

Supplementary Materials: Ethyl 4-(5-(methoxymethyl)furan-2-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

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Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

571 formula(e) evaluated with 27 results within limits (up to 3 best isotopic matches for each mass)

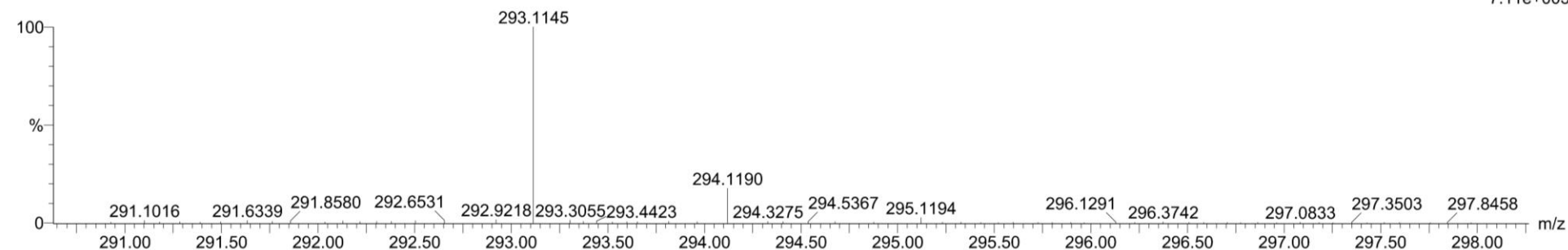
Elements Used:

C: 0-1000 H: 0-1000 N: 0-500 O: 0-500

standard

Salma-unair-DHPM8-neg 20 (0.679)

TOF MS ES-
7.11e+003



Minimum: -1.5
Maximum: 30.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
293.1145	293.1025	12.0	40.9	7.5	206.4	0.4	C15 H17 O6
	293.1137	0.8	2.7	7.5	207.1	1.2	C14 H17 N2 O5
	293.1250	-10.5	-35.8	7.5	210.1	4.1	C13 H17 N4 O4

Figure S1. HRESIMS spectra of Ethyl 4-(5-(methoxymethyl)furan-2-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate.

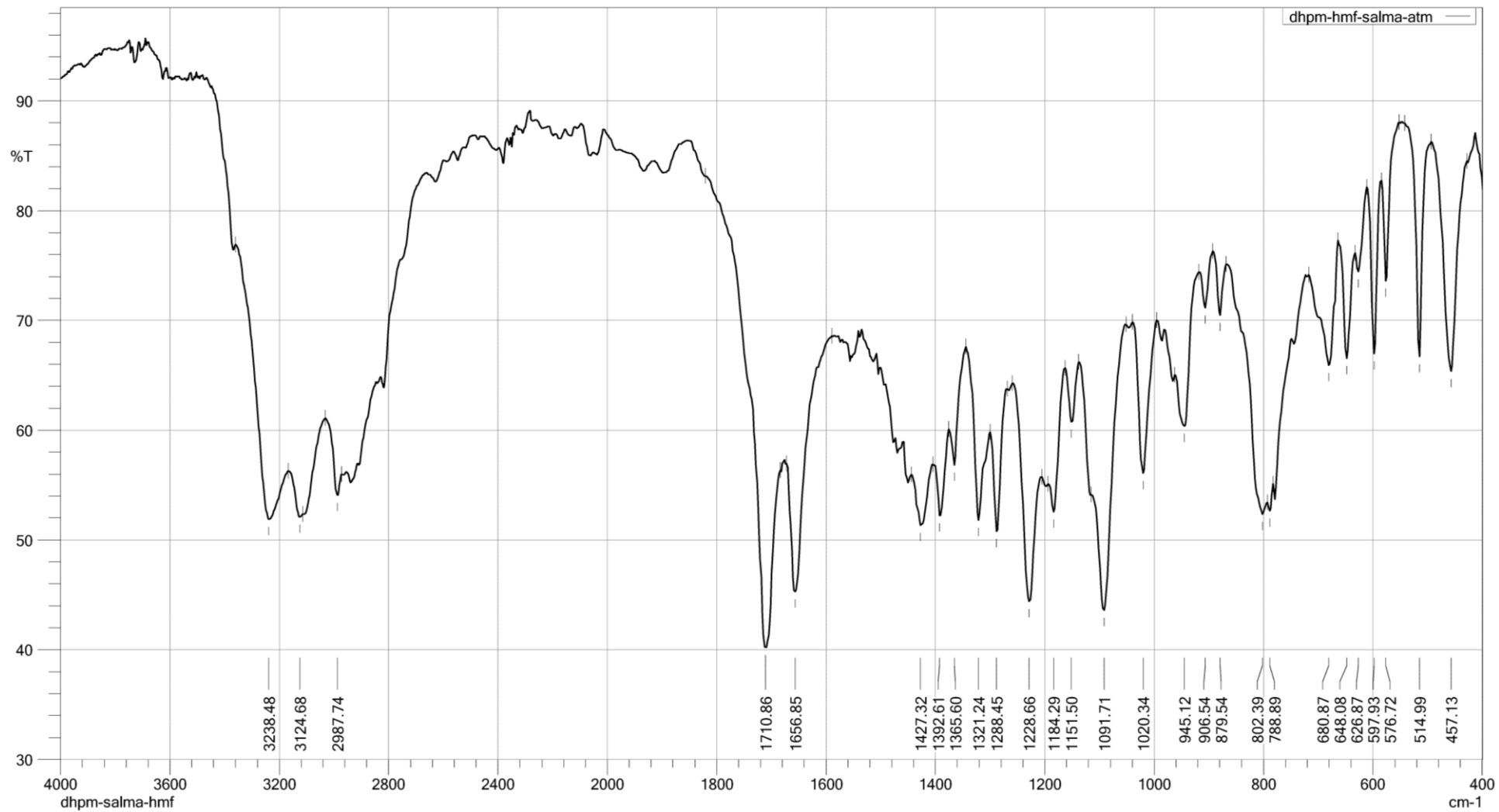


Figure S2. FTIR spectra of Ethyl 4-(5-(methoxymethyl)furan-2-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate.

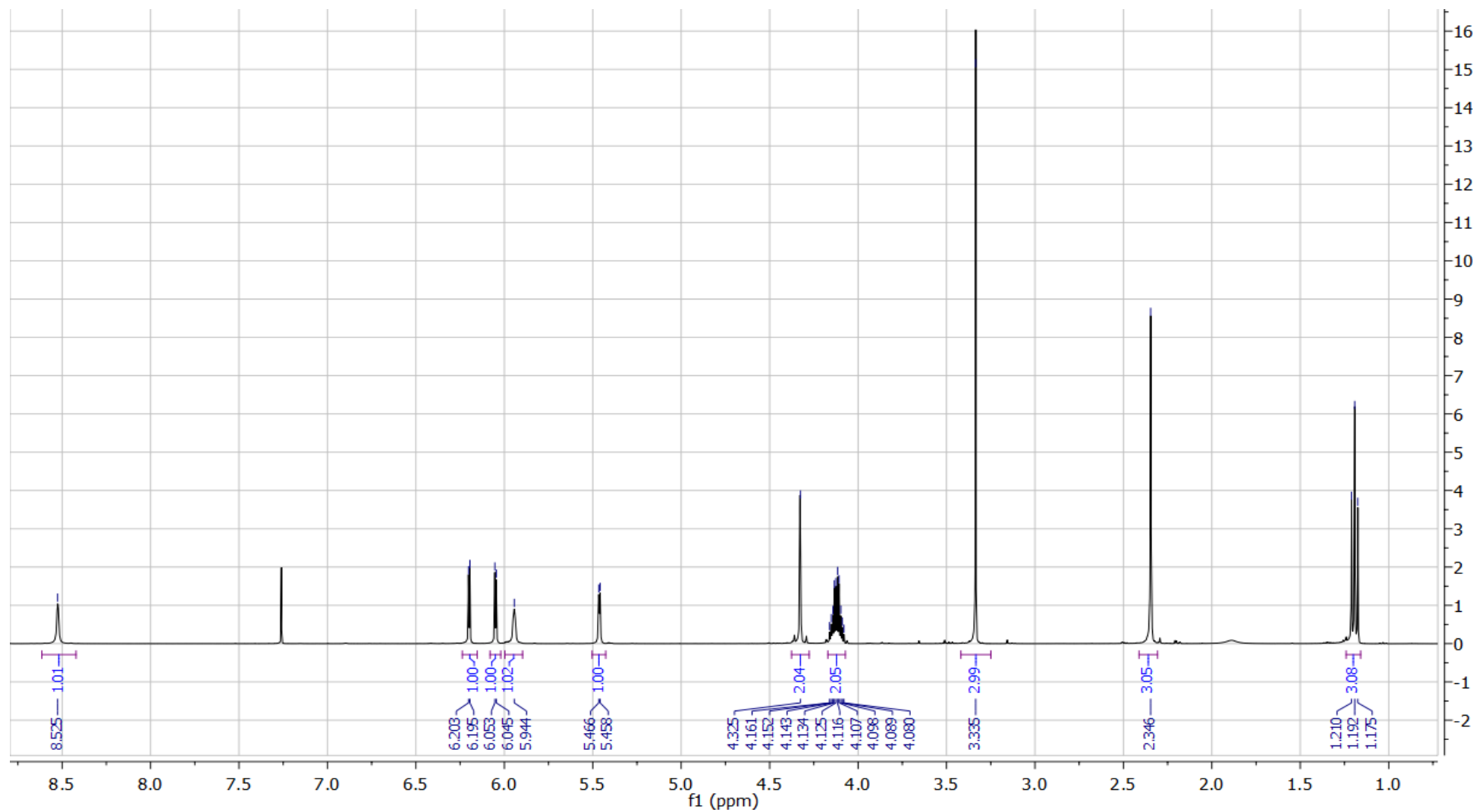


Figure S3. ¹H-NMR spectra of Ethyl 4-(5-(methoxymethyl)furan-2-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate in CDCl₃.

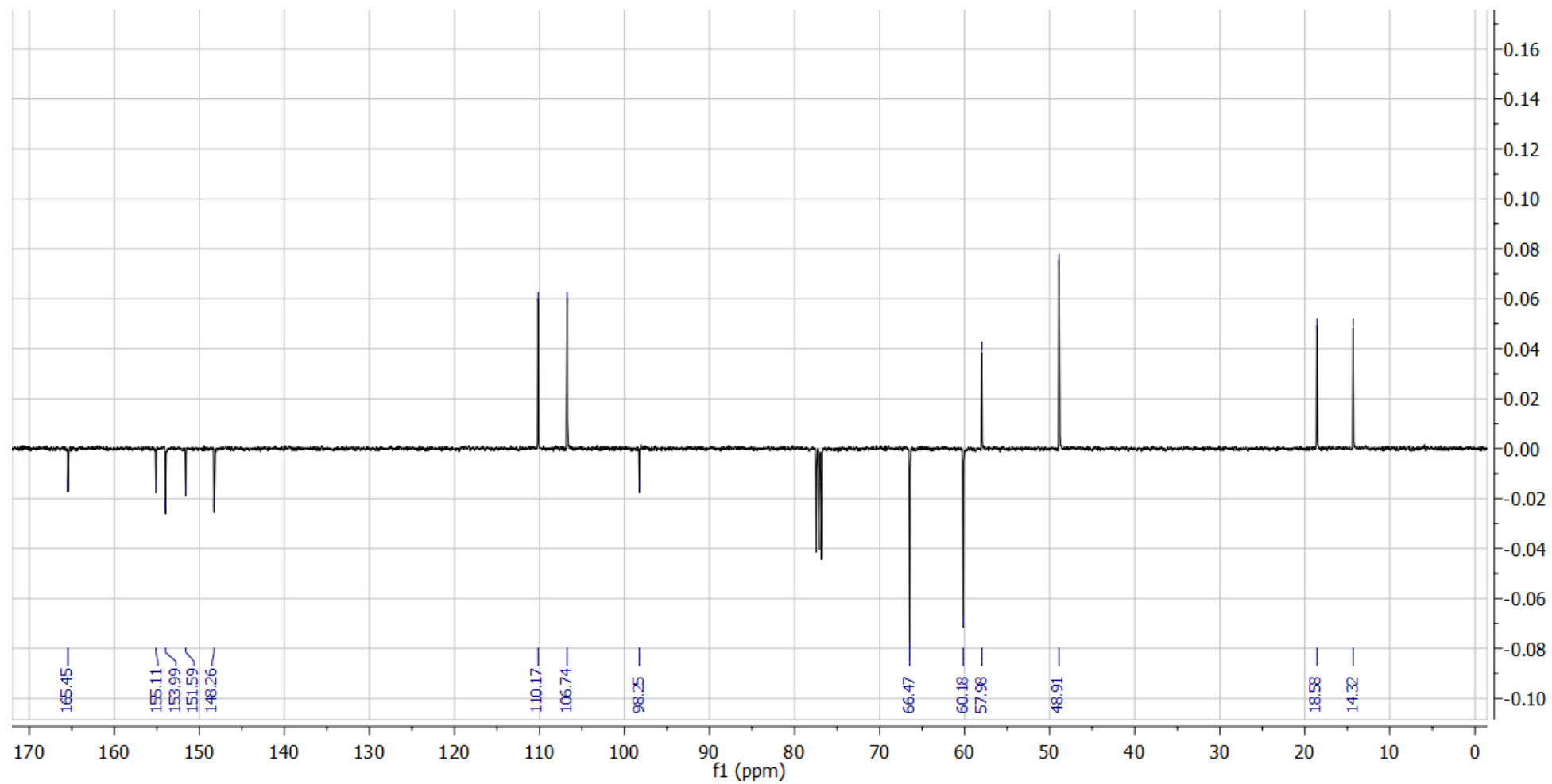


Figure S4. APT spectra of Ethyl 4-(5-(methoxymethyl)furan-2-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate in CDCl₃

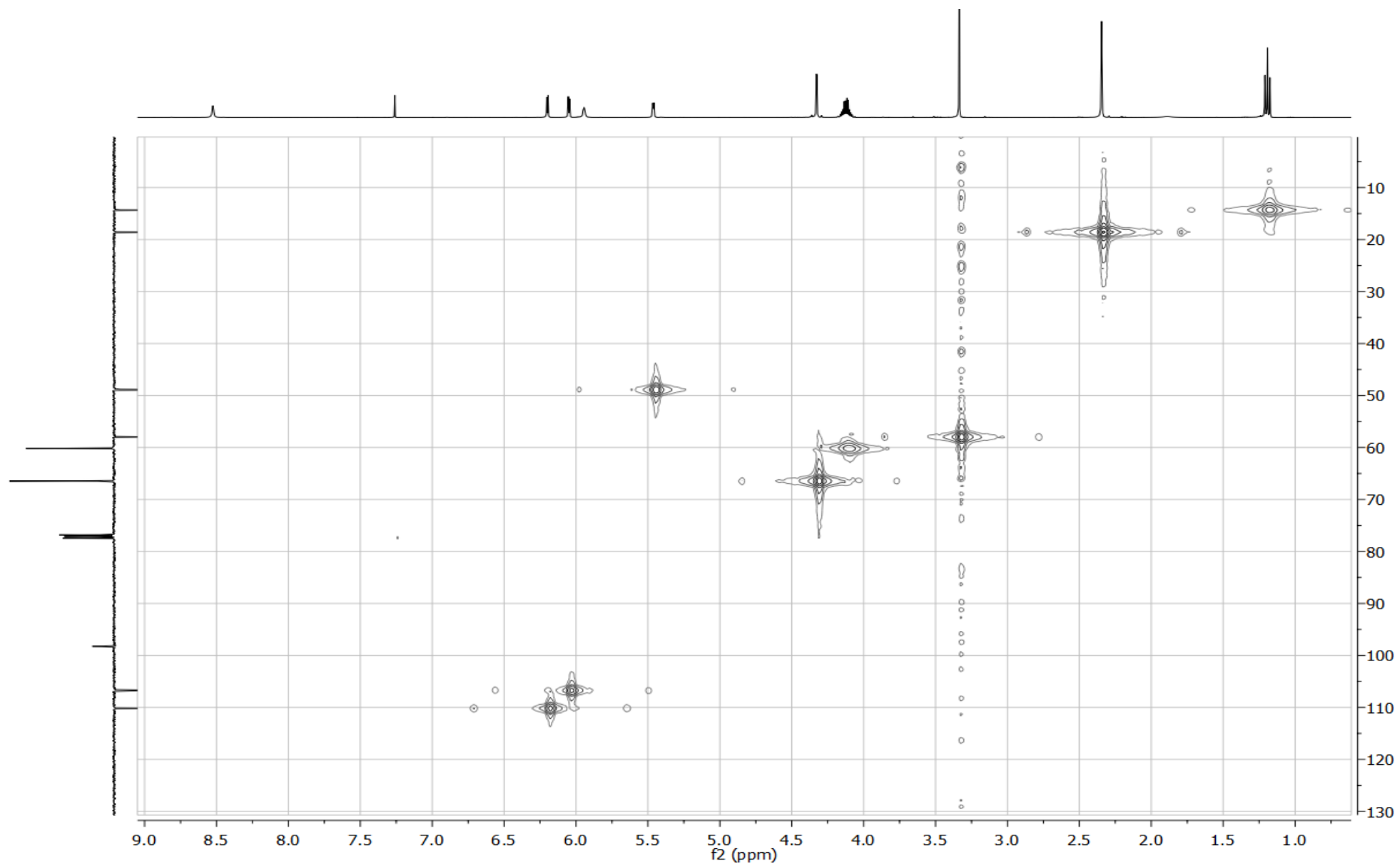


Figure S5. HMOC spectra of Ethyl 4-(5-(methoxymethyl)furan-2-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate.

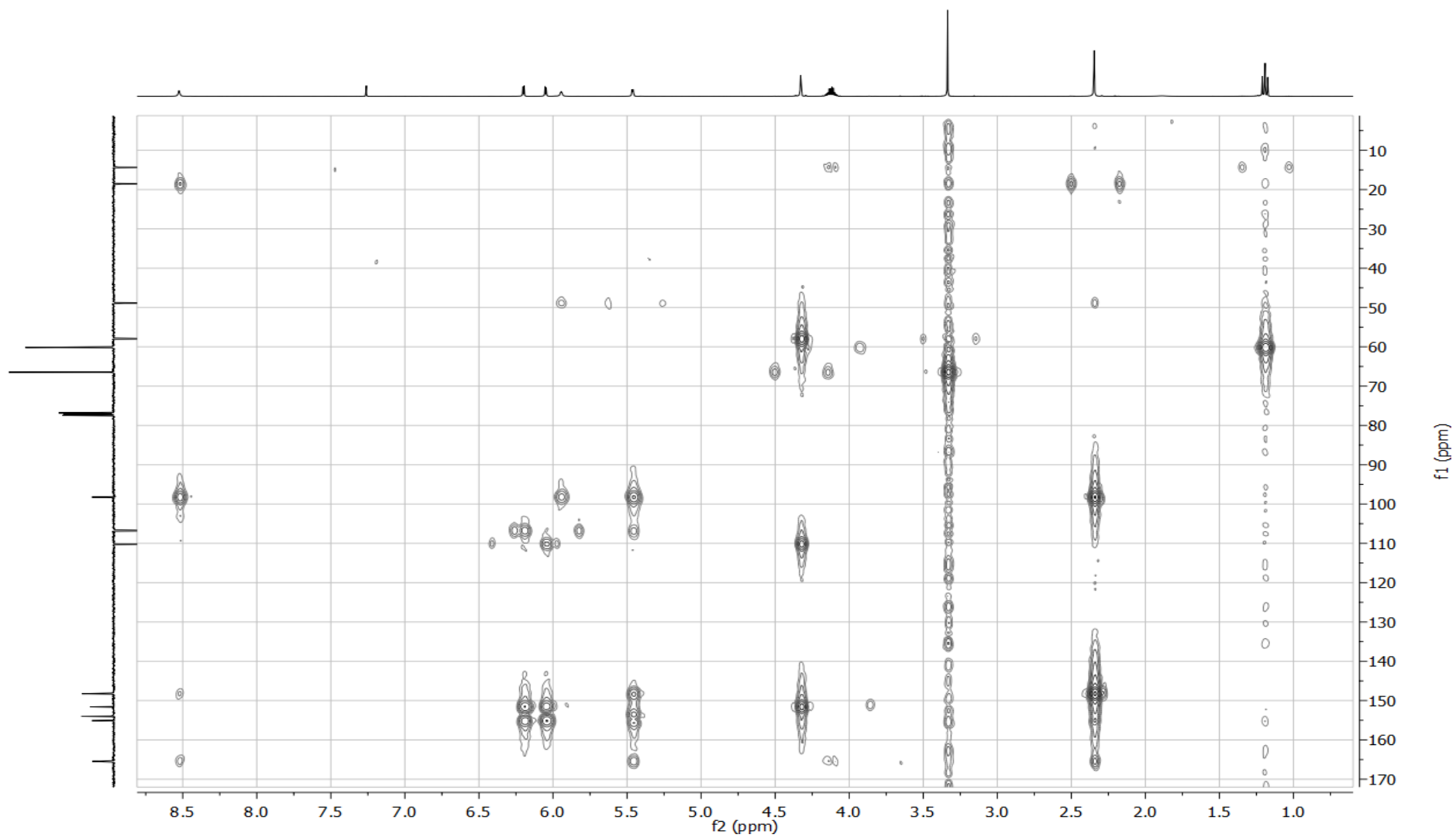


Figure S6. HMBC spectra of Ethyl 4-(5-(methoxymethyl)furan-2-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate.