

Supplementary data

Core–Shell Superparamagnetic Metal Organic Framework: A Recyclable and Green Catalyst for the Synthesis of Propargylamines

Elham Arefi, Amir Khojastehnezhad, and Ali Shiri*

Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran

E-mail: alishiri@um.ac.ir

Table of Content	Page Number
Particle size distribution diagram of Fe ₃ O ₄ @MOF	2
Elemental mapping of Fe ₃ O ₄ @MOF	3
EDX patterns of (a) Fe ₃ O ₄ and (b) Fe ₃ O ₄ @MOF	4
Nitrogen adsorption-desorption isotherms of bare Fe ₃ O ₄	5
Nitrogen adsorption-desorption isotherms of bare Fe ₃ O ₄ @HKUST-1	6
Hot filtration test diagram	7
FT-IR and NMR data	8
Original sepectrums of FT-IR and NMR	9-23

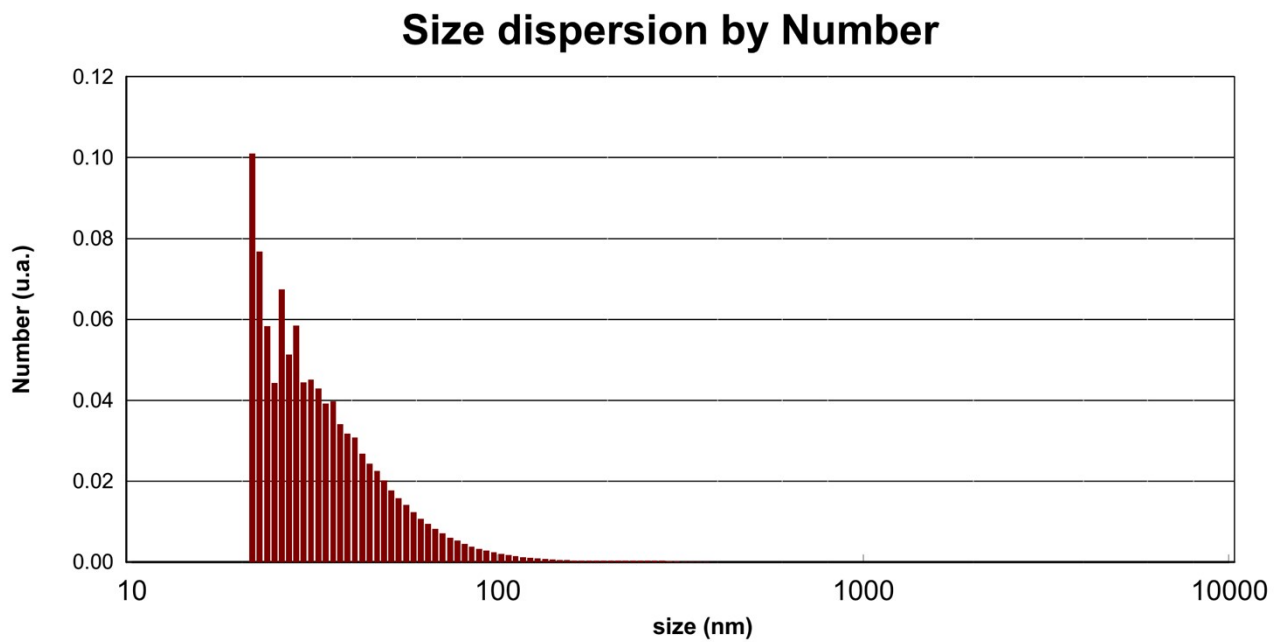


Figure S1. The particle size distribution diagram of $\text{Fe}_3\text{O}_4@\text{MOF}$

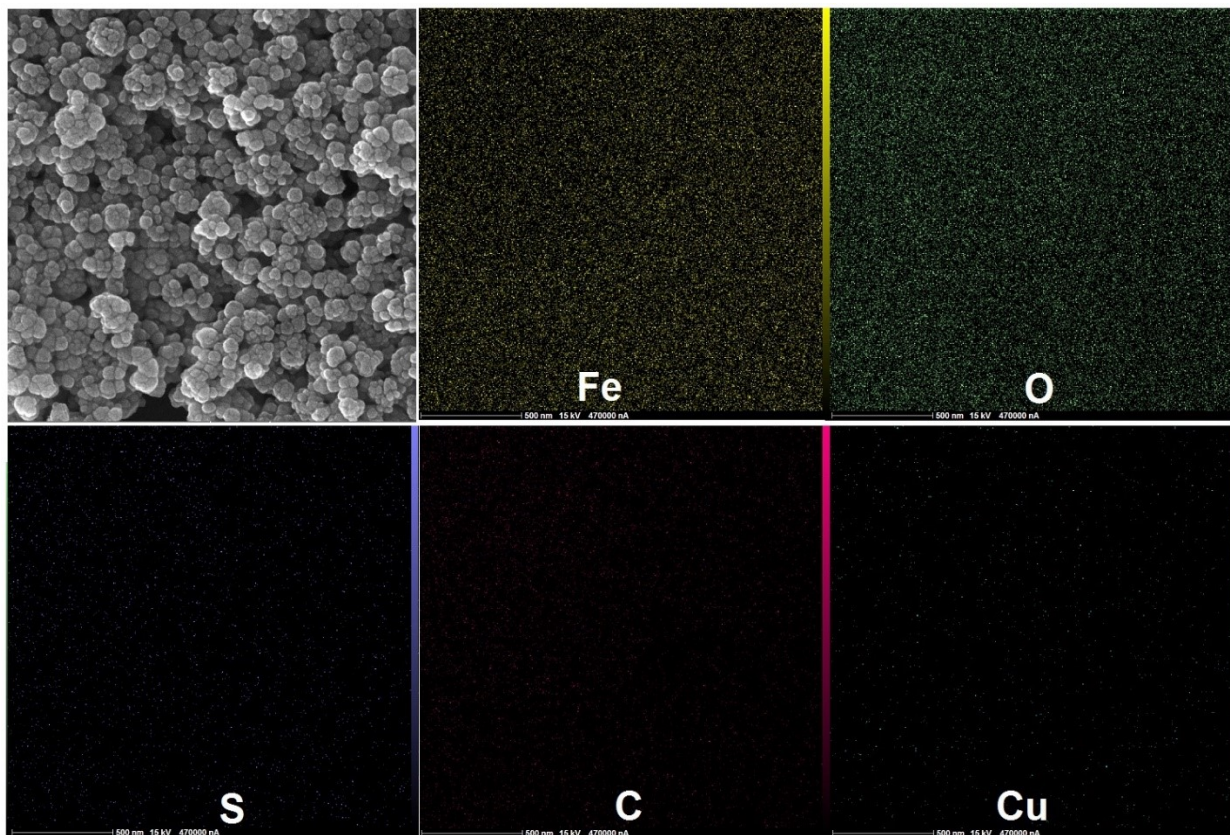


Figure S2. Elemental mapping of $\text{Fe}_3\text{O}_4@\text{MOF}$

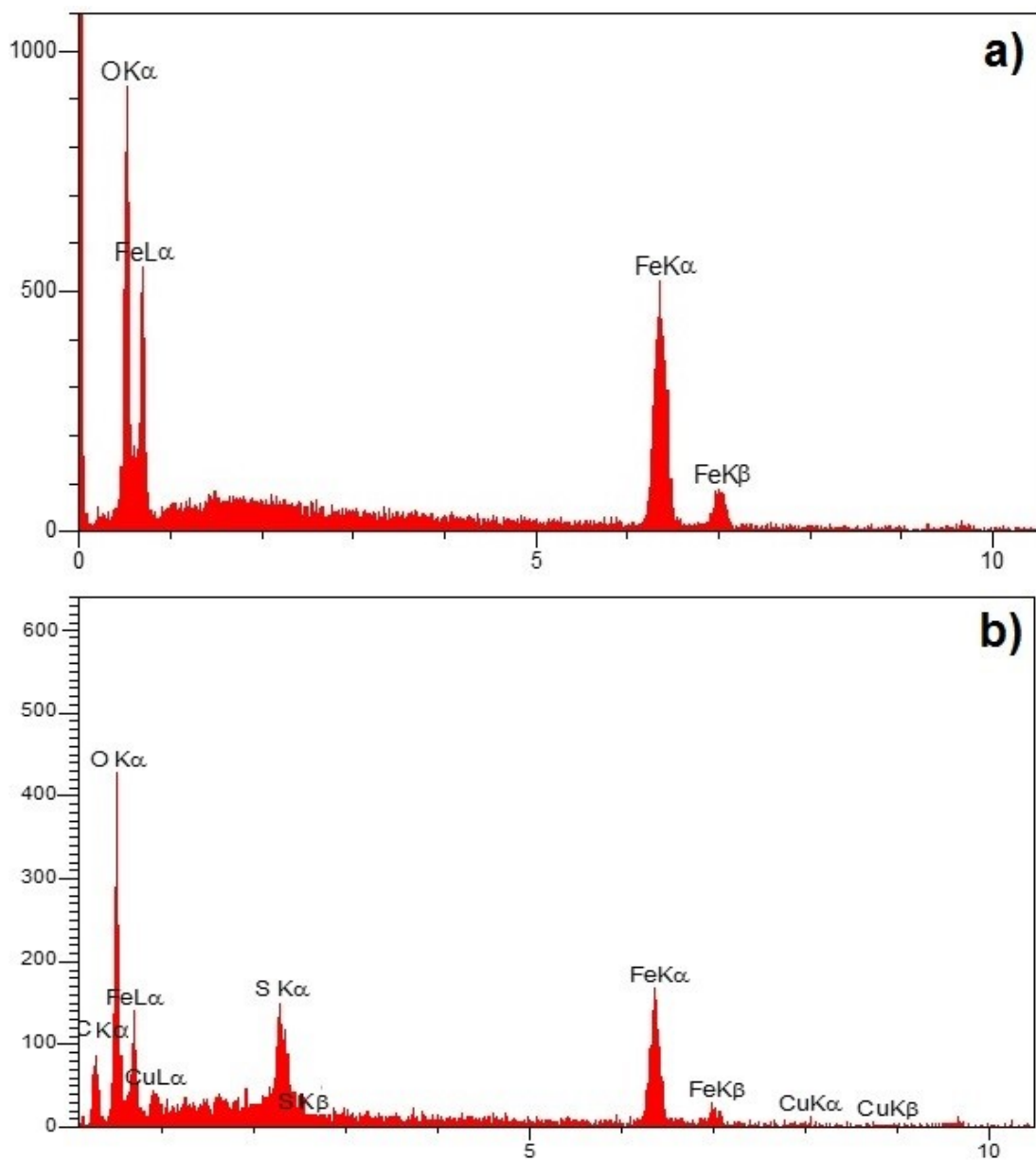


Figure S3. EDX patterns of (a) Fe_3O_4 and (b) $\text{Fe}_3\text{O}_4@\text{MOF}$

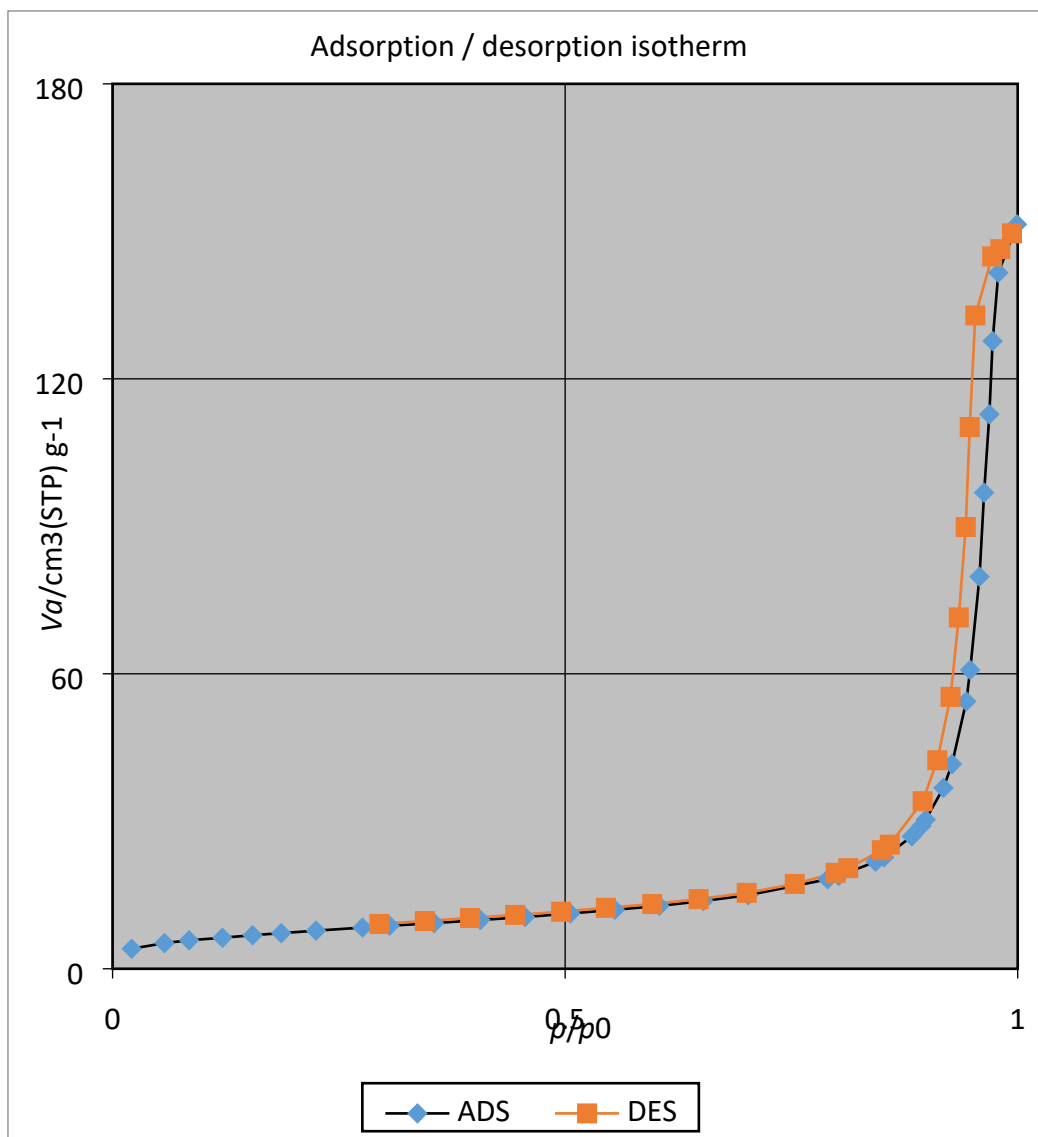


Figure S4. Nitrogen adsorption-desorption isotherms of bare Fe_3O_4

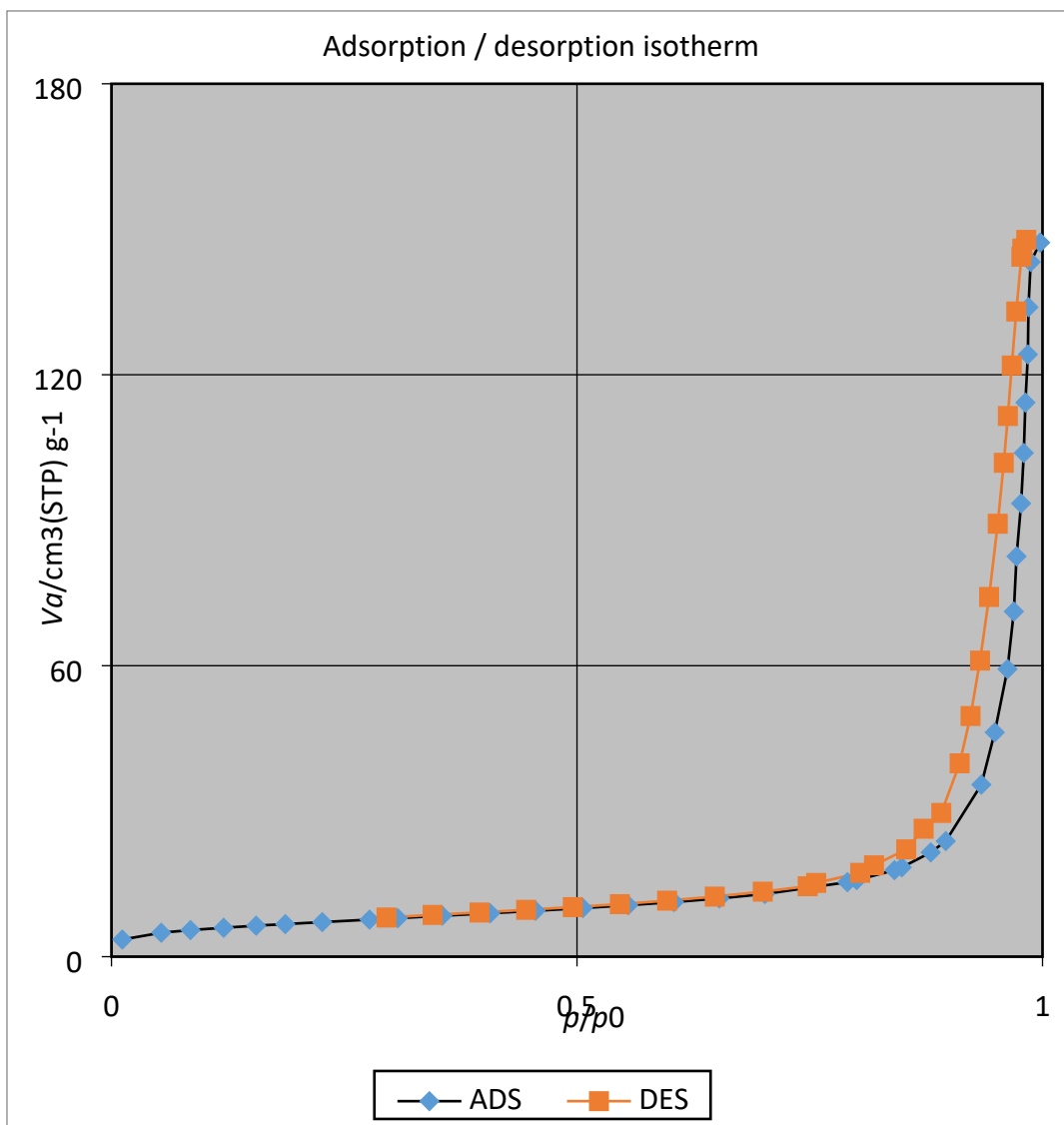


Figure S5. Nitrogen adsorption-desorption isotherms of Fe₃O₄@HKUST-1

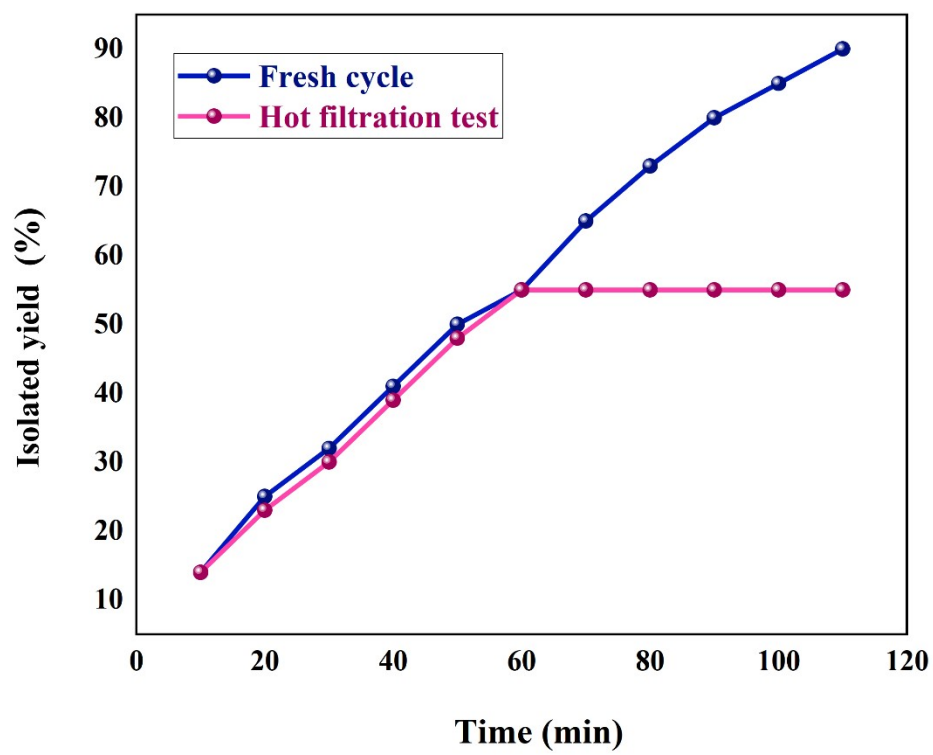


Figure S6. Hot filtration text diagram

4-(1,3-Diphenylprop-2-yn-1-yl)morpholine (Table 2, entry 1)

¹H-NMR (300 MHz, CDCl₃): δ= 2.69 (4H, t, *J*= 4.35), 3.76–3.80 (4H, m), 4.85 (1H, s), 7.35–7.42 (6H, m), 7.44–7.54 (2H, m), 7.69 (2H, d, *J*= 7.2); ¹³C-NMR (CDCl₃, 75 Hz): δ= 49.89, 62.06, 67.15, 85.01, 88.55, 122.98, 128.27, 128.30, 128.34, 128.65, 131.84, 137.74; M.S. (70 ev) *m/z* (%): 277 (M⁺, 100).

4-(1-(4-Methoxyphenyl)-3-phenylprop-2-yn-1-yl)morpholine (Table 2, entry 2)

¹H-NMR (300 MHz, CDCl₃): δ= 1.36 (4H, m), 2.73 (4H, m), 3.66 (3H, m), 4.86 (1H, s, *J*= 8.7), 6.93–6.96 (2H, m, *J*= 6.3), 7.37–7.39 (3H, m, *J*= 8.2), 7.55–7.57 (4H, m); ¹³C-NMR (CDCl₃, 75 Hz): δ= 49.76, 55.33, 61.60, 66.96, 84.60, 88.36, 113.71, 122.02, 127.76, 128.36, 130.02, 131.84, 159.47; M.S. (70 ev) *m/z* (%): 307 (M⁺, 100).

4-(3-phenyl-1-(*p*-tolyl)prop-2-yn-1-yl)morpholine (Table 2, entry 5)

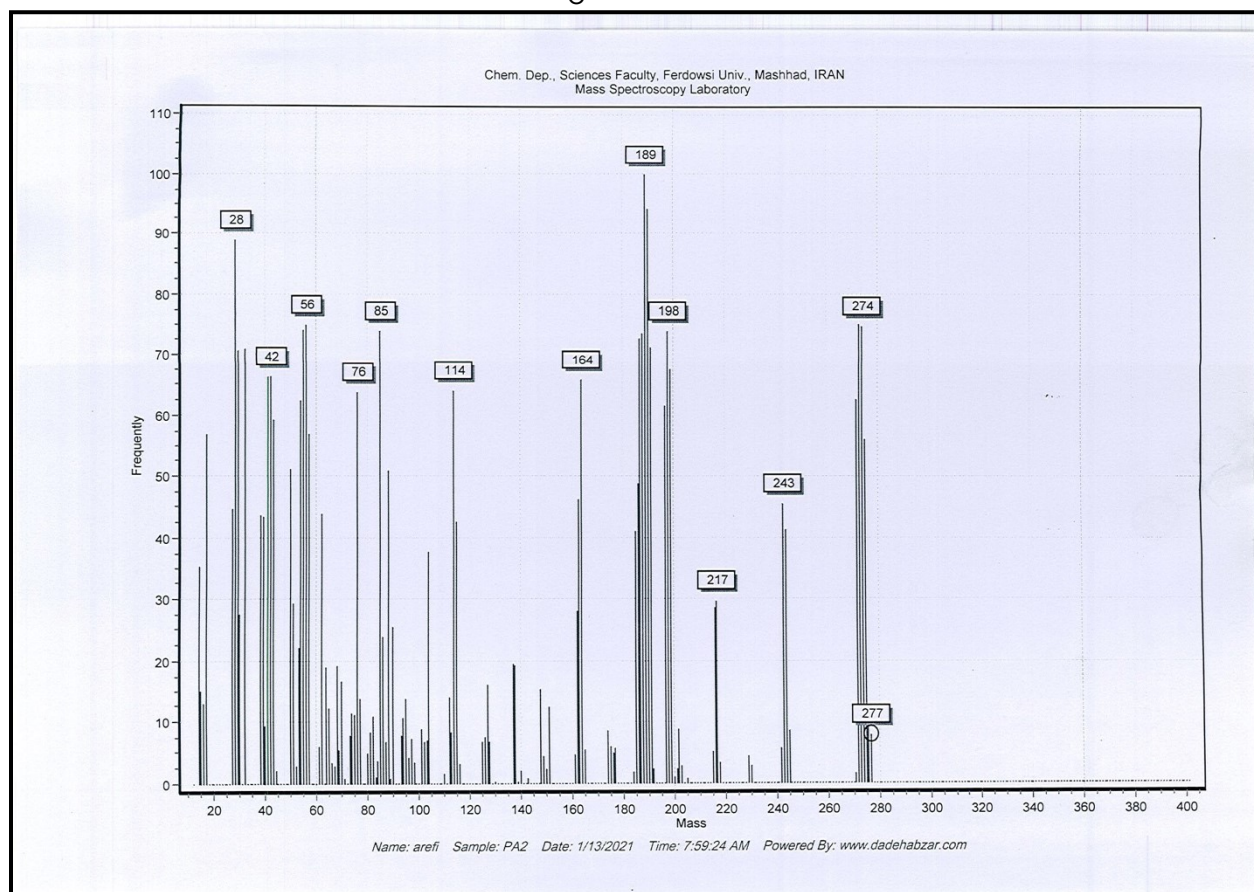
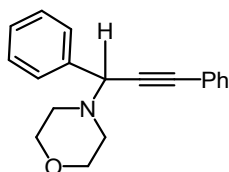
¹H-NMR (300 MHz, CDCl₃): δ= 2.29 (3H, s), 2.57–2.62 (4H, t, *J*= 4.3 Hz), 3.66–3.70 (4H, m), 4.72 (1H, s), 7.09 (2H, d, *J*= 7.9 Hz), 7.12 (2H, d, *J*= 7.3 Hz), 7.43–7.26 (5H, m); ¹³C-NMR (CDCl₃, 75 Hz): δ= 21.16, 49.84, 61.84, 67.03, 83.67, 88.33, 123.16, 128.21, 128.33, 128.66, 128.99, 131.84, 137.81; M.S. (70 ev) *m/z* (%): 291 (M⁺, 100).

1-(1,3-Diphenylprop-2-yn-1-yl)piperidine (Table 2, entry 6)

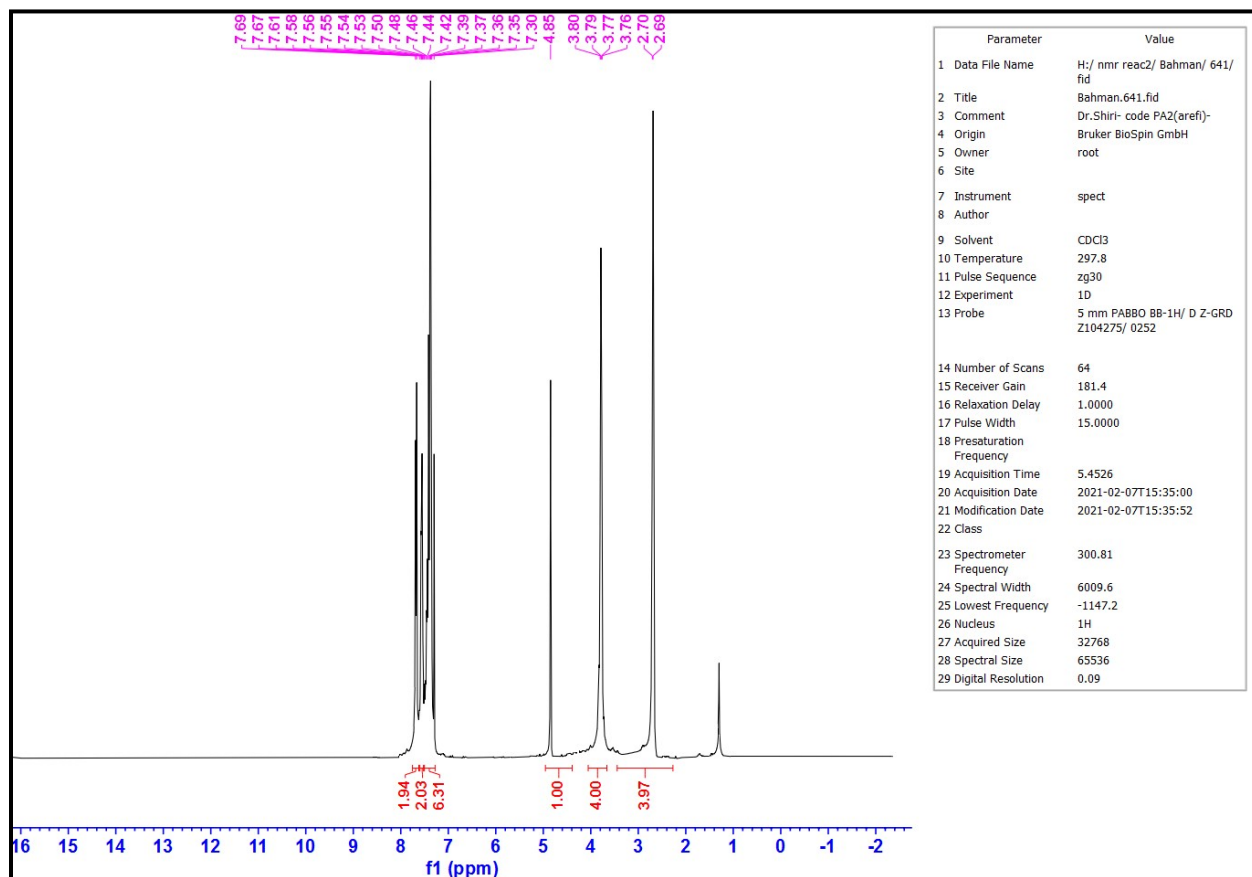
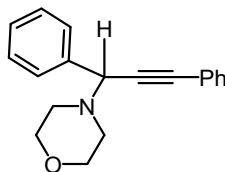
¹H-NMR (300 MHz, CDCl₃): δ= 1.49–1.66 (2H, m), 1.68–1.72 (4H, m), 2.67 (4H, t, *J*= 5.25), 4.89 (1H, s), 7.35–7.57 (6H, m), 7.58–7.69 (2H, m), 7.71–7.72 (2H, m); ¹³C-NMR (CDCl₃, 75 Hz): δ= 24.44, 26.13, 50.69, 62.38, 86.02, 87.95, 123.34, 127.57, 128.13, 128.33, 128.66, 131.86, 138.42.

1-(1-(phenylethynyl)cyclohexyl)piperidine (Table 2, entry 12)

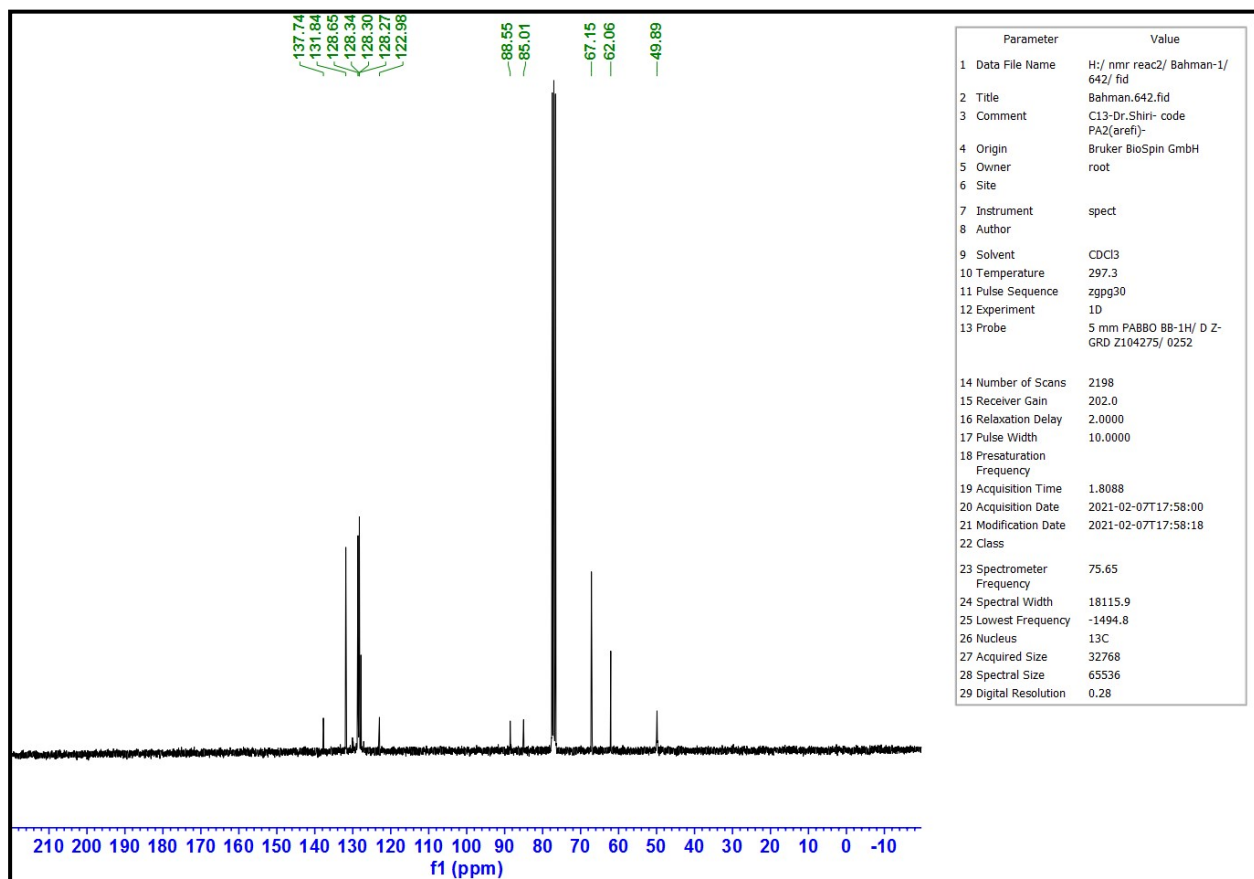
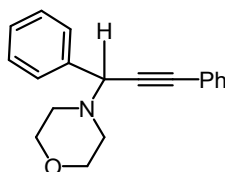
¹H-NMR (300 MHz, CDCl₃): δ= 1.42–1.63 (12H, m), 2.17–2.19 (4H, m), 3.30 (4H, t, *J*= 4.8 Hz), 7.24–7.29 (3H, m, *J*= 4.8 Hz), 7.43–7.47 (2H, m); ¹³C-NMR (CDCl₃, 75 Hz): δ= 23.12, 23.49, 24.55, 25.27, 33.38, 47.69, 73.96, 81.59, 87.48, 121.79, 128.48, 129.26, 132.51; M.S. (70 ev) *m/z* (%): 267 (M⁺, 100).



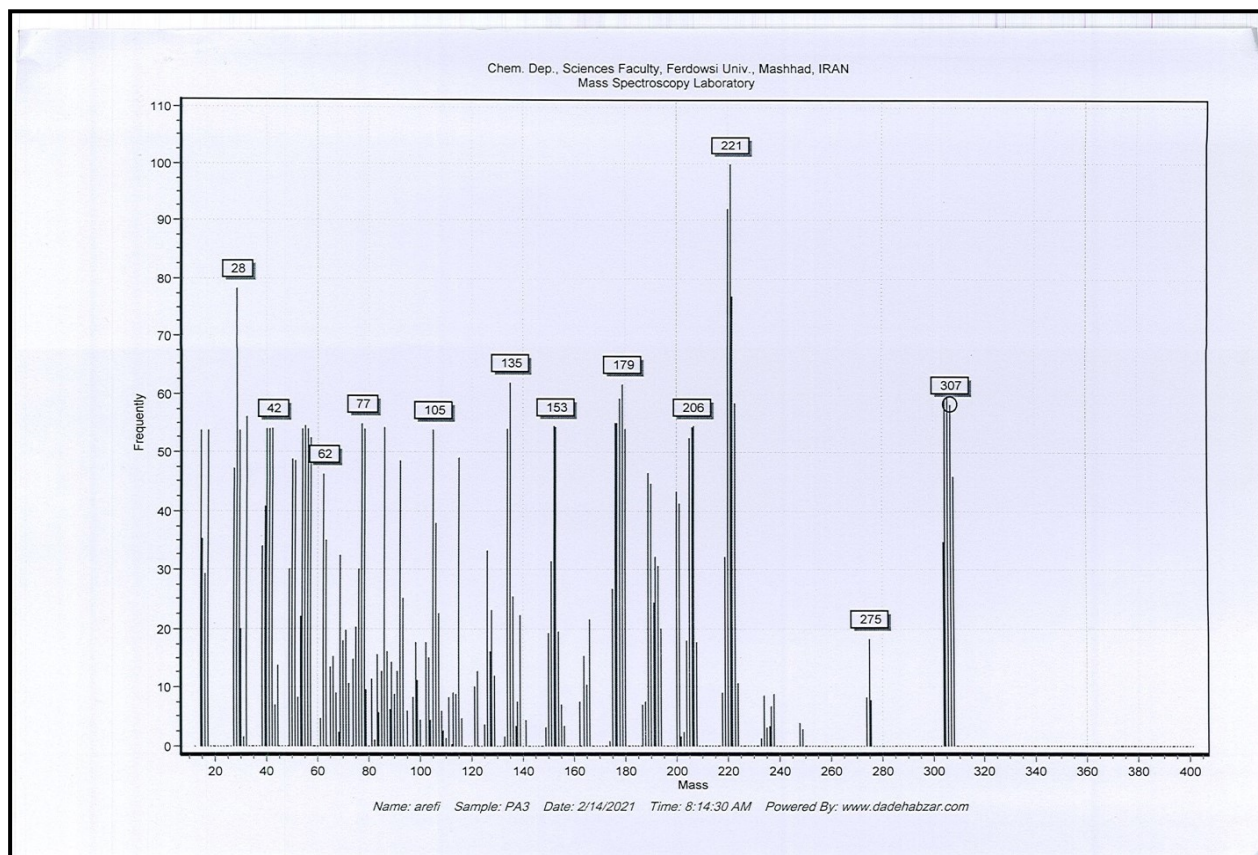
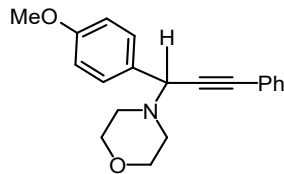
Mass spectrum of 4-(1,3-Diphenylprop-2-yn-1-yl)morpholine (Table 2, entry 1)



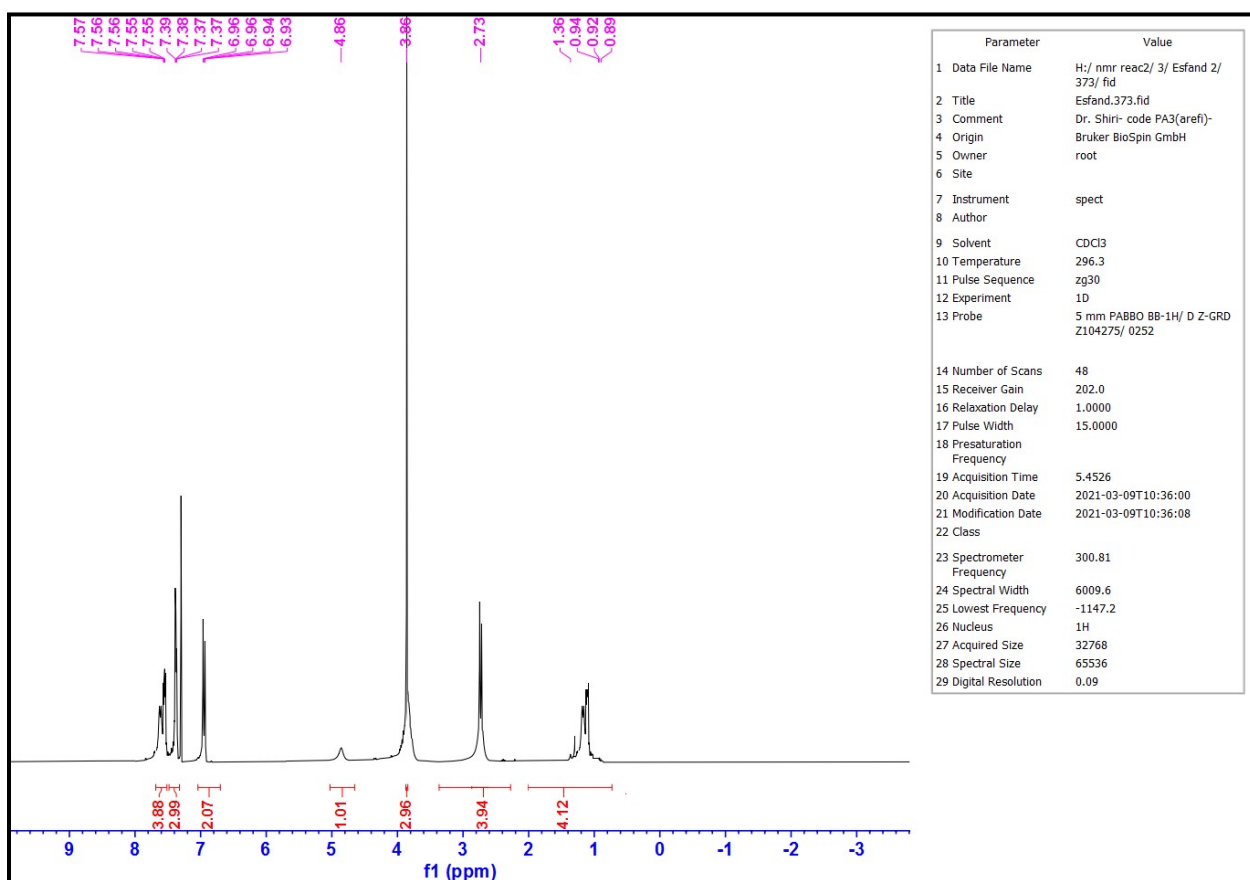
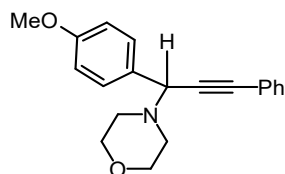
$^1\text{H-NMR}$ of 4-(1,3-Diphenylprop-2-yn-1-yl)morpholine (Table 2, entry 1)



^{13}C -NMR of 4-(1,3-Diphenylprop-2-yn-1-yl)morpholine (Table 2, entry 1)

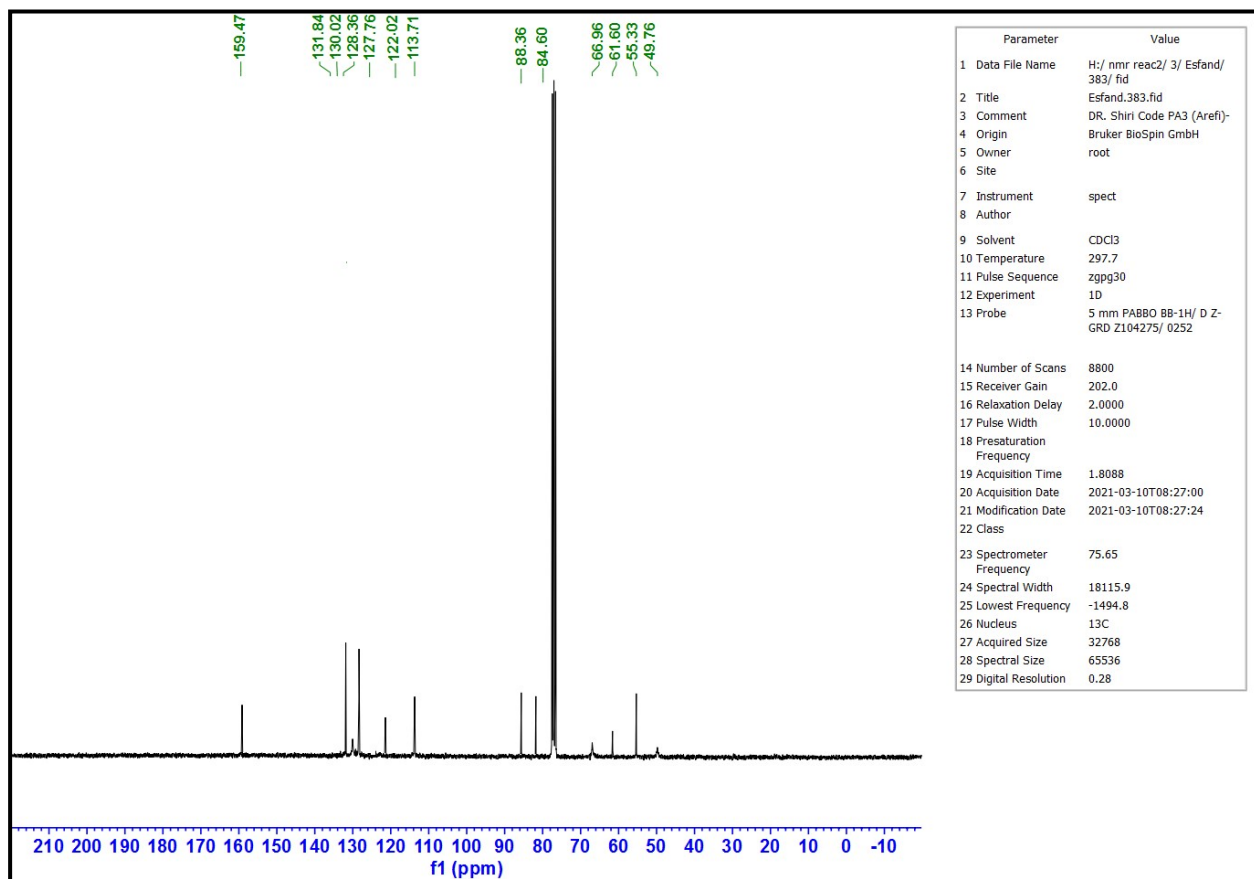
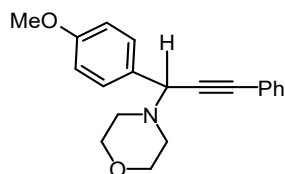


Mass spectrum of 4-(1-(4-Methoxyphenyl)-3-phenylprop-2-yn-1-yl) morpholine (Table 2, entry 2)

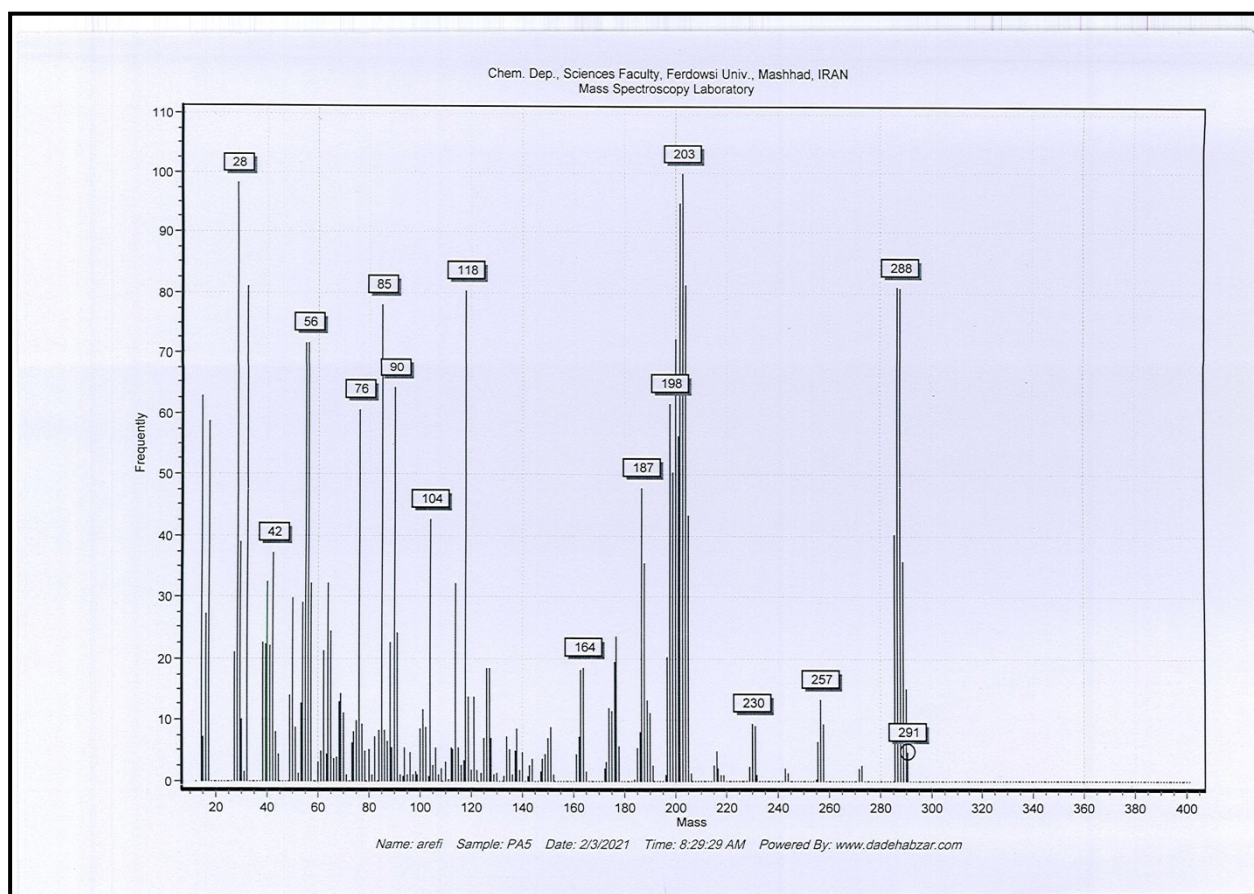
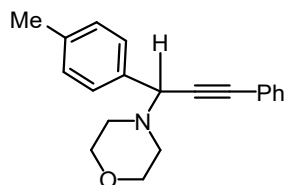


Parameter	Value
1 Data File Name	H:/ nmr reac2/ 3/ Esfond 2/ 373/ fid
2 Title	Esfond.373.fid
3 Comment	Dr. Shiri- code PA3(arefi)-
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB-1H/ D Z-GRD Z104275/ 0252
14 Number of Scans	48
15 Receiver Gain	202.0
16 Relaxation Delay	1.0000
17 Pulse Width	15.0000
18 Presaturation Frequency	
19 Acquisition Time	5.4526
20 Acquisition Date	2021-03-09T10:36:00
21 Modification Date	2021-03-09T10:36:08
22 Class	
23 Spectrometer Frequency	300.81
24 Spectral Width	6009.6
25 Lowest Frequency	-1147.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.09

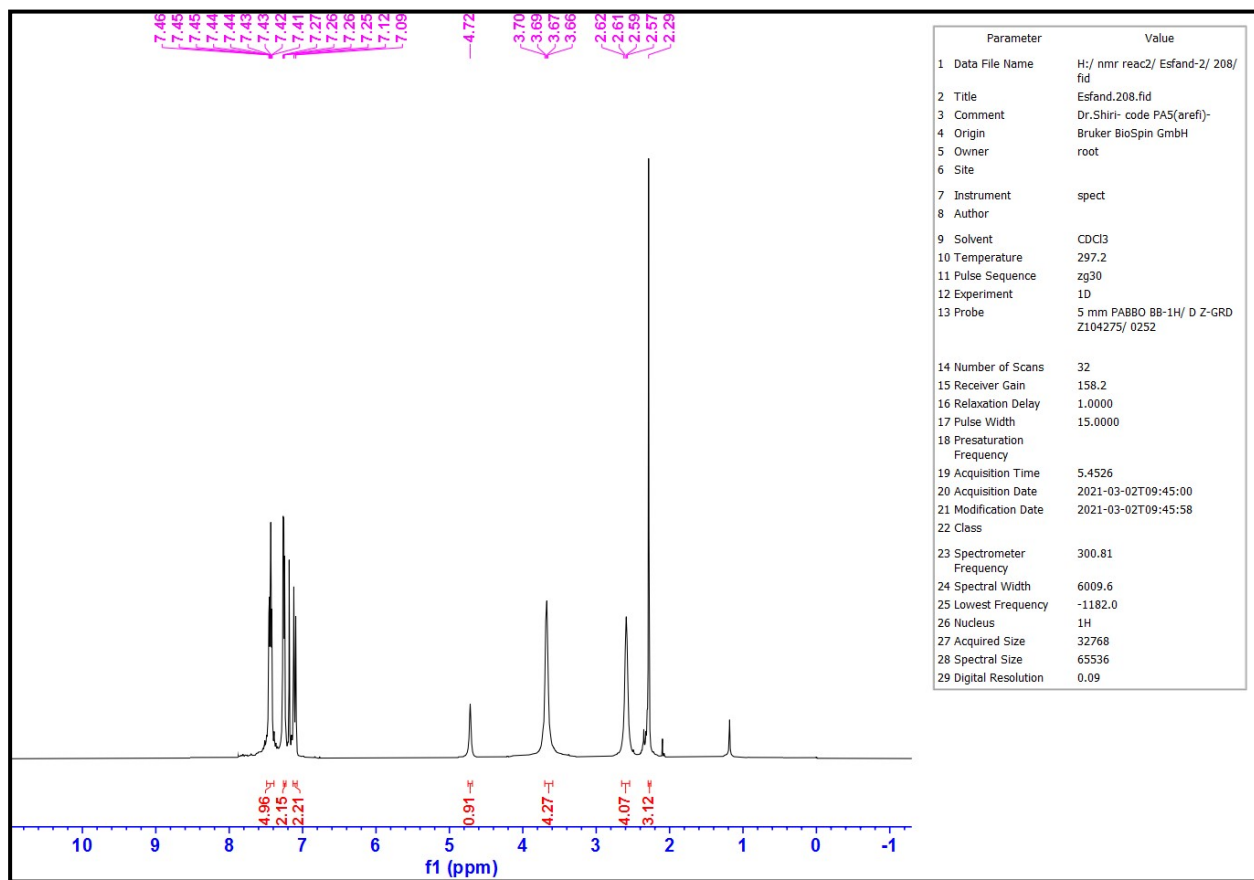
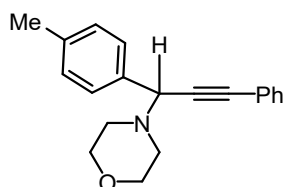
¹H NMR of 4-(1-(4-Methoxyphenyl)-3-phenylprop-2-yn-1-yl)morpholine (Table 2, entry 2)



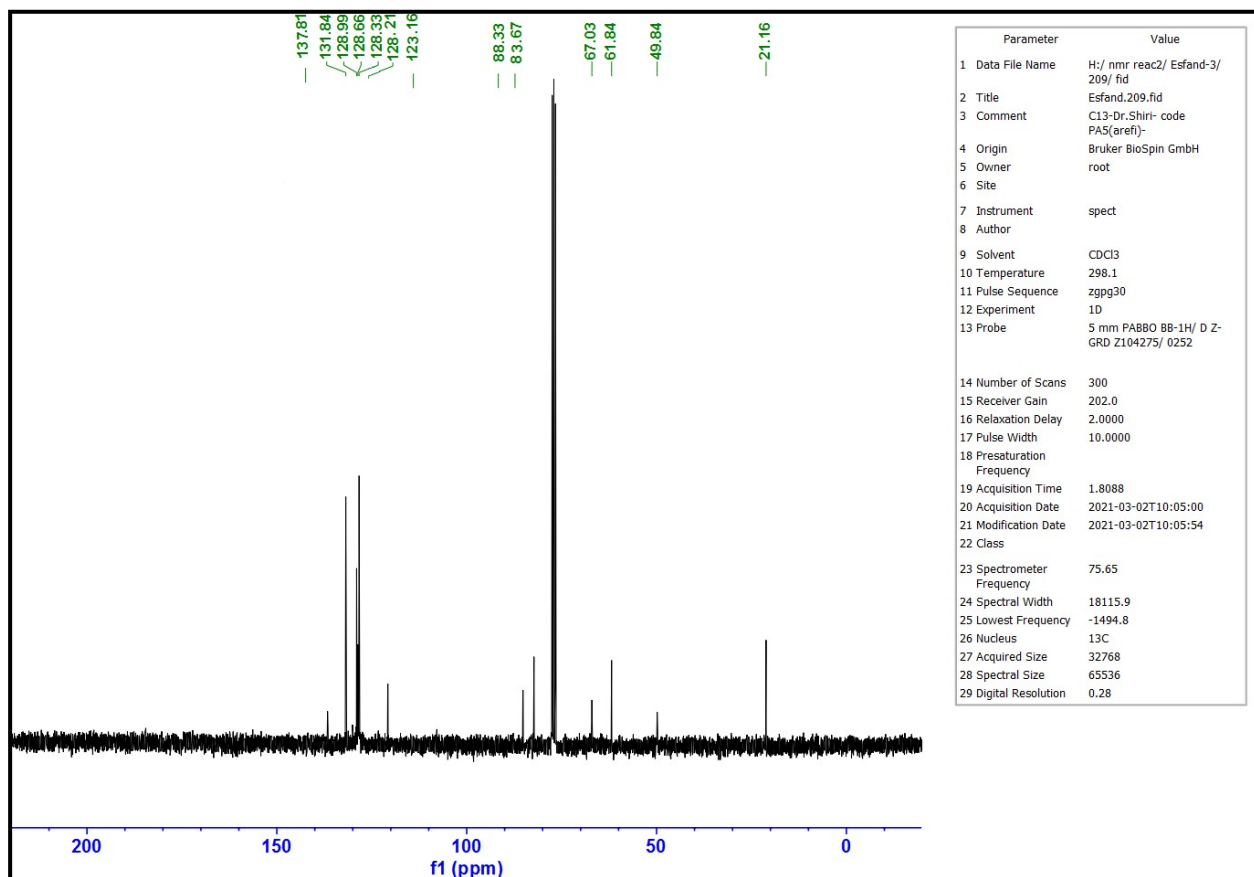
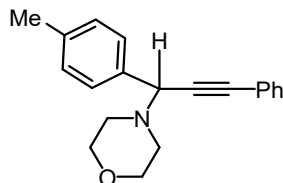
^{13}C -NMR of 4-(1-(4-Methoxyphenyl)-3-phenylprop-2-yn-1-yl) morpholine (Table 2, entry 2)



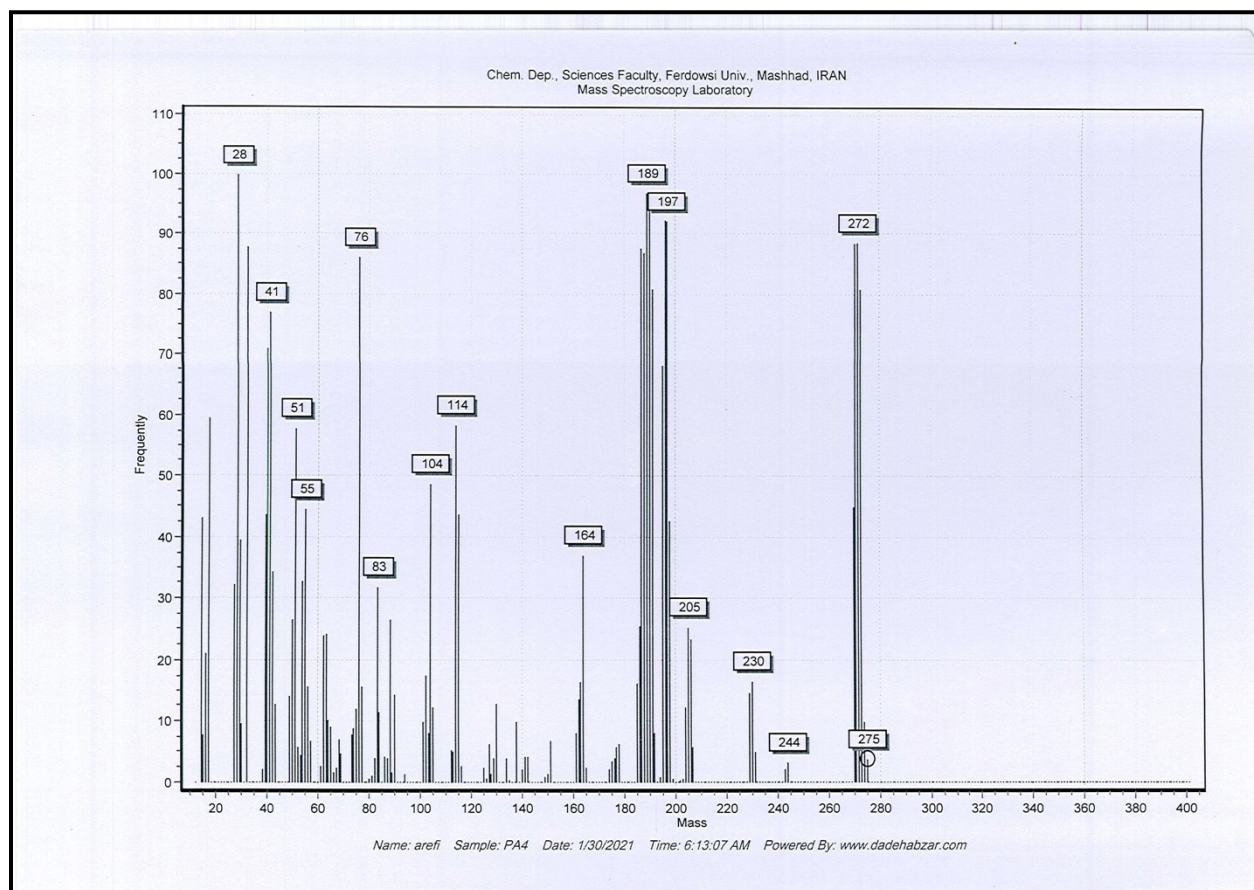
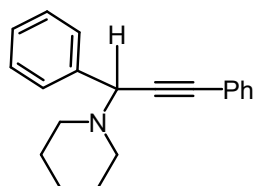
Mass spectrum of 4-(3-phenyl-1-(p-tolyl)prop-2-yn-1-yl)morpholine (Table 2, entry 5)



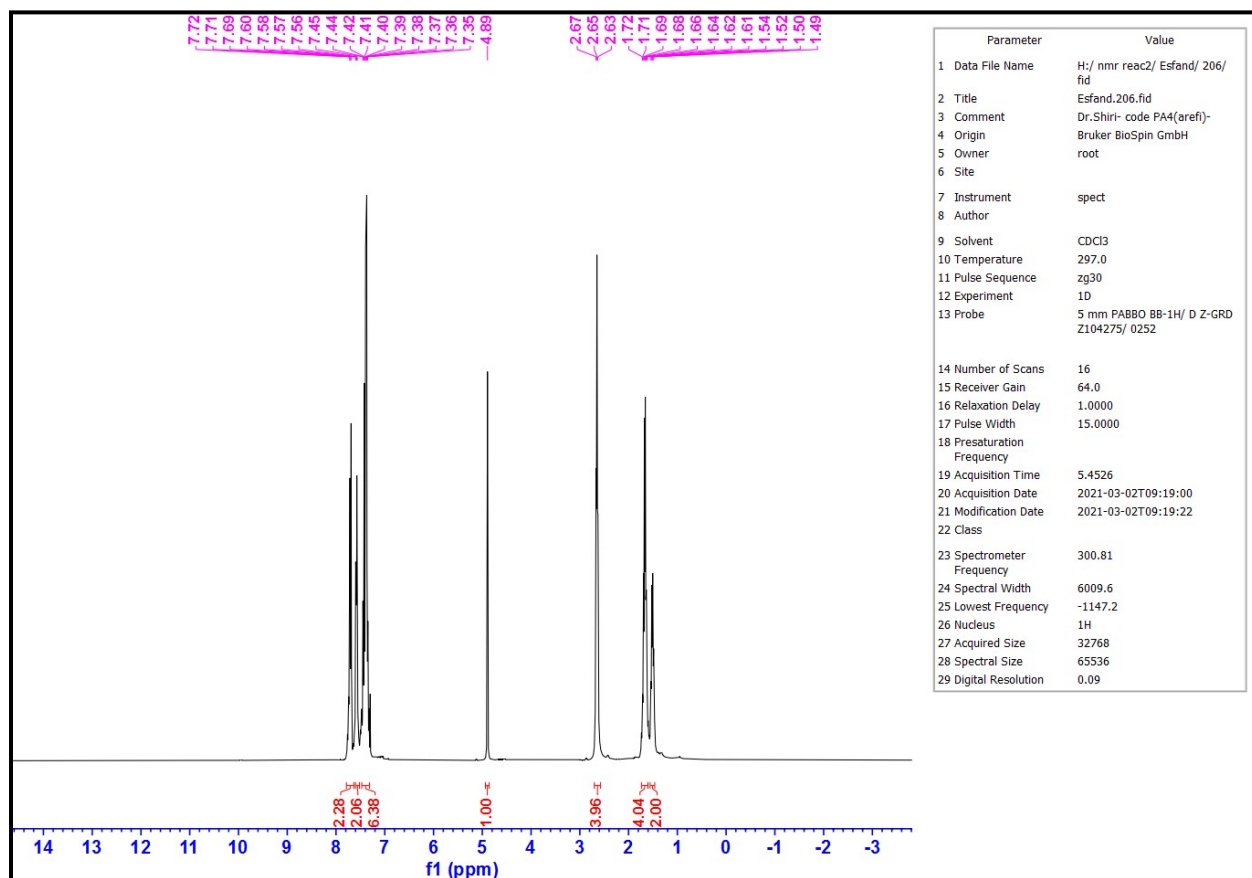
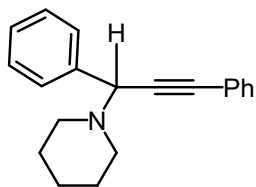
¹H-NMR of 4-(3-phenyl-1-(p-tolyl)prop-2-yn-1-yl)morpholine (Table 2, entry 5)



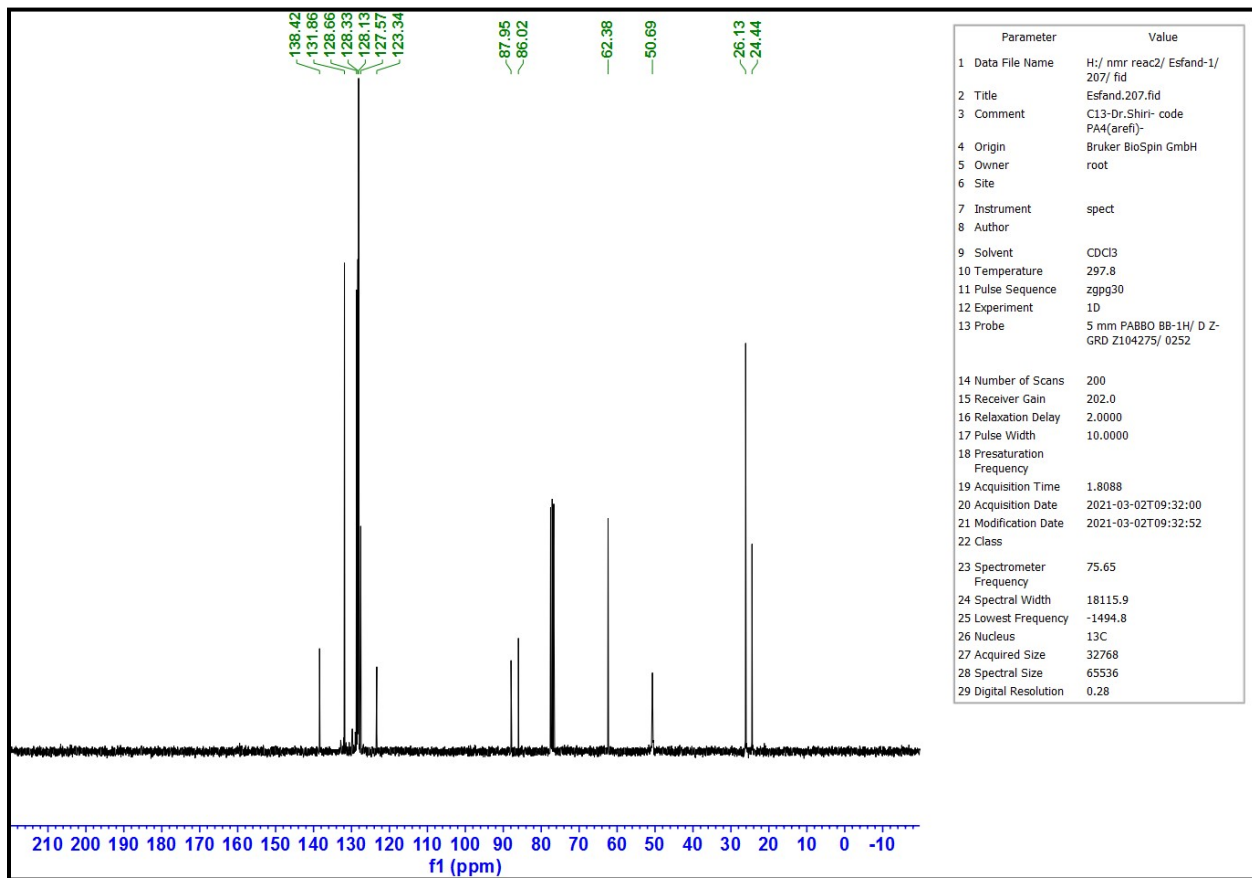
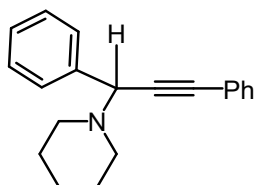
^{13}C -NMR of 4-(3-phenyl-1-(*p*-tolyl)prop-2-yn-1-yl)morpholine (Table 2, entry 5)



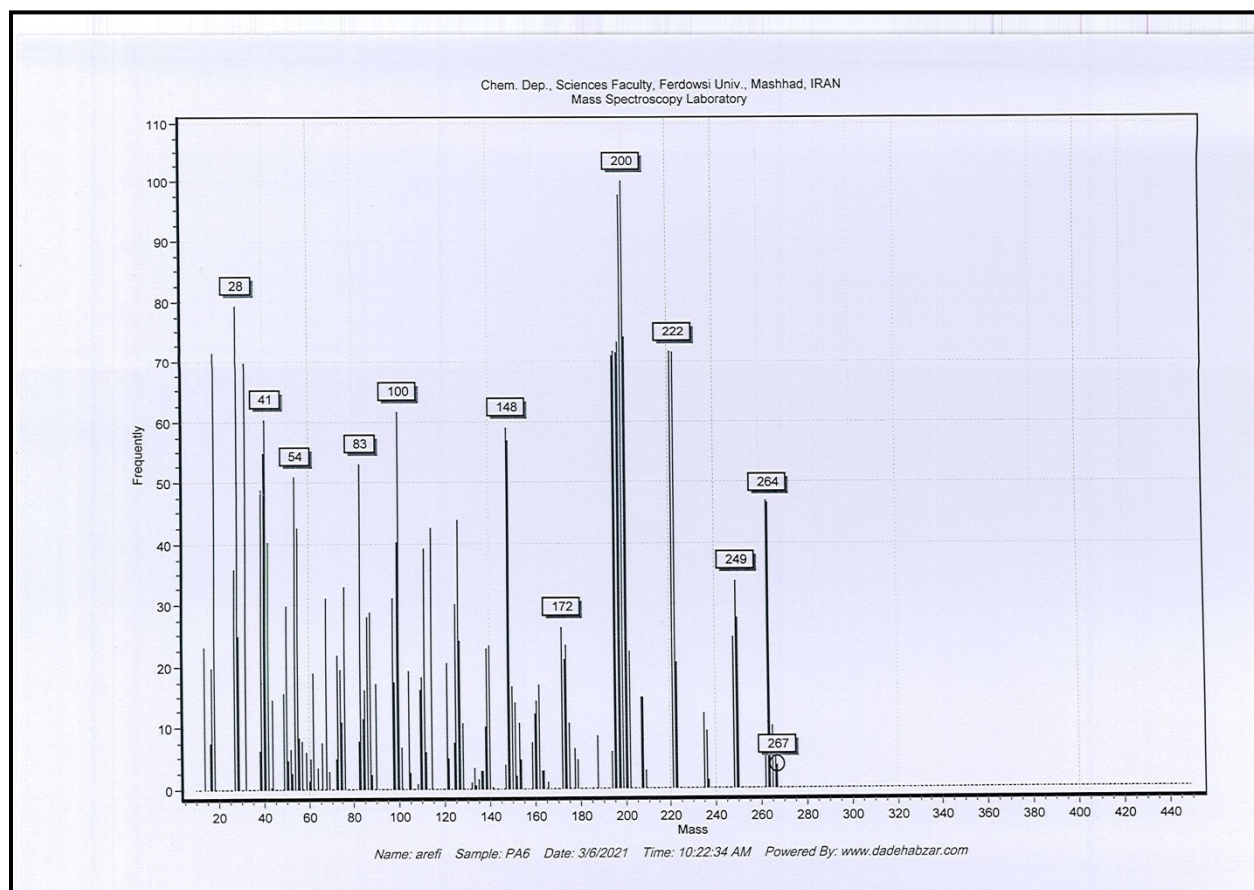
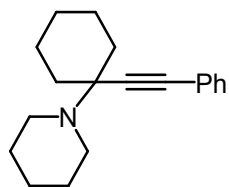
Mass spectrum of 1-(1,3-Diphenylprop-2-yn-1-yl) piperidine (Table 2, entry 6)



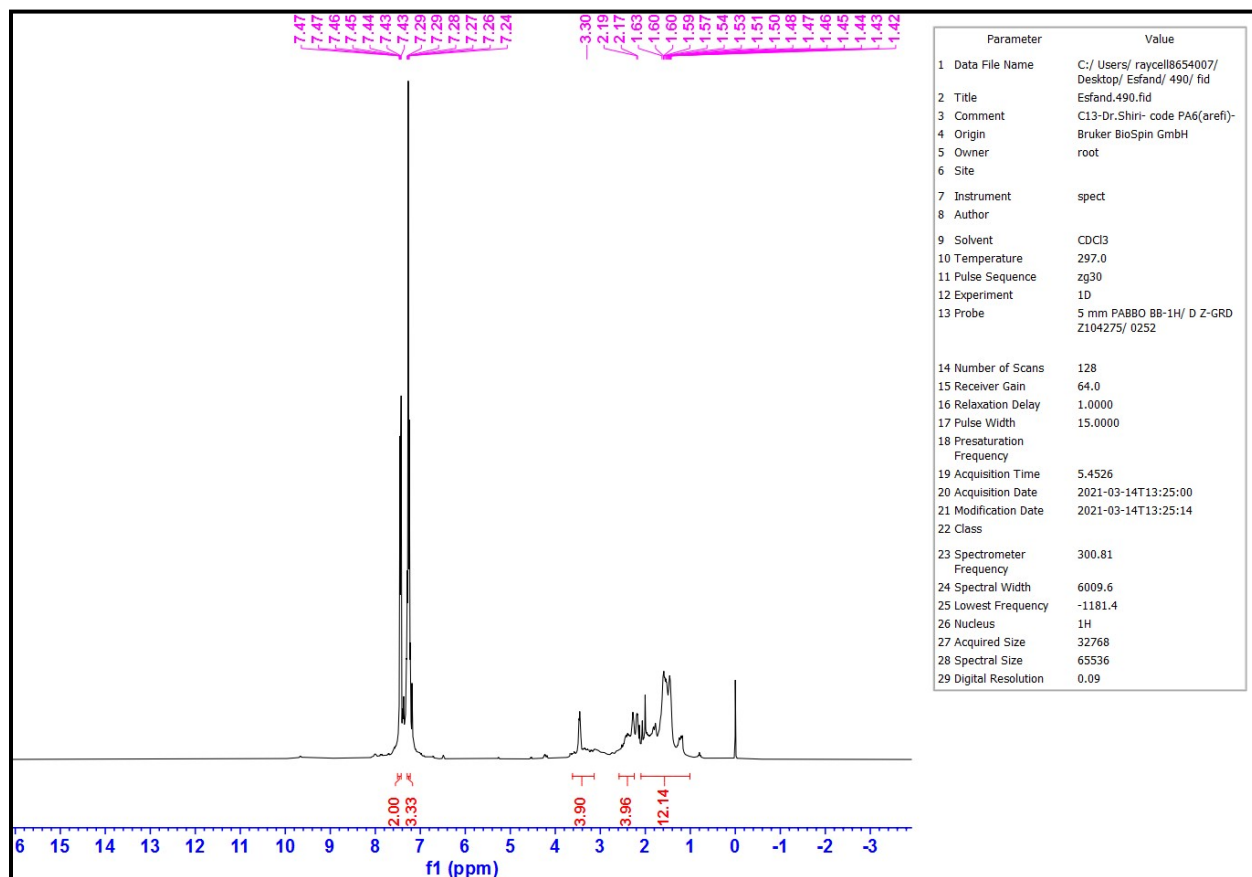
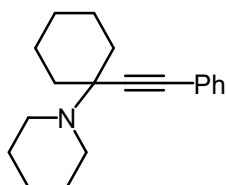
$^1\text{H-NMR}$ of 1-(1,3-Diphenylprop-2-yn-1-yl) piperidine (Table 2, entry 6)



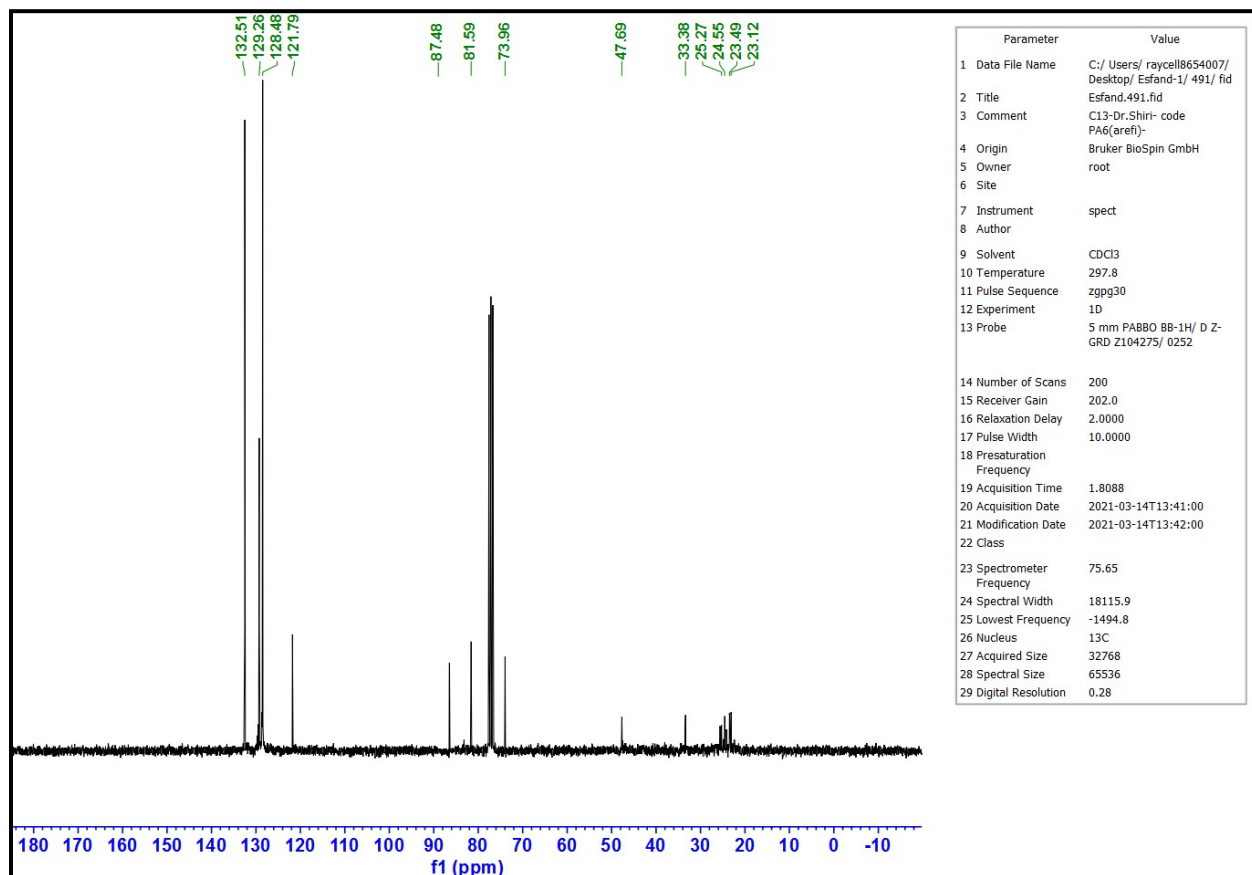
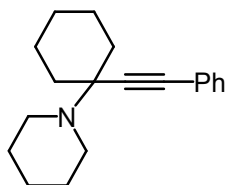
^{13}C -NMR of 1-(1,3-Diphenylprop-2-yn-1-yl) piperidine (Table 2, entry 6)



Mass spectrum of 1-(1-(phenylethynyl)cyclohexyl)piperidine (Table 2, entry 12)



¹H-NMR of 1-(1-(phenylethynyl)cyclohexyl)piperidine (Table 2, entry 12)



^{13}C -NMR of 1-(1-(phenylethynyl)cyclohexyl)piperidine (Table 2, entry 12)