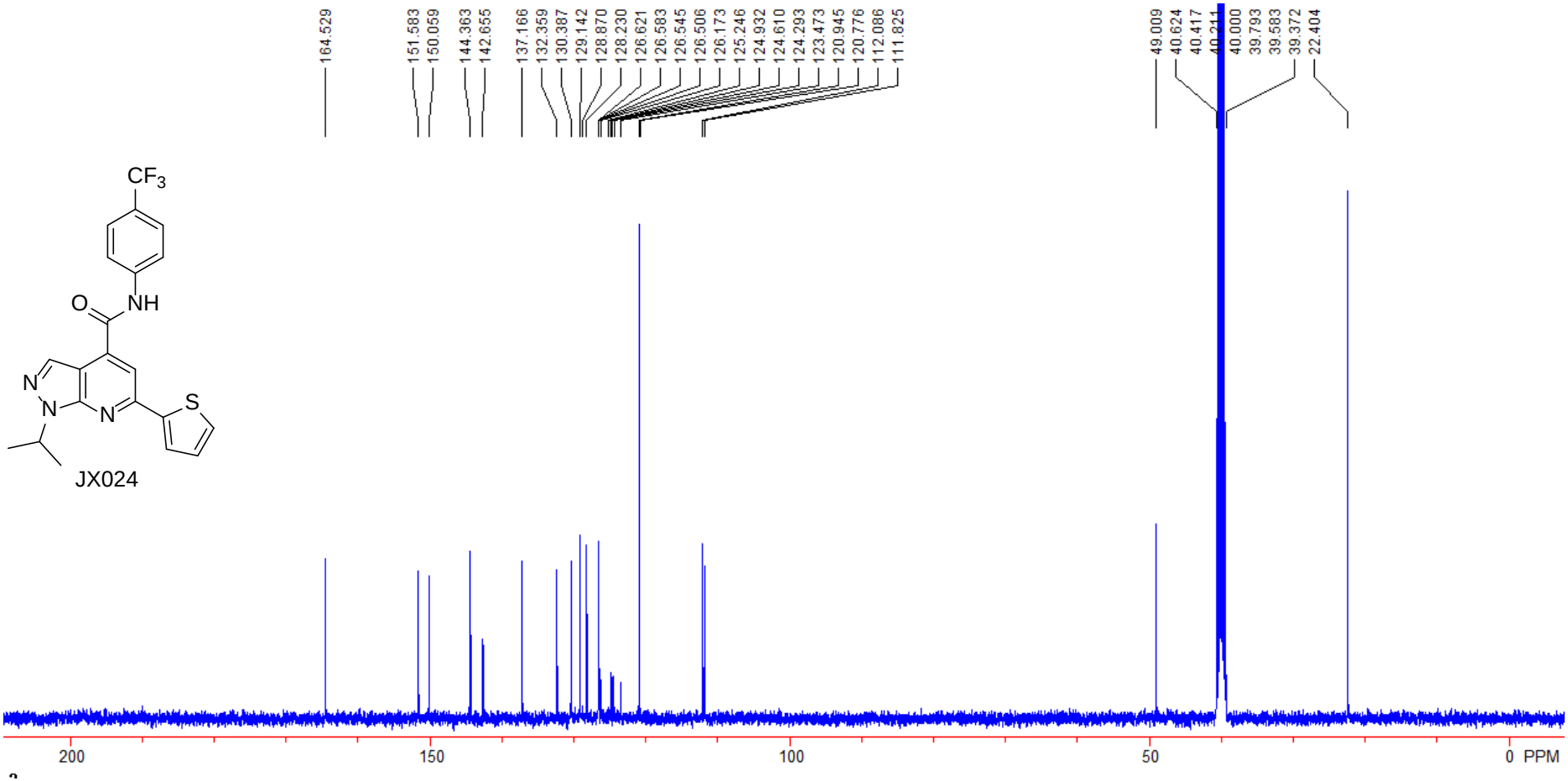

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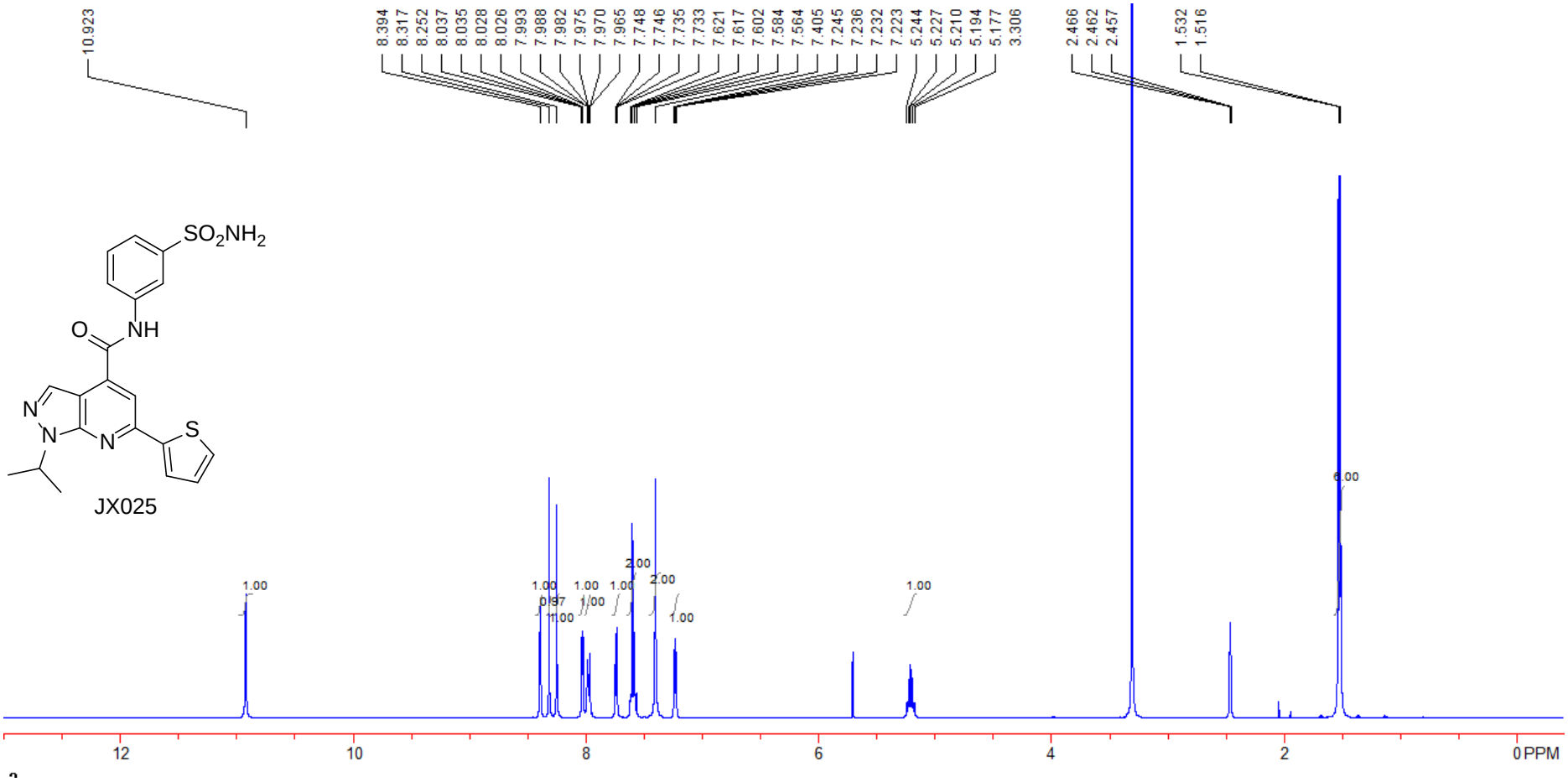

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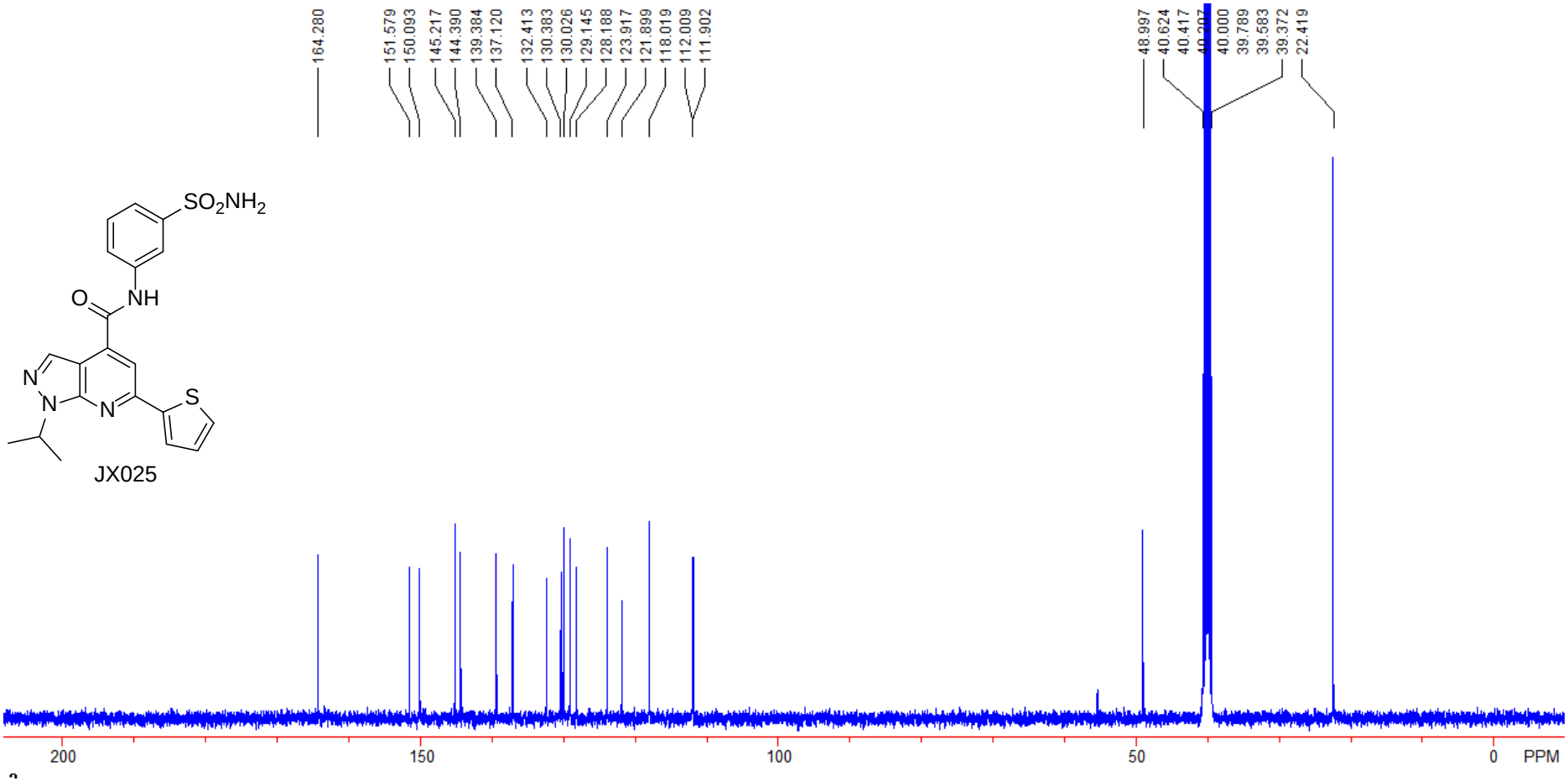

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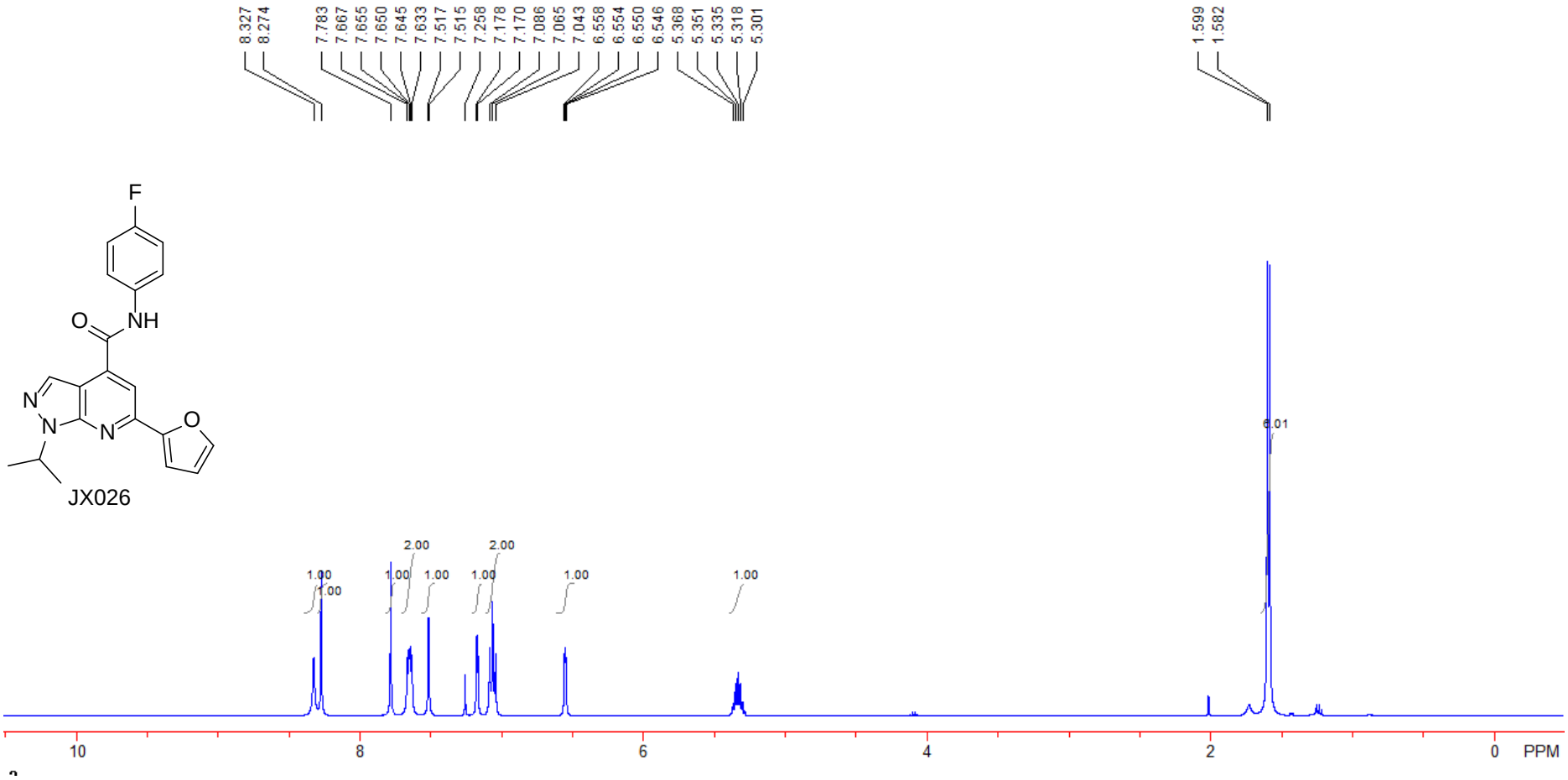

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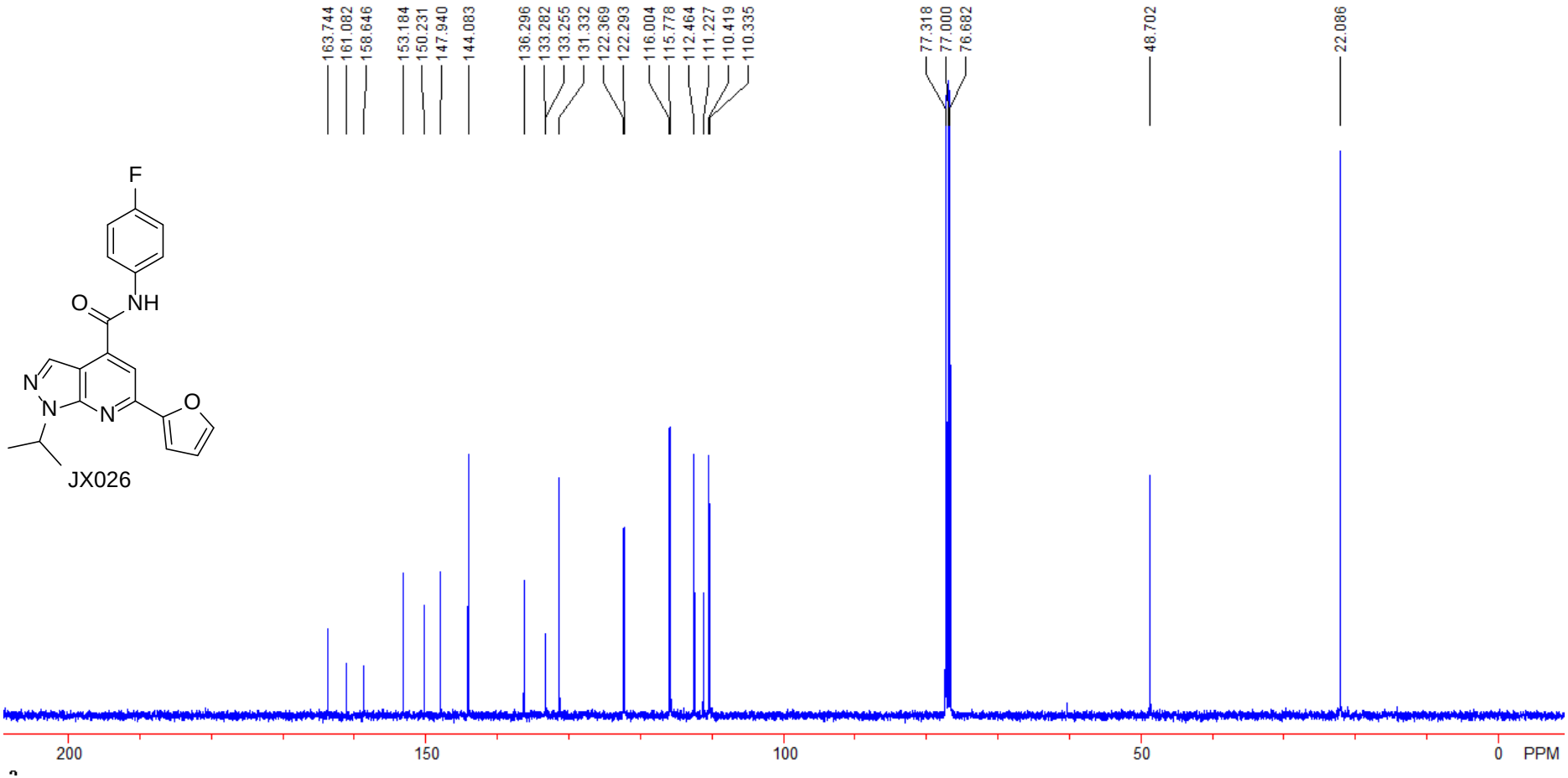

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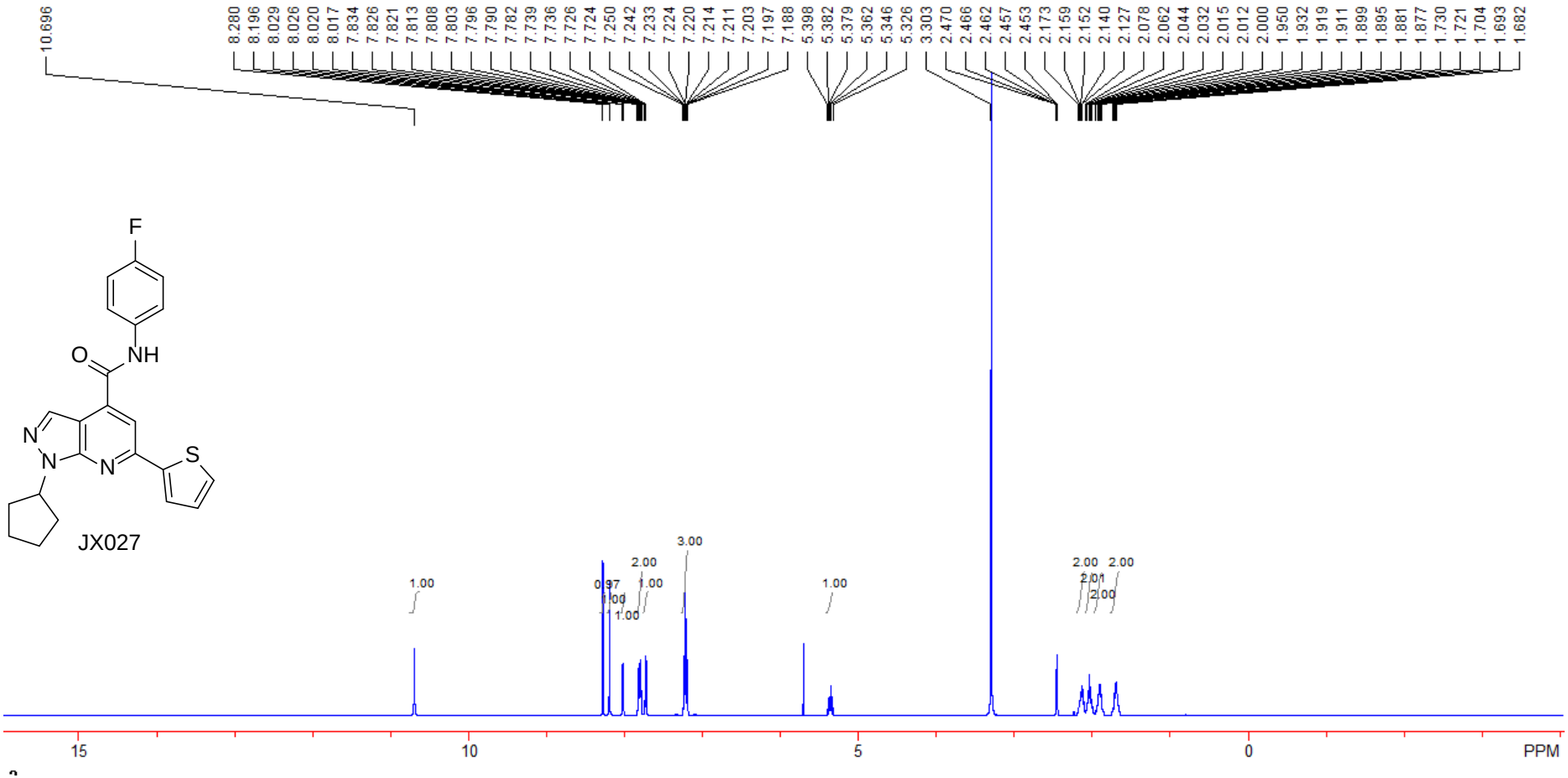

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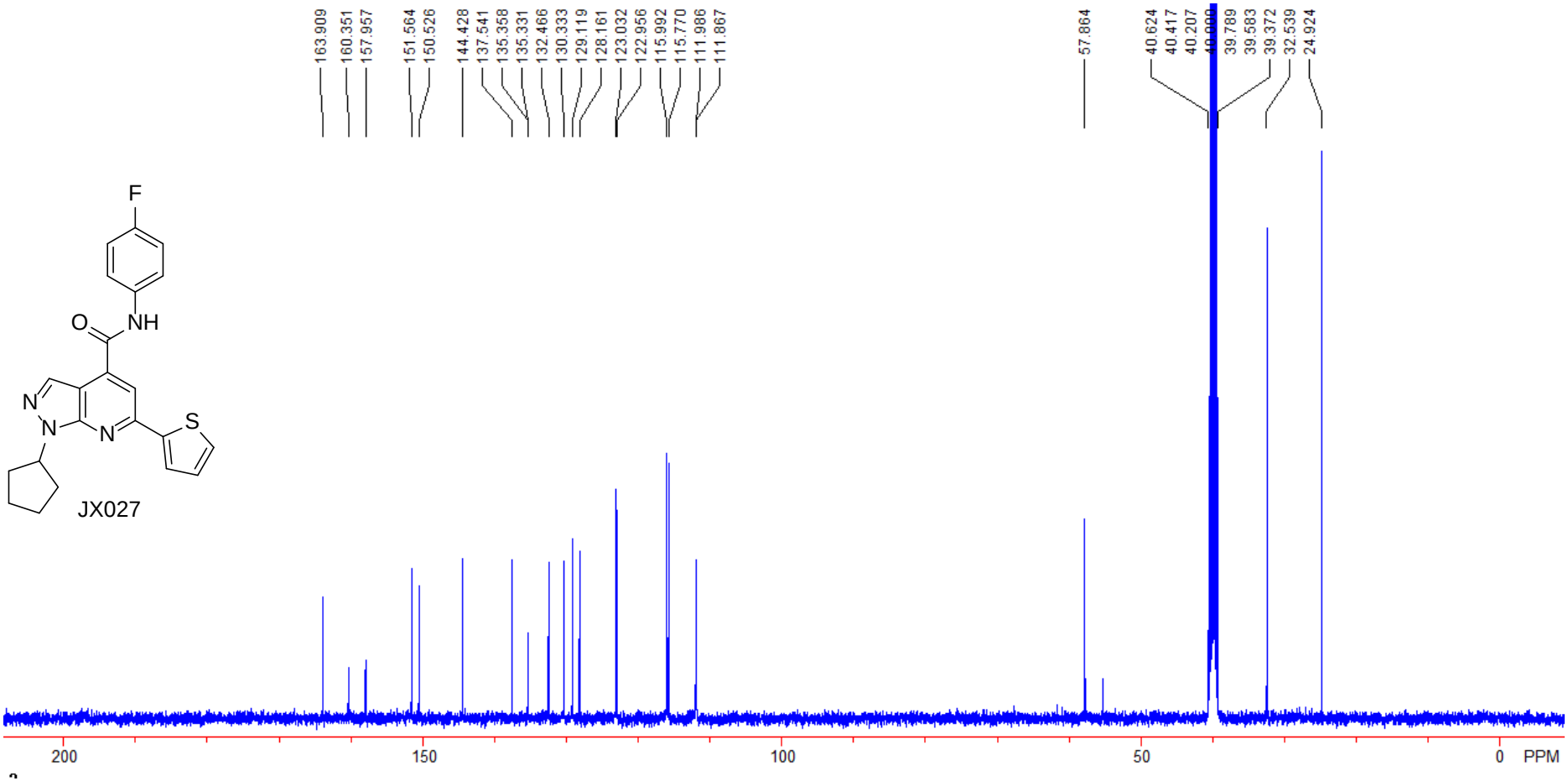

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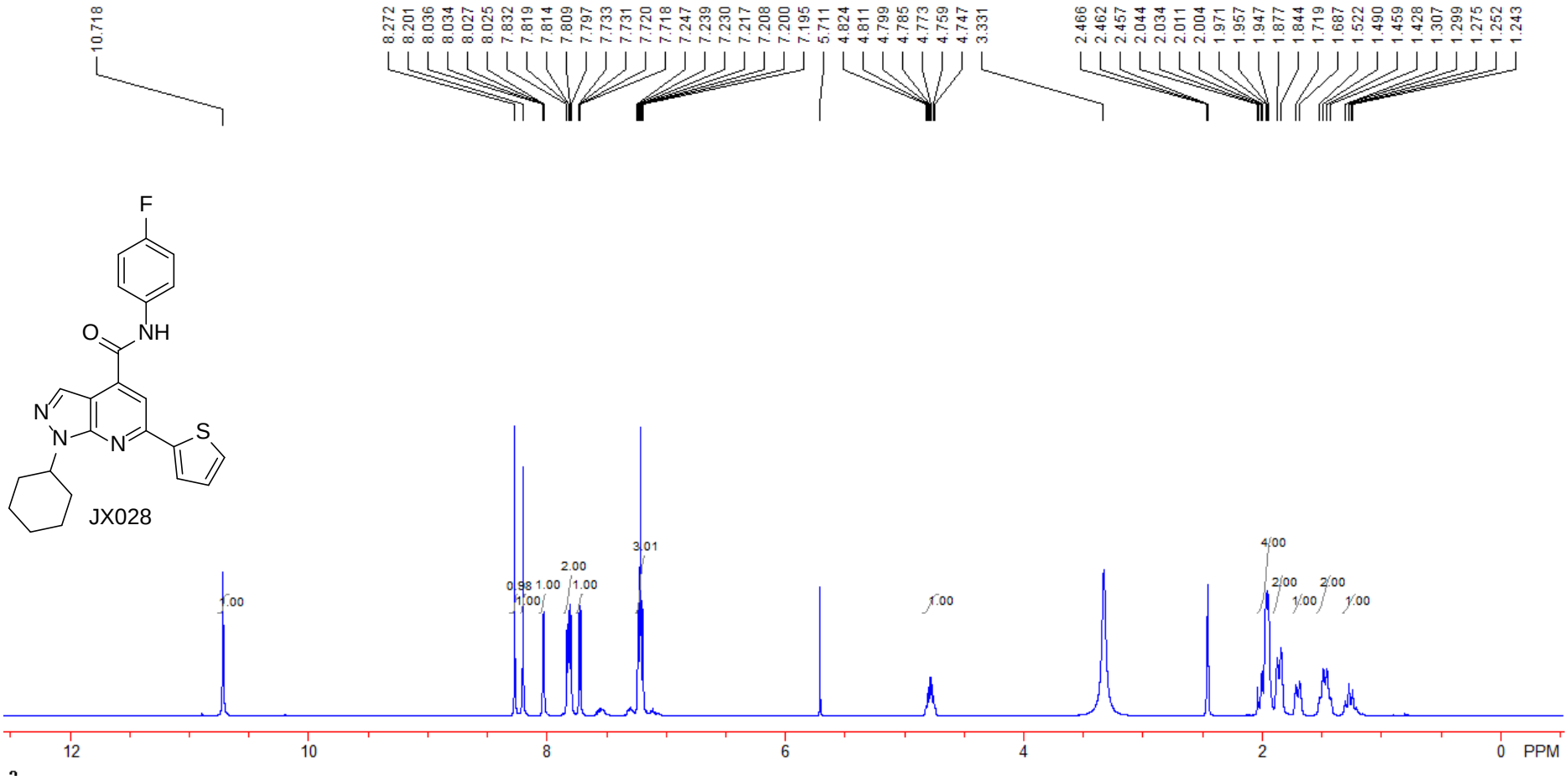

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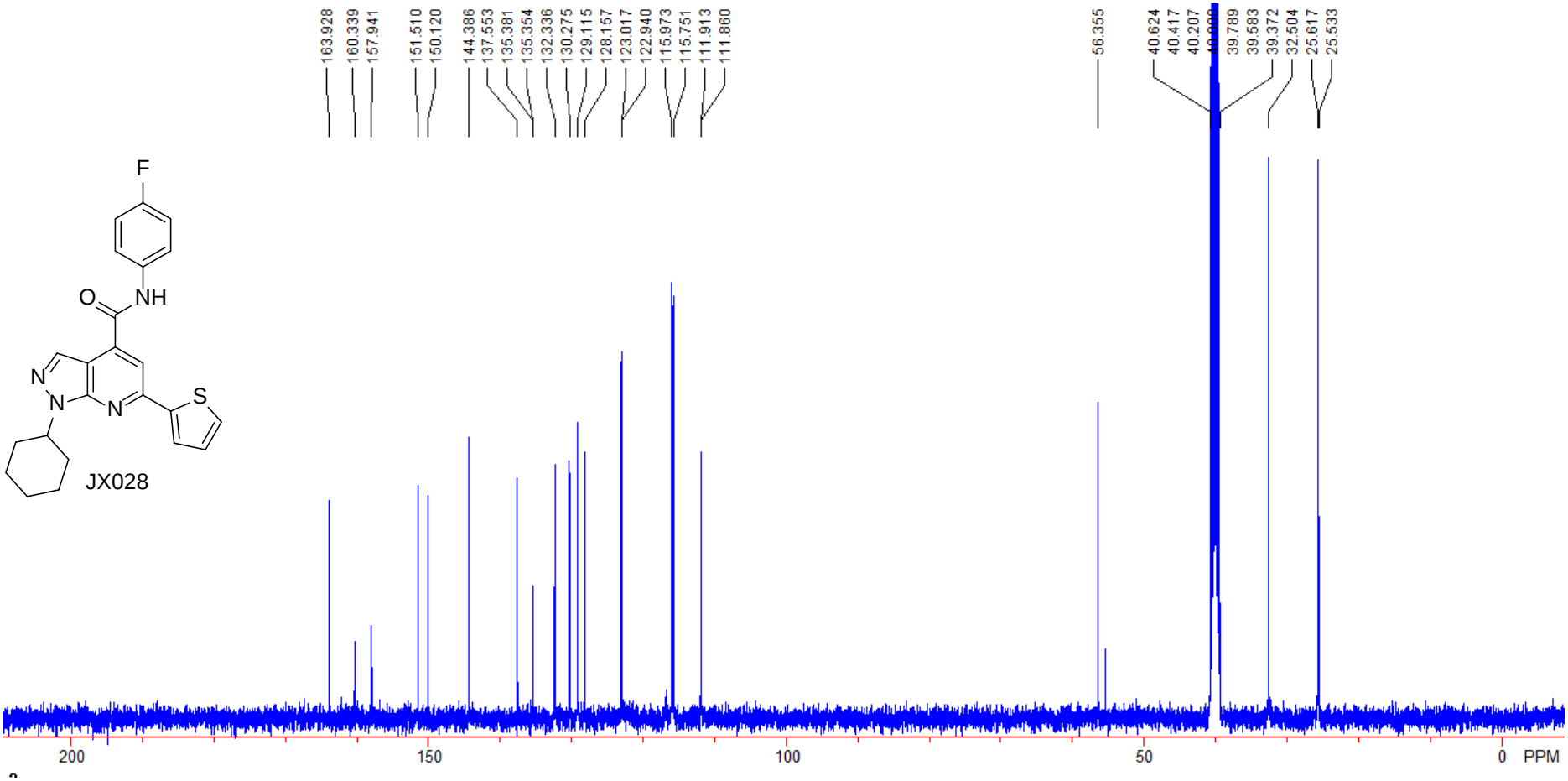

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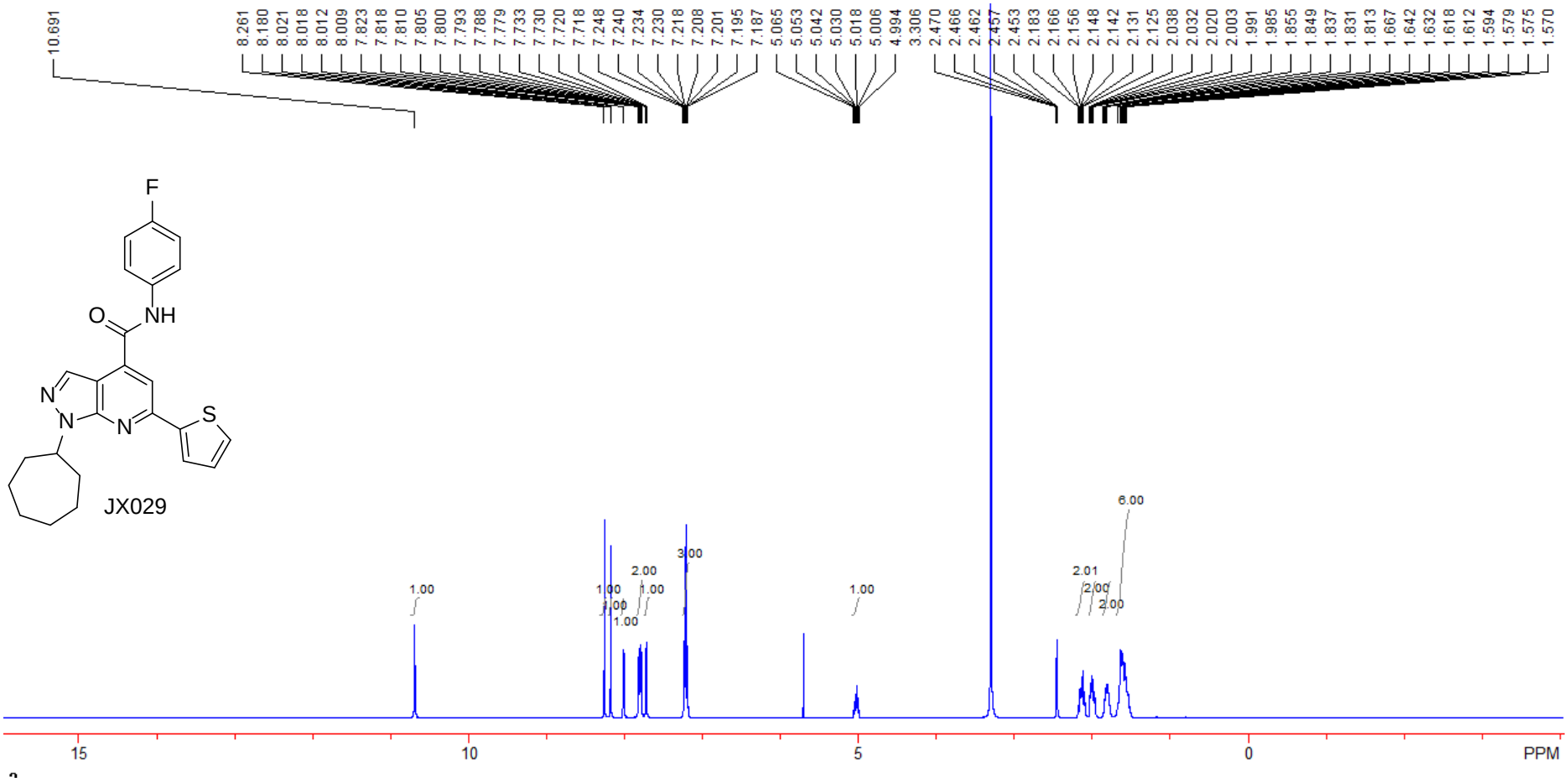

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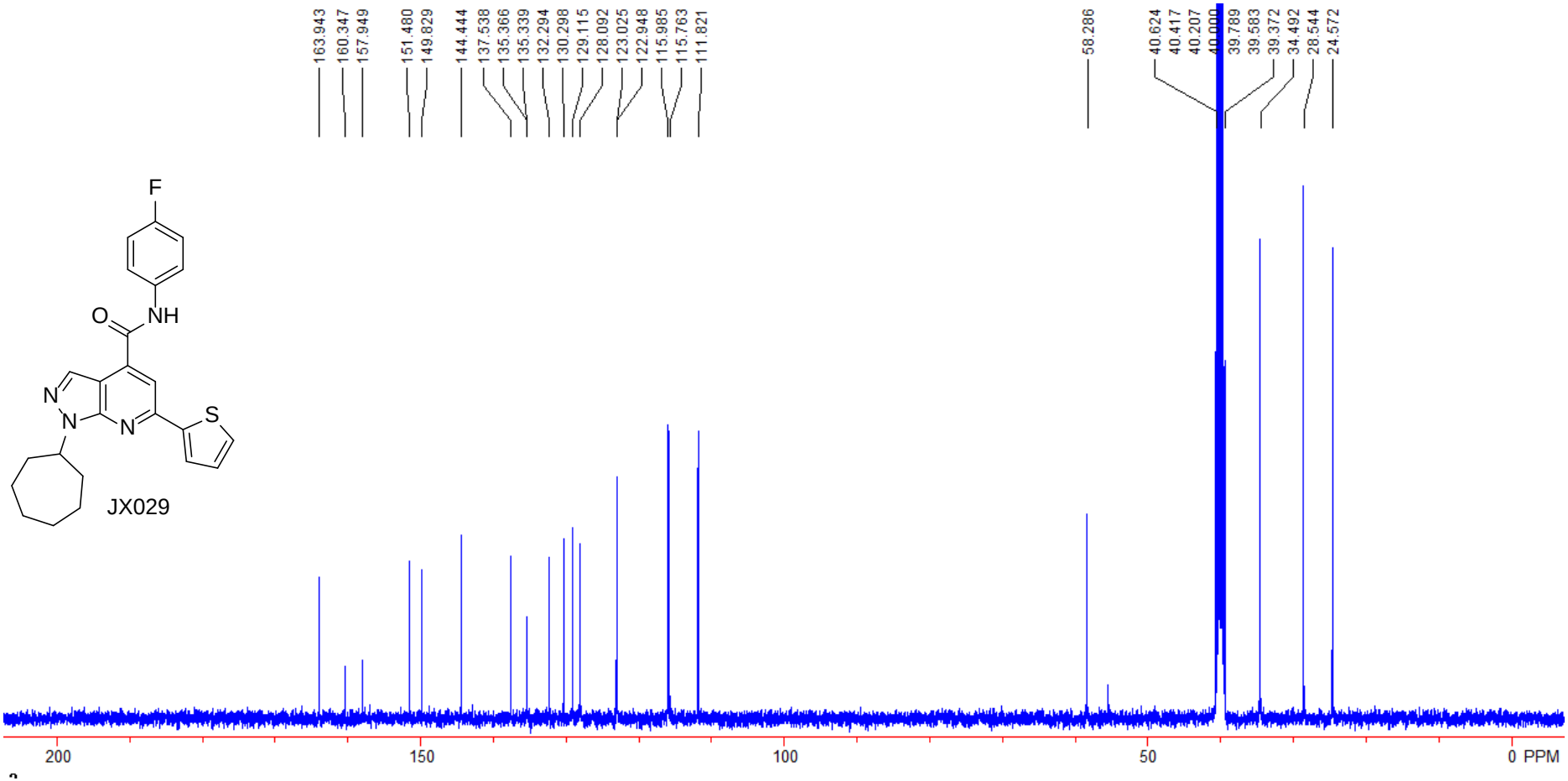

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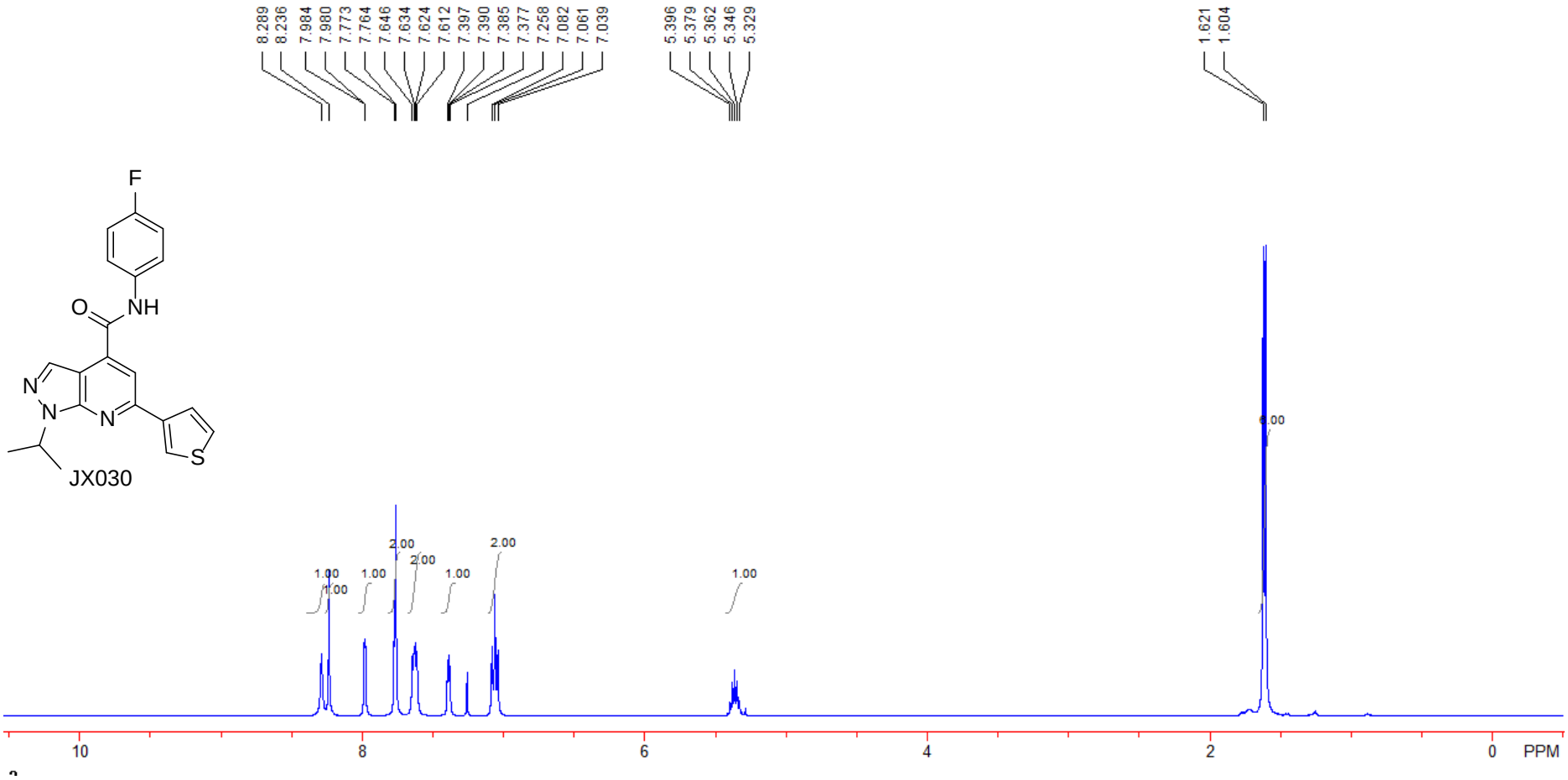

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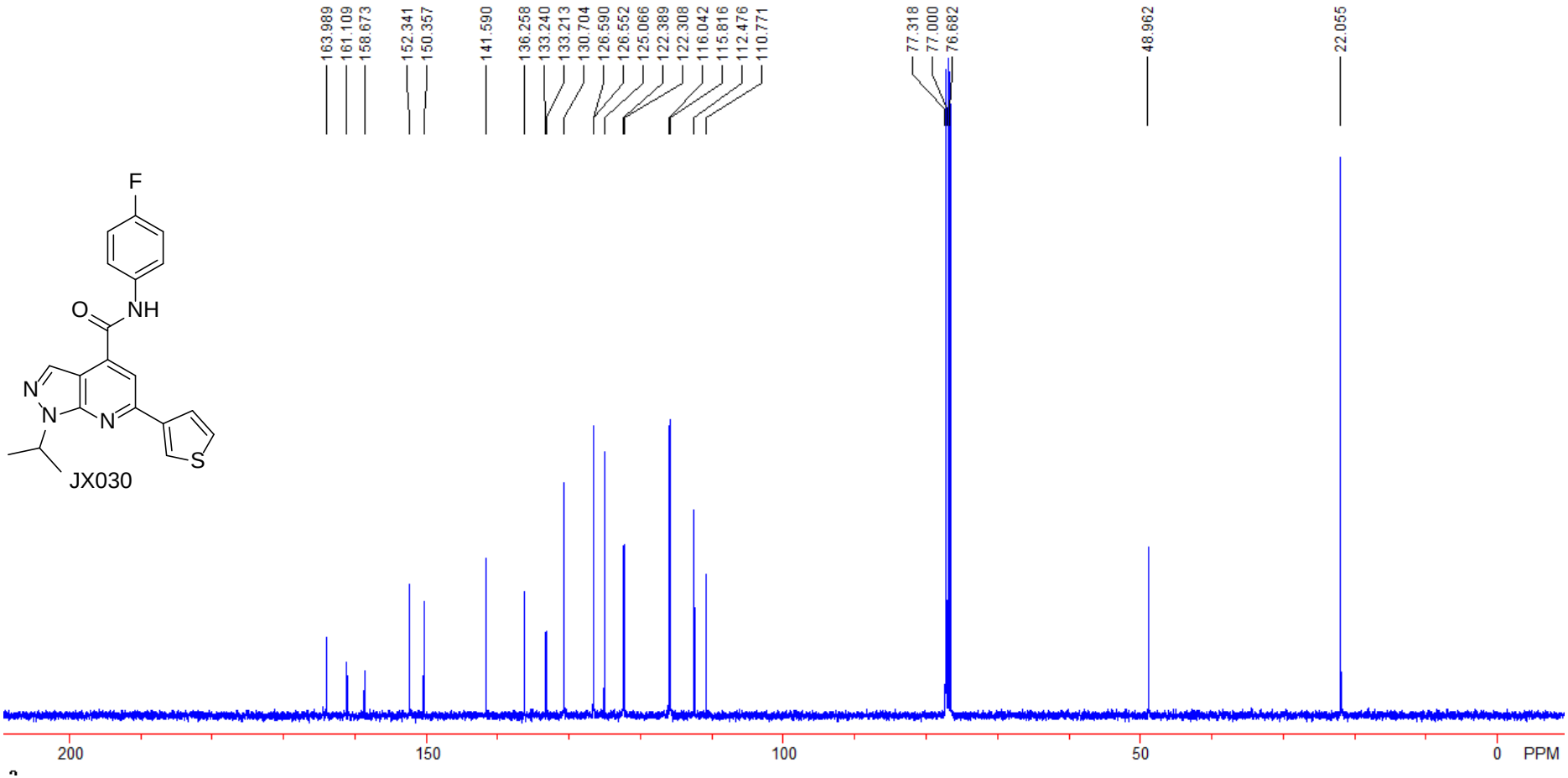

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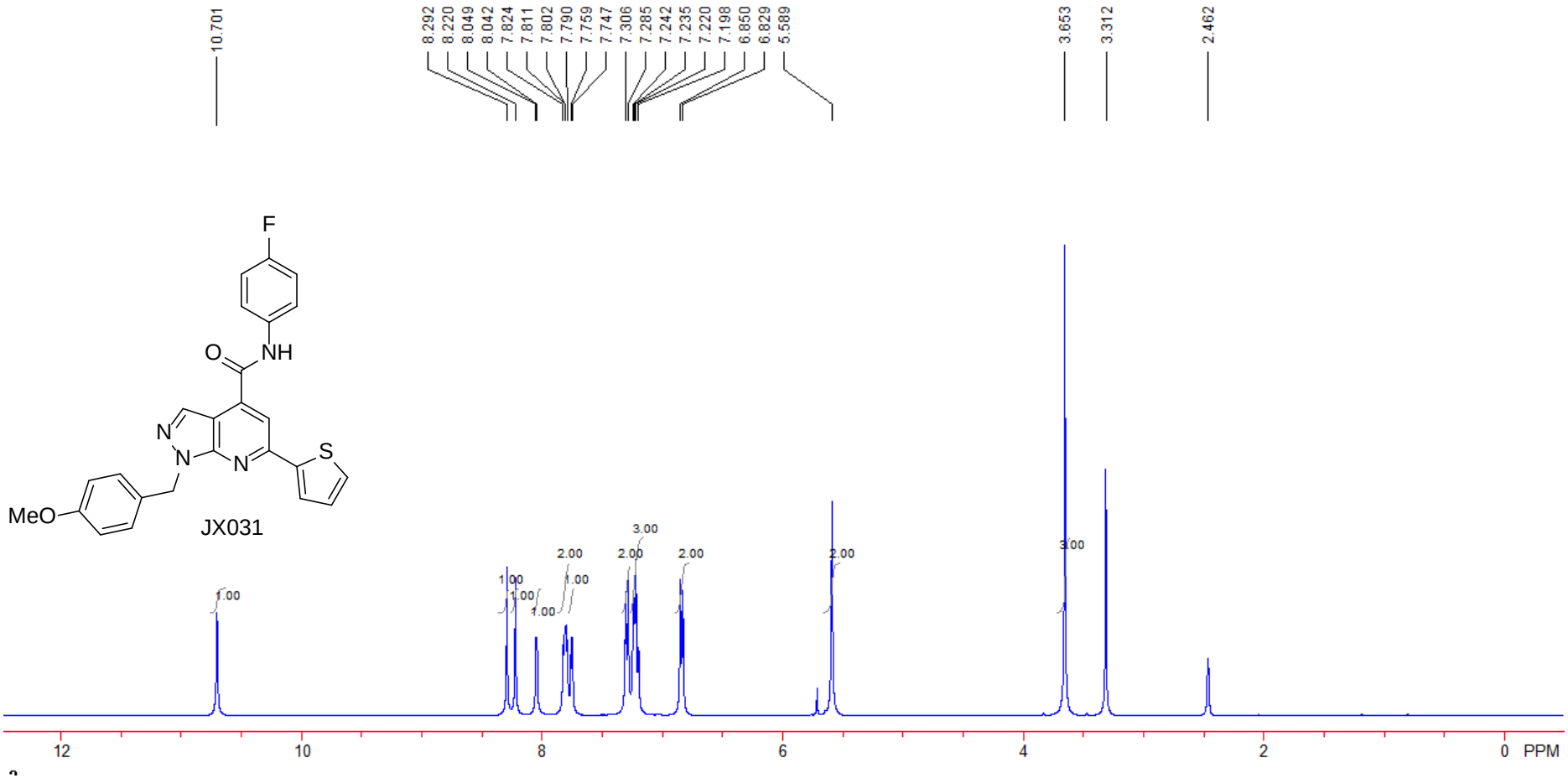

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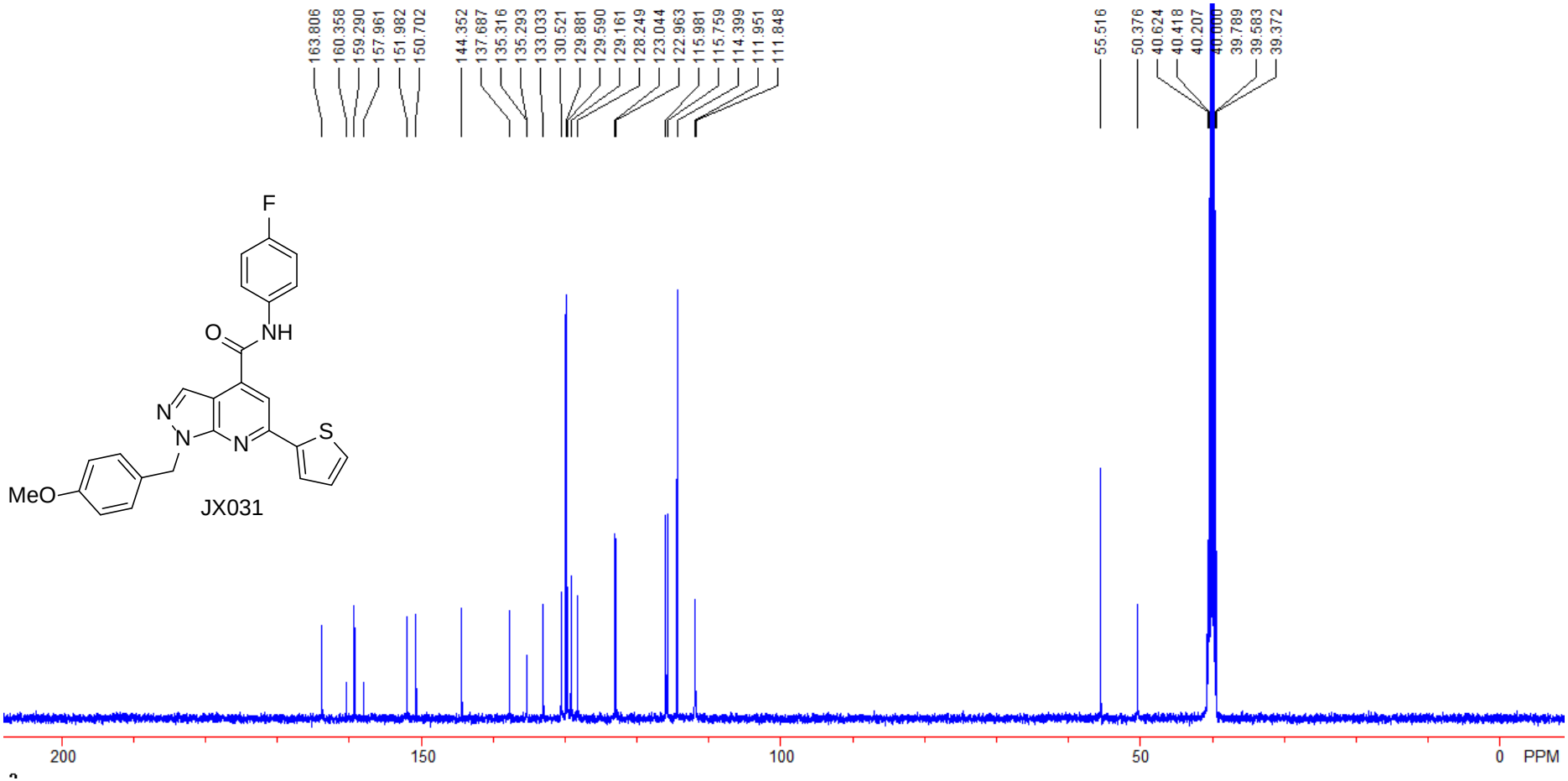

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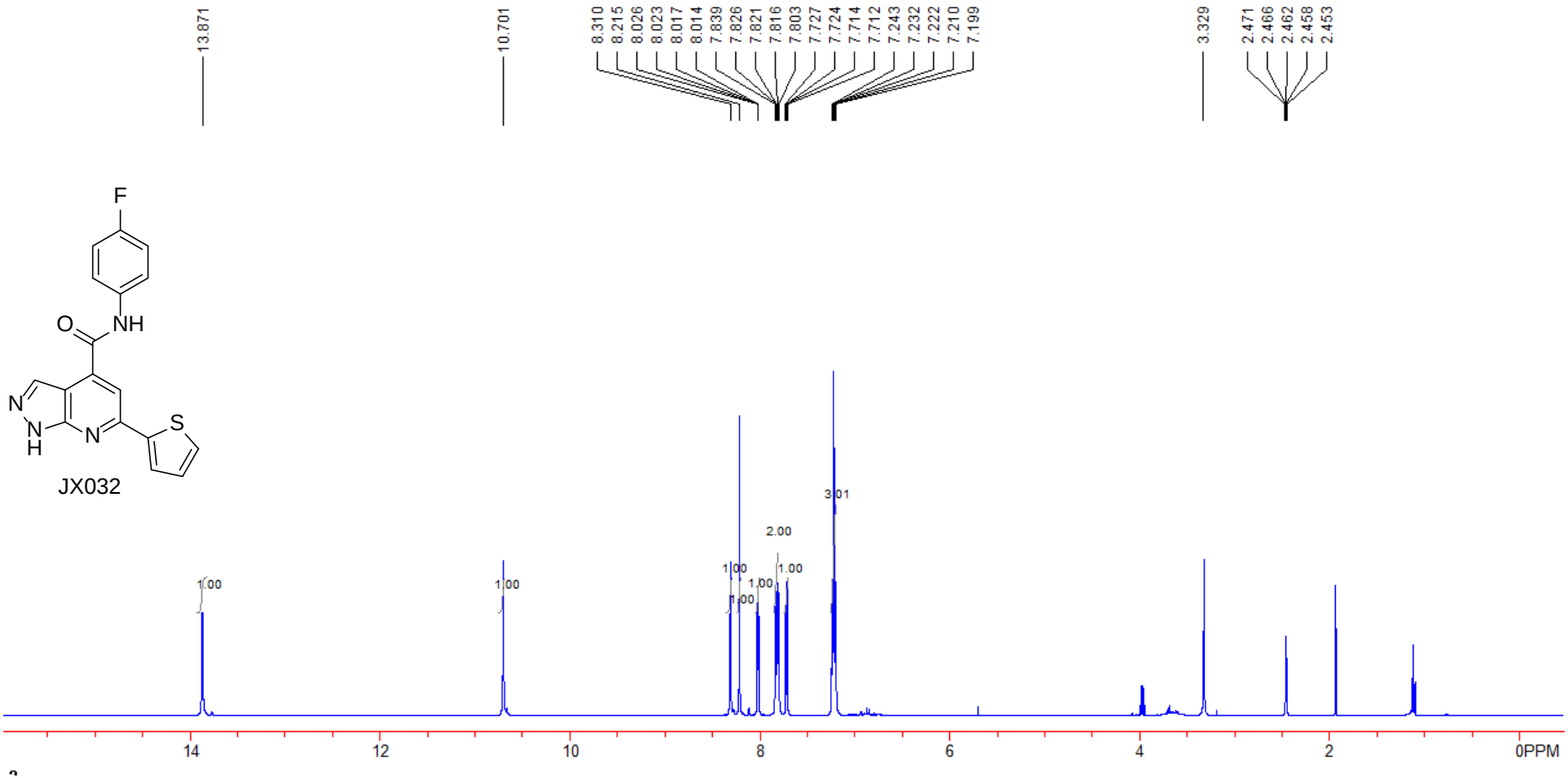

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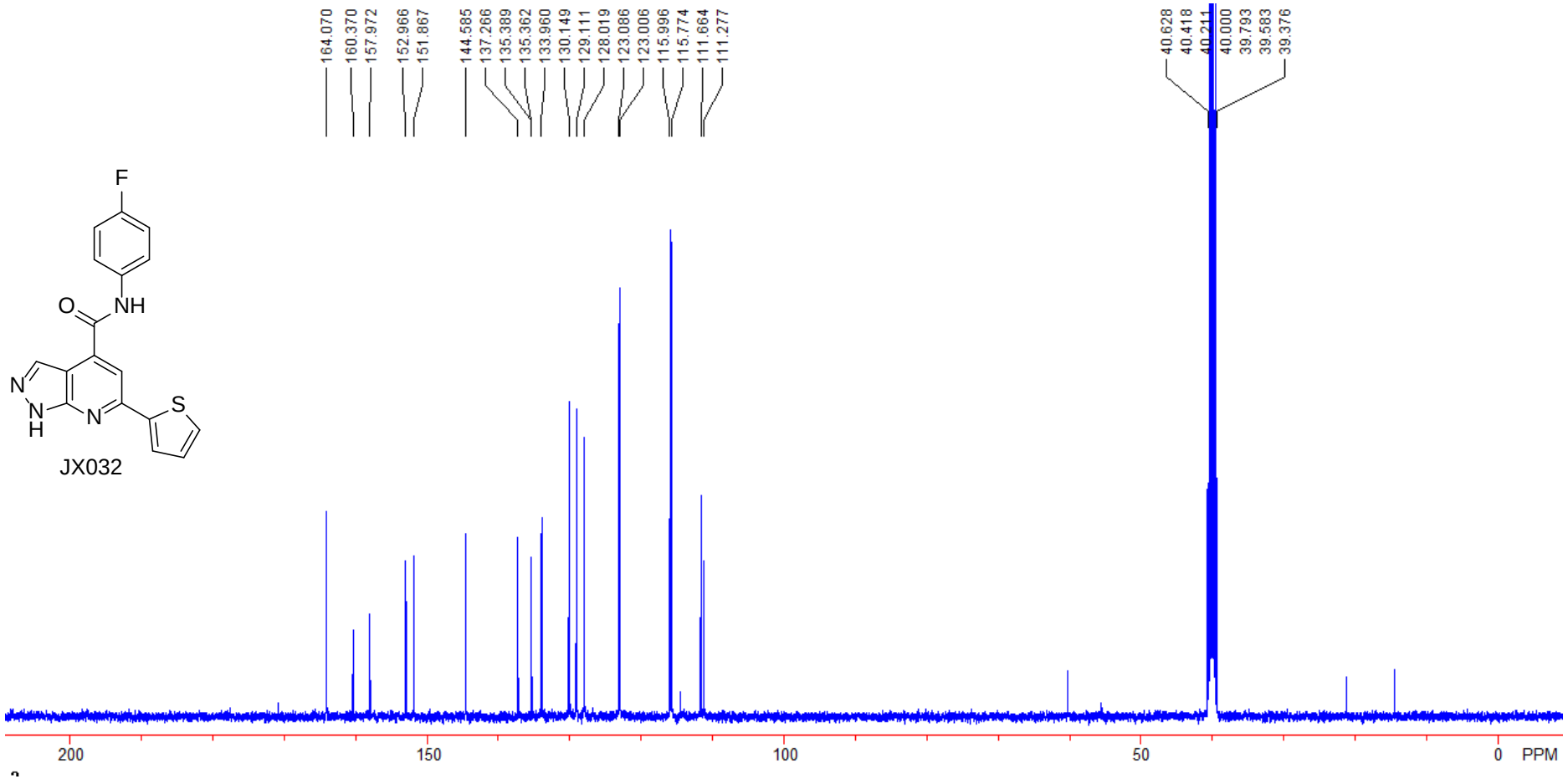

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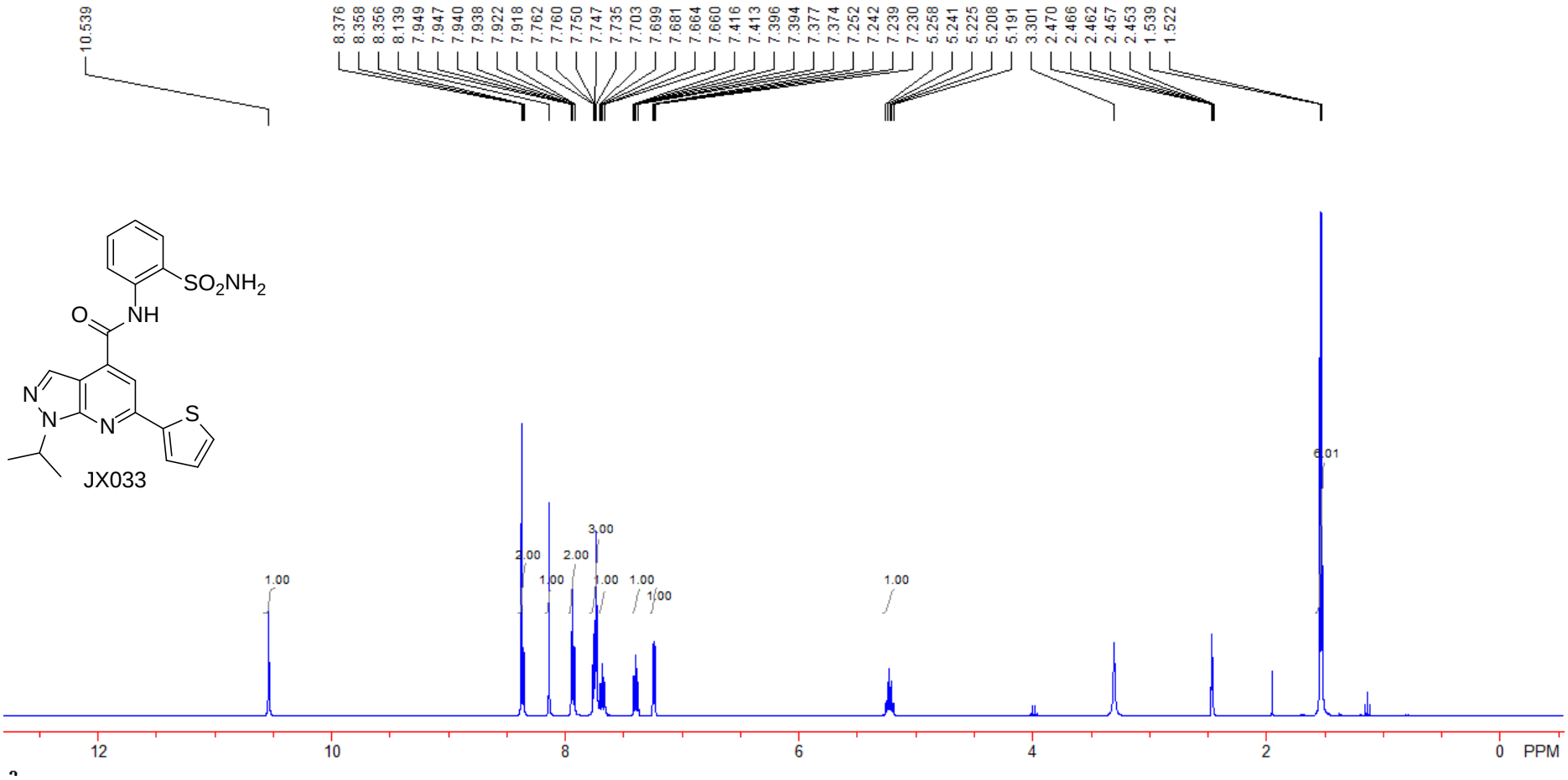

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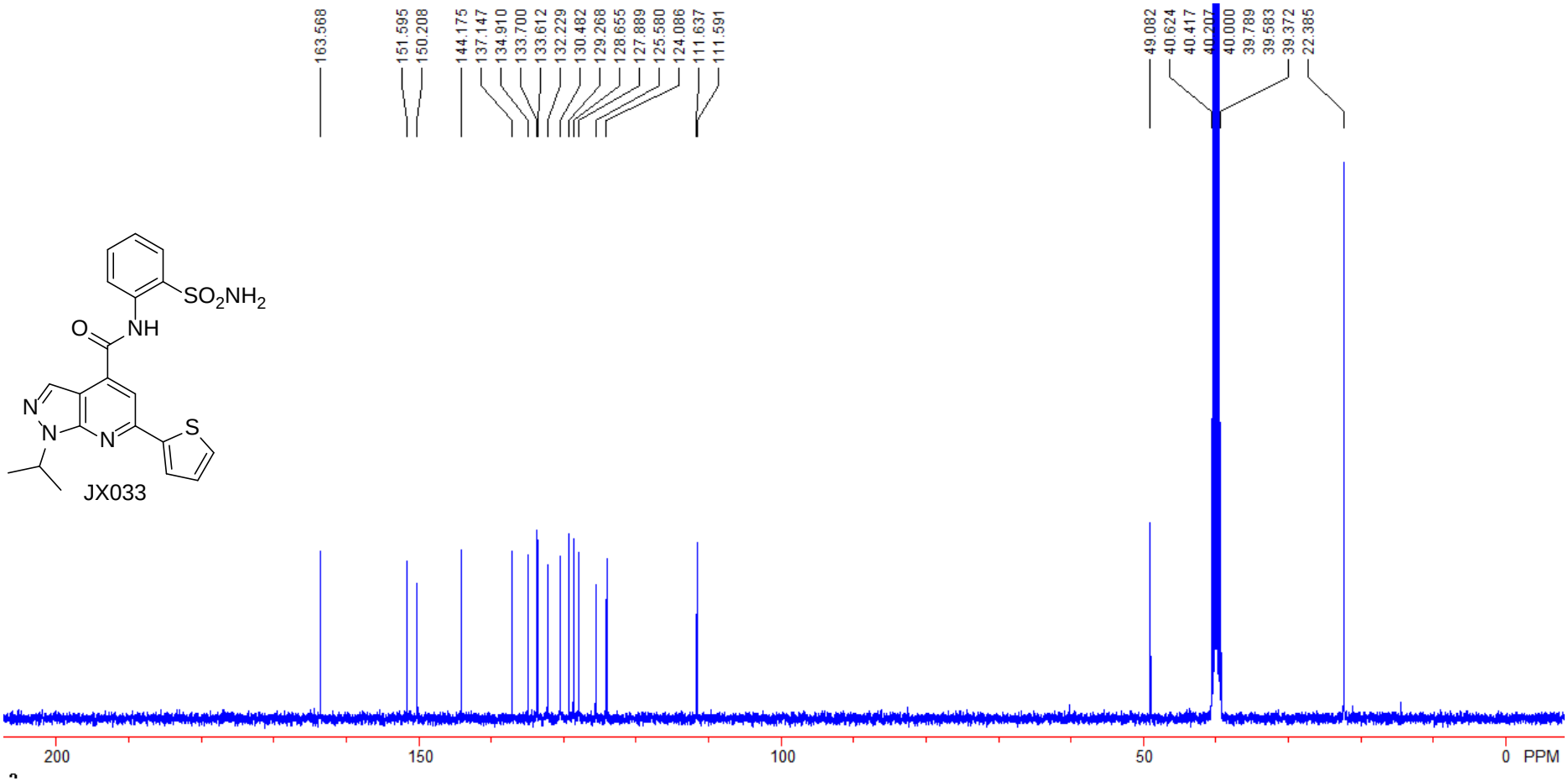

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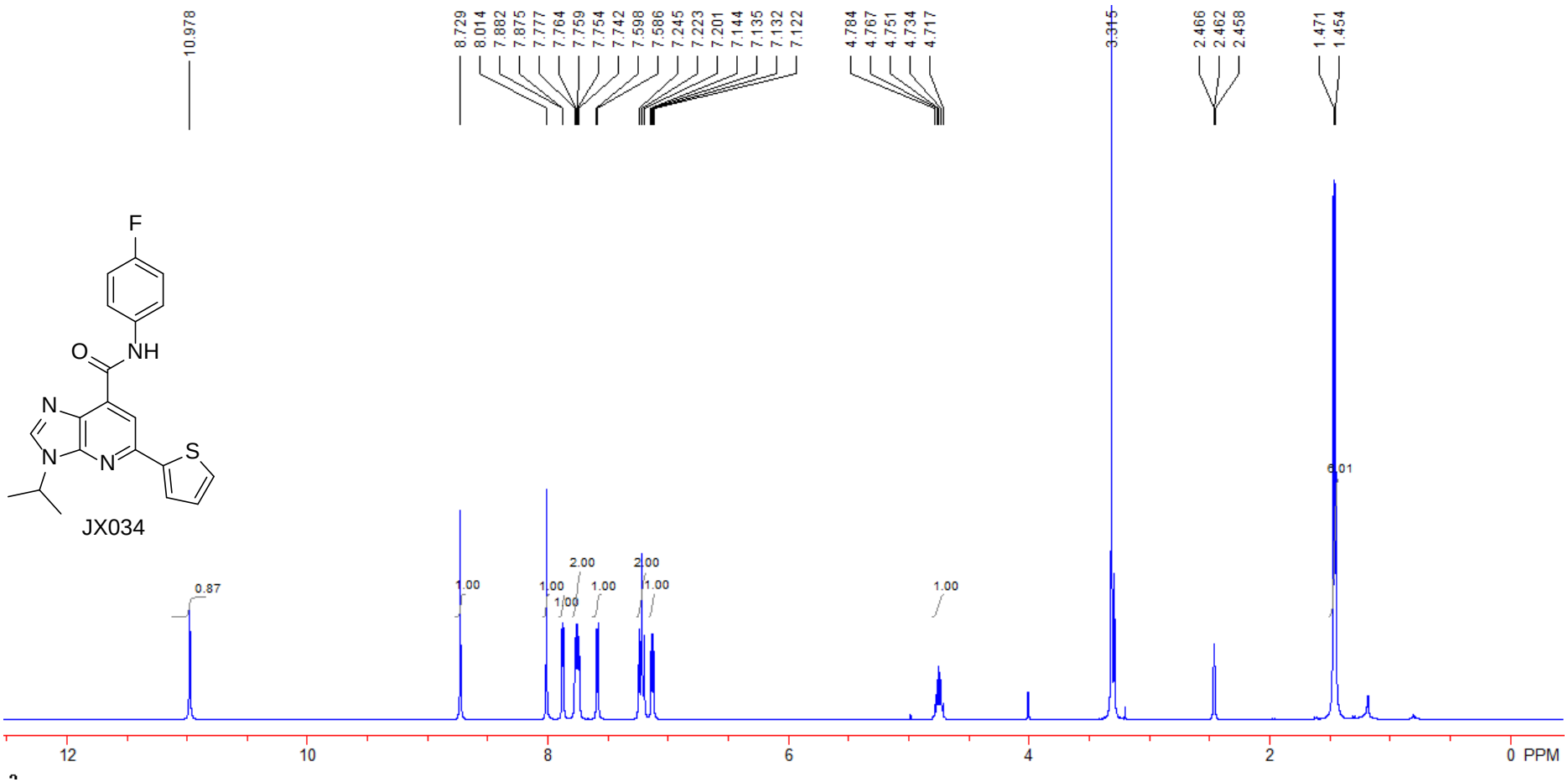

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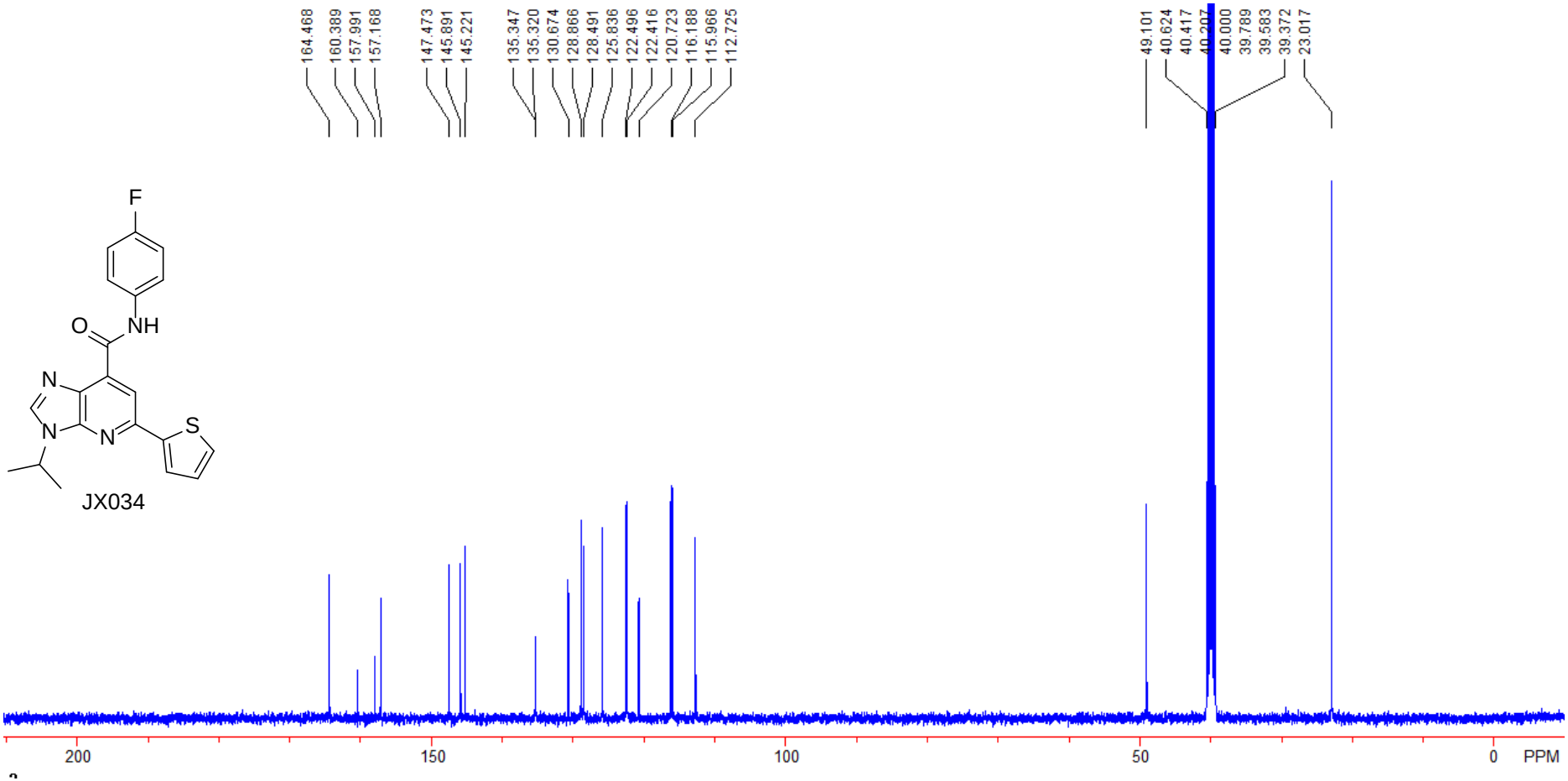

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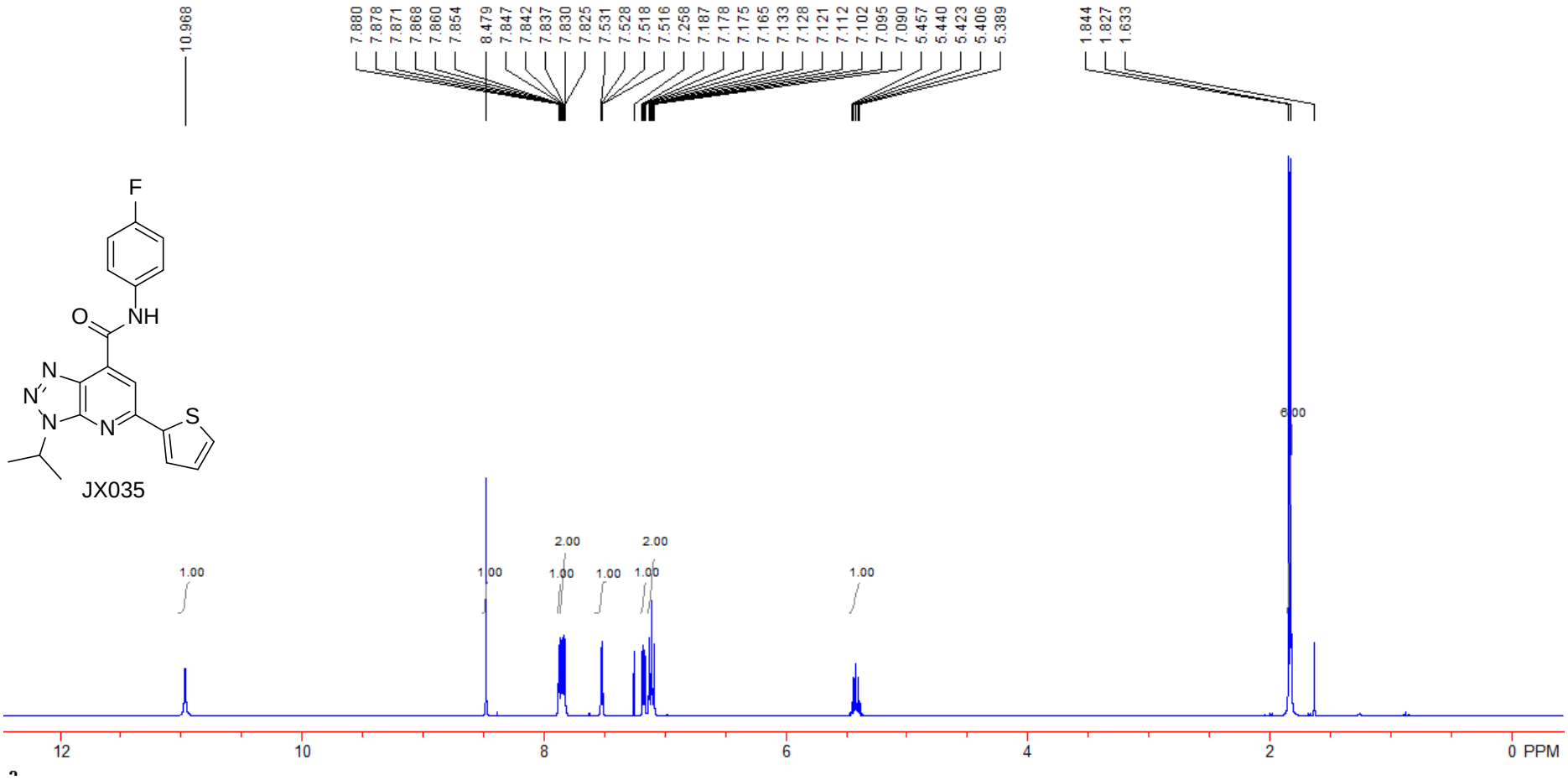

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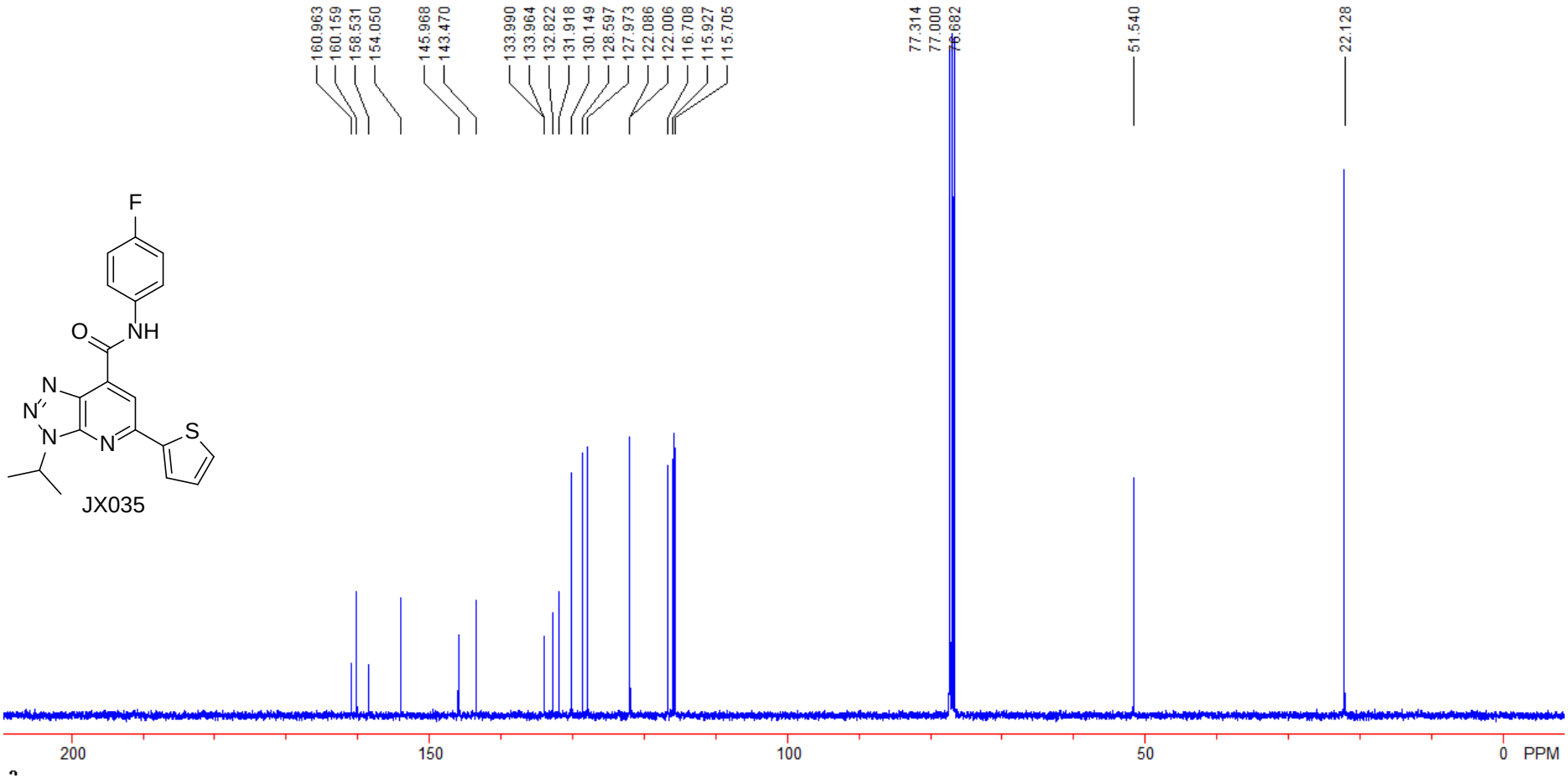

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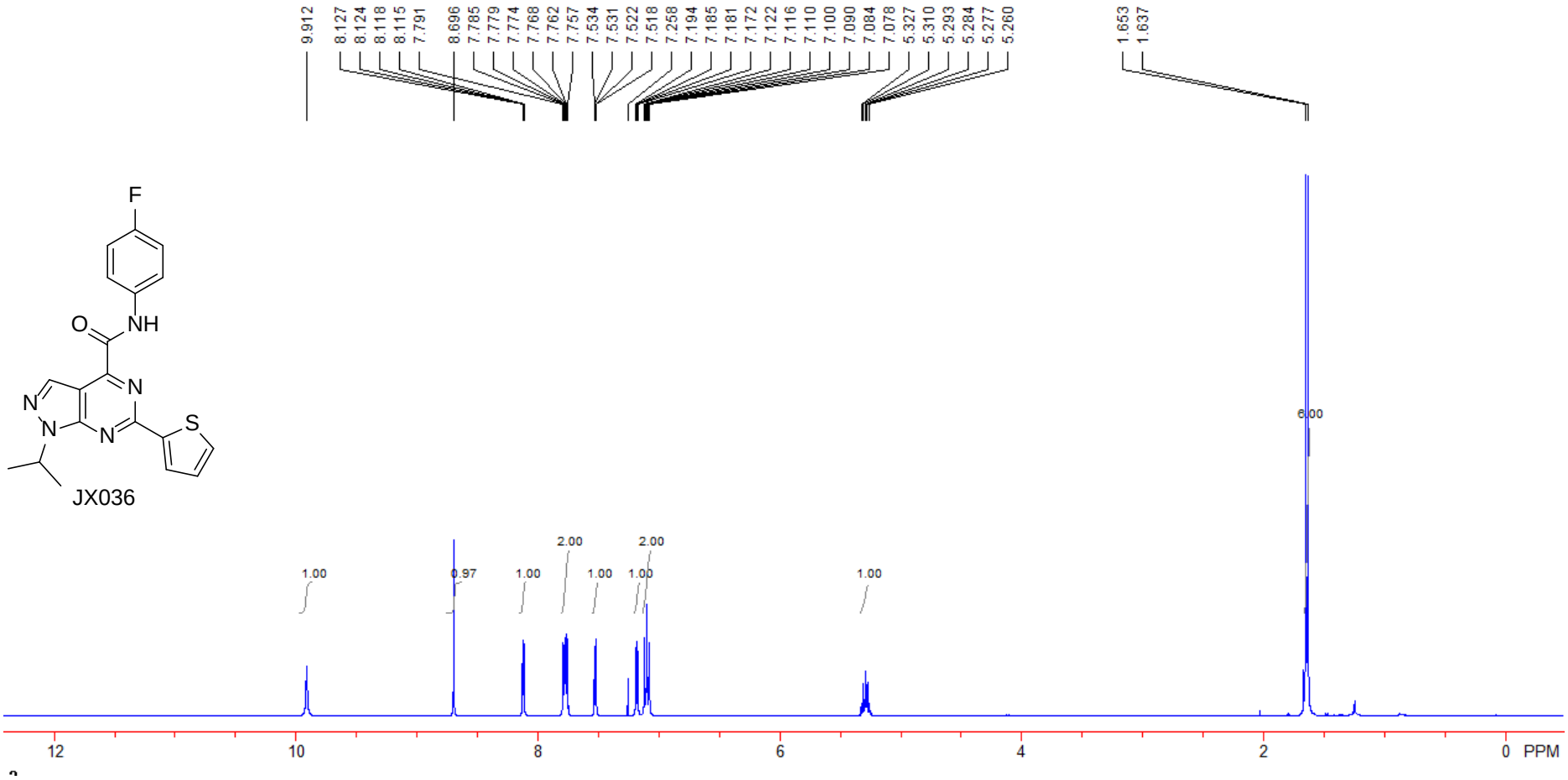

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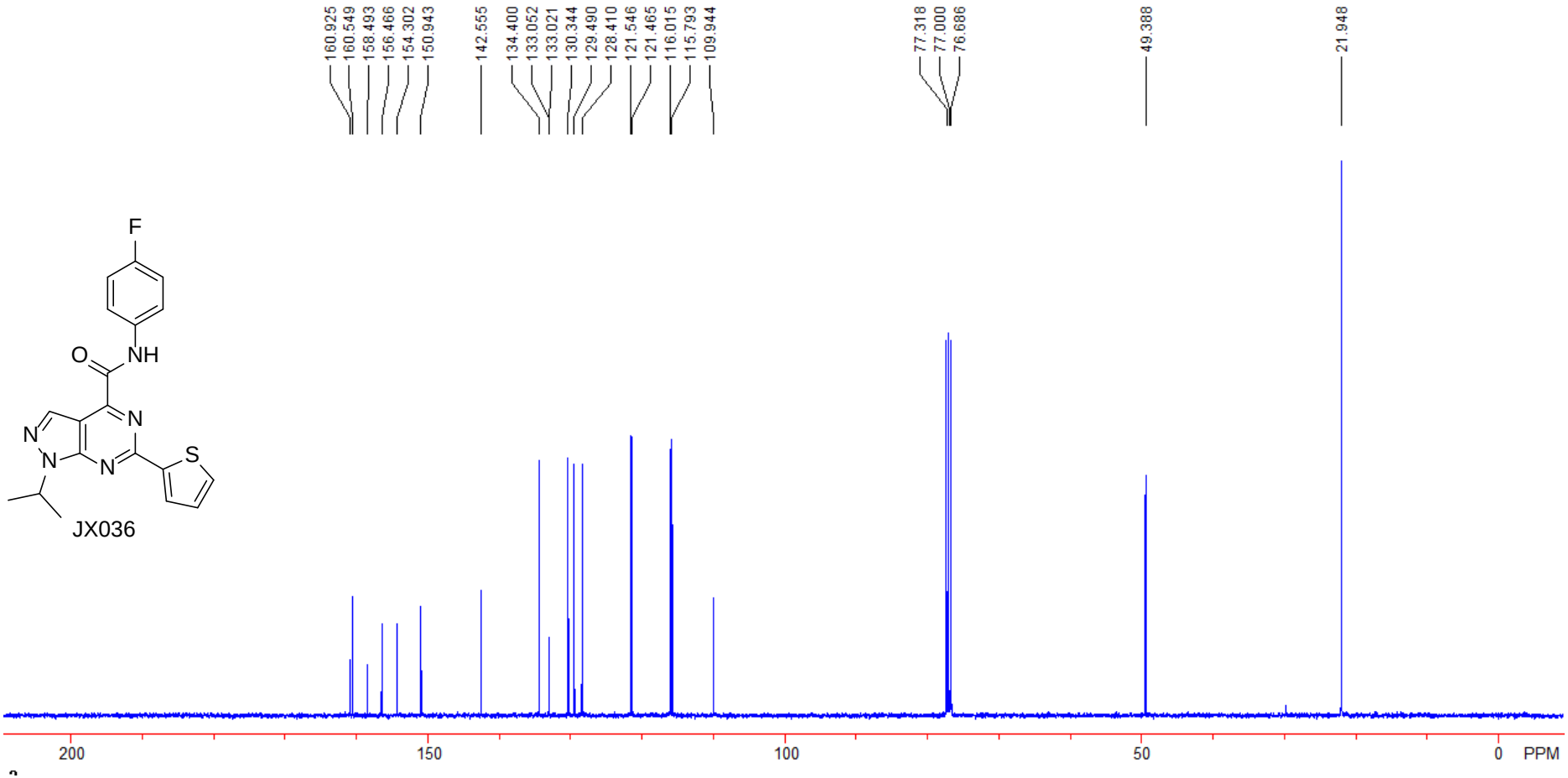

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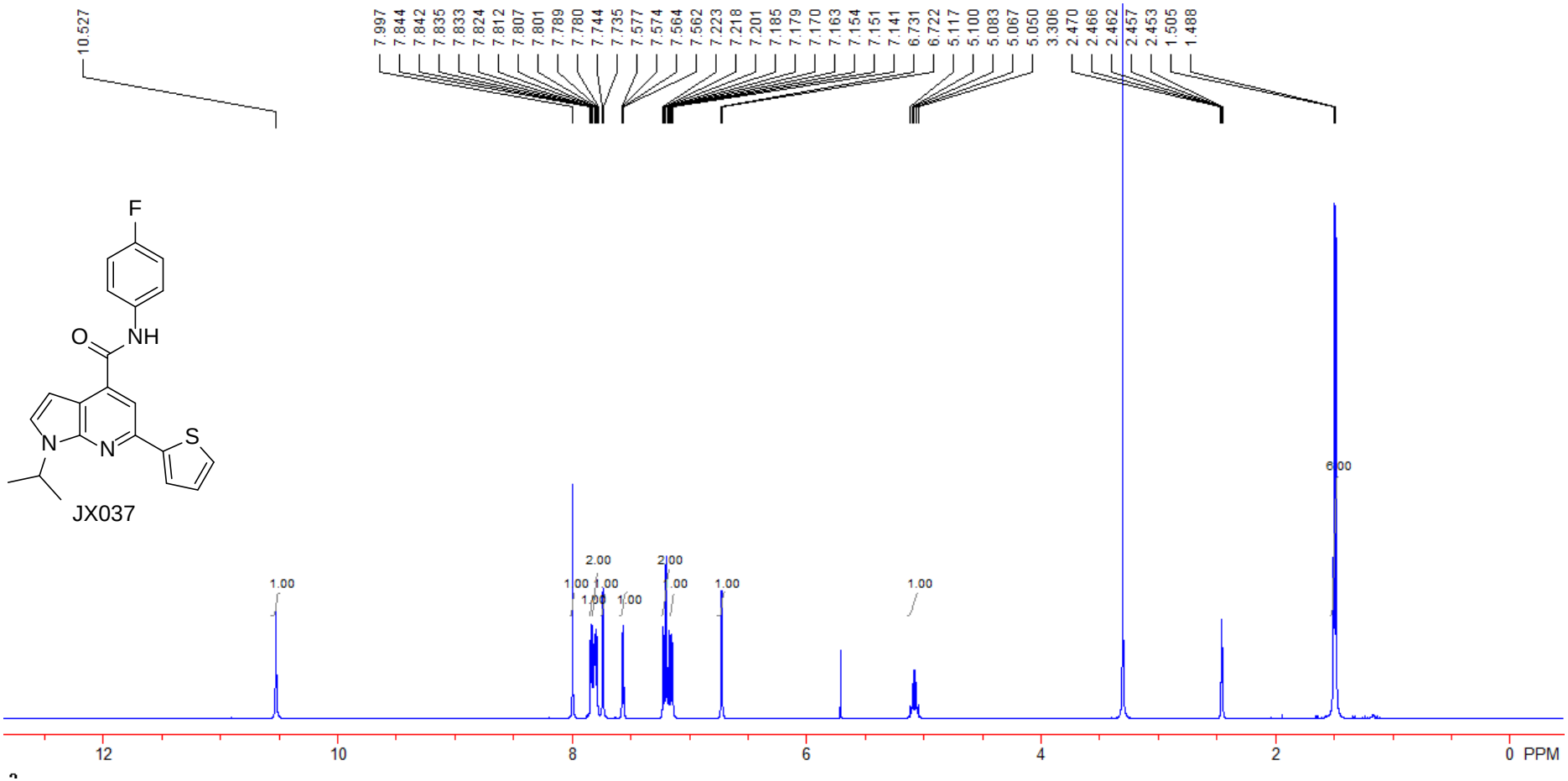

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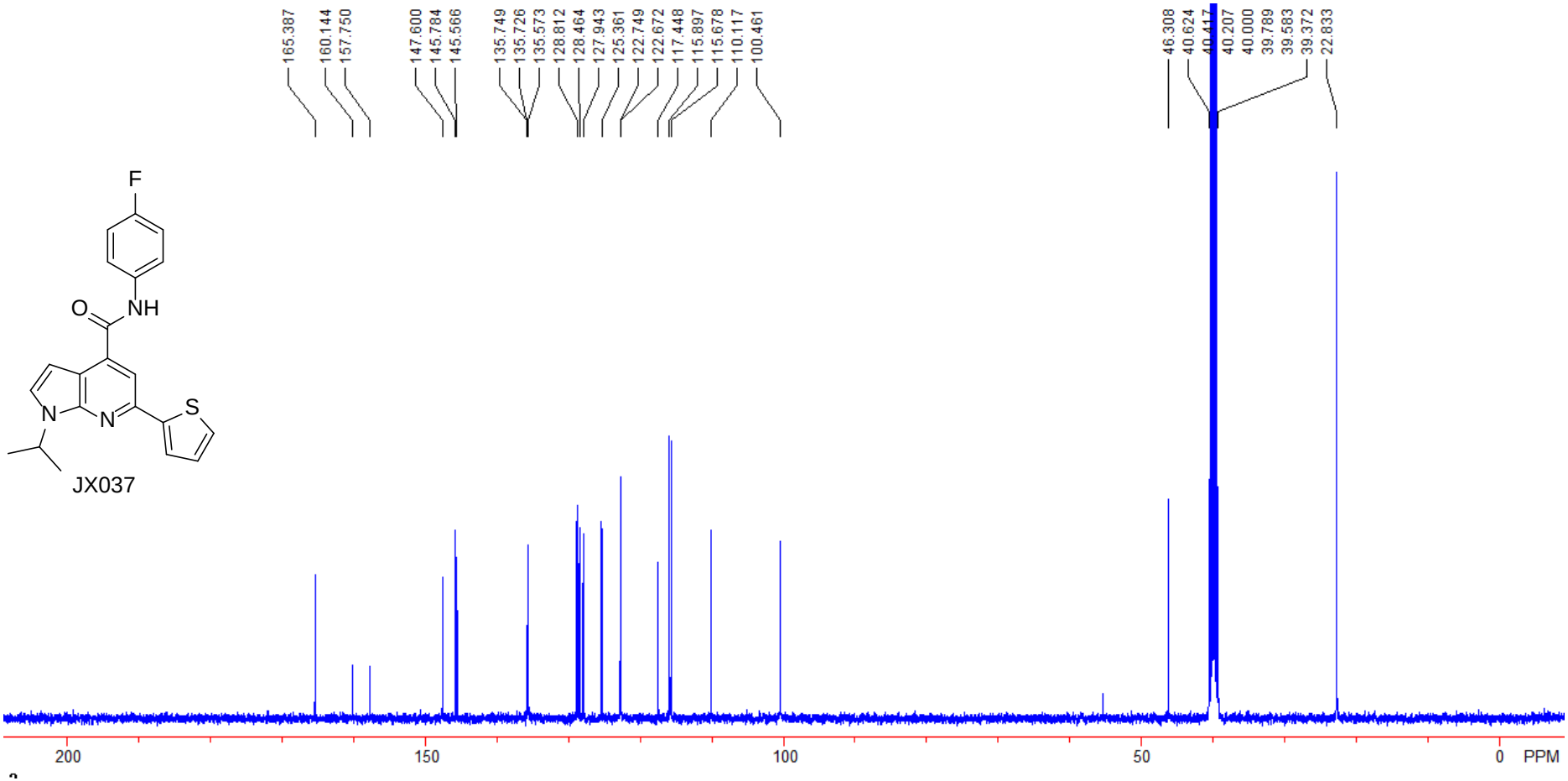

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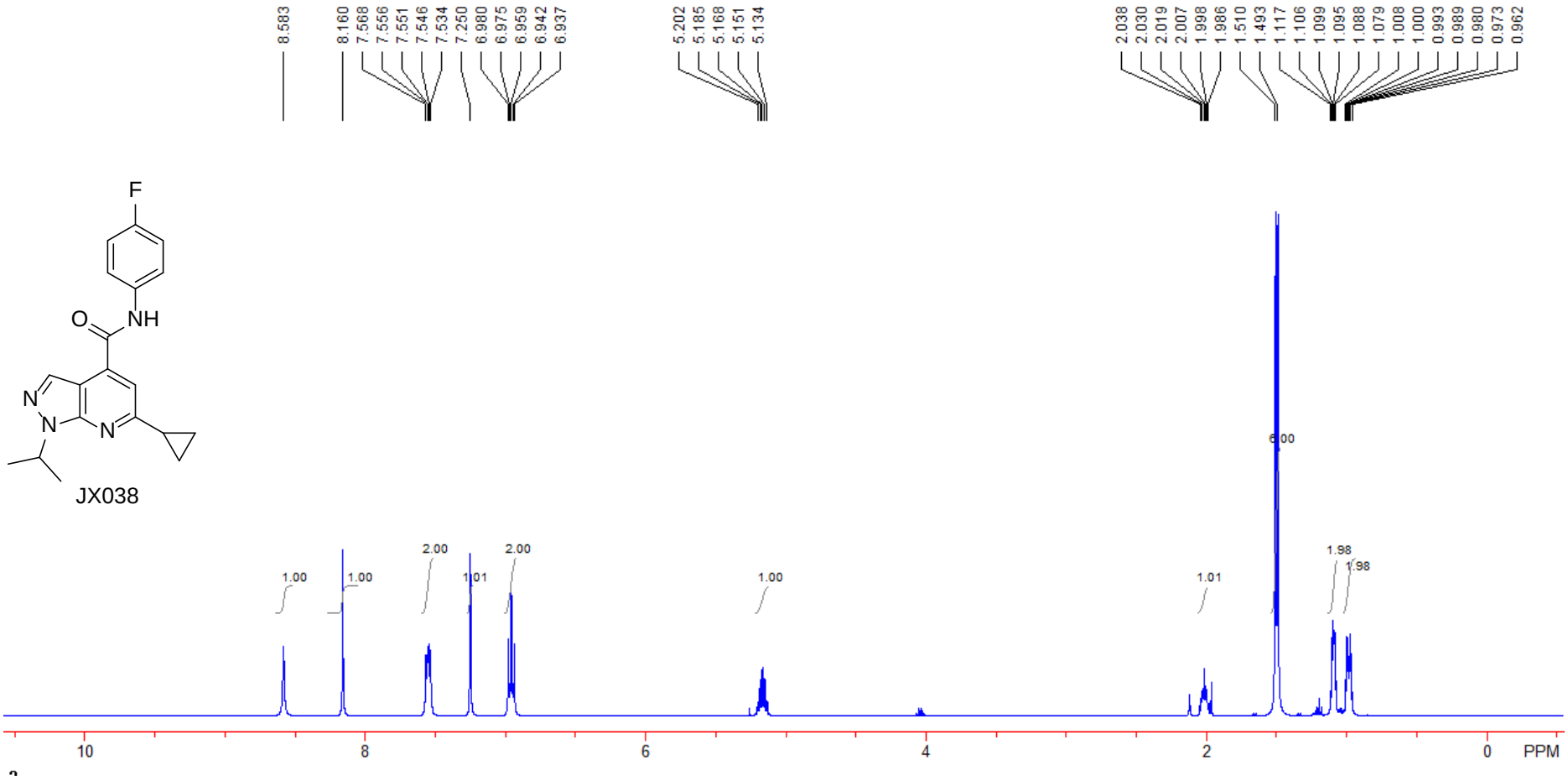

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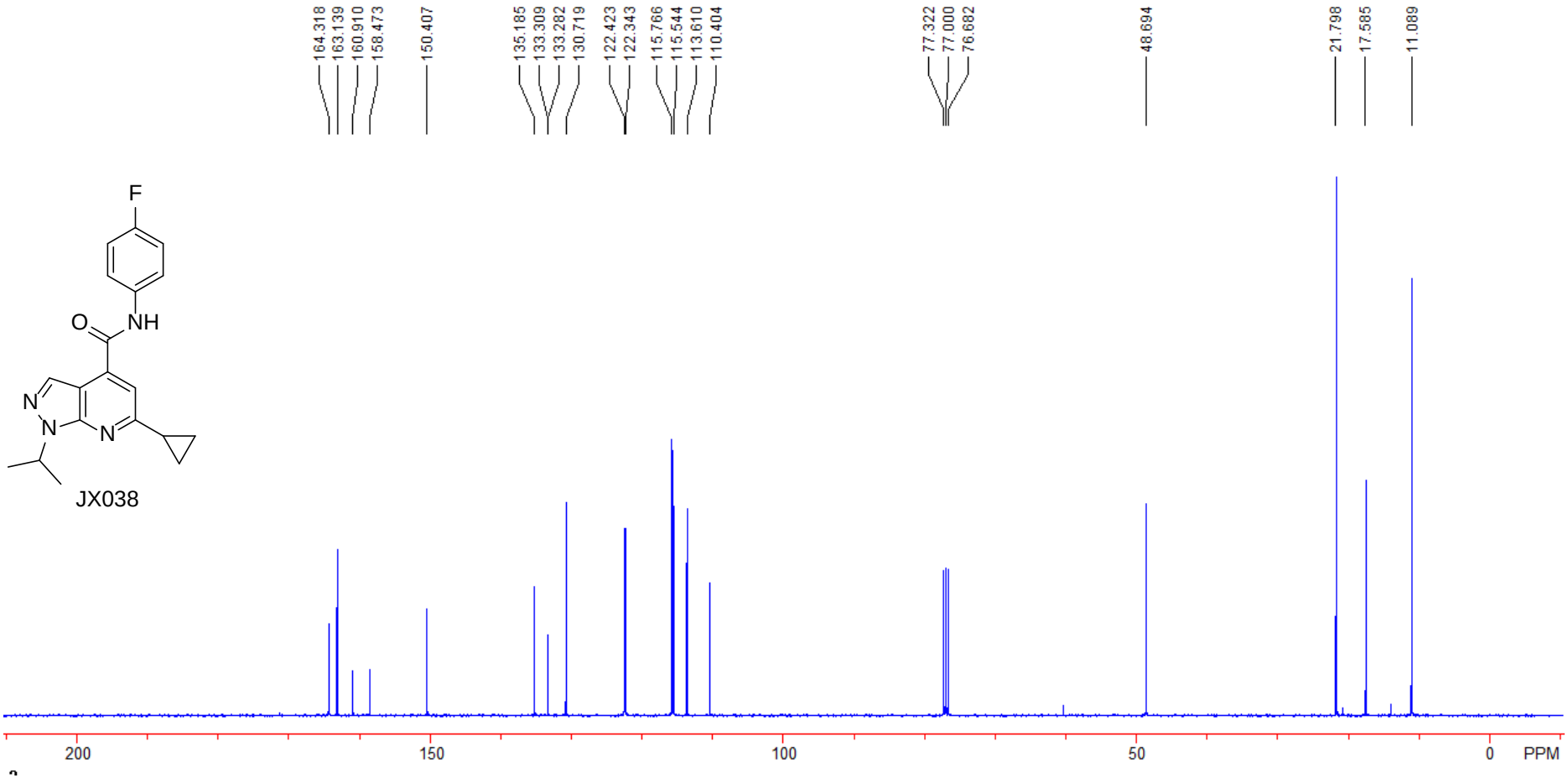

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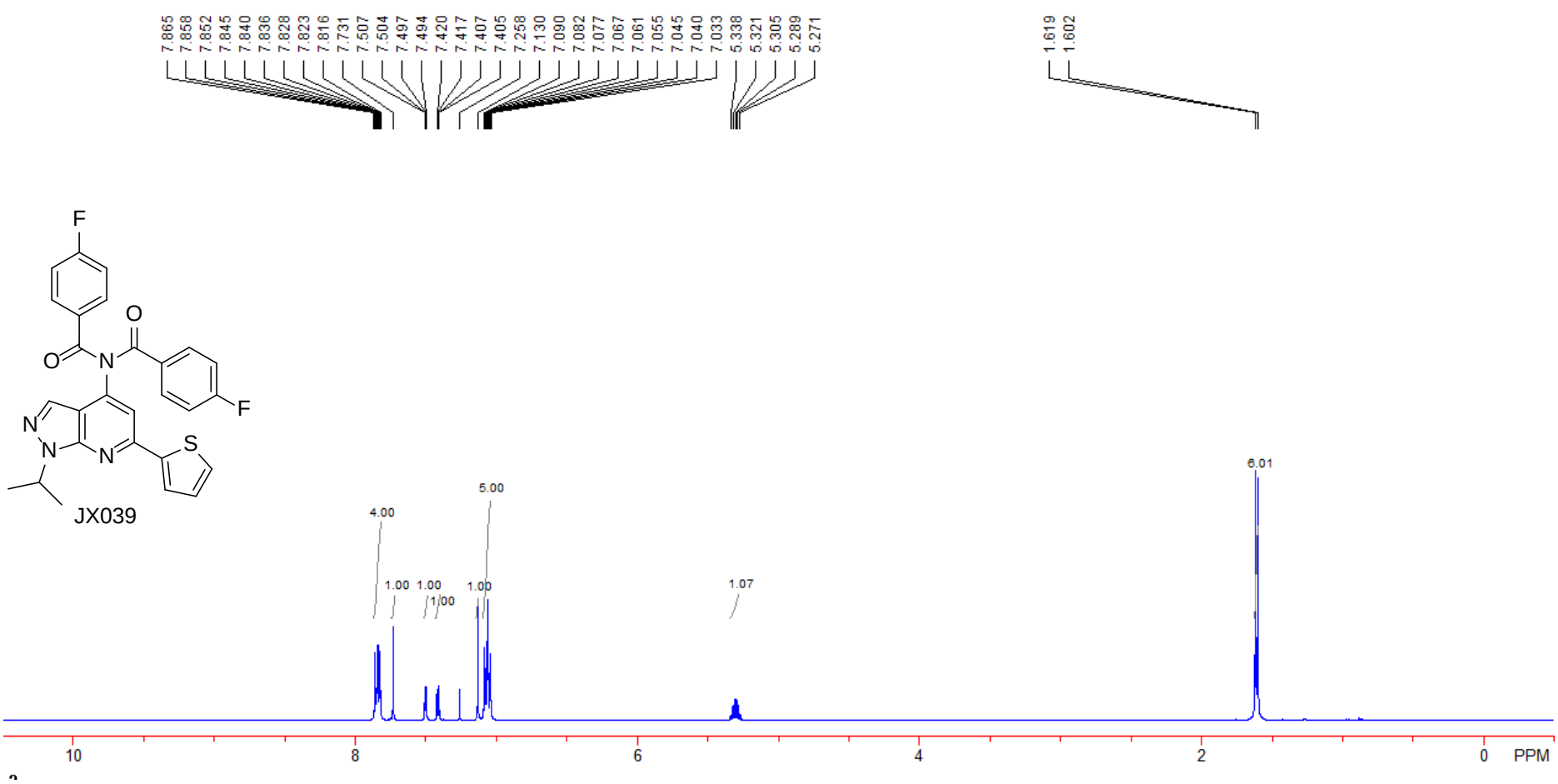

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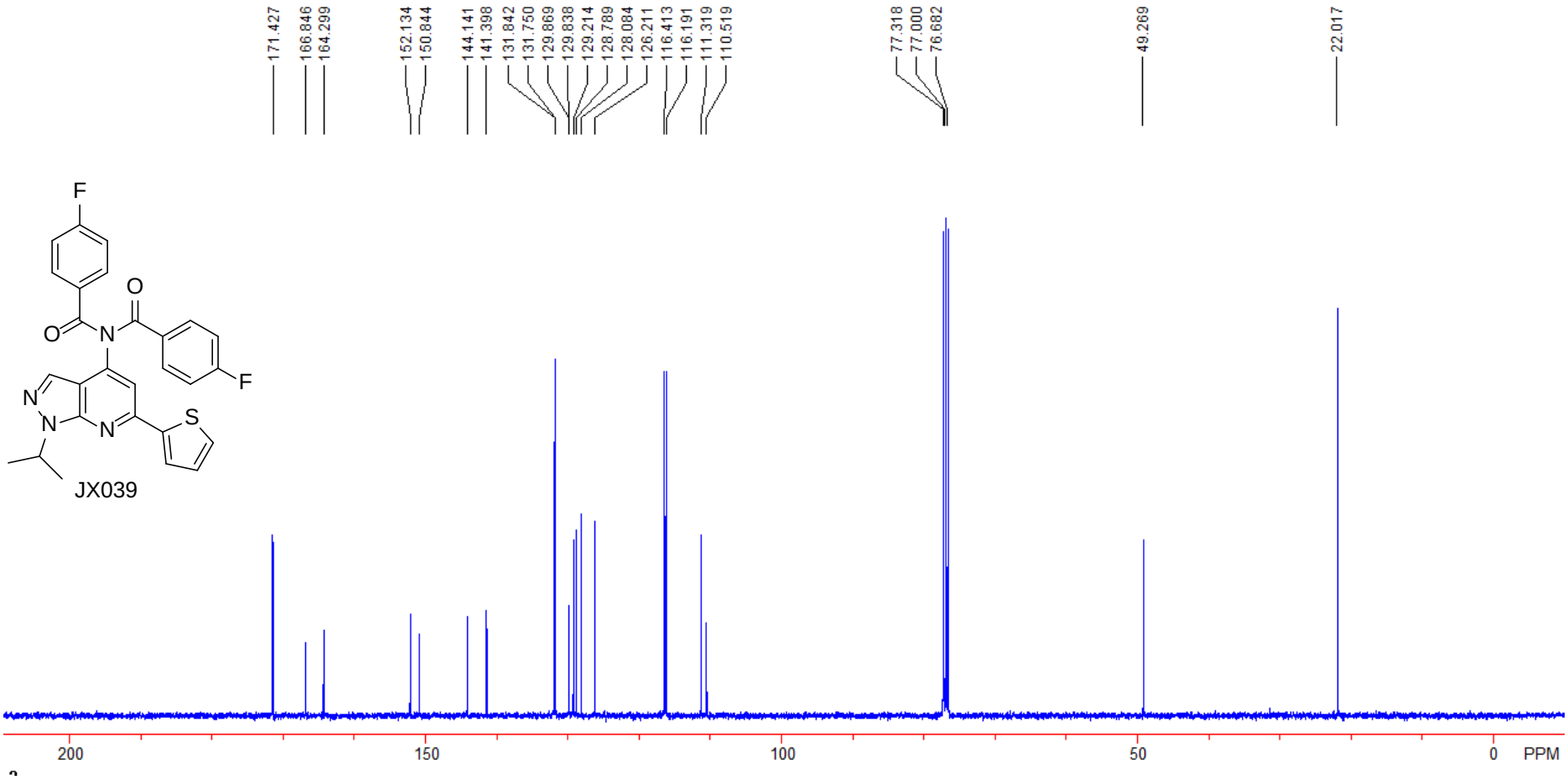

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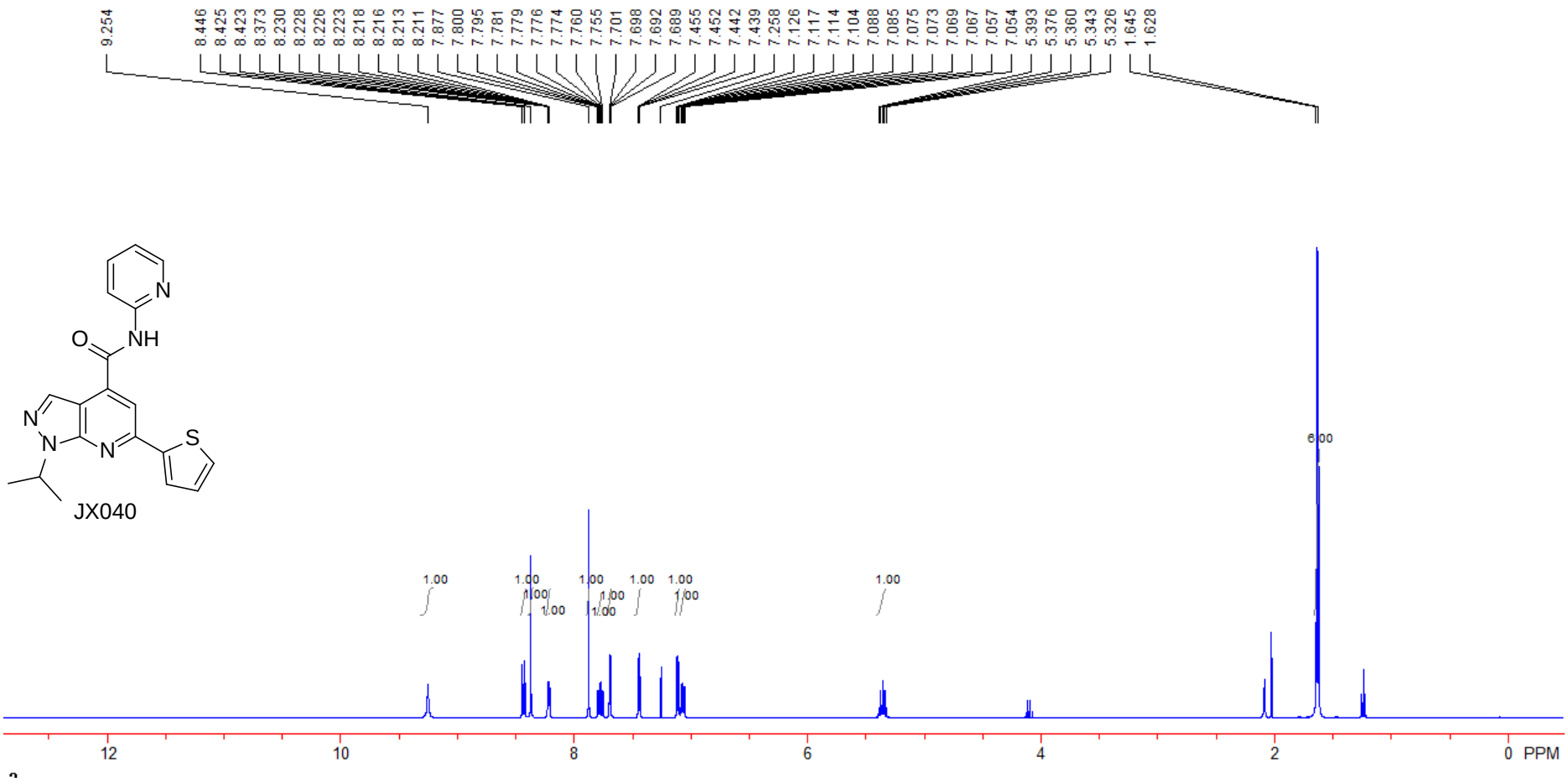

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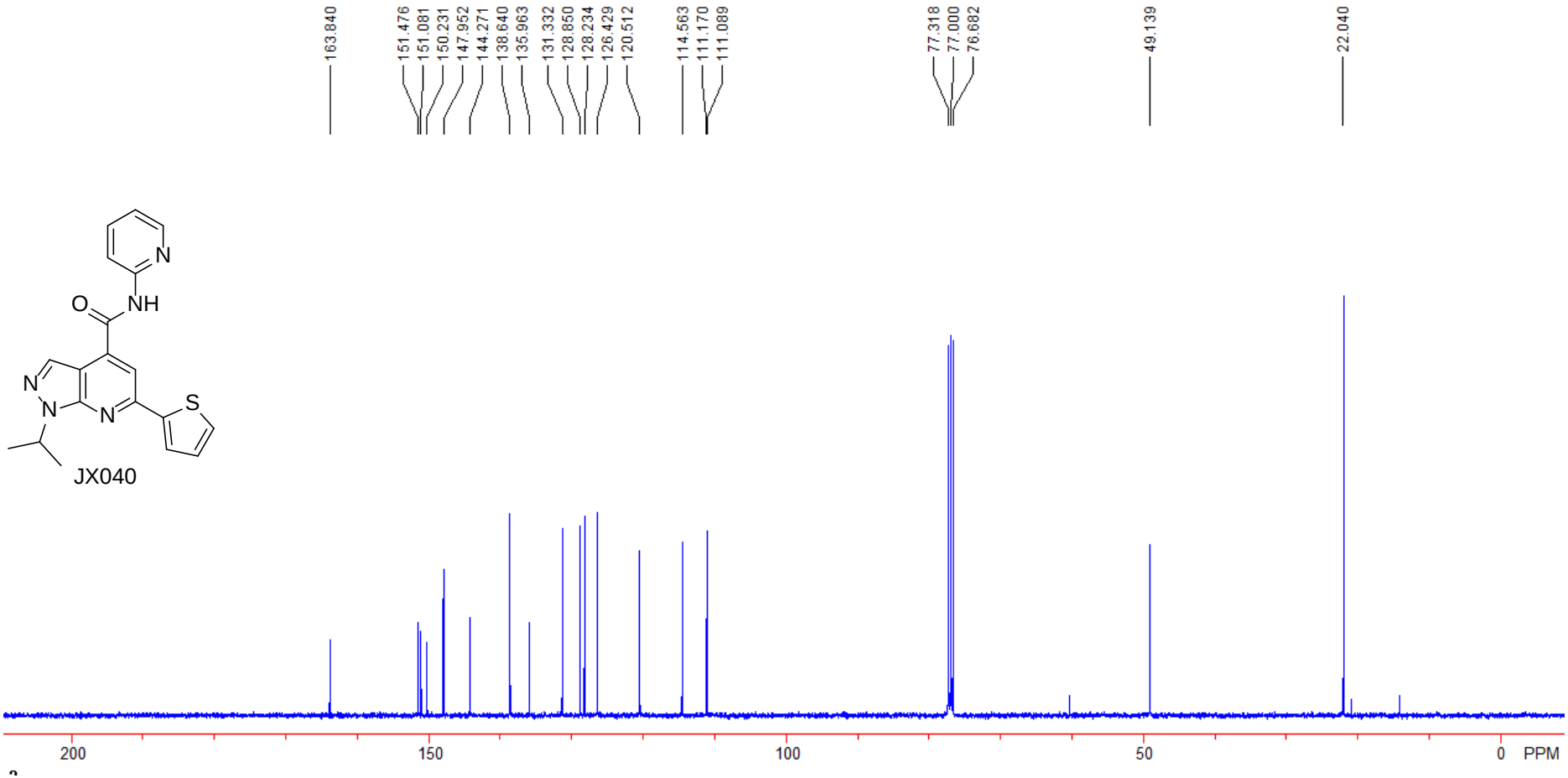

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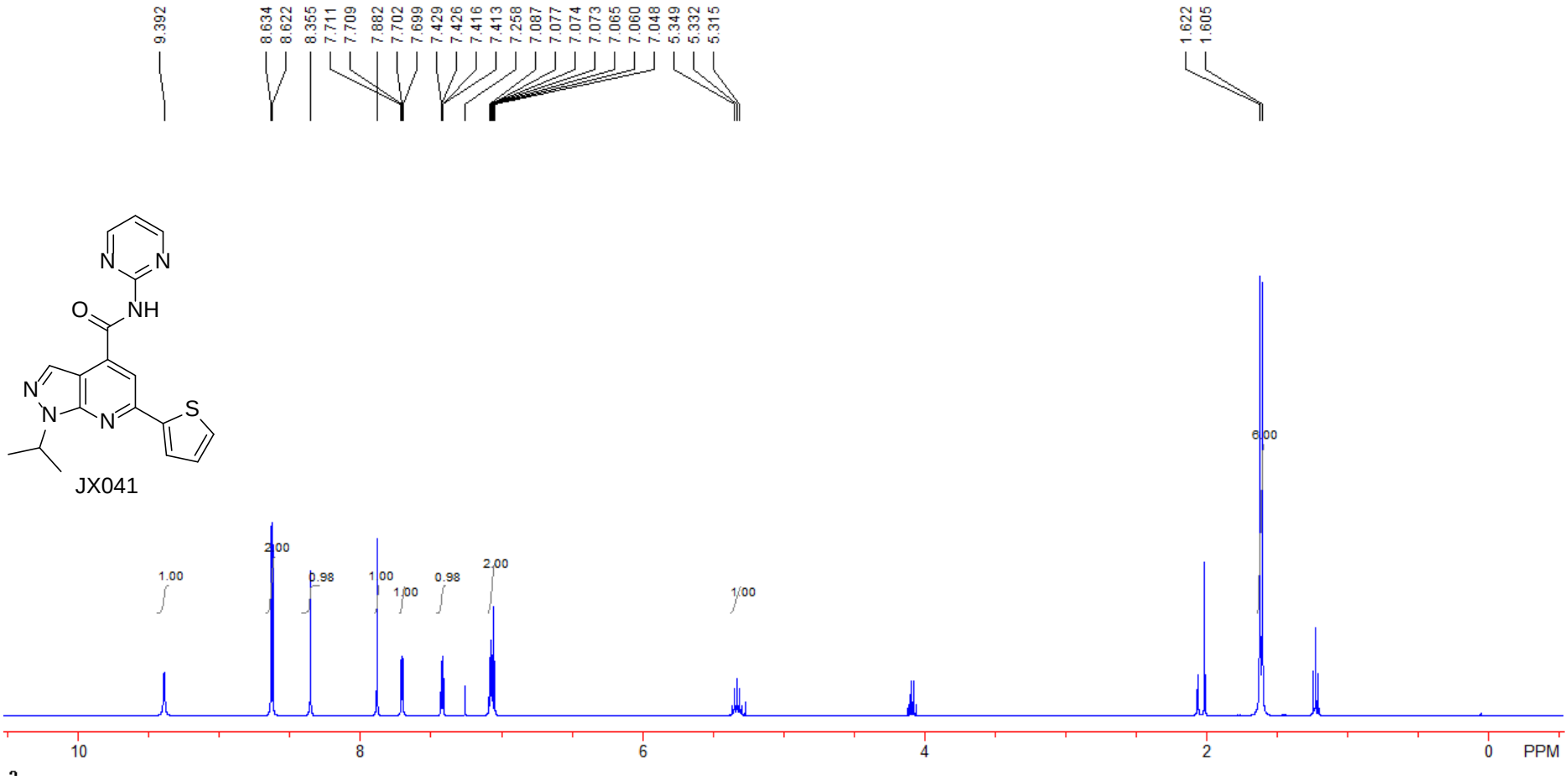

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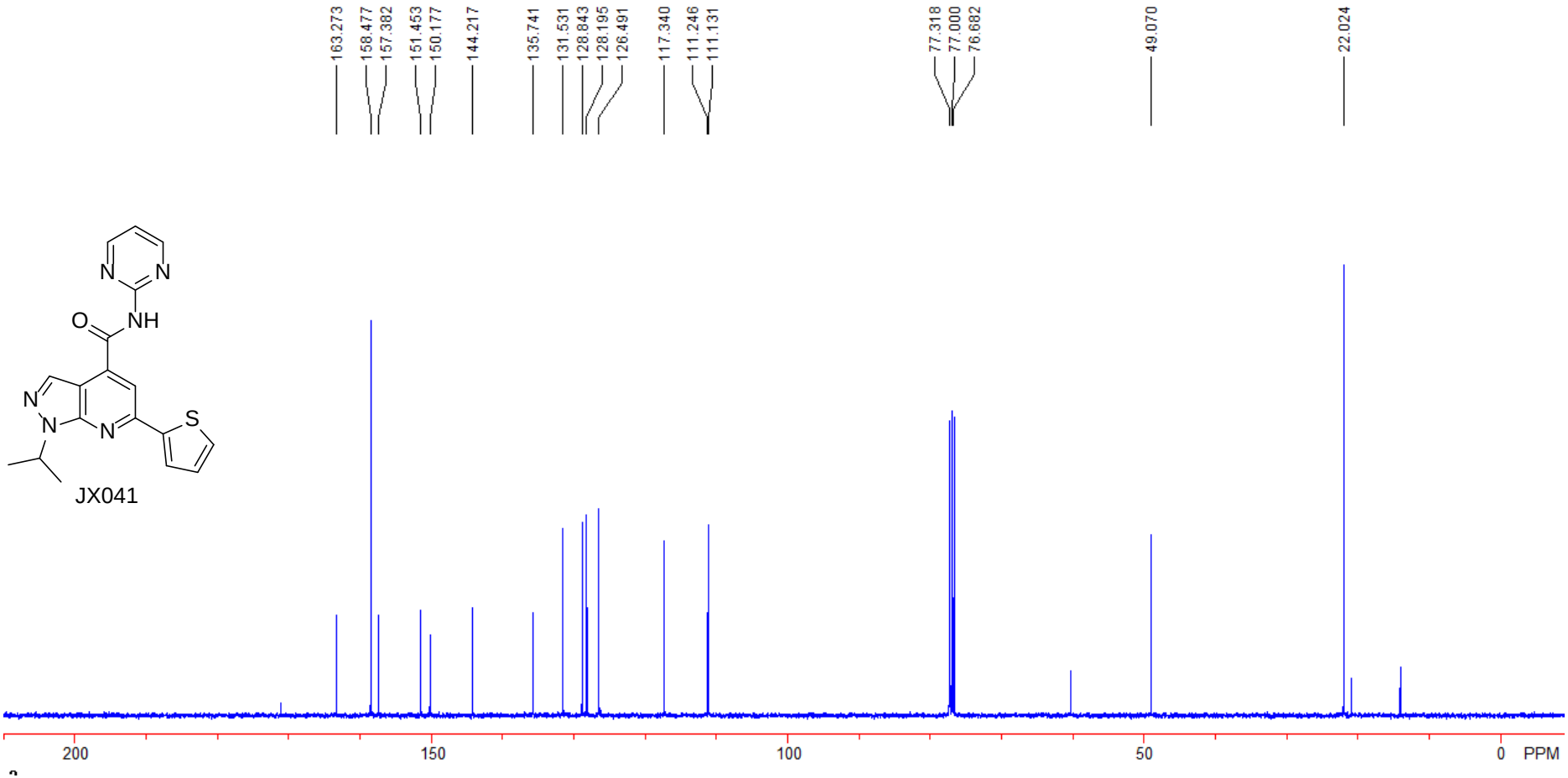

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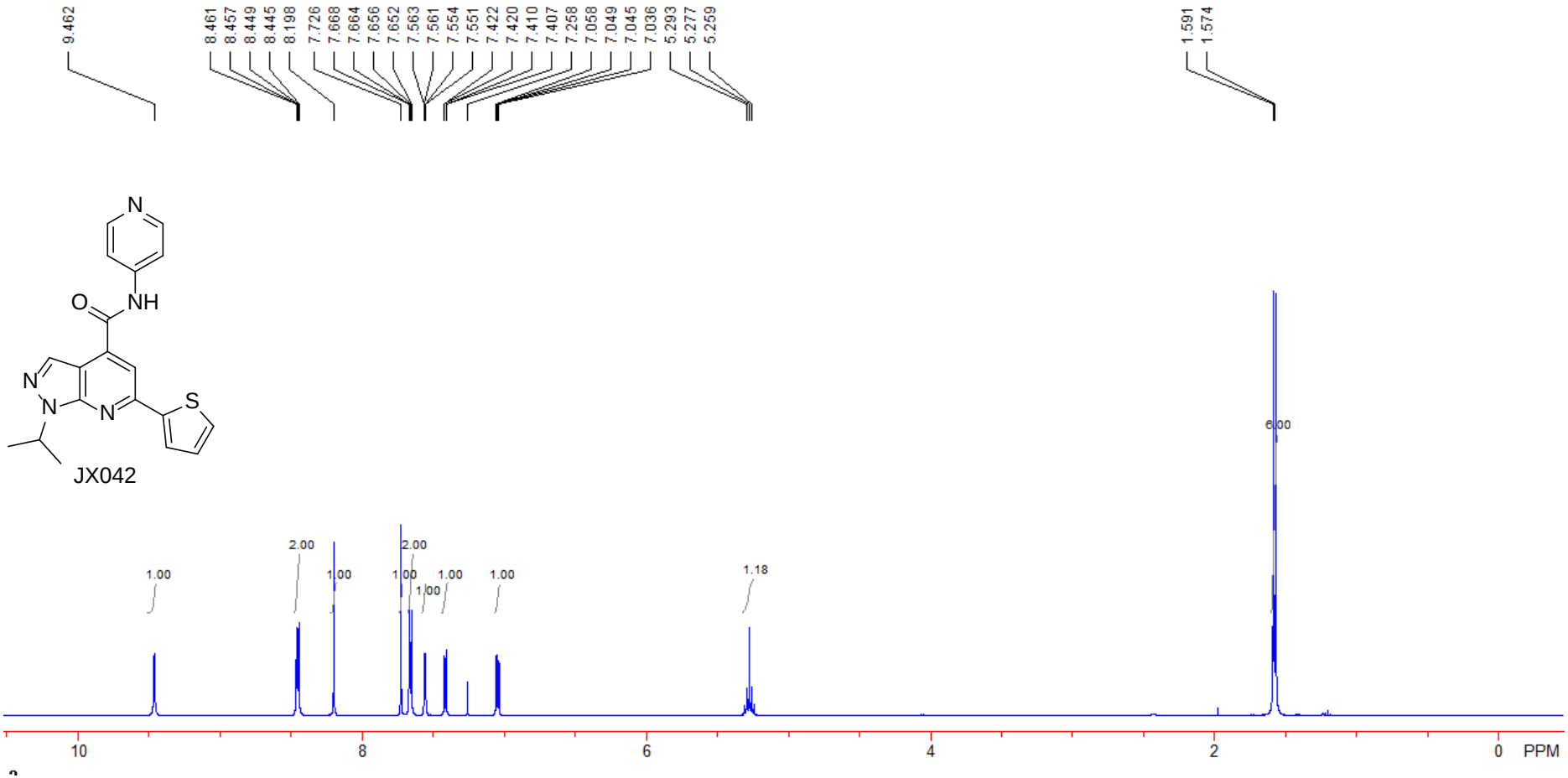

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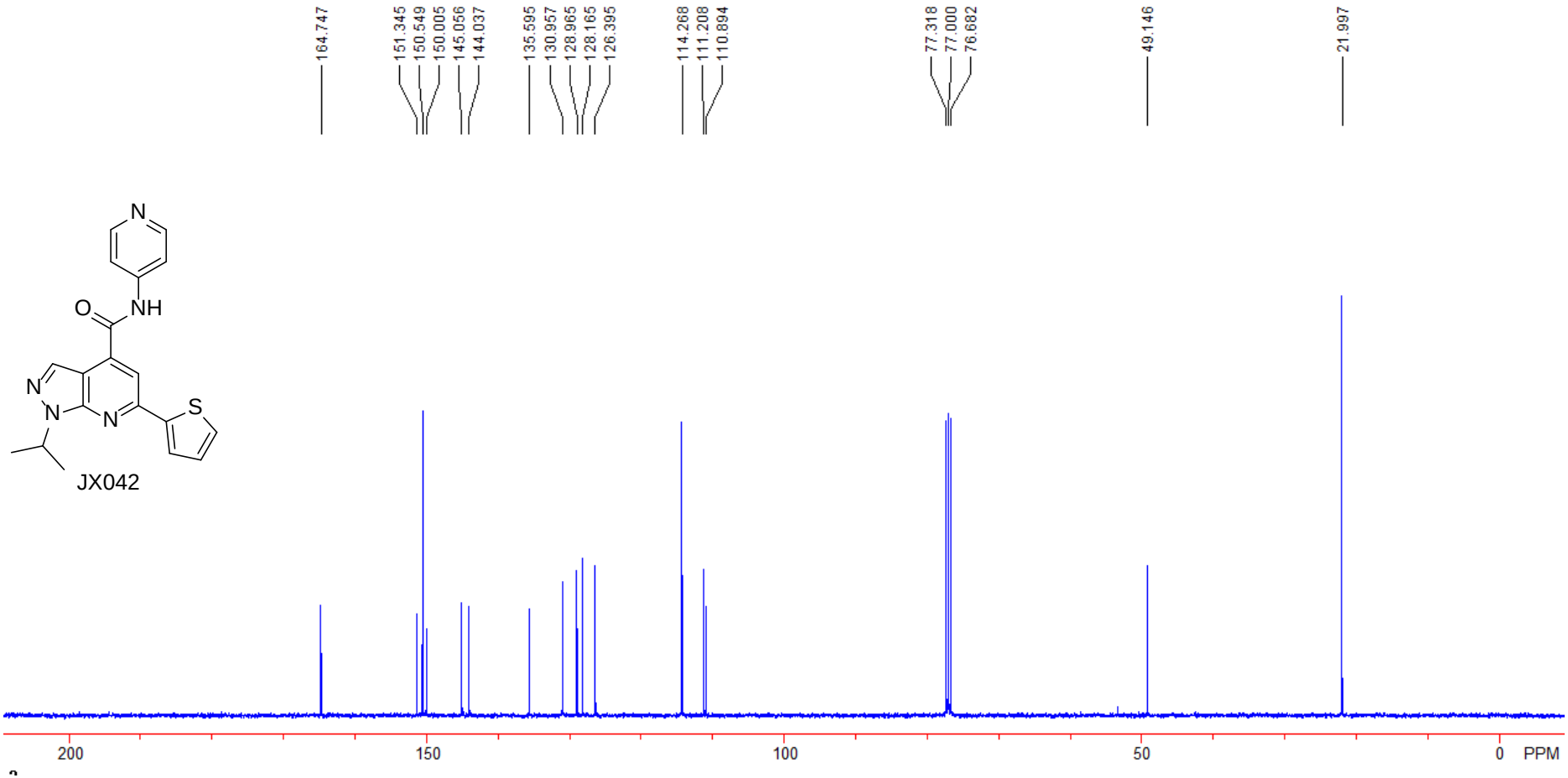

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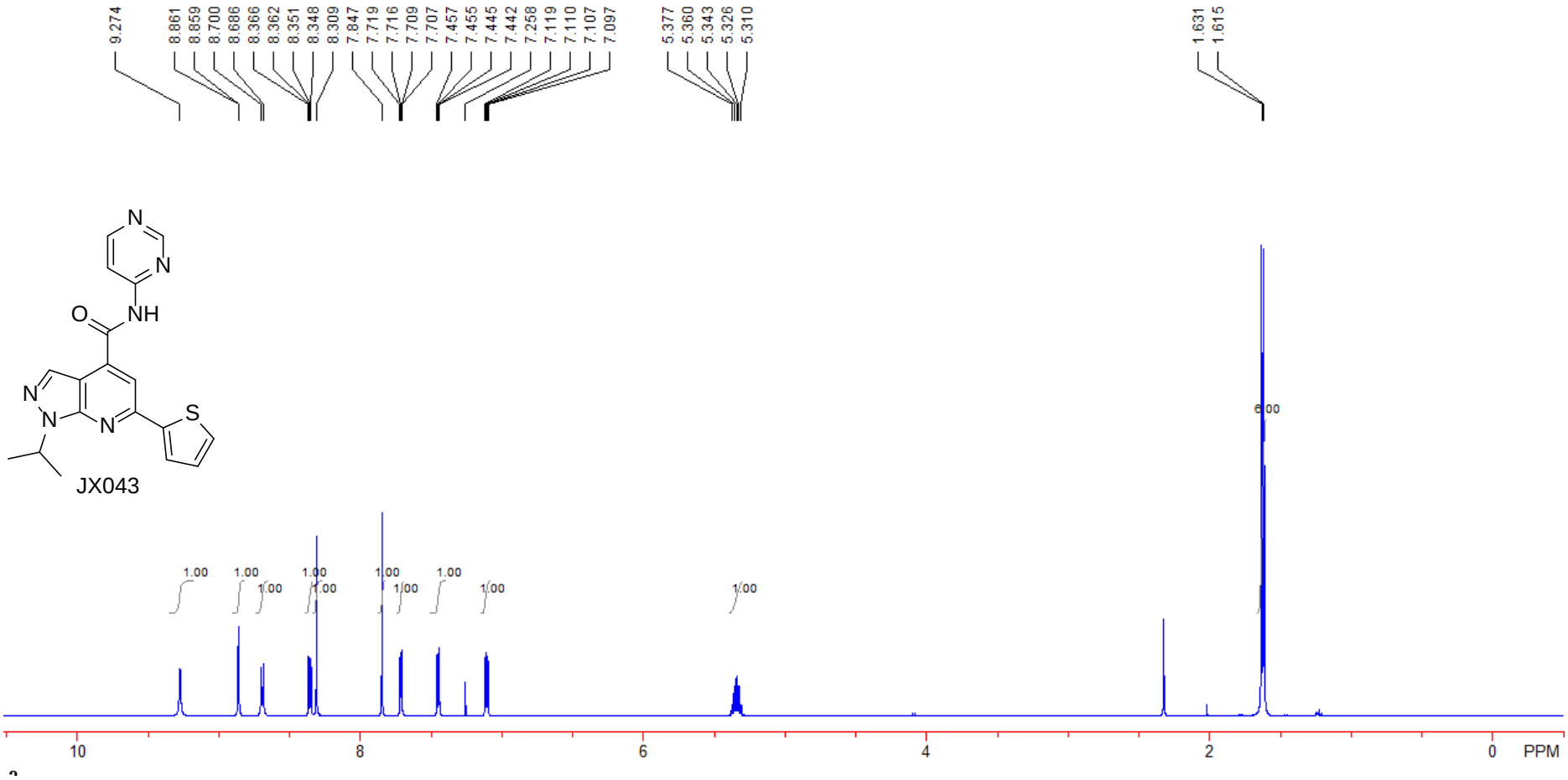

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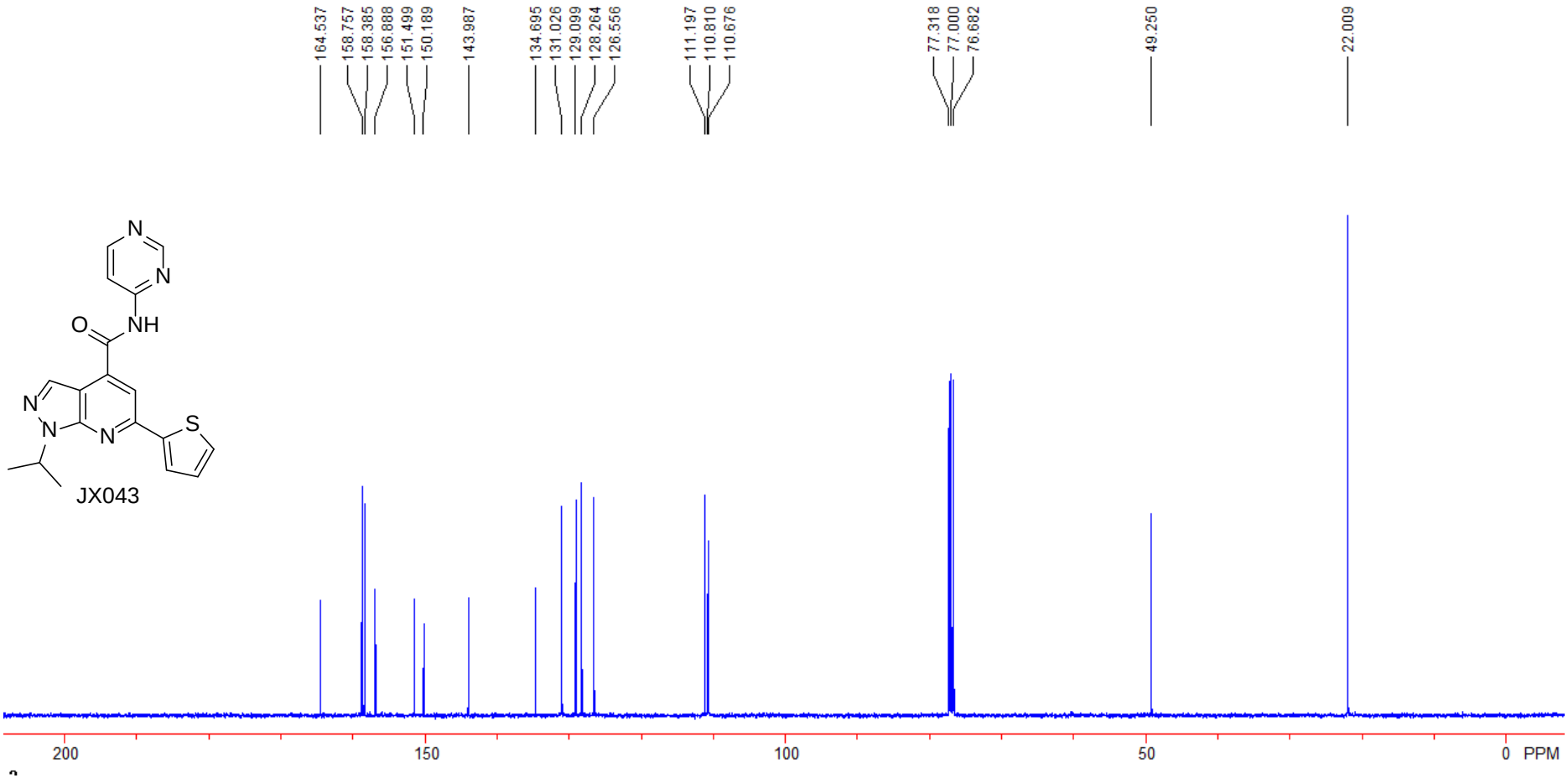

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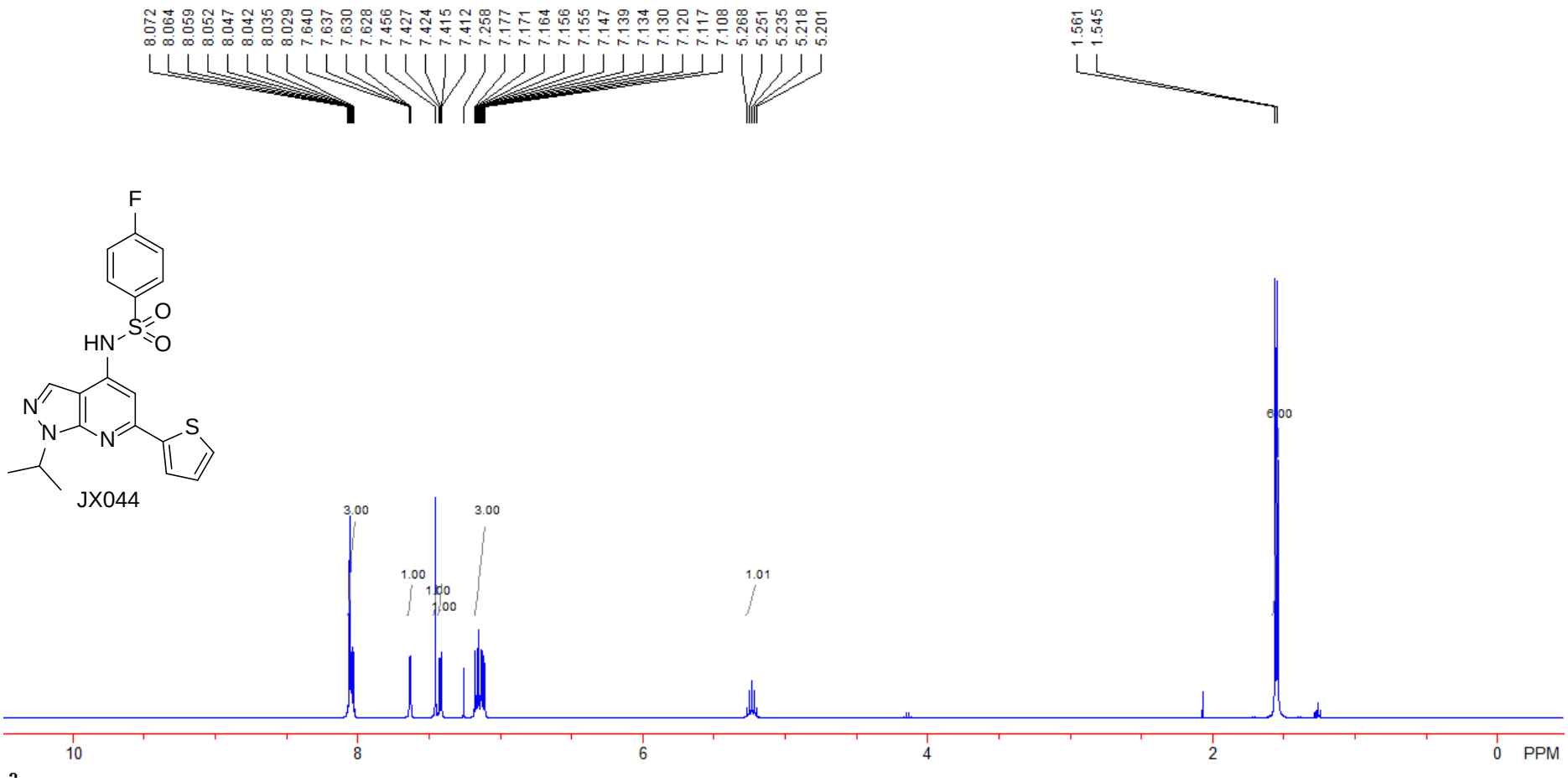

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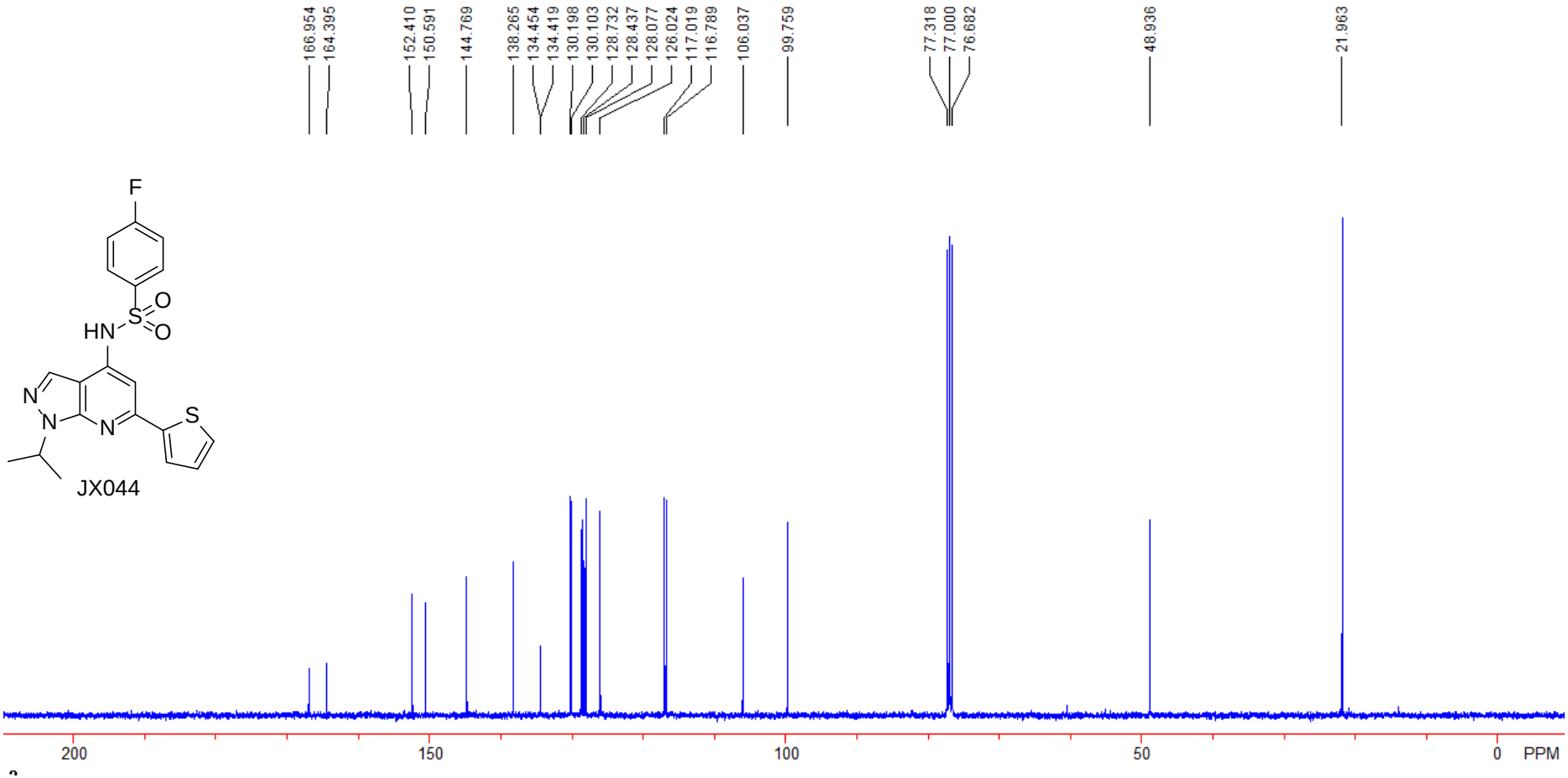

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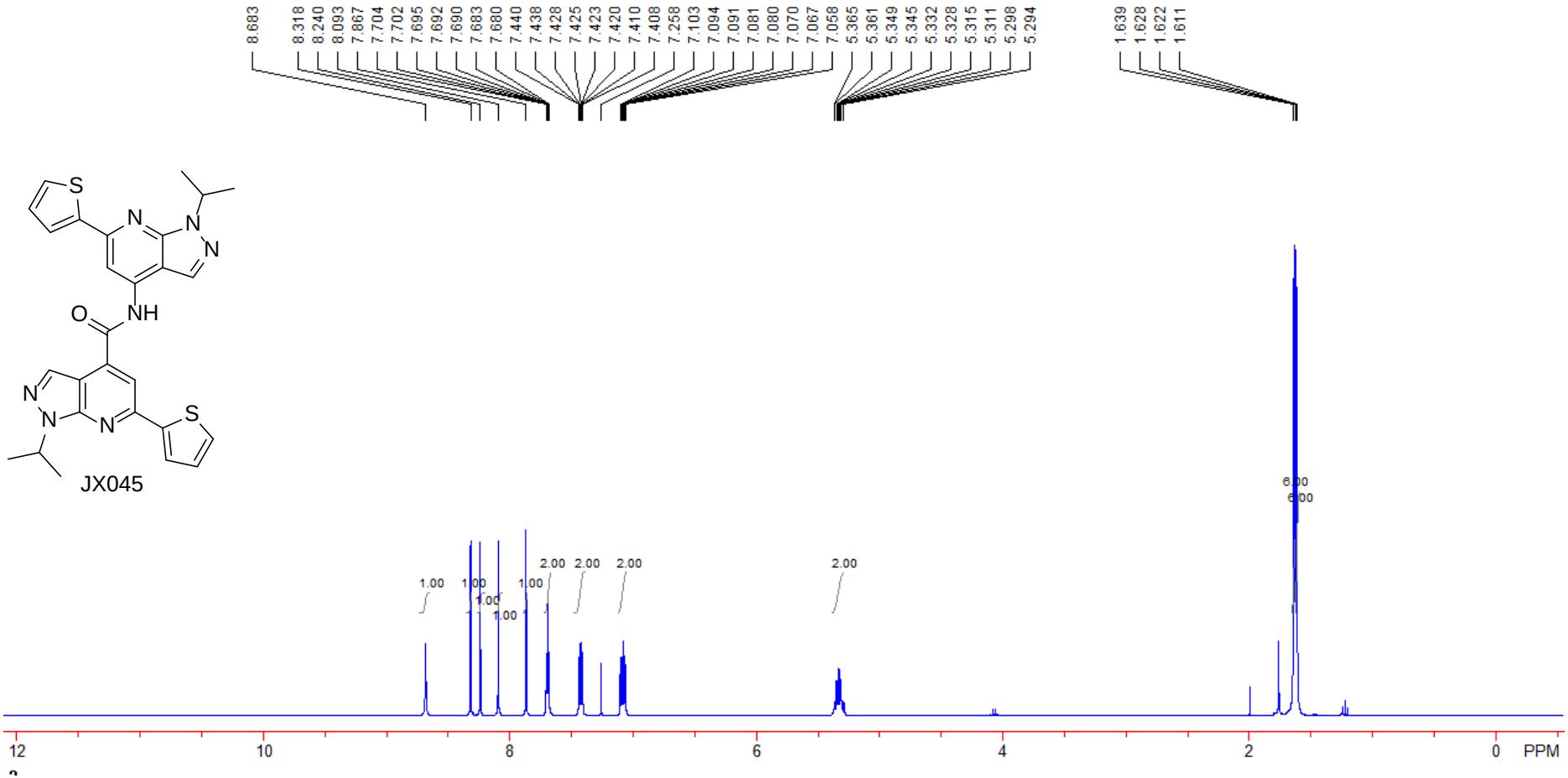

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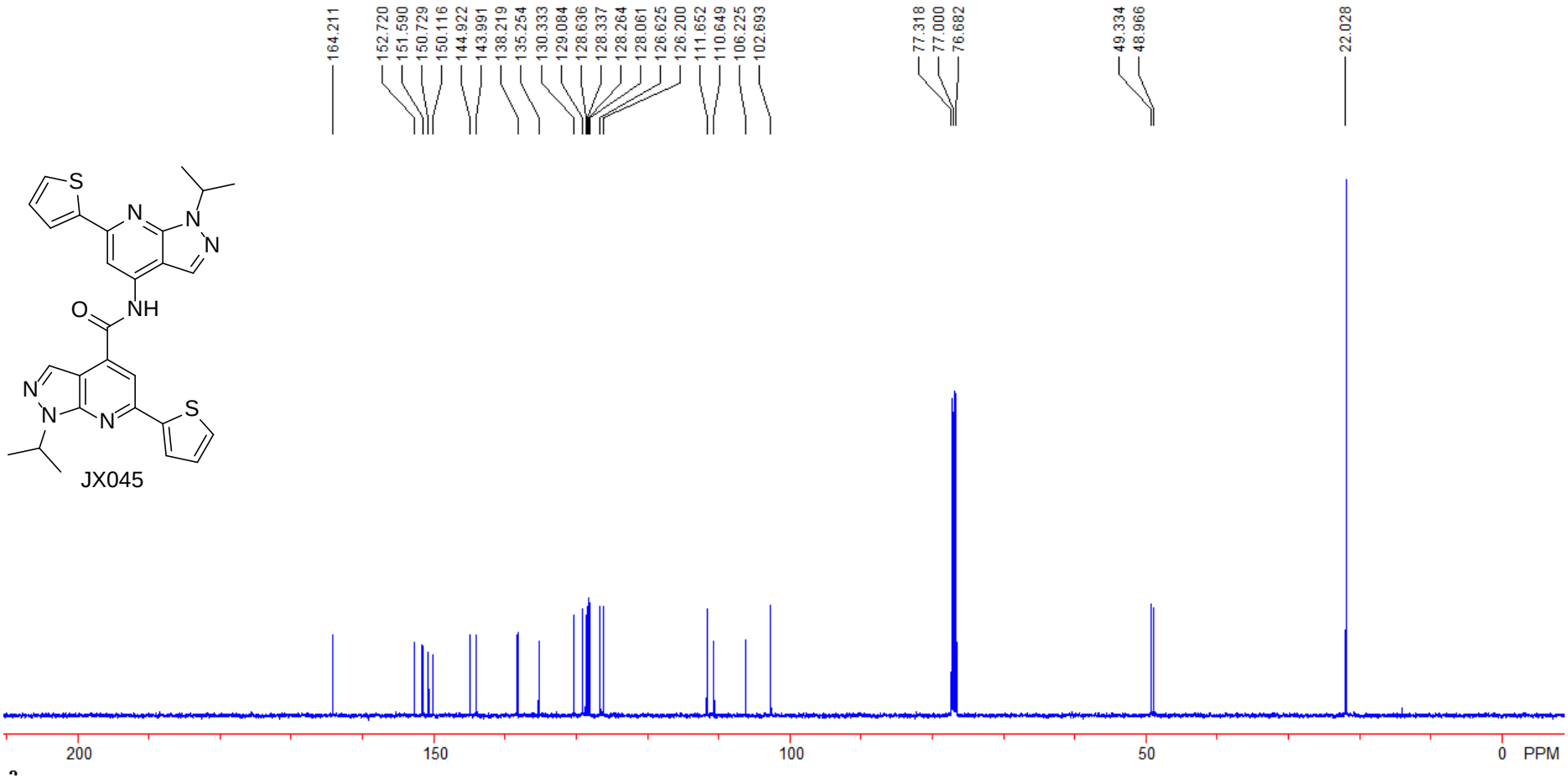

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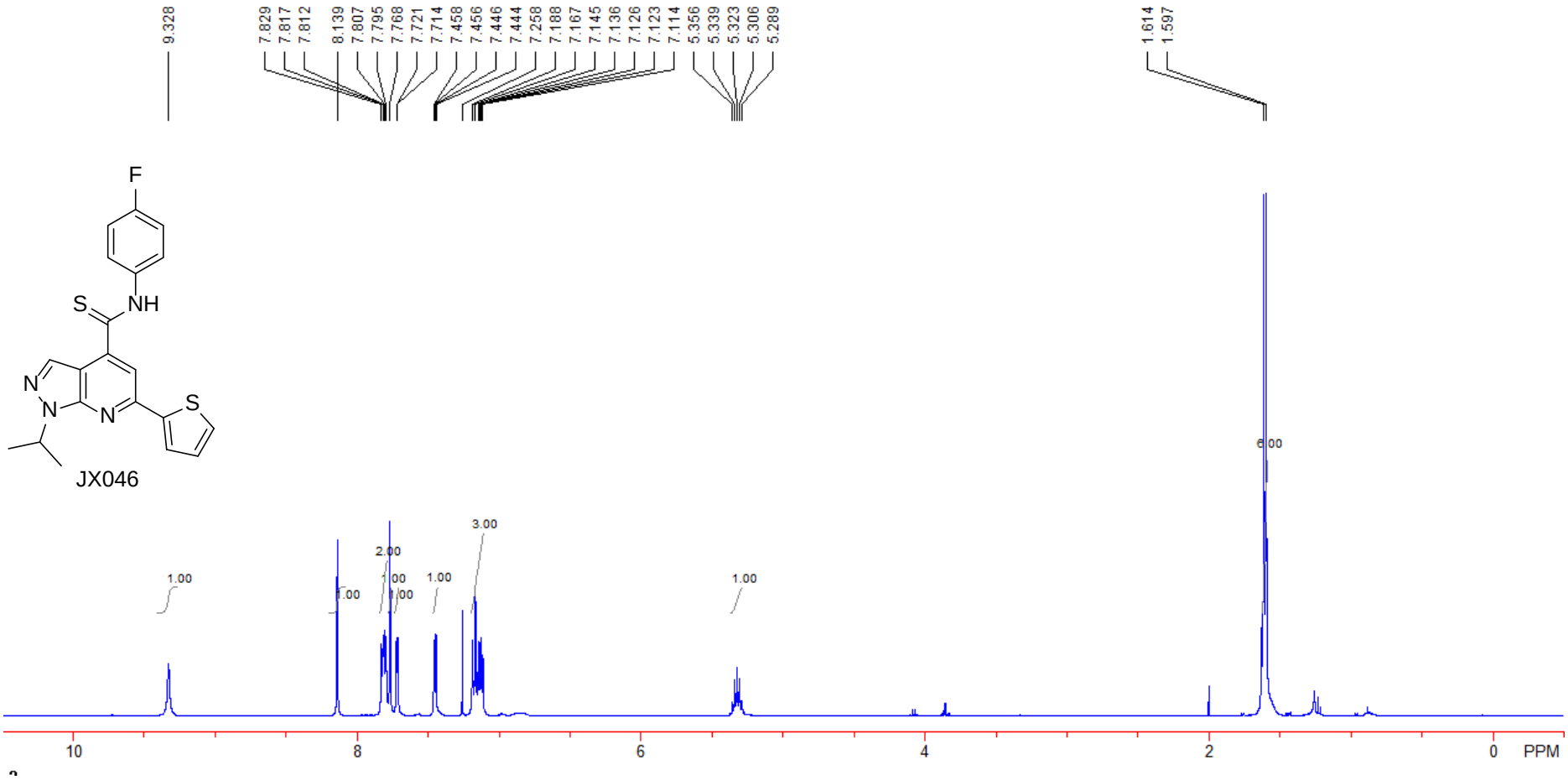

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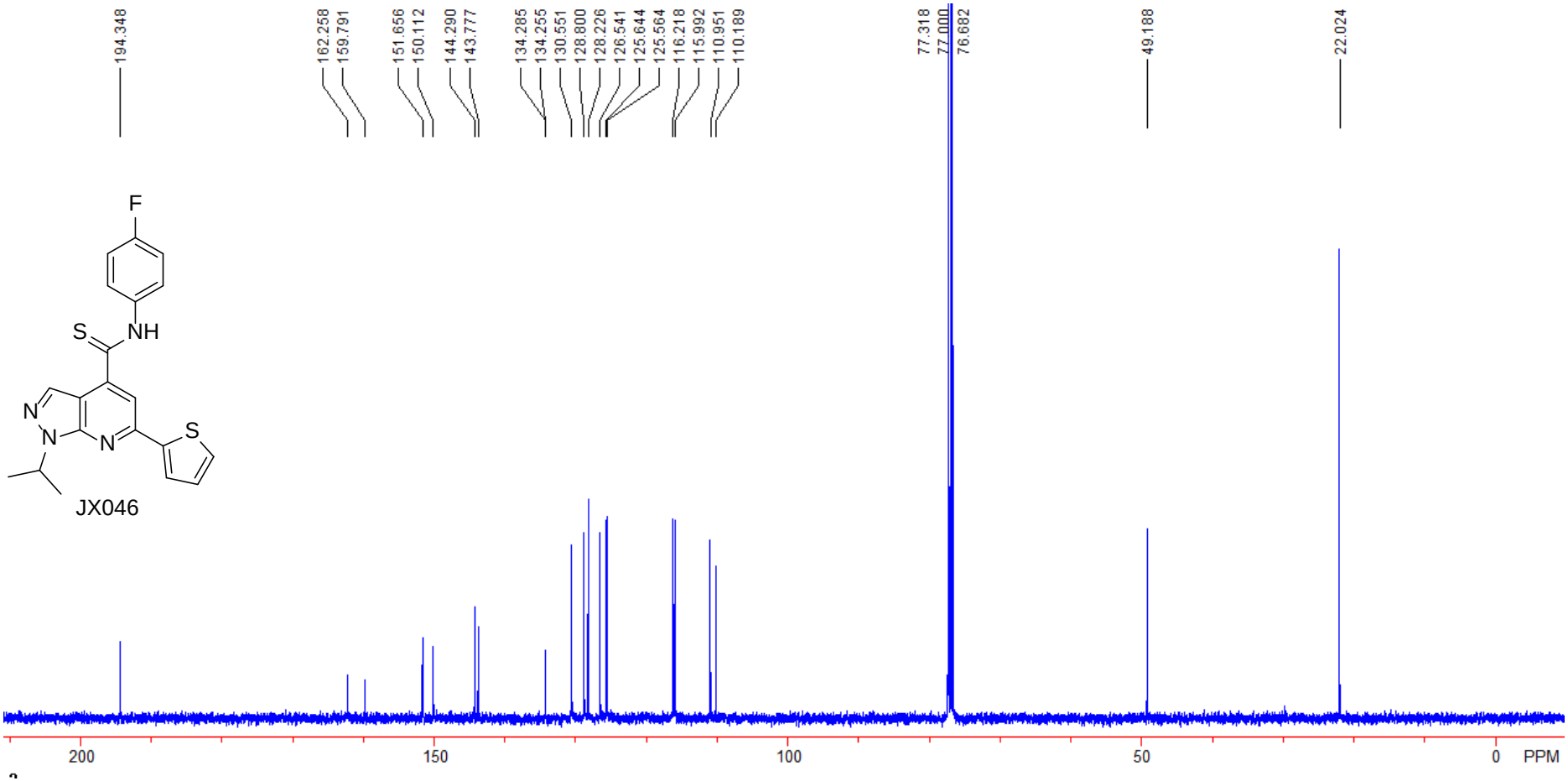

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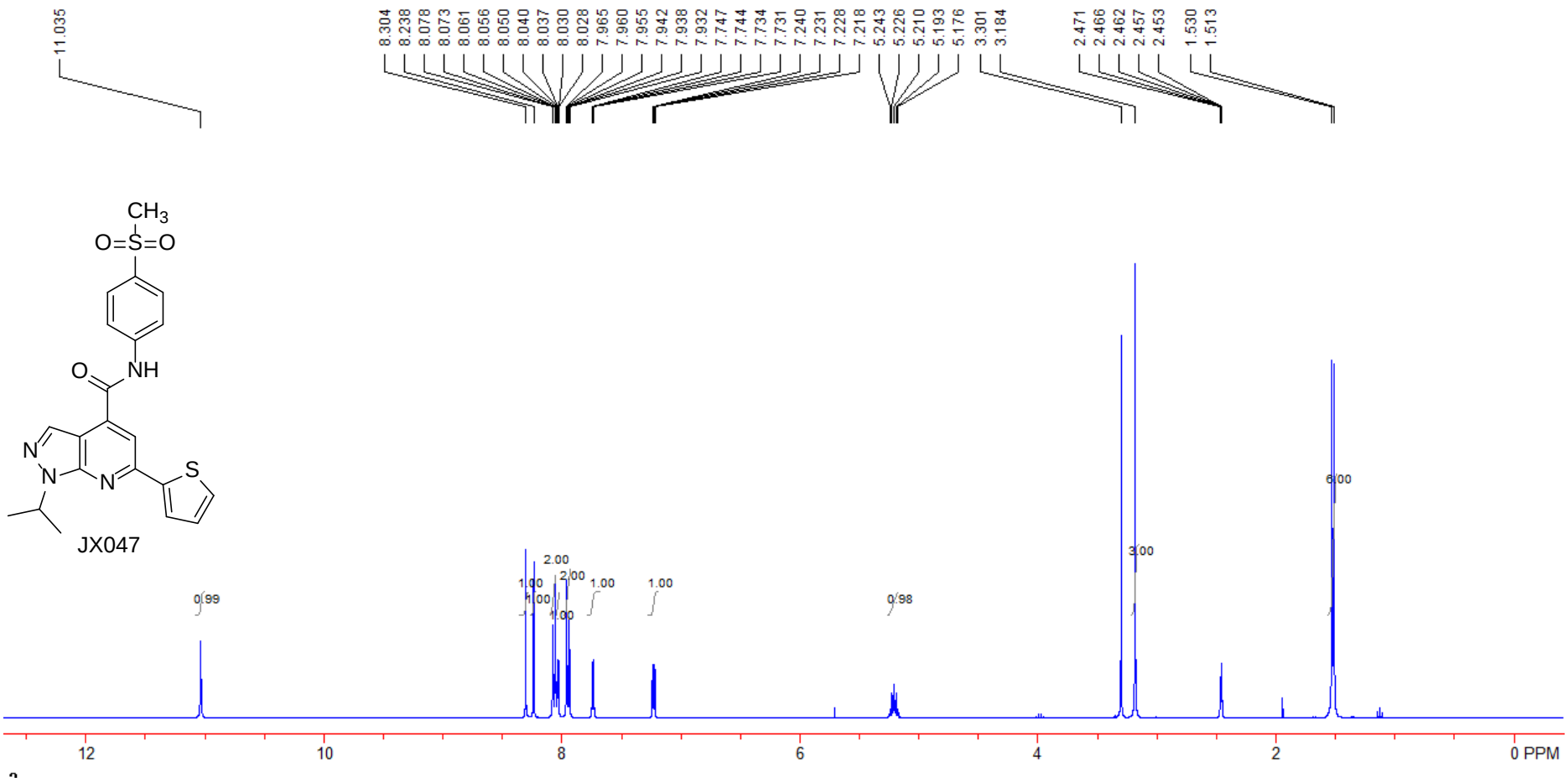

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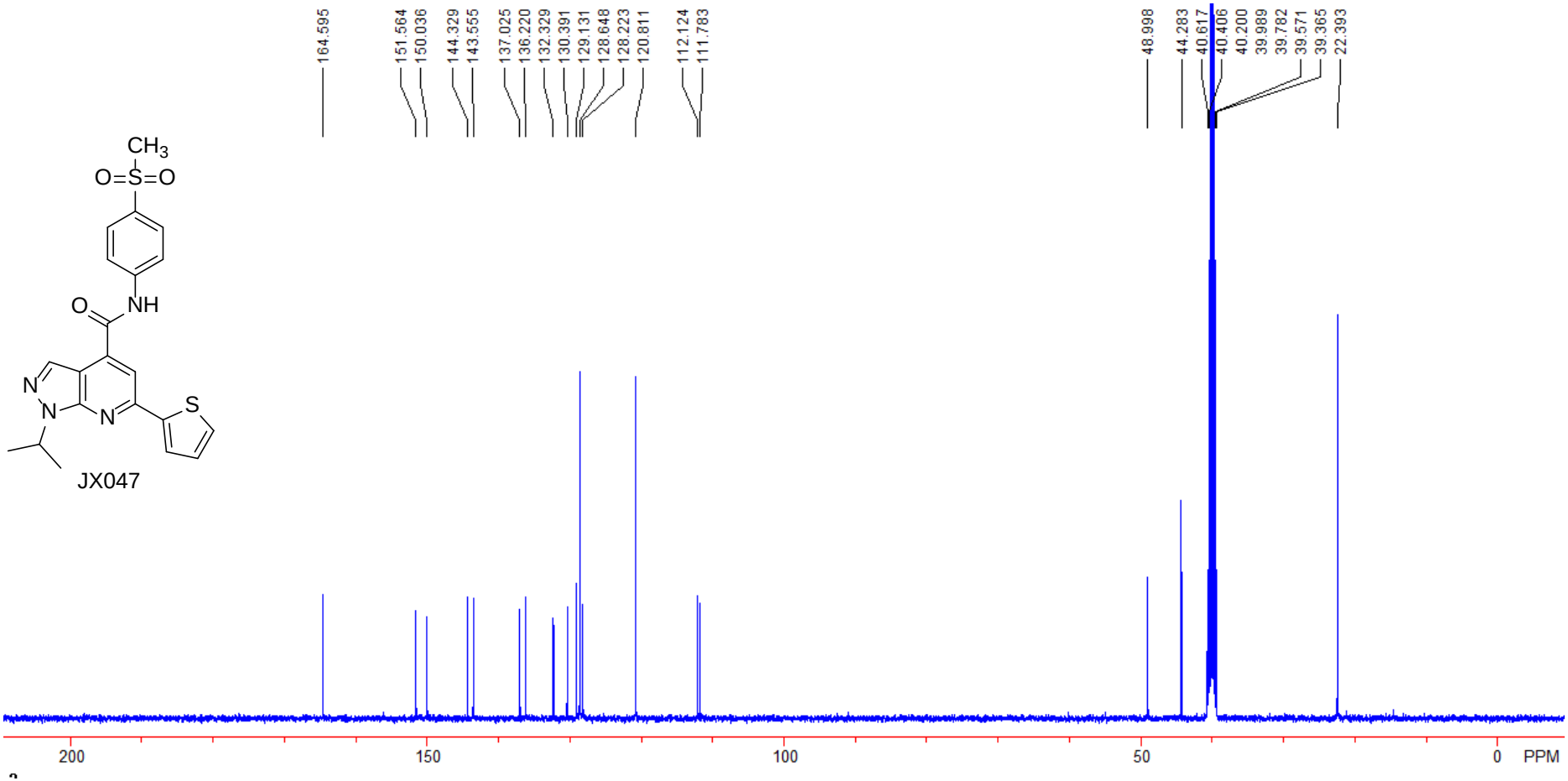

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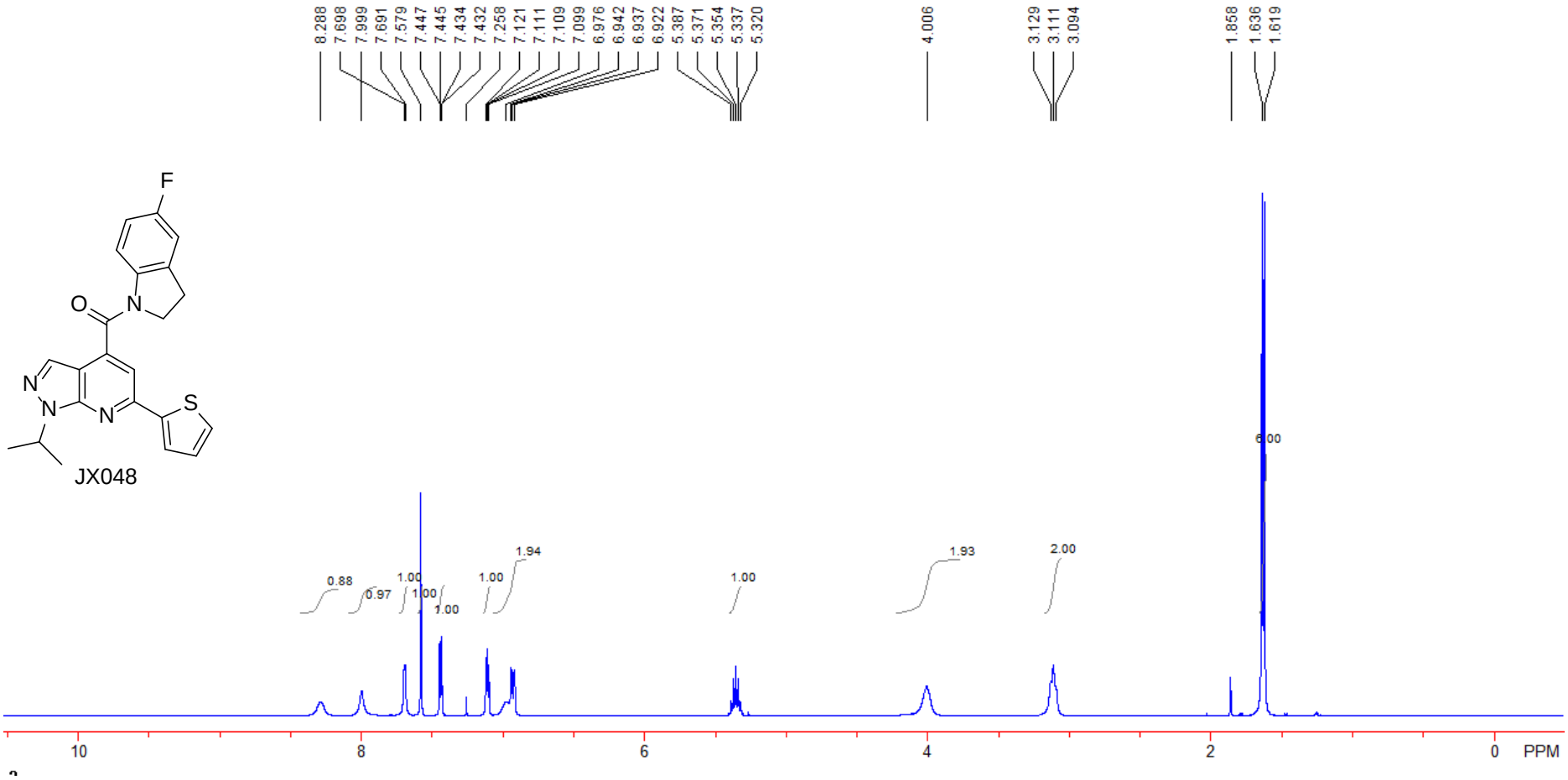

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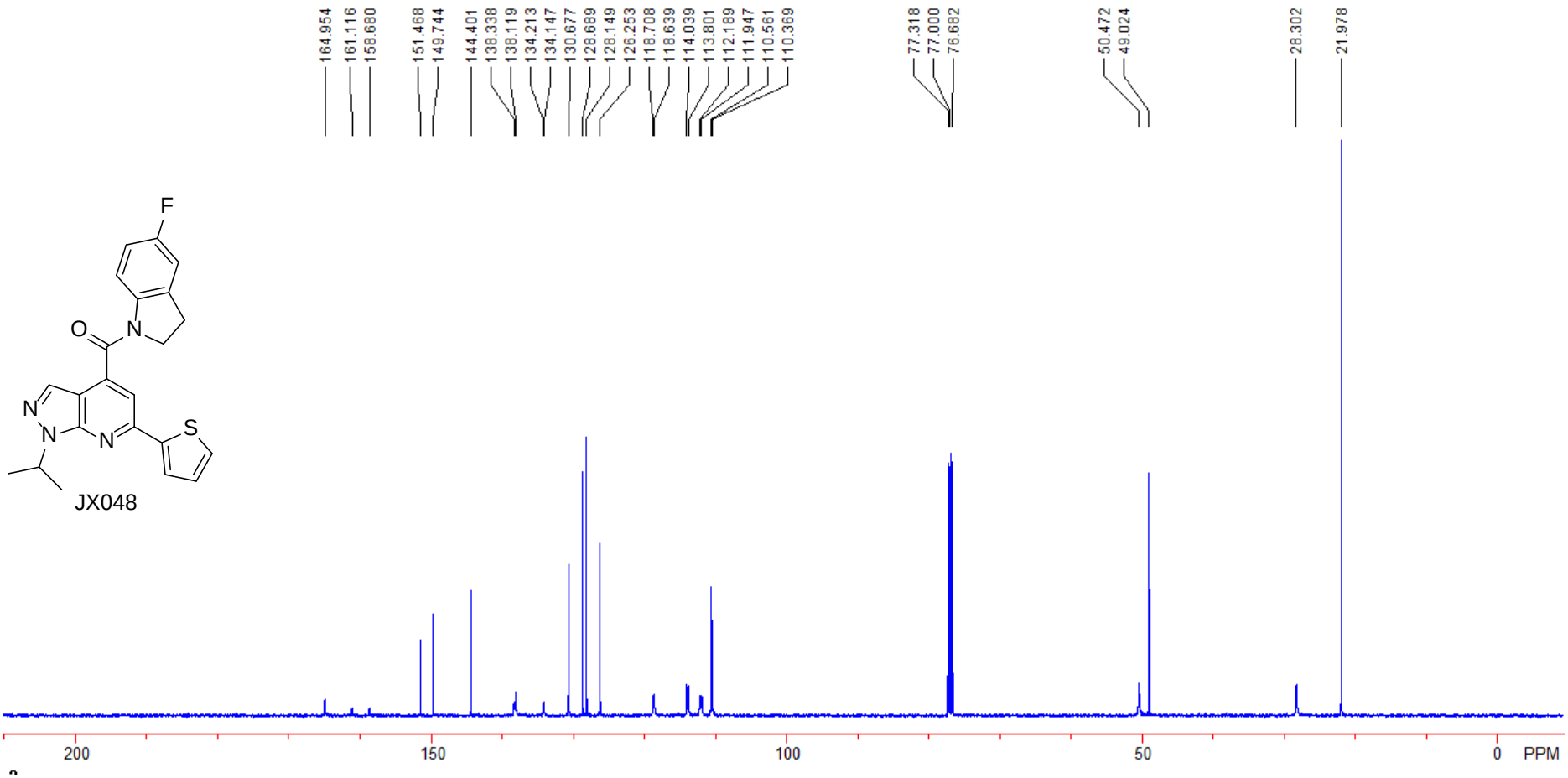

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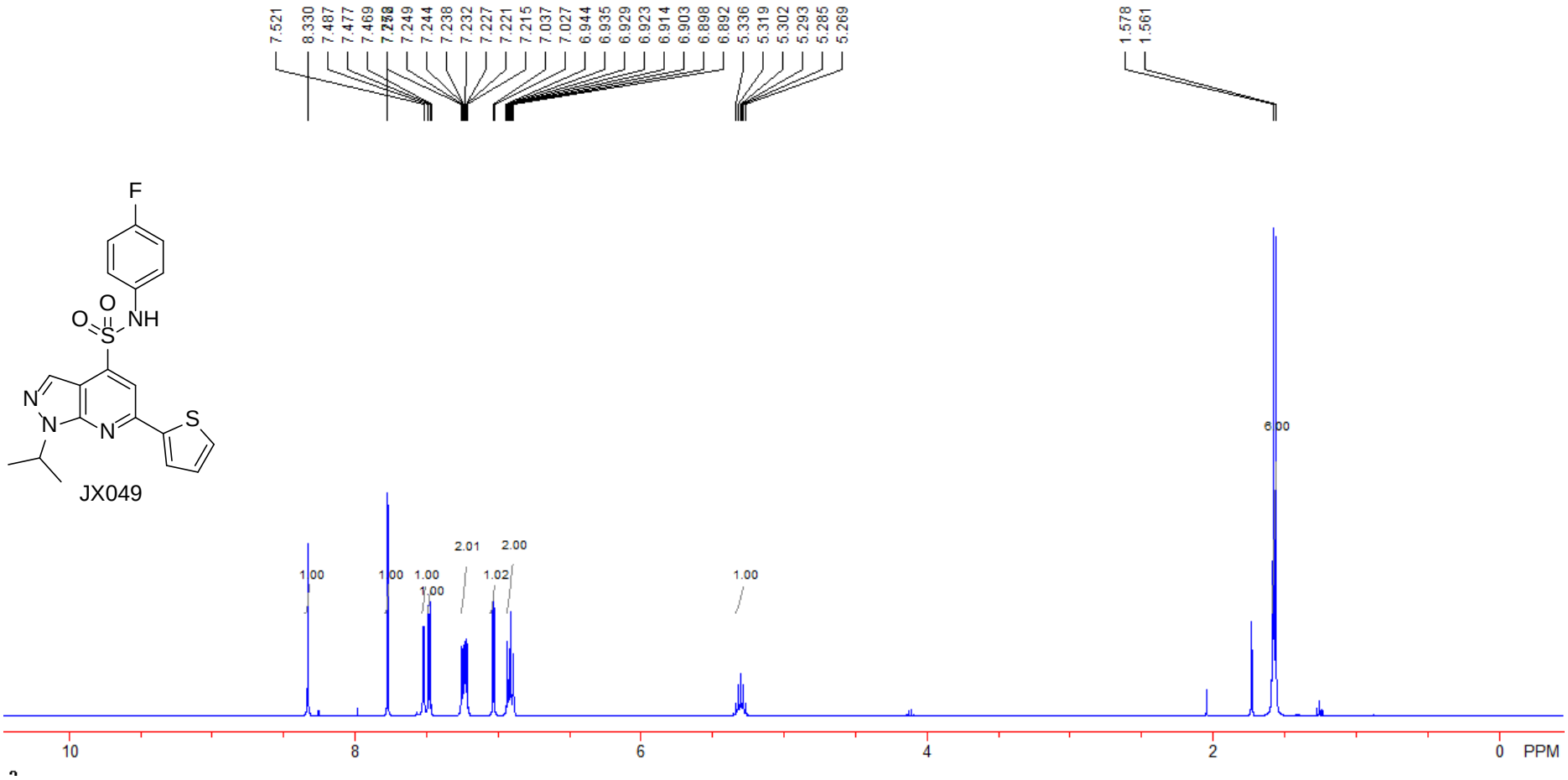

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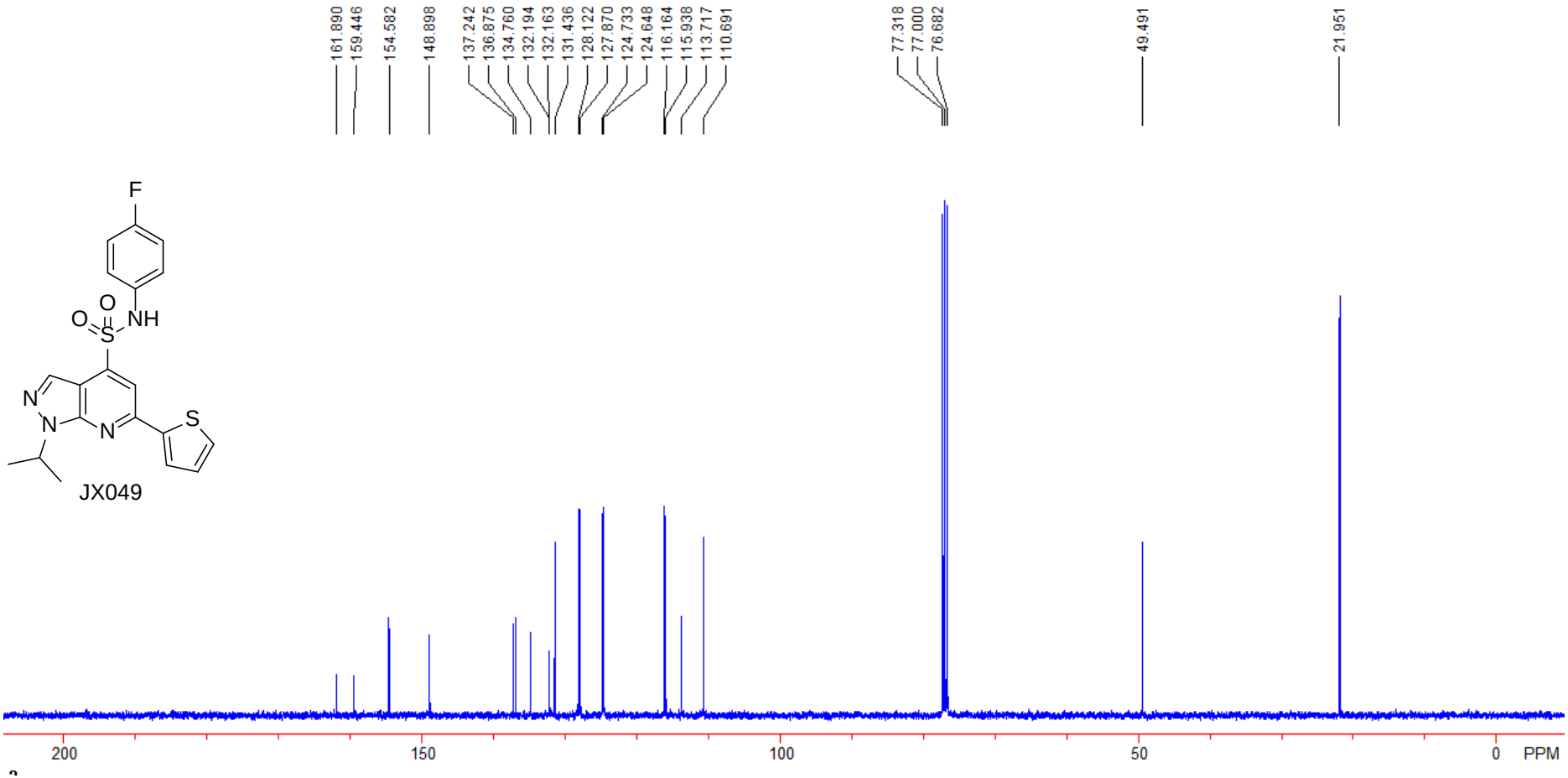

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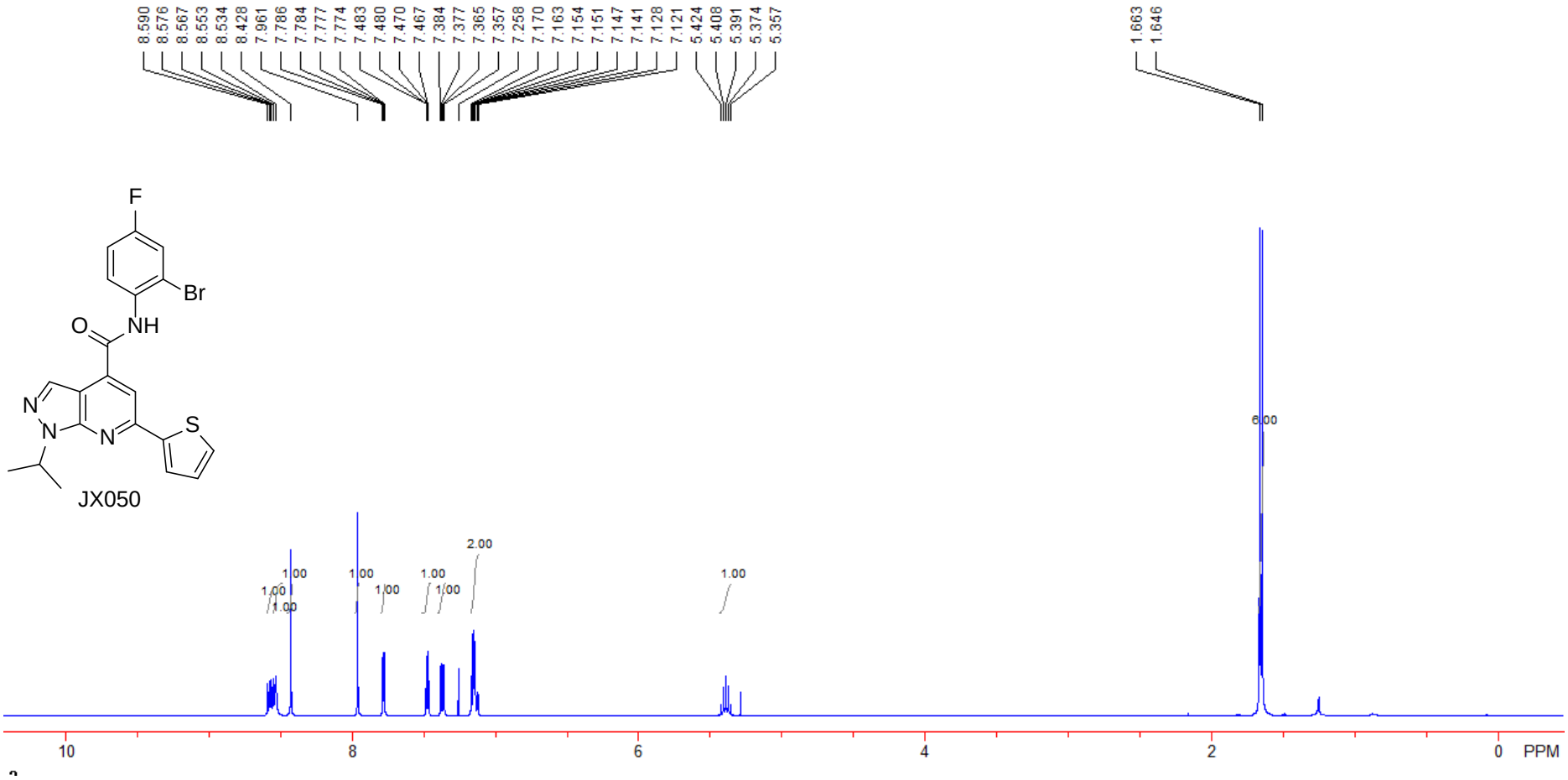

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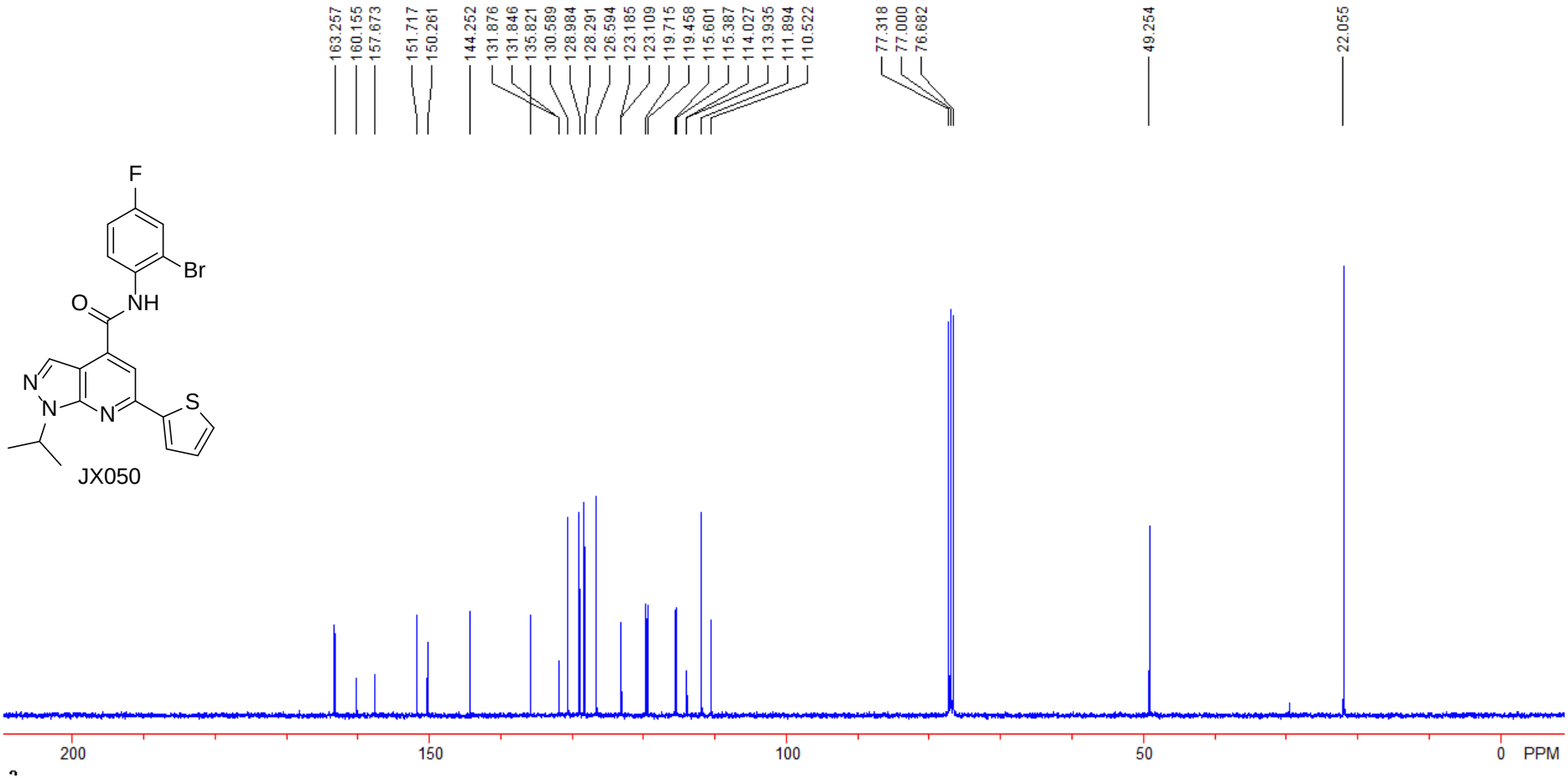

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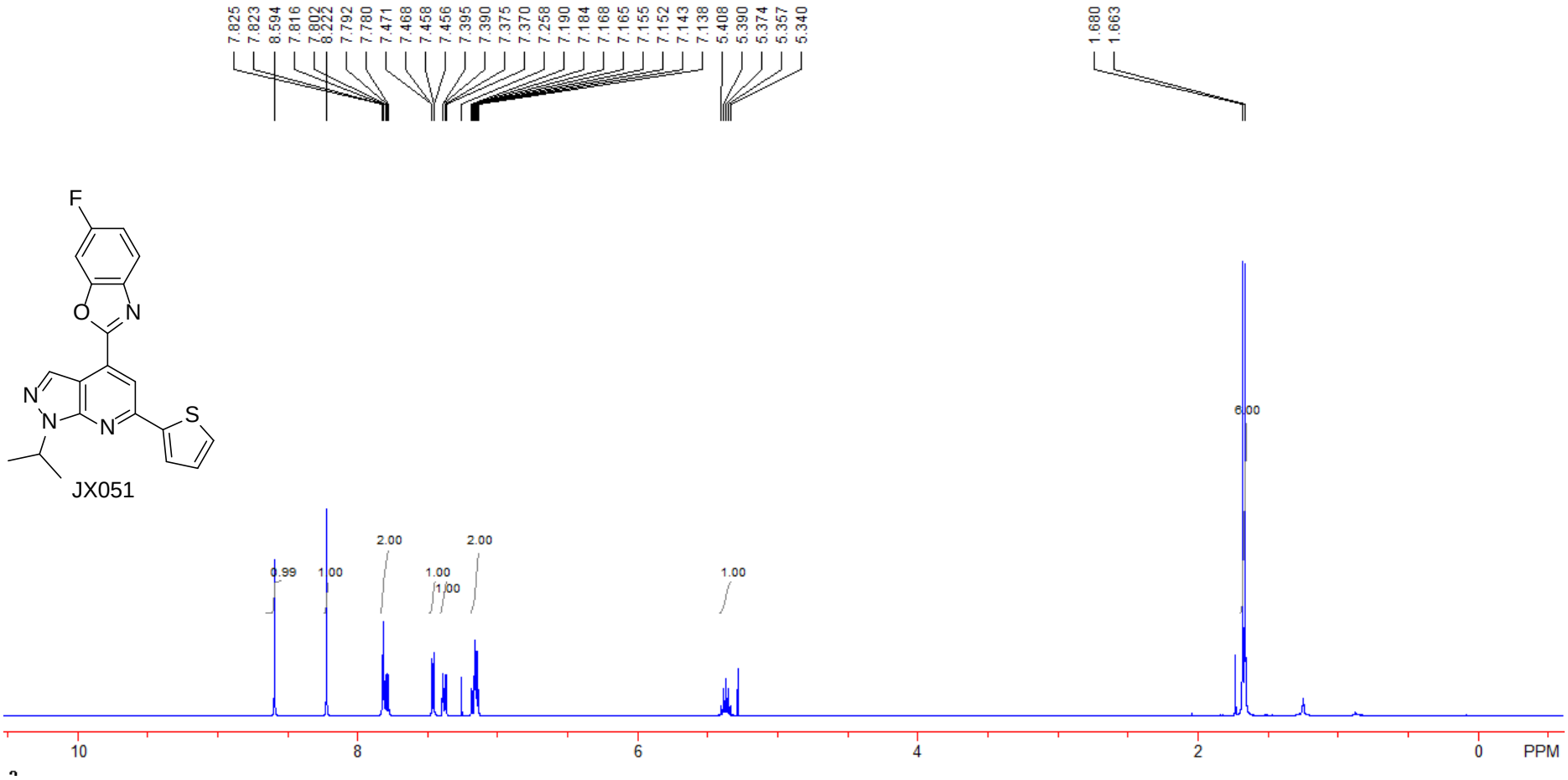

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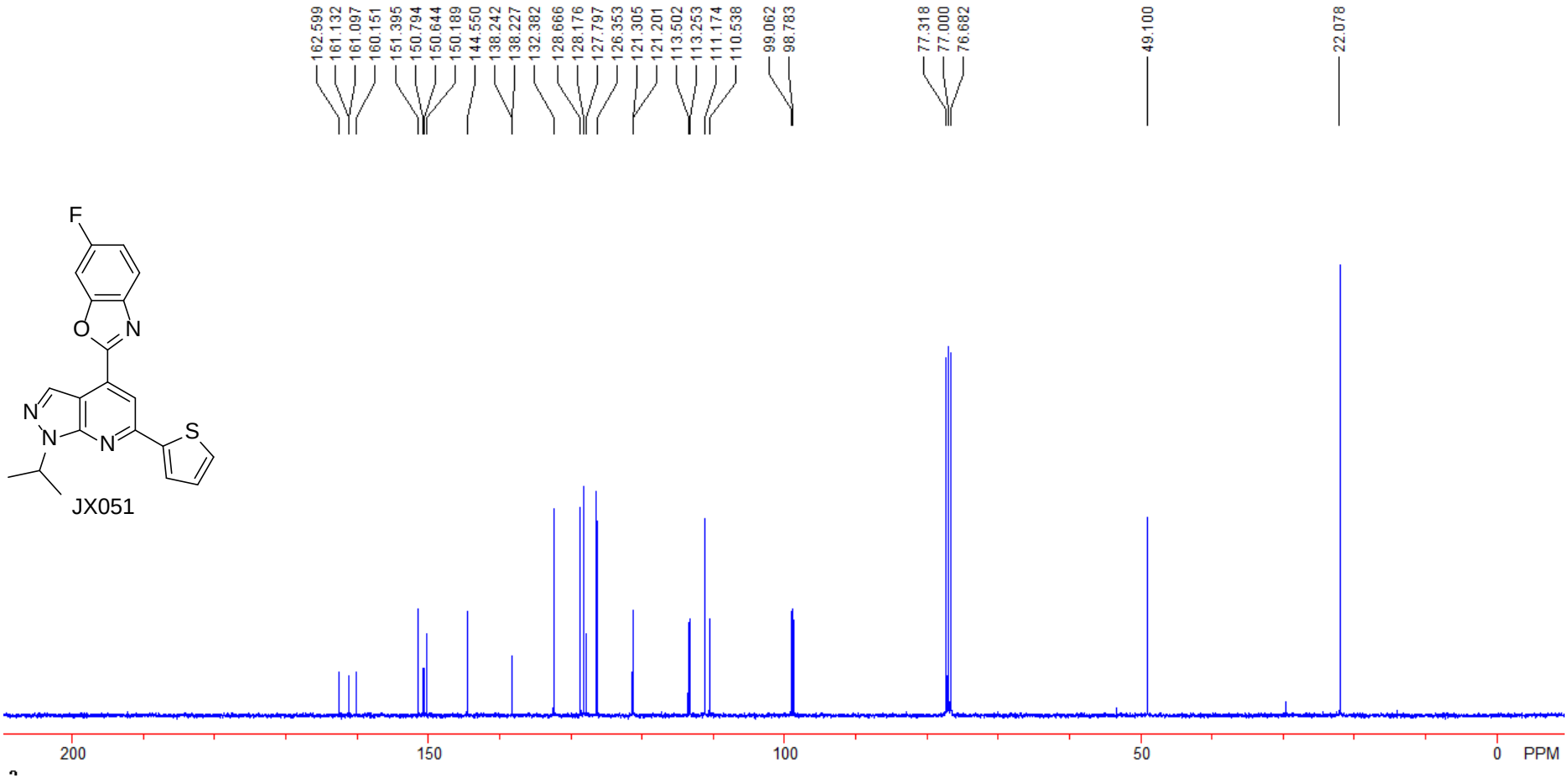

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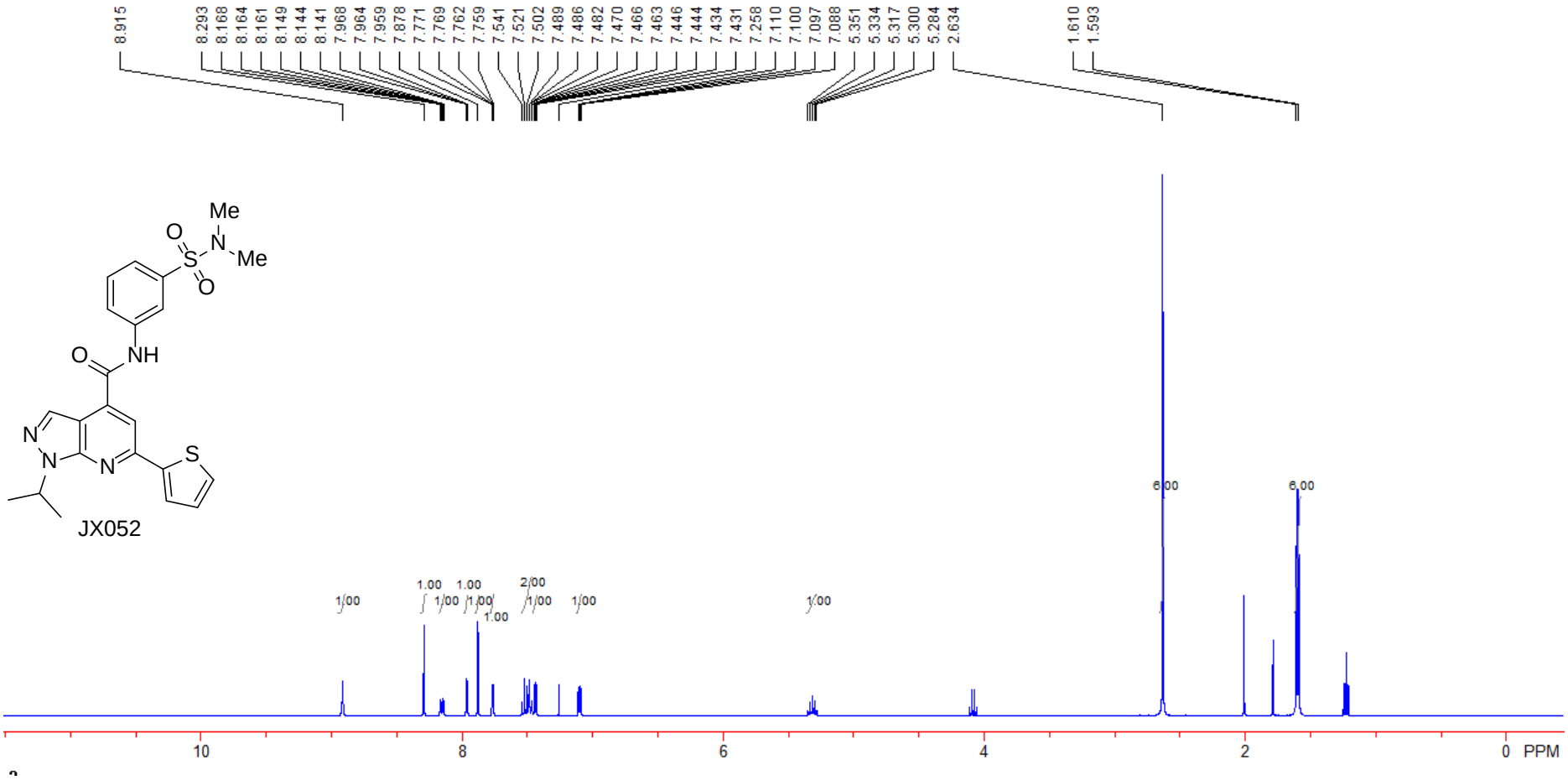

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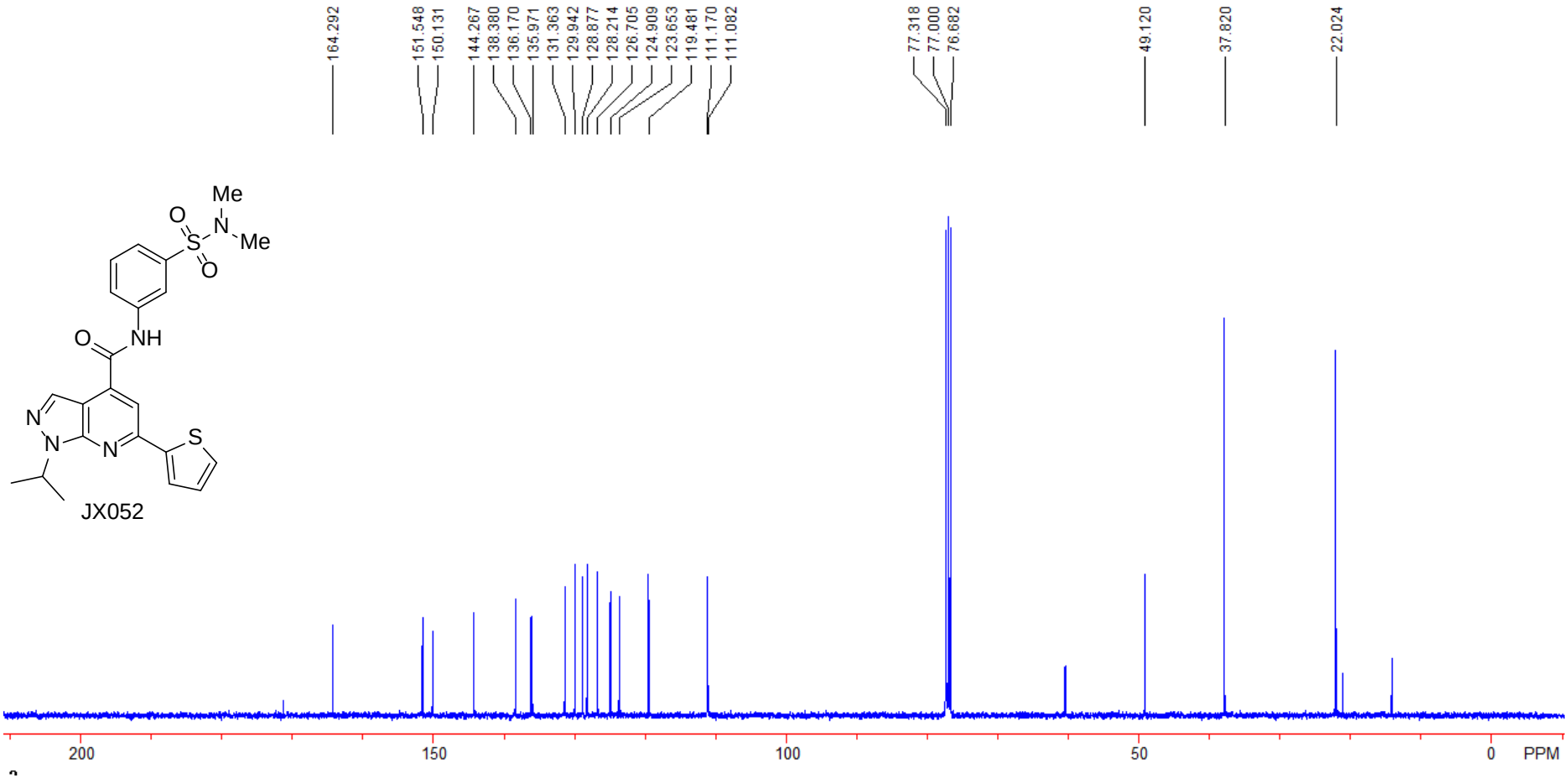

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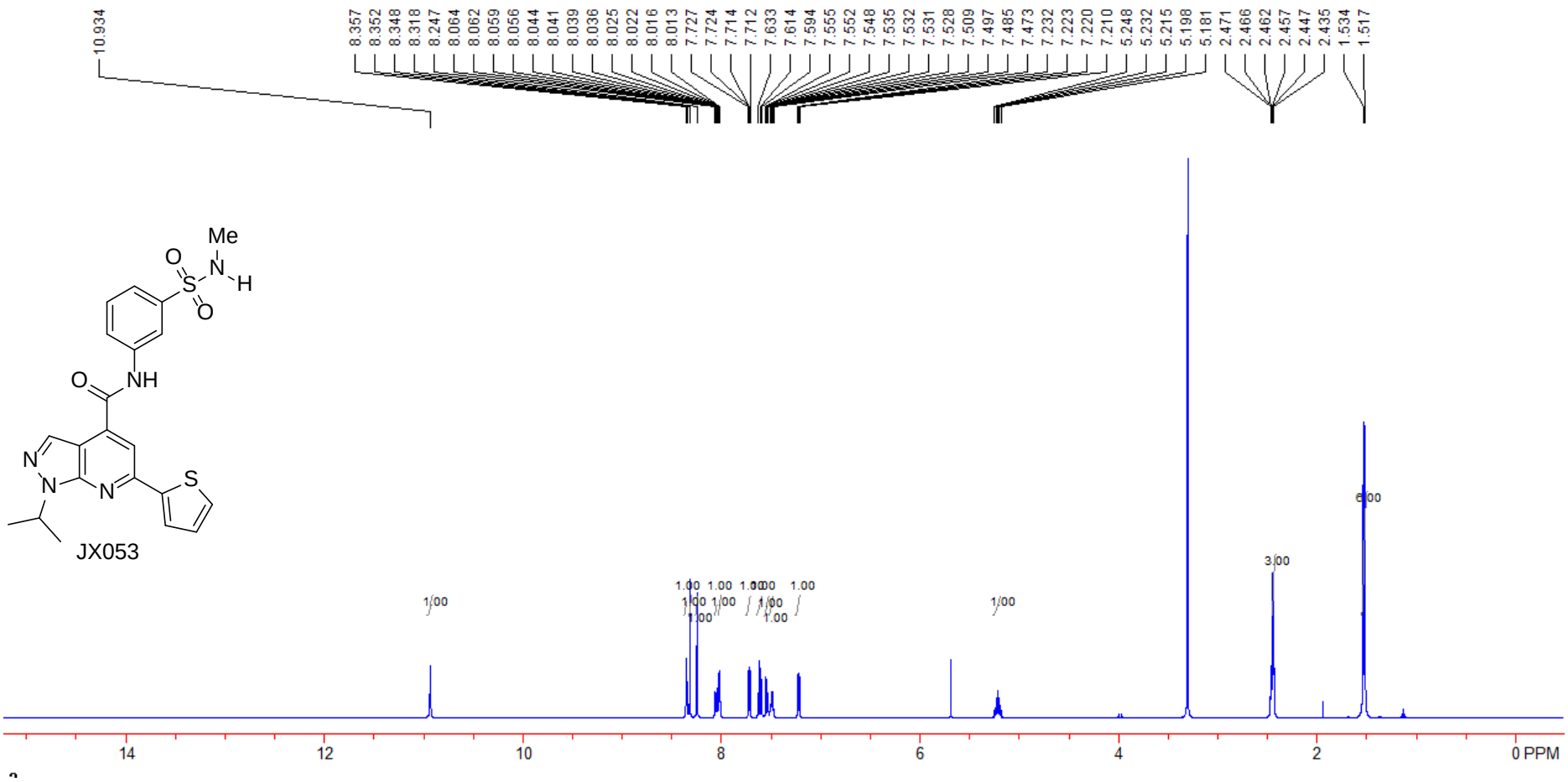

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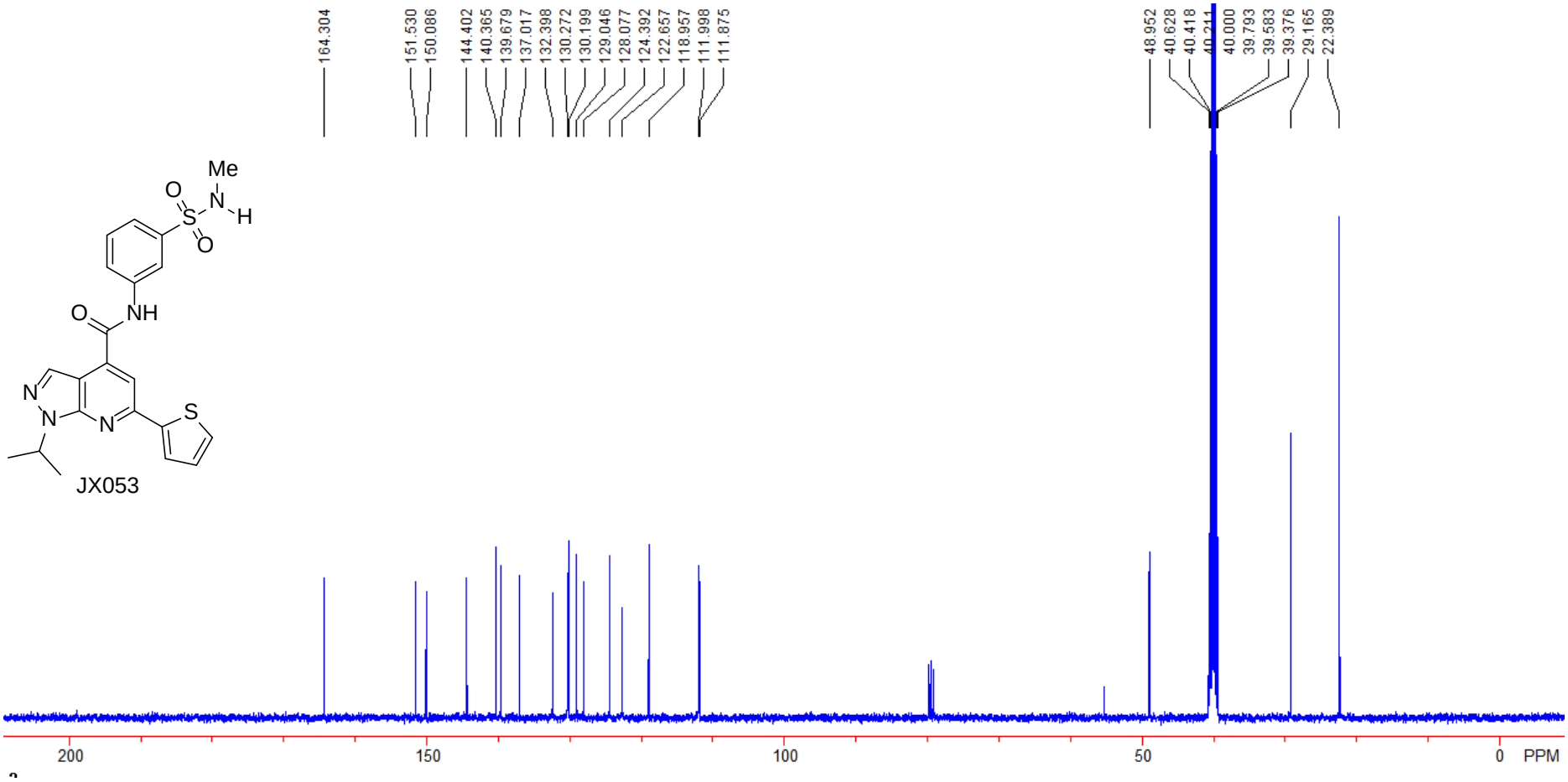

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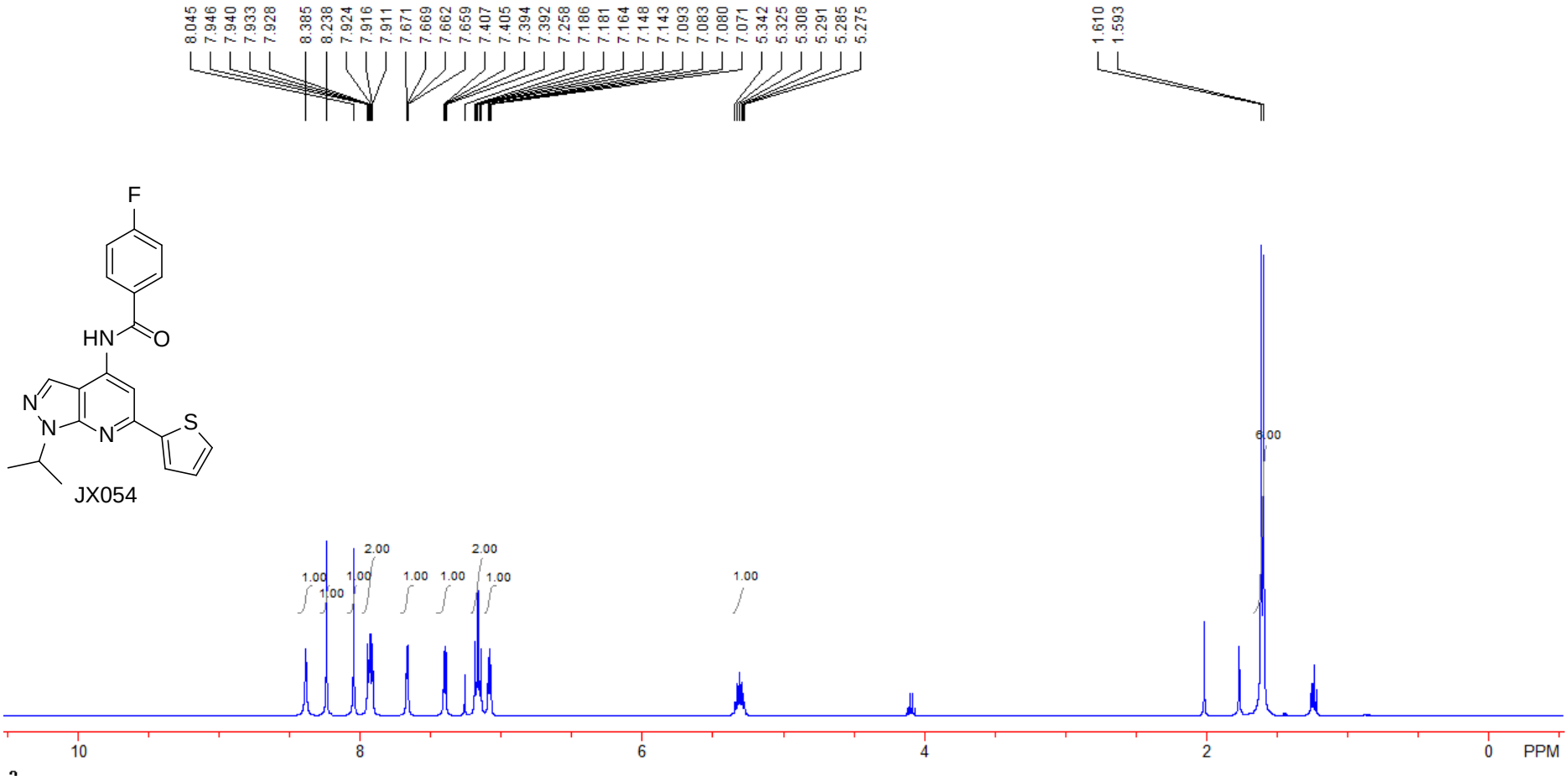

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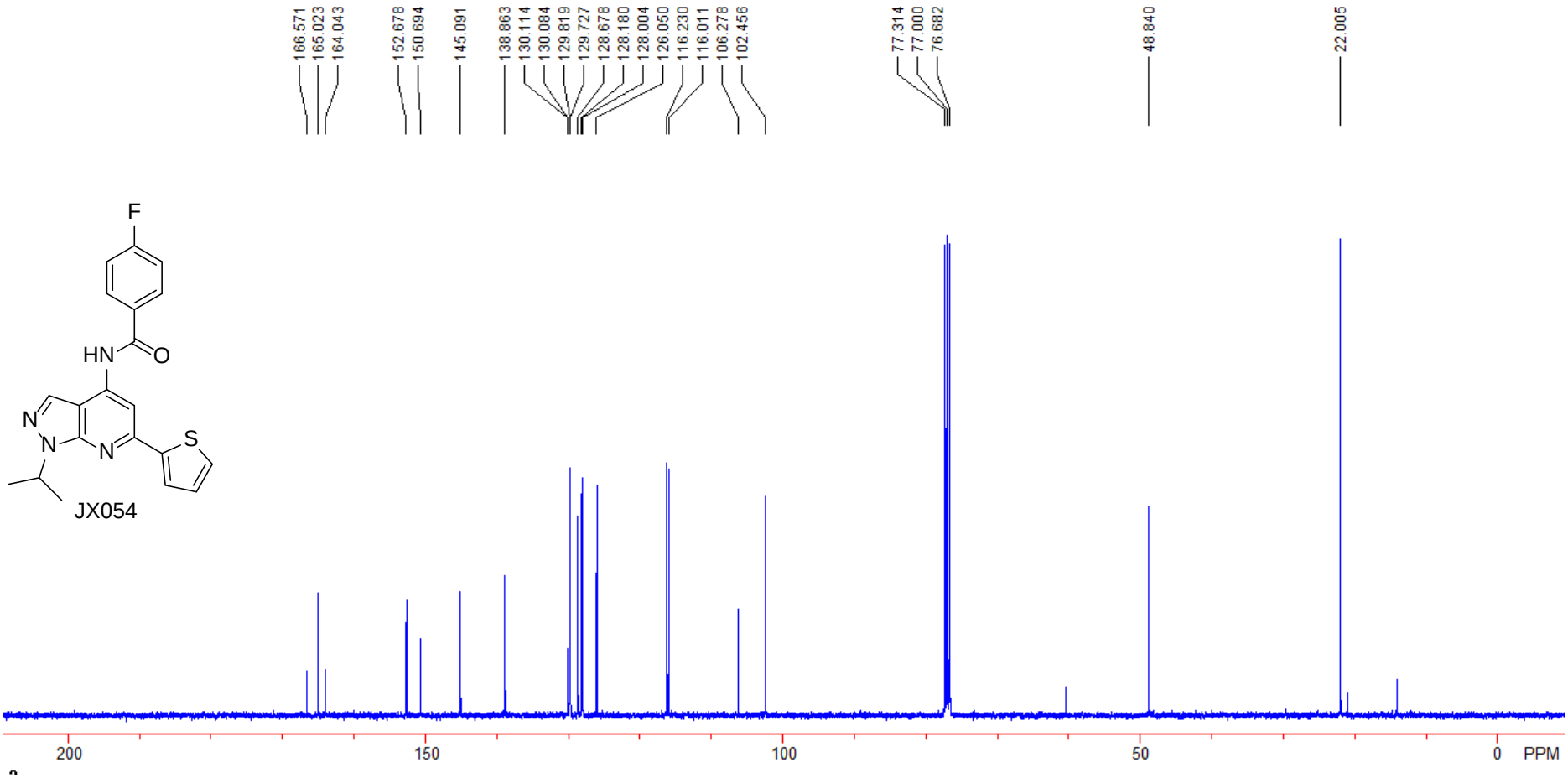

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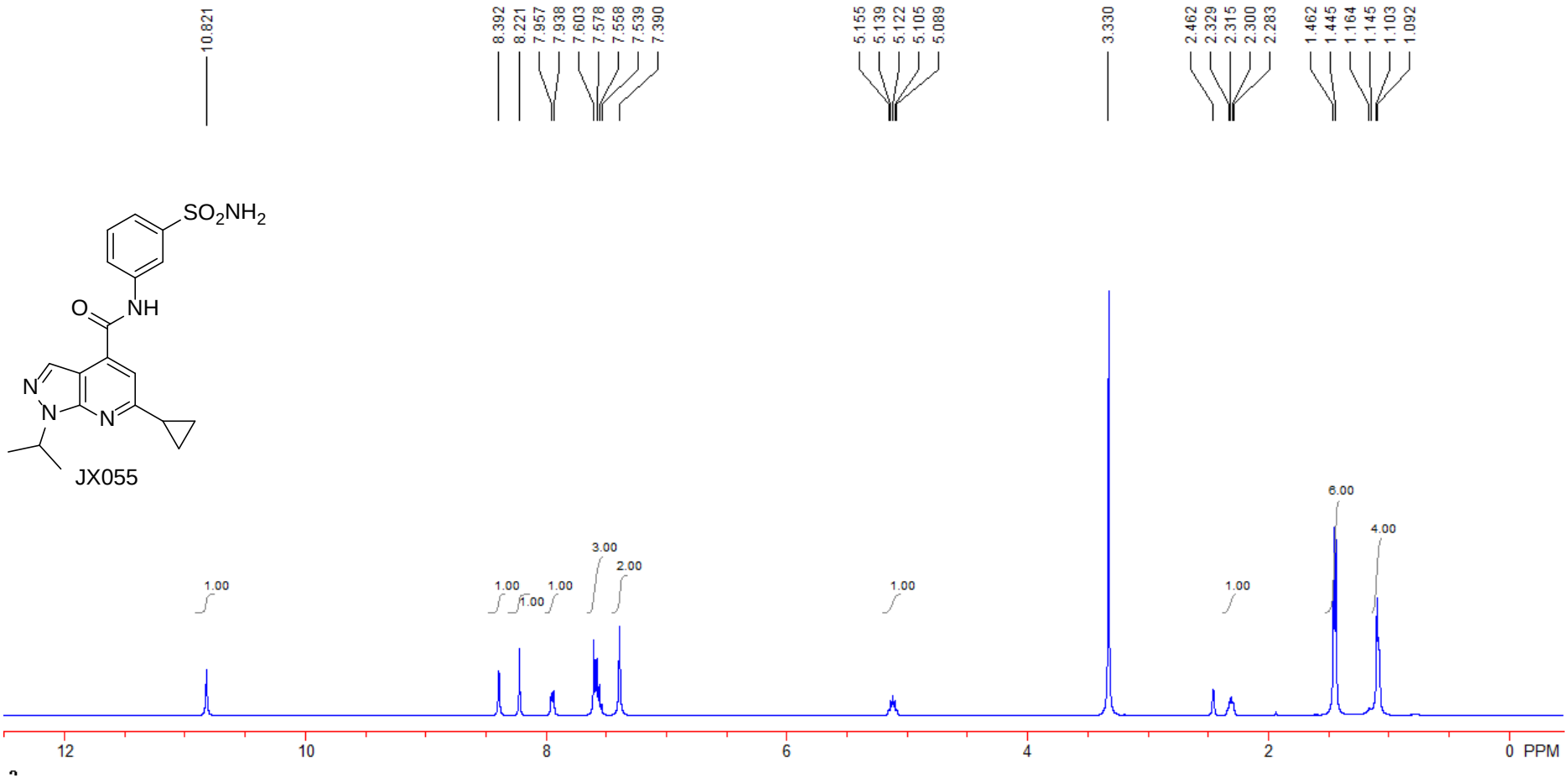

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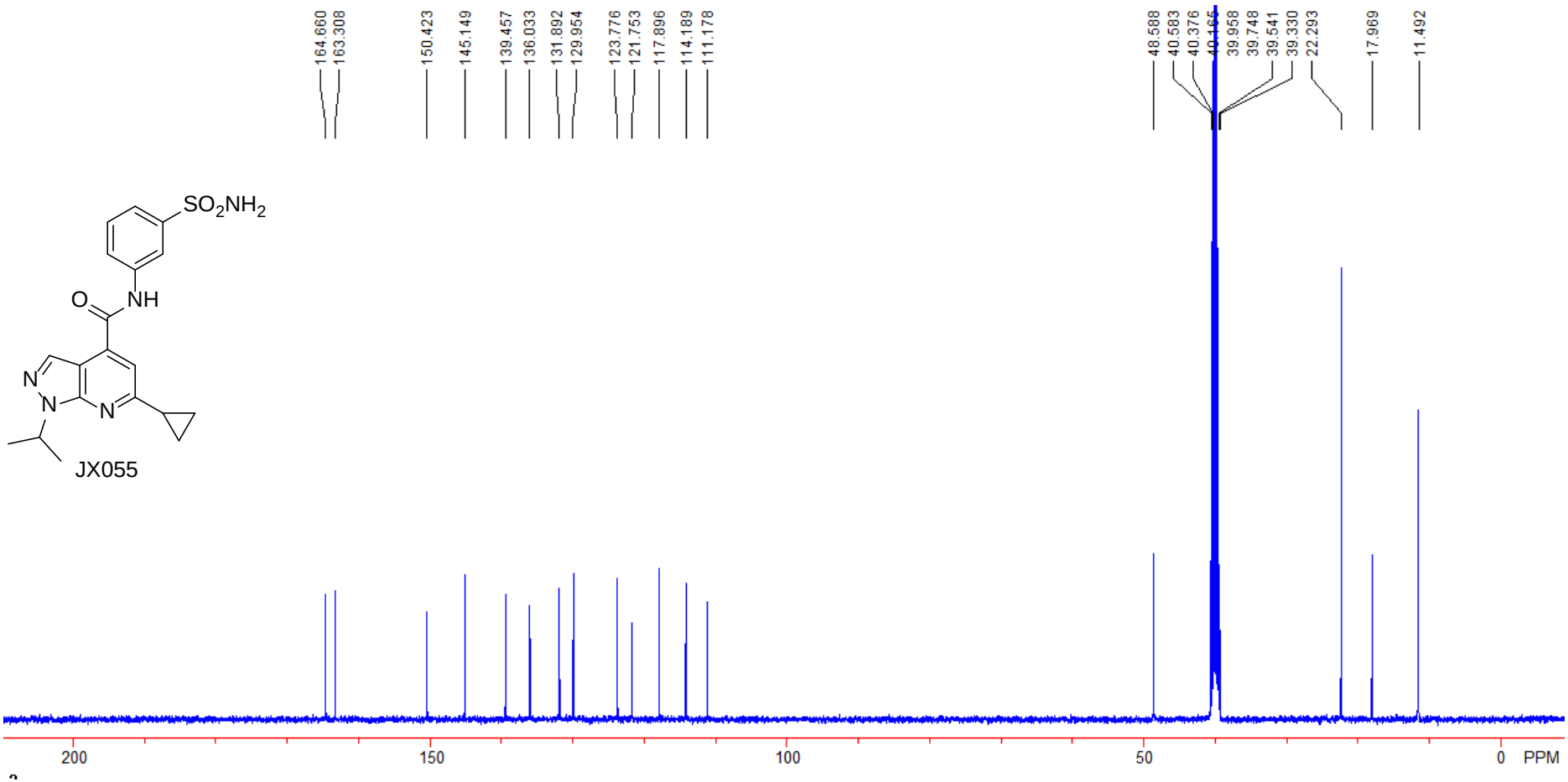

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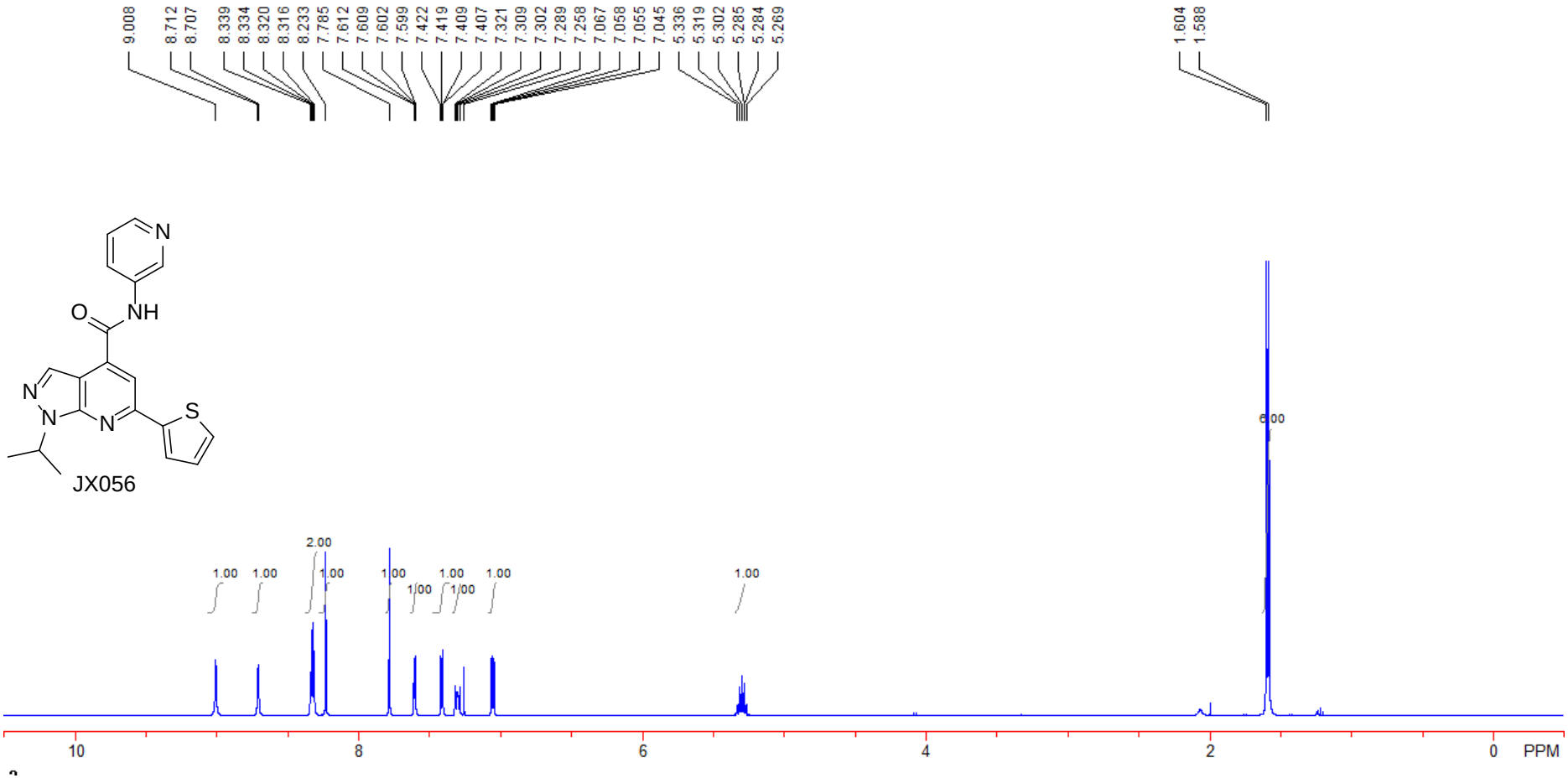

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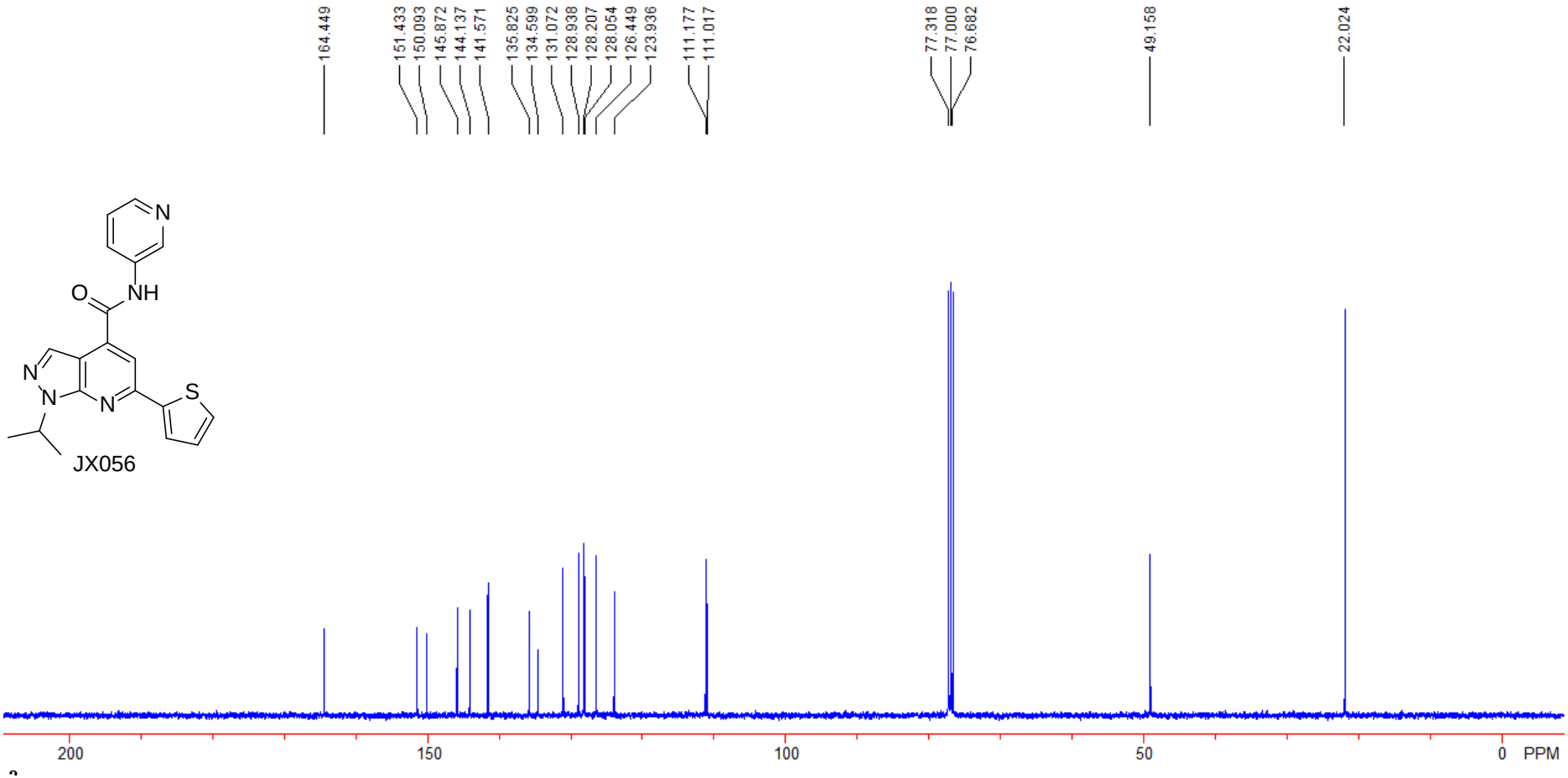

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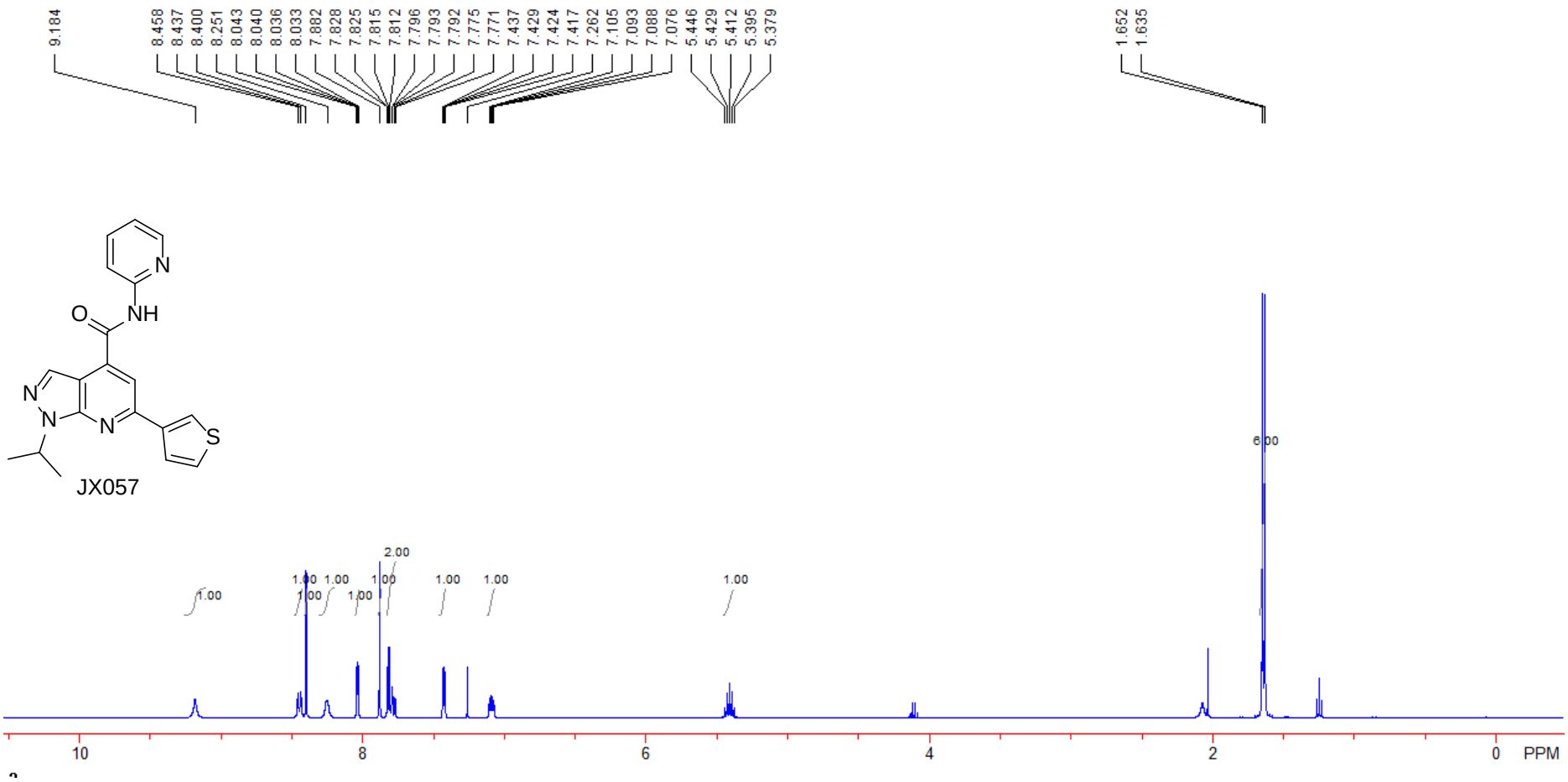

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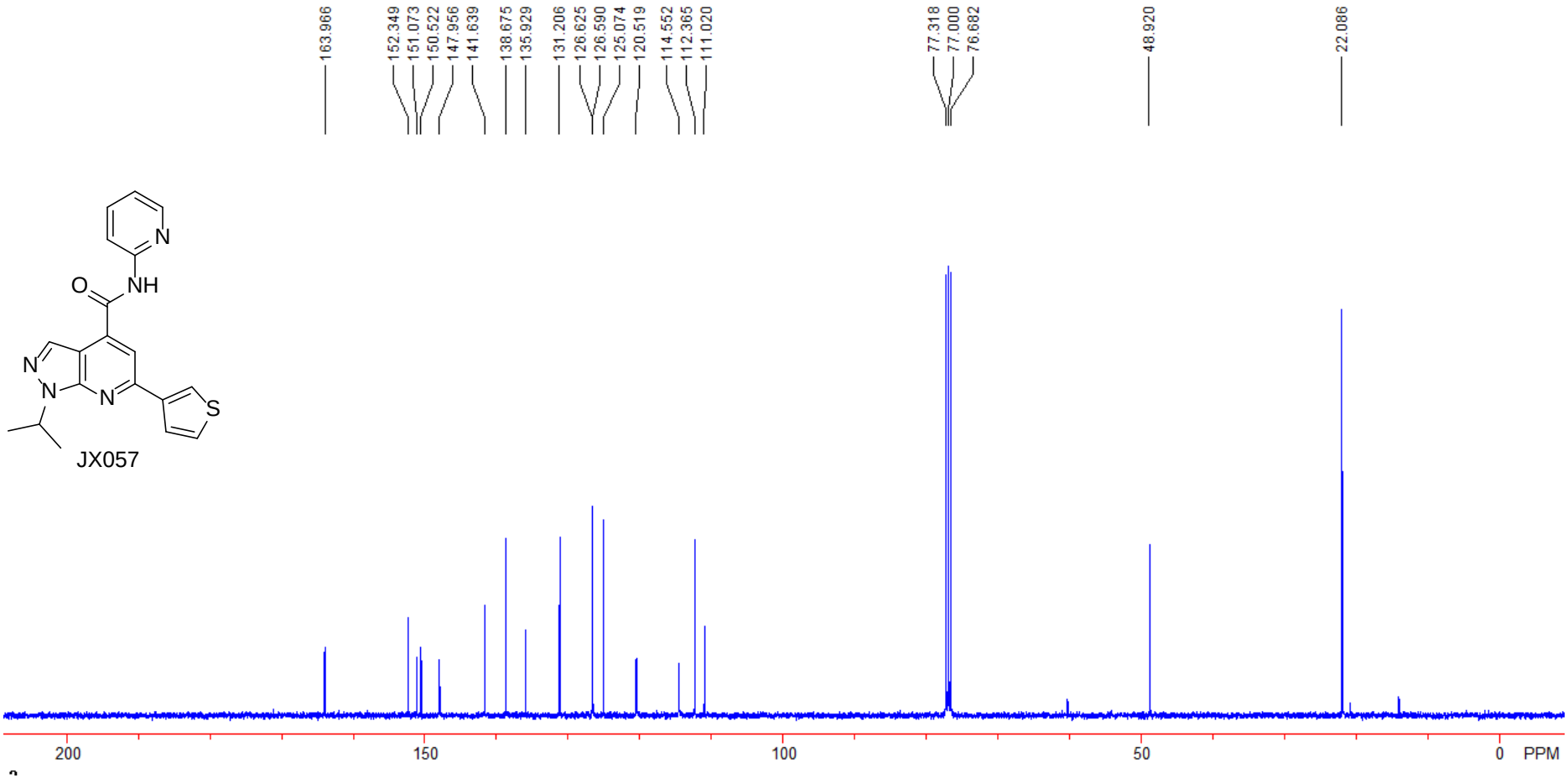

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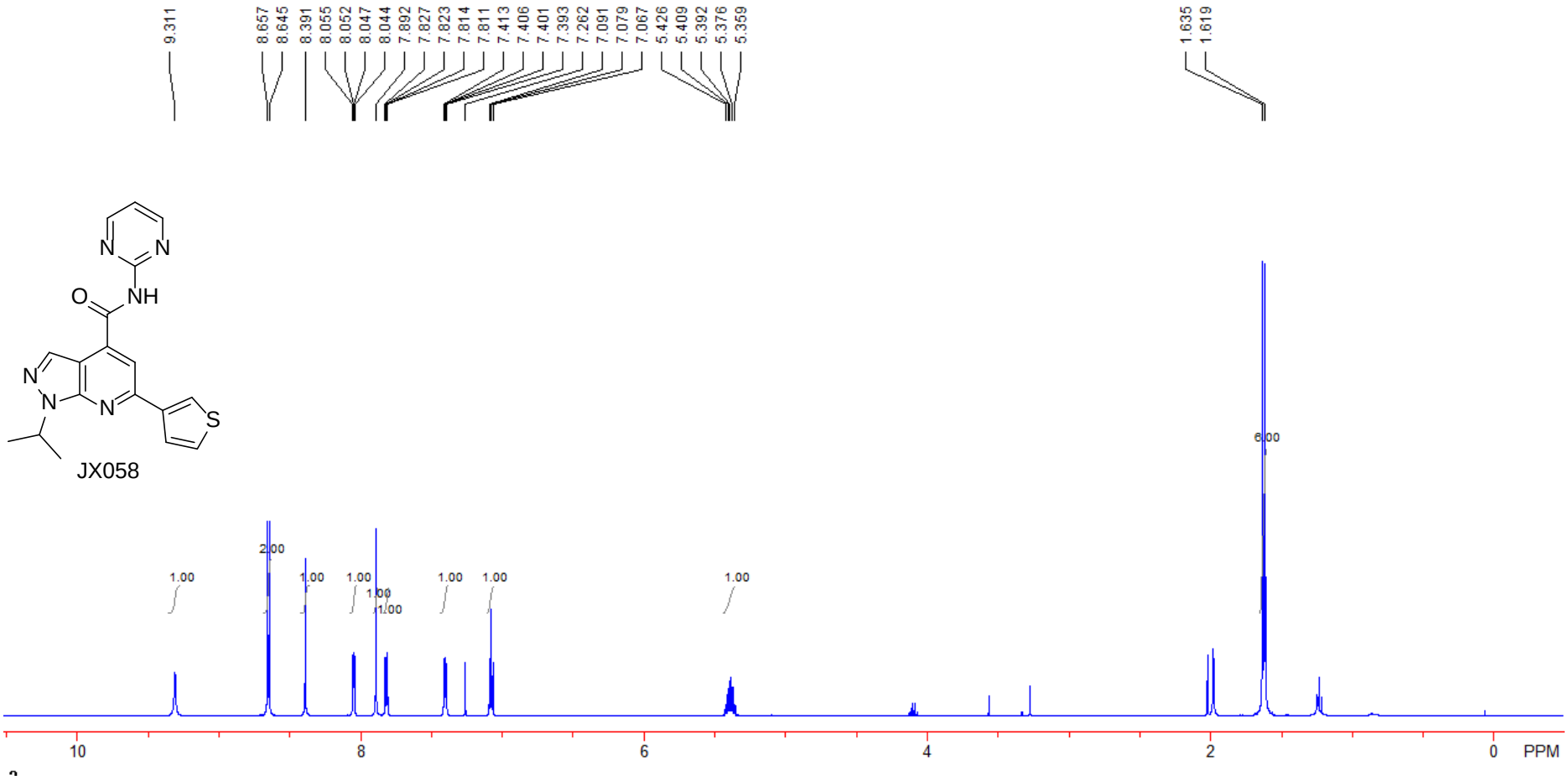

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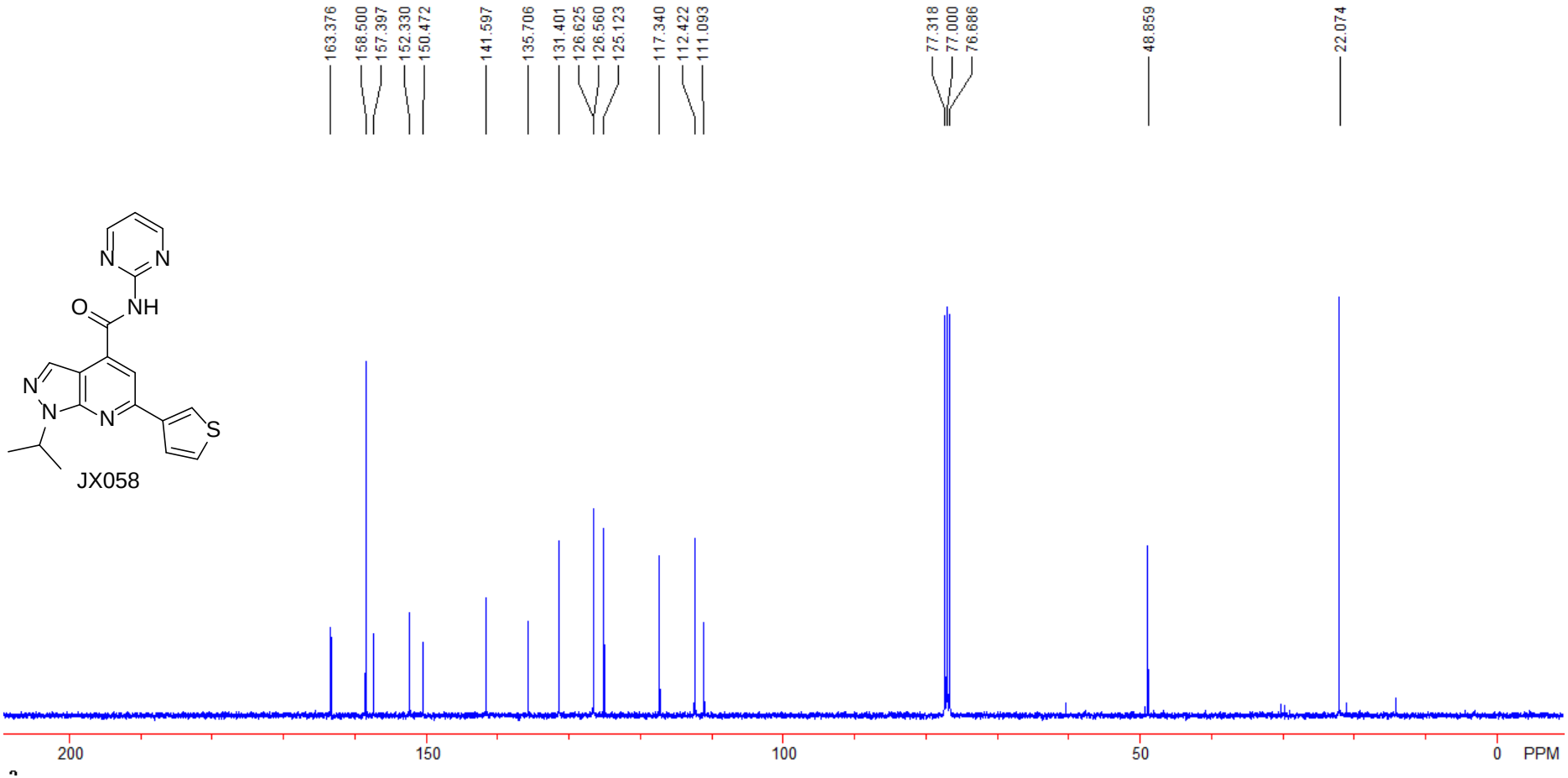

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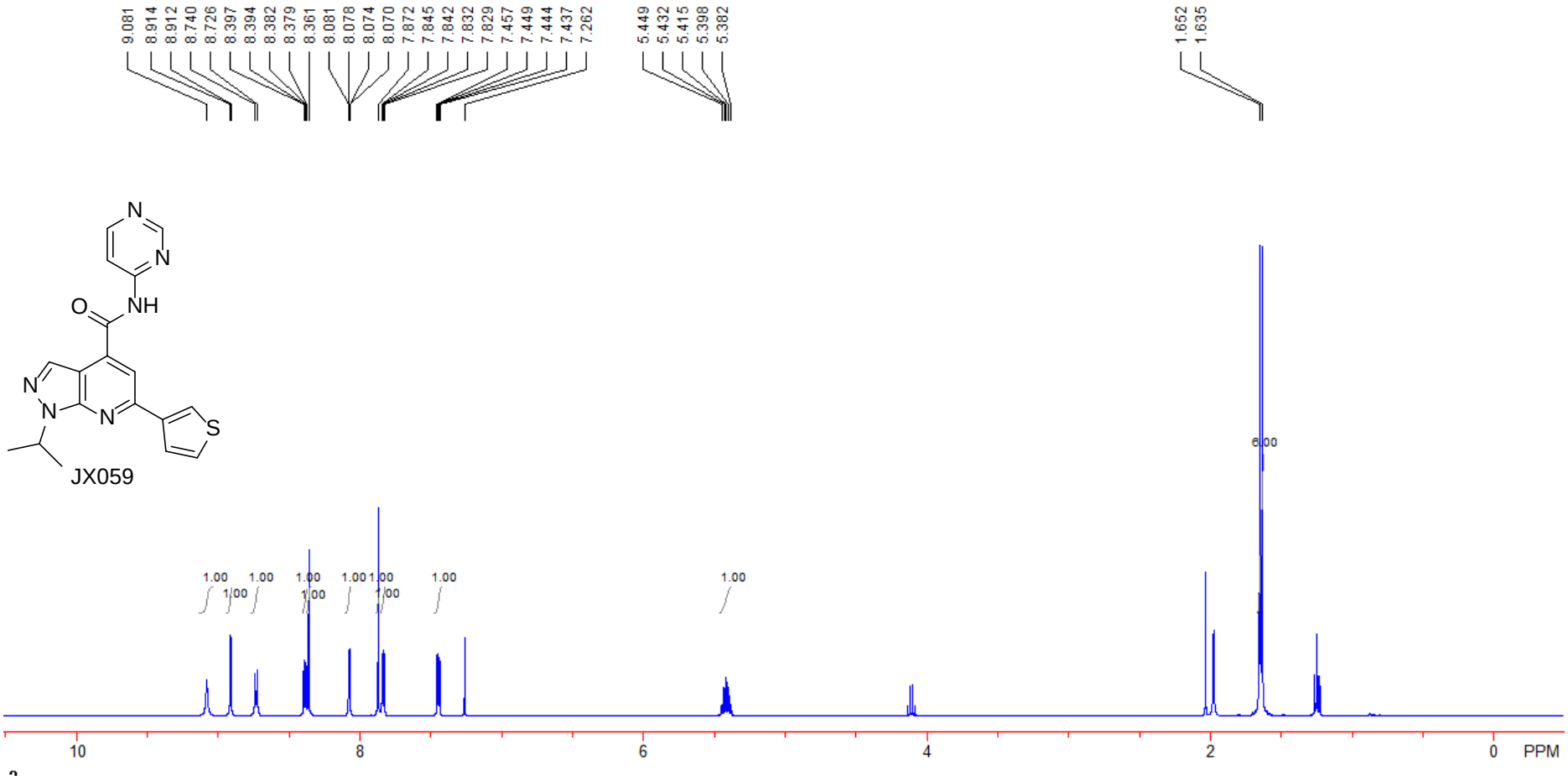

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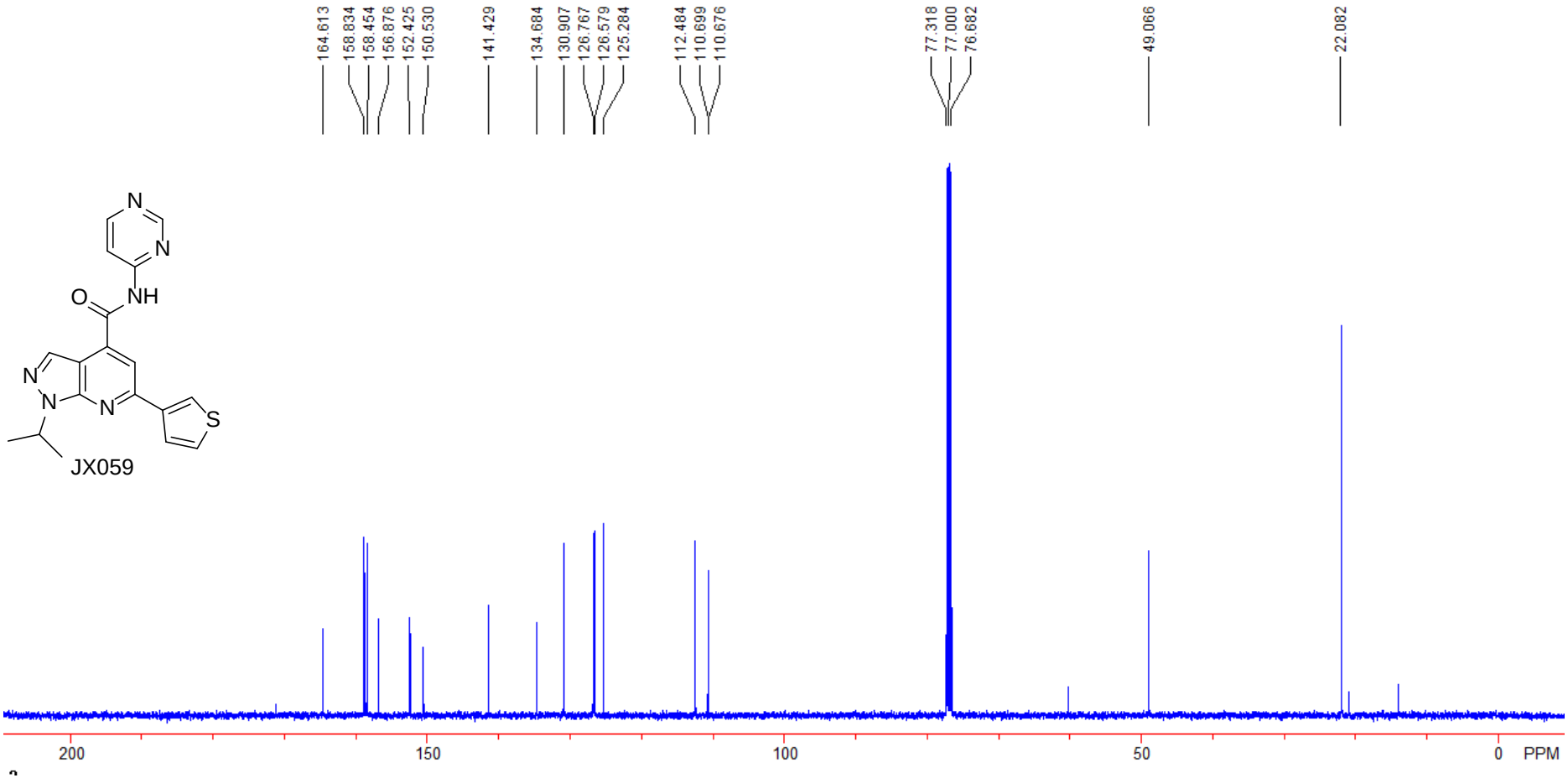

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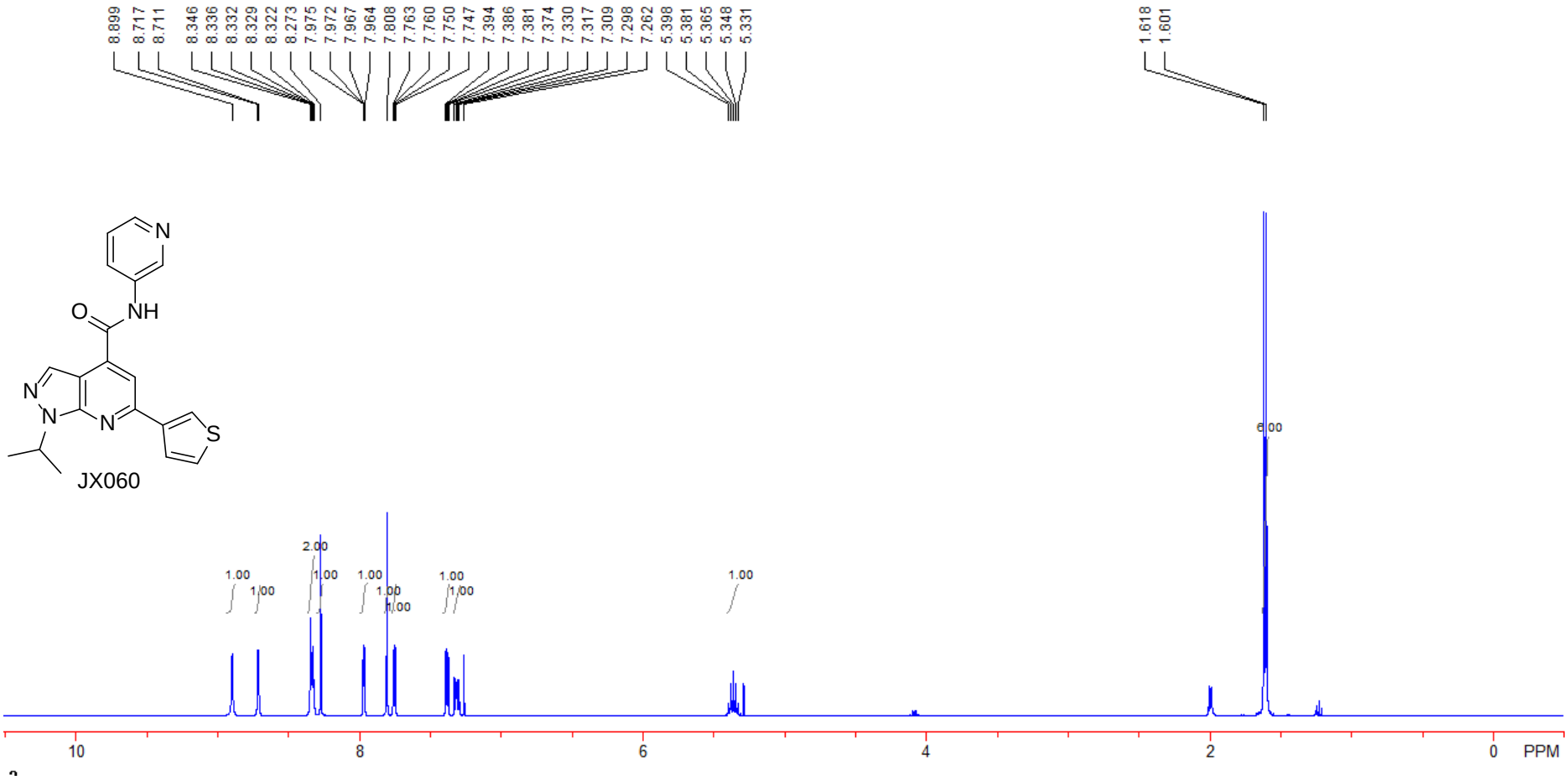

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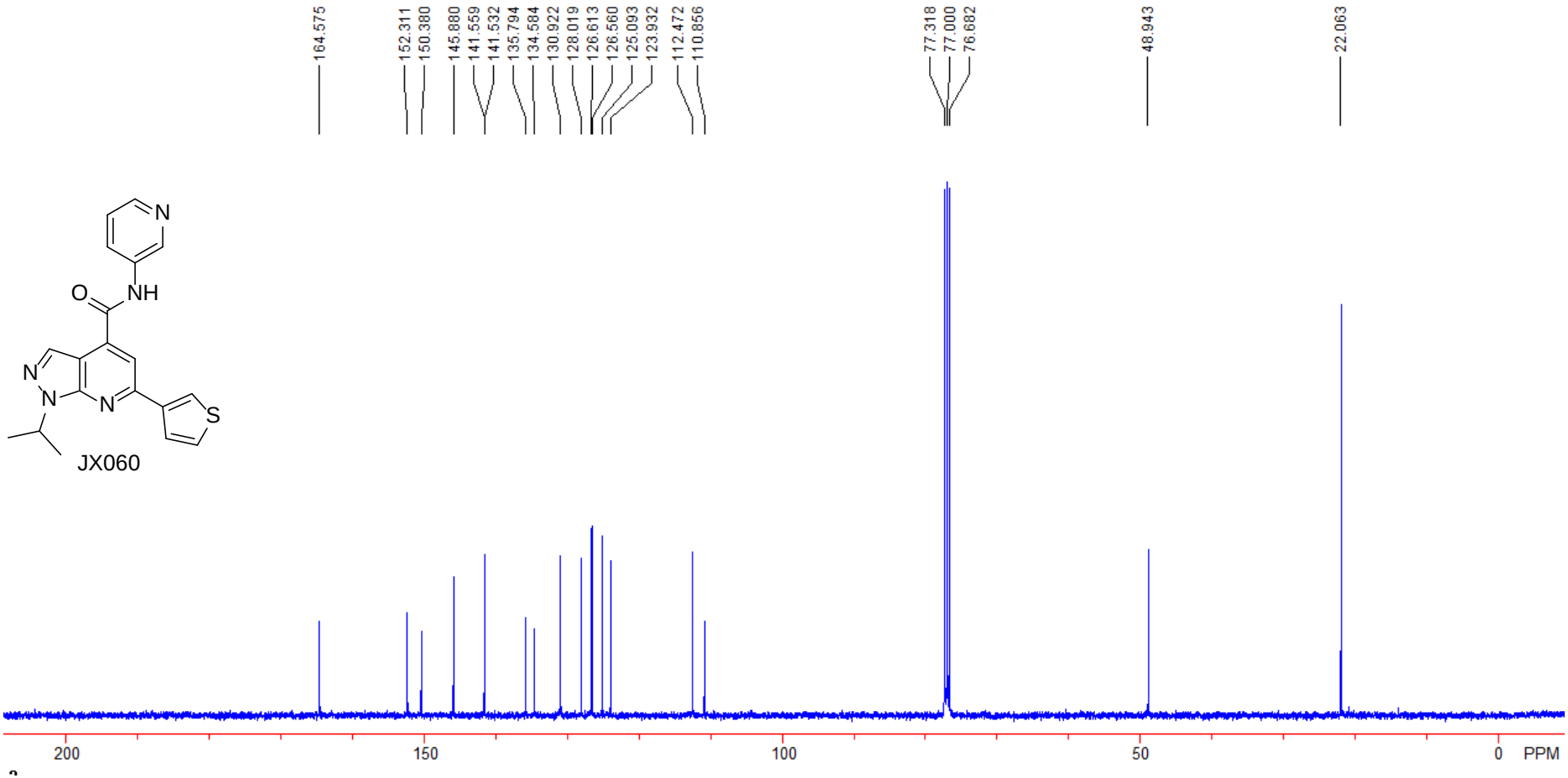

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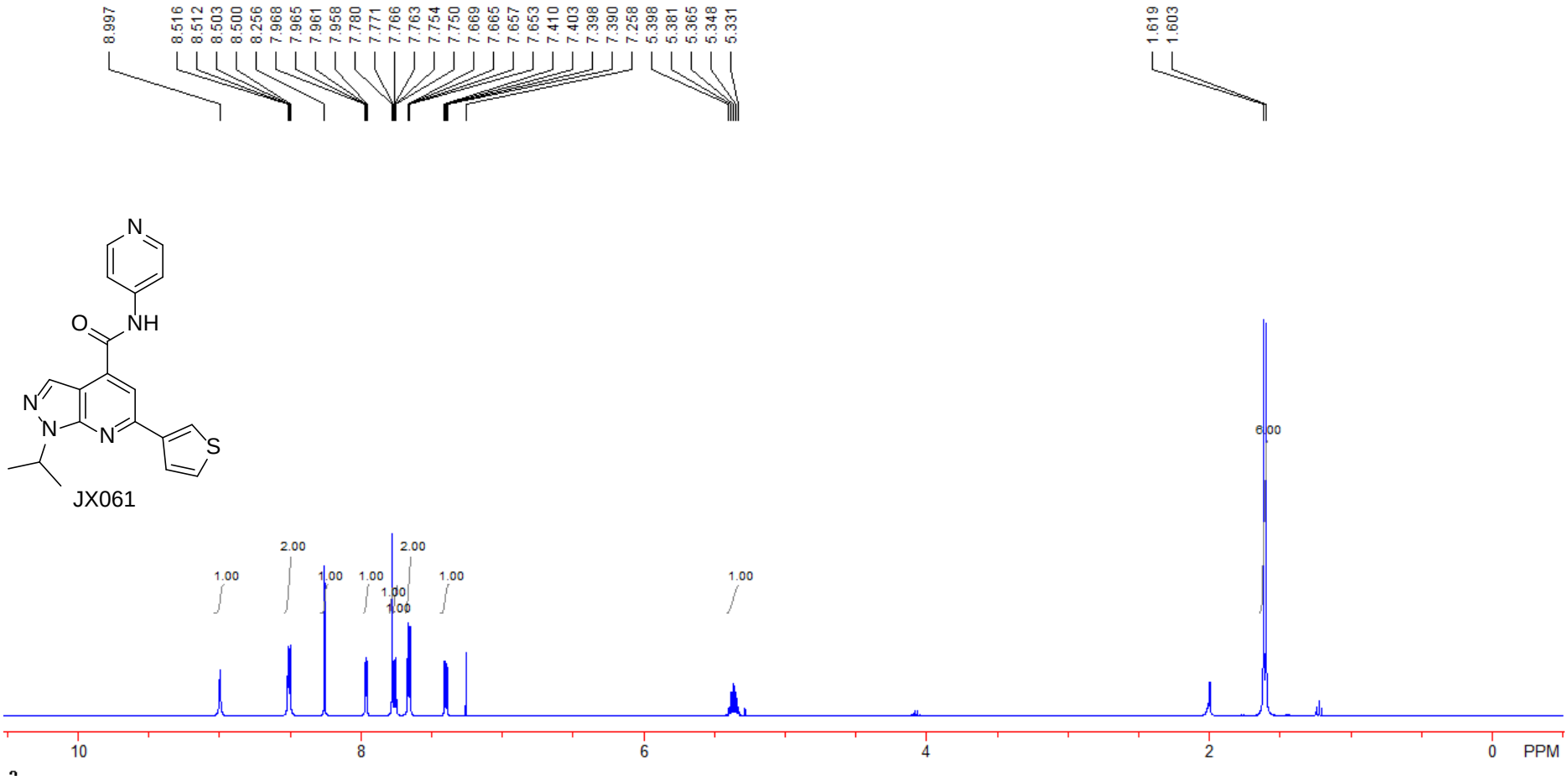

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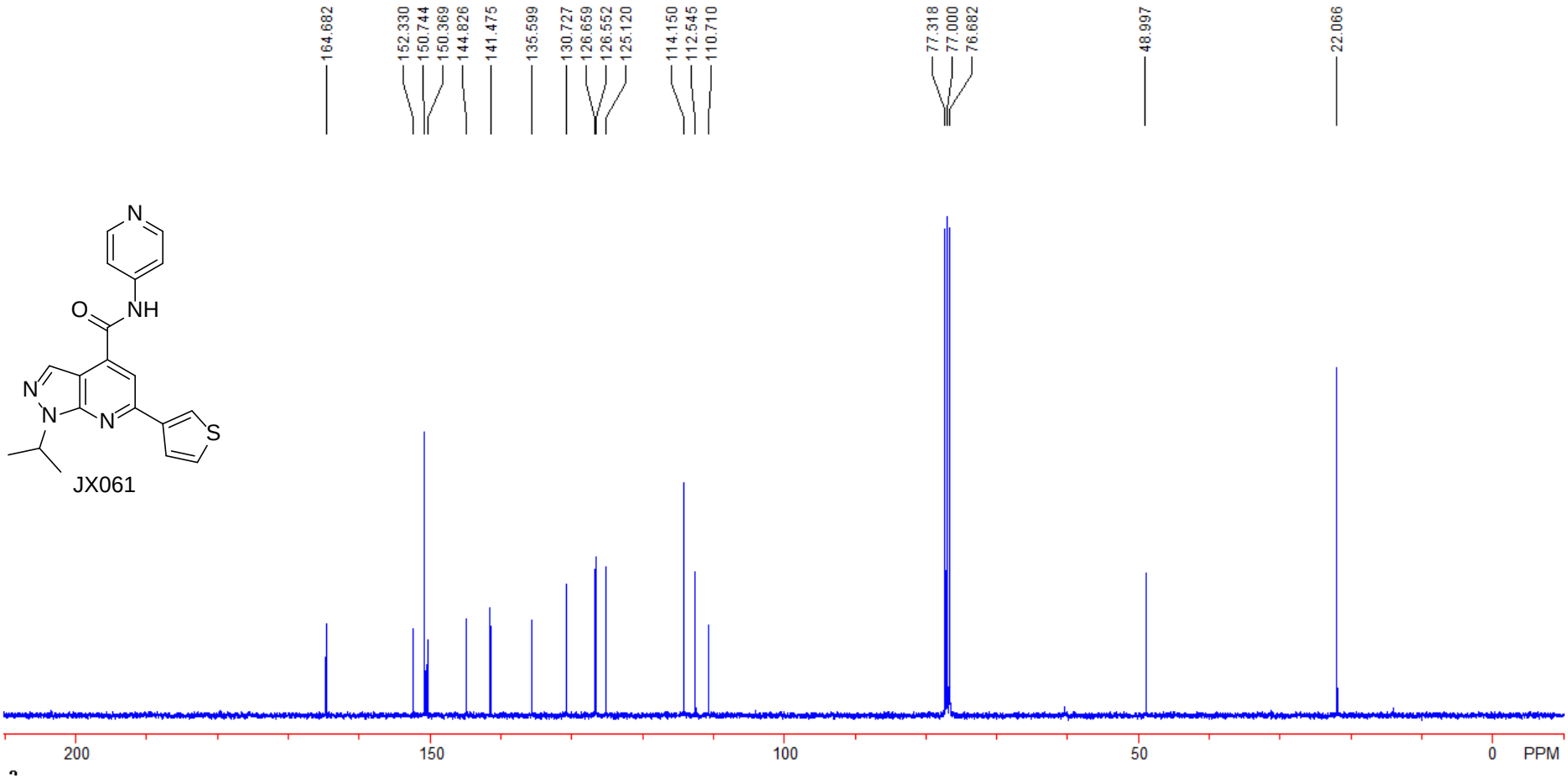

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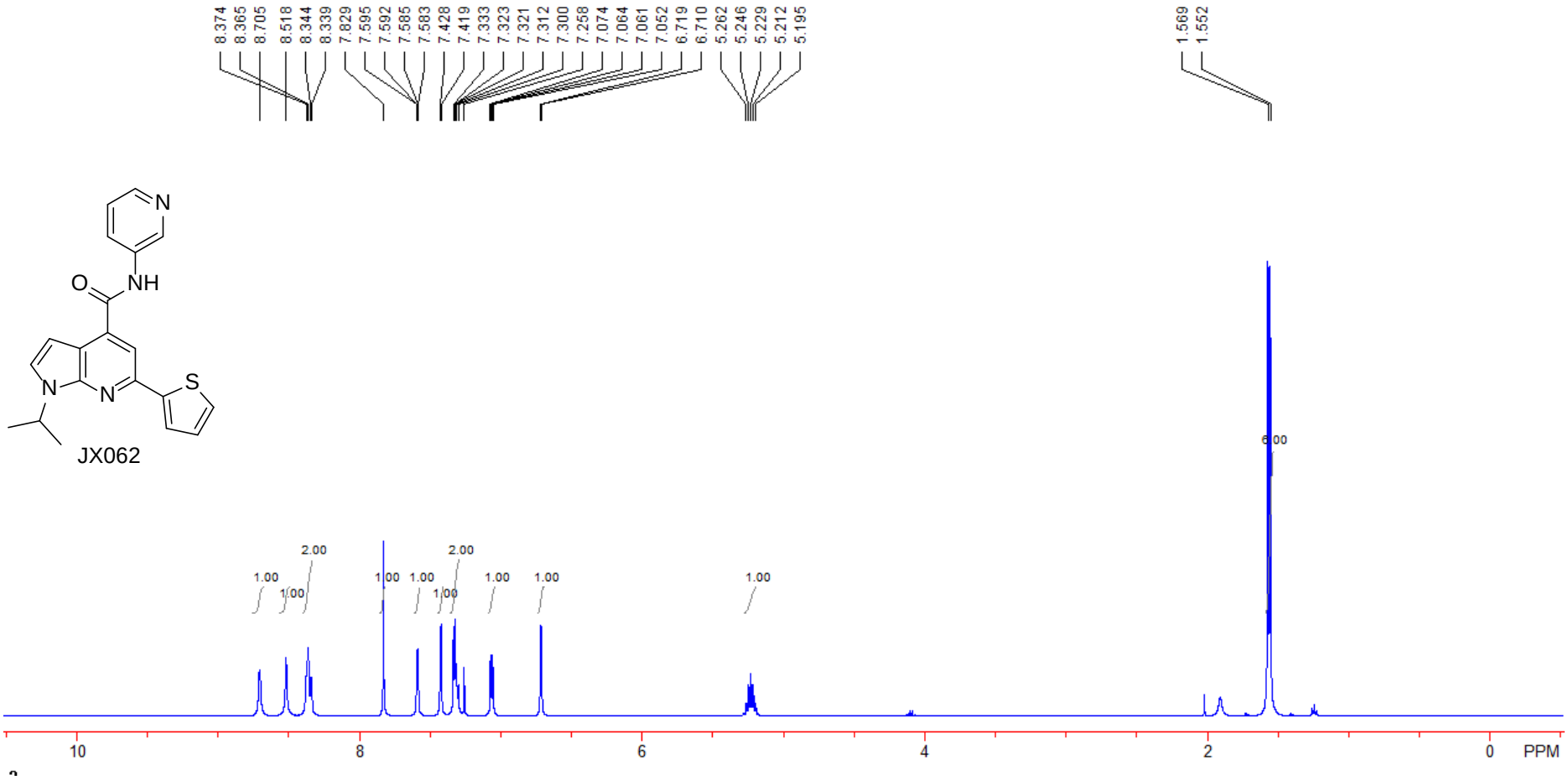

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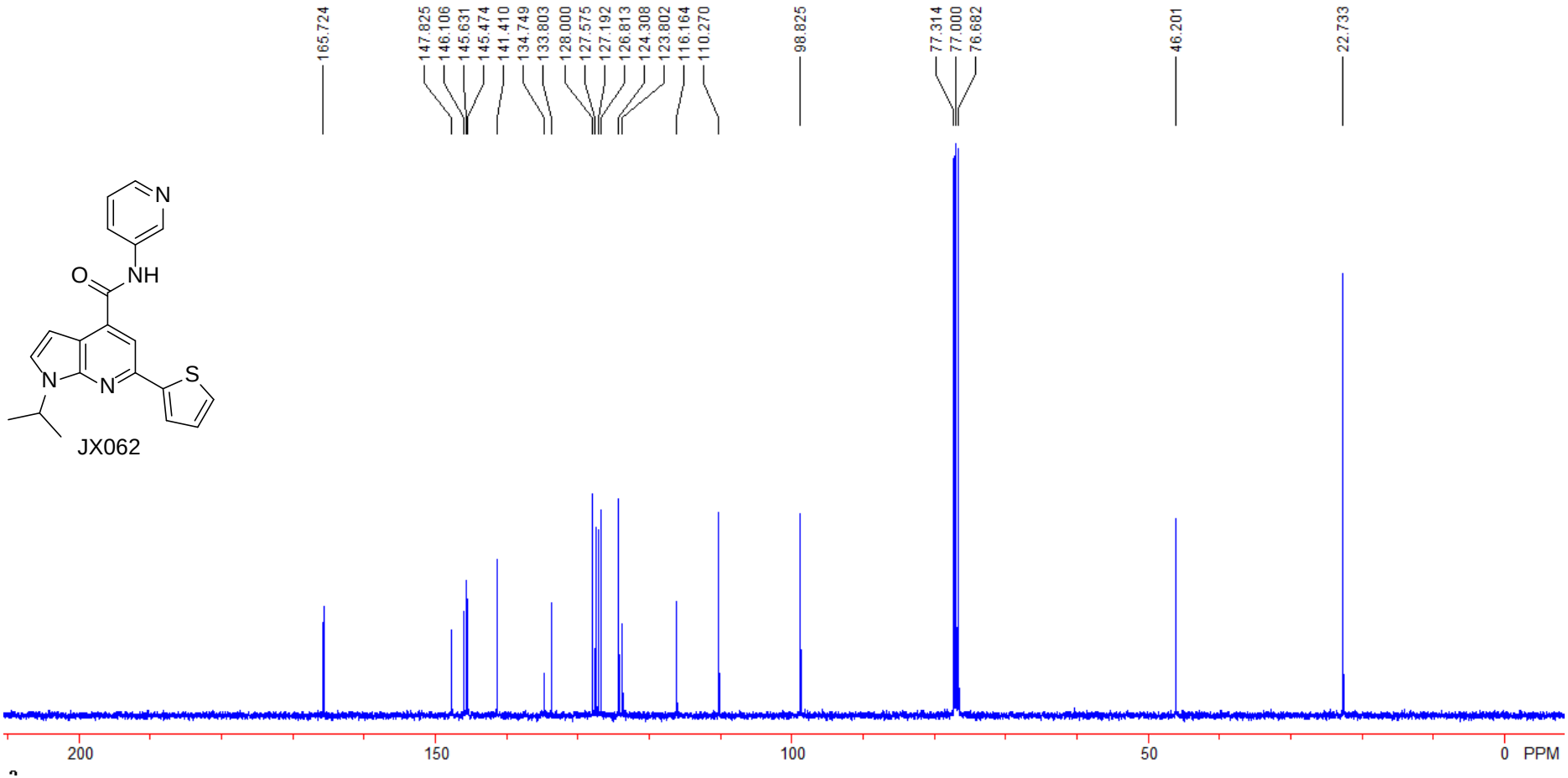

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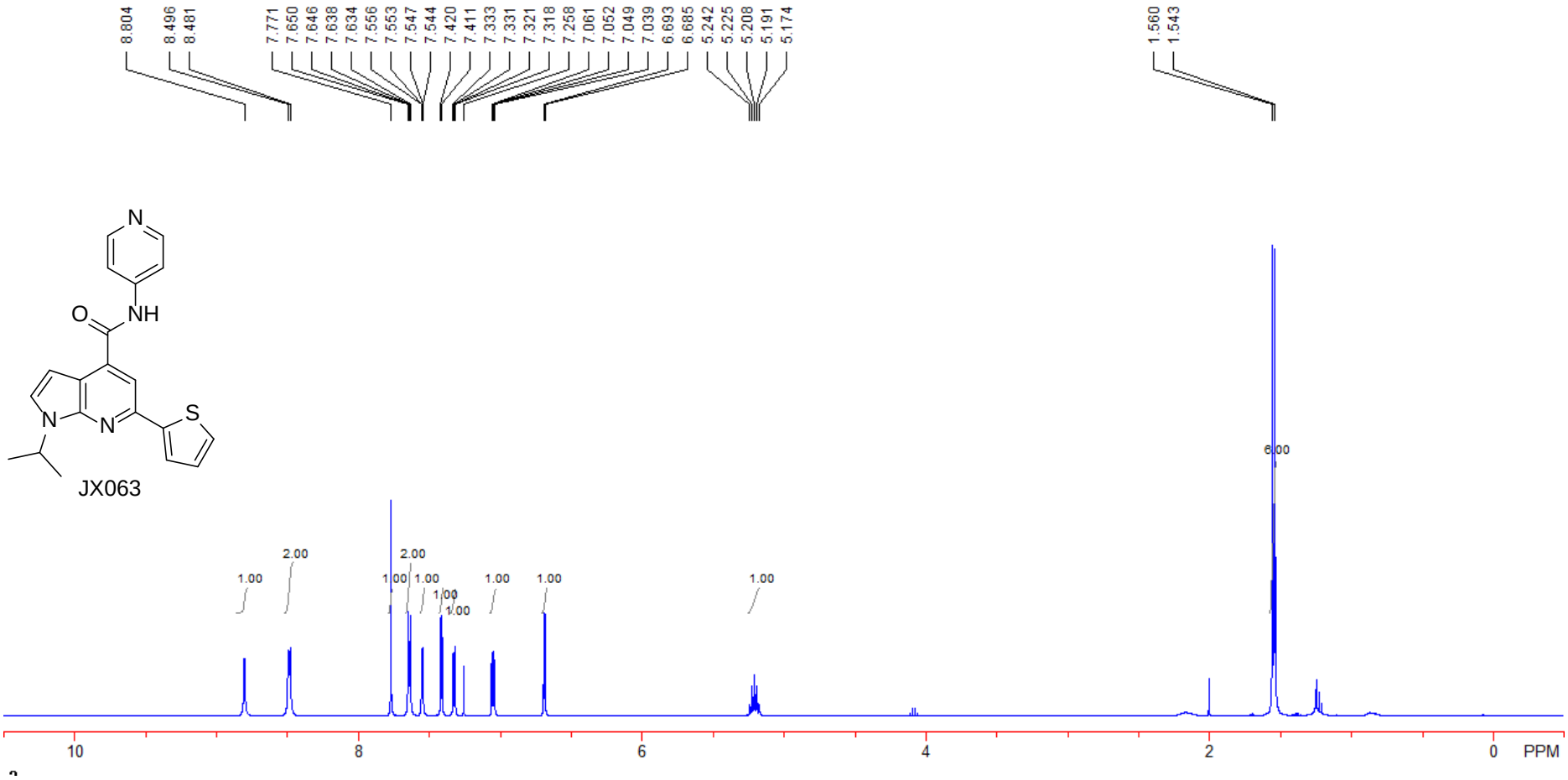

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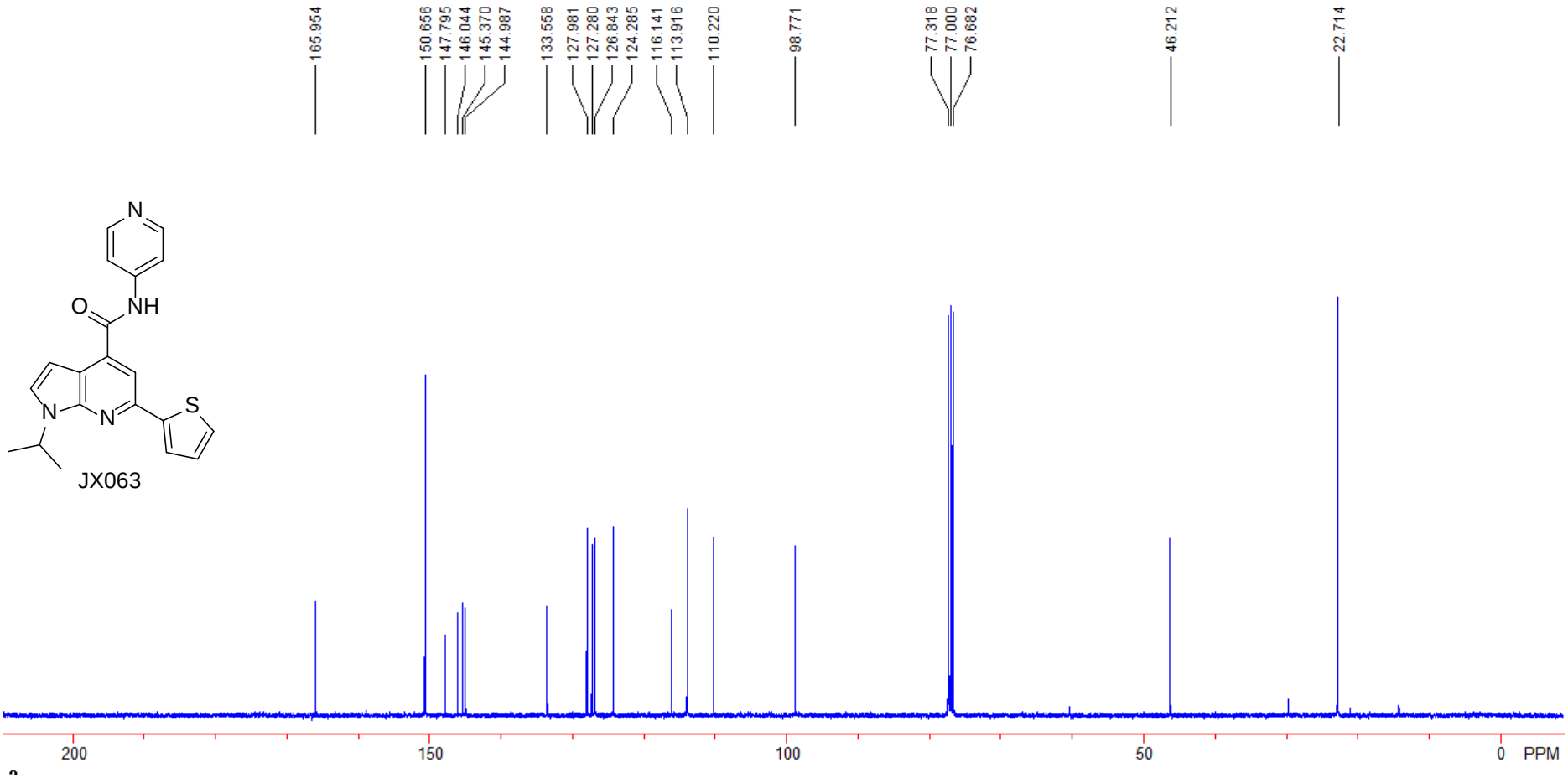

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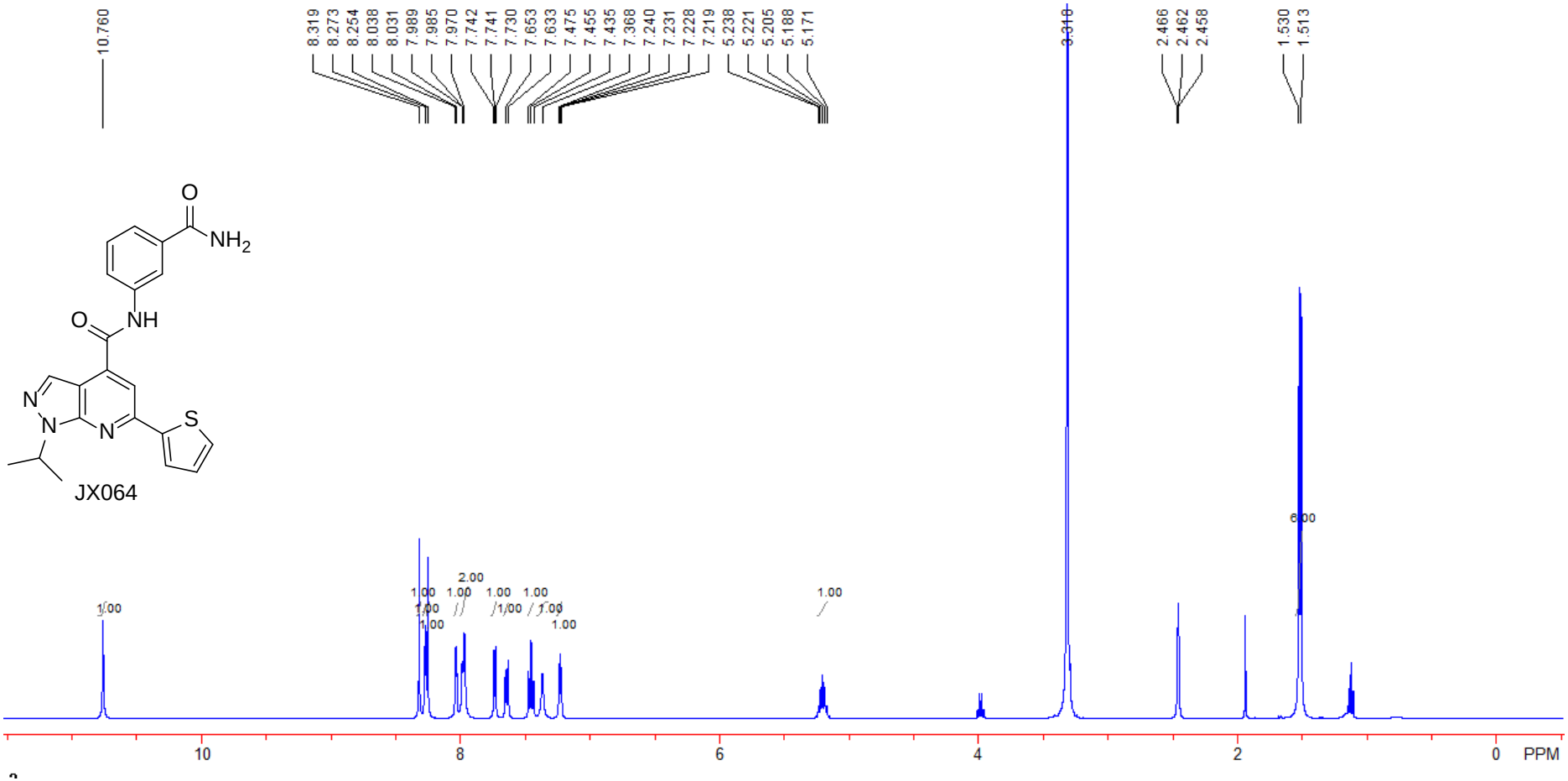

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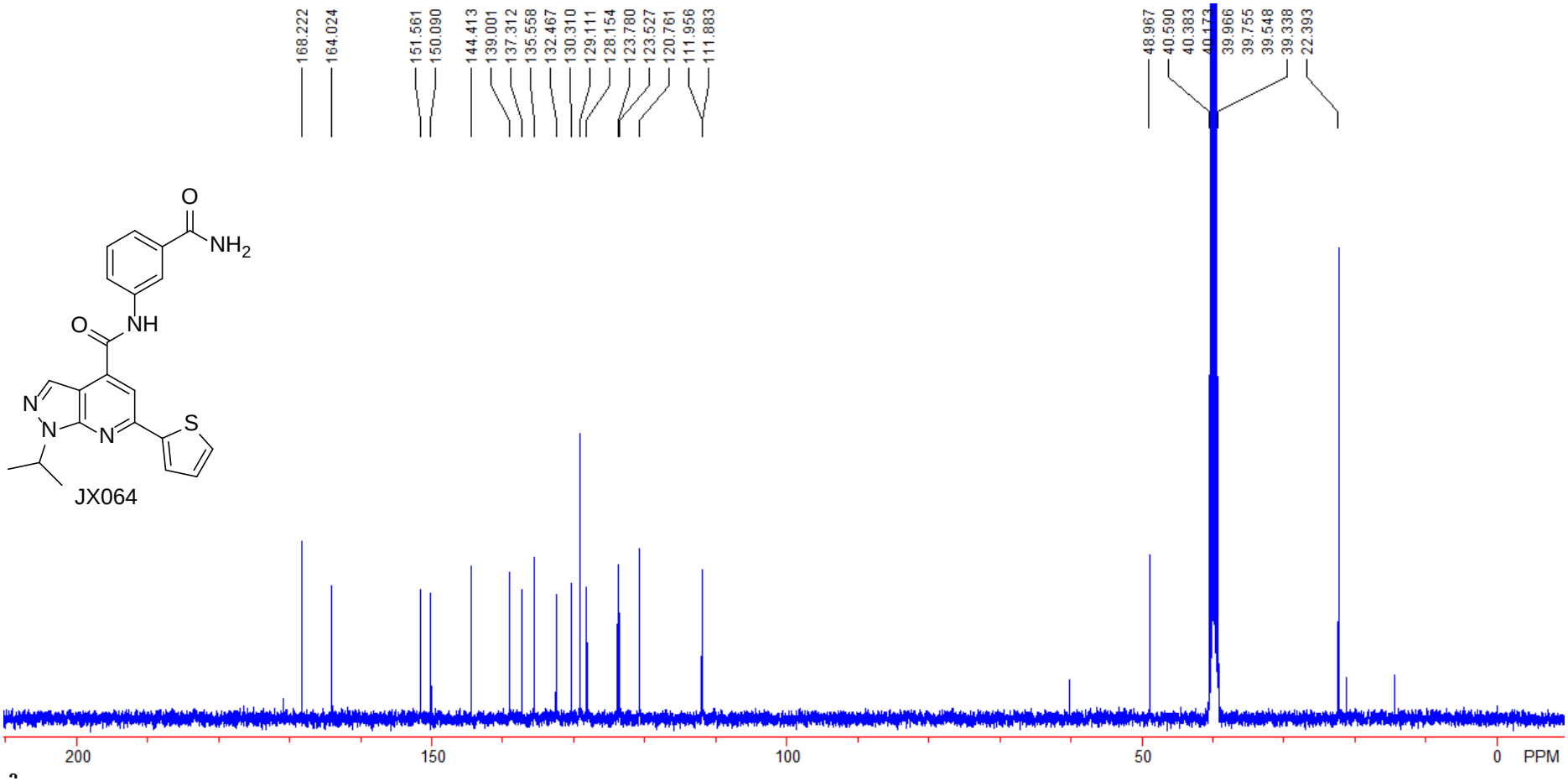

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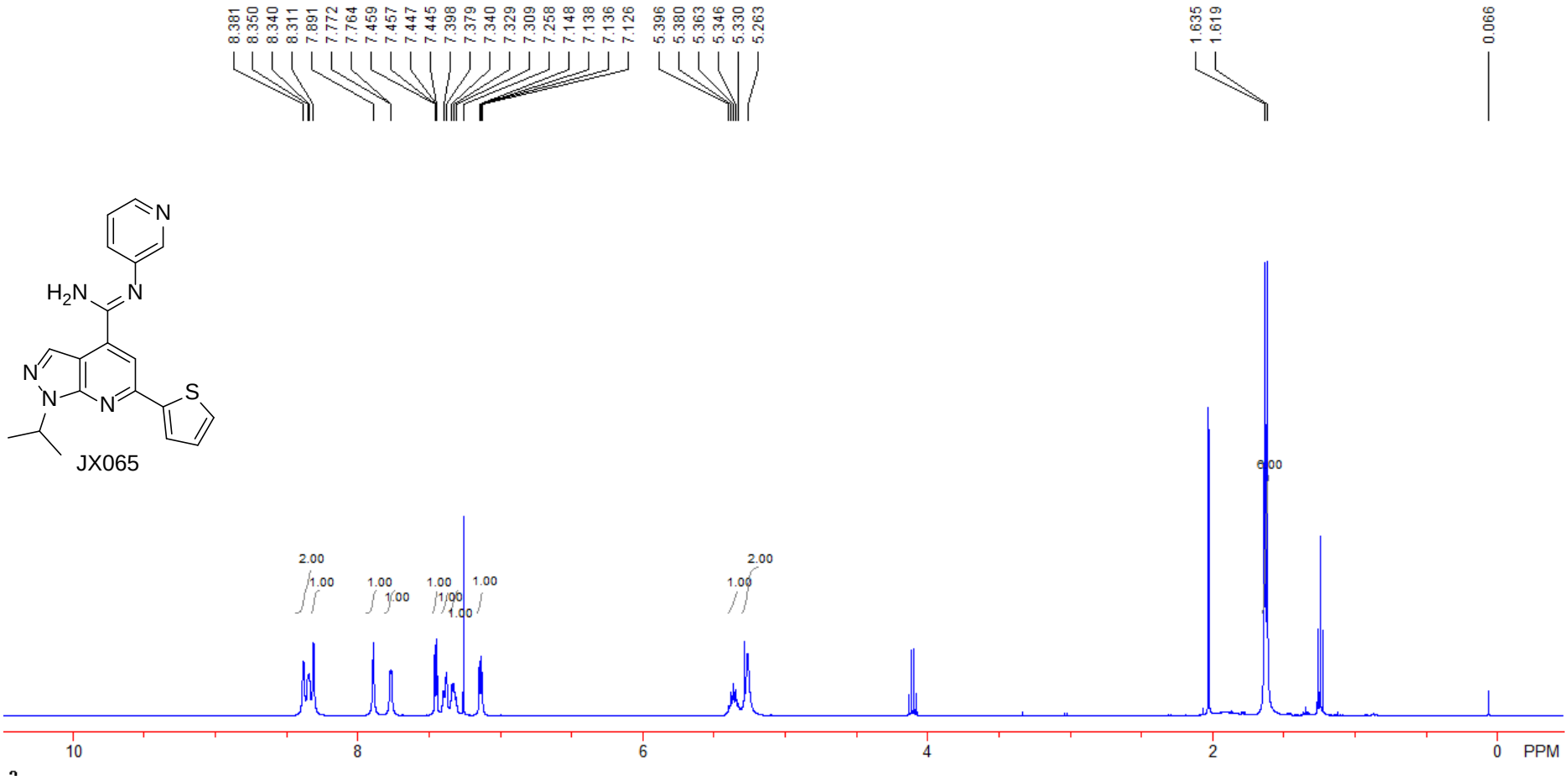

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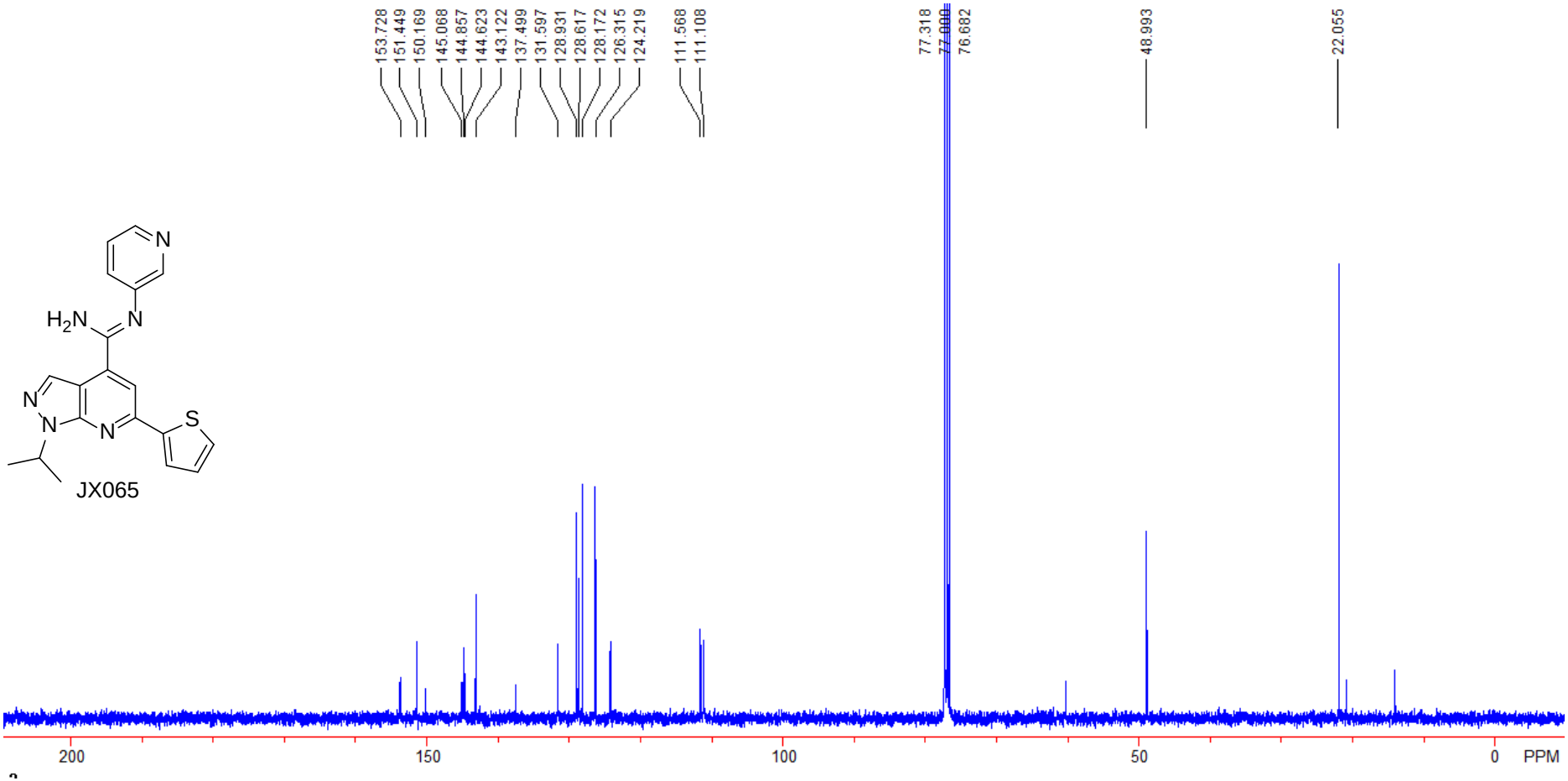

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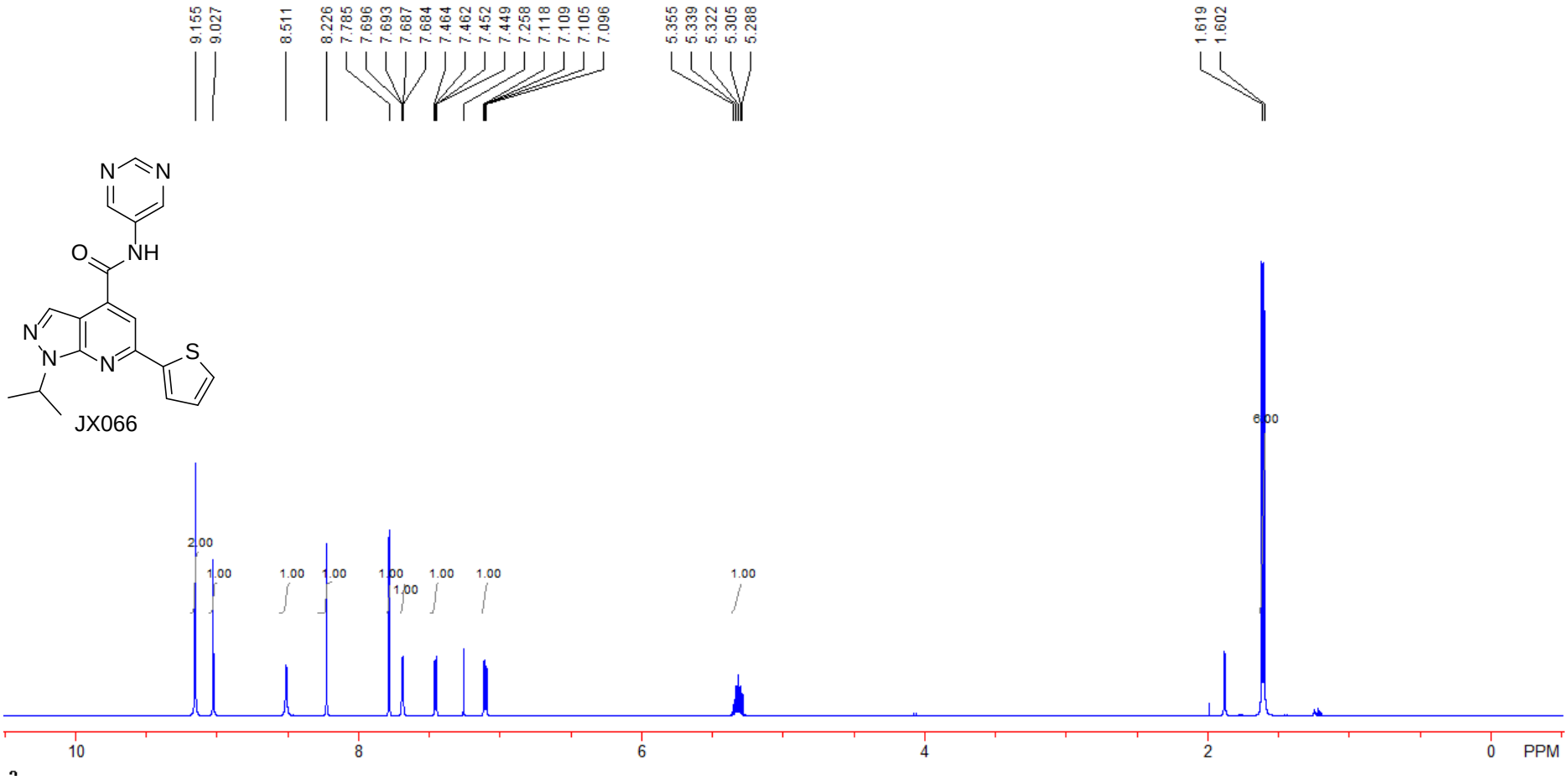

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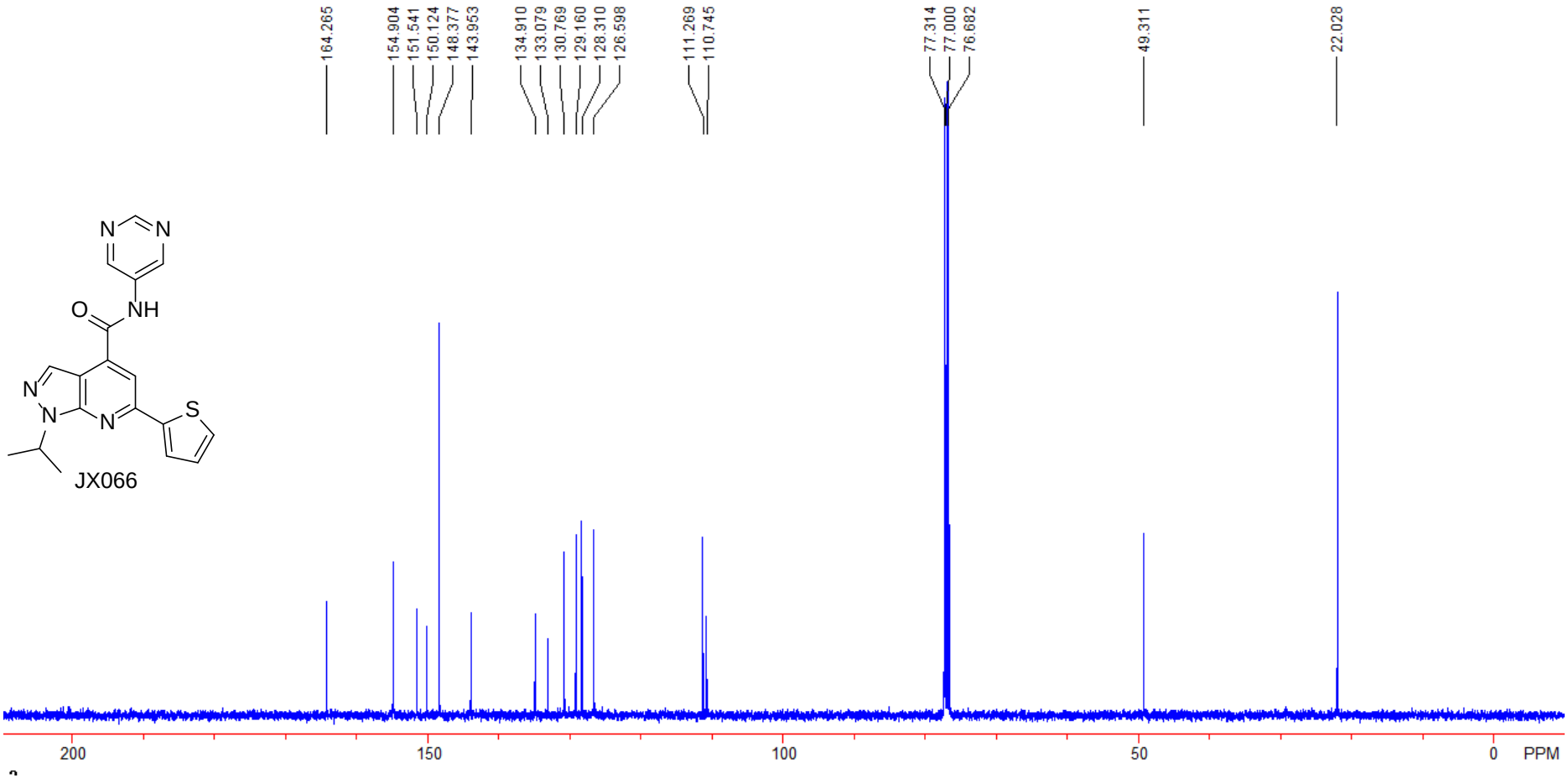

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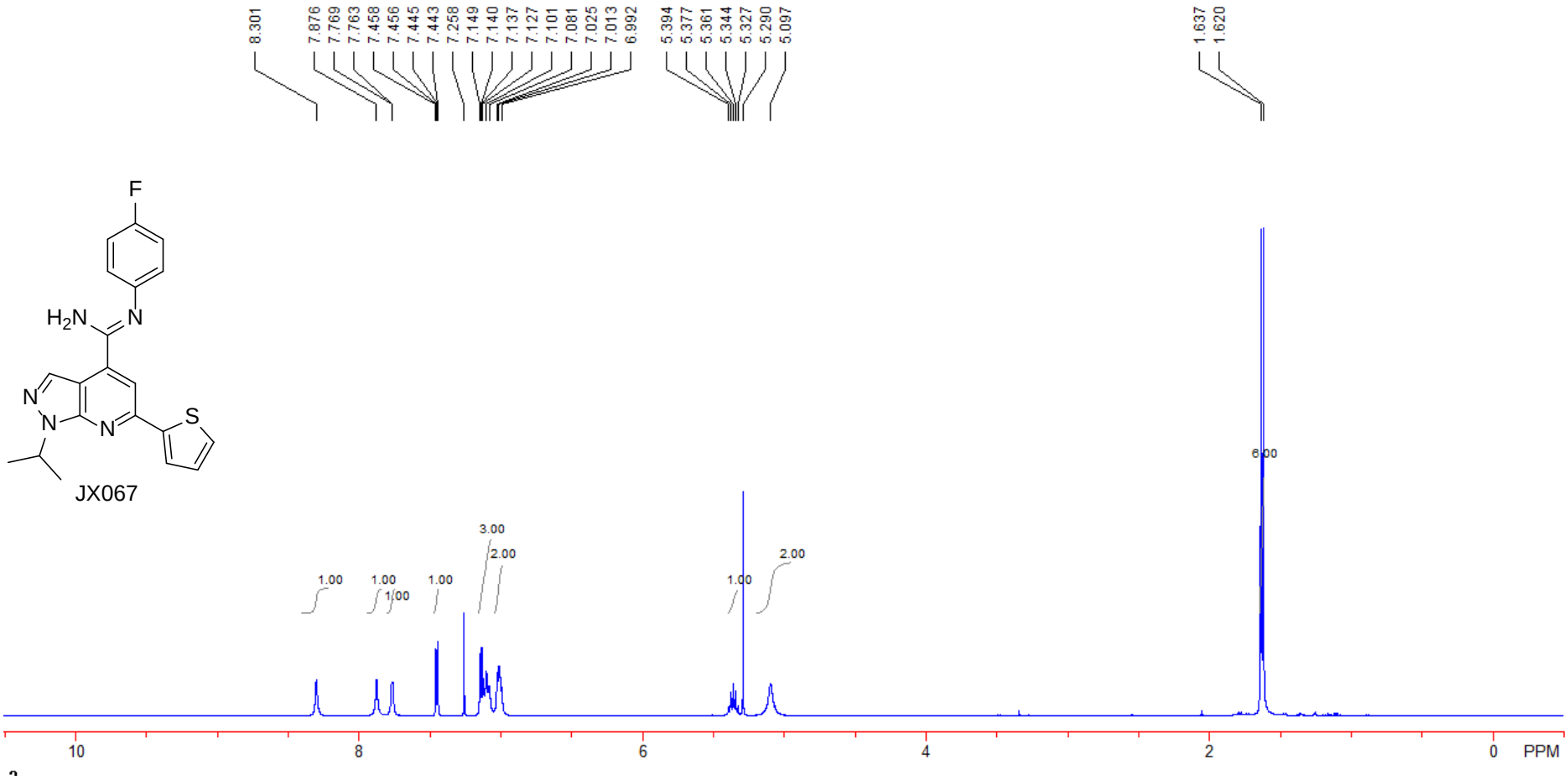

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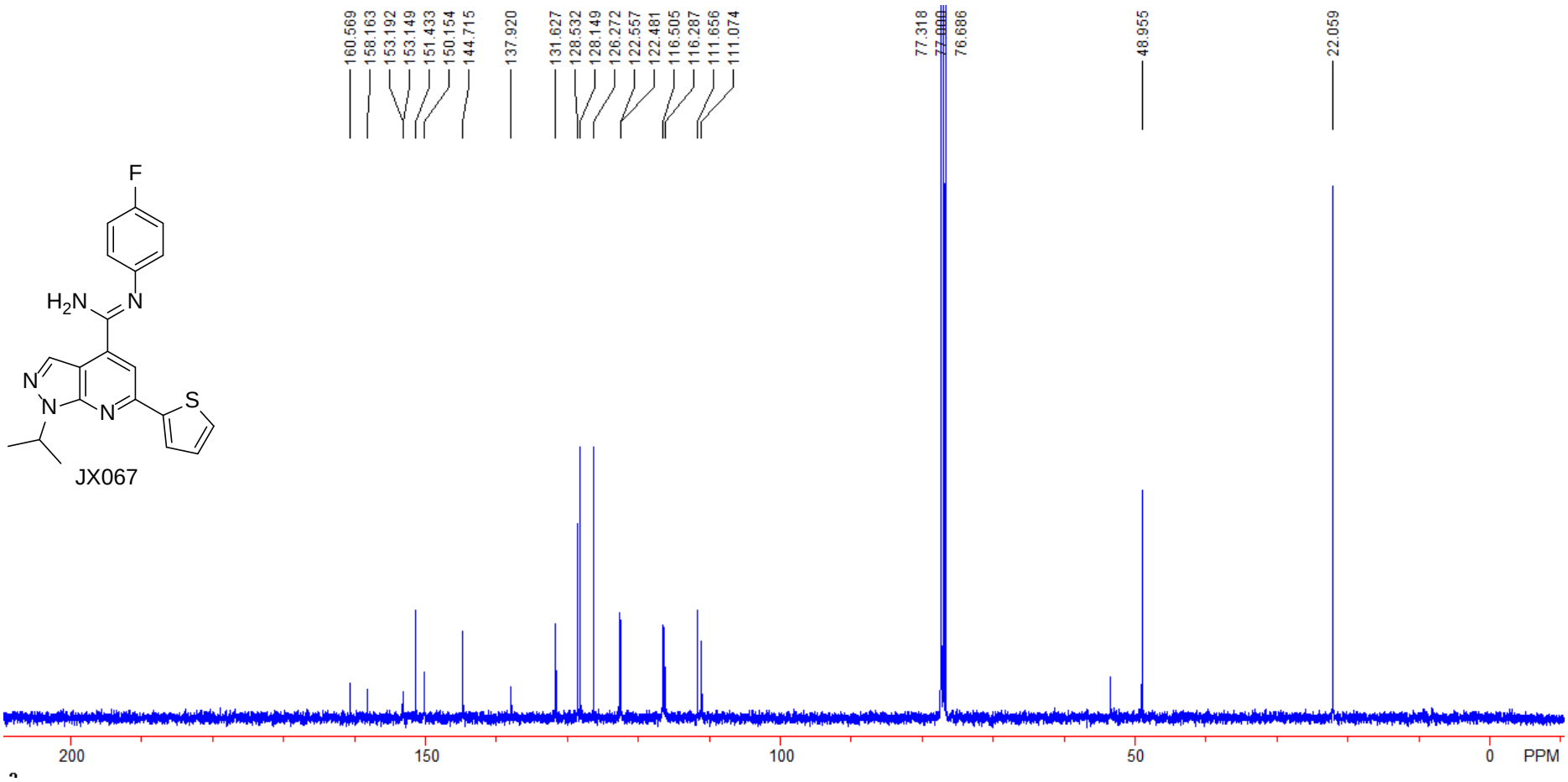

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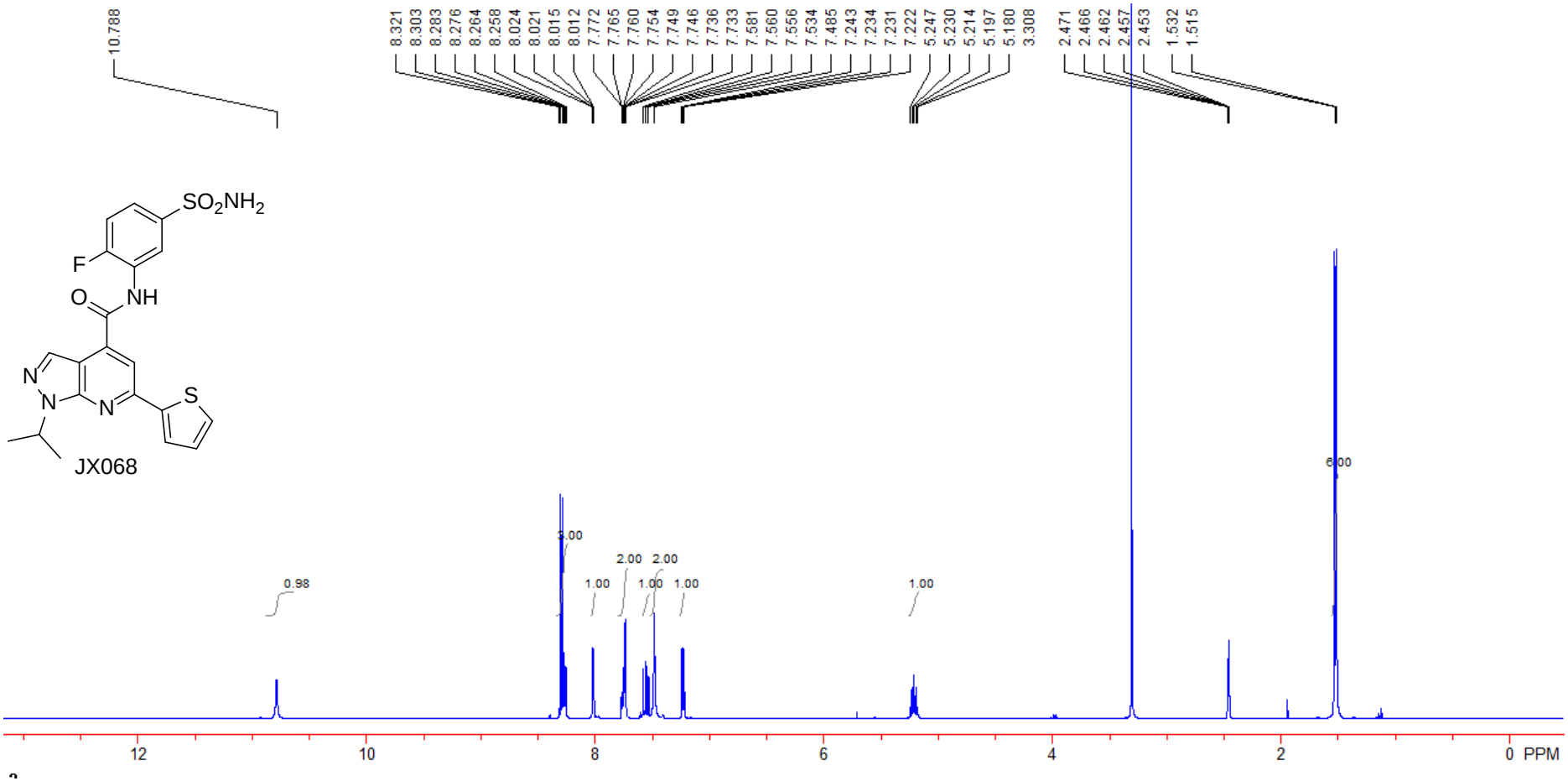

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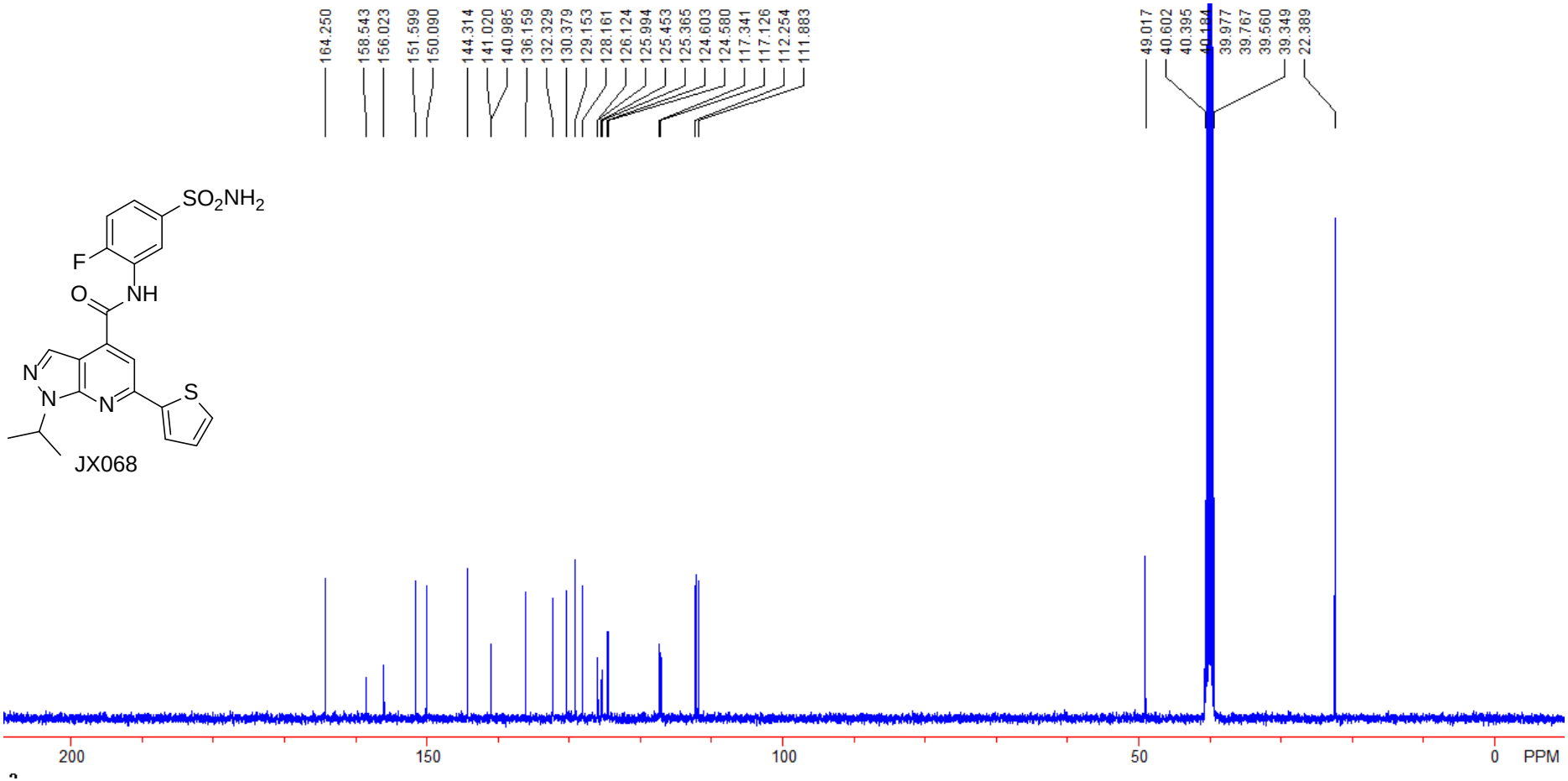

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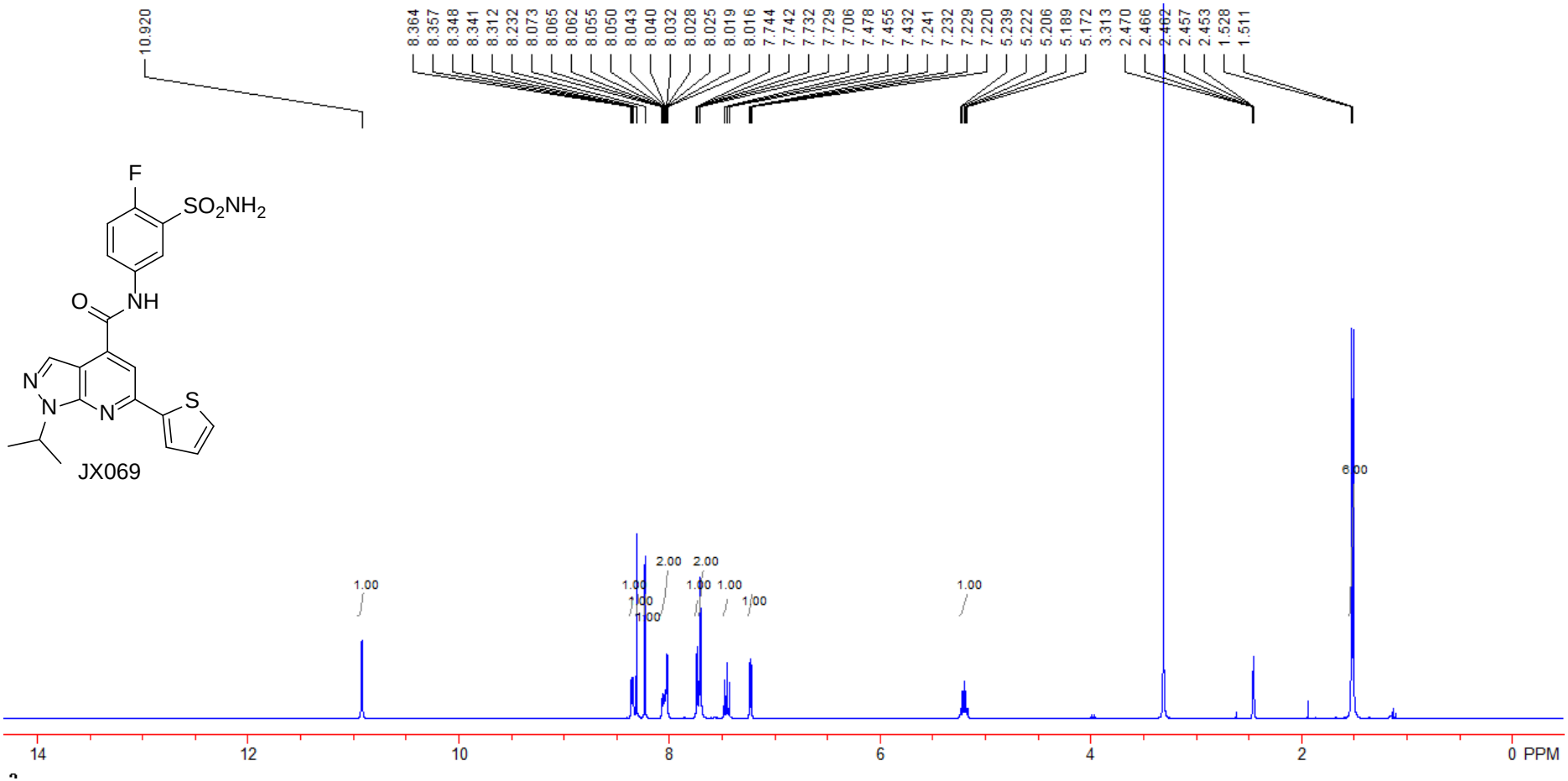

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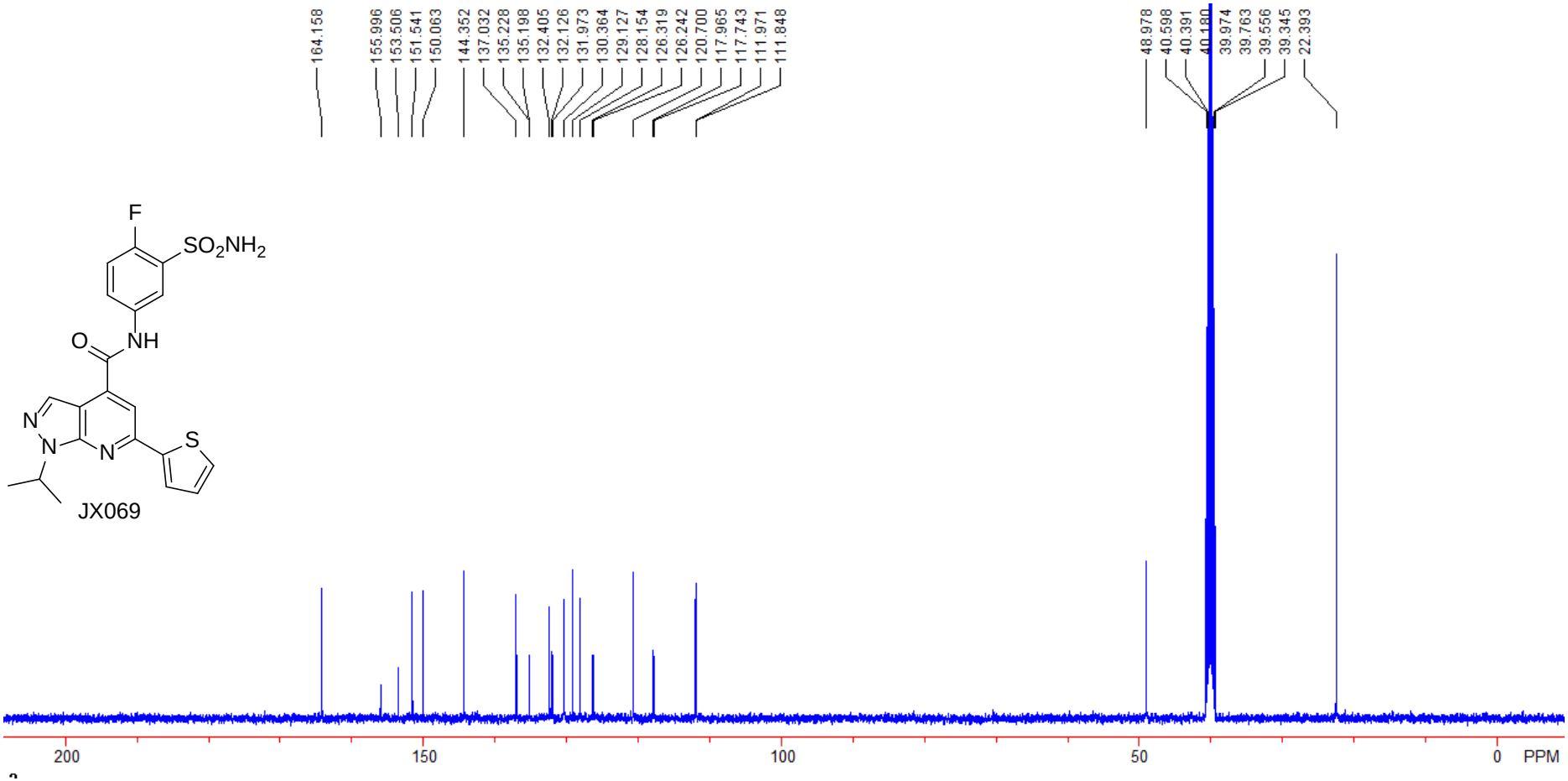

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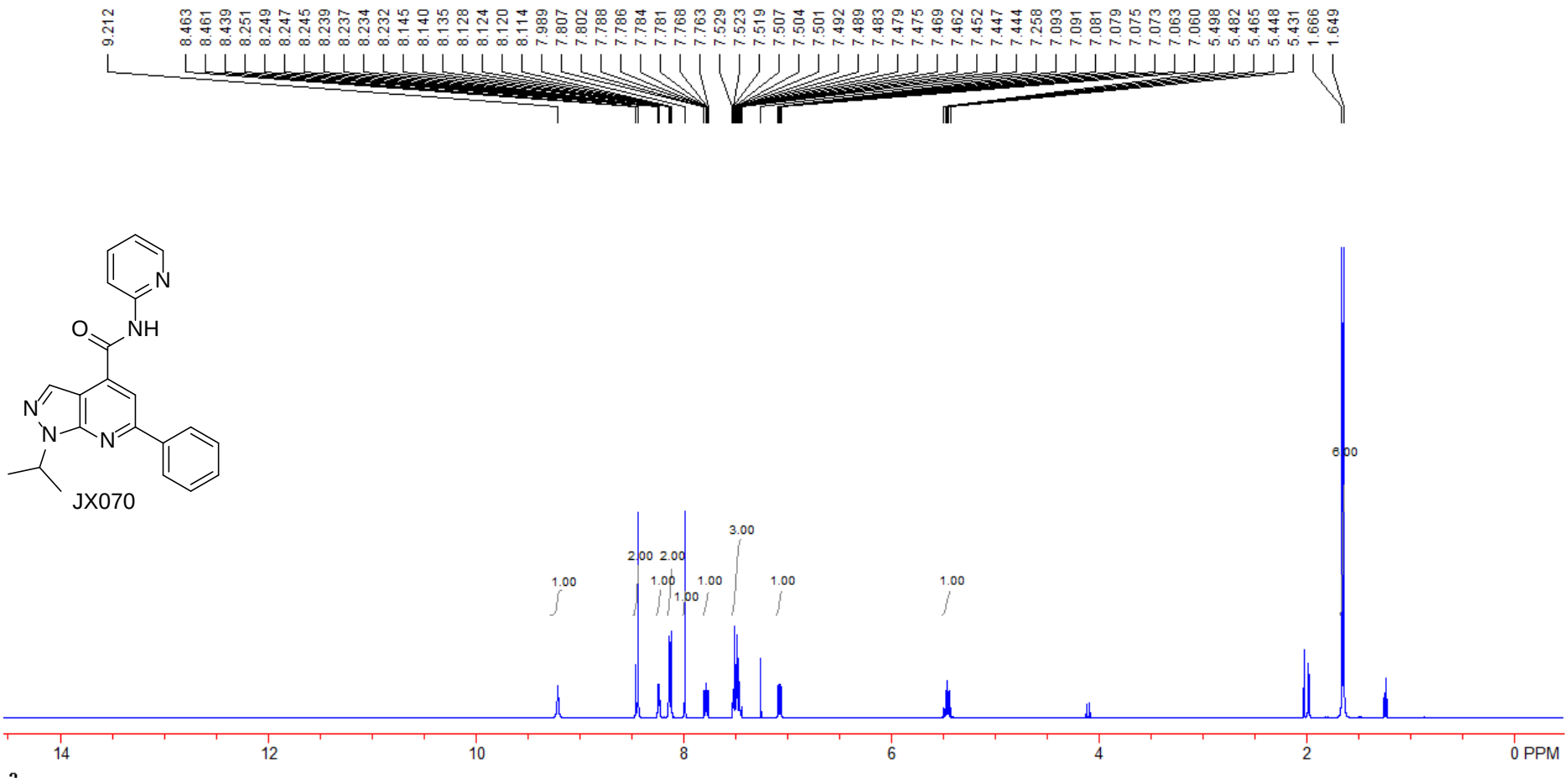

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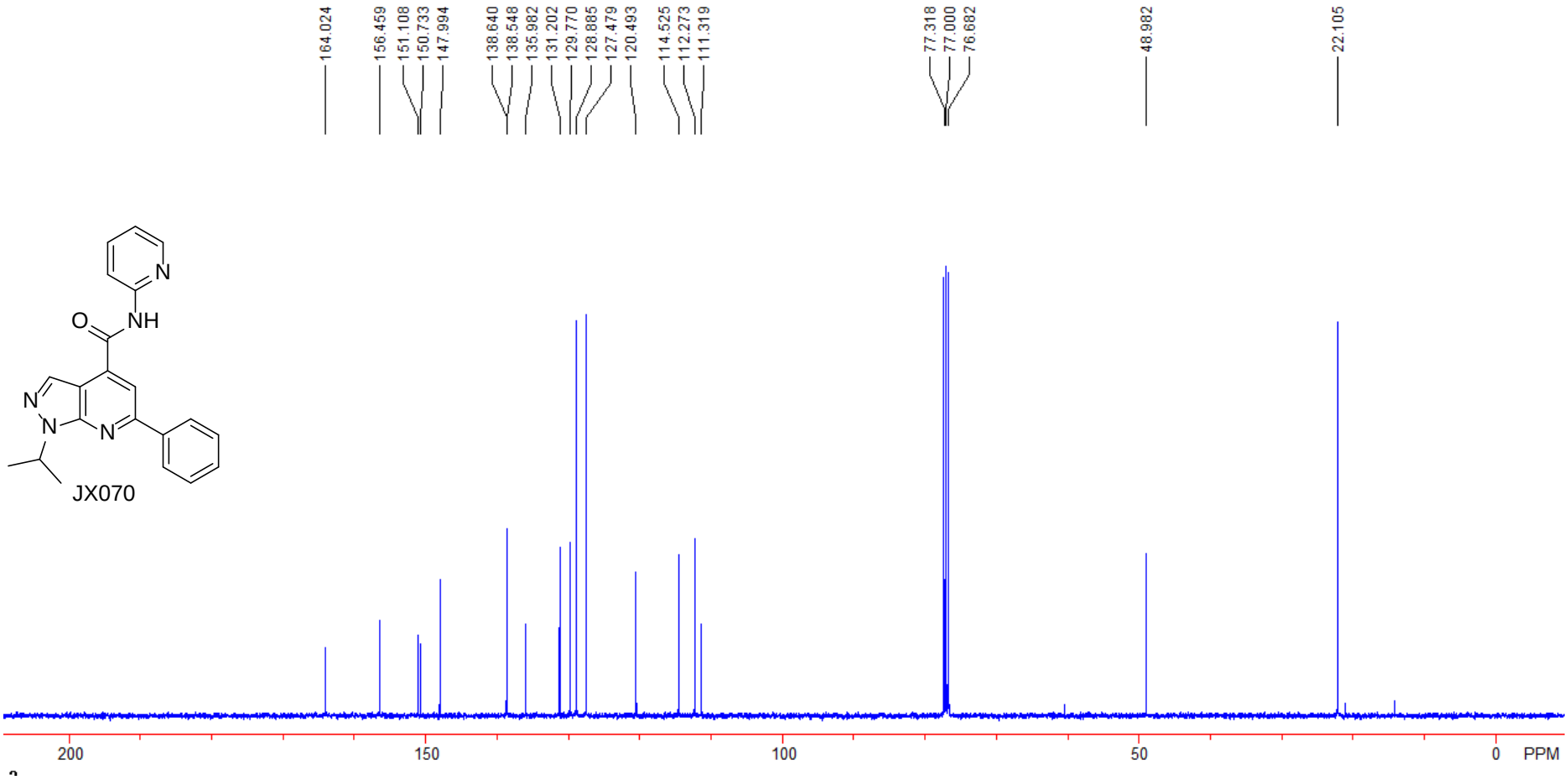

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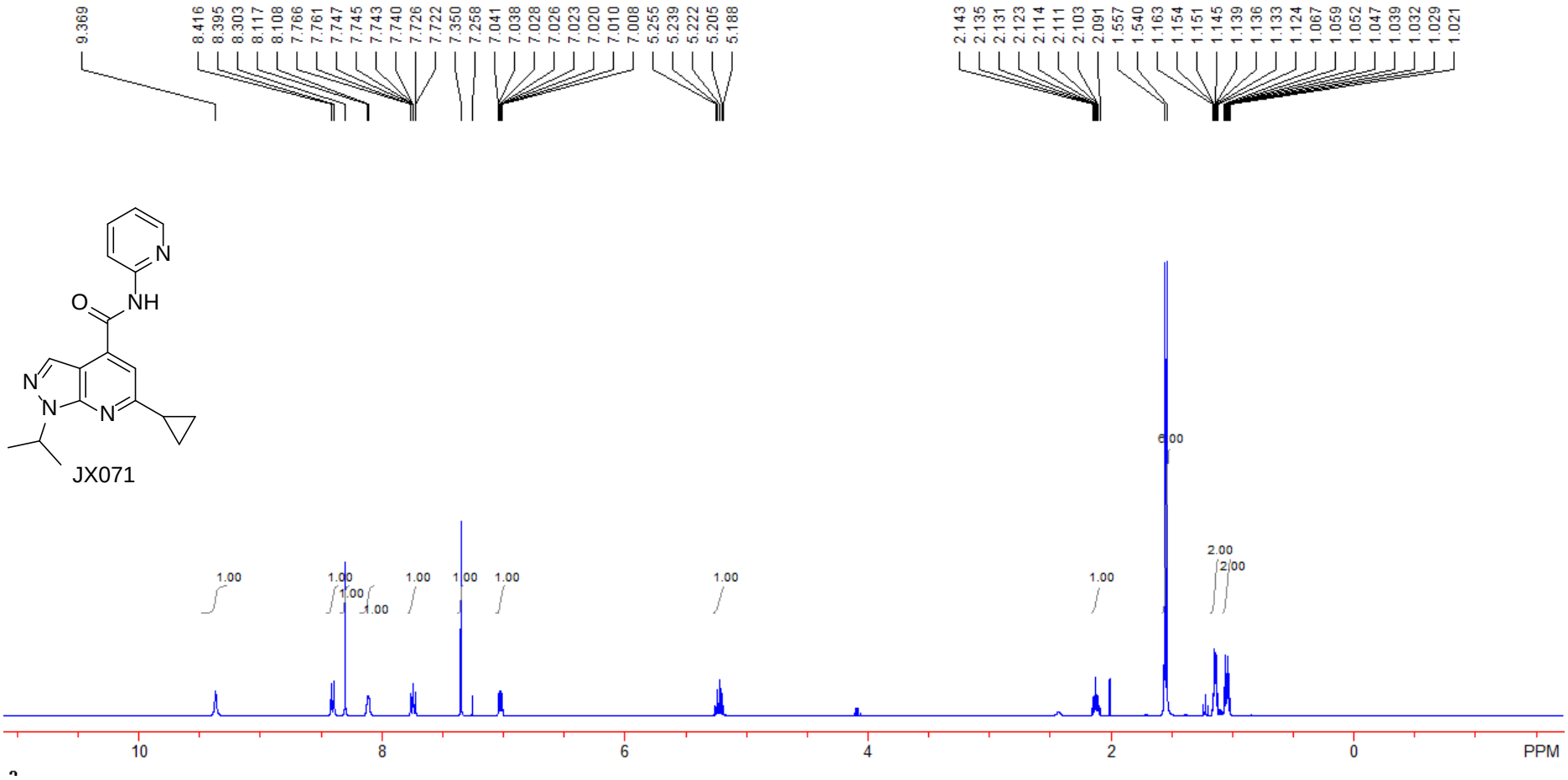

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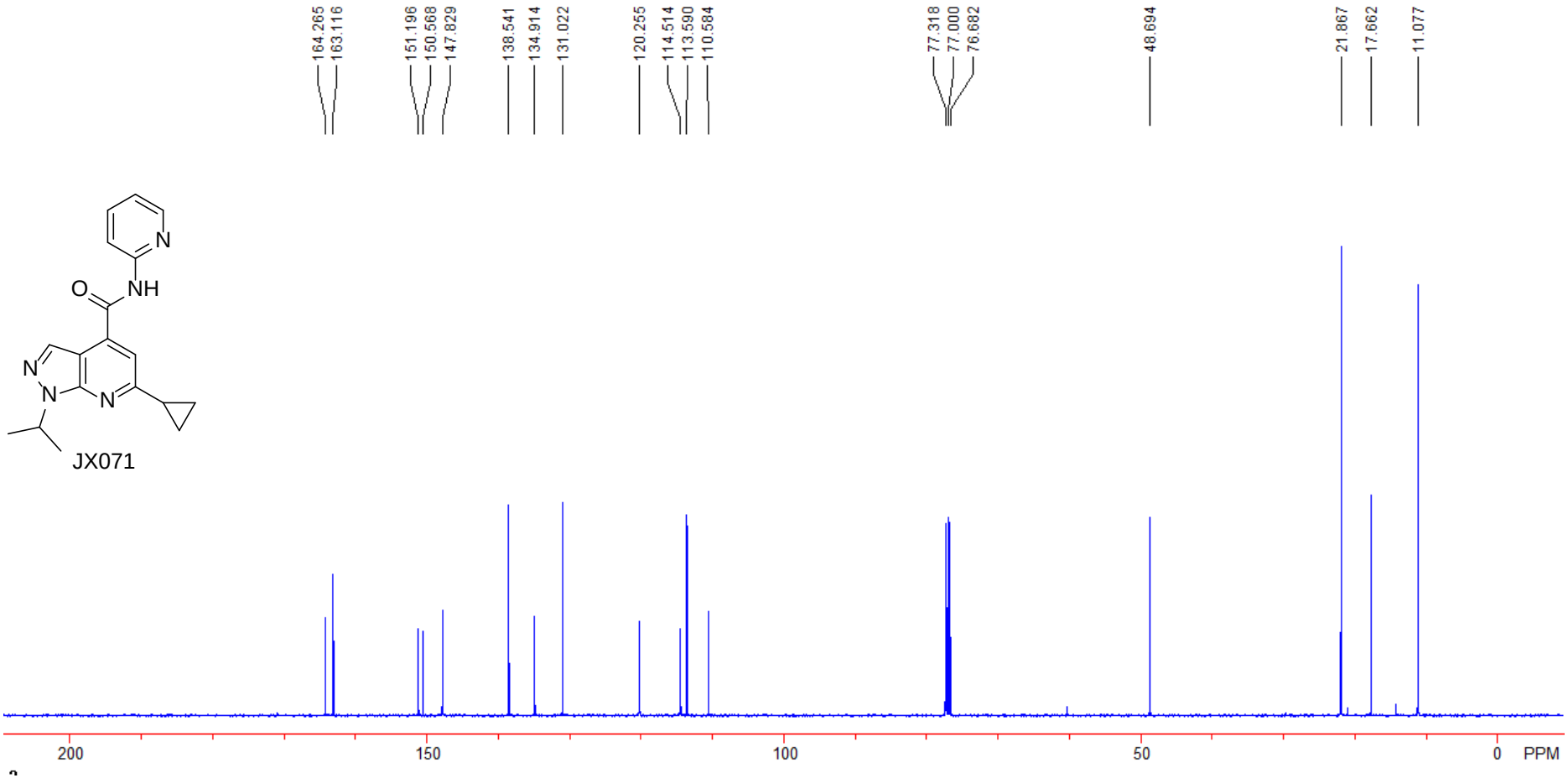

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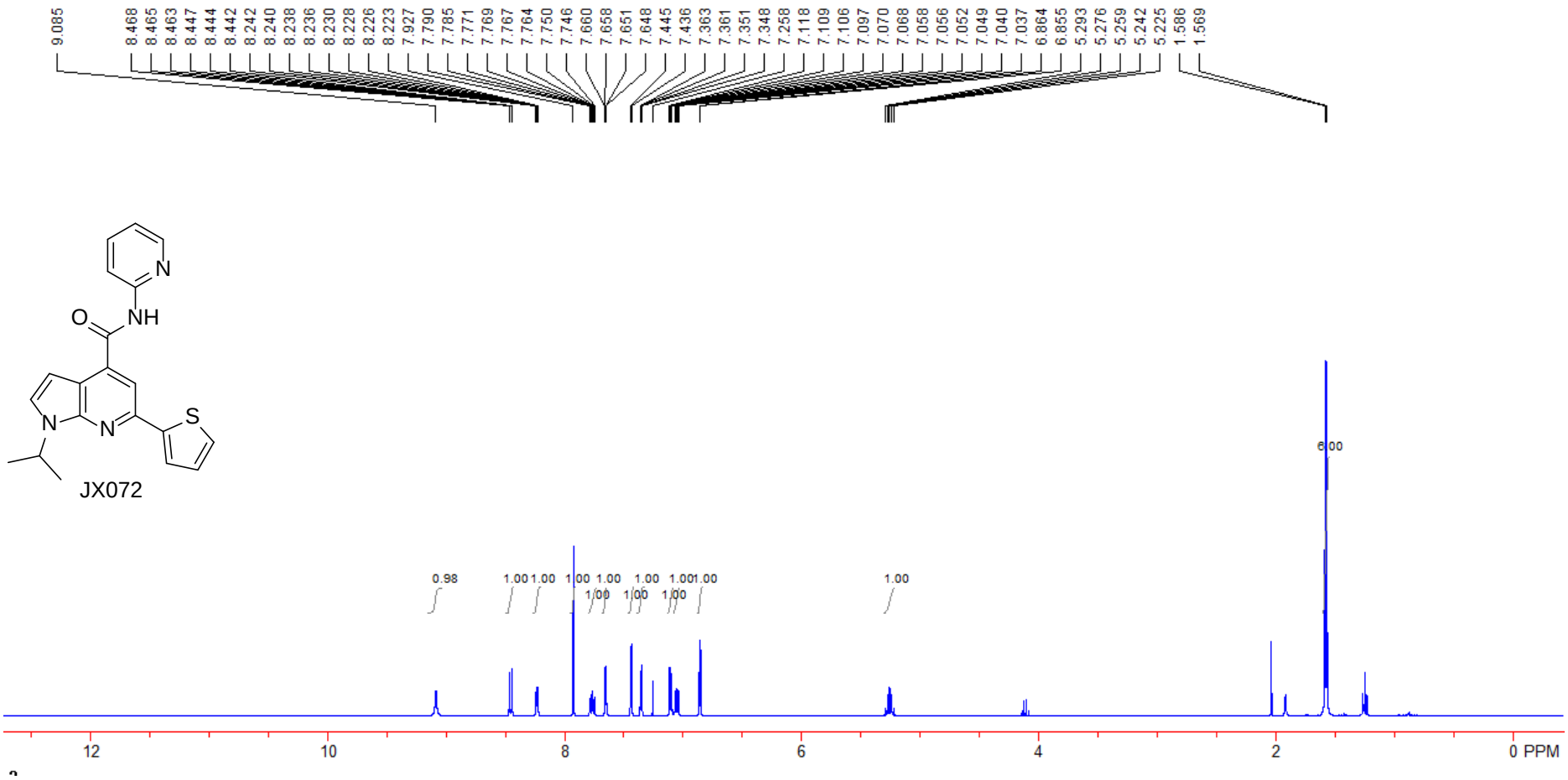

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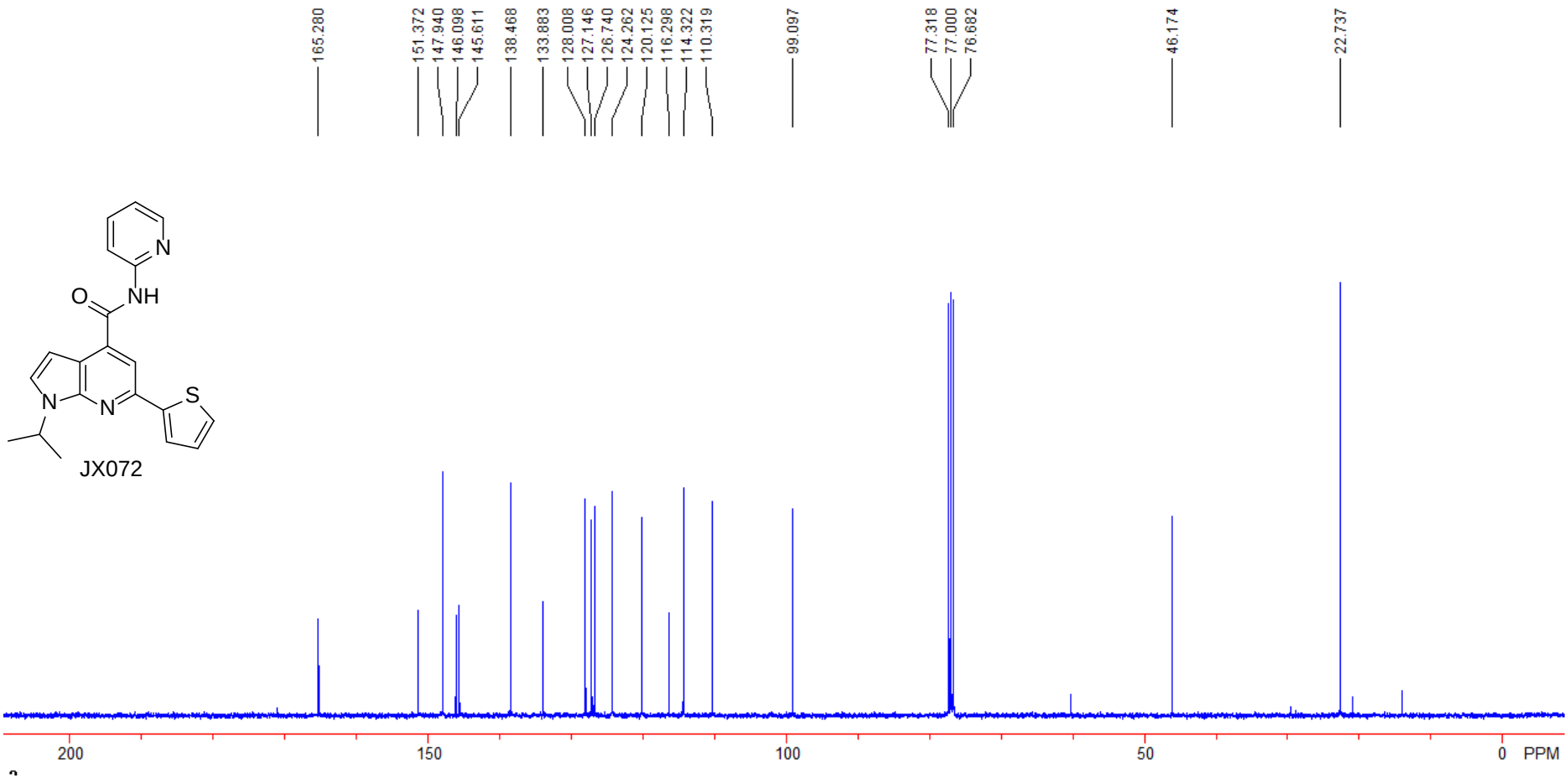

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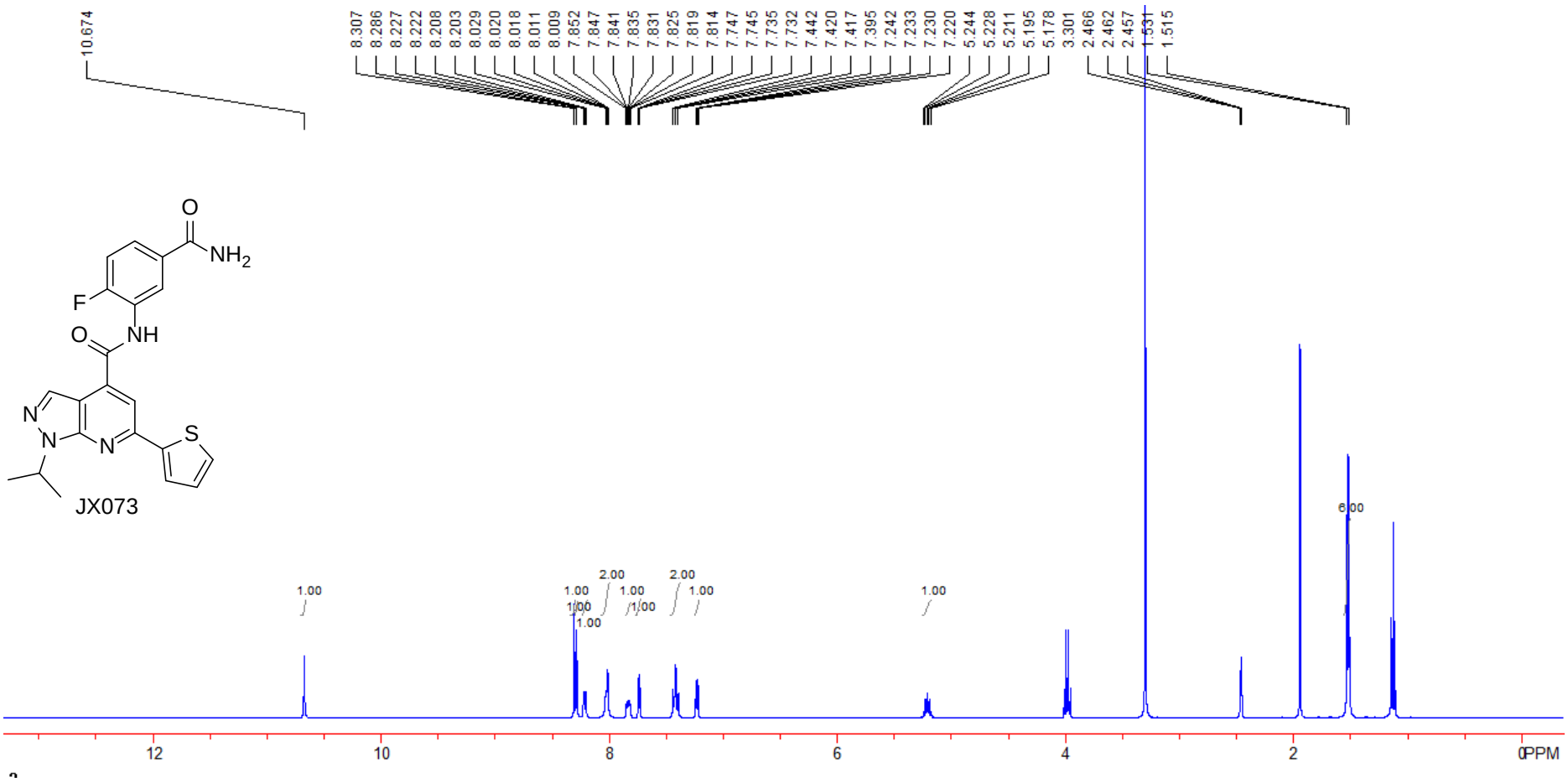

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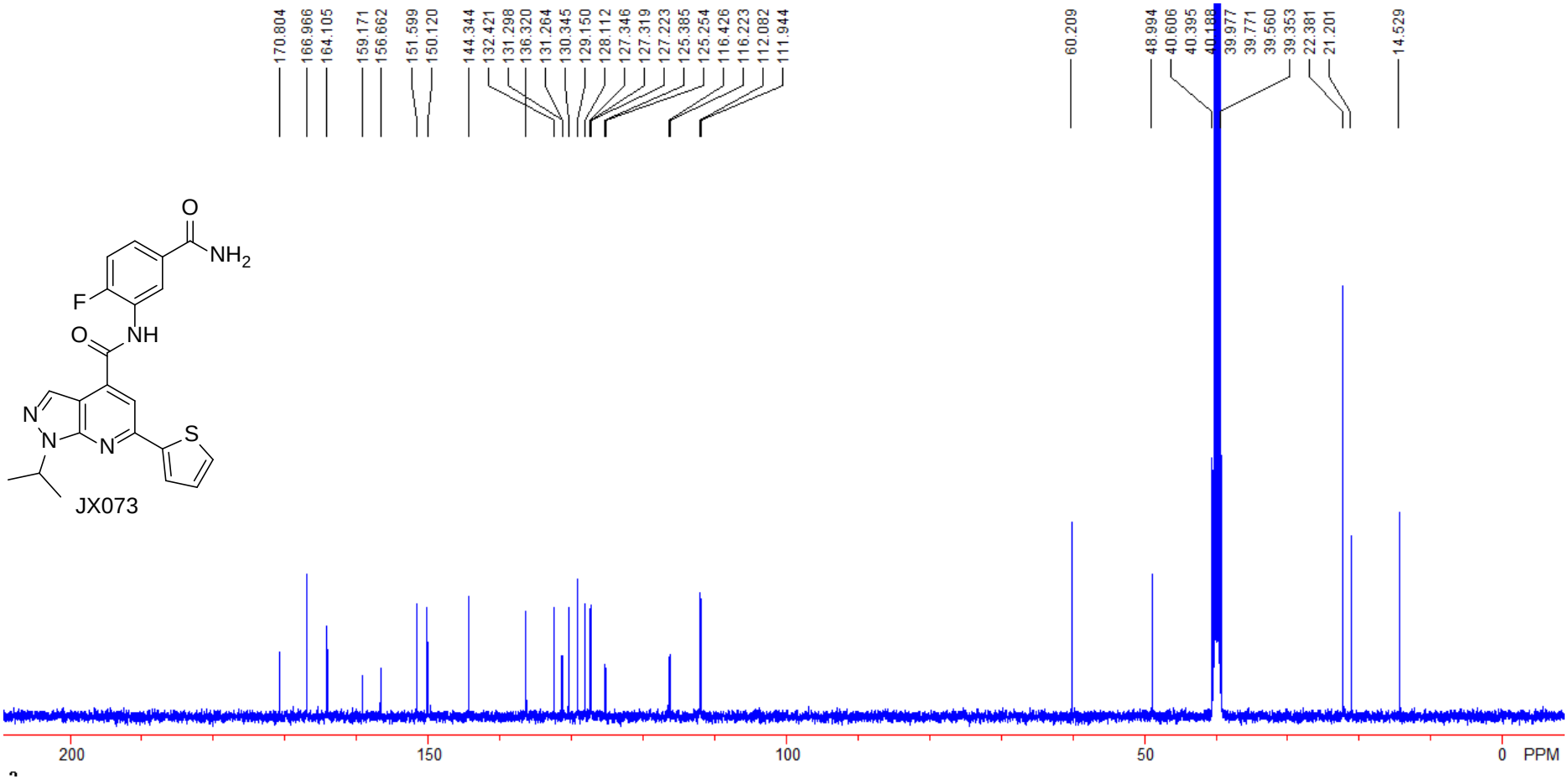

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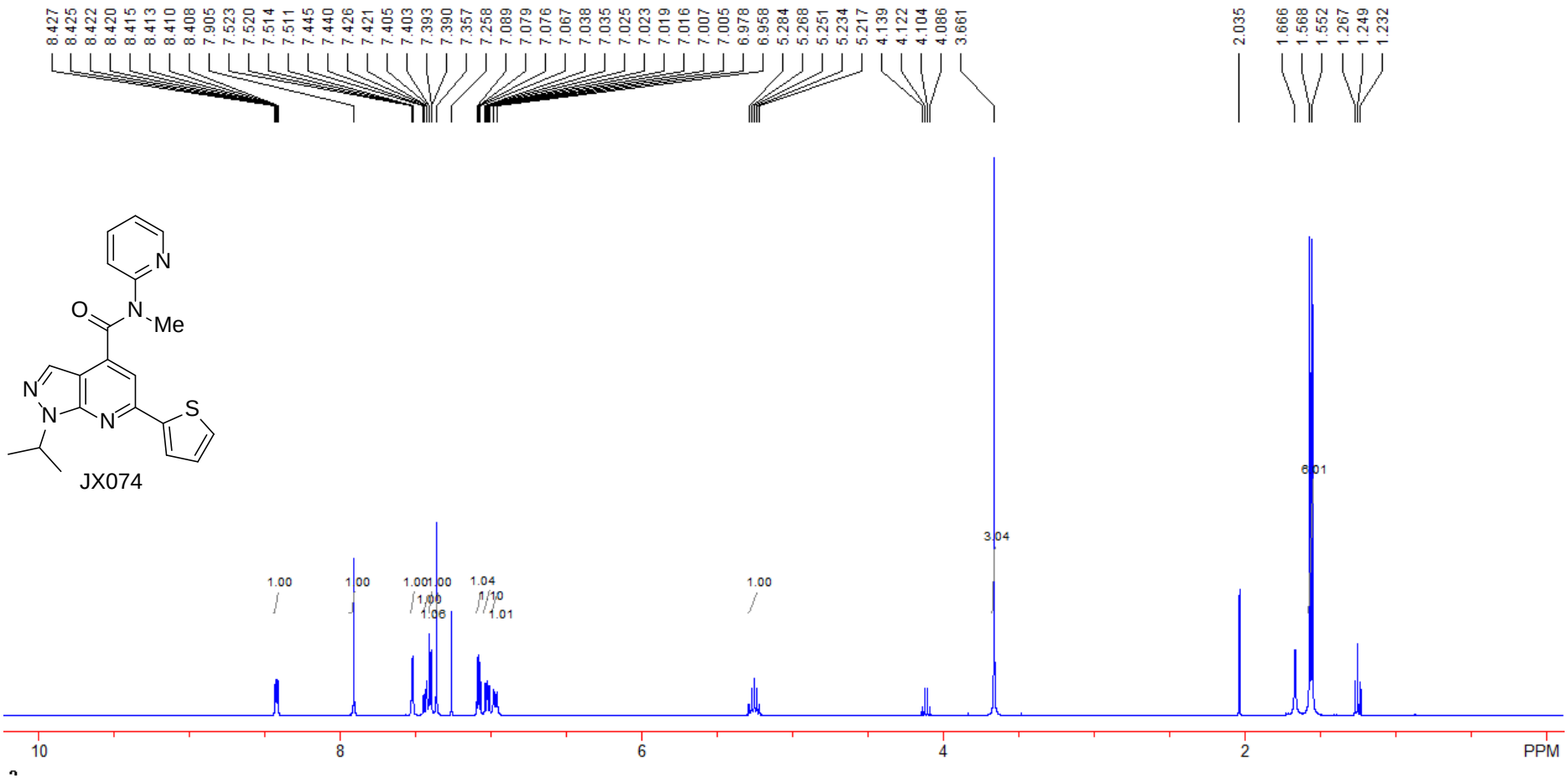

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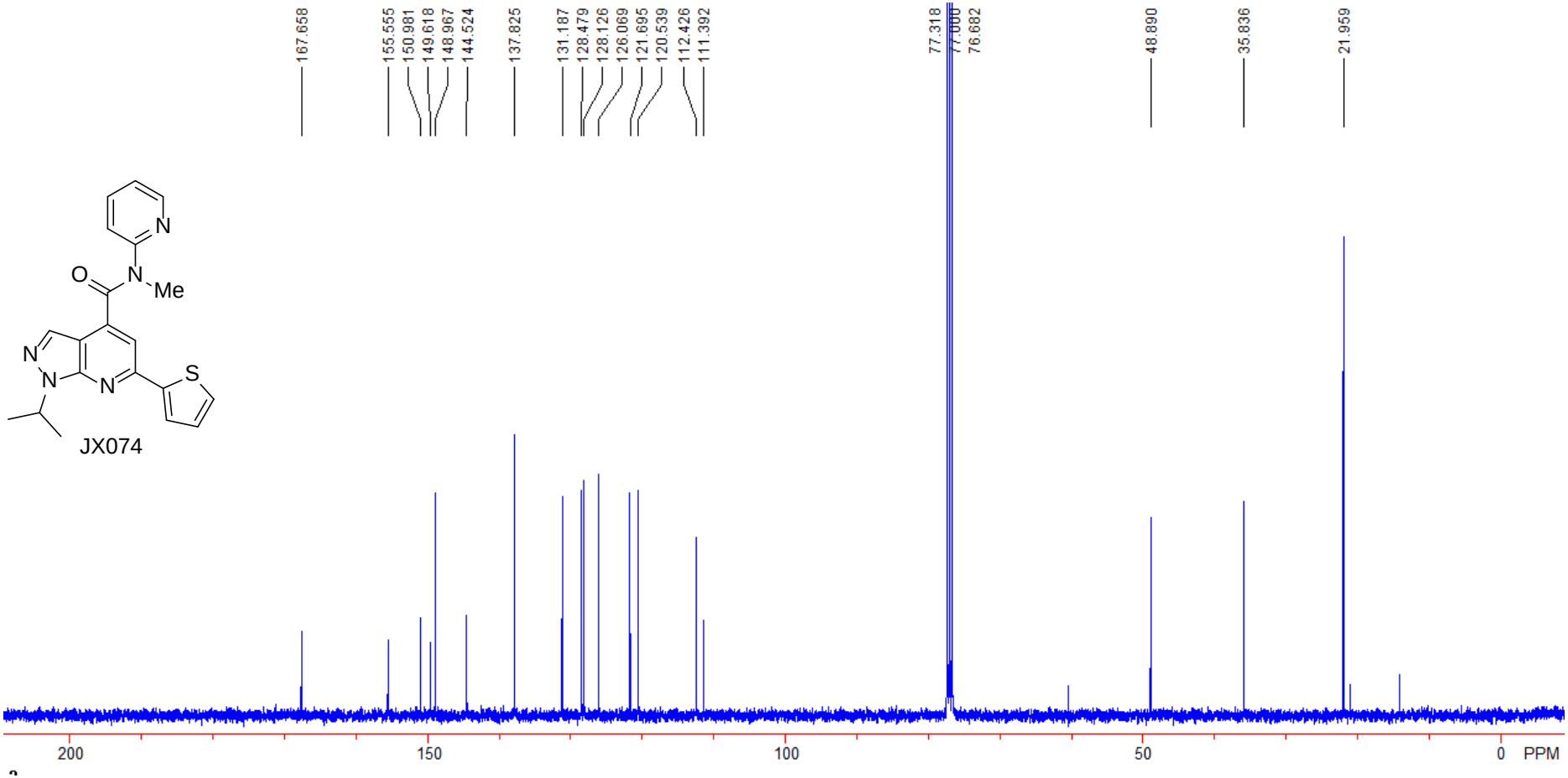

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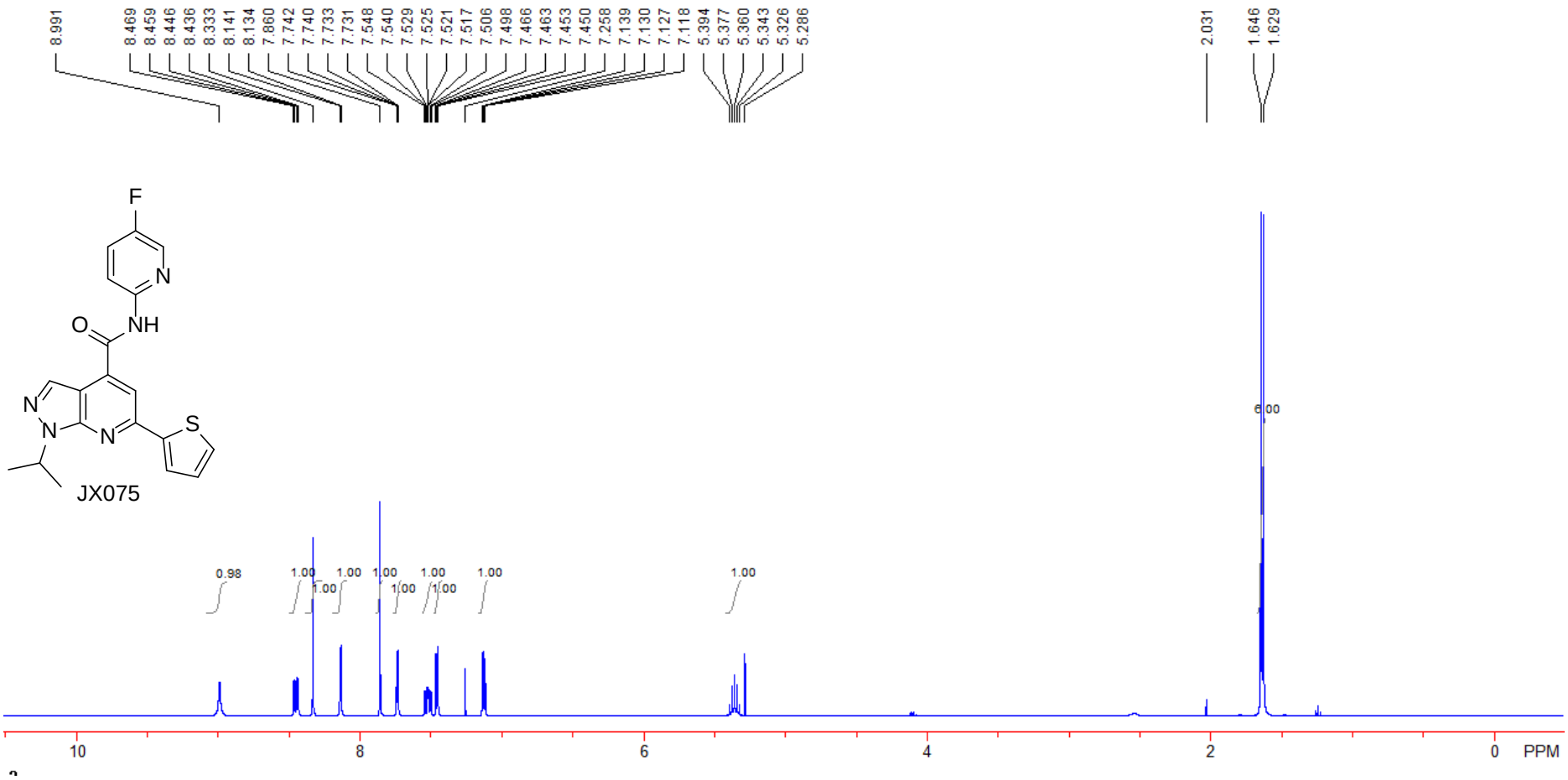

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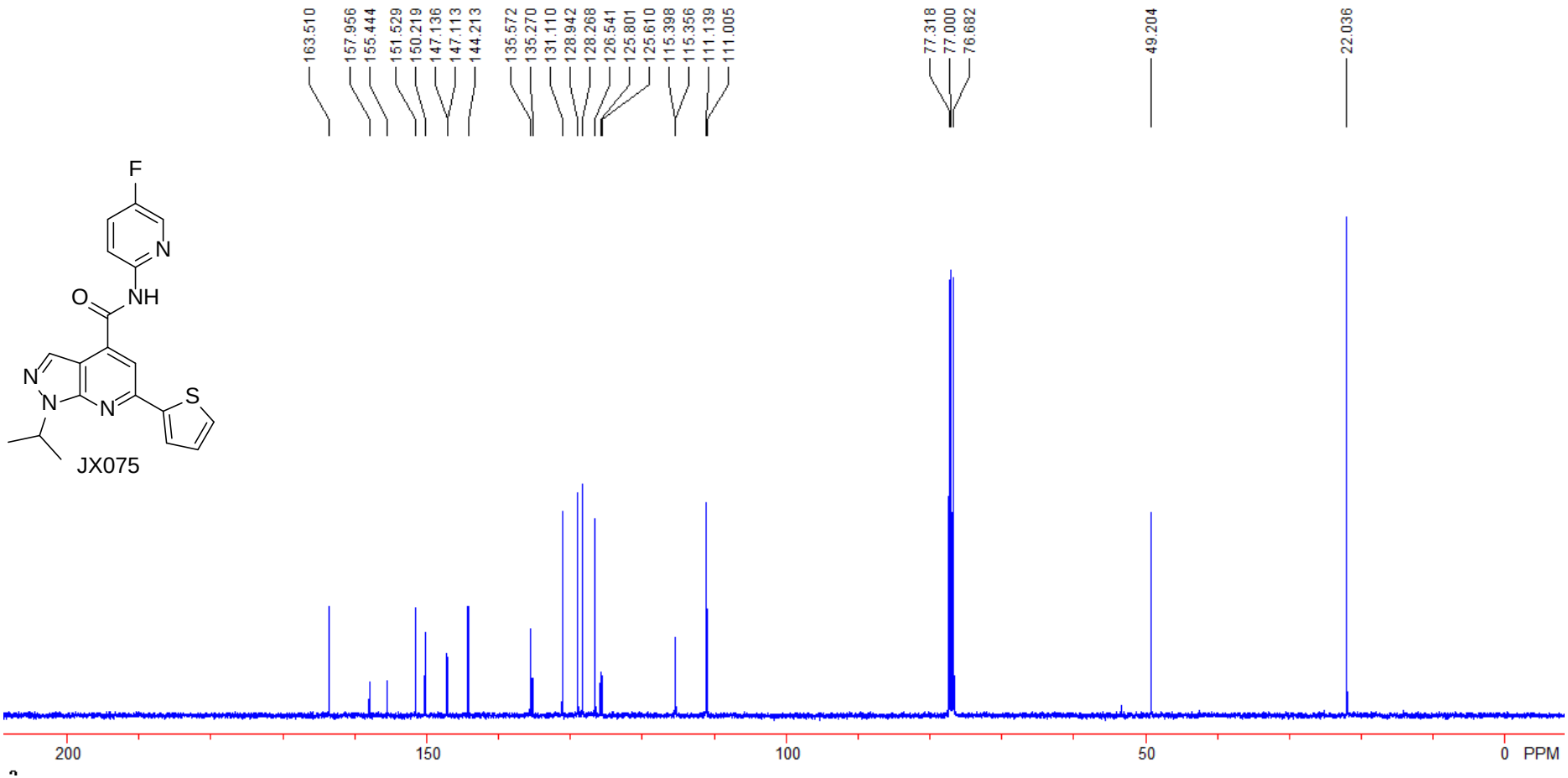

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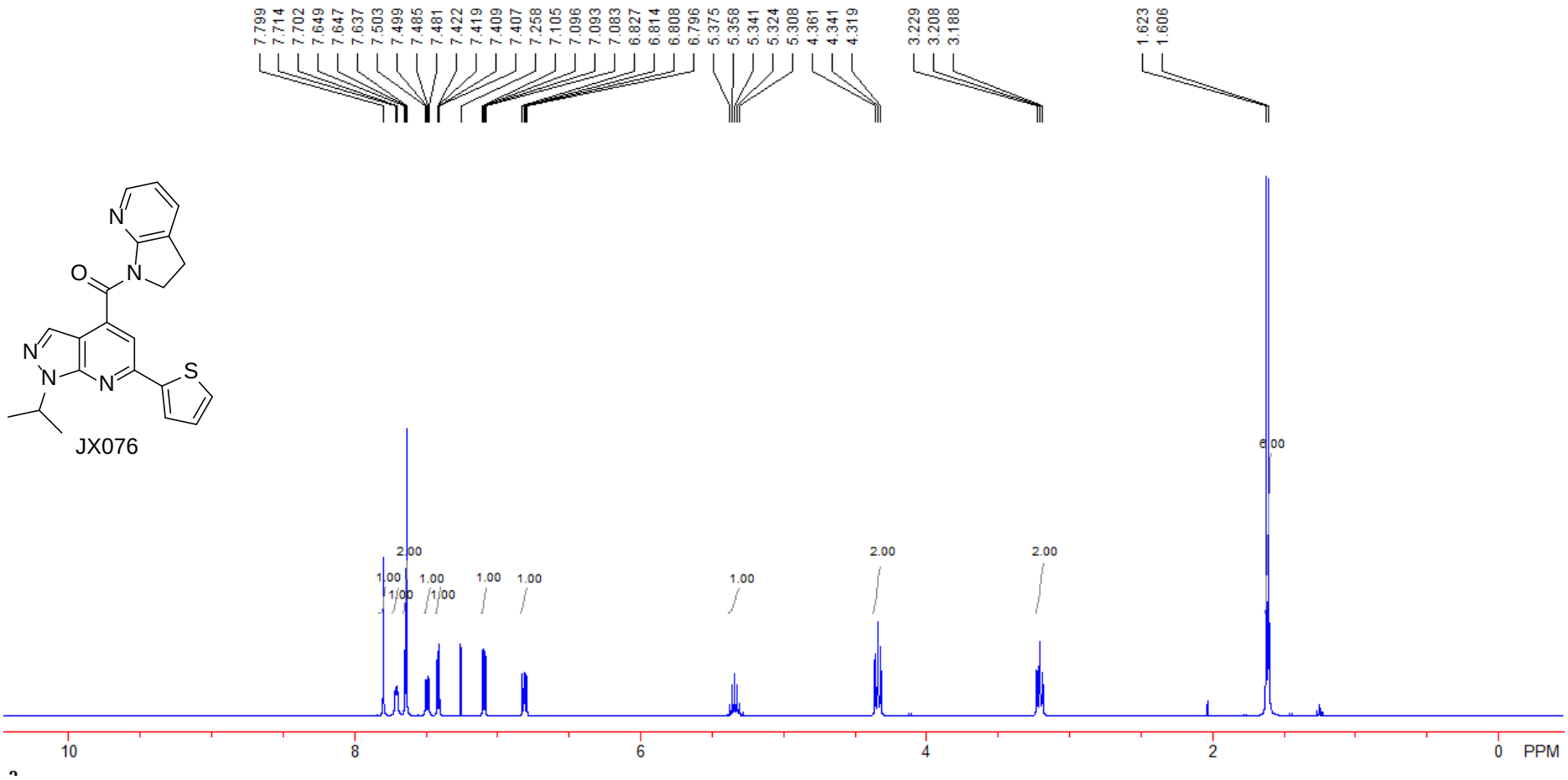

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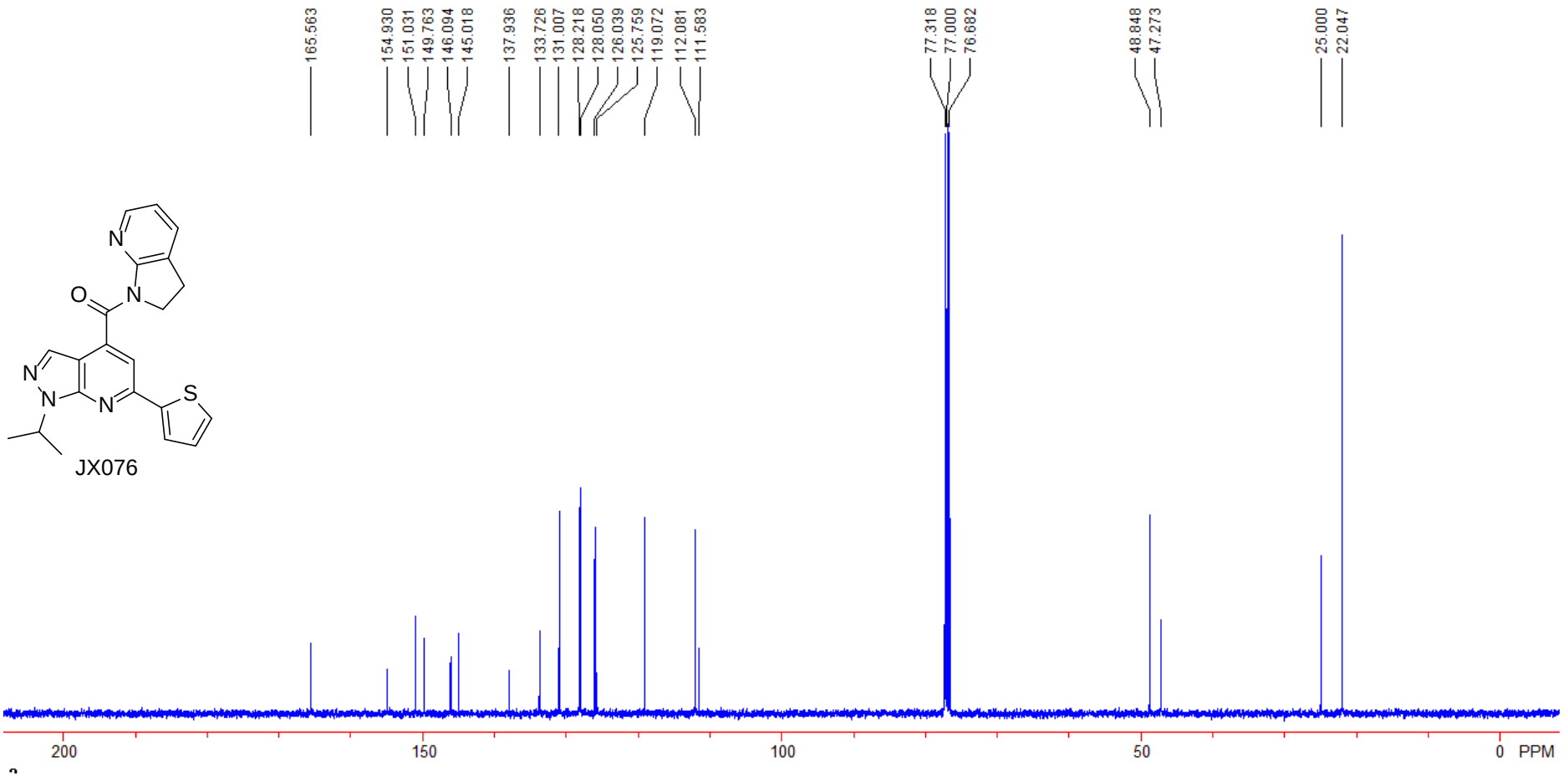

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PPM

Supplementary Table S1: SAR analysis of analogues in the original screening library.[a]

R[1]	**R[6]**	**C4**	**Activity[a]**	**Notes**
(4-chlorophenyl) methyl	phenyl	dimethyl	1.42	
1,1-dioxo-1-thiolan-3-yl	cyclopropyl	2-fluoro-4-methylphenyl	0.153	
		3-fluorophenyl	39.4, 2.54, 2.54	
		2,4-difluorophenyl	0.407	
benzyl	phenyl	dimethyl-	0.994	
		1-methyl-1*H*-pyrazol-3-yl	0.462	
ethyl	phenyl	1,3-thiazol-2-yl	0.111	
		5-methyl-1,3,4-thiadiazol-2-yl	1.51	
		5-methyl-1,3-thiazol-2-yl)	0.344	
		propan-2-yl	0.293	
	thiophen-2-yl	**4-cyanophenyl**	**118.0, 98.9, 98.9**	b
		4-methyl-3-sulfamoylphenyl	**155.0, 112.0**	b
		4-carbamoylphenyl	*144*	c
		4-fluoropheny	*113.0, 100.0, 100.0*	c
		1,3-benzothiazol-2-yl	0.212	
		2,3-dimethylphenyl	0.545, 2.04, 2.04	
		2,4-difluorophenyl	0.63, 0.275, 0.275	
		2,4-dimethylphenyl	0.153, 0.0549, 0.0549	
		2,6-dimethylphenyl	0.172	
		2-chloro-4-fluorophenyl	0.218	
		2-chloro-4-methylphenyl	0.246, 0.199, 0.199	
		2-fluorophenyl	0.64	
		2-iodophenyl	0.416	
		3-methoxyphenyl	13.8, 29.8, 29.8	

		4-chloro-2-fluorophenyl	0.169, 0.399, 0.399	
		5-chloro-2-methoxyphenyl	0.202, 0.5, 0.5	
		5-fluoro-2-methylphenyl	0.861	
		5-methyl-1,3-thiazol-2-yl	0.152	
		phenyl-	3.45, 1.61, 1.61	
methyl	cyclopropyl	4-chloro-2-fluorophenyl	0.173	
		5-fluoro-2-methylphenyl	0.646	
	phenyl	3-[2-(pyridin-2-yl)ethynyl]phenyl	0.123	
		pyridin-3-yl	0.28	
	propan-2-yl	2,3,4-trifluorophenyl)	0.195	
	thiophen-2-yl	4-(cyanomethyl)phenyl	1.52, 1.26	
pyridin-3-ylmethyl	phenyl	2,4,6-trimethylphenyl)	0.653, 0.241	
		2-chloro-4-fluorophenyl	0.309	
		2-fluoro-5-methylphenyl	0.329	
thiophen-2-ylmethyl	methyl	2-chlorophenyl	0.323	
		3,4-difluorophenyl	0.104	
		4-ethylphenyl	0.161, 0.0732, 0.0732	
		2-chloro-4,6-dimethylphenyl	0.156	
propan-2-yl	2,3-dihydro-1,4-benzodioxin-6-yl	5-methylpyridin-2-yl	0.227	
		dimethyl	0.229	
	2,5-dimethylthiophen-3-yl	4,5-dihydro-1,3-thiazol-2-yl	0.238	
		6-chloro-2*H*-1,3-benzodioxol-5-yl	0.238	
	2-methylphenyl	1,3-thiazol-2-yl	0.119, 1.78	
		5-methyl-1,3,4-thiadiazol-2-yl	0.272	
	cyclopropyl	2-methyl-3-oxo-3,4-dihydro-2*H*-1,4-benzoxazin-6-yl	**130**	b
		3-{5*H*,6*H*,7*H*,8*H*,9*H*-[1,2,4]triazolo[4,3-	**96.5, 79.3**	b

		a]azepin-3-yl}phenyl		
		4-methyl-3-sulfamoylphenyl	**143**	b
		5-methanesulfonyl-2-methylphenyl	**139.0, 70.6, 70.6**	b
		2-methylphenyl	*62.2*	c
		3-methoxyphenyl	*96.2*	c
		3-methylphenyl	*82.6*	c
		4-fluoro-2-methylphenyl	*112*	c
		pyridin-3-yl	*170.0, 107.0*	c
		(4-ethylphenyl	0.505, 4.07, 4.07	
		2-(methylsulfanyl)phenyl	0.34	
		2,3-dimethylphenyl	0.164	
		2,4,6-trimethylphenyl	0.132	
		2,4-dibromophenyl	0.59	
		2,5-dimethylphenyl	0.152	
		2-carbamoylphenyl	5.57	
		2-chloro-4,6-dimethylphenyl	0.304	
		2-chloro-4-methylphenyl	0.4	
		2-ethylphenyl	0.135	
		2-fluorophenyl	0.256	
		2-methoxyphenyl	0.344	
		2-methyl-6-(propan-2-yl)phenyl	0.323, 0.846, 0.846	
		3-(2-methyl-1,3-thiazol-4-yl)phenyl	0.19, 0.542	
		3-(methylsulfanyl)phenyl	0.284	
		3,4-dimethylphenyl	1.47	
		3,5-dimethylphenyl	0.44, 0.463, 0.463	
		3-ethylphenyl	0.447, 0.218, 0.218	
		4-bromo-2-fluorophenyl	0.23	

		4-bromo-2-methylphenyl	1.04	
		4-bromophenyl	0.296, 1.02, 1.02	
		4-chlorophenyl	147.0, 0.644, 0.644	
		4-methoxyphenyl	13.7, 1.49, 1.49	
		5-chloro-2-methylphenyl	0.211, 0.179	
		methylsulfanyl)phenyl	117.0, 29.2, 29.2	
	methyl	(3,5-dichlorophenyl	0.11	
		(3-methoxyphenyl	0.187	
		2-(methylsulfanyl)phenyl	0.886	
		2,3-dichlorophenyl	0.177	
		2,3-dimethylphenyl	0.168	
		2,4-bis(morpholin-4-yl)phenyl	0.155	
		2,5-dimethoxyphenyl	6.53, 0.184	
		2,5-dimethylphenyl	0.278	
		2,6-bis(propan-2-yl)phenyl	0.129	
		2,6-diethylphenyl	0.192	
		2-bromo-4-methylphenyl	0.252	
		2-bromophenyl	0.097	
		2-fluoro-4-methylphenyl	0.136	
		2-fluoro-5-methylphenyl)	0.453	
		2-fluorophenyl	0.348, 2.18, 2.18	
		2-iodophenyl	0.136	
		2-methoxy-5-methylphenyl	0.19, 0.271	
		2-methyl-6-(propan-2-yl)phenyl	0.202	
		3-(methylsulfanyl)phenyl	0.17, 0.215, 0.215	
		3,5-dimethylphenyl	0.136	
		3-chloro-2-methylphenyl	0.2	

		3-chloro-4-methylphenyl	14.1	
		3-chlorophenyl	0.76	
		3-fluorophenyl	0.518, 1.19, 1.19	
		3-iodo-4-methylphenyl	0.357, 6.47, 6.47	
		3-methylphenyl	1.21, 0.119, 0.119	
		4-(dimethylcarbamoyl)phenyl	0.337	
		4-bromo-3-methylphenyl	0.798, 0.279, 0.279	
		4-chloro-2,5-dimethoxyphenyl	0.142	
		4-fluorophenyl	3.16	
		4-iodophenyl	0.161, 0.119, 0.119	
		5-chloro-2,4-dimethoxyphenyl	1.41	
		5-chloro-2-fluorophenyl	0.26, 0.12, 0.12	
		5-fluoro-2-methylphenyl	0.116	
		5-methylpyridin-2-yl	0.238, 1.12	
		benzoic acid	0.34	
		quinolin-8-yl	0.688, 0.332	
	phenyl	2*H*-1,3-benzodioxol-5-yl	**112**	b
		3-(1,3,4-oxadiazol-2-yl)phenyl	**128.0, 67.4**	b
		phenyl	**127**	b
	propan-2-yl	2-(4-methylpiperazin-1-yl)phenyl	**115**	b
		3-(2-oxopyrrolidin-1-yl)phenyl	**156**	b
		2,3-dimethylphenyl	4.61	
		2,4,6-trimethylphenyl)	0.36	
		2,6-dimethylphenyl	0.136	
		2-ethyl-6-methylphenyl	0.225	
		2-fluorophenyl	11.6	

		2-methyl-6-(propan-2-yl)phenyl	0.6	
	thiophen-2-yl	2-chloro-4-fluorophenyl	**121.0, 90.9, 90.9**	b
		2-fluoro-4-methylphenyl	**116.0, 100.0**	b
		2-fluorophenyl	**174.0, 110.0**	b
		2-methylphenyl	**157**	b
		3-methanesulfonylphenyl	**199**	b
		3-methoxyphenyl	**106.0, 51.6**	b
		4-fluoro-2-methylphenyl	**150.0, 85.1**	b
		4-methoxyphenyl	**103.0, 45.7**	b
		4-methyl-3-sulfamoylphenyl	**158**	b
		5-fluoro-2-methylphenyl	**125**	b
		2,6-dimethylphenyl	*196.0, 135.0*	c
		2-chlorophenyl	*108.0, 69.3*	c
		2-bromophenyl	99.3, 12.0, 12.0	

a) The biological activities of 144 1*H*-pyrazolo[3,4-*b*]pyridine-4-carboxamide compounds identified in our initial screening against CVB3–-H3 replication in HeLa-RW cells was performed as described[15] and expressed as percentage of anti-CVB3-H3 activity of a positive control guanidine. Numbers represent single results and some compounds were tested more than once. b) Bold numbers indicate positive hits that have been disclosed previously.[15] c) Italic numbers indicate false positives that failed secondary tests later.