

Discovering potent inhibitors against c-Met kinase: molecular design, organic synthesis and bioassay

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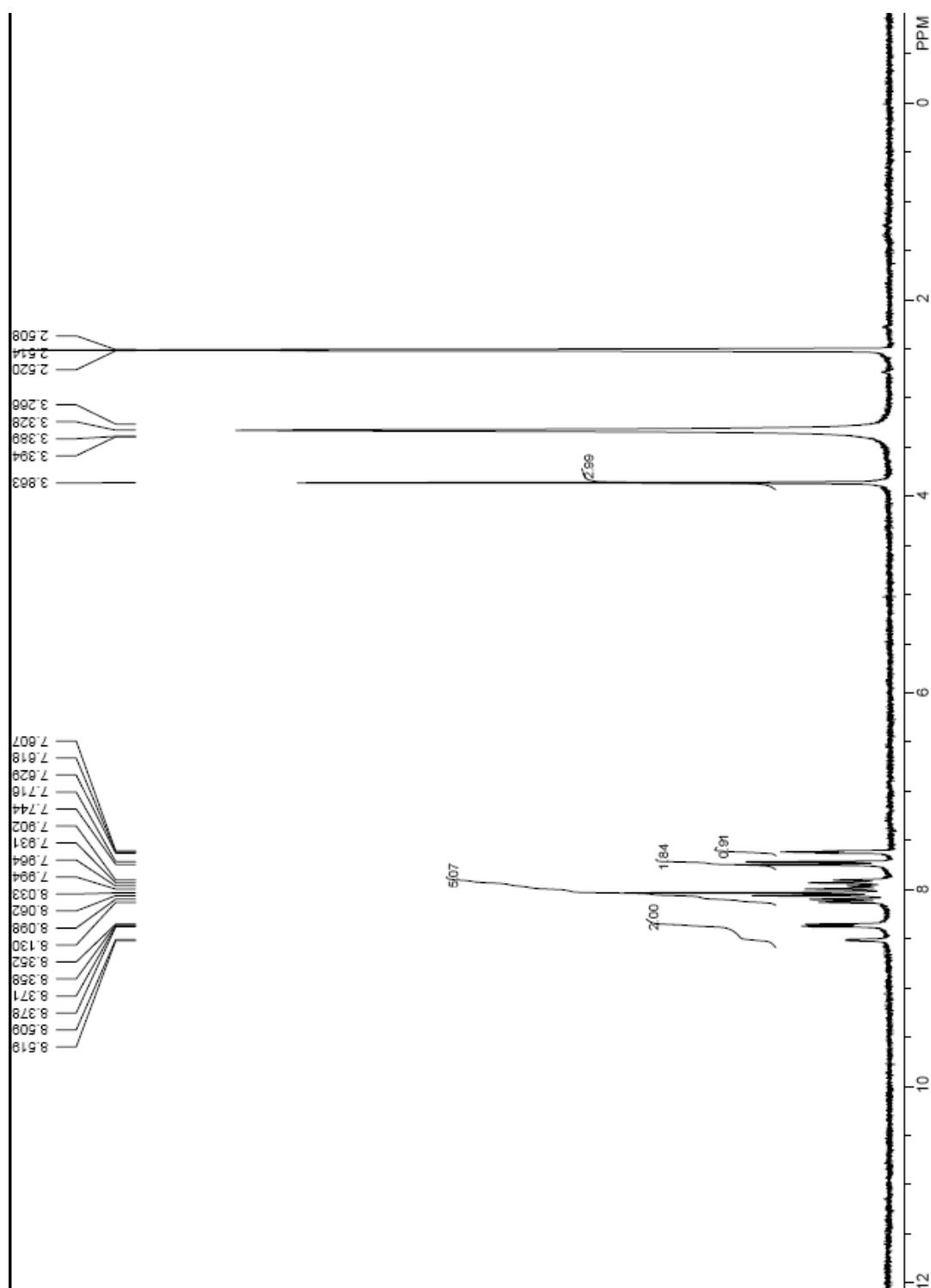
Table S1 The HPLC analyses of all the target compounds. The purity of identified compounds that was essential to the conclusions drawn in the text and determined by the instrumentation with one system given in the following table. The peak purity was checked with UV spectra.

	Method		
Equipment	Agilent 1100 with binary pump, photodiode array detector (DAD), ESI and APCI mass spectrometer		
Column	Agilent Zorbax Eclipse SB-C ₁₈ (25×4.6mm, 5µm particle size)		
System condition	CH ₃ OH / H ₂ O, 80 %(v/v) of CH ₃ OH gradient, flow rate: 1.0 ml/min, calculated the relative purity of each compound at 254 nm		
Results	Compd	Retention time (min)	Relative purity (%)
	1a	1.428	100.00
	1b	1.562	100.00
	1c	1.125	98.22
	1d	6.235	96.12
	1e	6.336	97.55
	1f	1.978	100.00
	1g	1.235	100.00
	1h	1.637	100.00
	1i	1.542	97.46
	1j	1.723	100
	1k	5.359	100
	1l	5.369	95.26
	1m	1.023	100.00
	1n	1.365	95.29
	1o	1.412	98.22
	1p	1.725	97.81

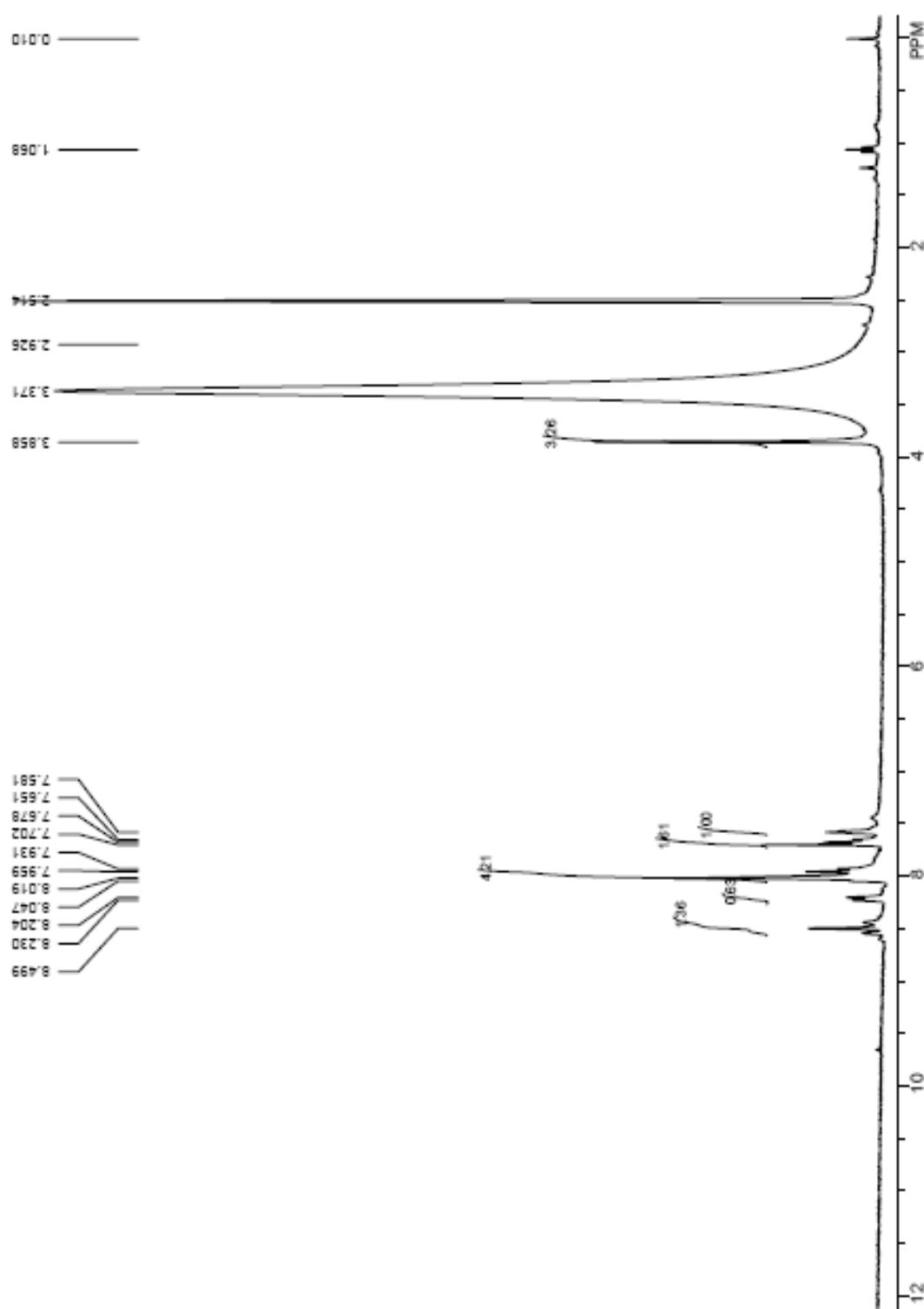
	1q	1.685	97.36
	1r	1.632	100.00
	5a	1.874	100.00
	5b	1.123	95.13
	5c	5.892	95.96
	5d	5.356	96.23
	5e	1.215	100.00
	5f	1.921	100.00
	5g	1.326	99.15

Copies of ^1H NMR of all the target compounds

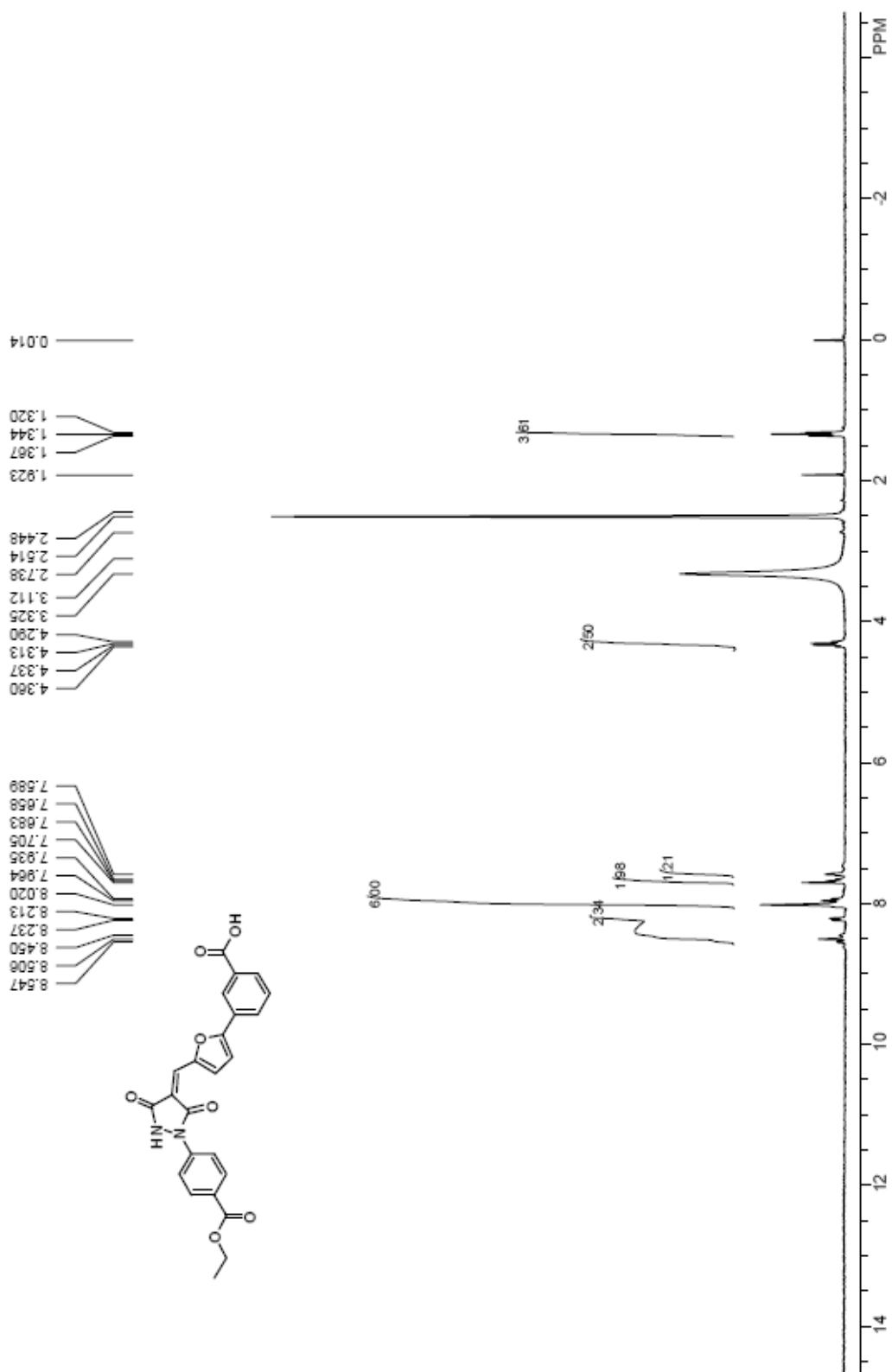
2-chloro-5-((1-(4-(methoxycarbonyl)phenyl)-3,5-dioxopyrazolin-4-ylidene)methyl)furan-2-yl)benzoic acid (No. 1a).



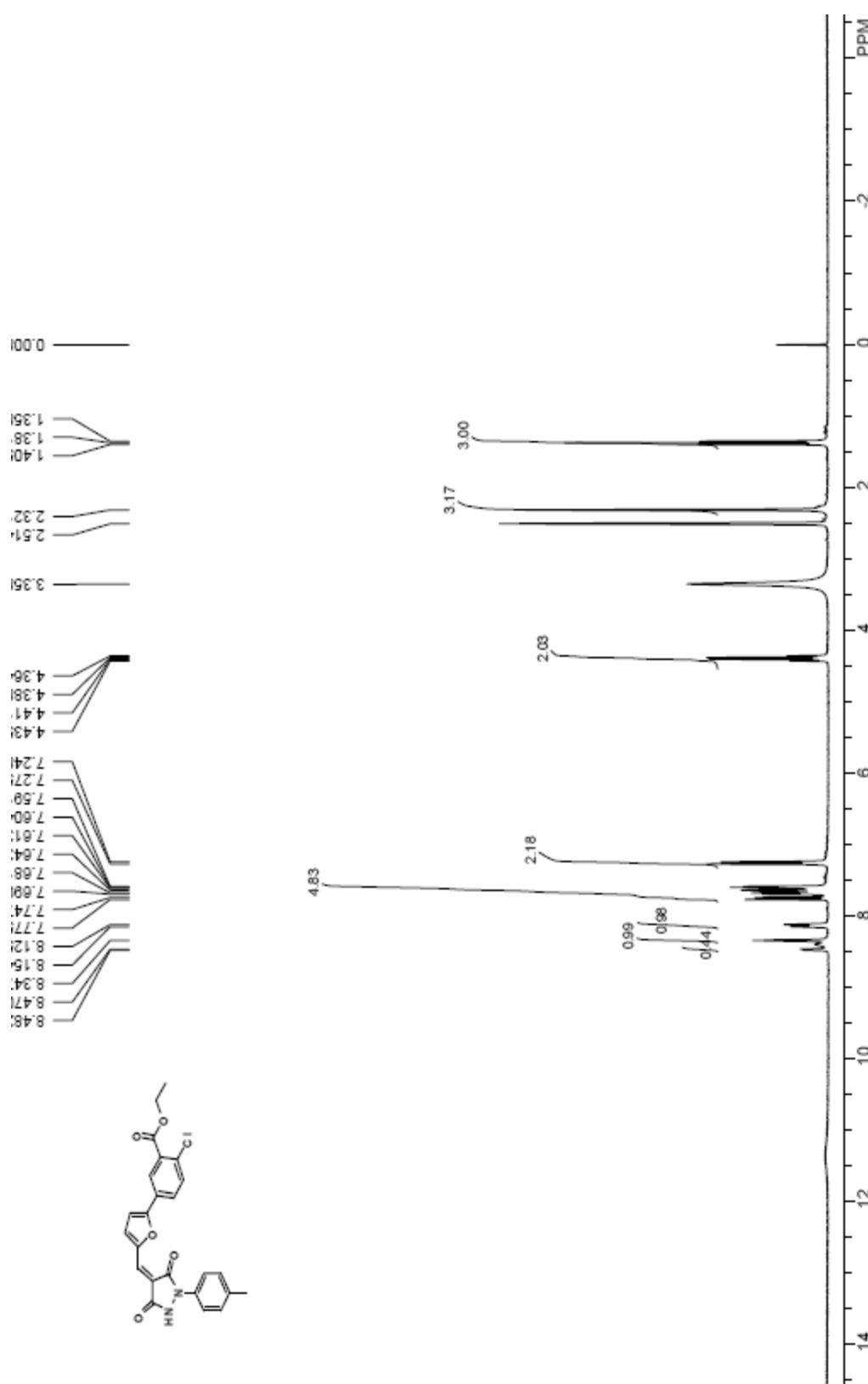
3-((5-((1-(4-(Methoxycarbonyl)phenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan-2-yl)benzoic acid (No. 1b).



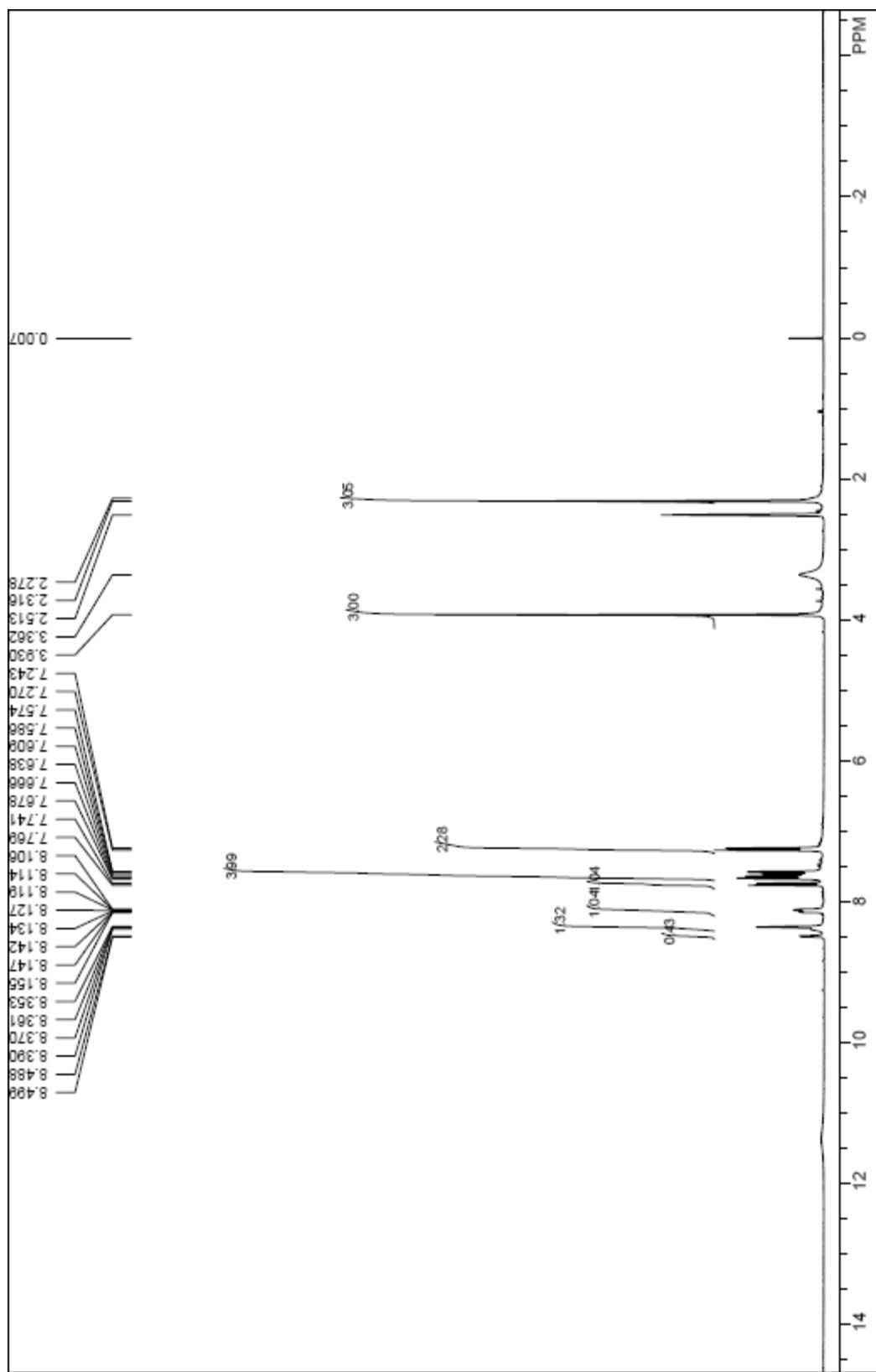
3-((1-(4-(Ethoxycarbonyl)phenyl)-3,5-dioxopyrazolin-4-ylidene)methyl)furan-2-carboxylic acid (No. 1c).



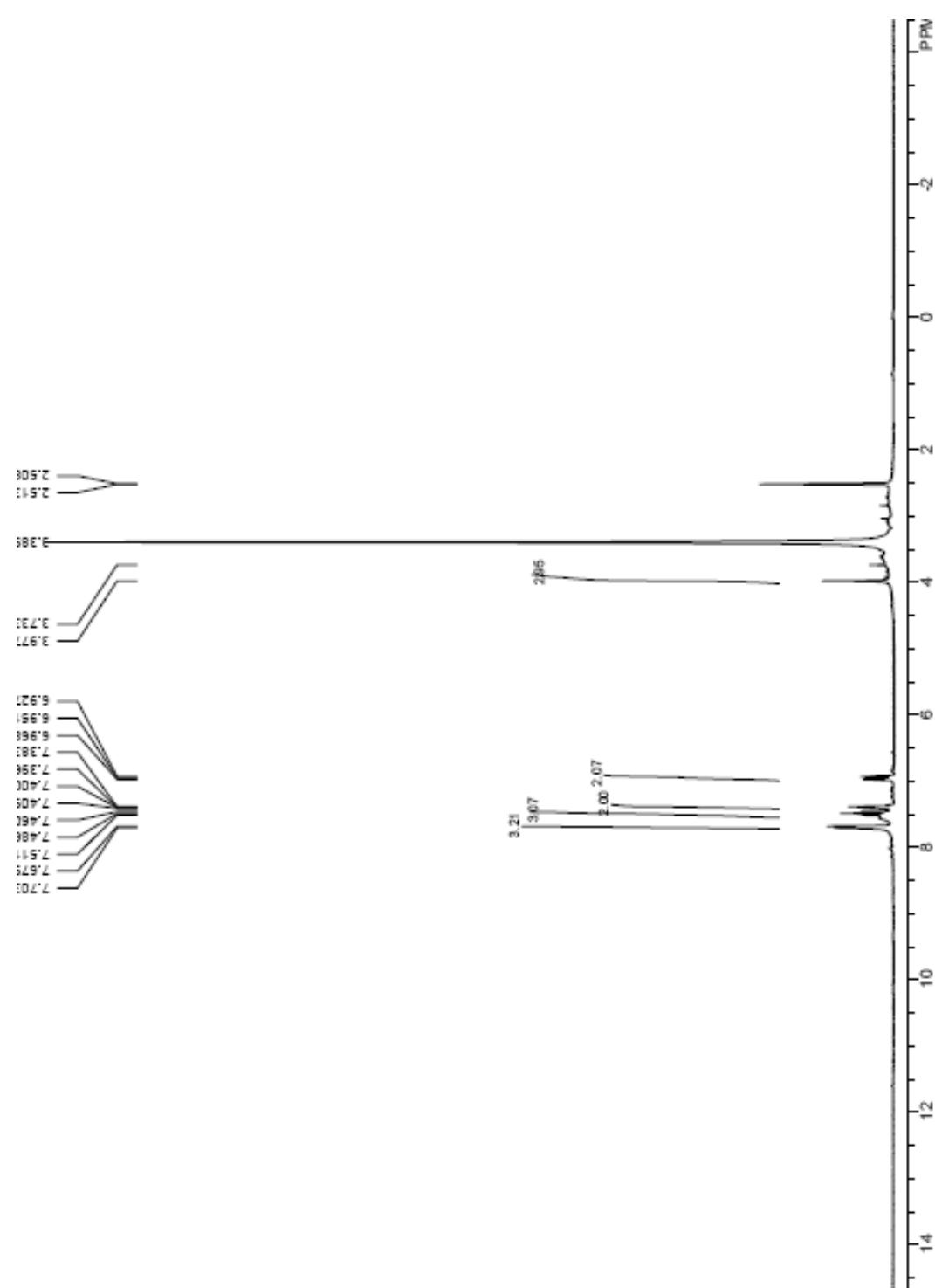
Ethyl 2-chloro-5-(5-((3,5-dioxo-1-p-tolylpyrazolin-4-ylidene)methyl)furan-2-yl)benzoate (No. 1d).



Methyl 2-chloro-5-((5-(3,5-dioxo-1-p-tolylpyrazolidin-4-ylidene)methyl)furan-2-yl)benzoate (No. 1e).

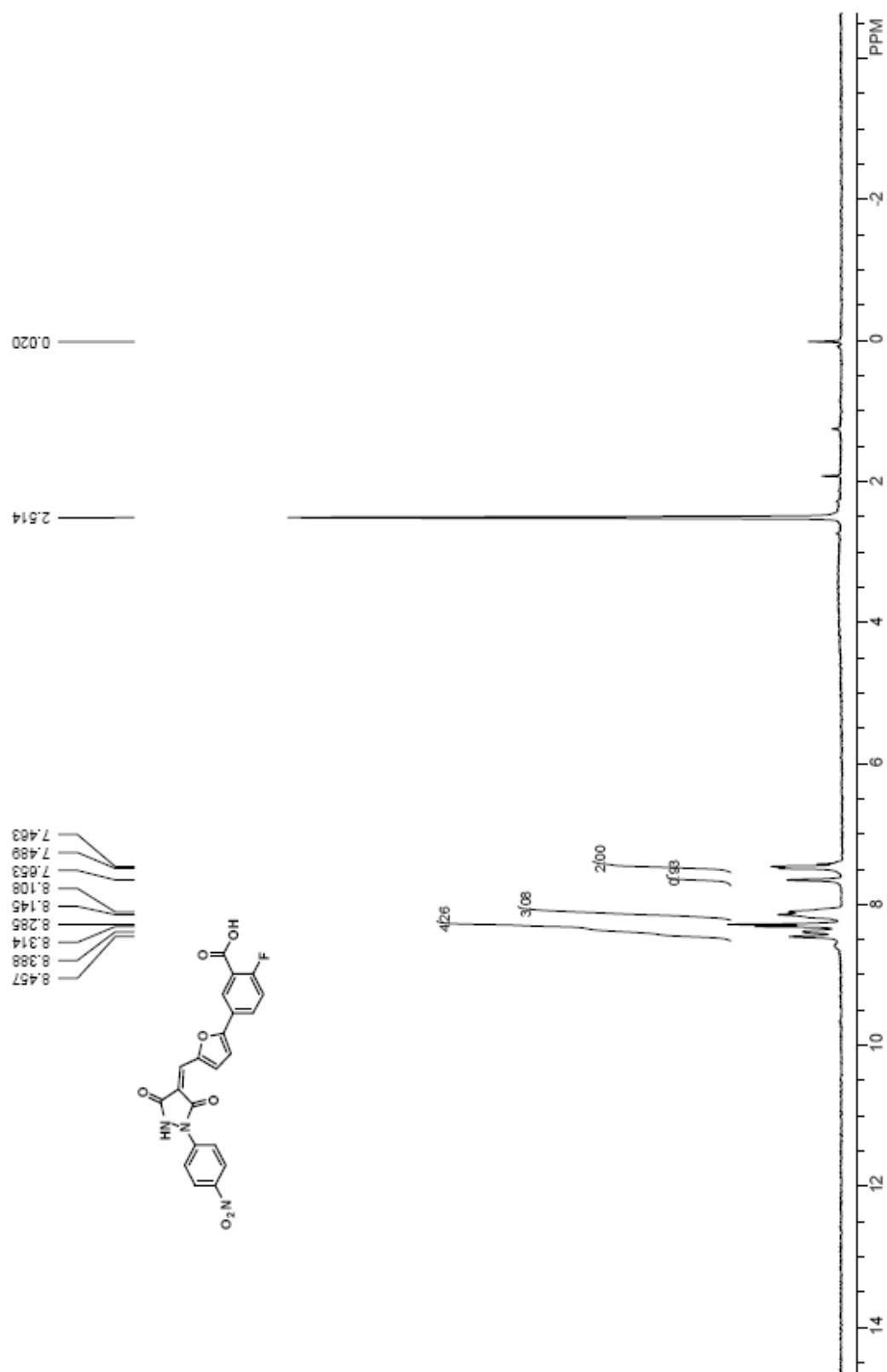


2-Fluoro-5-((1-(4-methoxyphenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan-2-yl)benzoic acid (No. 1f).



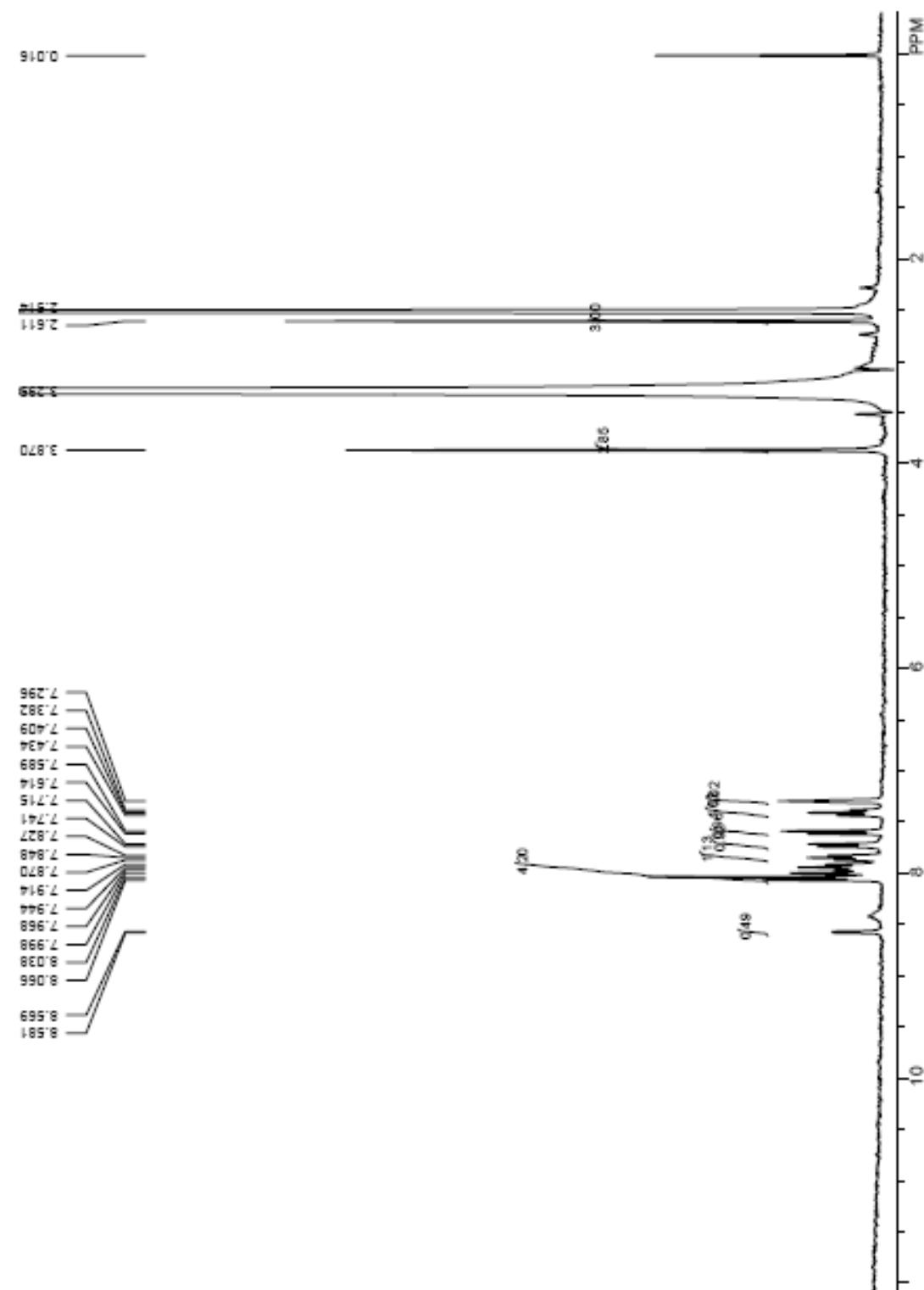
2-Fluoro-5-((1-(4-nitrophenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan-2-yl)benzoic

acid (No. 1g).



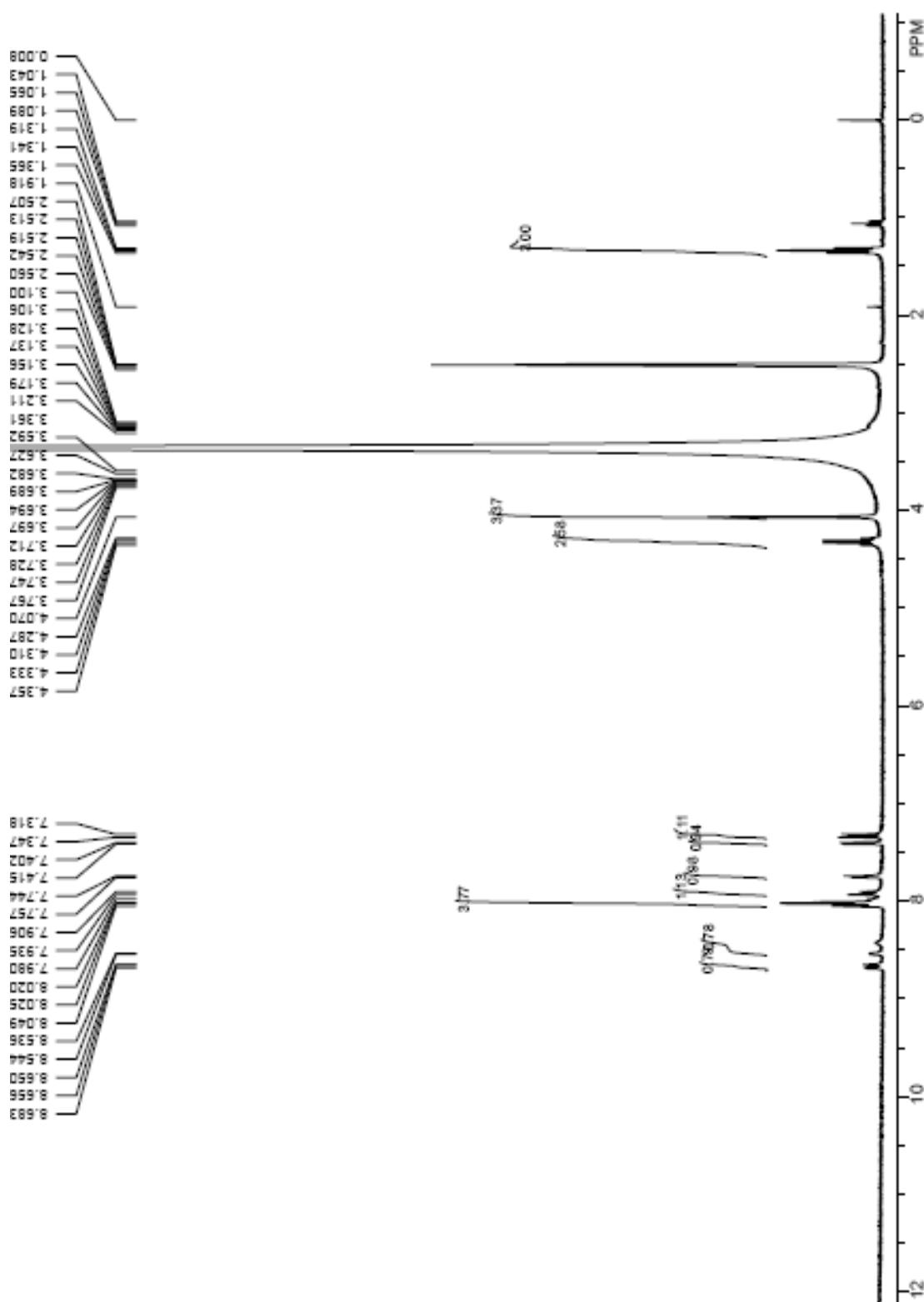
3-((1-(4-(Methoxycarbonyl)phenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan-2-yl)-4-

methylbenzoic acid (No. 1h).



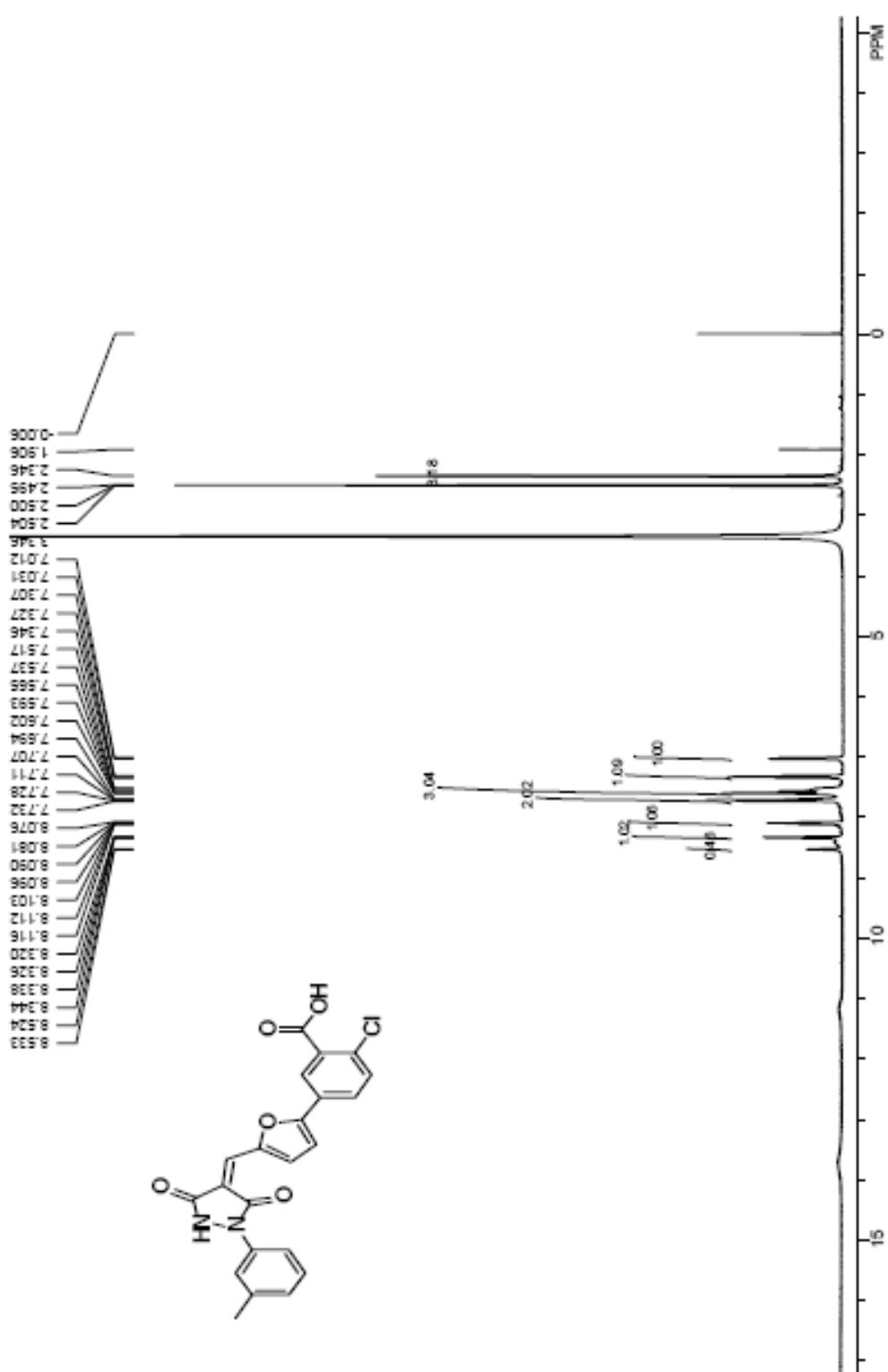
3-(5-((1-(4-(Ethoxycarbonyl)phenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan-2-yl)-4-me

thoxybenzoic acid (No. 1i).



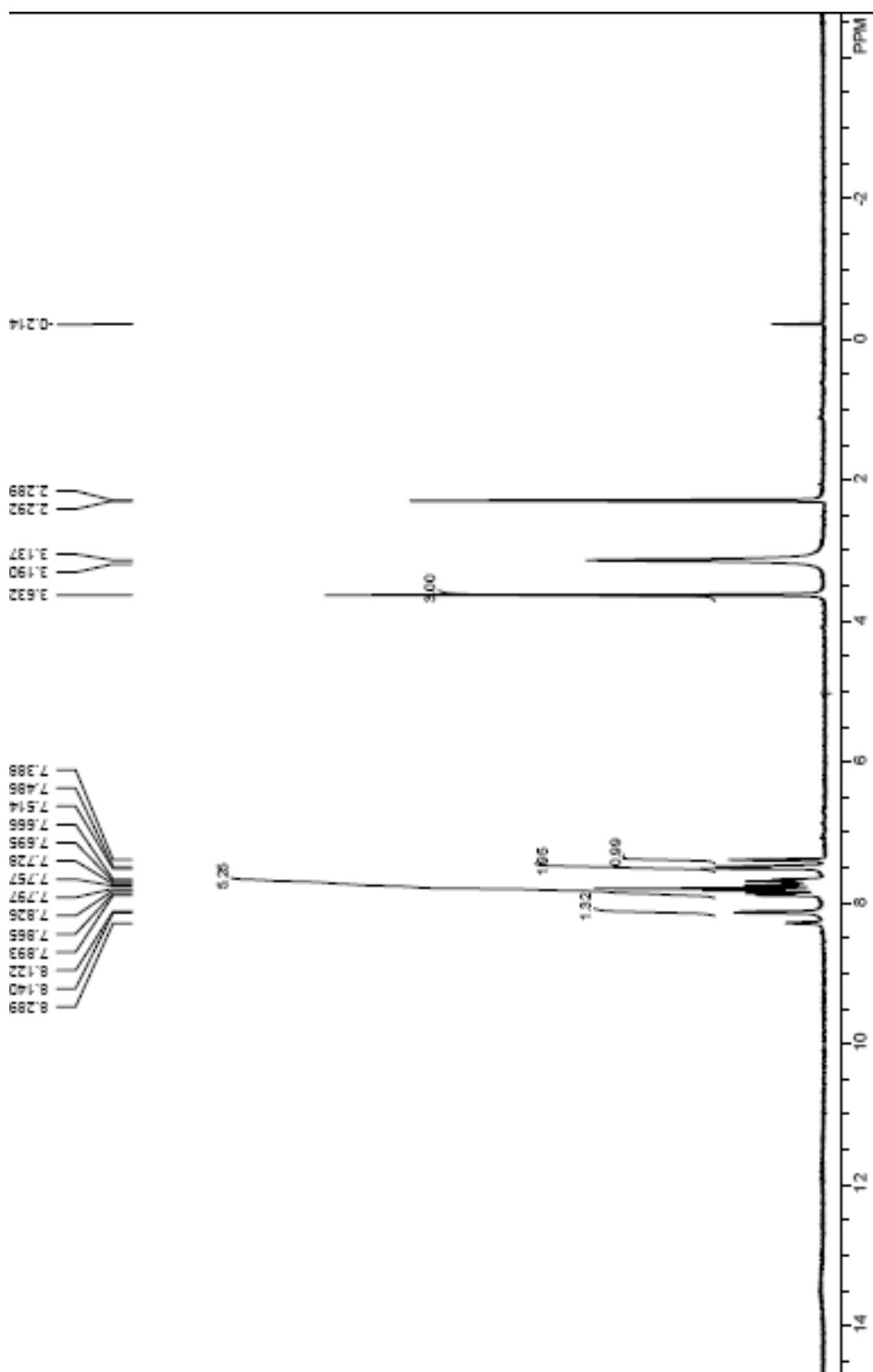
2-Chloro-5-((3,5-dioxo-1-(m-tolyl)pyrazolidin-4-ylidene)methyl)furan-2-ylben-

zoic acid (No. 1j).



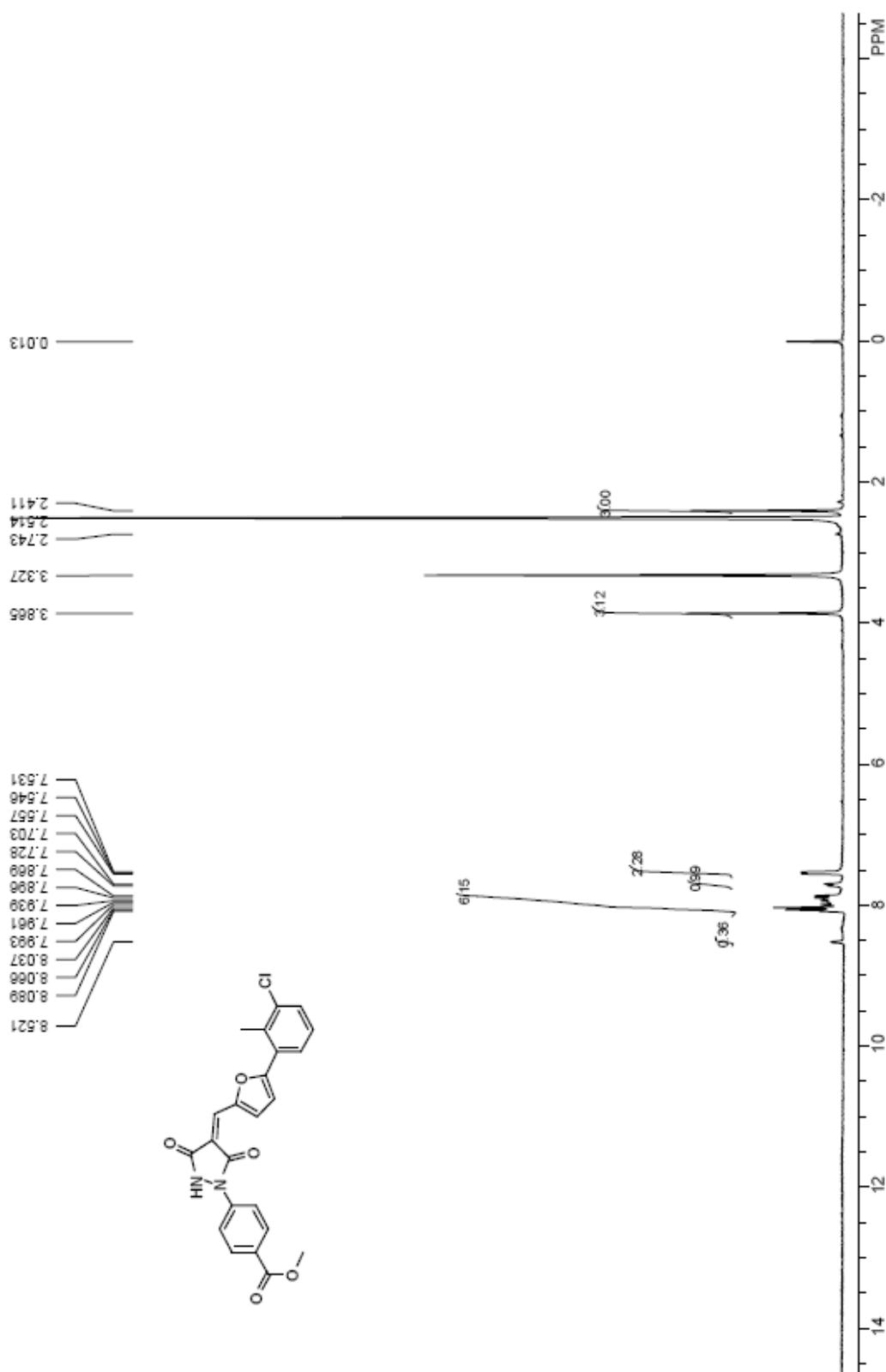
Methyl 4-((4-((5-(3-chlorophenyl)furan-2-yl)methylene)-3,5-dioxopyrazolidin-1-yl)benzoate

(No. 1k).



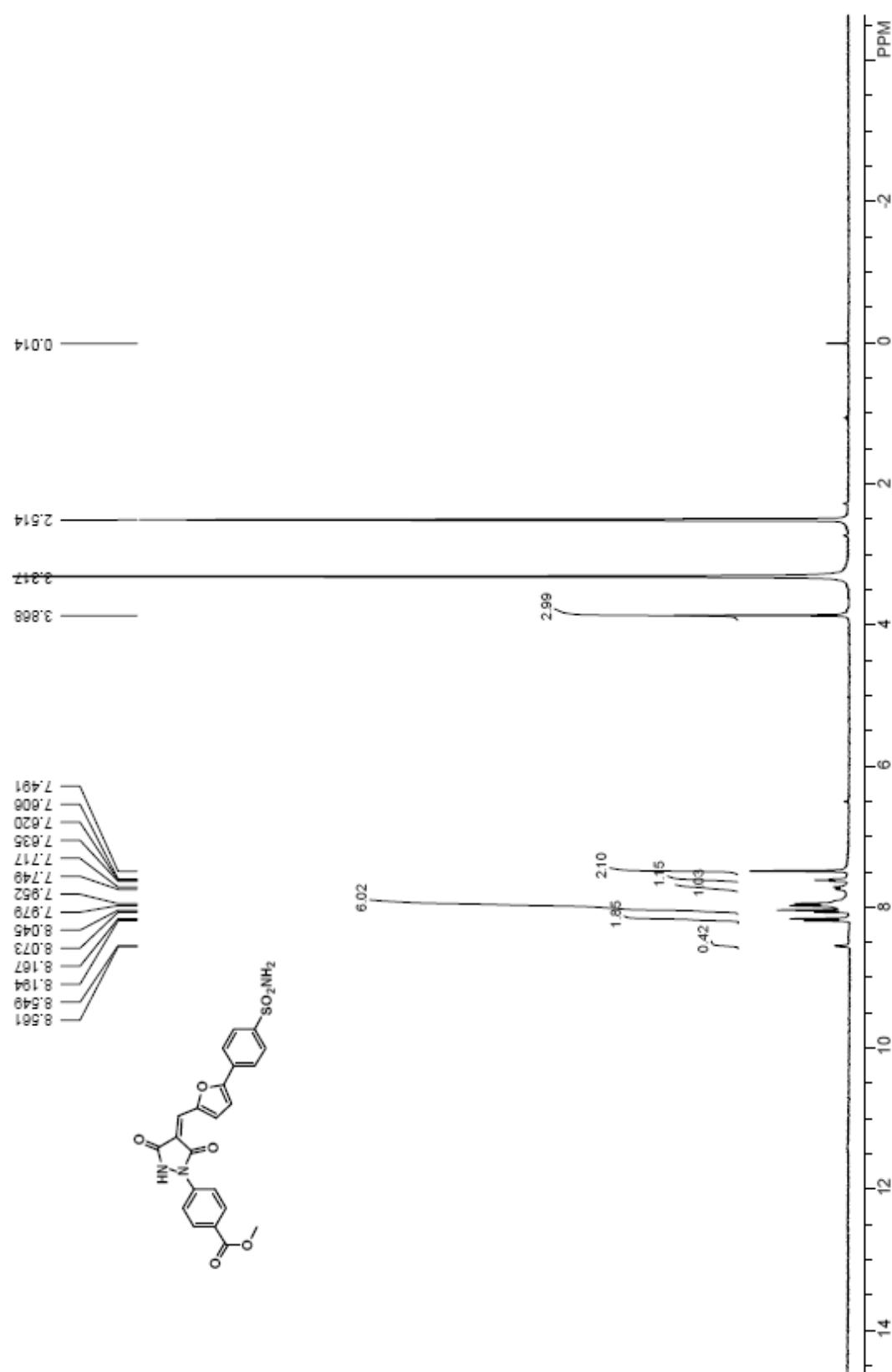
Methyl 4-((4-(3-chloro-2-methylphenyl)furan-2-yl)methylene)-3,5-dioxopyra

zolidin-1-yl)-benzoate (No. 1*I*).



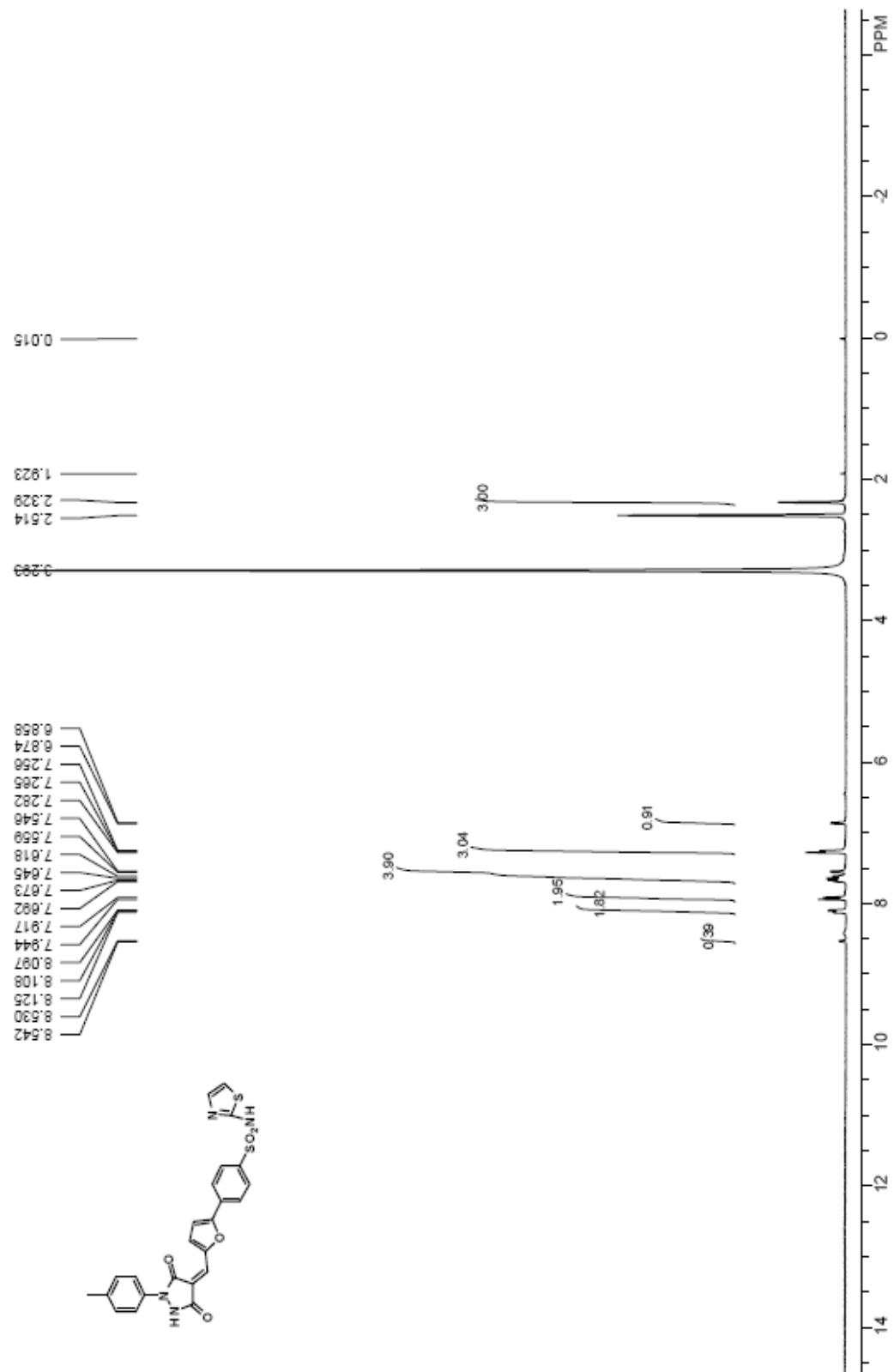
Methyl 4-(3,5-dioxo-4-((5-(4-sulfamoylphenyl)furan-2-yl)methylene)pyrazolidin-1-yl)-

benzoate (No. 1m).



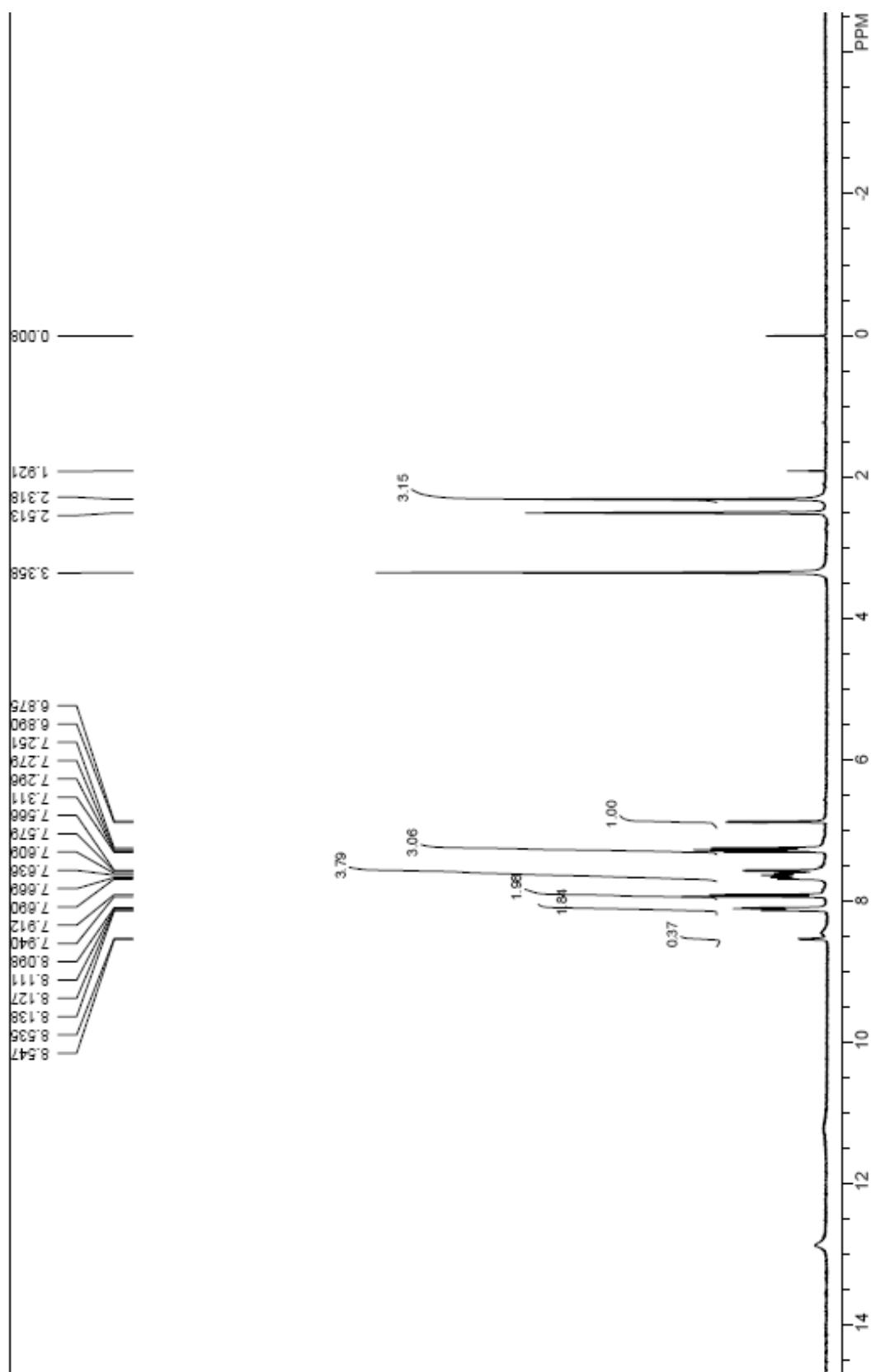
4-((3,5-Dioxo-1-p-tolylpyrazolidin-4-ylidene)methyl)furan-2-yl)-N-(thiazol-2-yl)benzenesu

Ifonamide (No. 1n).



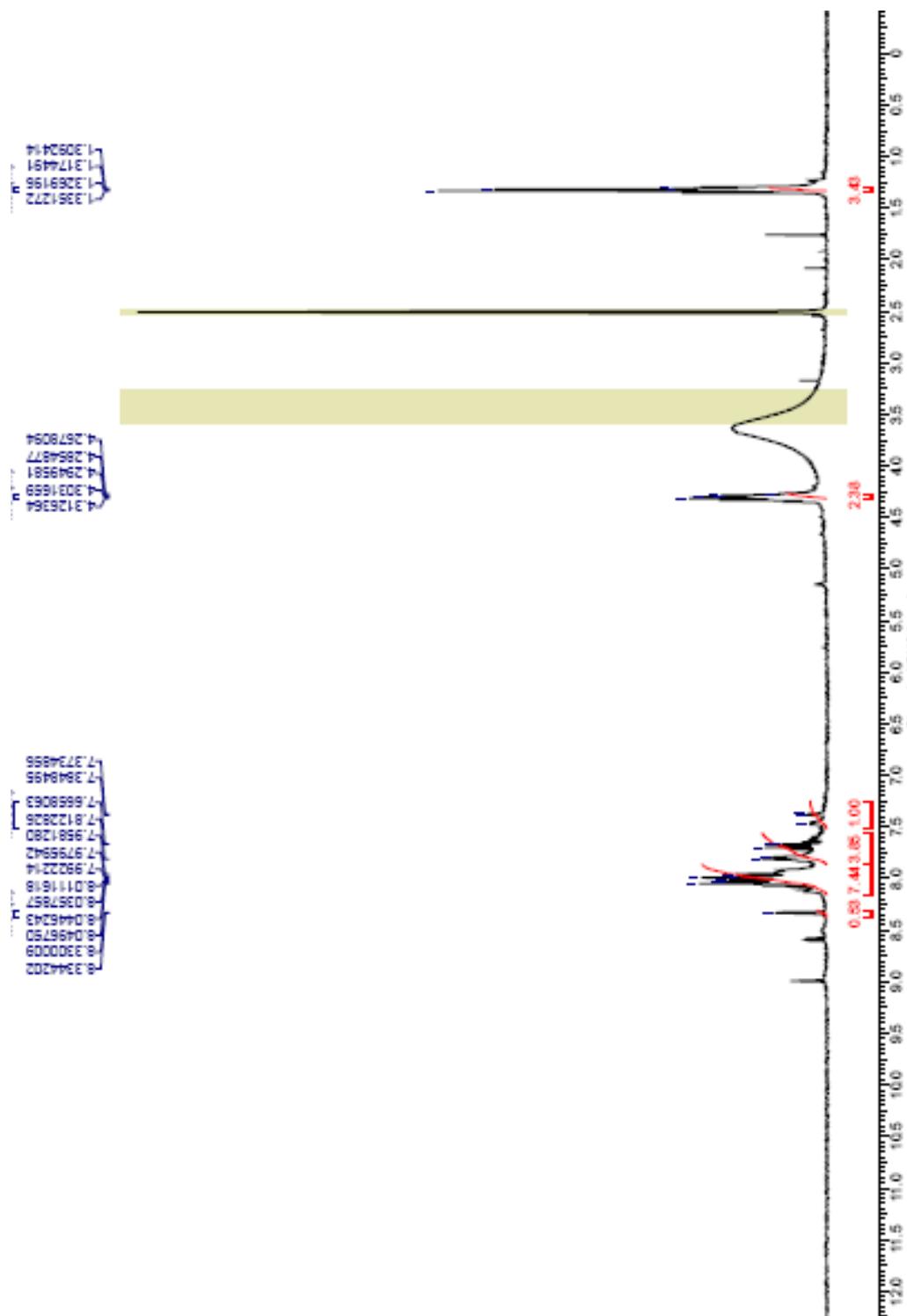
4-(5-((1-(3-Chloro-4-methylphenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan-2-yl)-N-(thi

azol-2-yl)benzenesulfonamide (No. 1o).



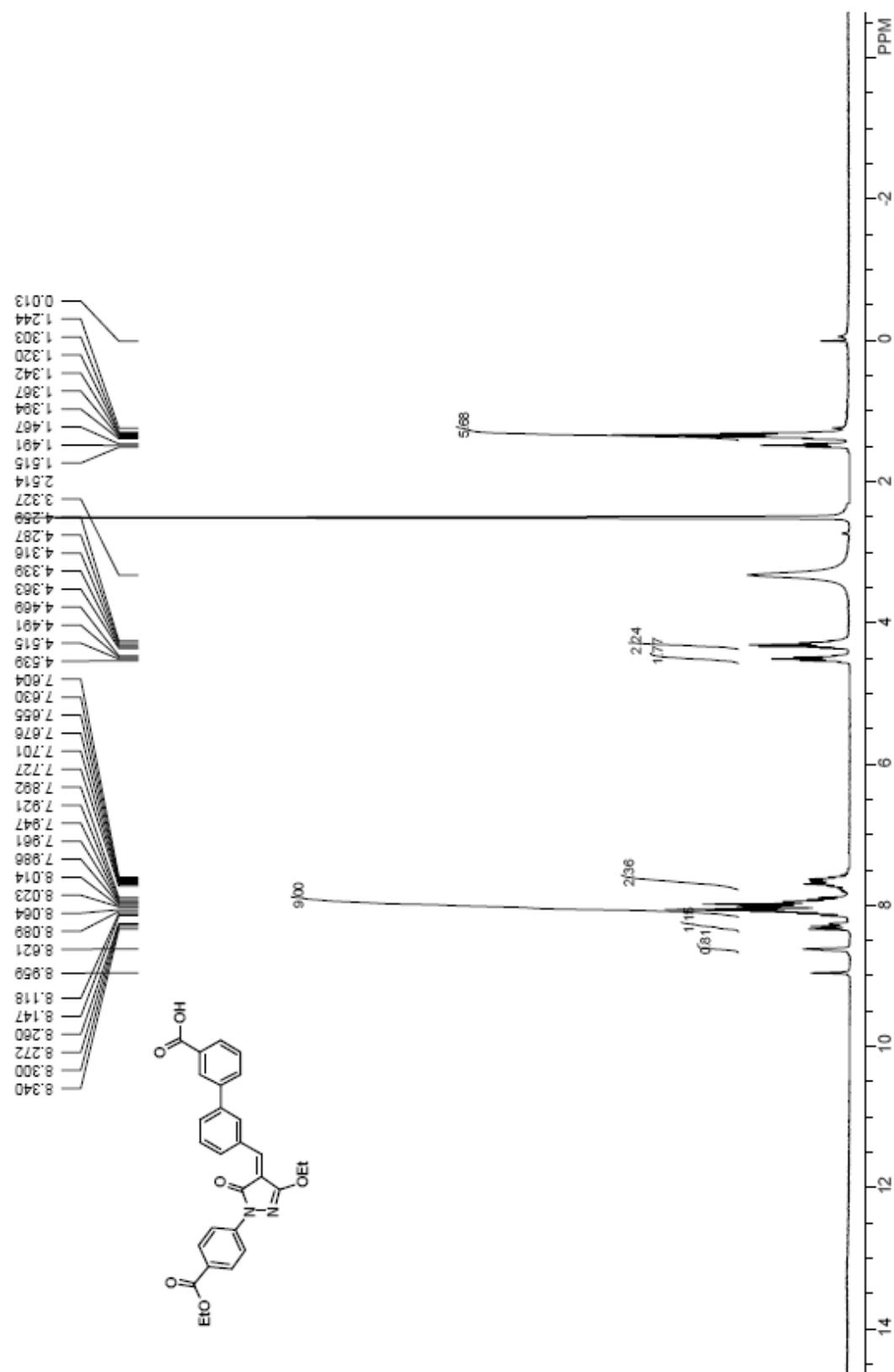
3'-(1-(4-(Ethoxycarbonyl)phenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)biphenyl-3-carbox

yllic acid (No. 1p).



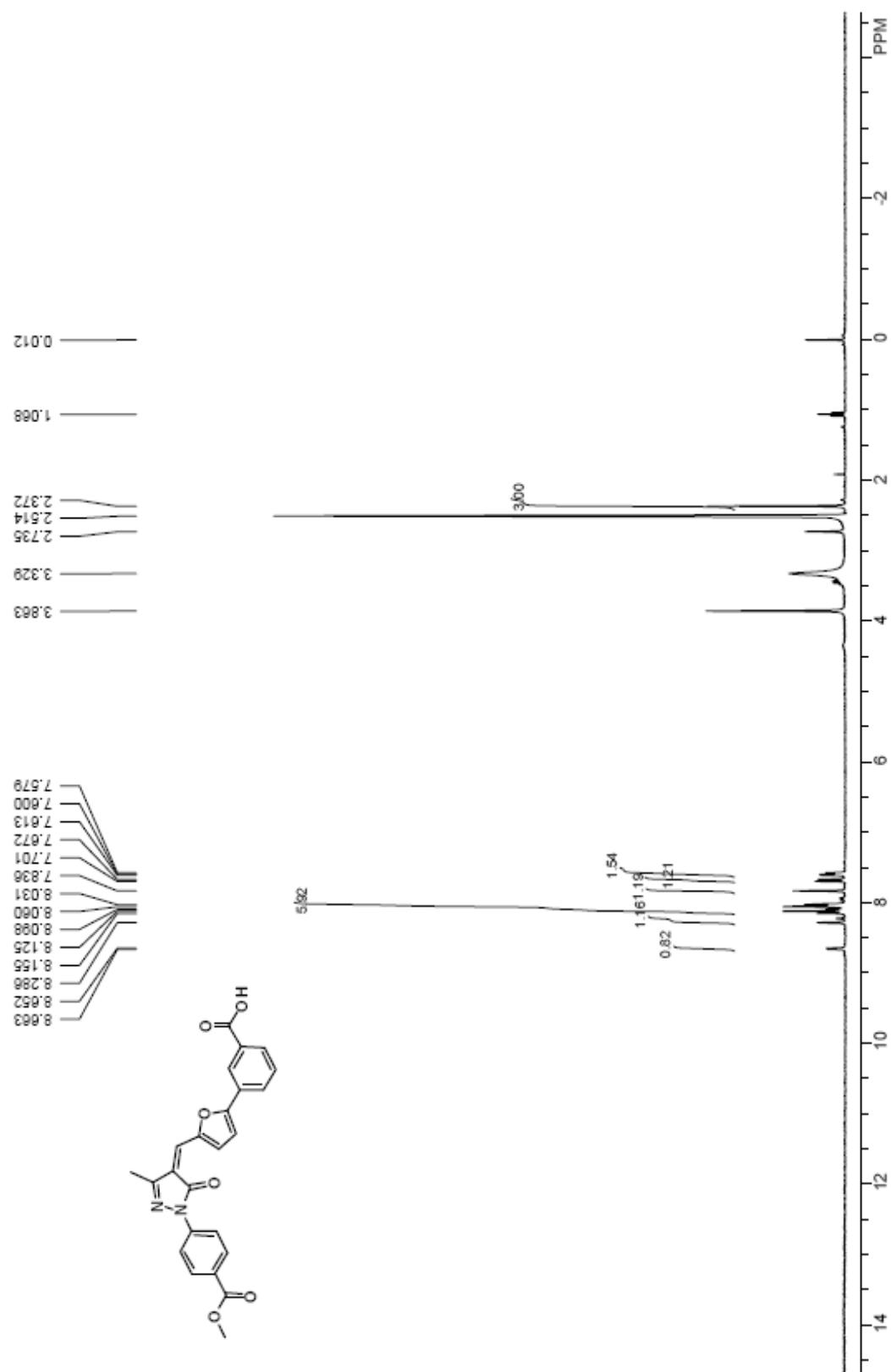
3'-(3-Ethoxy-1-(4-(ethoxycarbonyl)phenyl)-5-oxo-1H-pyrazol-4(5H)-ylidene)methyl)biphenyl

1-3-carboxylic acid (No. 1q).



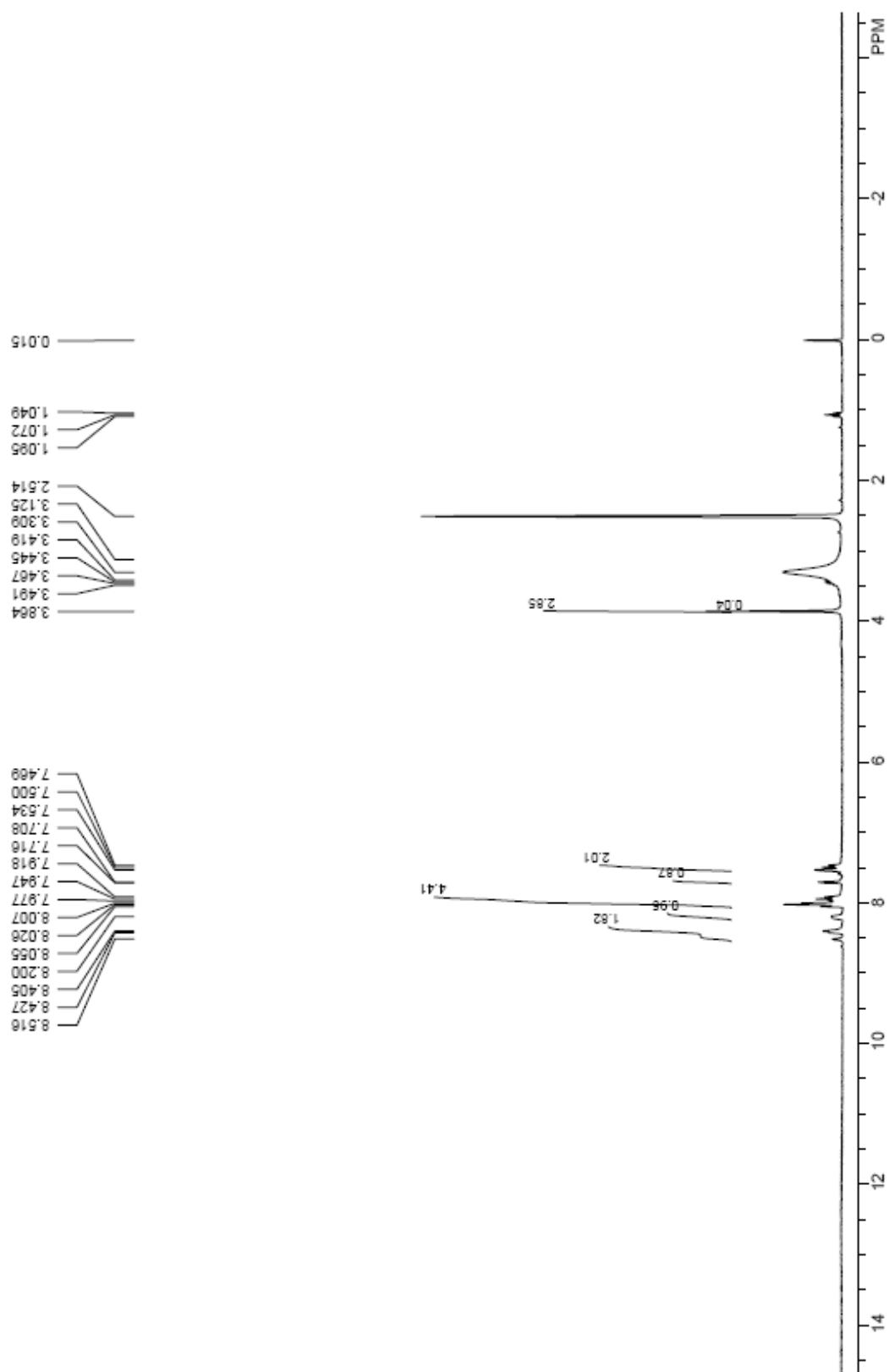
3-((1-(4-(Methoxycarbonyl)phenyl)-3-methyl-5-oxo-1H-pyrazol-4(5H)-ylidene)methyl)furan

an-2-yl)benzoic acid (No. 1r).



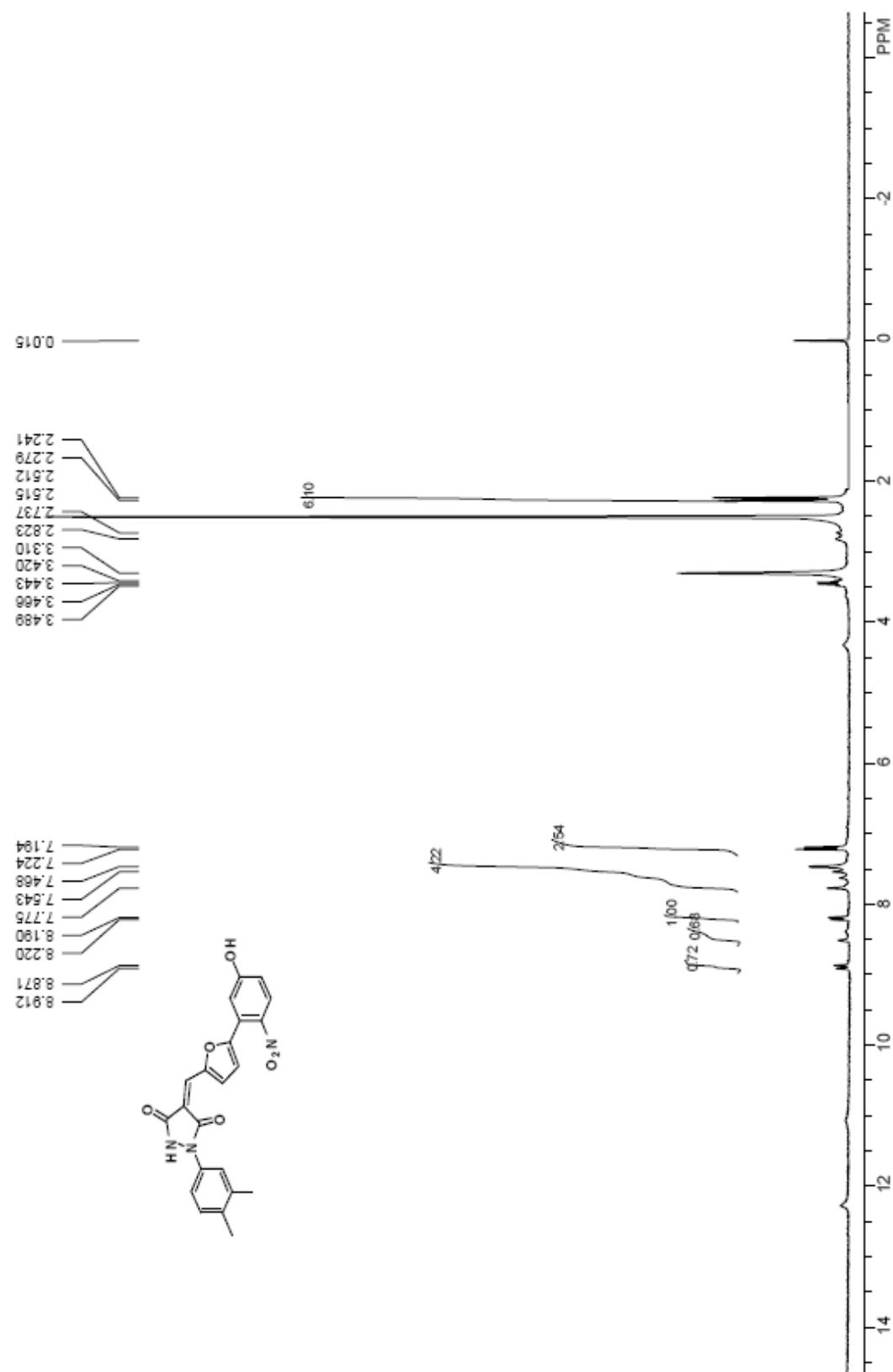
2-Fluoro-5-((1-(4-(methoxycarbonyl)phenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan

-2-yl)benzoic acid (No. 5a).



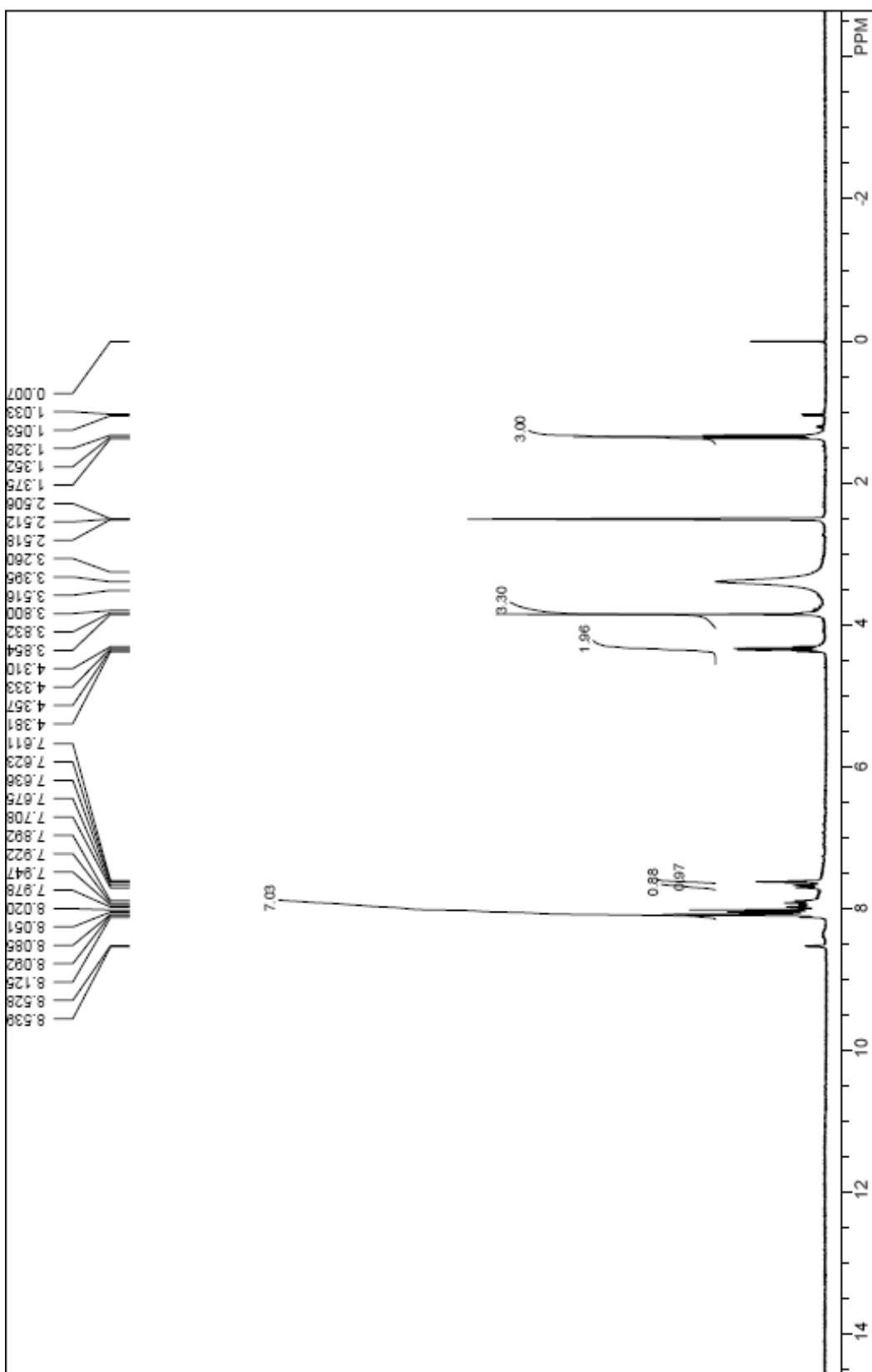
1-(3,4-Dimethylphenyl)-4-((5-(5-hydroxy-2-nitrophenyl)furan-2-yl)methylene)pyrazolidine-3

,5-dione (No. 5b).



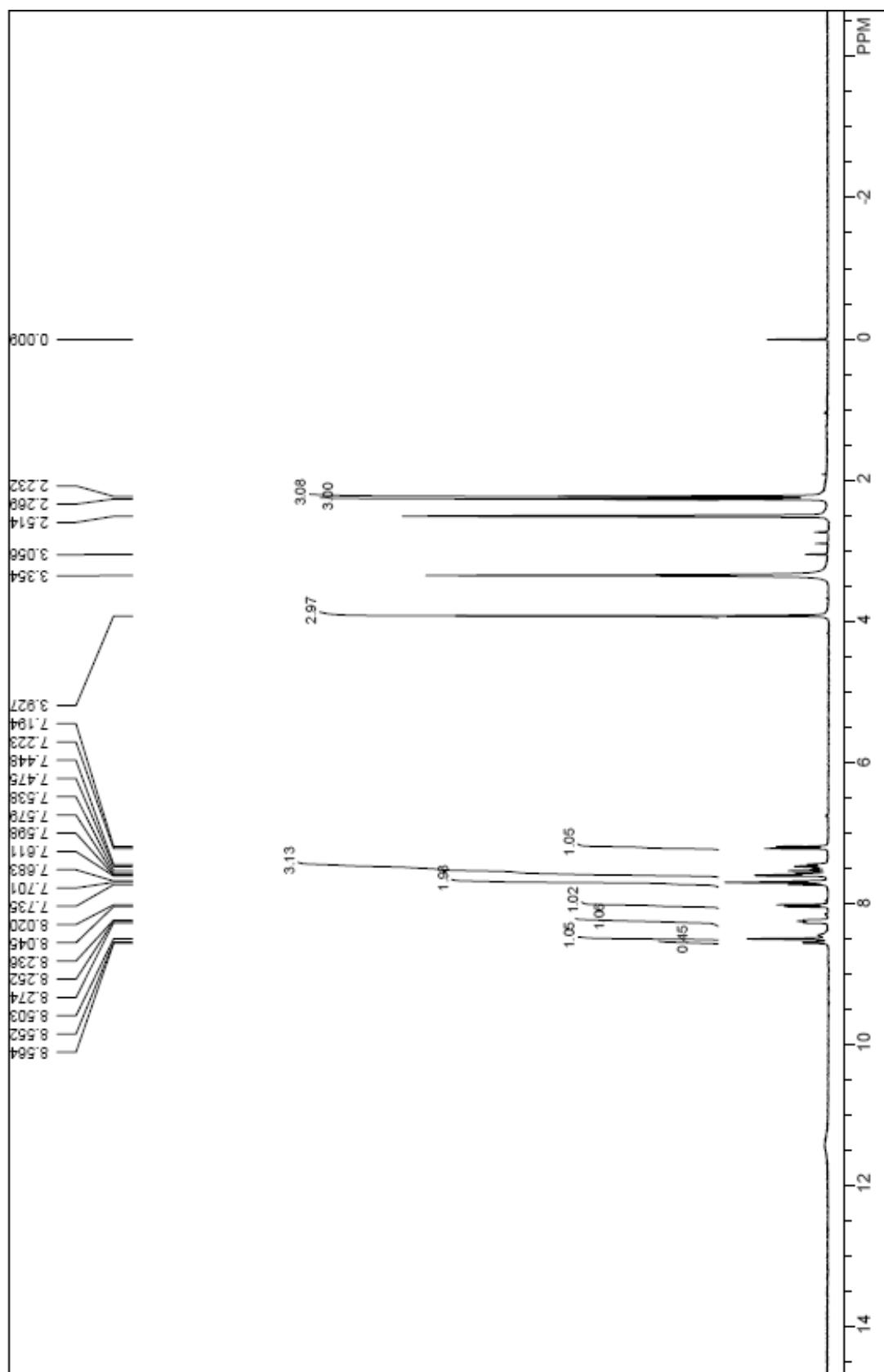
Ethyl 4-((1-(4-(methoxycarbonyl)phenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan-2-

yl)benzoate (No. 5c).



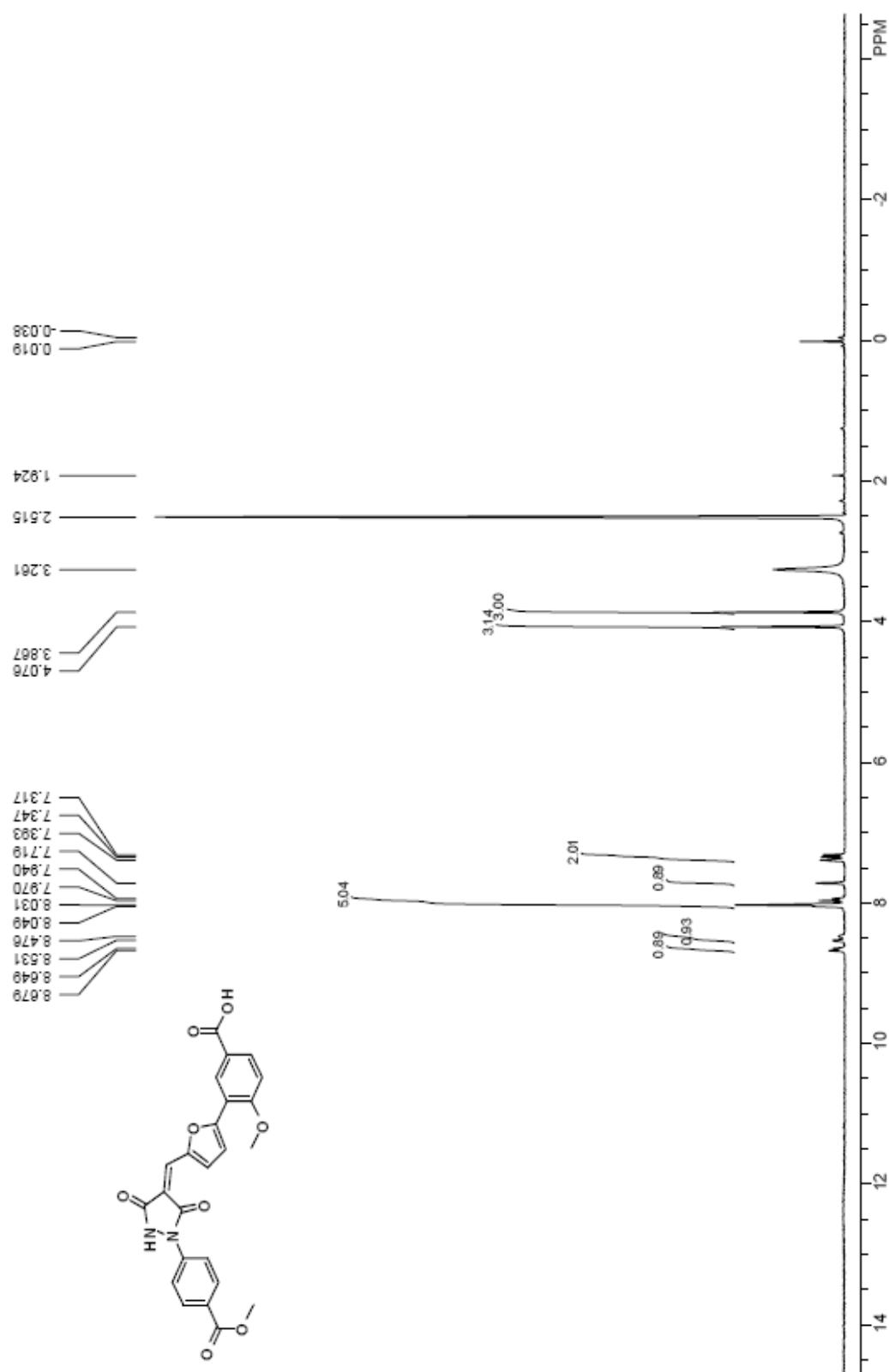
Methyl 3-((1-(3,4-dimethylphenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan-2-yl

benzoate (No. 5d).



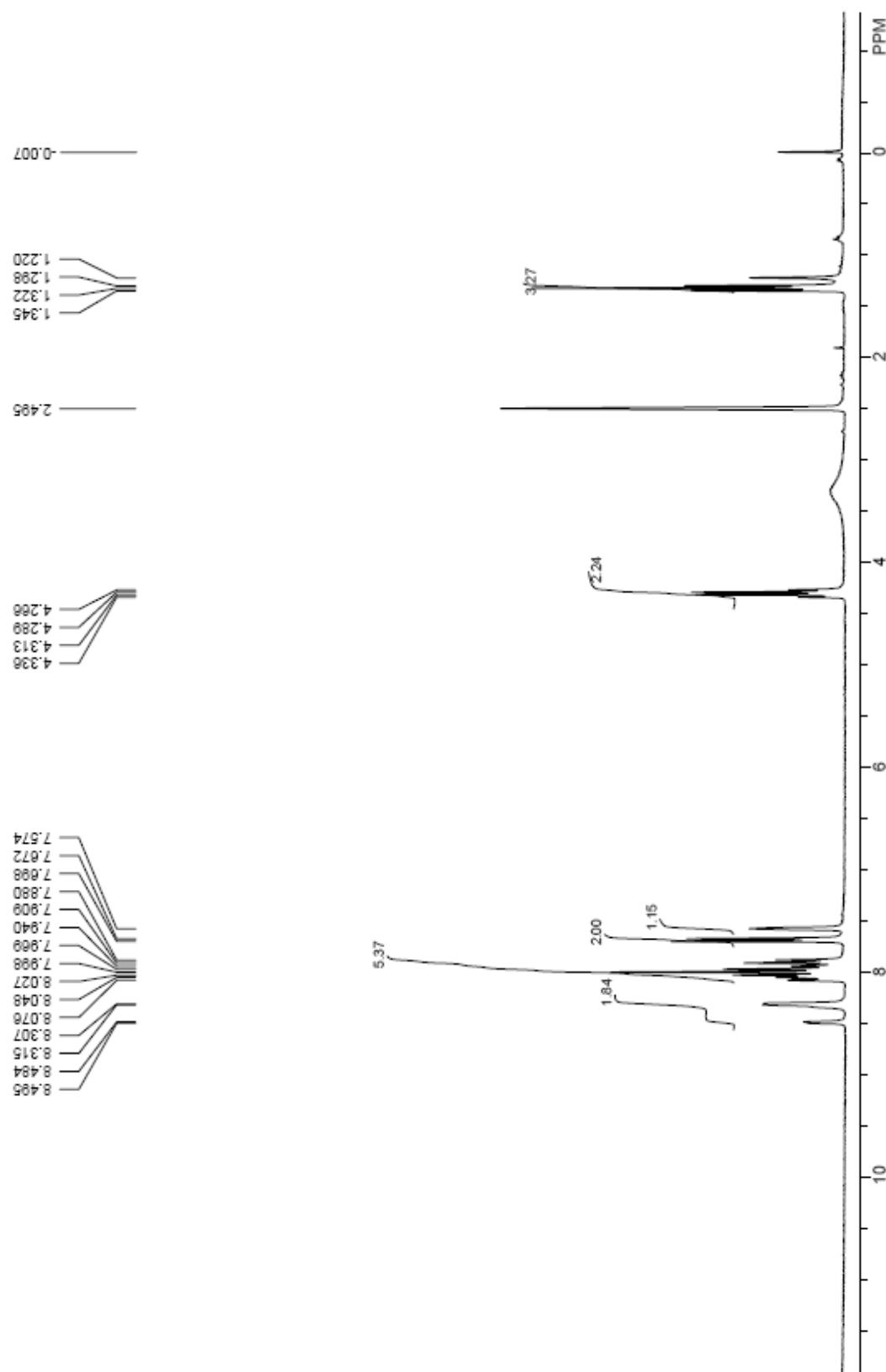
4-Methoxy-3-((1-(4-(methoxycarbonyl)phenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan

an-2-yl)benzoic acid (No. 5e).



5-((1-(4-(ethoxycarbonyl)phenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)furan-2-yl)-2-fluorobenzoic acid (No. 5e).

orobenzoic acid (No. 5f).



3'-(1-(4-(methoxycarbonyl)phenyl)-3,5-dioxopyrazolidin-4-ylidene)methyl)biphenyl-3-carbo

xrylic acid (No. 5g).

