

UiO-67 Metal-organic framework immobilized Fe³⁺ catalyst for efficient Morita-Baylis-Hillman reaction

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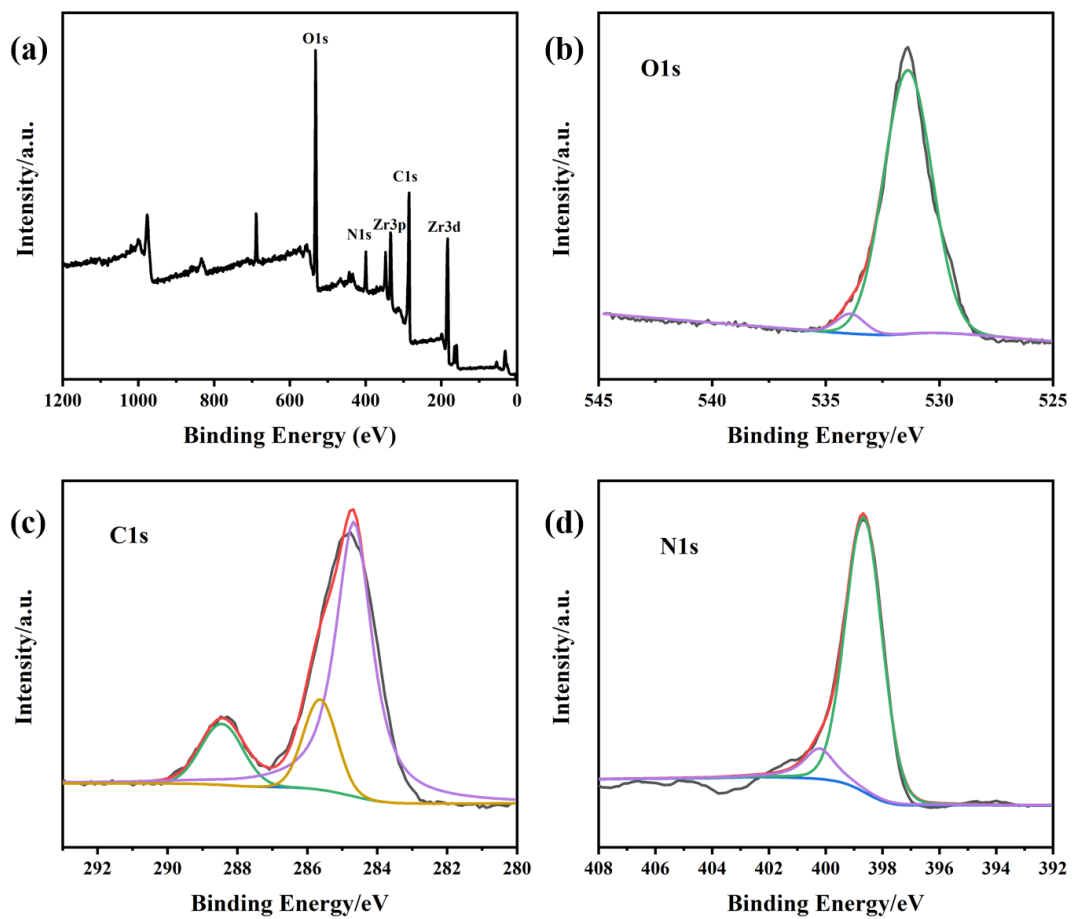


Fig. S1 XPS spectra of UiO-67

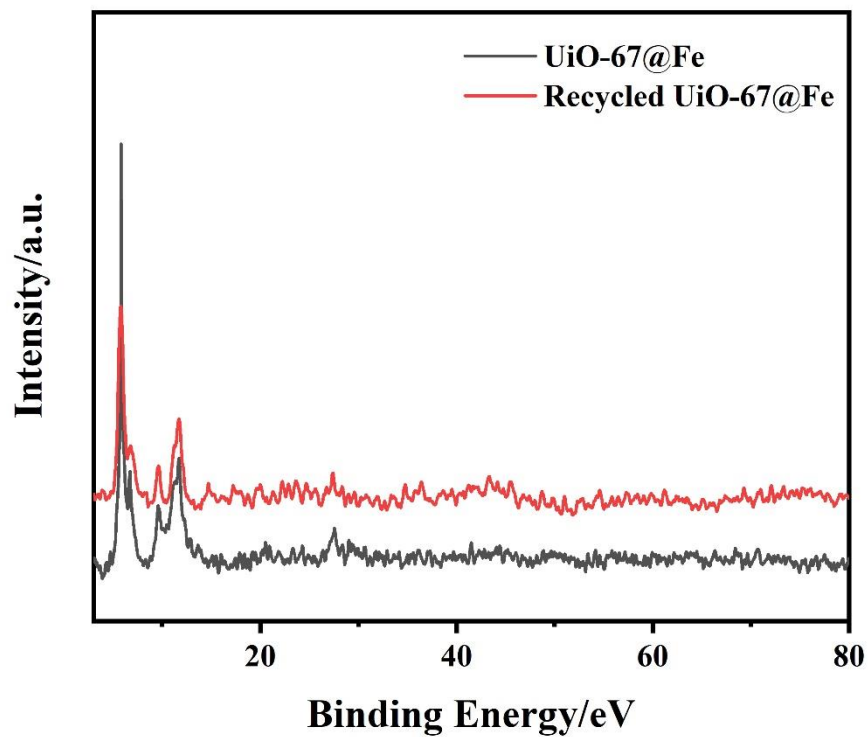


Fig. S2 PXRD pattern of UiO-67@Fe and recycled UiO-67@Fe

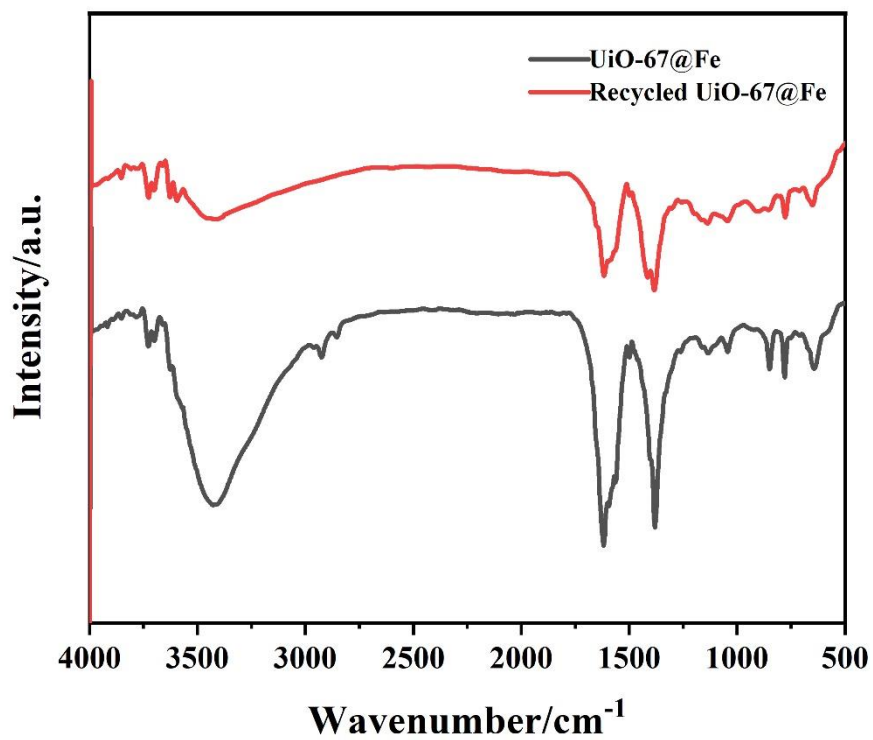


Fig. S3 FT-IR pattern of UiO-67@Fe and recycled UiO-67@Fe

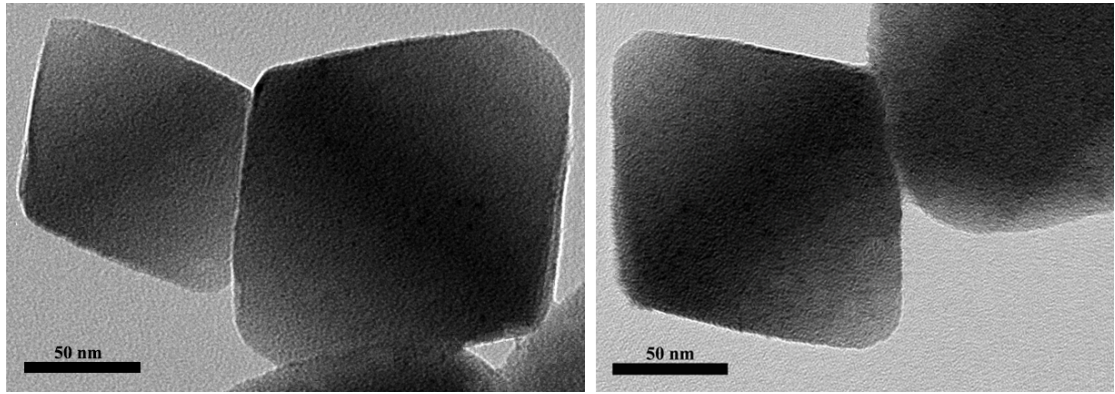
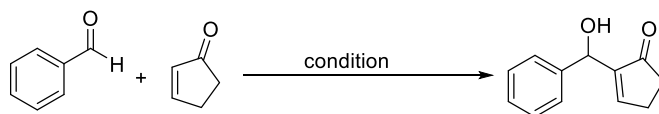


Fig. S4 TEM observation of UiO-67

Table S1 Various catalysts of MBH reaction of cyclopentenone with benzaldehyde.

Entry	Catalyst	Solvent	Time (h)	Temp. (°C)	Yield (%)	TON ^a	TOF (h ⁻¹) ^b	References
1	UiO-67@Fe (1.0 mol%)	THF	6	23	93	93	15.5	This work
2	NMP (5.0 mol%)/Ba(OH) ₂ (1.5 mol%) ^[1]	CH ₃ OH /CH ₂ Cl ₂	9	0	72	48	5.3	[1]
3	α-ZrP/Uracil/Cu ²⁺ (20mg) ^[2]	DMF	15	r.t.	74	-	-	[2]
4	Fu (+)-DMAP/(10mol%) MgI ₂ (50mol%) ^[3]	<i>i</i> -PrOH	24	-20	87	8.7	0.36	[3]
5	IRMOF-3-thiourea (2 mol%) ^[4]	THF	24	4	73	36.5	1.52	[4]

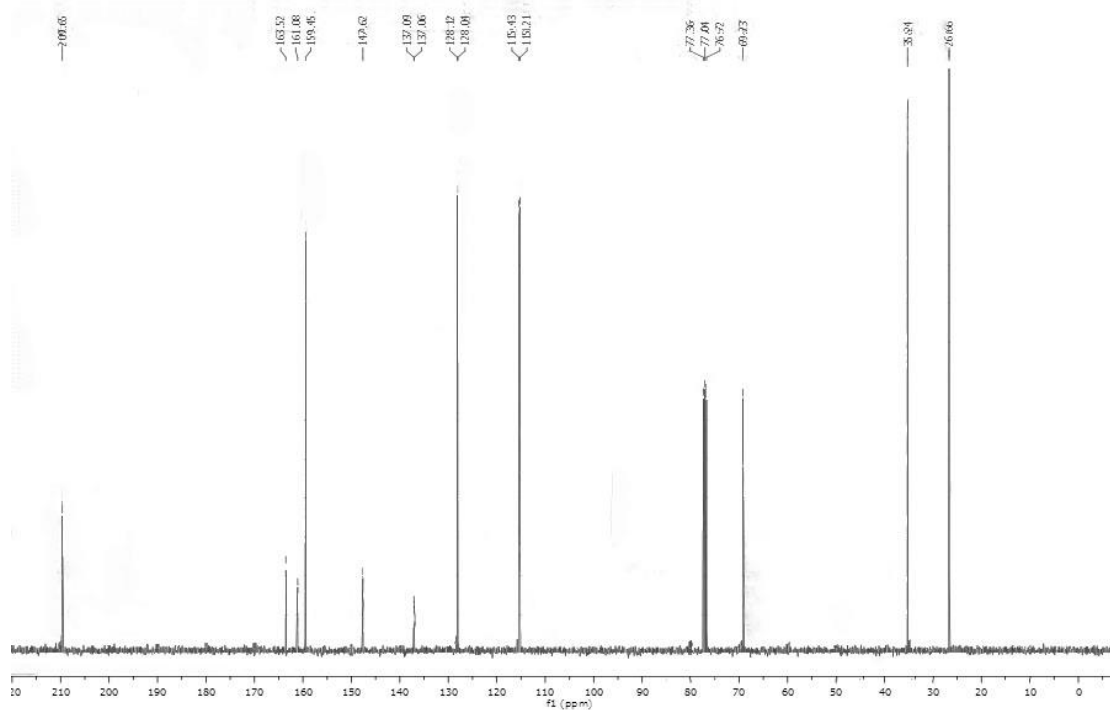
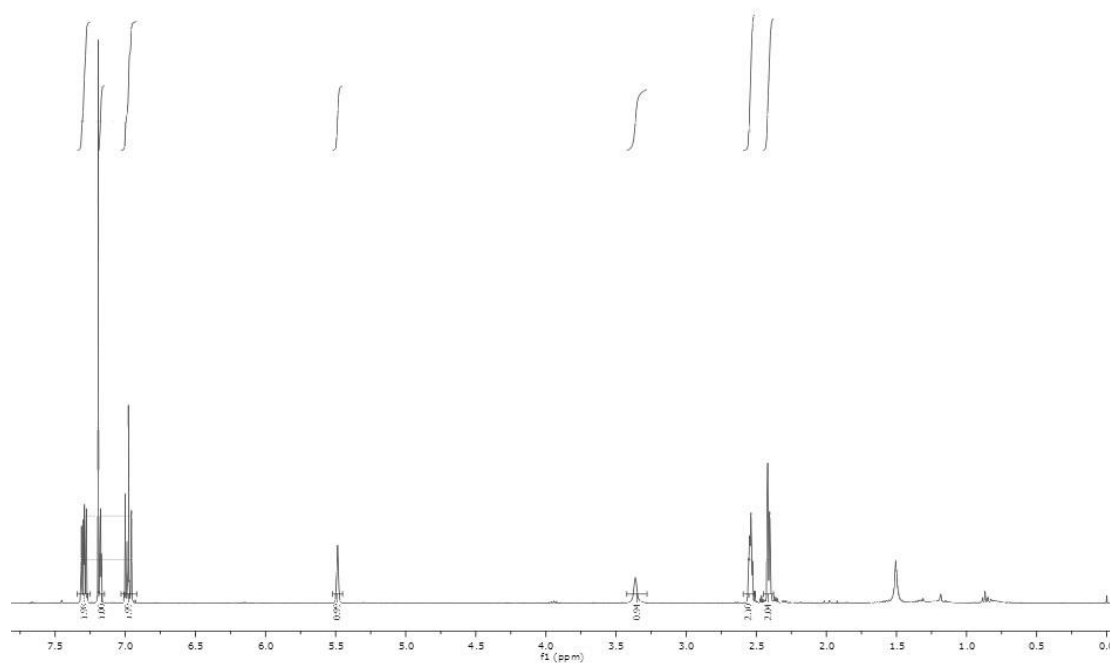
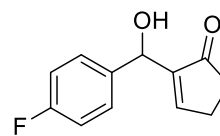
^a Turnover number = mol converted/mol of active sites. ^b Turnover frequency = Turnover number/reaction time.

References

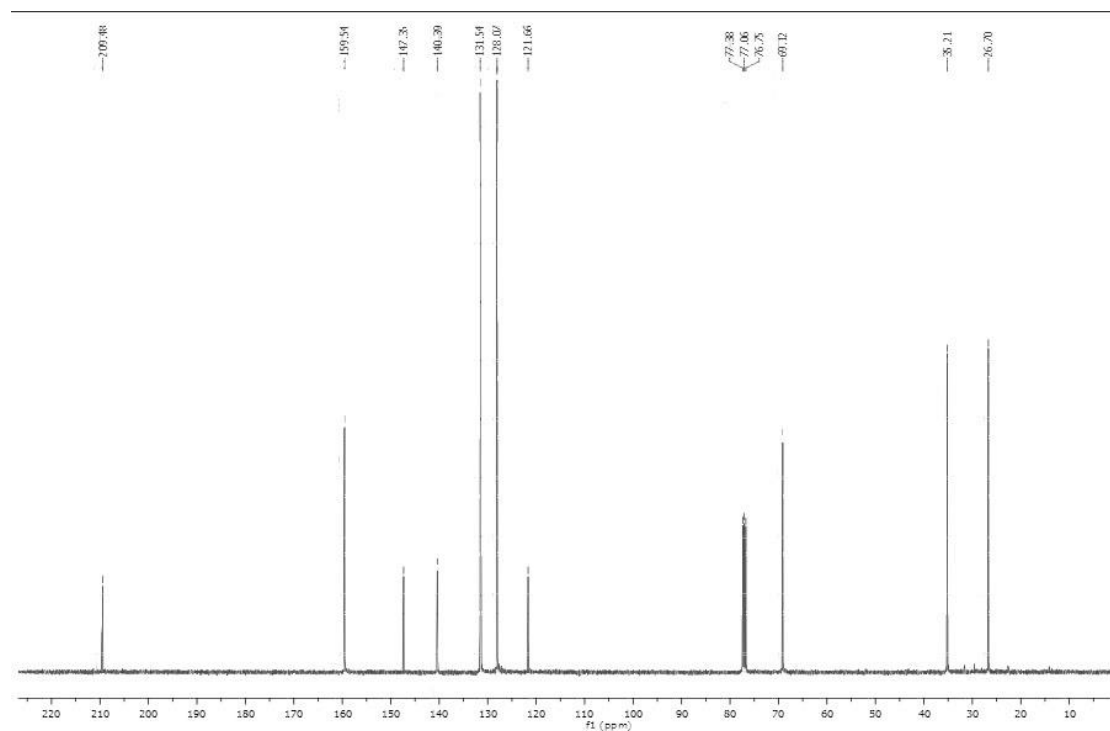
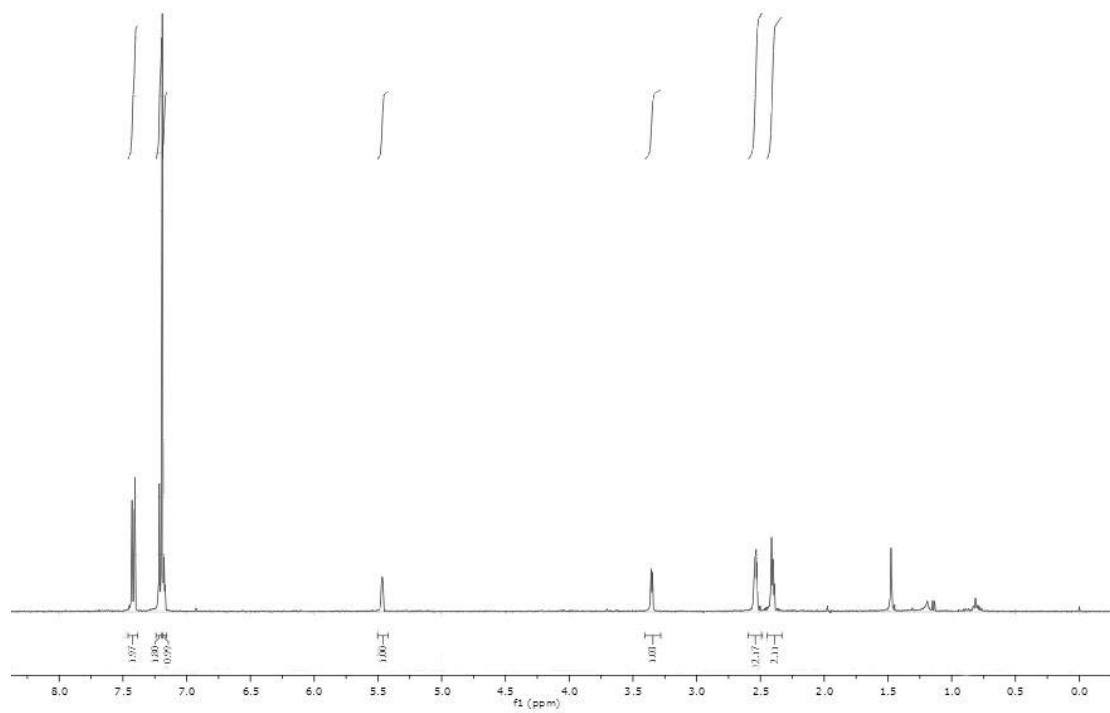
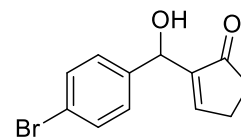
- [1] K. P. Guerra, C. A. M. Afonso, *Tetrahedron*, 2011, 67, 2562-2569.
- [2] R. Hajipour, S. Zakery, *Appl Organometal Chem.*, 2018, 32, e4487.
- [3] Bugarin, B. T. Connell, *Chem. Commun.*, 2010, 46, 2644–2646.
- [4] Y. Luan, N. Zheng, Y. Qi, J. Tang, G. Wang, *Catal. Sci. Technol.*, 2014, 4, 925-929.

NMR spectra:

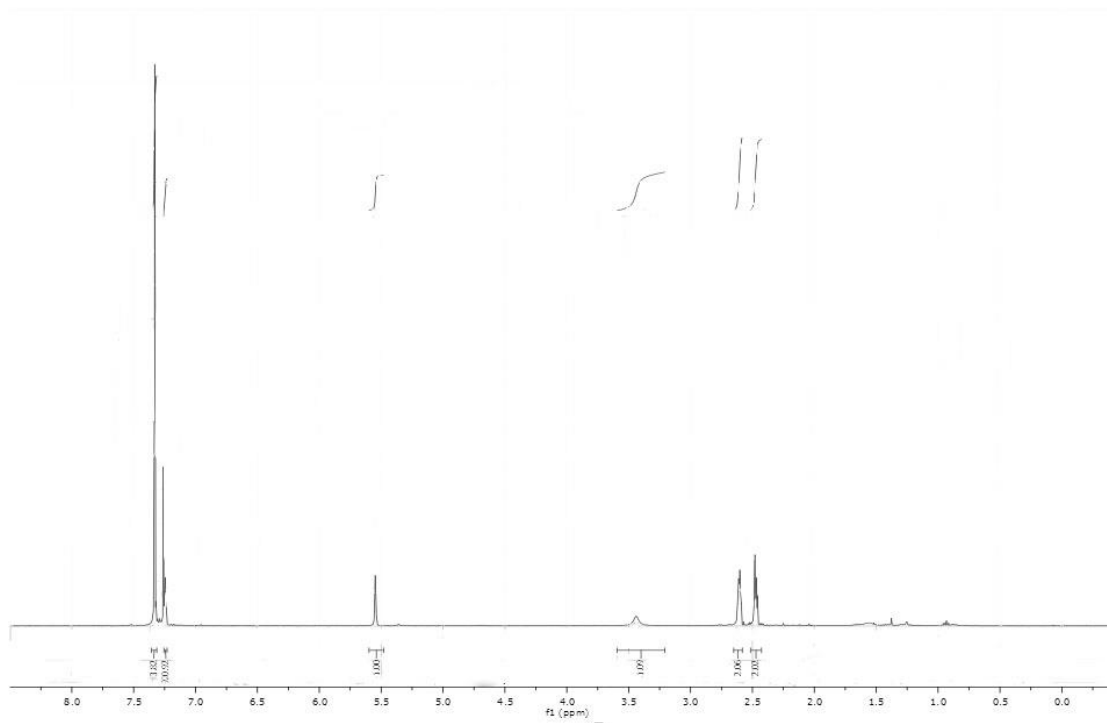
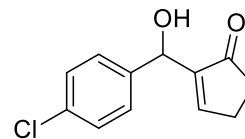
3a 2-[(4-Fluoro-phenyl)-hydroxy-methyl]-cyclopent-2-enone



3b 2-[(4-Bromo-phenyl)-hydroxy-methyl]-cyclopent-2-enone



3d 2-[(4-Chloro-phenyl)-hydroxy-methyl]-cyclopent-2-enone



— 209.73

— 159.73

— 147.58

— 140.01

— 133.69

— 128.78

— 127.91

— 77.55

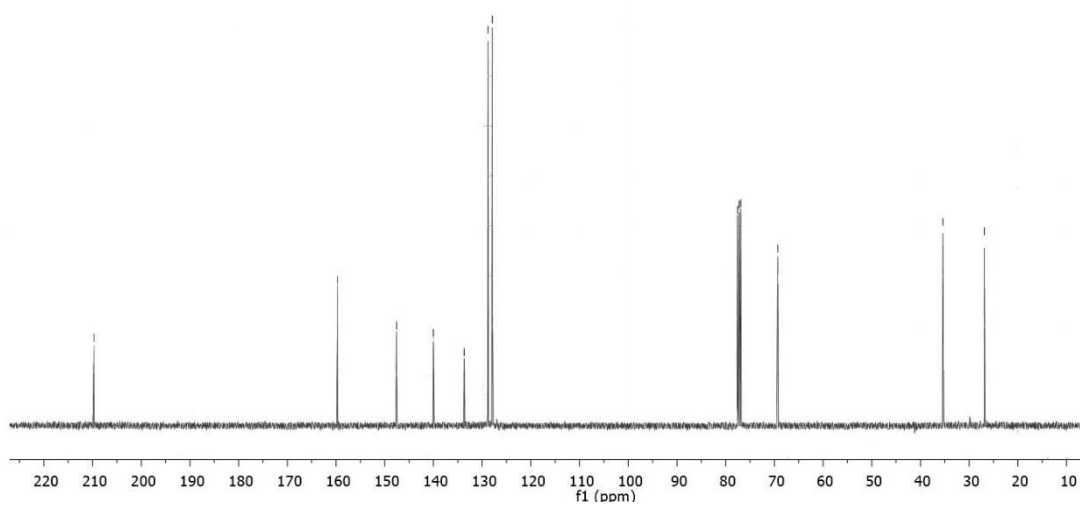
— 77.23

— 76.91

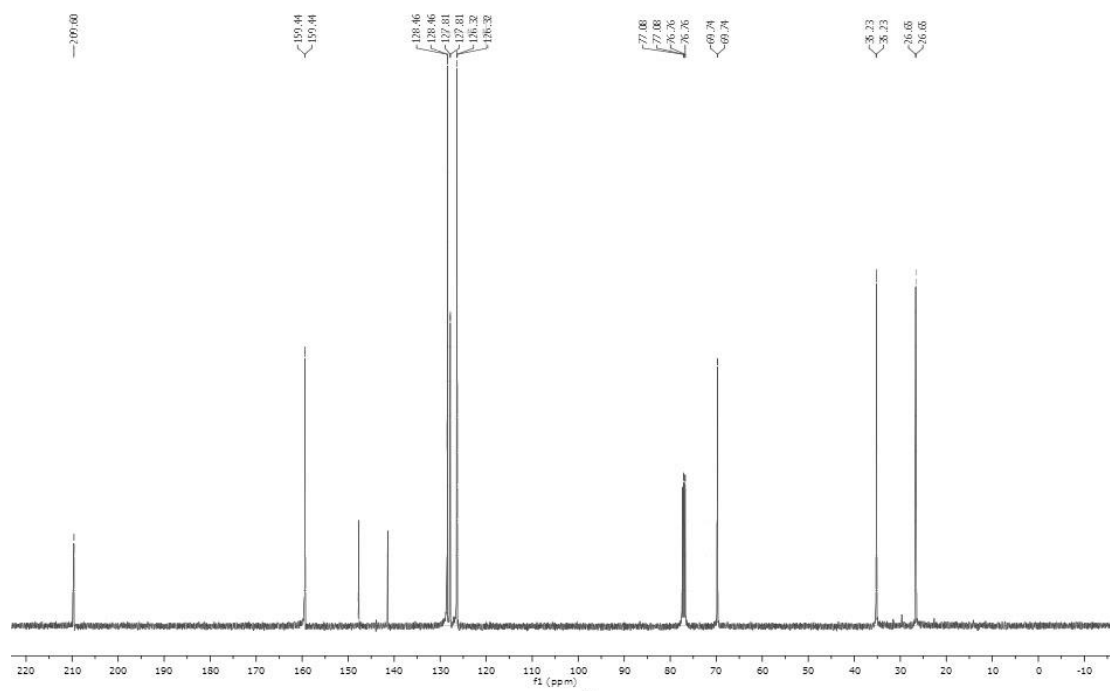
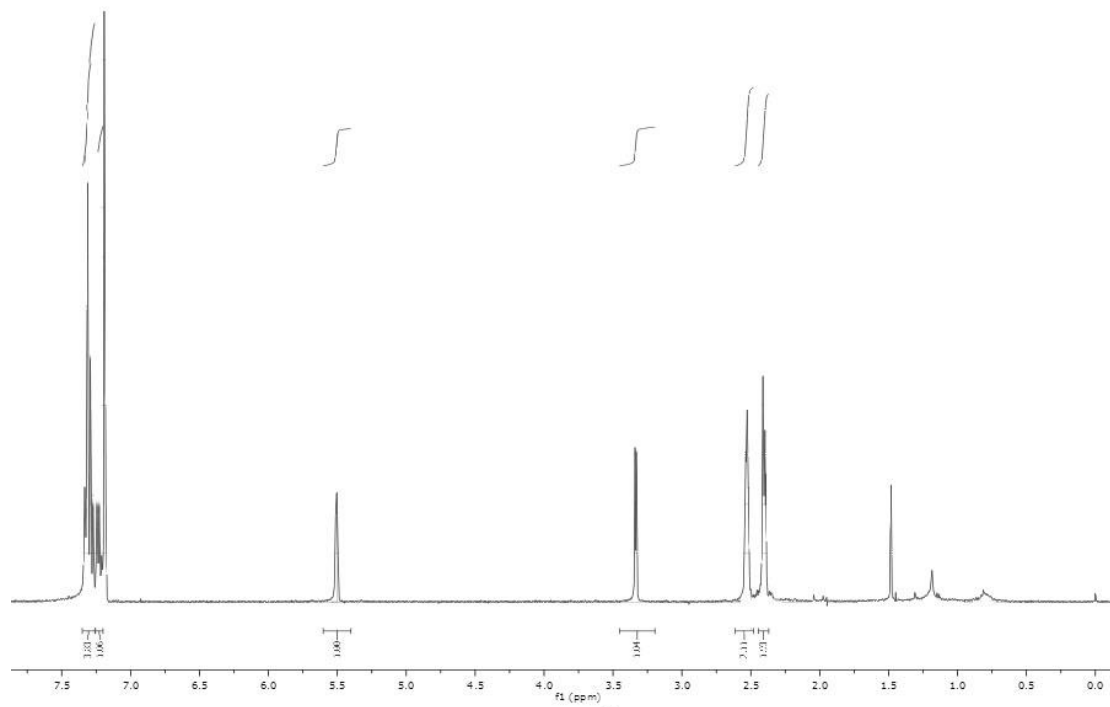
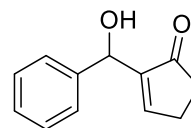
— 69.29

— 35.39

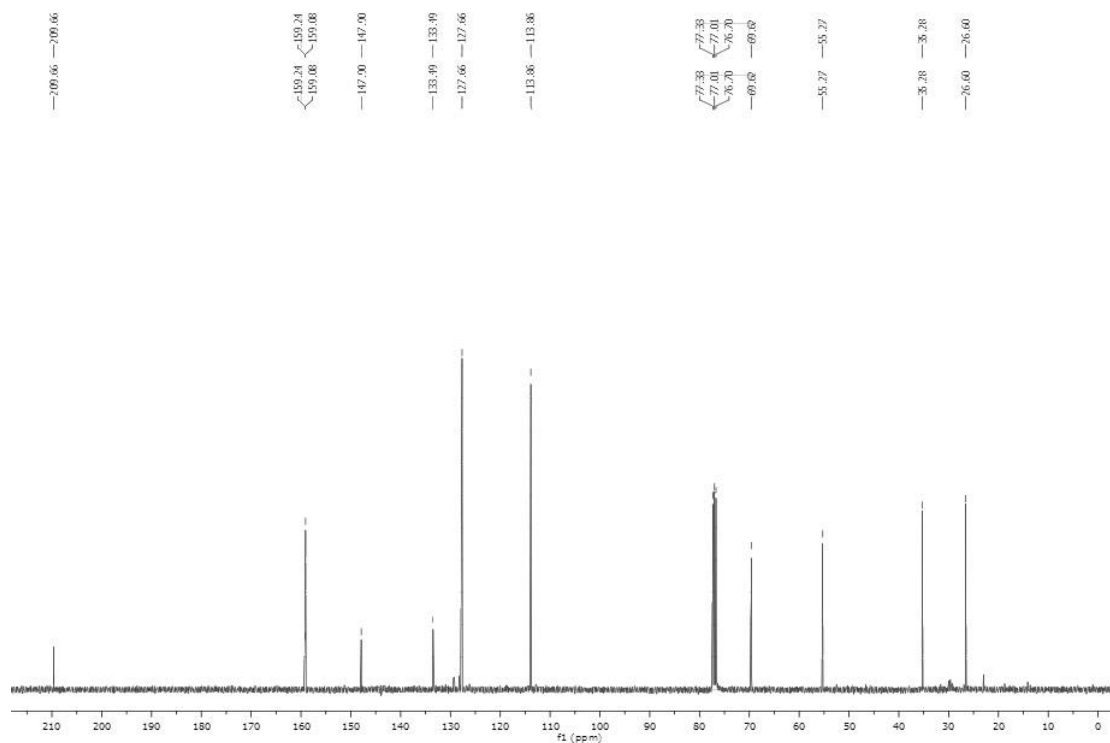
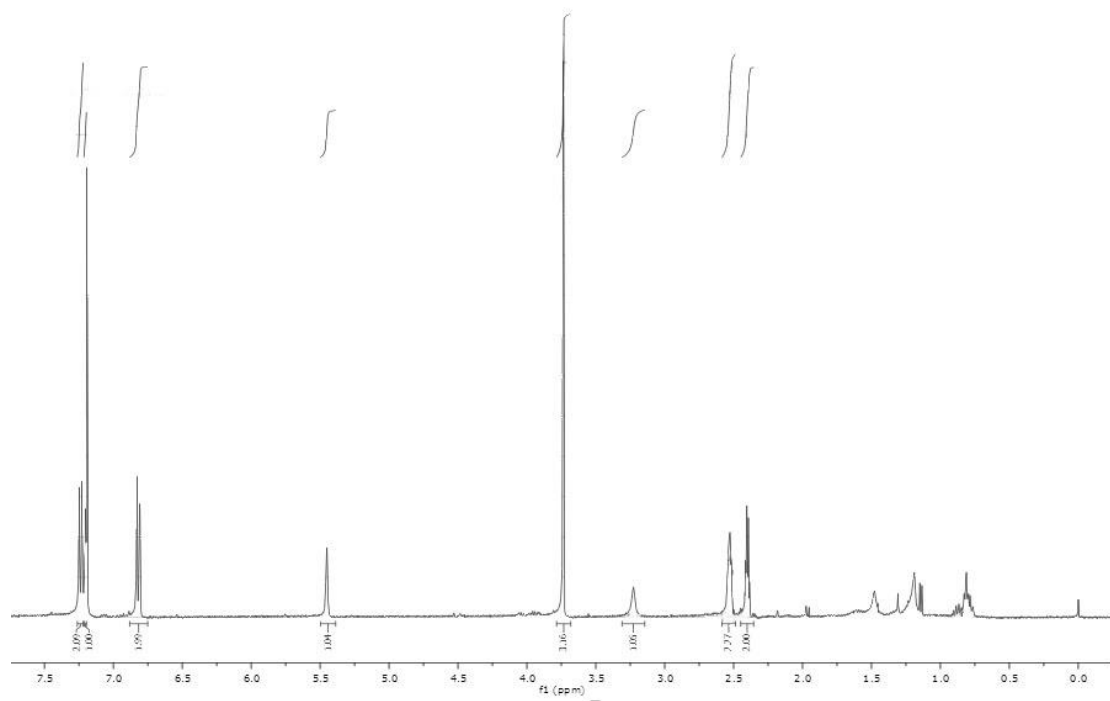
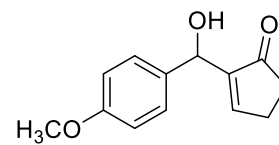
— 26.87



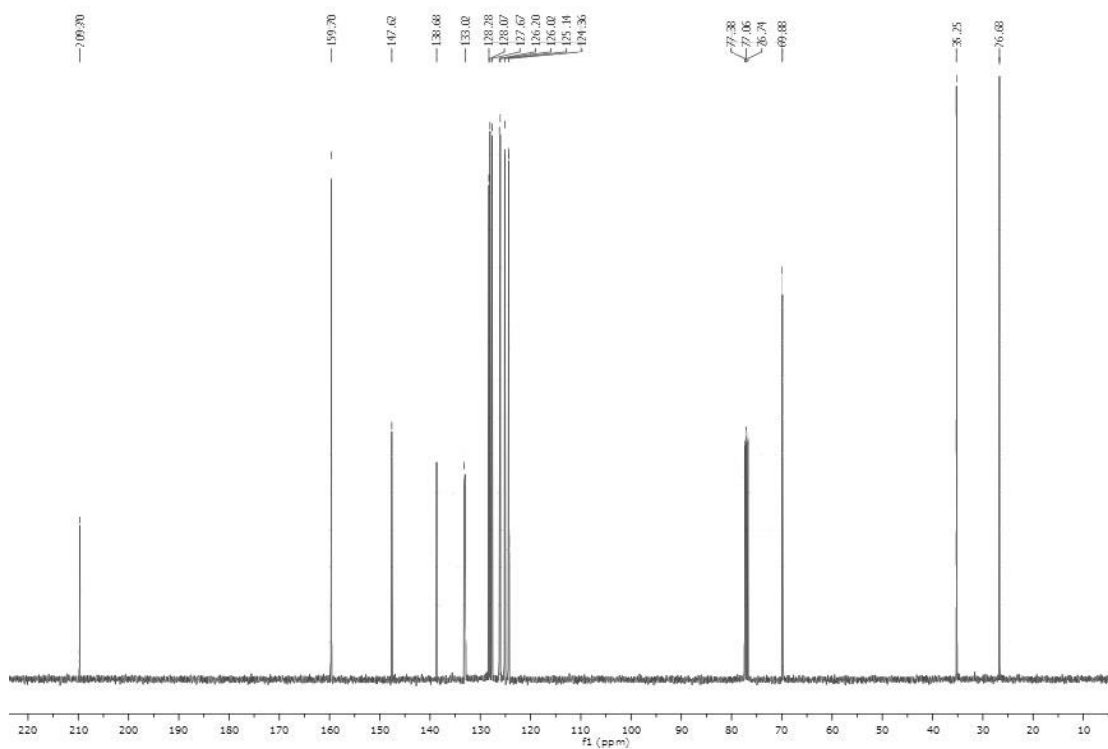
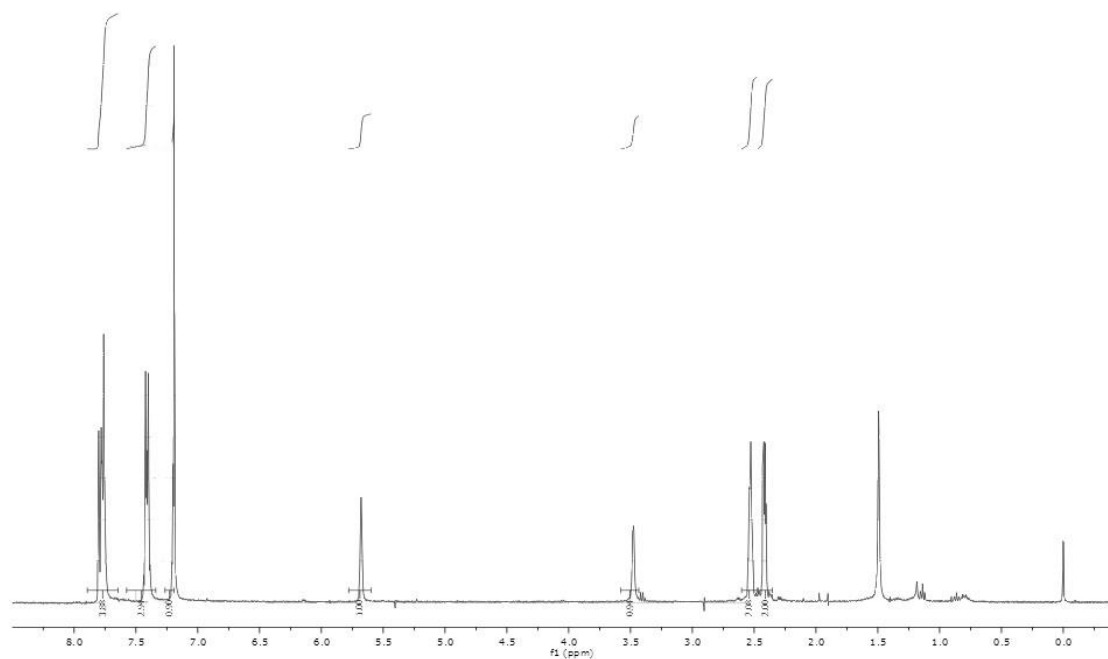
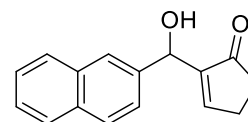
3e 2-(Hydroxy-phenyl-methyl)-cyclopent-2-enone



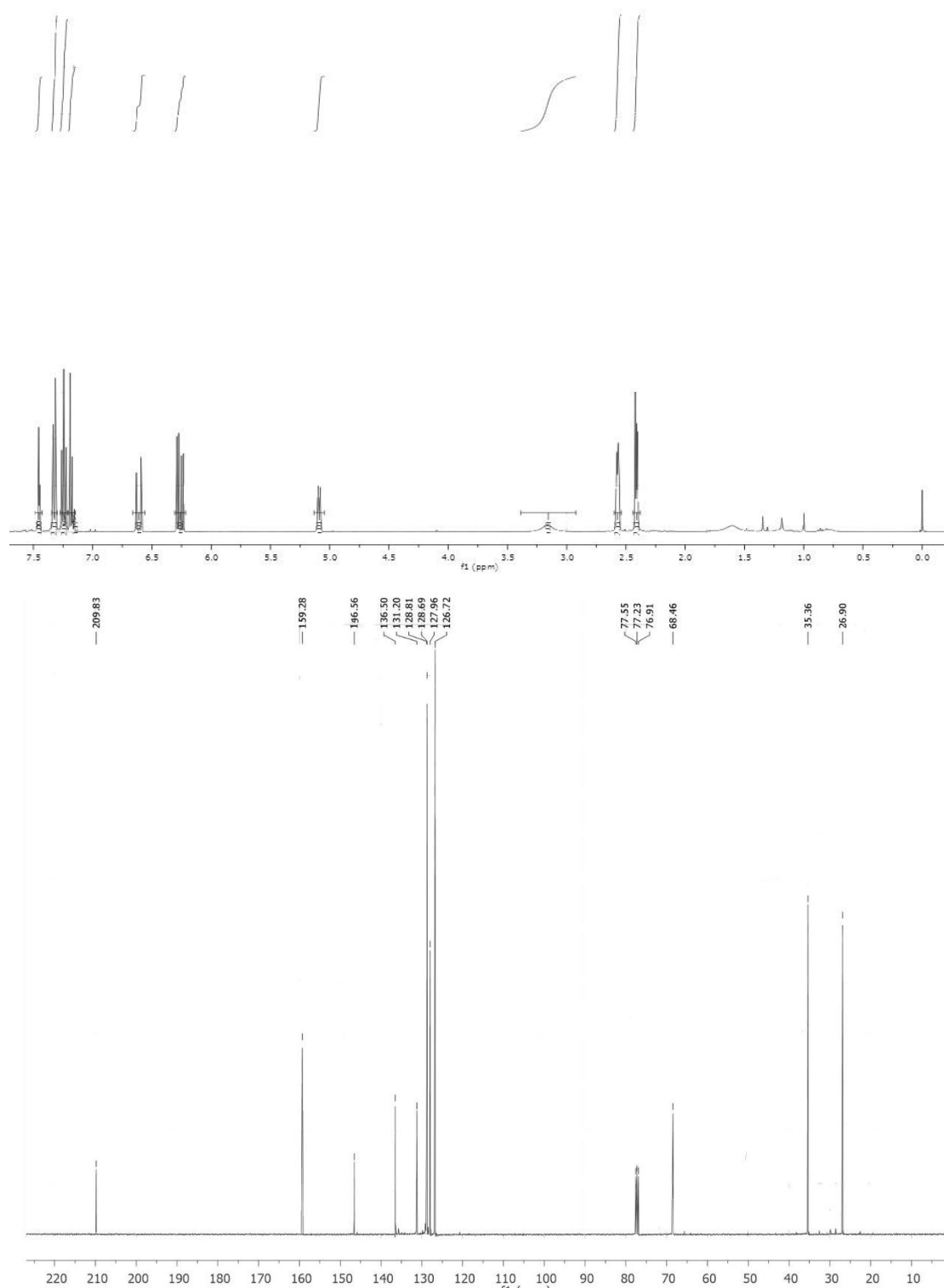
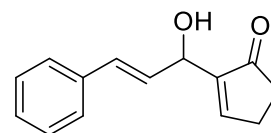
3g 2-[Hydroxy-(4-methoxy-phenyl)-methyl]-cyclopent-2-enone



3h 2-(Hydroxy-naphthalen-2-yl-methyl)-cyclopent-2-enone



3i 2-(1-Hydroxy-3-phenyl-allyl)-cyclopent-2-enone



3j 2-(1-Hydroxy-3-phenyl-propyl)-cyclopent-2-enone

