

Supplementary Materials

# **(E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one**

Nicholas Bailey and Bradley O. Ashburn\*

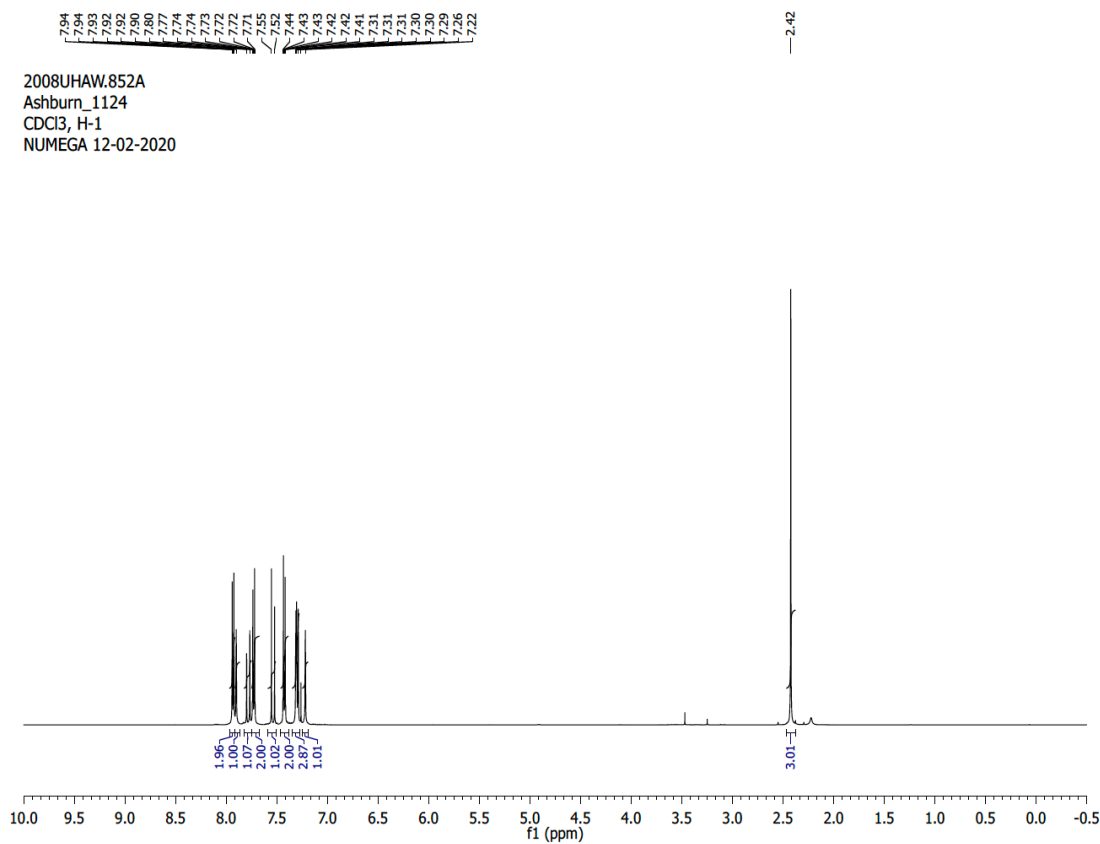


Figure S1. <sup>1</sup>H NMR of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (whole spectrum).

2008UHAW.852A  
 Ashburn\_1124  
 CDCl<sub>3</sub>, H-1  
 NUMEGA 12-02-2020

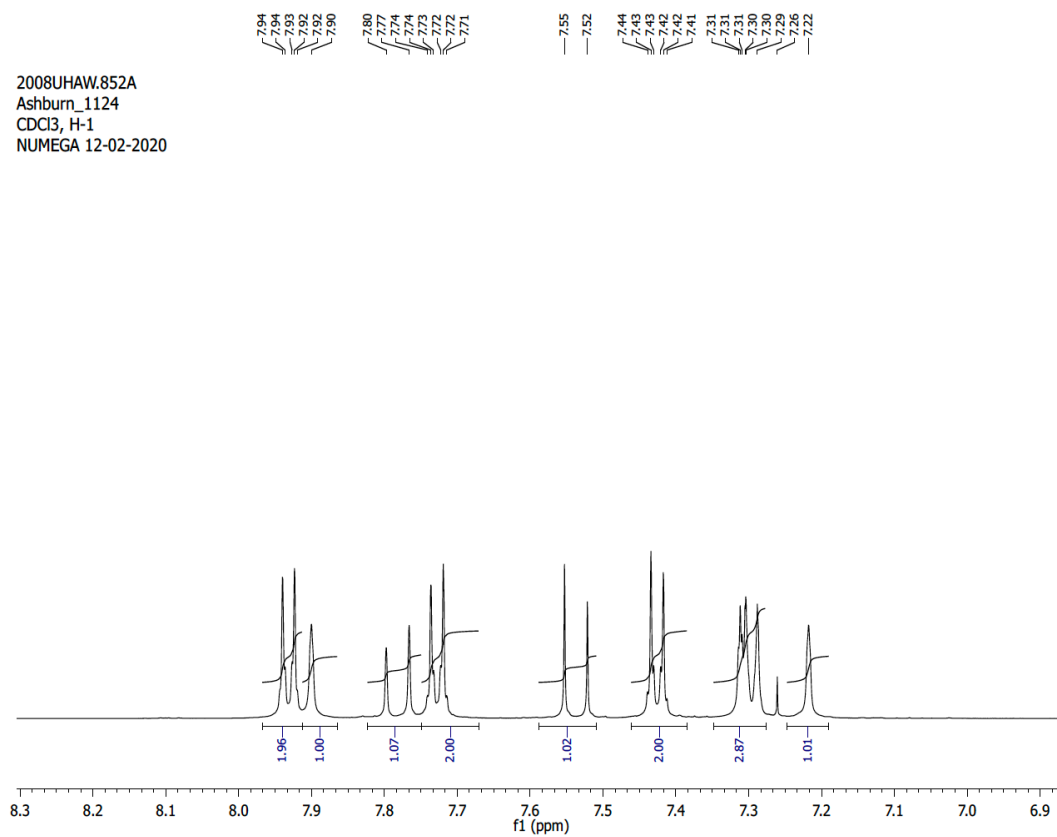


Figure S2. <sup>1</sup>H NMR of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (close up spectrum).

2008UHAW.852A  
 Ashburn\_1124  
 CDCl<sub>3</sub>, H-1  
 NUMEGA 12-02-2020

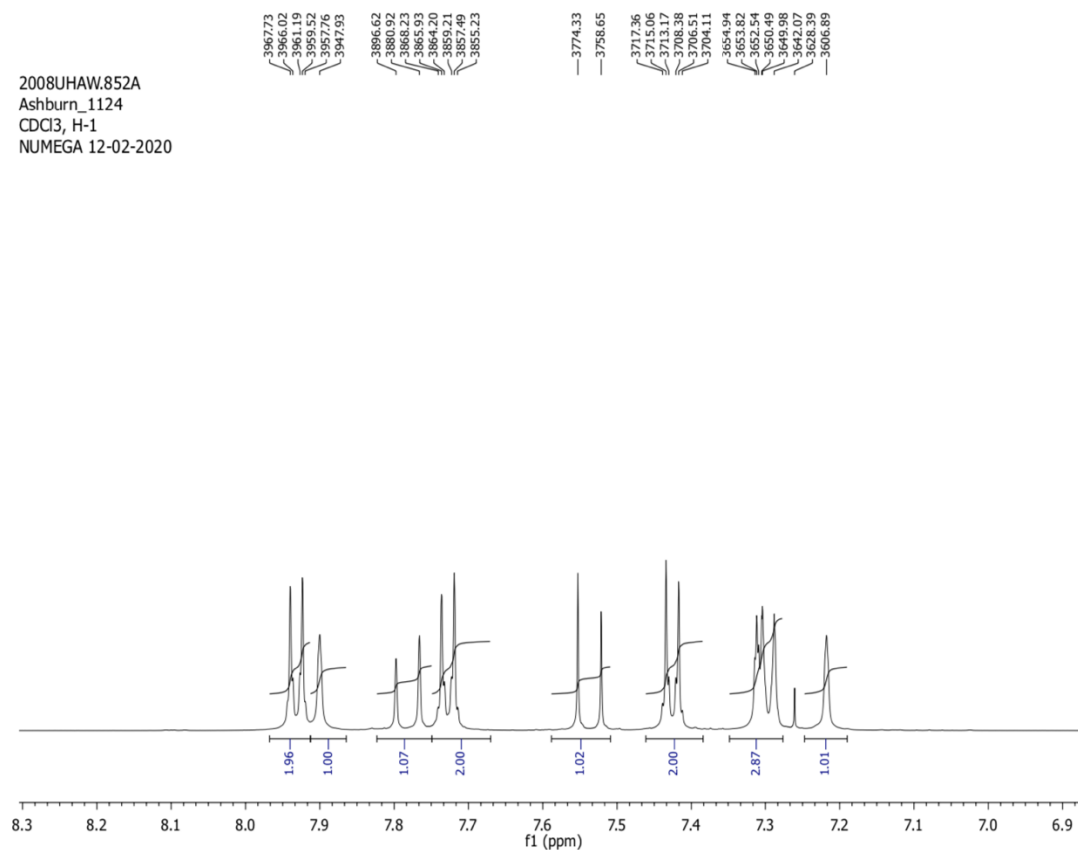


Figure S3. <sup>1</sup>H NMR of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (close up spectrum shown in Hz).

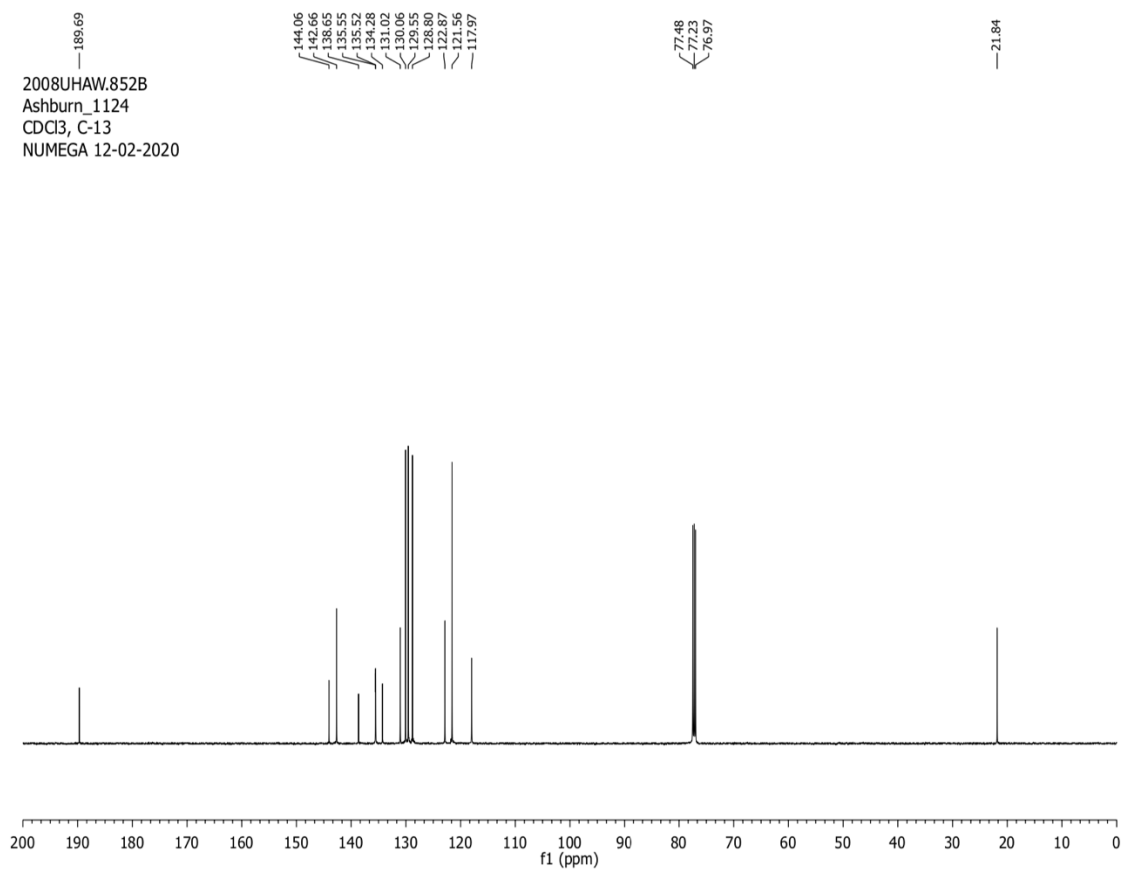


Figure S4. <sup>13</sup>C NMR of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (whole spectrum).

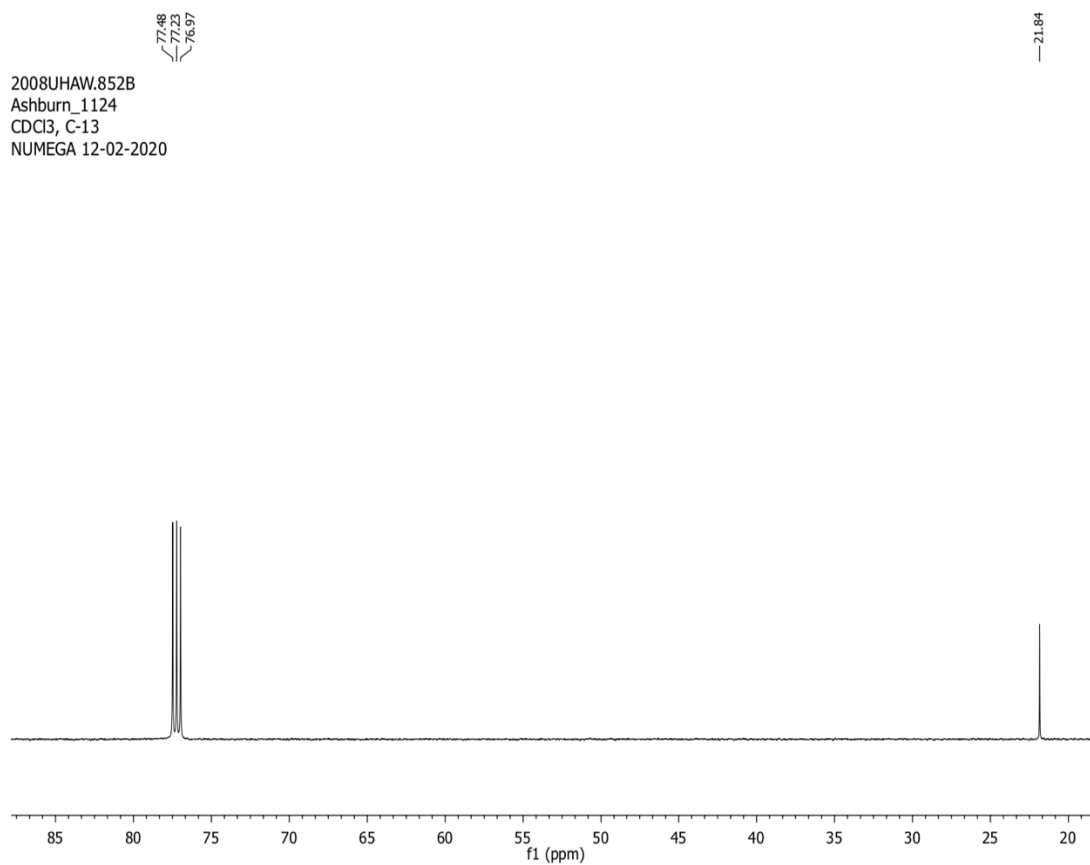


Figure S5. <sup>13</sup>C NMR of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (close up spectrum).

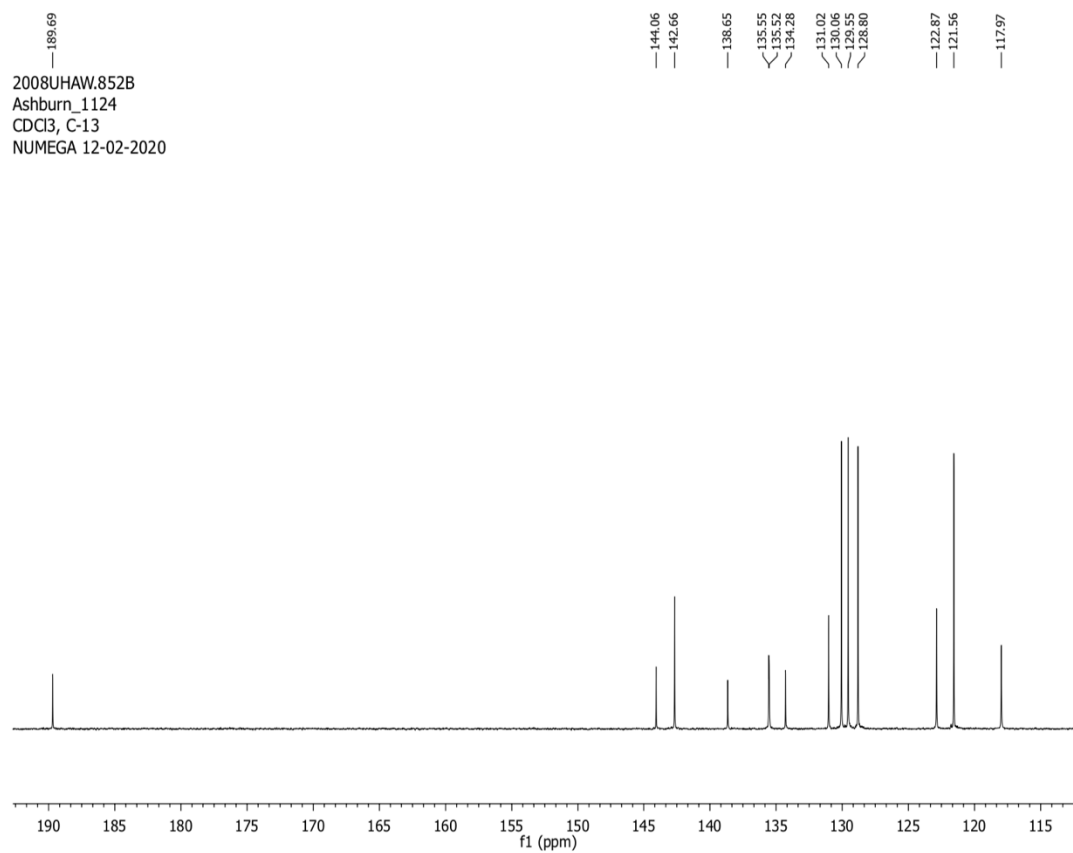


Figure S6. <sup>13</sup>C NMR of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (whole spectrum).

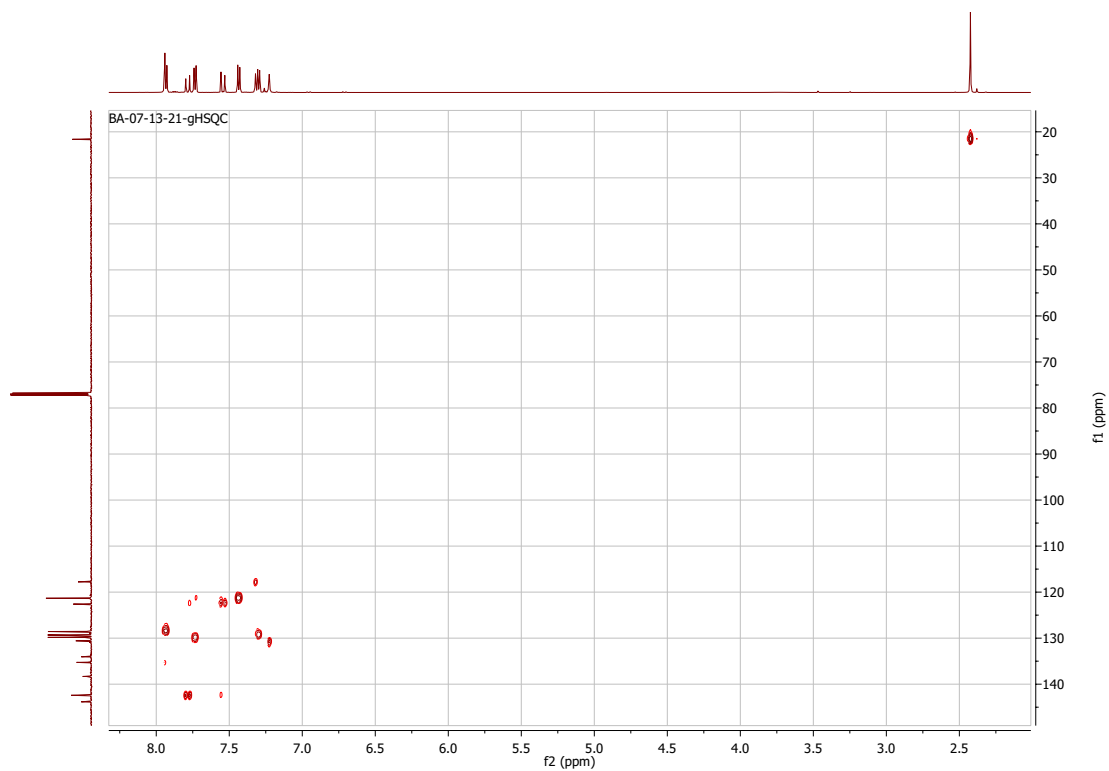


Figure S7. HSQC NMR of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (whole spectrum).

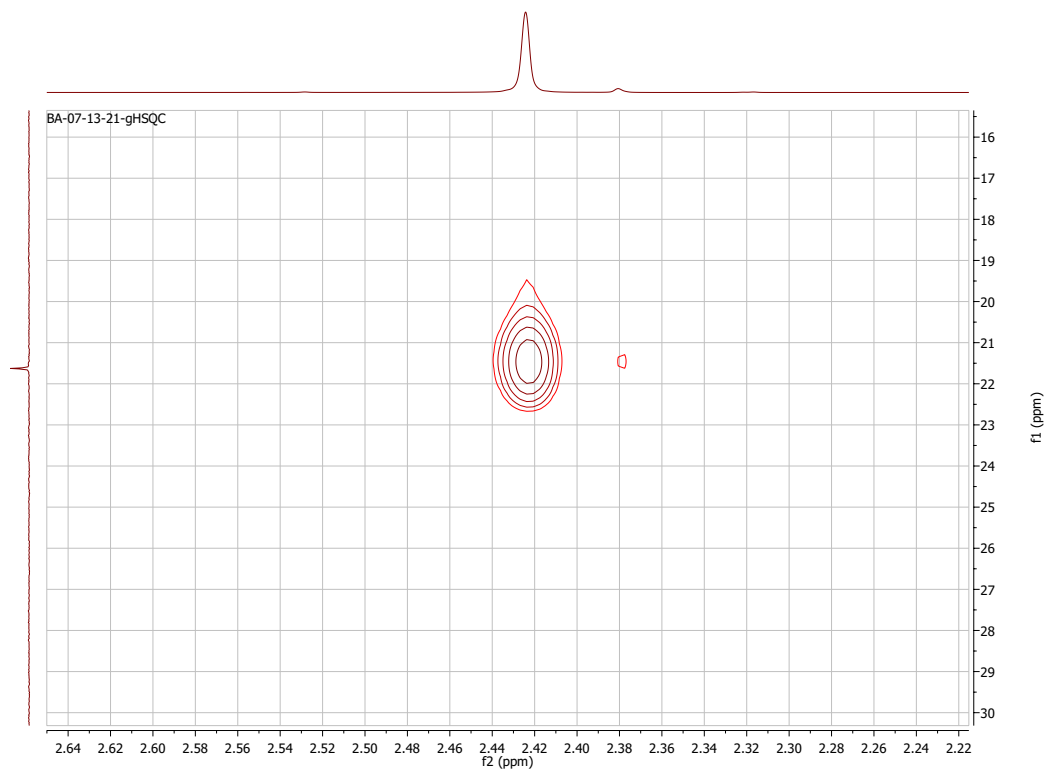


Figure S8. HSQC NMR of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (close up spectrum).



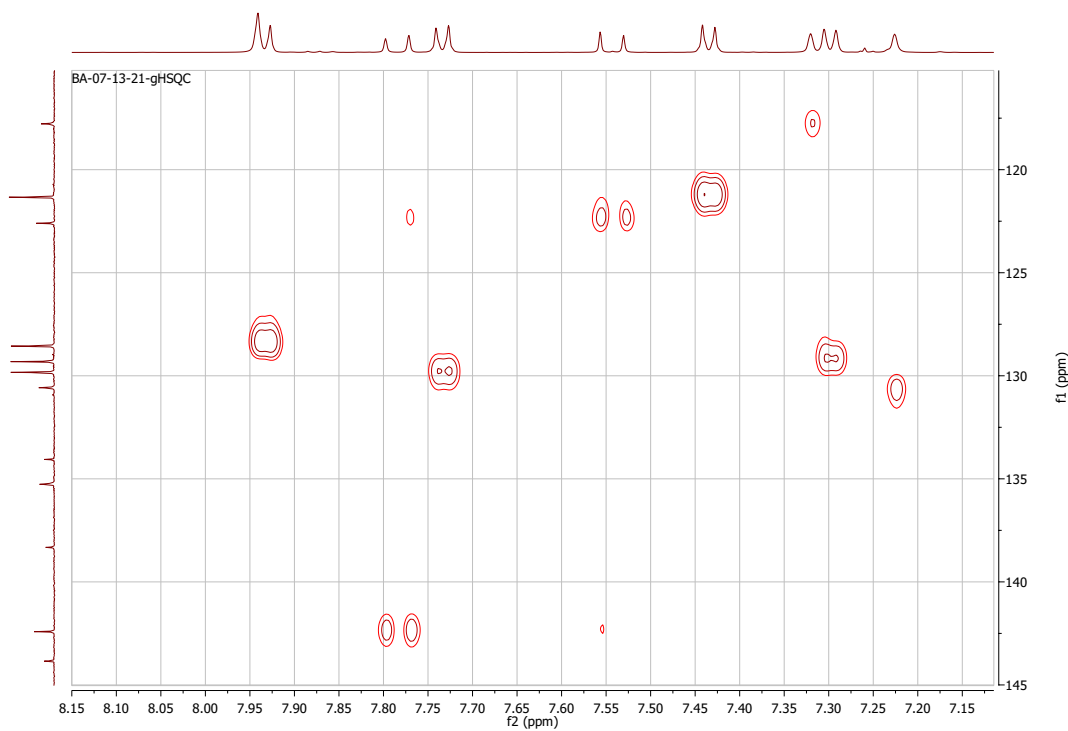


Figure S9. HSQC of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (close up spectrum)

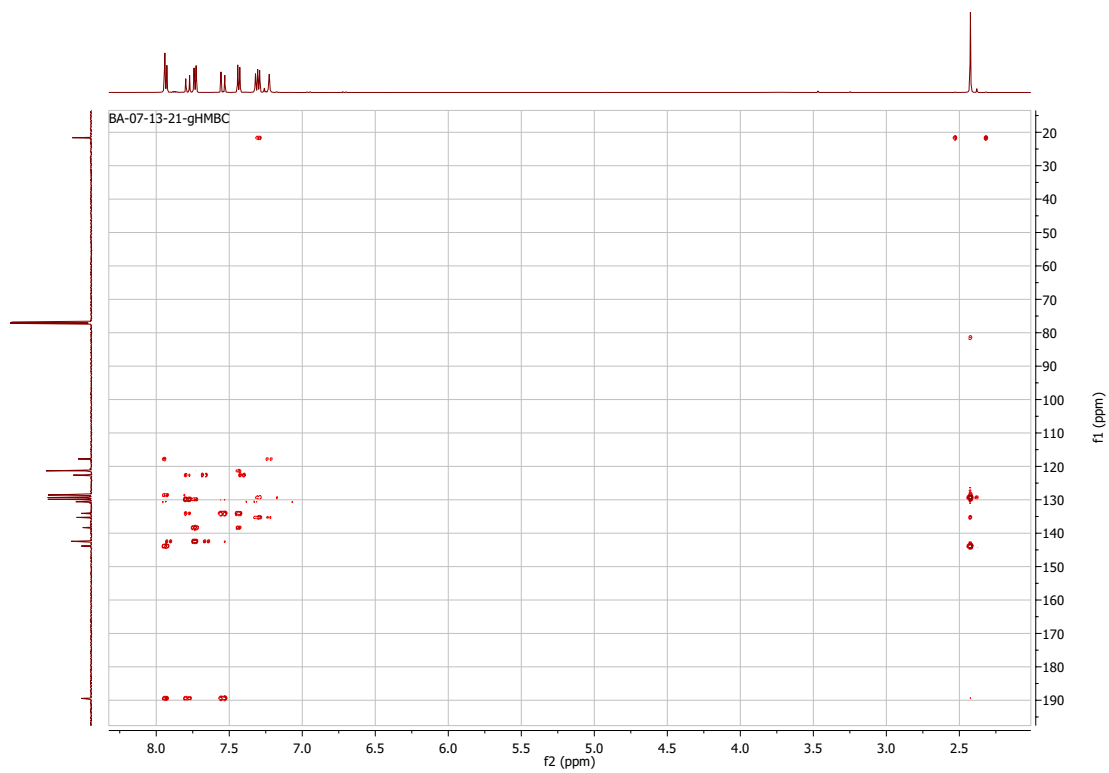


Figure S10. HMBC of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (whole spectrum)

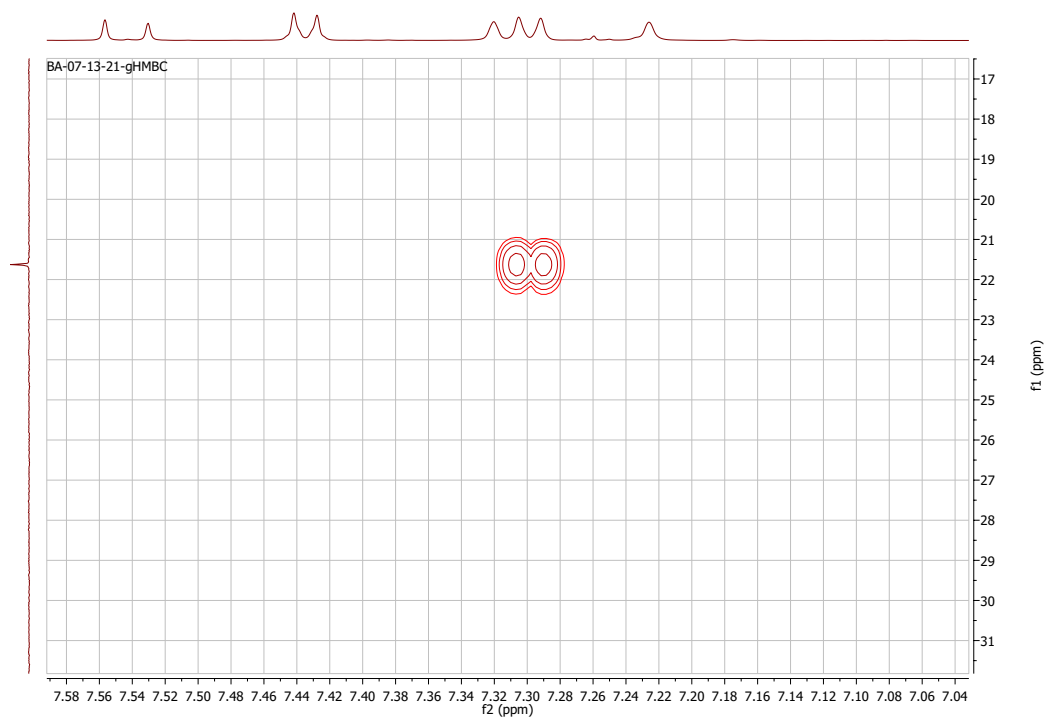


Figure S11. HMBC of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (close up spectrum)

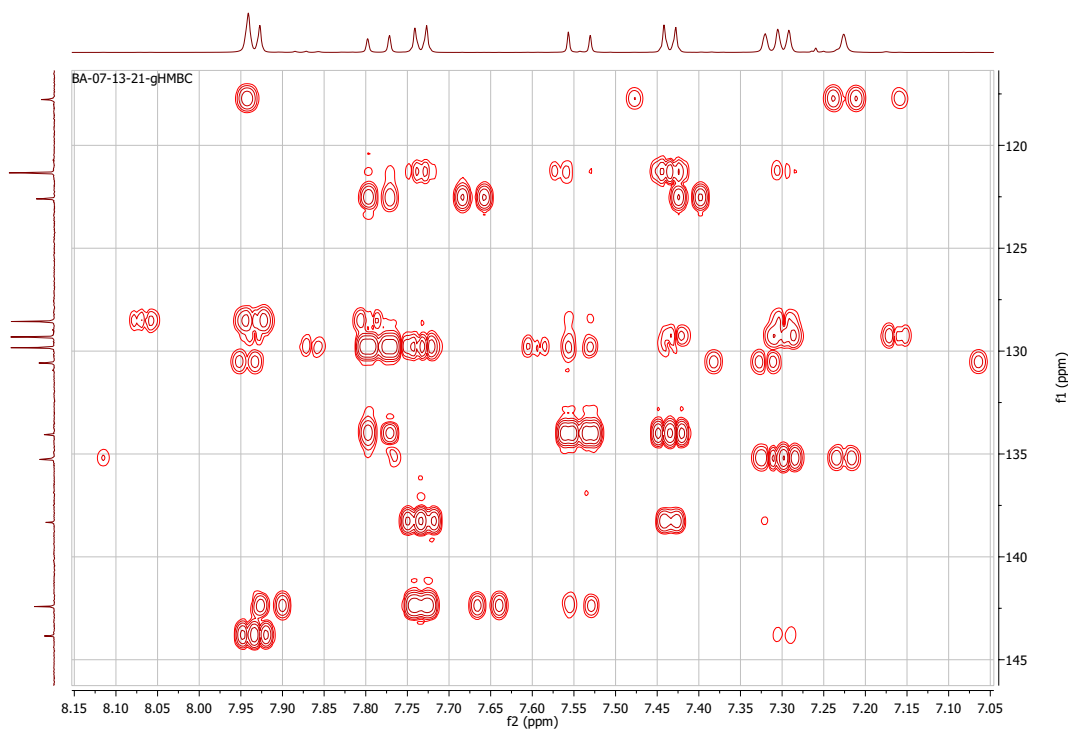


Figure S12. HMBC of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one (close up spectrum)

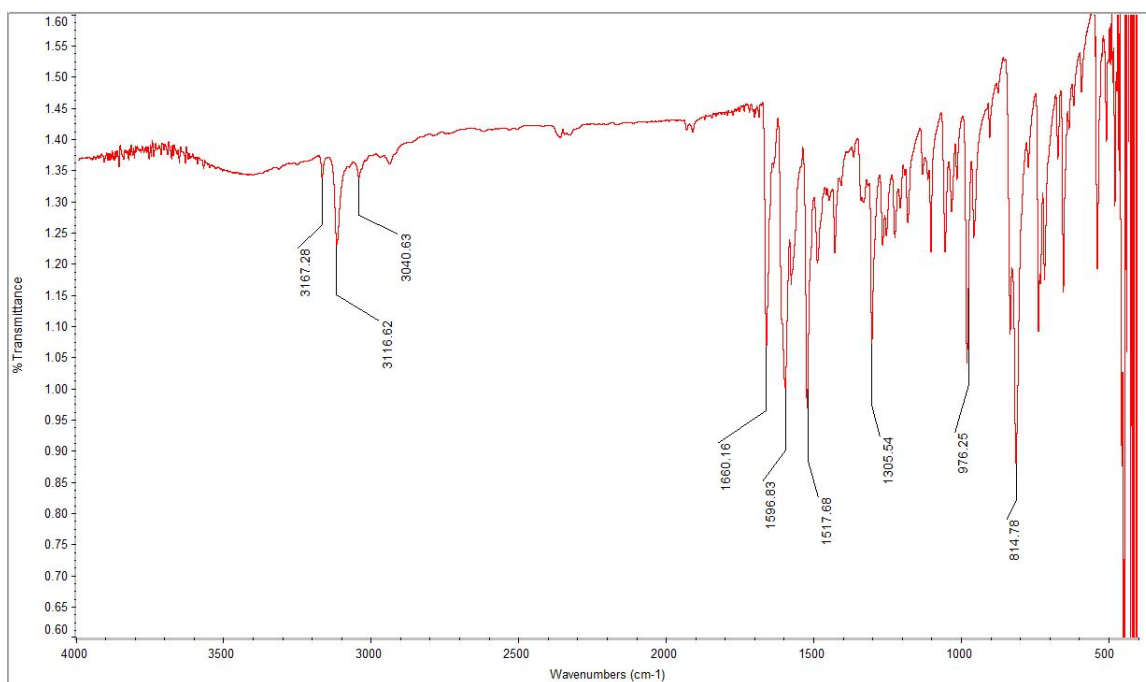
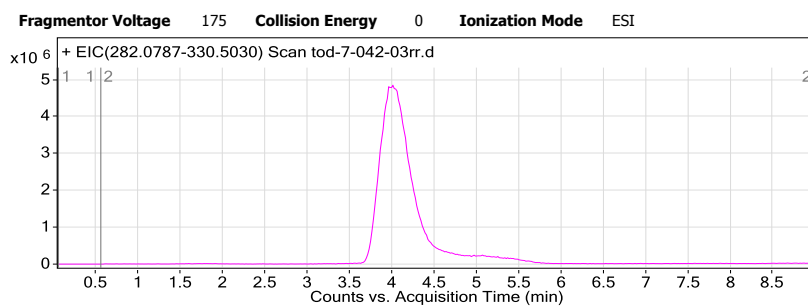
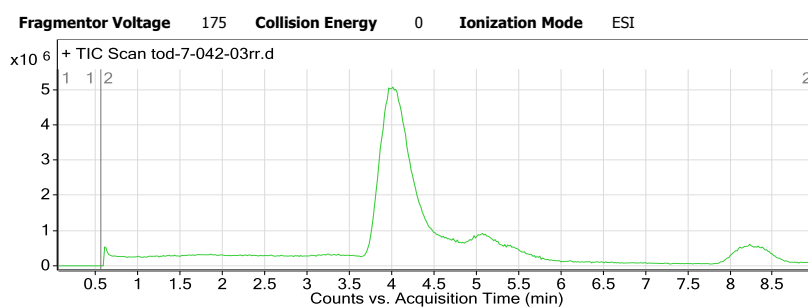


Figure S13. FTIR of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one.

## Qualitative Compound Report

<b>Data File</b>	tod-7-042-03rr.d	<b>Sample Name</b>	tod-7-042-03
<b>Sample Type</b>	Sample	<b>Position</b>	P1-D3
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	MS1-9min.m	<b>Acquired Time</b>	7/13/2021 4:31:34 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Metabolomics-Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Stream Name</b>	LC 1	<b>Acquisition SW</b>	6200 series TOF/6500 series
		<b>Version</b>	Q-TOF B.06.01 (B6157)



**Compound Table**

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C19 H16 N2 O	4.017	288.12531	1463320	C19 H16 N2 O	288.12626	-3.3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H16 N2 O	289.1325	4.017	Find By Formula	288.12531

Figure S14. ESI-MS of (E)-3-[4-(1H-imidazol-1-yl)phenyl]-1-(4-methylphenyl)prop-2-en-1-one.