Electronic Supplementary Material (ESI) for Green Chemistry
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Supplementary Information

Elimination of the negative effect of nitrogen compounds by CO_2/water in the hydrocracking of anthracene

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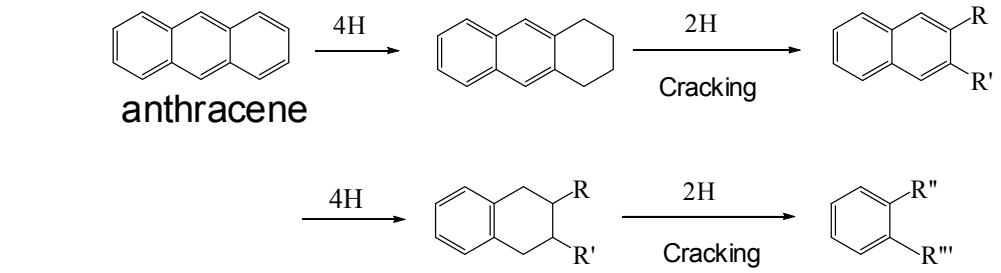
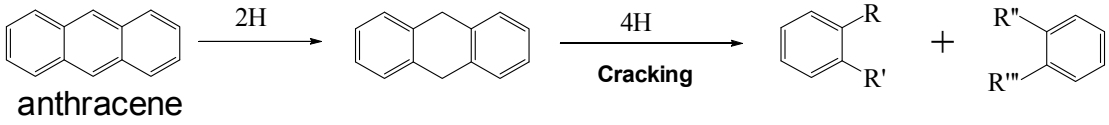
1. Hydrocracking pathways of anthracene



(**A**)



(**B**)

Scheme S1 Hydrocracking pathways of anthracene; (**A**) hydrocracking from terminal ring and (**B**) hydrocracking of anthracene from central ring

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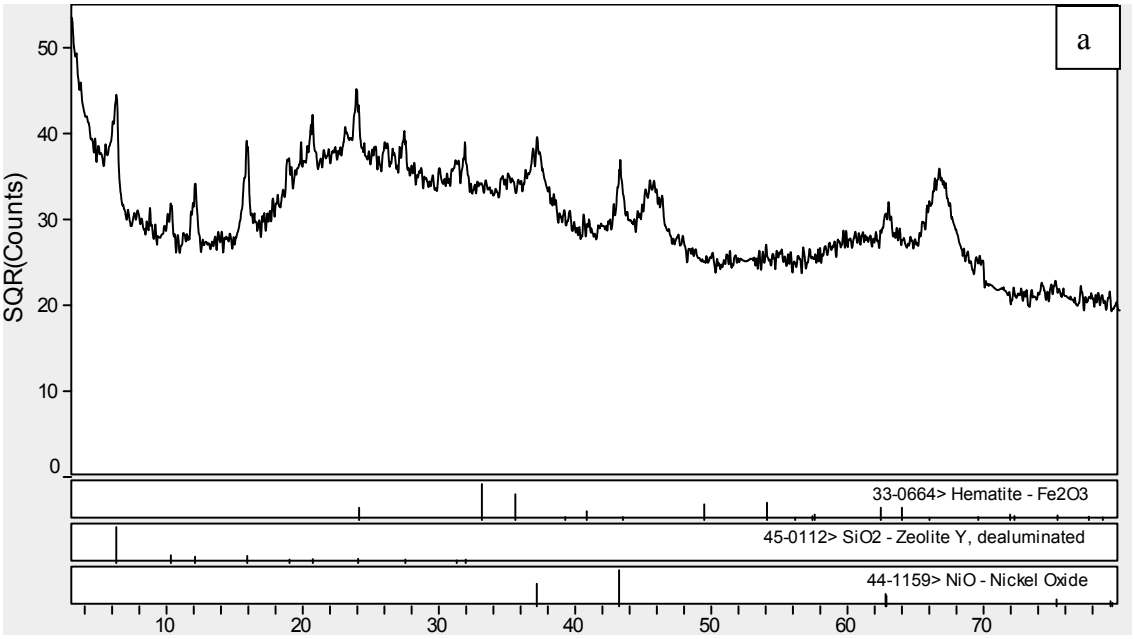
2. Experimental

Preparation of the NiFe catalyst: The NiFe catalyst was prepared using the method reported in the literature[S1]. Briefly, NiO and Fe_2O_3 with molar ratio of 1:1 were supported on dealuminated Y zeolite to get the NiFe catalyst. The mass ratio of the metal oxides and the support Y zeolite was 1:20. In this work, the supported catalyst is denoted as NiFe.

XRD patterns of the catalysts The XRD pattern of the NiFe-based catalyst is presented in Figure S1(a). The (111), (200) and (220) peaks are attributed to the characteristic peaks of NiO, and (012), (104) and (110) peaks belong to hematite. Other peaks are corresponding to the peaks of dealuminated Y zeolite. The XRD pattern of the HZSM-5 is given in Figure S1(b), which is consistent with that in the JCPDS database.



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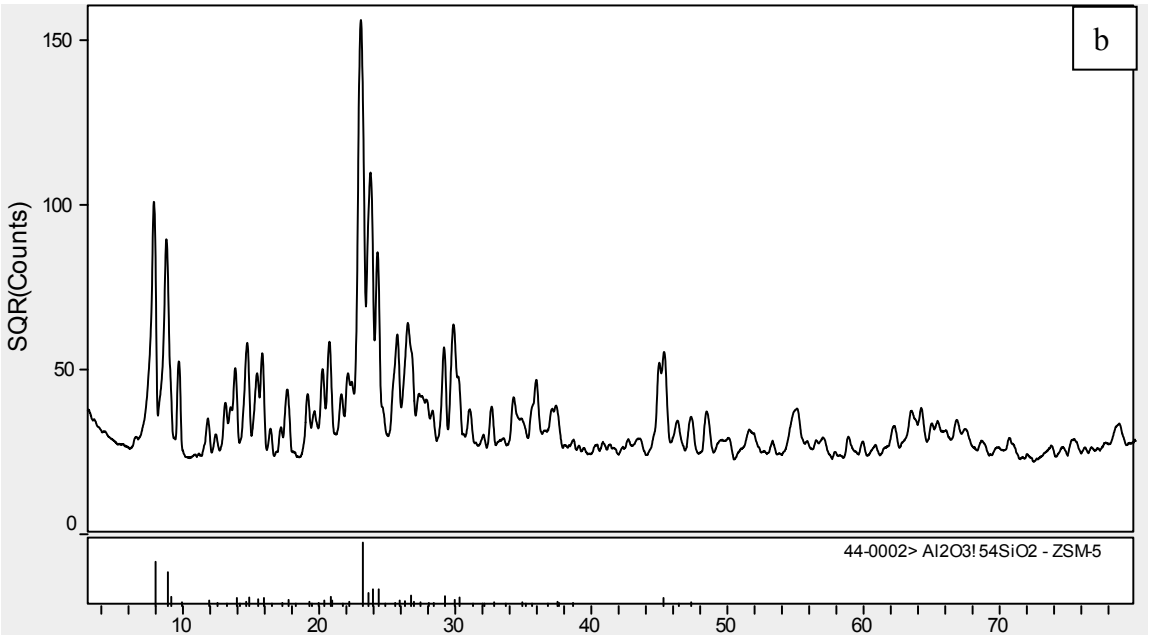


Figure S1. XRD patterns of the NiFe-based catalyst(a) and HZSM-5(b)

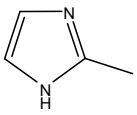
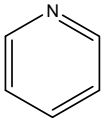
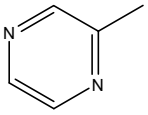
Structural parameters of the HZSM-5 The structural parameters of the HZSM-5 measured by the N_2 adsorption-desorption isotherm method are given in Table S1. The BET surface area was calculated from BET equation. The pore size distribution was calculated using Original Density Functional Theory.

Table S1 Structural parameters of HZSM-5(Si/Al molar ratio=15)

Sample	BET surface Area (m^2/g)	Pore volume (cm^3/g)	Average pore width (nm)
HZSM-5	359.4	0.064	5.0

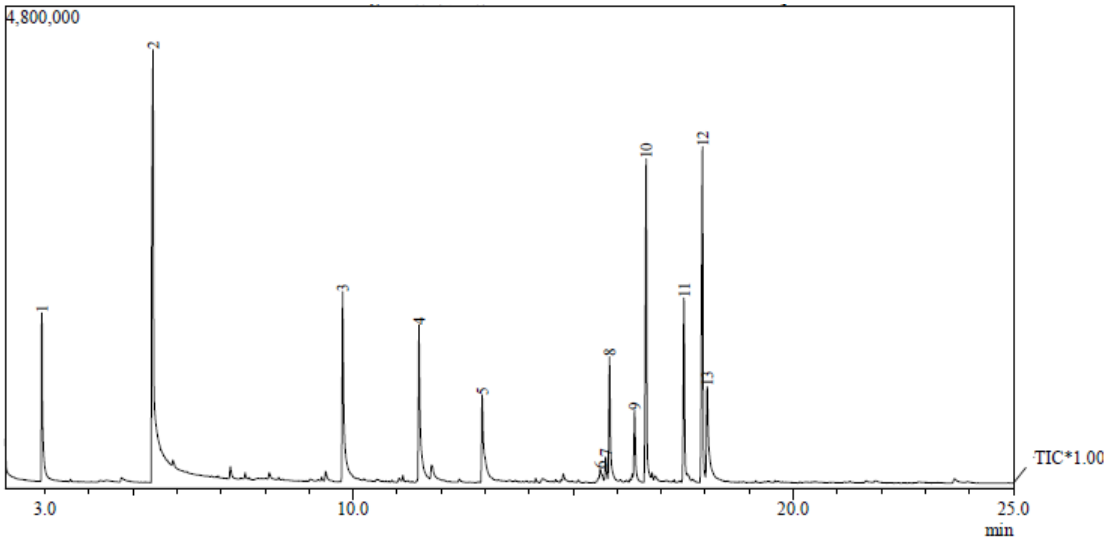
3. Chemical structures of nitrogen compounds in our work

Table S2 Chemical structures of nitrogen compounds used

Name	2-methyl imidazole	pyrrole	pyridine	2-methyl pyrazine
Structural formula				

4. Identification of the main products under different reaction conditions

Figure S2 presents the GC-MS spectra of the hydrocracking products of anthracene at 415°C. The main compounds include 2-methyl imidazole, ethyl biphenyl, dihydrophenanthrene, sym-octahydrophenanthrene, sym-octahydroanthracene, tetrahydroanthracene, alkylnaphthalenes, alkyltetralin.



Peak Report TIC

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	2.930	2.908	3.100	3373693	5.30	1689091	7.71	1.99	MI	
2	5.455	5.417	6.592	20856367	32.75	4351537	19.86	4.79	MI	
3	9.766	9.725	10.050	5518530	8.67	1908348	8.71	2.89	MI	
4	11.499	11.467	11.708	4471047	7.02	1560495	7.12	2.86	MI	
5	12.936	12.900	13.167	3194908	5.02	876474	4.00	3.64	MI	
6	15.617	15.583	15.700	320971	0.50	101832	0.46	3.17	MI	
7	15.739	15.708	15.783	469872	0.74	226546	1.03	2.07	MI	
8	15.827	15.783	15.958	2867590	4.50	1224298	5.59	2.34	MI	
9	16.397	16.367	16.467	1381328	2.17	661474	3.02	2.08	MI	
10	16.659	16.600	16.767	6919338	10.87	3239062	14.78	2.13	MI	
11	17.520	17.475	17.583	3750330	5.89	1818836	8.30	2.05	MI	
12	17.938	17.883	18.008	7605395	11.94	3348977	15.28	2.27	MI	
13	18.045	18.008	18.200	2945775	4.63	906801	4.14	3.24	MI	
				63675144	100.00	21913771	100.00			

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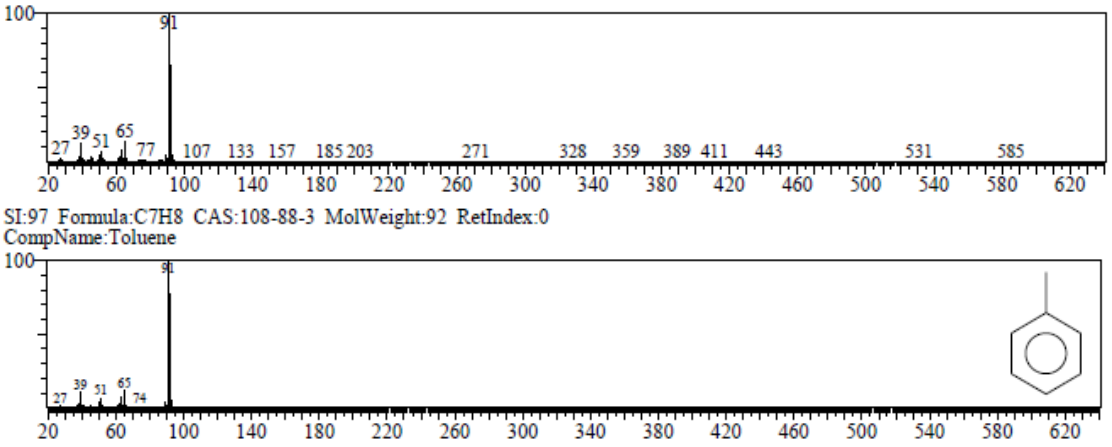

SI:97 Formula:C7H8 CAS:108-88-3 MolWeight:92 RetIndex:0
CompName:Toluene

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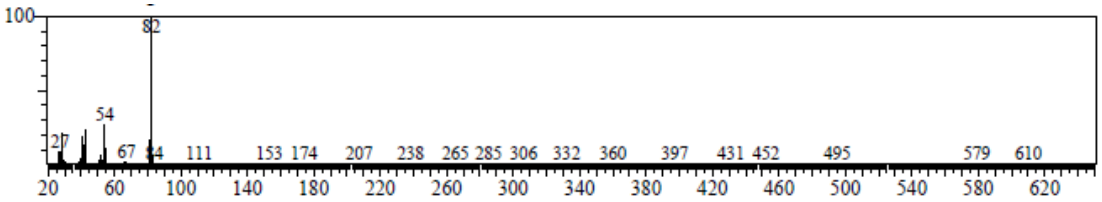
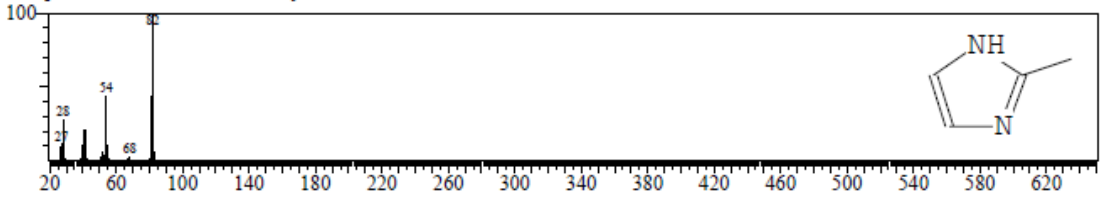


SI:93 Formula:C4H6N2 CAS:693-98-1 MolWeight:82 RetIndex:0
CompName:1H-Imidazole, 2-methyl-



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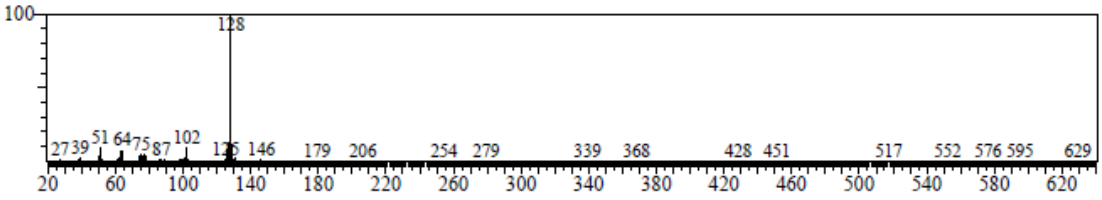
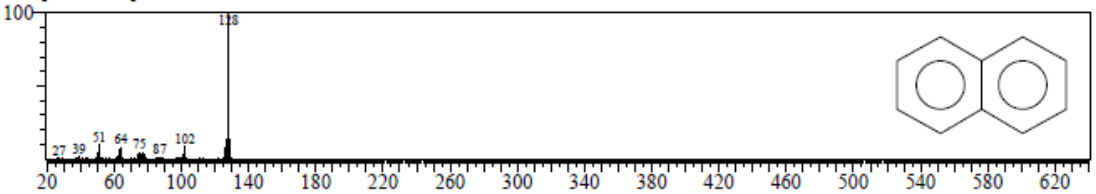


SI:98 Formula:C10H8 CAS:91-20-3 MolWeight:128 RetIndex:0
CompName:Naphthalene



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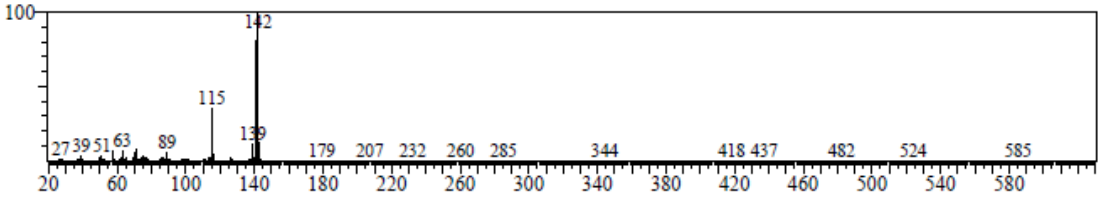

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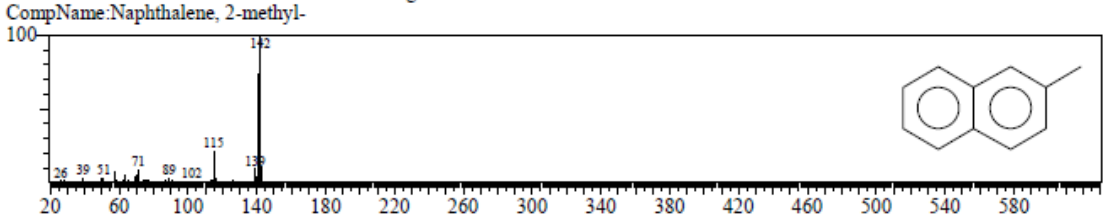

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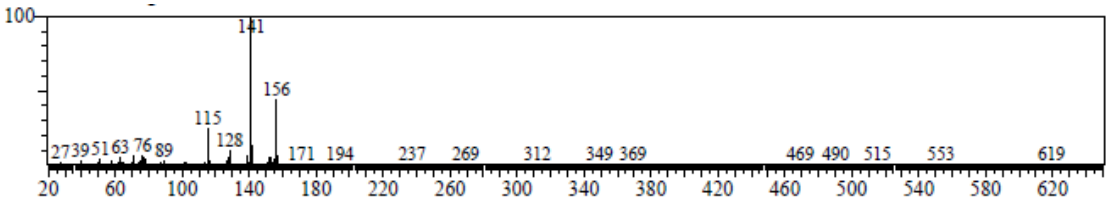

SI:96 Formula:C12H12 CAS:1127-76-0 MolWeight:156 RetIndex:0
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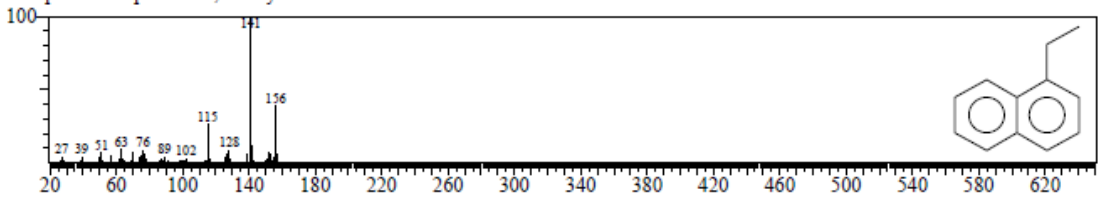

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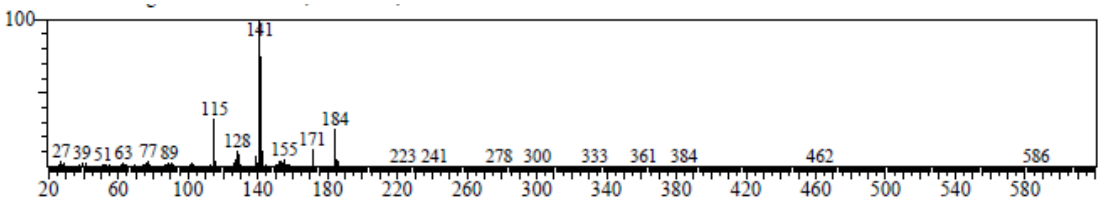

SI:91 Formula:C14H16 CAS:1134-62-9 MolWeight:184 RetIndex:0
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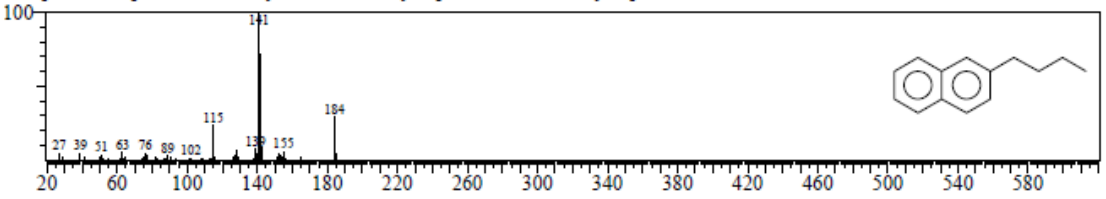

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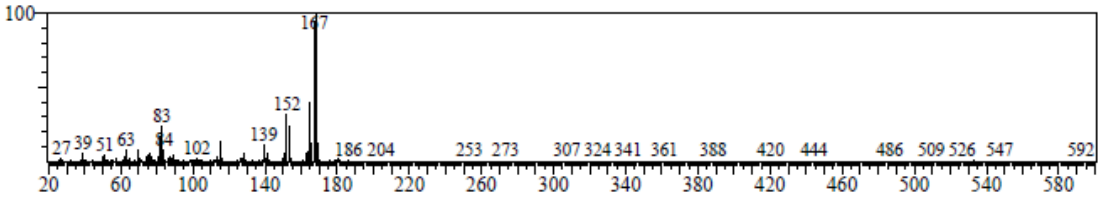
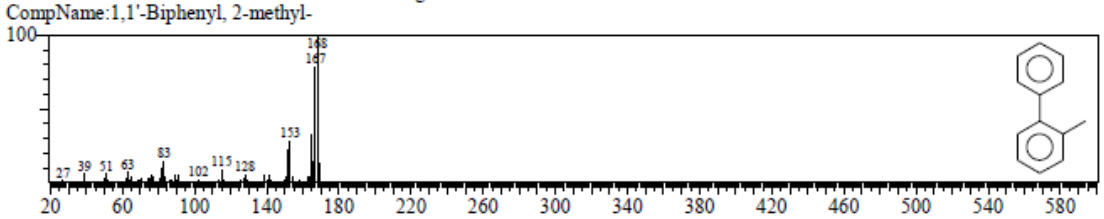


SI:92 Formula:C13H12 CAS:643-58-3 MolWeight:168 RetIndex:0
CompName:1,1'-Biphenyl, 2-methyl-



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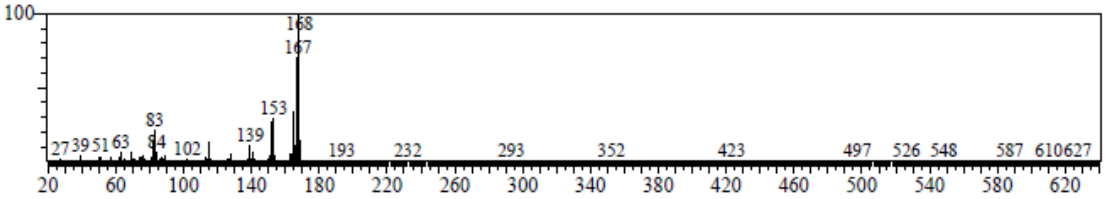
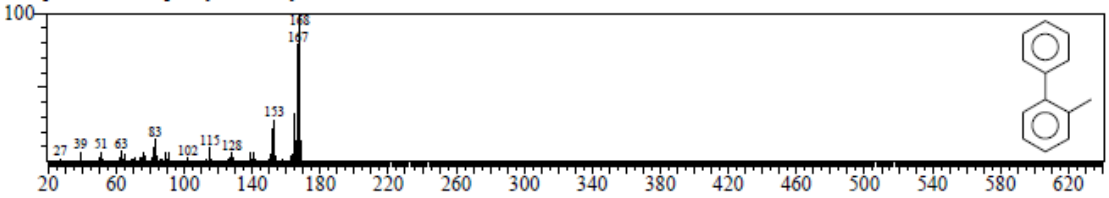


SI:94 Formula:C13H12 CAS:643-58-3 MolWeight:168 RetIndex:0
CompName:1,1'-Biphenyl, 2-methyl-



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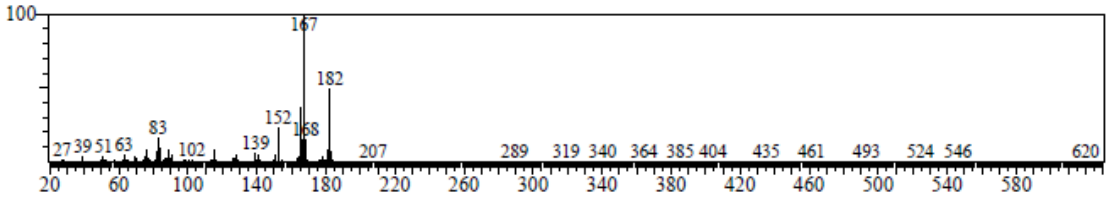
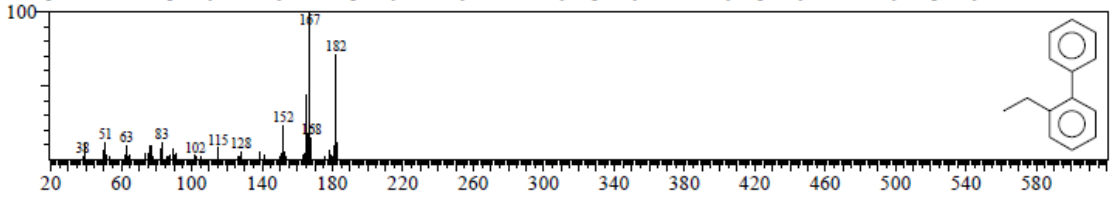


SI:90 Formula:C14H14 CAS:1812-51-7 MolWeight:182 RetIndex:0
CompName:1,1'-Biphenyl, 2-ethyl- $$ Biphenyl, 2-ethyl- $$ o-Ethylbiphenyl $$ 2-Ethylbiphenyl $$ 1-Ethyl-2-phenylbenzene $$



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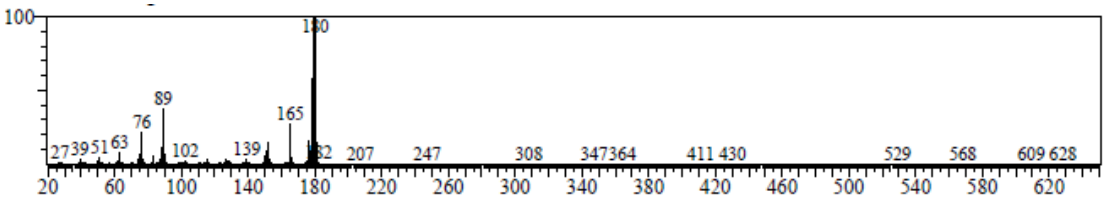
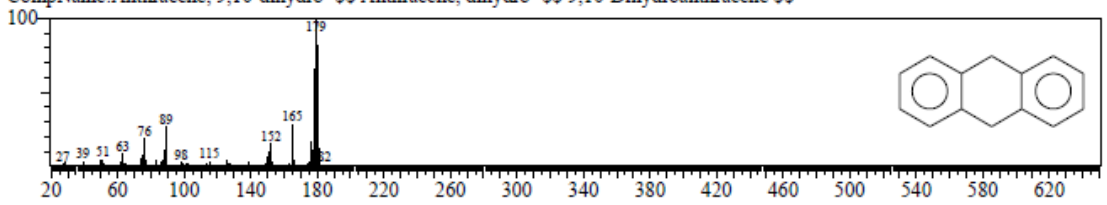


SI:94 Formula:C14H12 CAS:613-31-0 MolWeight:180 RetIndex:0
CompName:Anthracene, 9,10-dihydro- $$ Anthracene, dihydro- $$ 9,10-Dihydroanthracene $$



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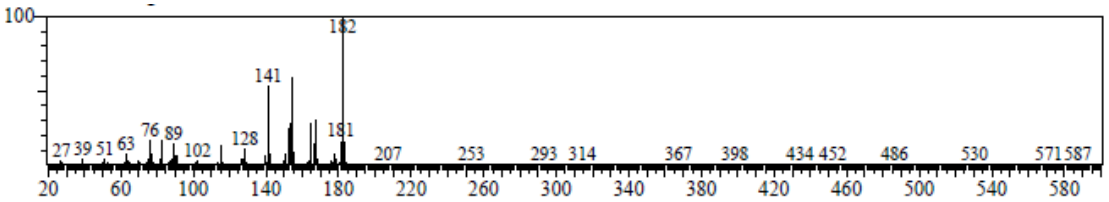

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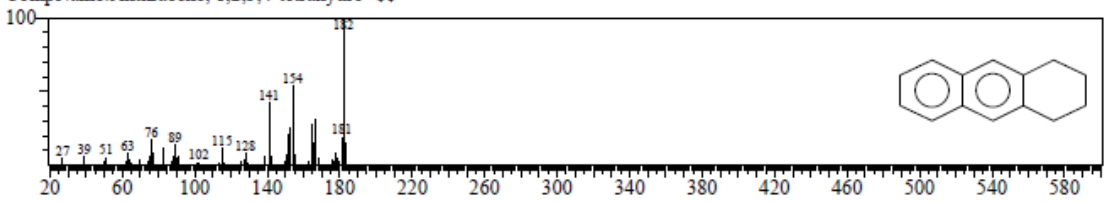

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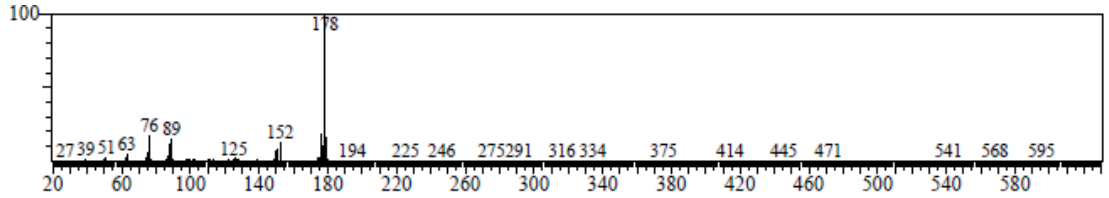
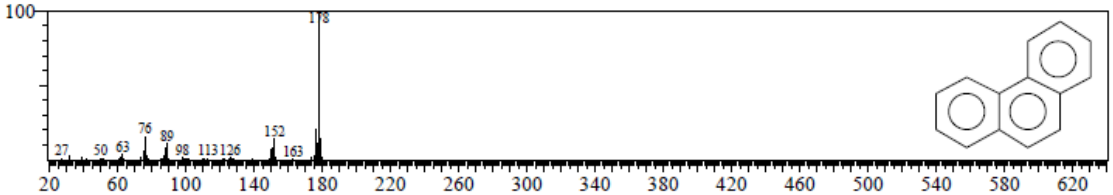


SI:94 Formula:C14H10 CAS:85-1-8 MolWeight:178 RetIndex:0
CompName:Phenanthrene



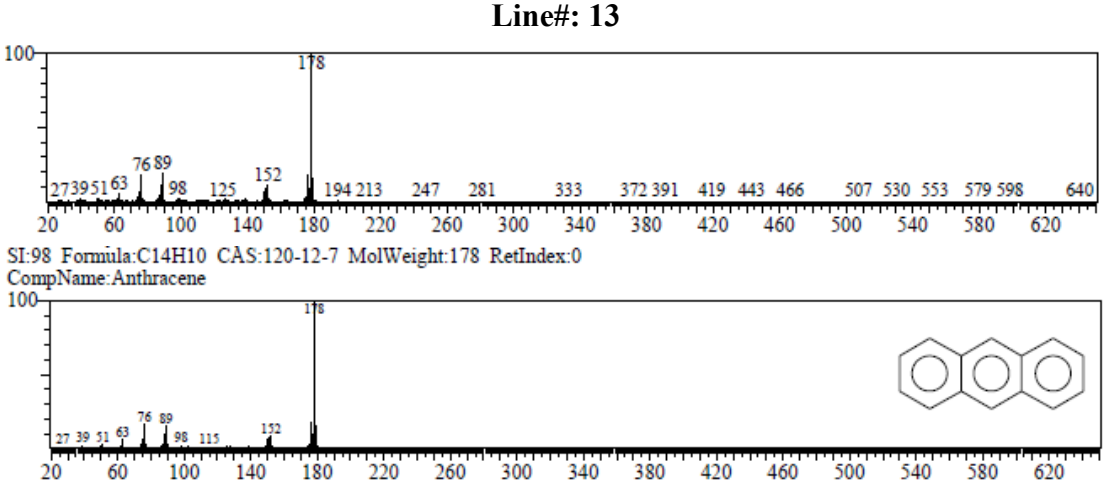


Figure S2. GC-MS spectra of the main products for hydrocracking of anthracene at 415°C. Reaction conditions: anthracene 0.05 g, NiFe 0.003 g, HZSM-5 0.013 g (Si/Al molar ratio=15), sulfur 0.06 g, formic acid 0.5 mL, 2-methyl imidazole 0.012 g, reaction time 2.5 h, reaction temperature 415°C, volume of the reactor 5 mL.

References

S1. C. M. Lee and C. N. Satterfield, *Energy Fuels*, 1993, **7**, 978-980.