

Supplementary Material for

Selectivity-tunable iron nanoparticles from lignocellulosic components for the reductive amination of carbonyl compounds towards switchable products

Xiuzheng Zhuang, Xiangqian Wei, Xiaohong Hu, Qi Zhang, Xinghua Zhang, Lungang Chen,

Jianguo Liu*, Longlong Ma*

¹Key Laboratory of Energy Thermal Conversion and Control of Ministry of Education, School of Energy and Environment, Southeast University, Nanjing 210096, People's Republic of China

** Corresponding authors e-mail: liujg@seu.edu.cn, mall@seu.edu.cn*

This document includes:

Fig. S1 Schematic layout of the experimental setup.

Fig. S2 SEM images of the hydrochars carbonized at different time.

Fig. S3 TEM images of the hydrochars carbonized prepared at water or glycol solvents.

Fig. S4 FTIR spectra of the hydrochars derived from different feedstock.

Fig. S5 TEM images of the $\text{Fe}_x\text{O}_y@\text{HC}$ at different hydrothermal temperatures.

Fig. S6 SEM images of the $\text{Fe}@\text{HC}$ at different pyrolysis temperatures.

Fig. S7 The XPS spectra of the $\text{Fe}@\text{HC}_{700}$.

Fig. S8 The control experiments under similar conditions.

Table S1 Yields of the hydrothermally synthesized nanosphere with crosslinker.

Table S2 Surface areas, average diameter, and total pore volumes of the $\text{Fe}_x\text{O}_y@\text{HC}$

S1. ^1H NMR and GC-MS spectra

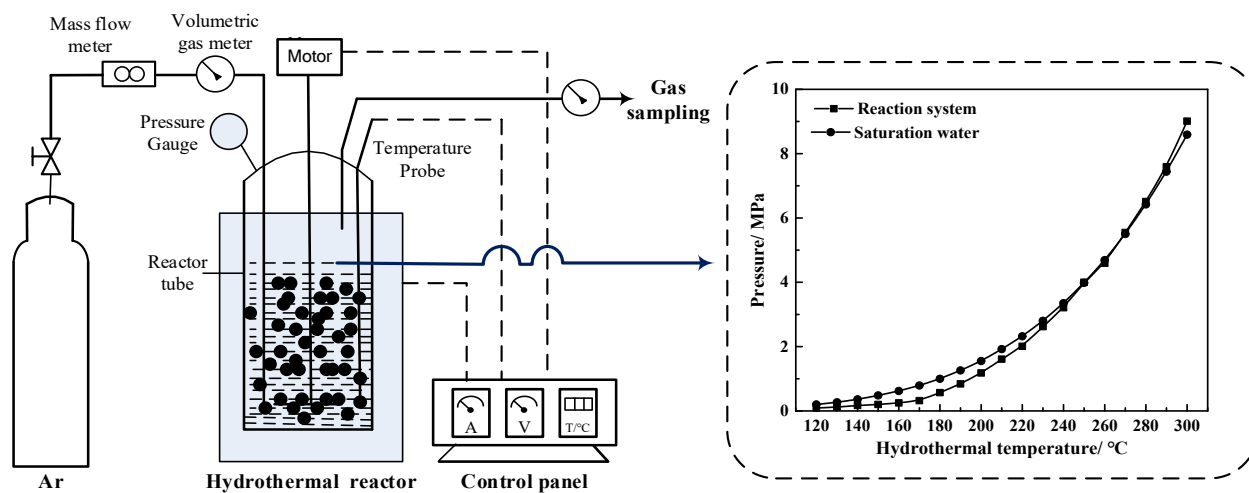


Fig. S1 Schematic layout of experimental setup

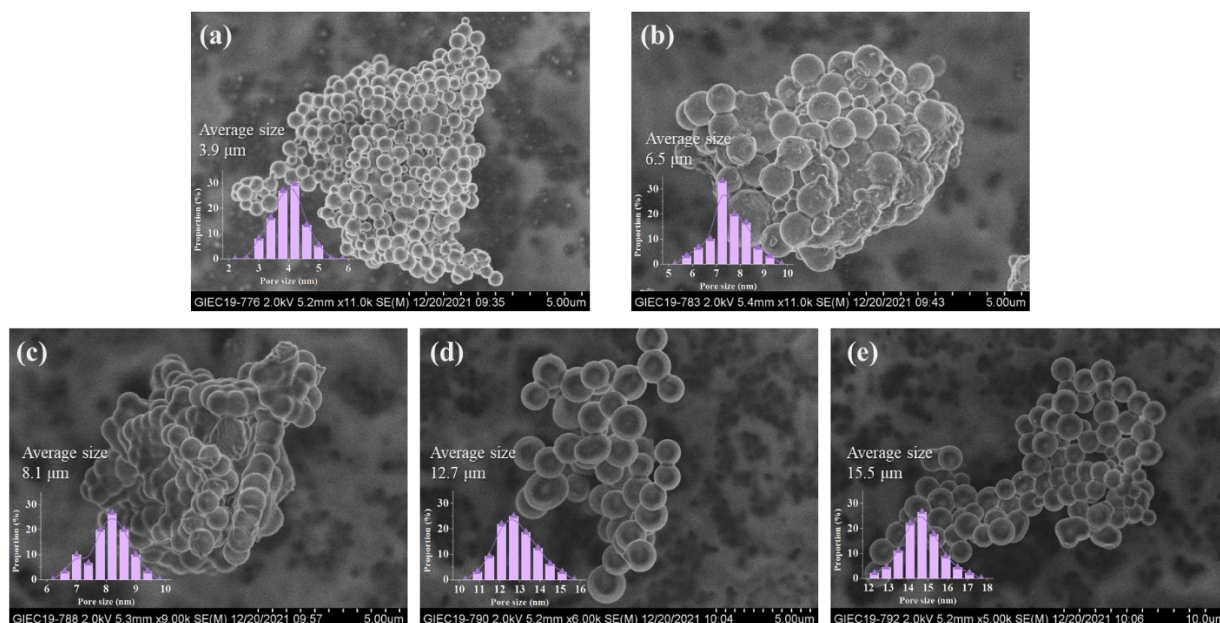


Fig. S2 SEM images of the hydrochars carbonized at different time. (a) 2 h; (b) 6 h; (c) 10 h; (d) 16 h; (e) 24 h. Note, the other conditions are 180 °C and 10 wt%.

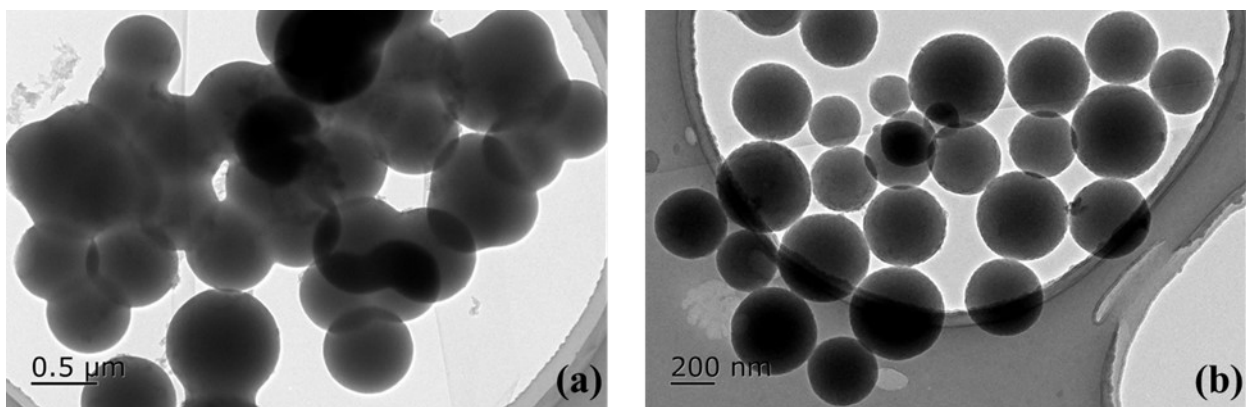


Fig. S3 TEM images of the hydrochars prepared at different solvents. (a) water; (b) glycol.

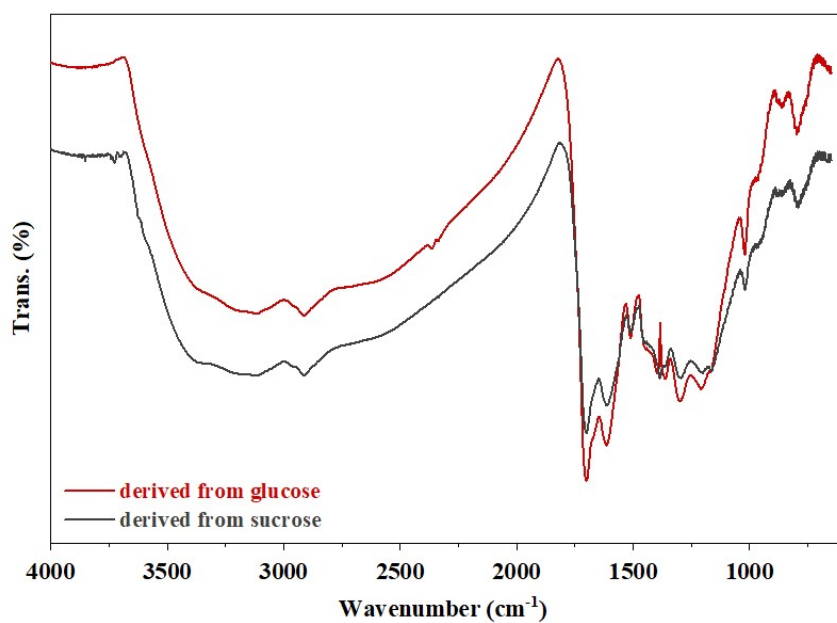


Fig. S4 FTIR spectra of the hydrochars derived from different feedstock. (a) glucose; (b) sucrose.

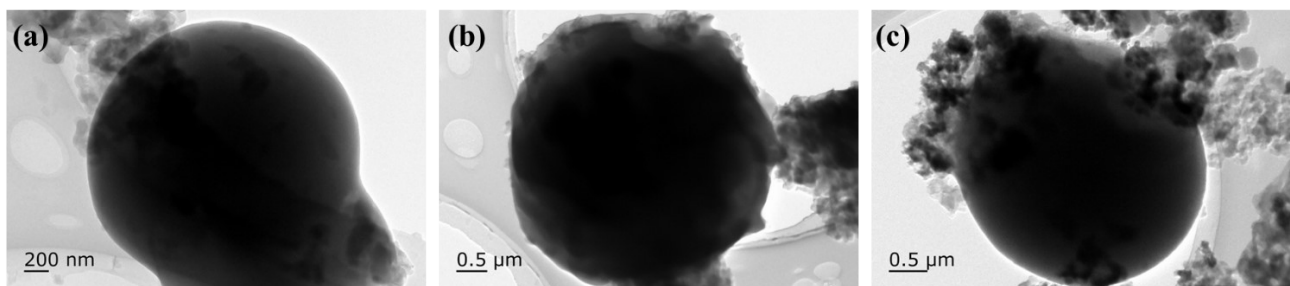


Fig. S5 TEM images of the $\text{Fe}_x\text{O}_y@\text{HC}$ at different hydrothermal temperatures. (a) 150 °C; (b) 180 °C; (c) 210 °C.

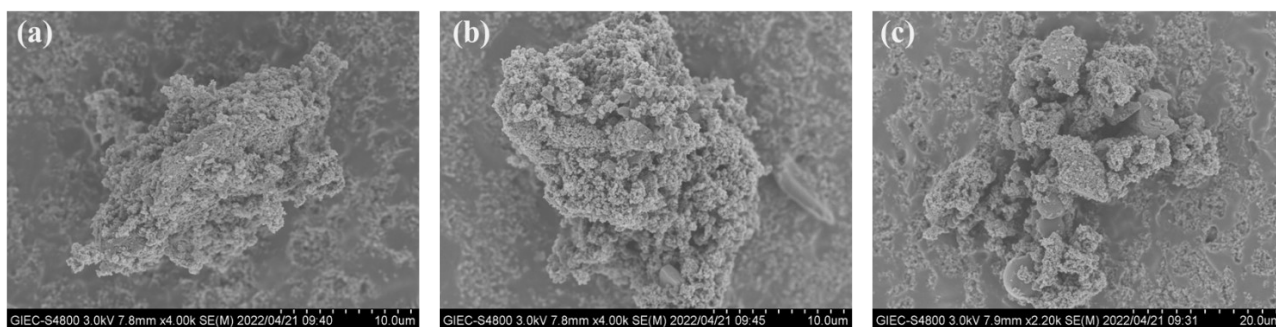


Fig. S6 SEM images of the Fe@HC at different pyrolysis temperatures. (a) 600 °C; (b) 700 °C; (c) 800 °C.

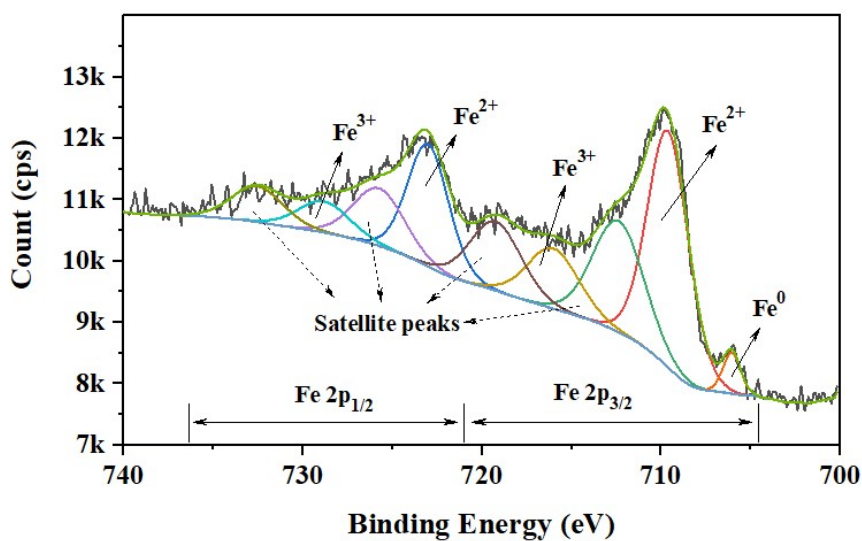


Fig. S7 The XPS spectra of the Fe@HC₇₀₀.

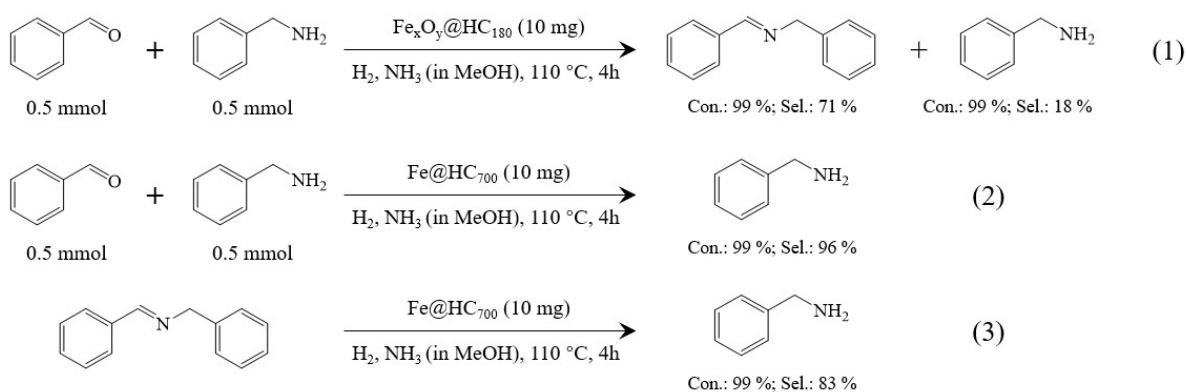


Fig. S8 The control experiments under similar conditions

Table S1 Yields of the hydrothermally synthesized nanosphere with crosslinker

Type of crosslinker	Ultimate analysis $w_{db}/\%$			Yield $w_{db}/\%$	Carbon conversion/ %
	C	H	O		
Citric acid	65.3	4.7	30.0	51.0	83.2
Graphene sheet	70.4	4.2	25.4	48.5	85.3
Gallic acid	66.3	4.8	28.9	47.8	79.2

Note: VM, volatile matters; FC, fixed carbon; O (oxygen) was calculated by difference based on dry base. Both of N and ash were not detected in the ultimate and proximate analysis, respectively. The reaction conditions are 180 °C, 16 h and 10 $wt\%$.

Table S2 Surface areas, average diameter, and total pore volumes of the $Fe_xO_y@HC$

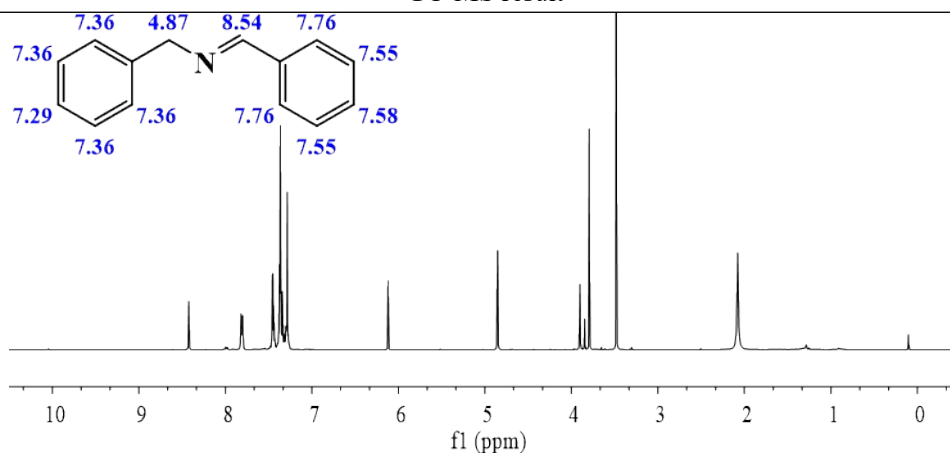
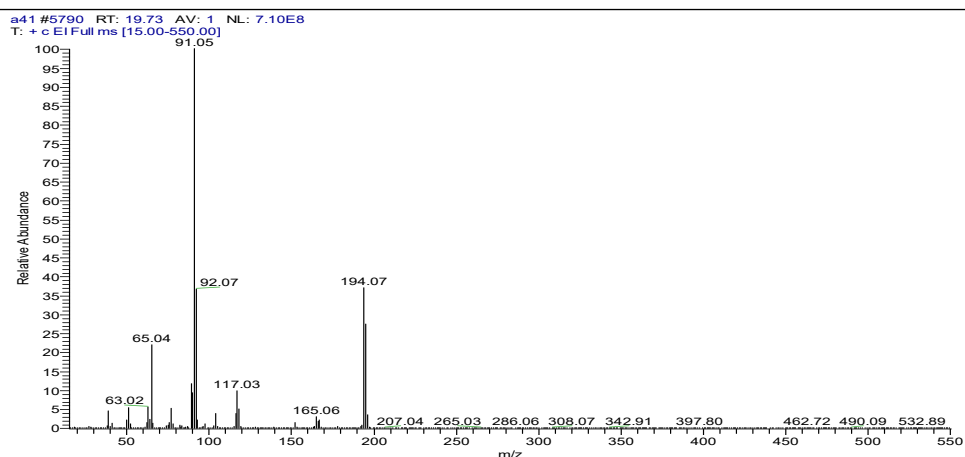
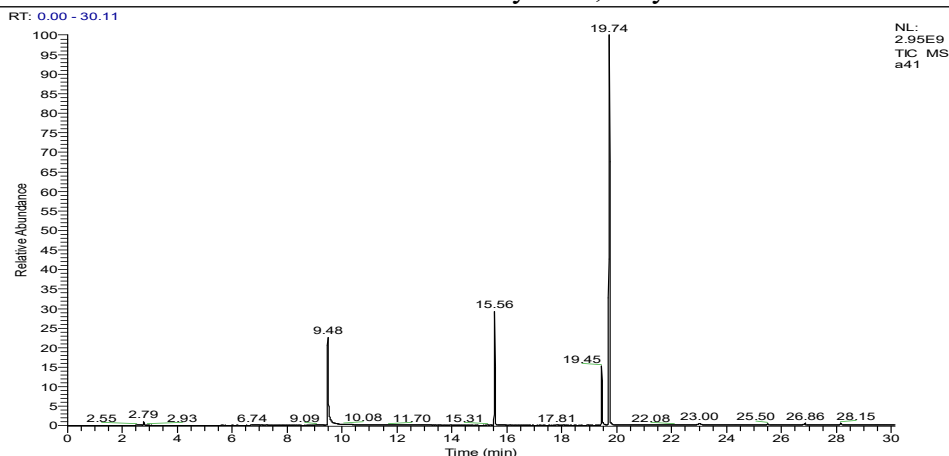
Catalyst	Specific surfaces area (m^2/g)	Average diameter (nm)	Pore volume (cm^3/g)
$Fe_xO_y@HC_{150}$	9.72	1.92	0.030
$Fe_xO_y@HC_{180}$	14.4	1.91	0.043
$Fe_xO_y@HC_{210}$	16.8	1.71	0.037

S1. ^1H NMR and GC-MS spectra

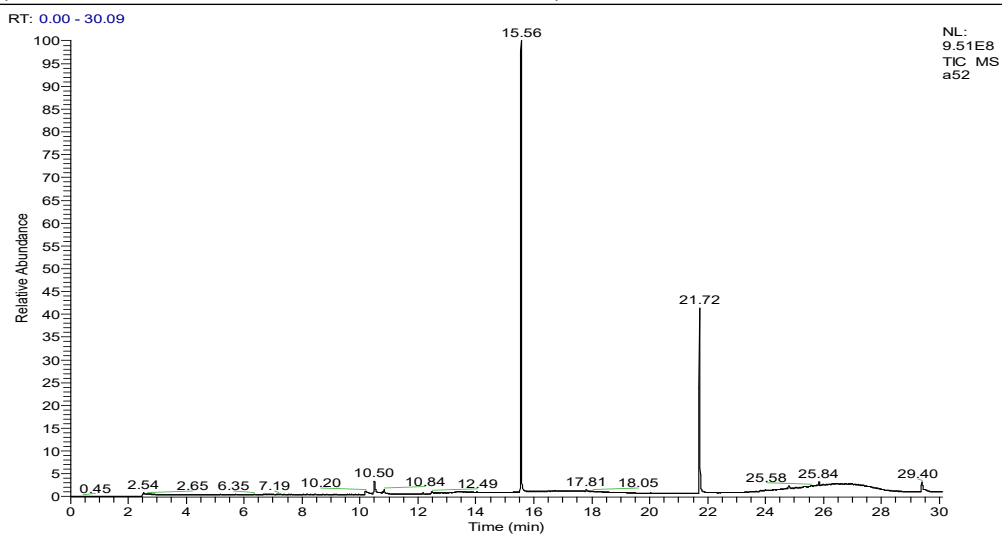
(In this GC-MS procedure, the first 2 min is held at 40 °C to stabilize the baseline and to evaporate the methanol solution, so that the huge peak in this period is not included in the calculation. Note, the peaks at 15.6 min (GC result) and 3.81/6.07 ppm (NMR result) represents 1,3,5-trimethoxybenzene.)

Entry 12 (CAS: 780-25-6; MW: 195.26; RT: 19.74 min).

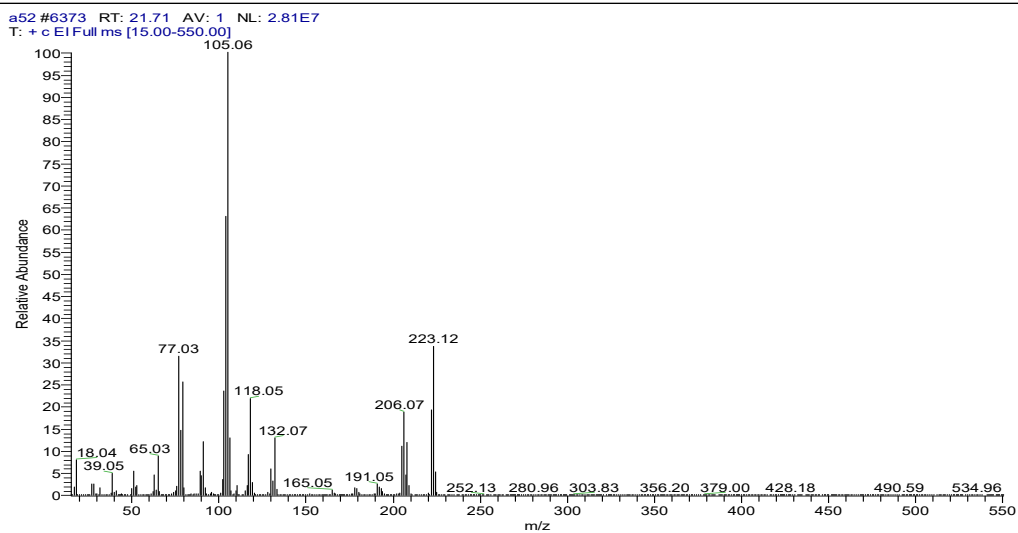
Please note that the similar substance is used in Entry 1-21, only the reaction conditions are different.



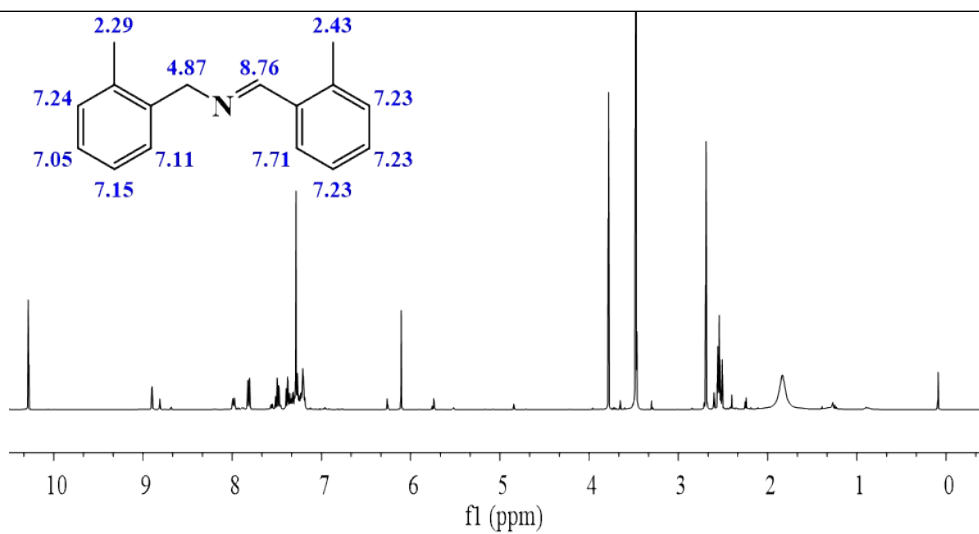
Entry 22 (CAS: N.D.; MW: 223.26; RT: 21.72 min)



GC result

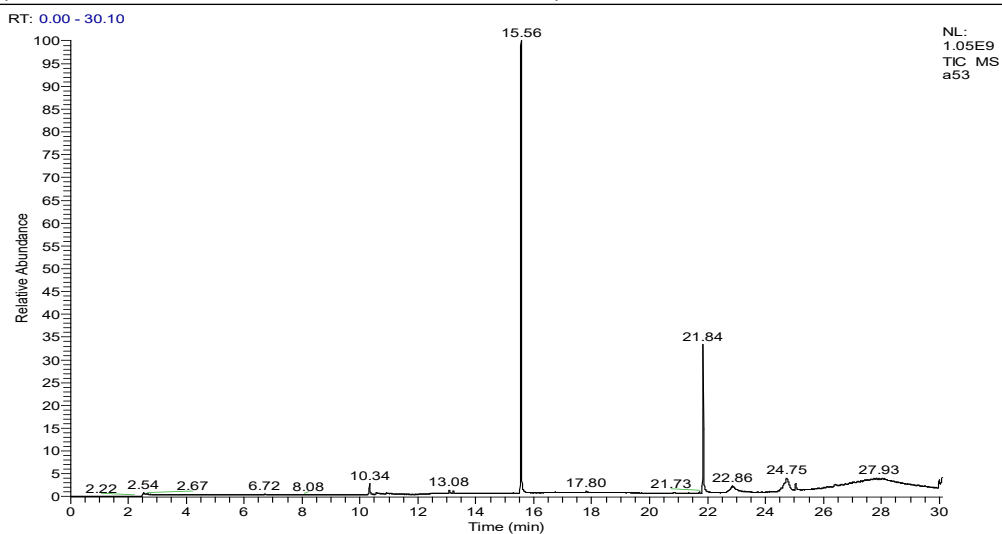


GC-MS result

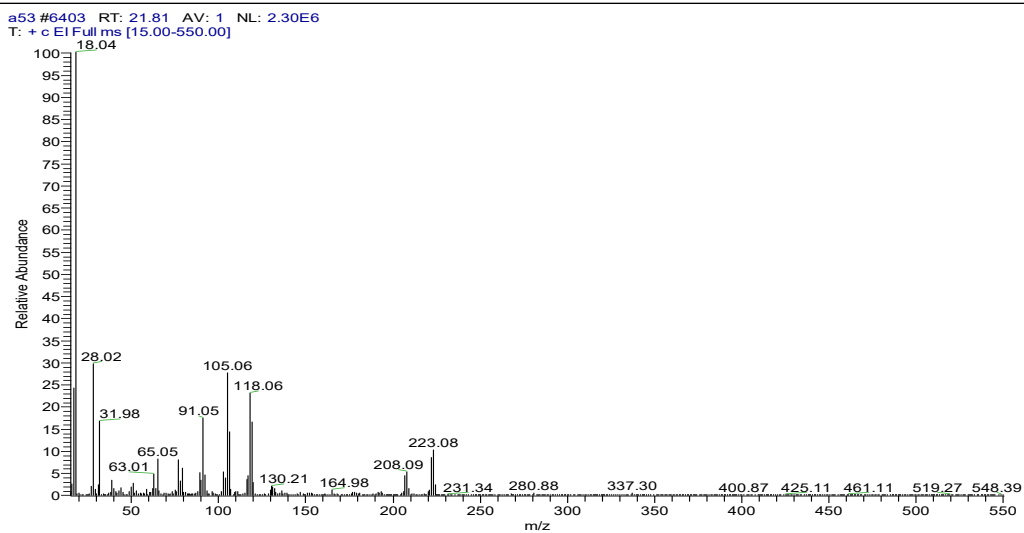


¹H NMR result

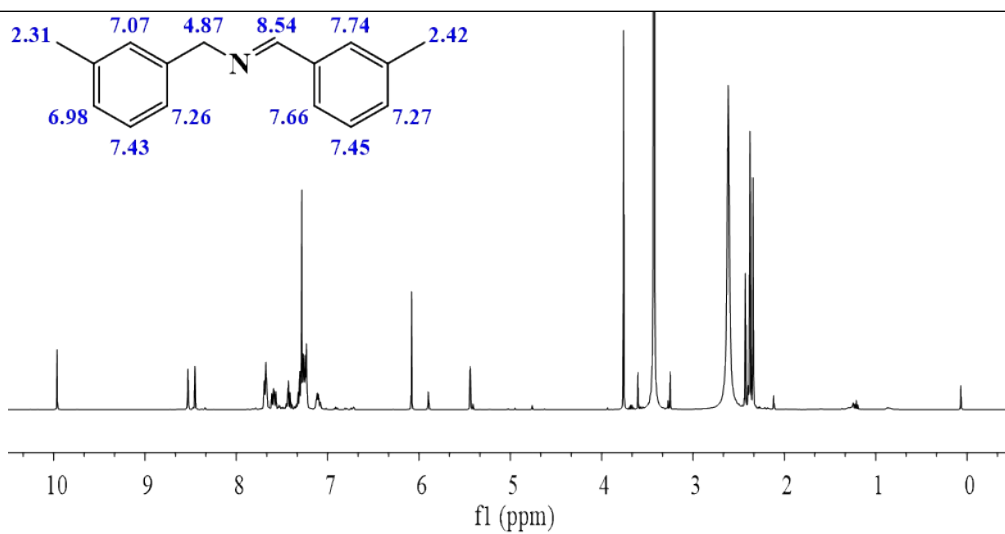
Entry 23 (CAS: N.D.; MW: 223.26; RT: 21.84 min)



GC result

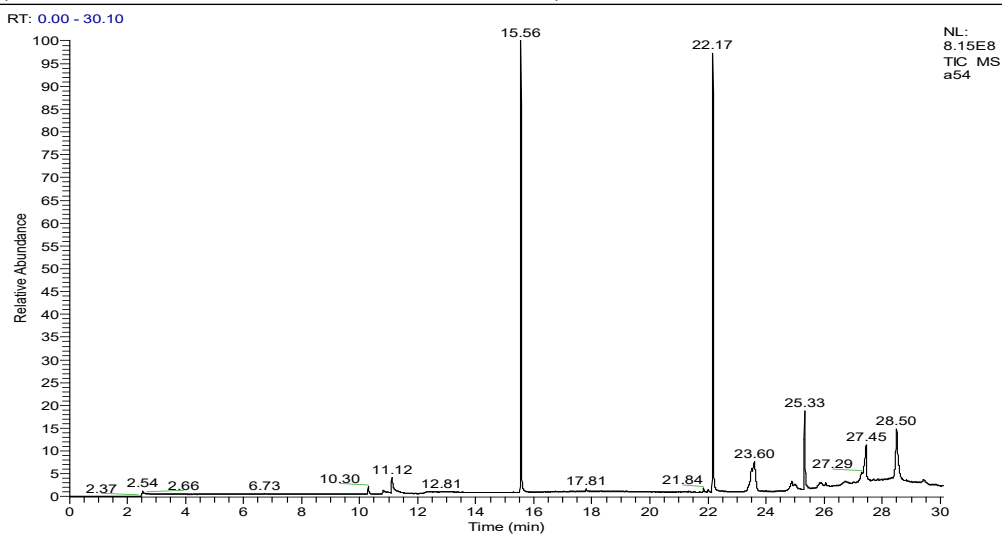


GC-MS result

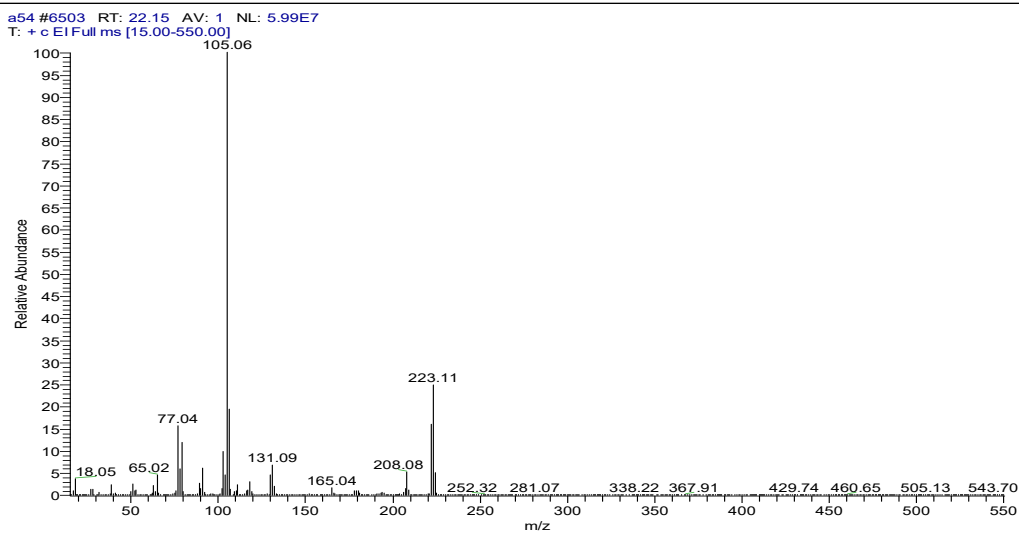


¹H NMR result

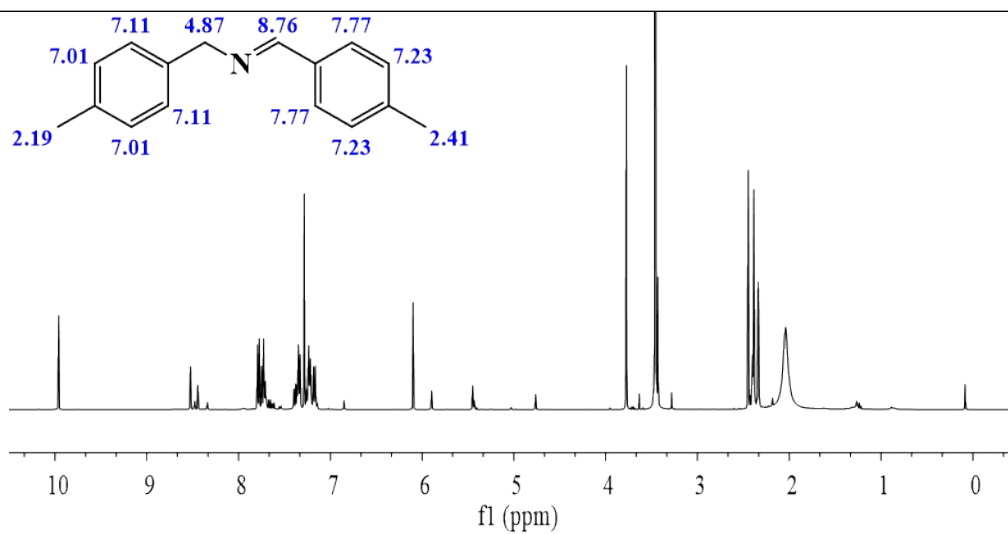
Entry 24 (CAS: N.D.; MW: 223.26; RT: 22.17 min)



GC result

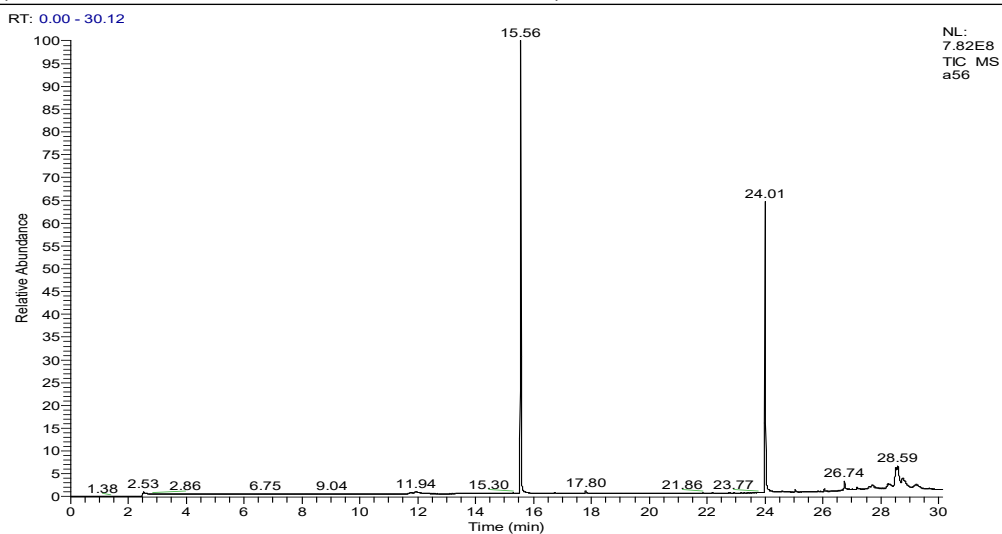


GC-MS result

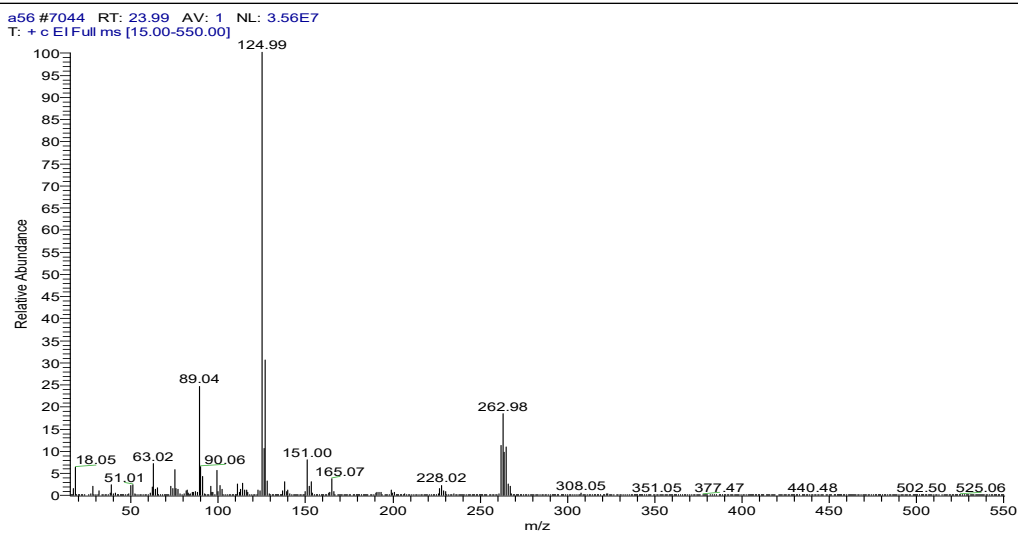


¹H NMR result

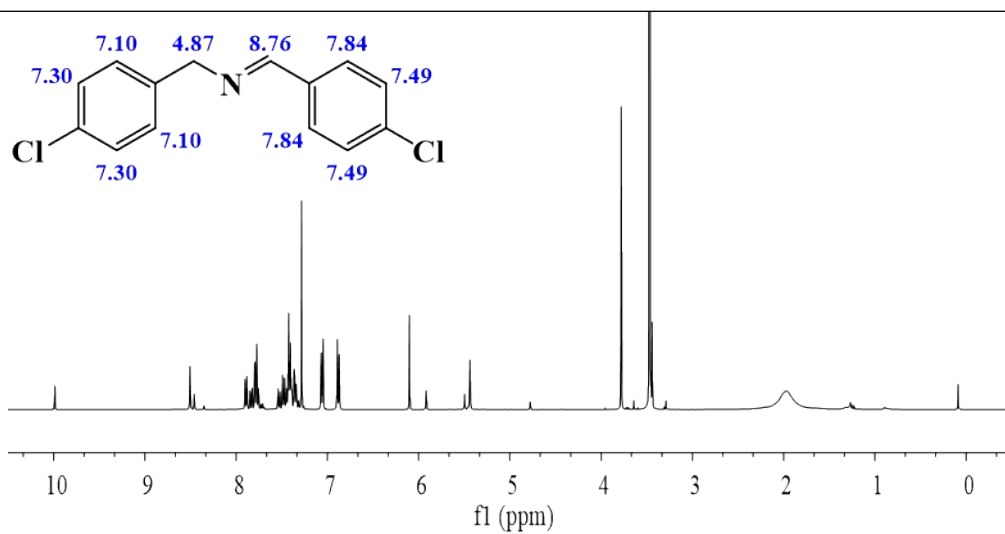
Entry 25 (CAS: N.D.; MW: 264.14; RT: 24.01 min)



GC result

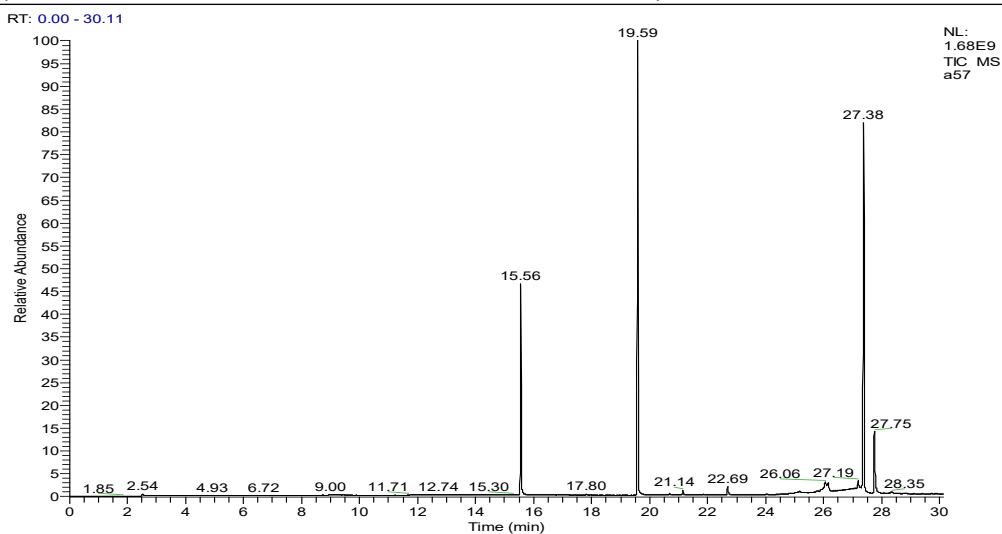


GC-MS result

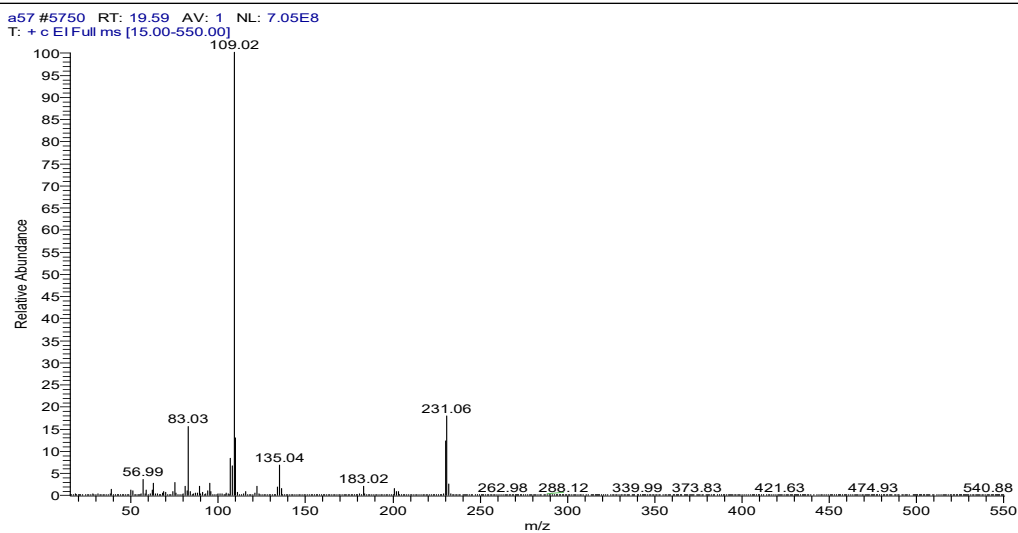


¹H NMR result

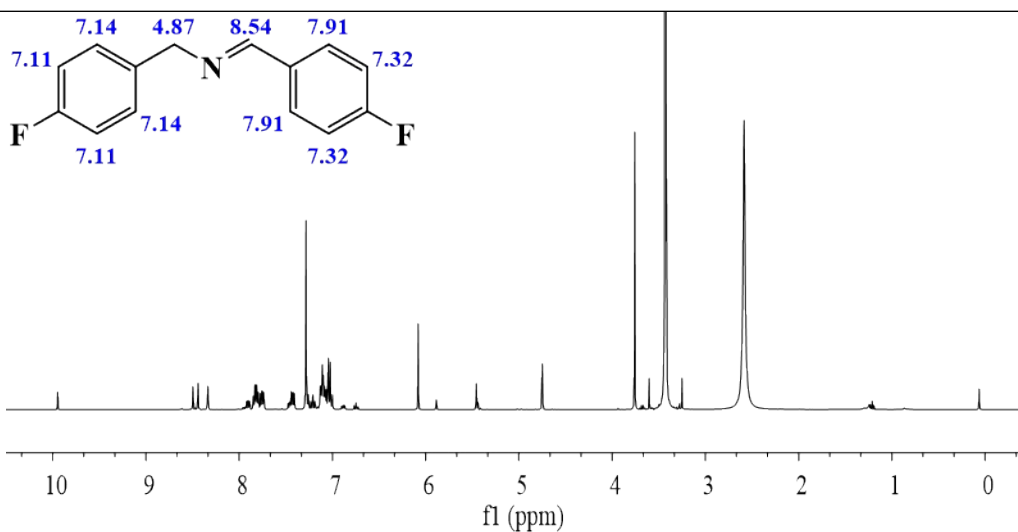
Entry 26 (CAS: 428819-12-9; MW: 231.24; RT: 19.59 min)



GC result

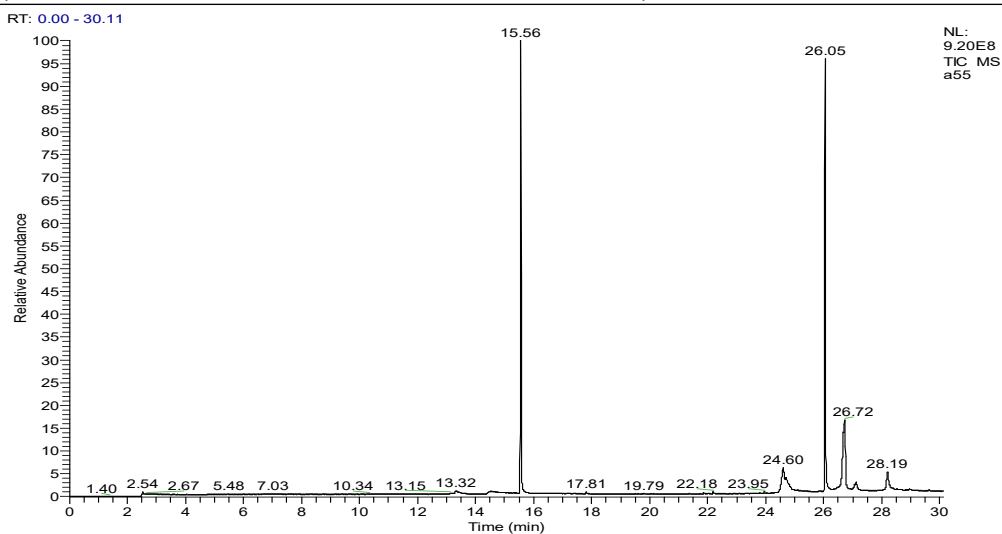


GC-MS result

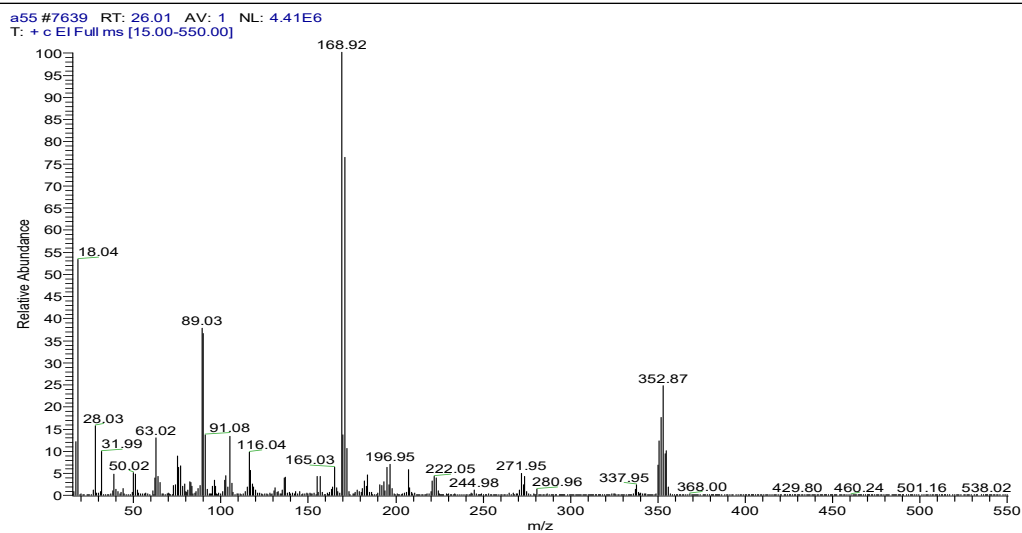


¹H NMR result

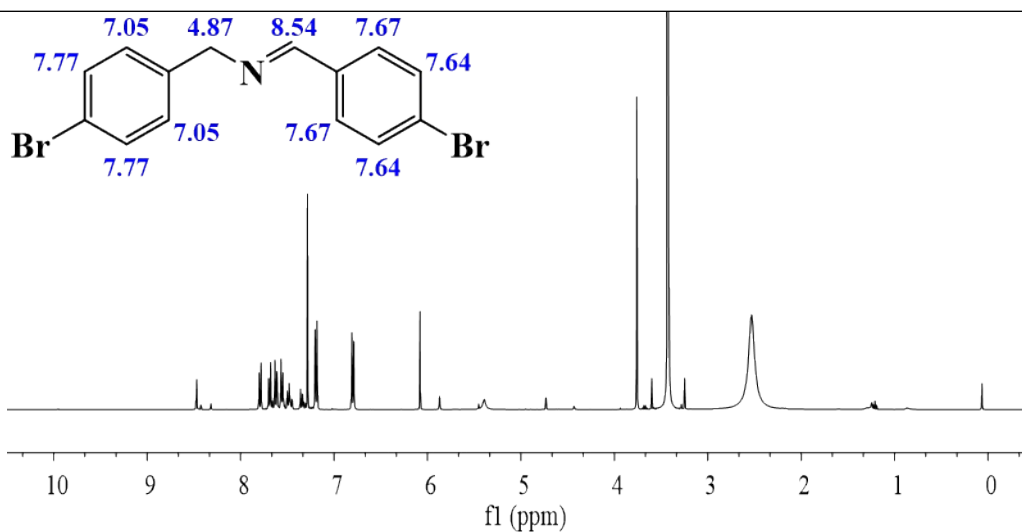
Entry 27 (CAS: 54560-80-4; MW: 353.05; RT: 26.05 min)



GC result



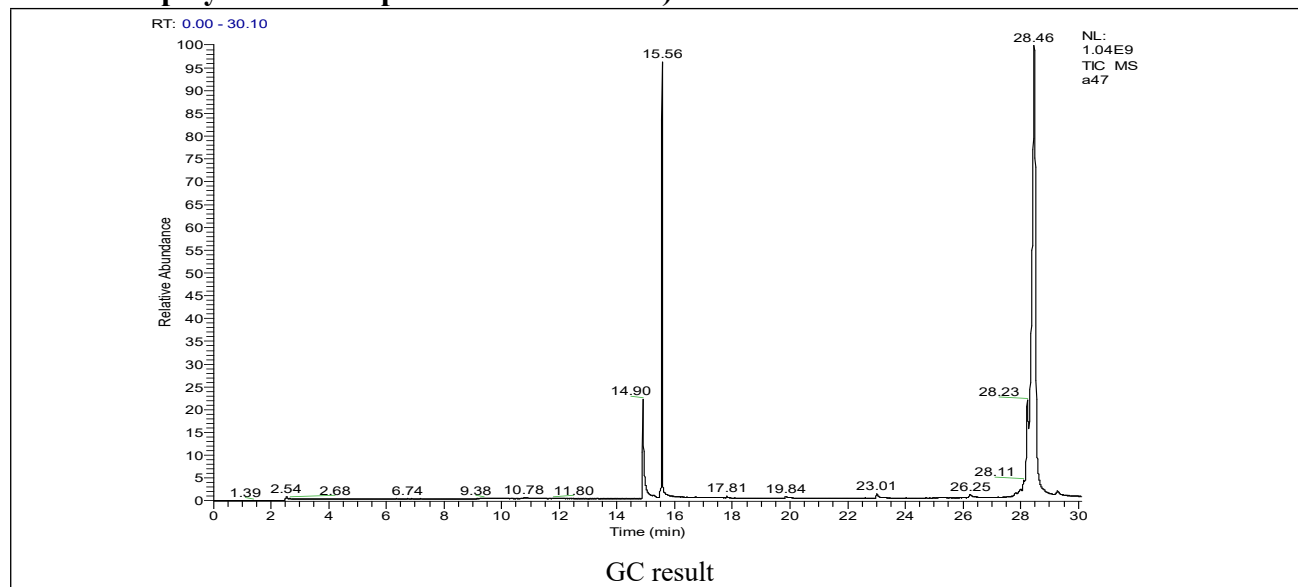
GC-MS result



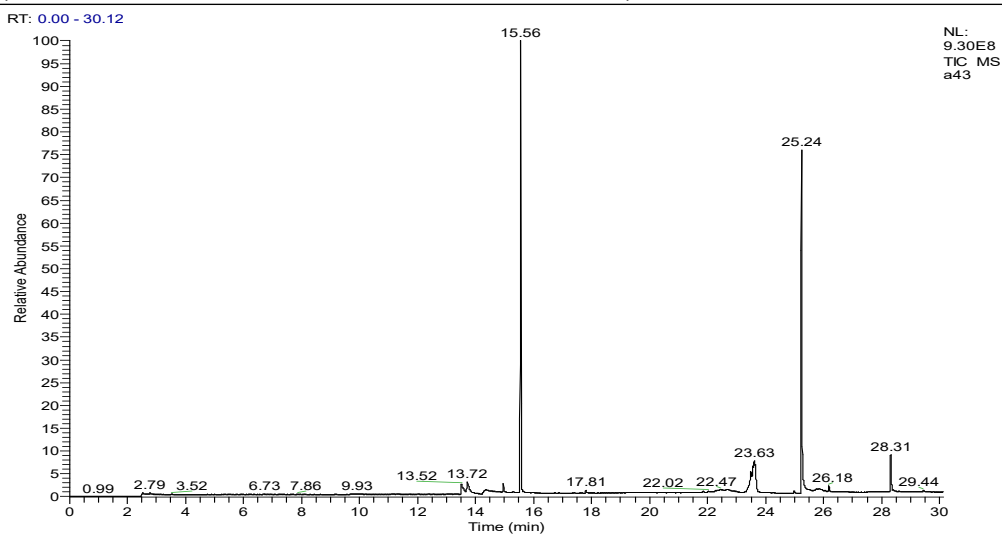
¹H NMR result

Entry 28

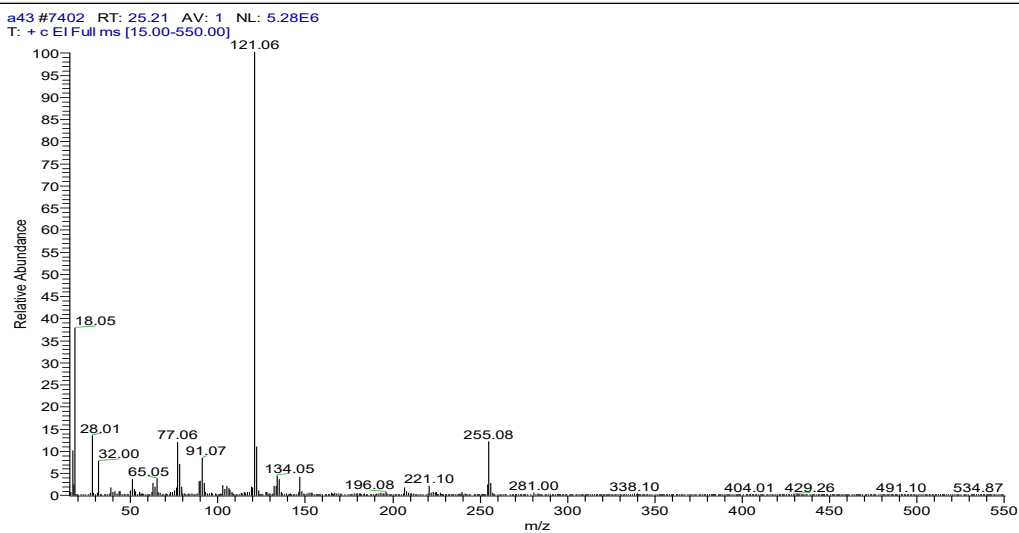
(Target product is not detected, and because of the unstable functional groups of -OH, a large number of polymers overlap between 27-29 min)



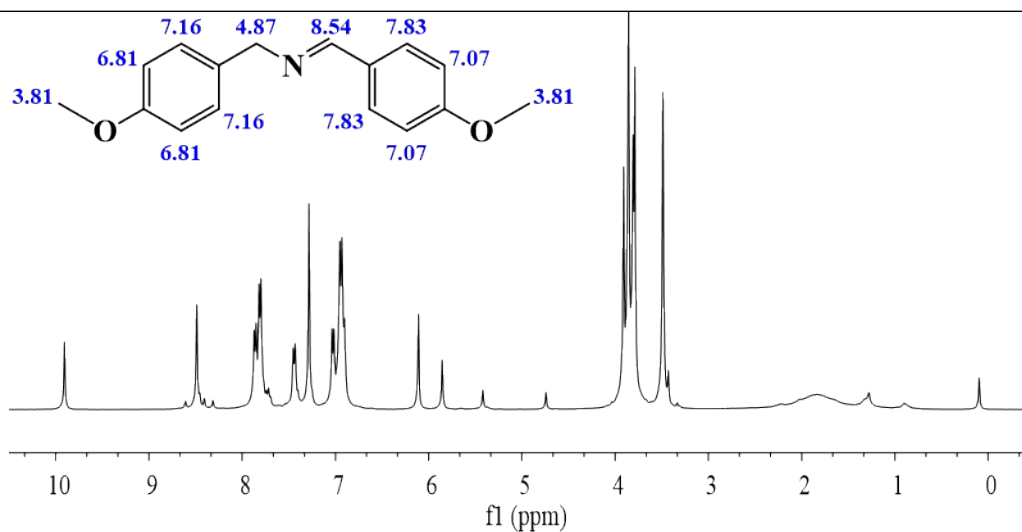
Entry 29 (CAS: 3261-60-7; MW: 255.31; RT: 25.24 min)



GC result

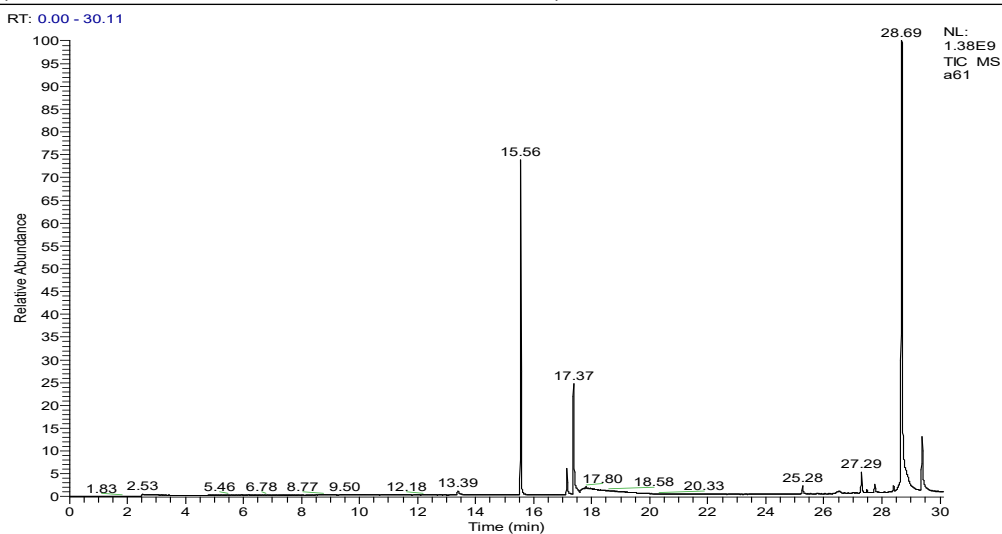


GC-MS result

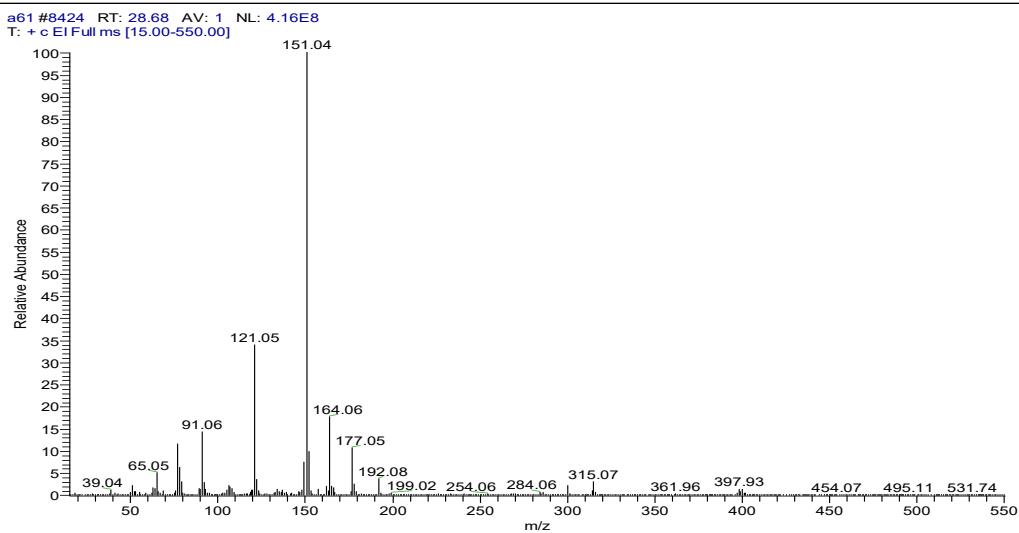


¹H NMR result

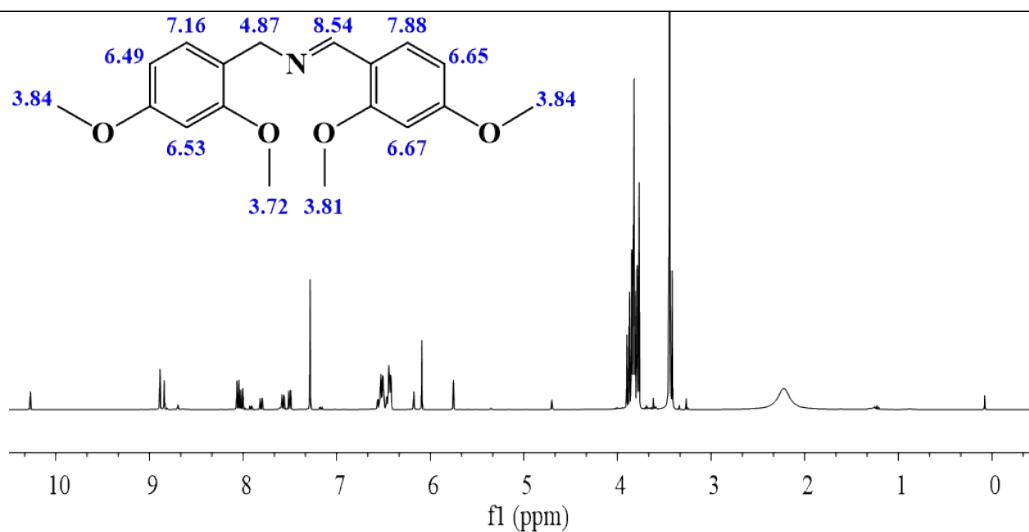
Entry 30 (CAS: N.D.; MW: 315.25; RT: 28.69 min)



GC result

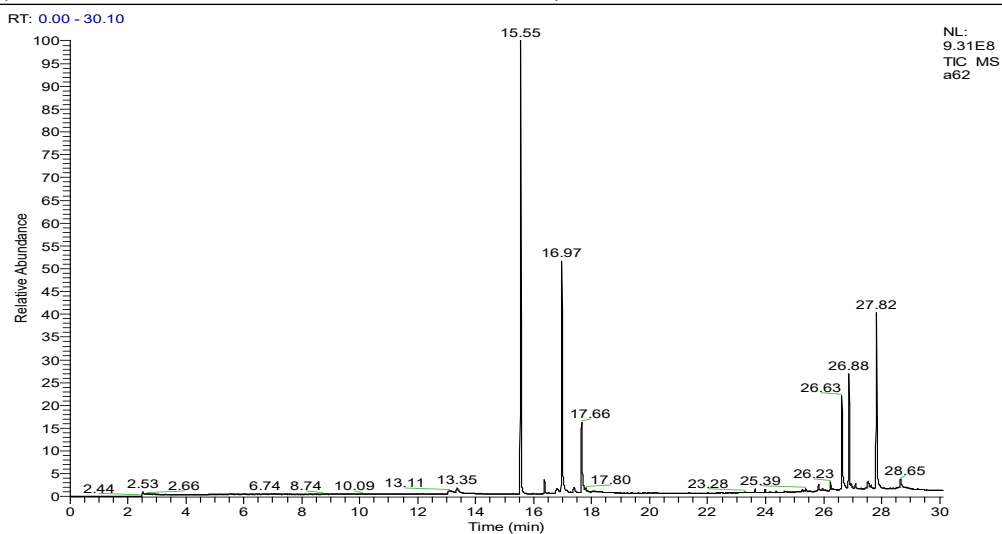


GC-MS result

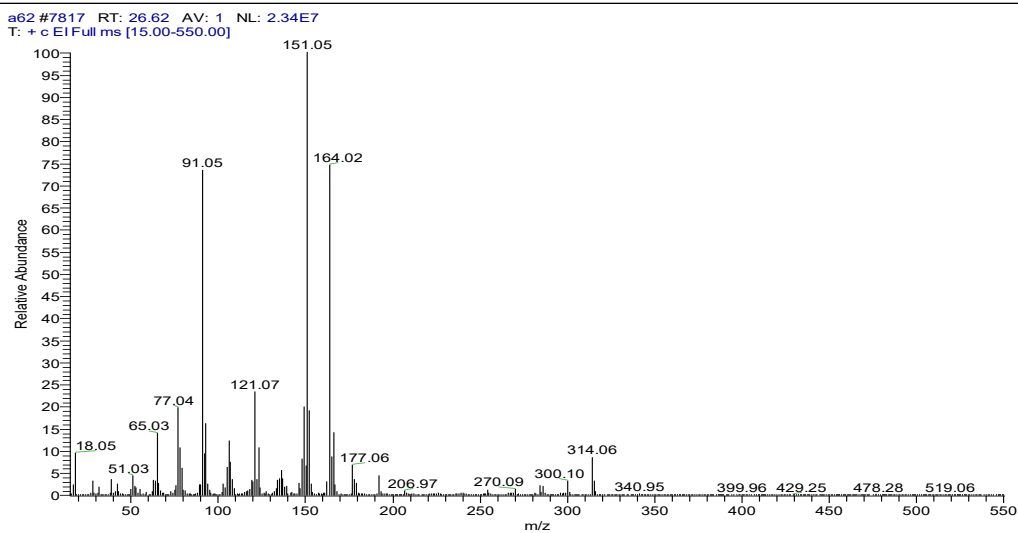


¹H NMR result

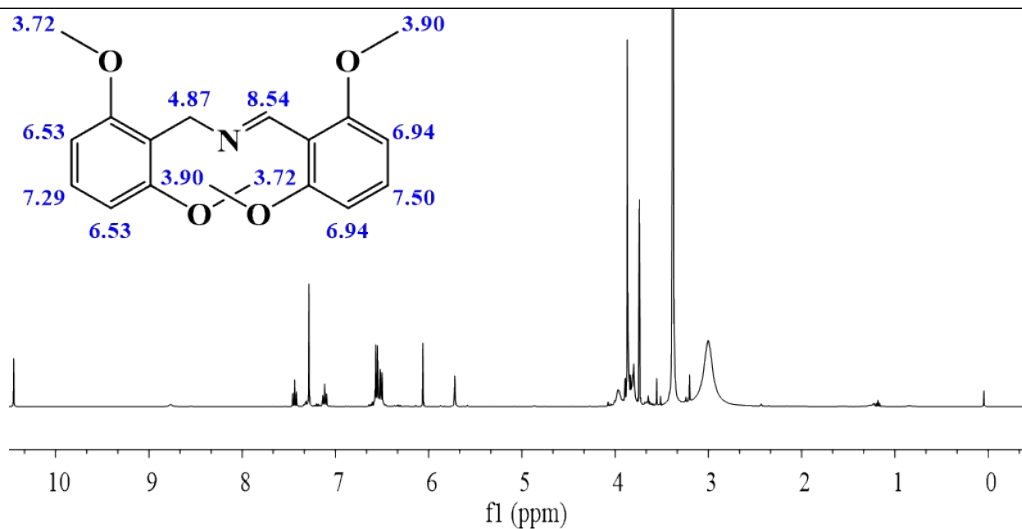
Entry 31 (CAS: N.D.; MW: 315.25; RT: 26.63 min)



GC result

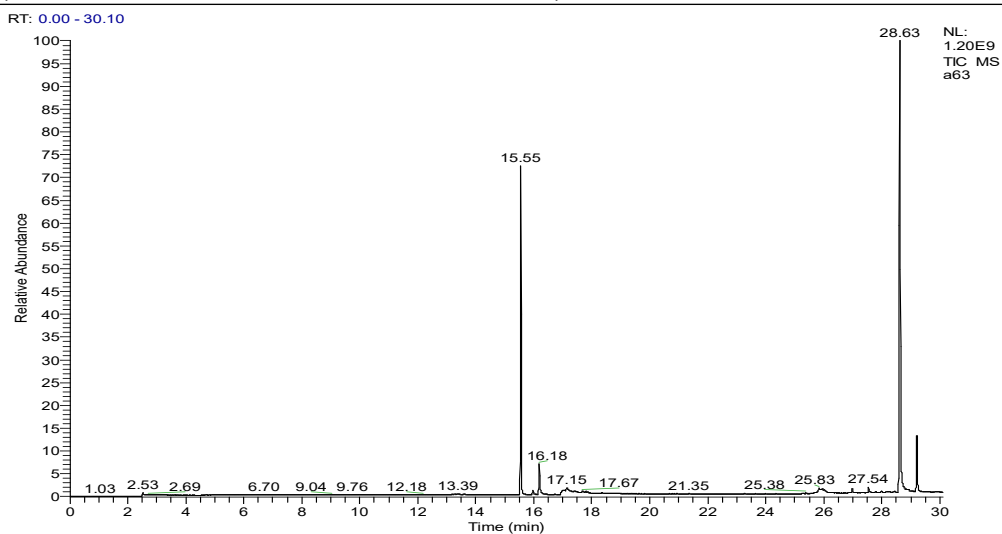


GC-MS result

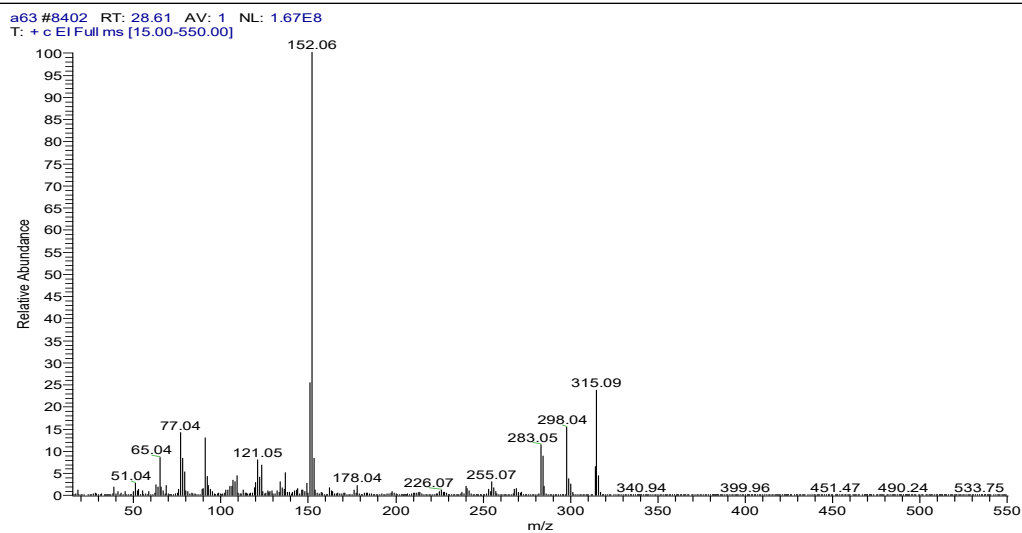


¹H NMR result

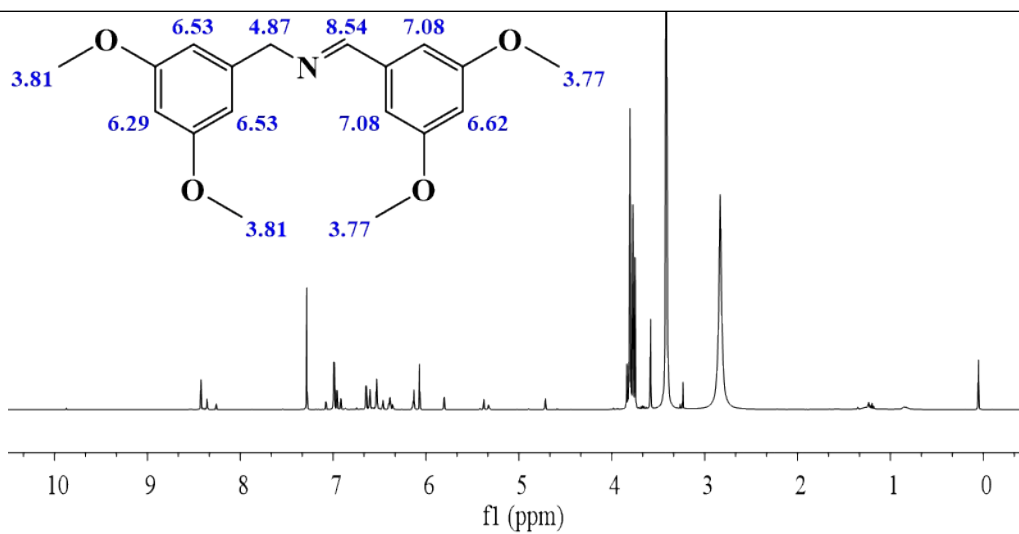
Entry 32 (CAS: N.D.; MW: 315.25; RT: 28.63 min)



GC result



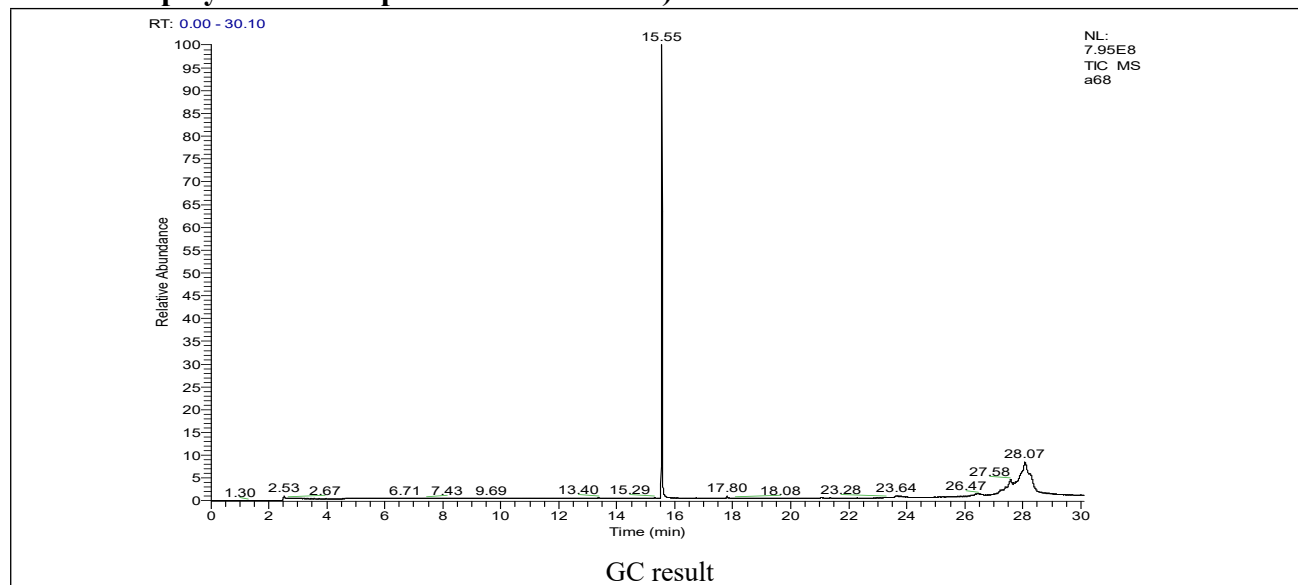
GC-MS result



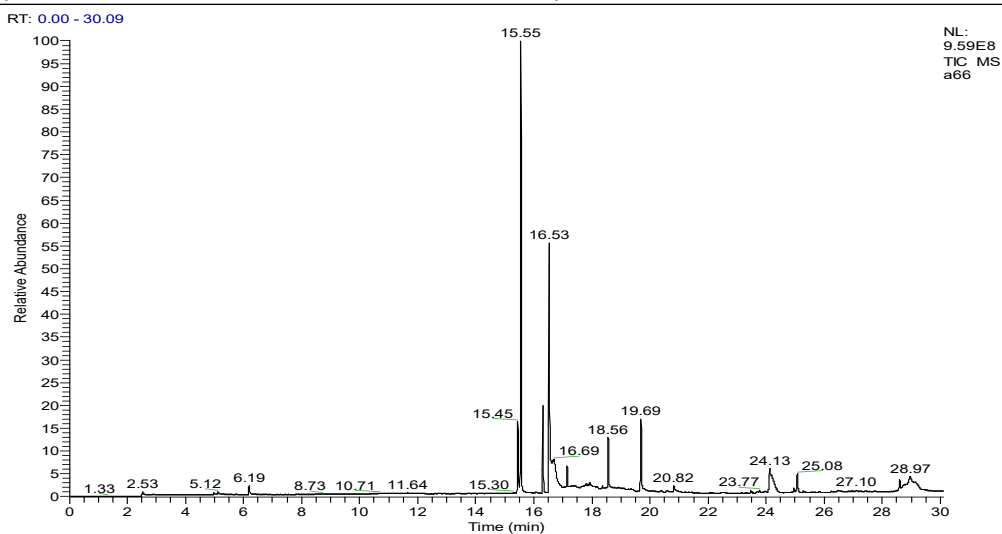
^1H NMR result

Entry 33

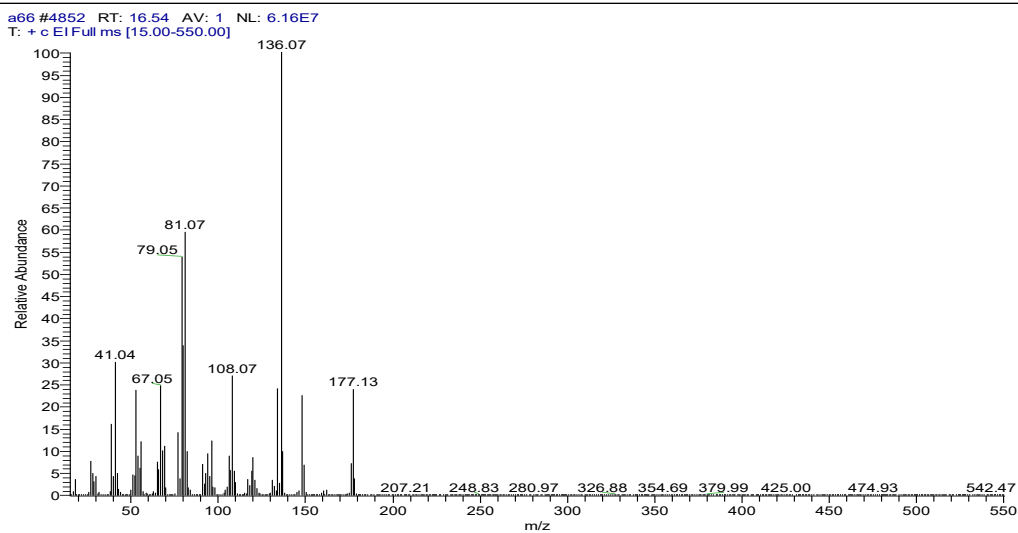
(Target product is not detected, and because of the unstable functional groups of -OH, a large number of polymers overlap between 26-29 min)



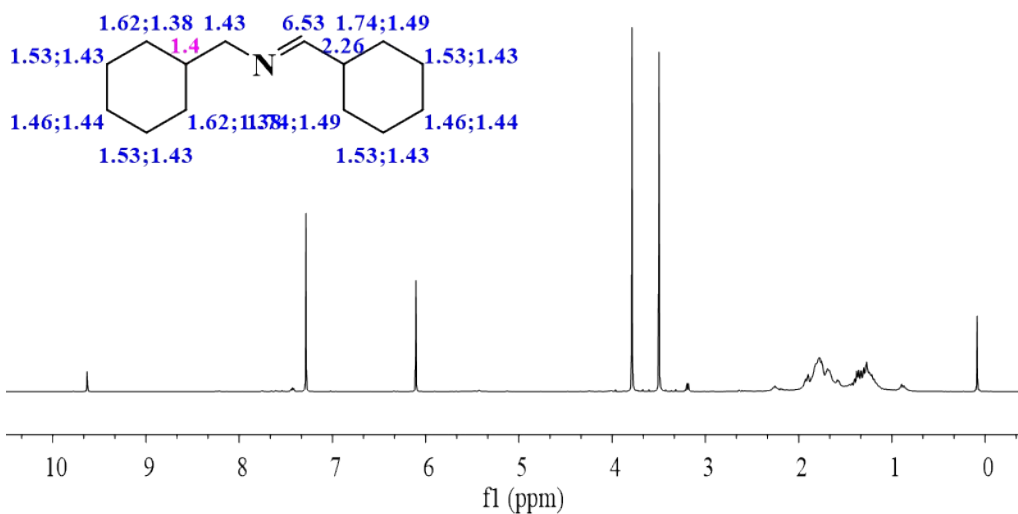
Entry 34 (CAS: N.D.; MW: 179.25; RT: 16.53 min)



GC result

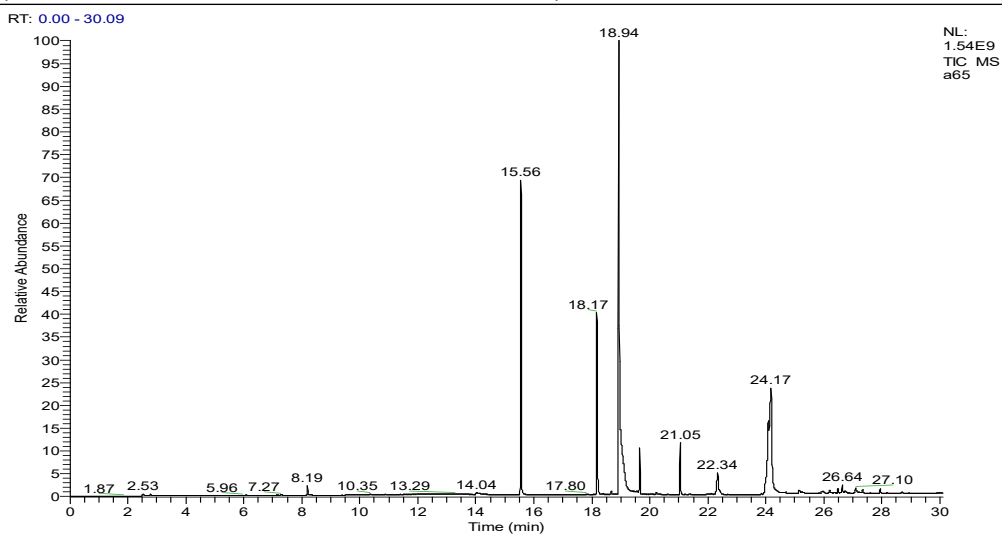


GC-MS result

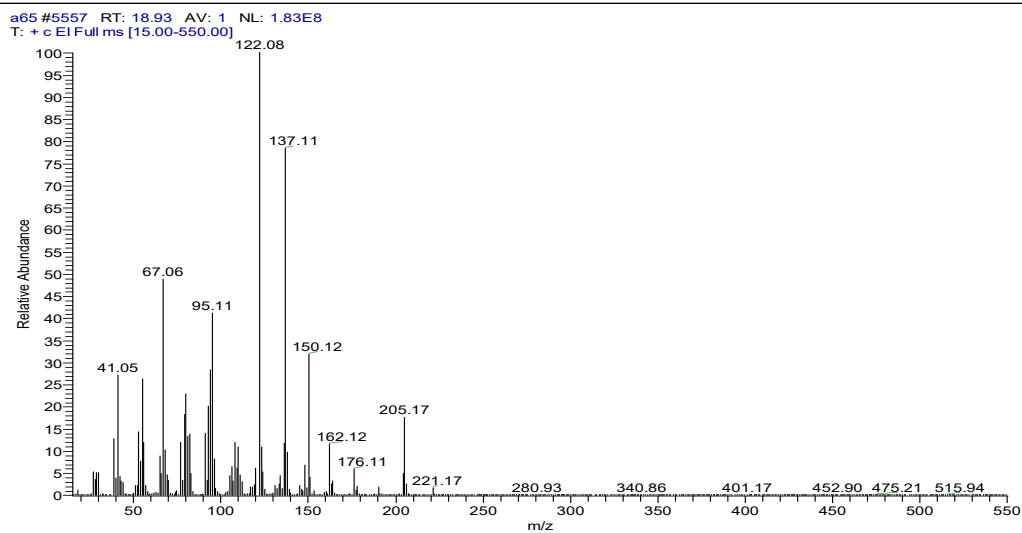


¹H NMR result

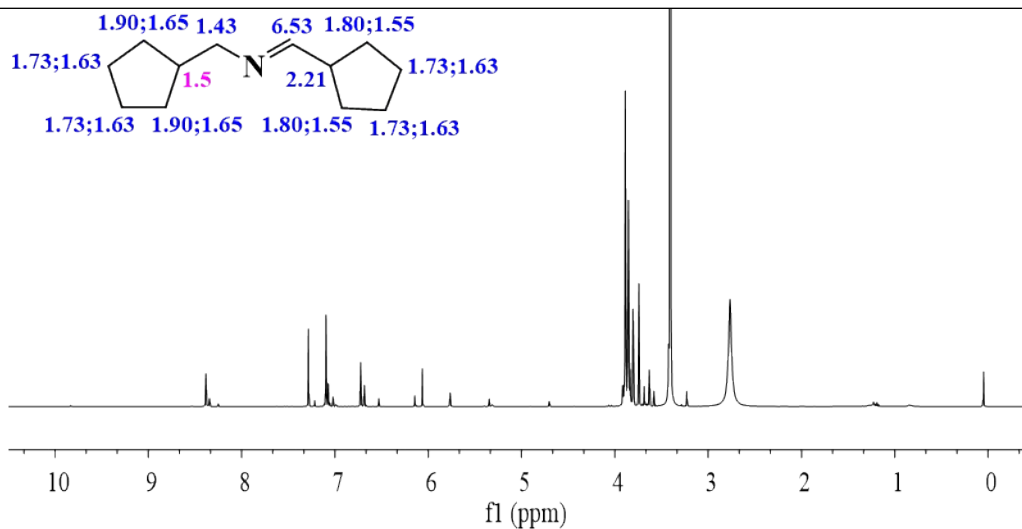
Entry 35 (CAS: N.D.; MW: 207.25; RT: 18.94 min)



GC result



GC-MS result



¹H NMR result