

Supporting Information

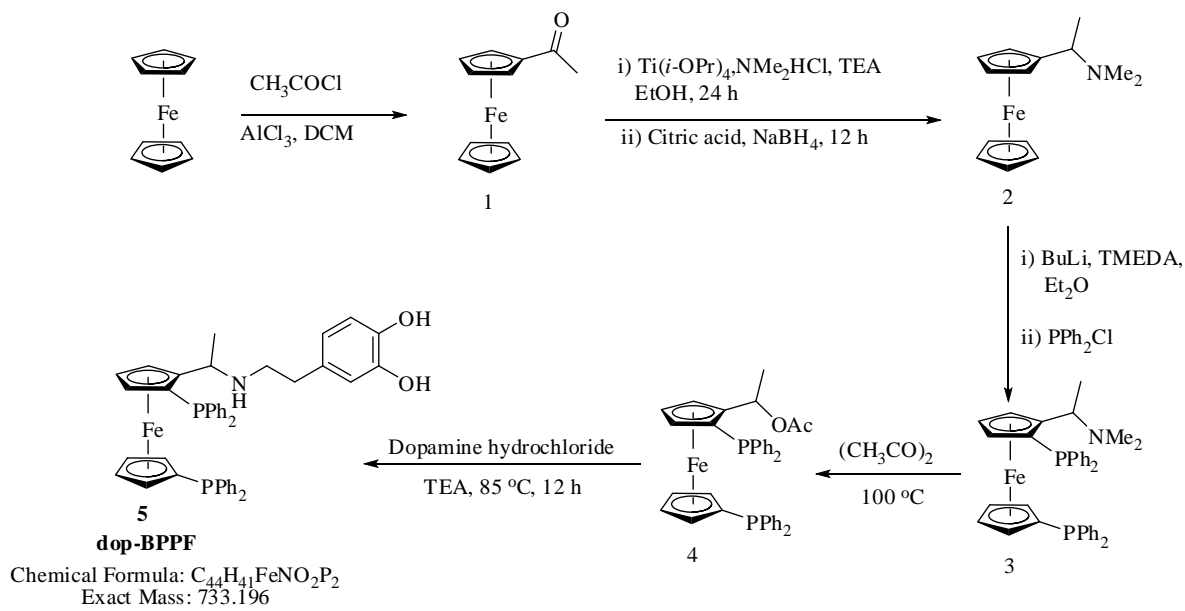
Magnetic Nanoparticle-Supported Ferrocenylphosphine: A Reusable Catalyst for Hydroformylation of Alkene and Mizoroki-Heck Olefination

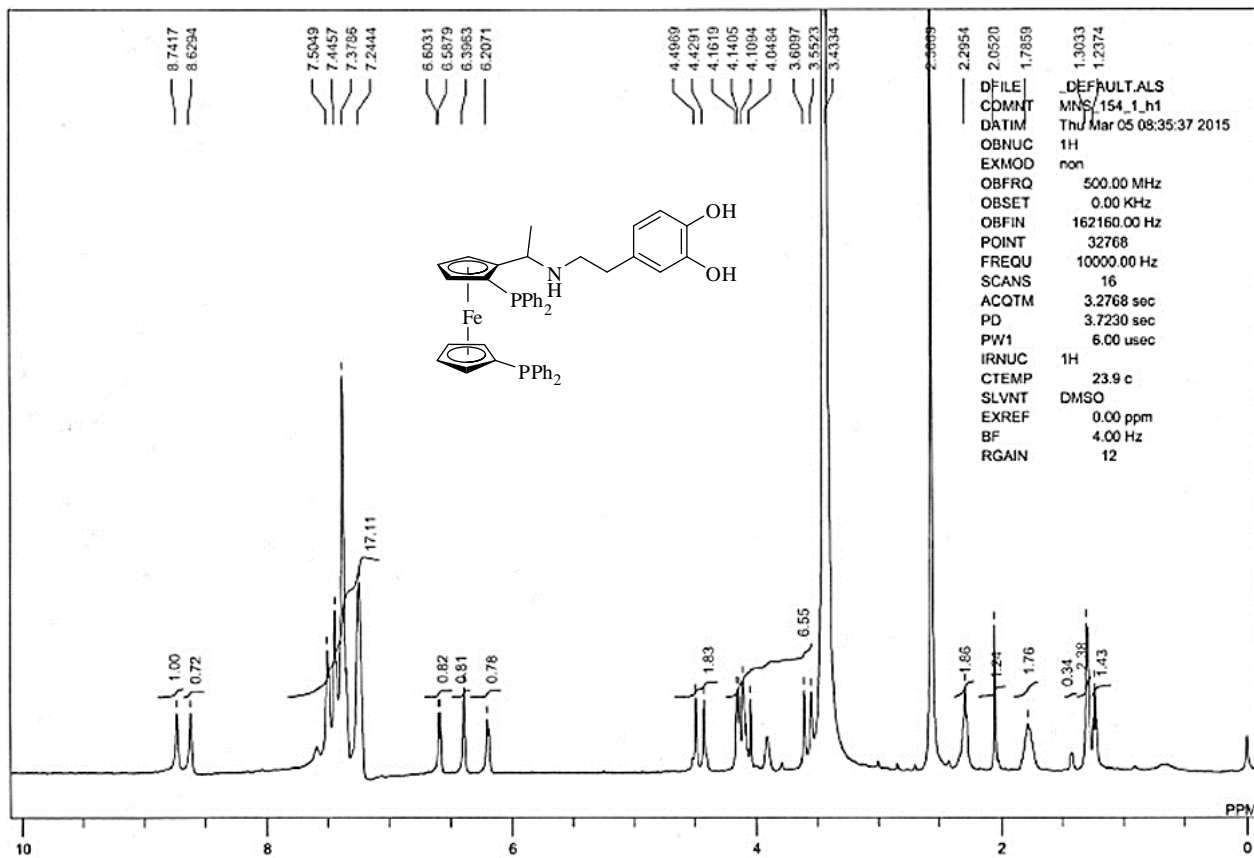
M. Nasiruzzaman Shaikh,^{*,a} Md. Abdul Aziz,^a Aasif Helal,^a Mohamed Bououdina,^b Zain H. Yamani^a and Tae-Jeong Kim^c

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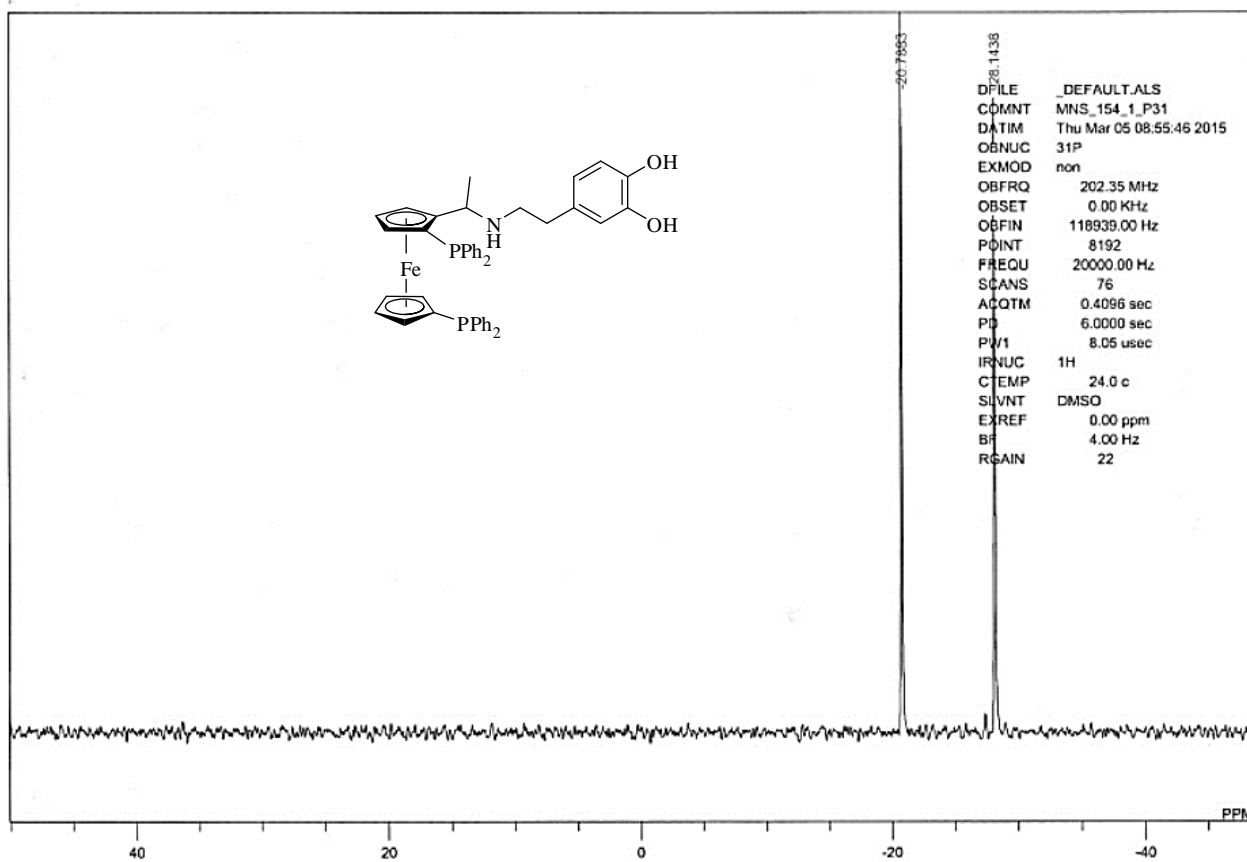
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Scheme 1



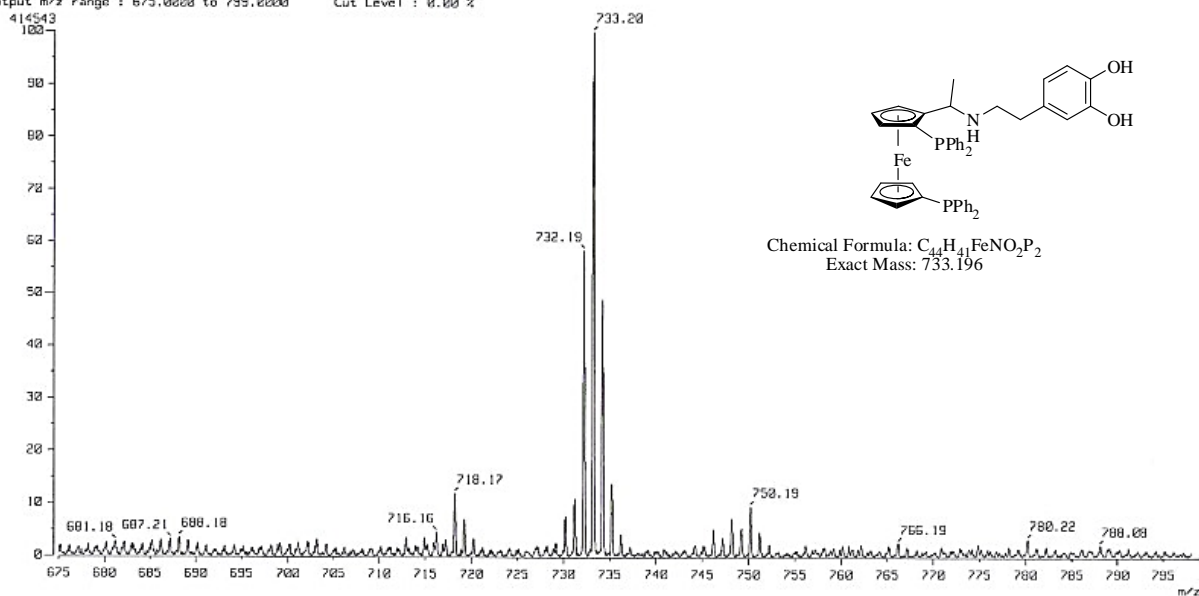


S1: ^1H NMR of the **dop-BPPF** in $\text{DMSO-}d_6$

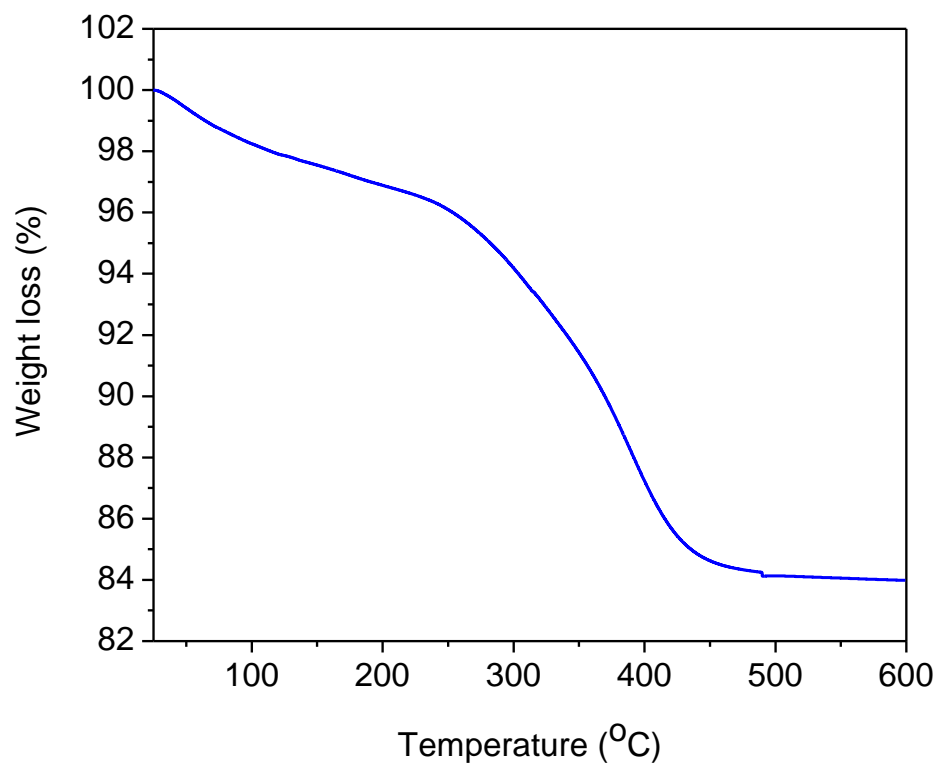


S2: ^{31}P NMR of the **dop-BPPF** in $\text{DMSO-}d_6$

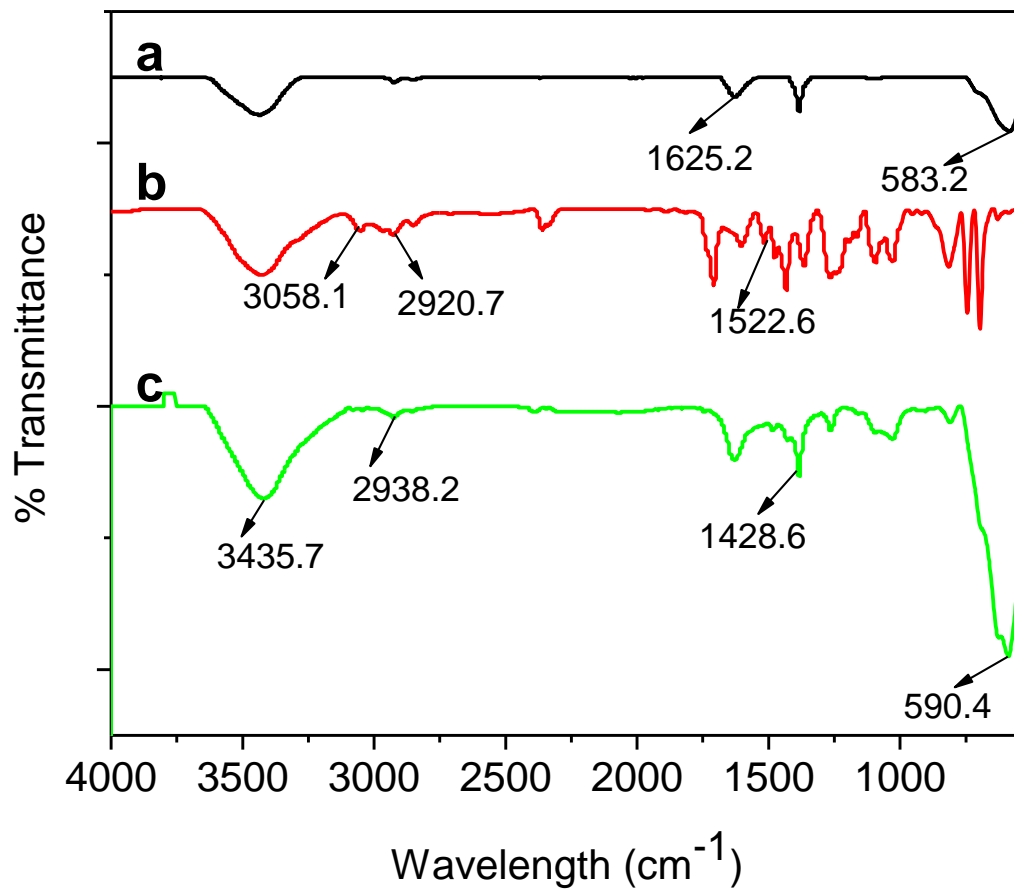
[Mass Spectrum]
 Data : MNS-154-C44H41FeNO2P2 Date : 20-May-2015 21:56
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.68 min Scan# : (14,15)
 BP : m/z 733.1961 Int. : 19.77
 Output m/z range : 675.0000 to 799.0000 Cut Level : 0.00 %



S3: FAB-Mass spectrum of the **dop-BPPF**



S4: TGA of **Fe₃O₄@dop-BPPF** under argon atmosphere



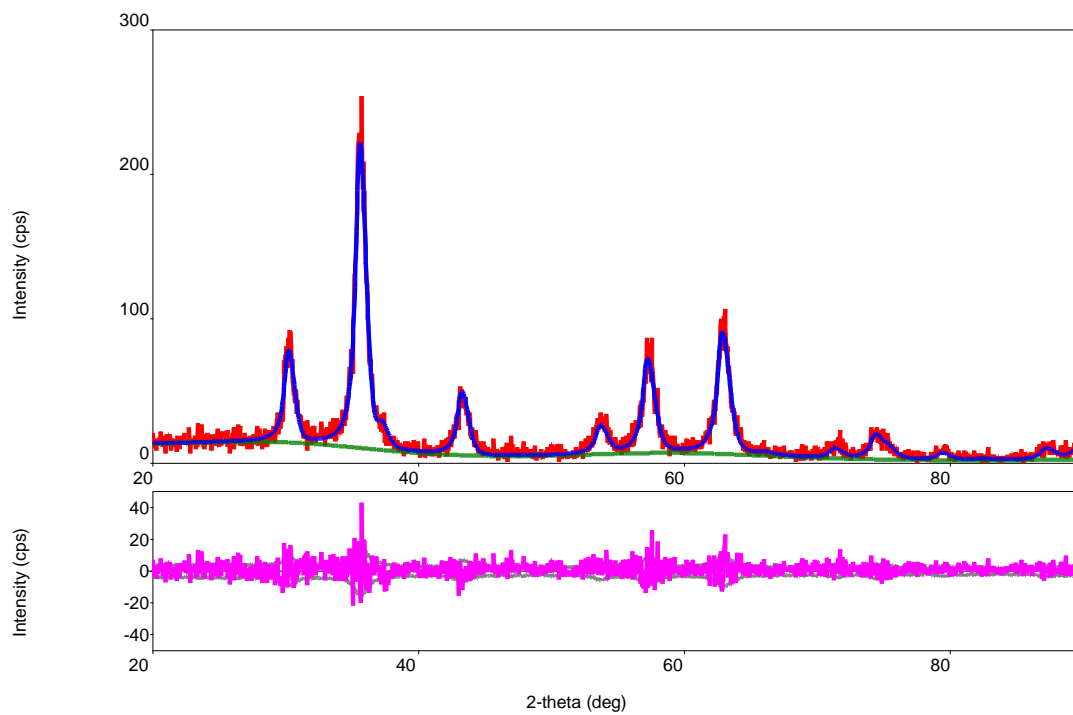
S5: FT-IR spectrum of a) Fe₃O₄ b) dop-BPPF c) Fe₃O₄@dop-BPPF with KBr pallet

Table 1. Structural, microstructural of magnetite Fe₃O₄ before and after coating and complexation with Pd and Rh.

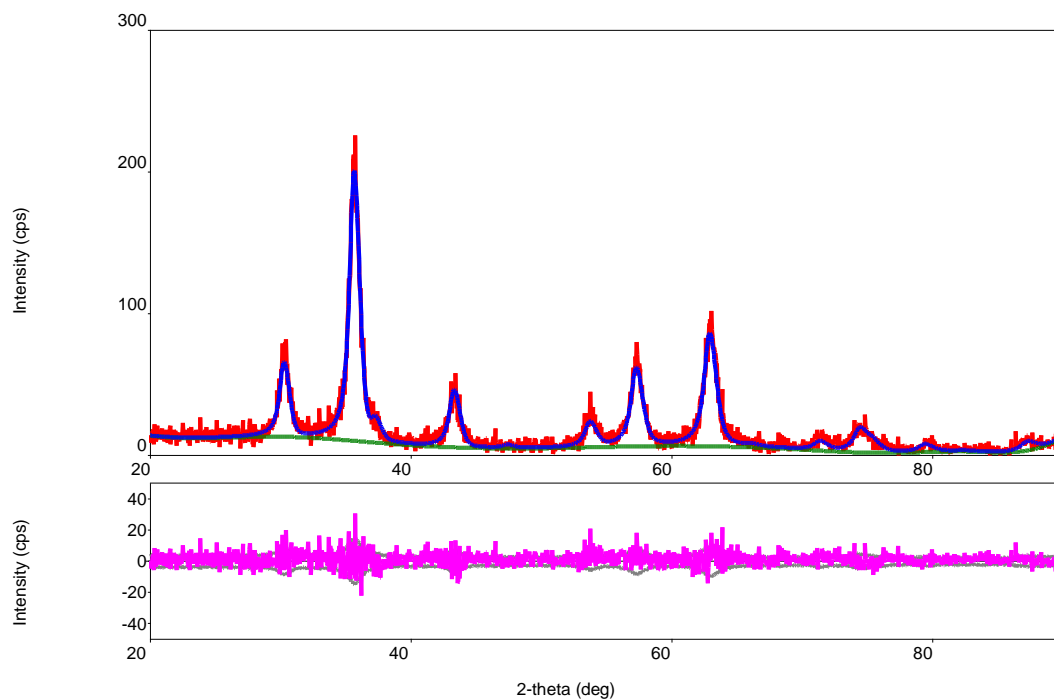
	Crystallite size (nm)	Microstrain (%)	Lattice parameter (Å)	Goodness of fit
Fe ₃ O ₄	8.4	0.360	8.372(4)	1.0726
Fe₃O₄@dop-BPPF	8.5	0.478	8.365(4)	1.1276
Fe₃O₄@dop-BPPF-Pd	8.6	0.500	8.363(4)	1.1079
Fe₃O₄@dop-BPPF-Rh	8.4	0.340	8.359(4)	1.1300

Table 2. Magnetic properties investigation data of magnetite Fe₃O₄ before and after coating and complexation with Pd and Rh.

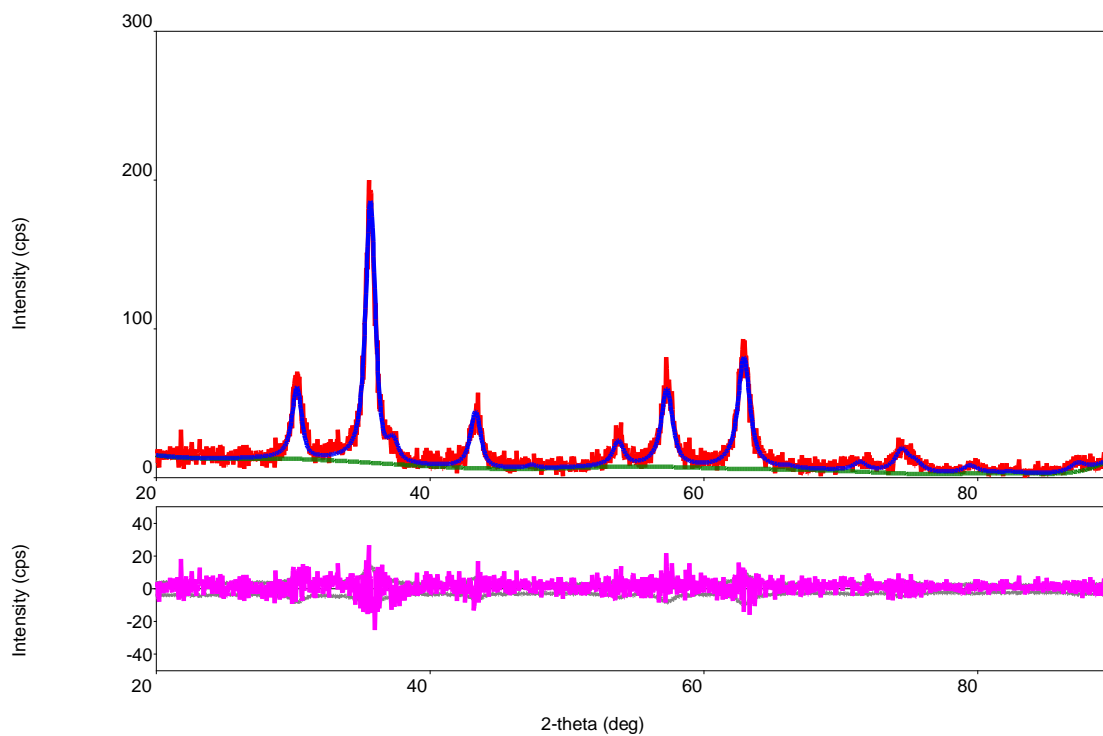
	Coercivity, H_c (Oe)	Remanence, M_r (emu/g)	Saturation magnetization, M_s (emu/g)
Fe ₃ O ₄	3.965	0.802	68.03
Fe₃O₄@dop-BPPF	4.322	0.645	58.75
Fe₃O₄@dop-BPPF-Rh	4.480	0.708	56.00
Fe₃O₄@dop-BPPF-Pd	4.614	0.722	54.15



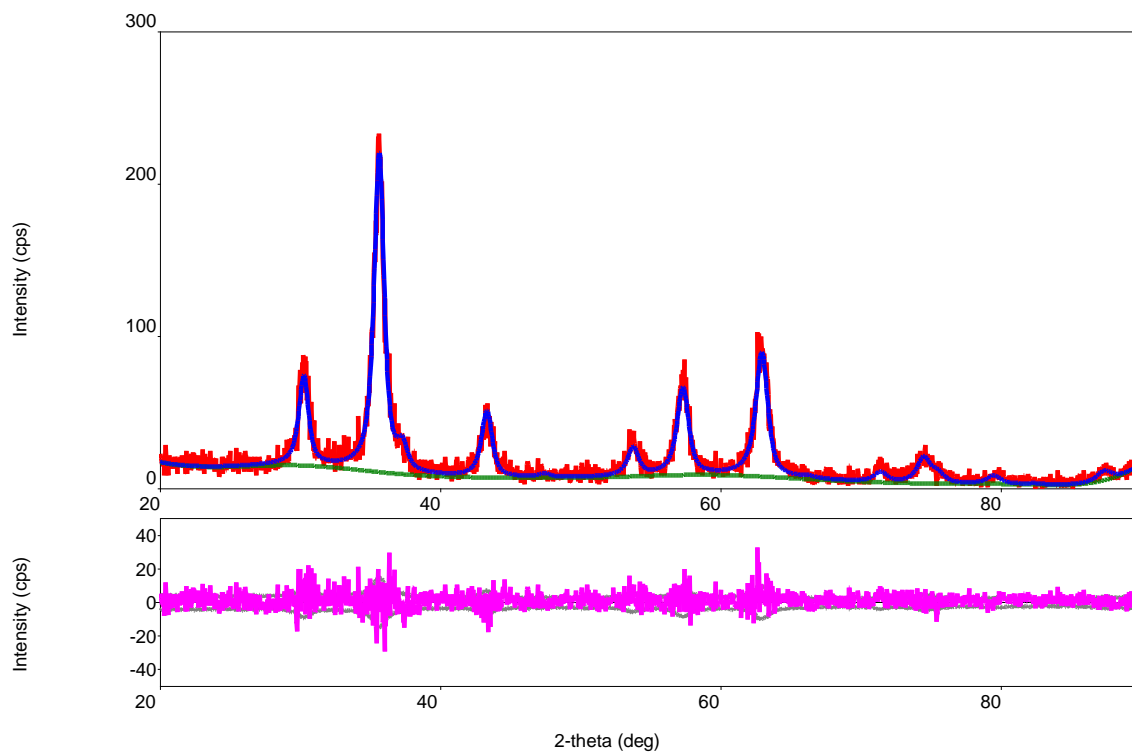
S6. XRD pattern refinement using the Rietveld method of Fe₃O₄



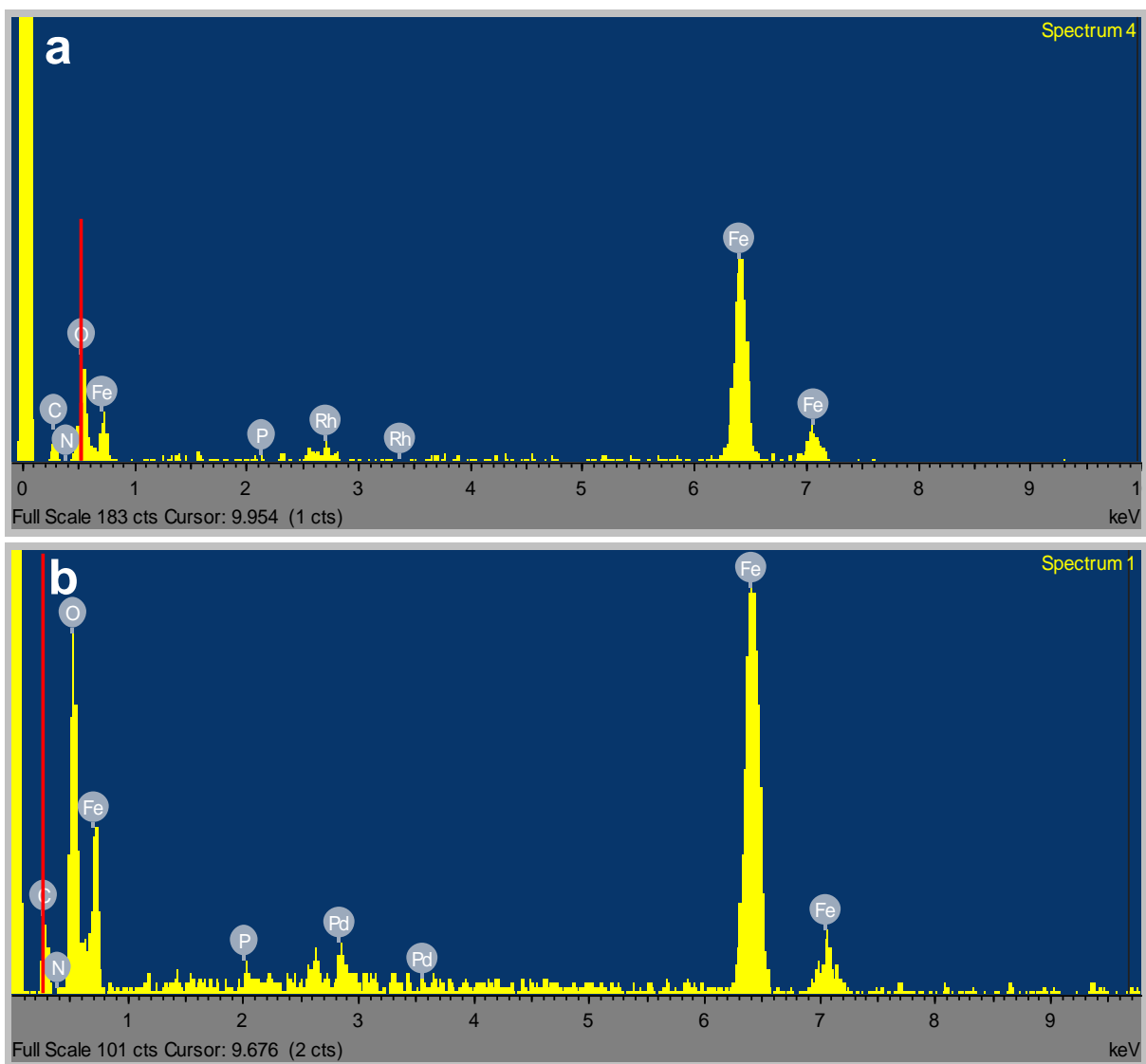
S7. XRD pattern refinement using the Rietveld method of Fe_3O_4 @dop-BPPF



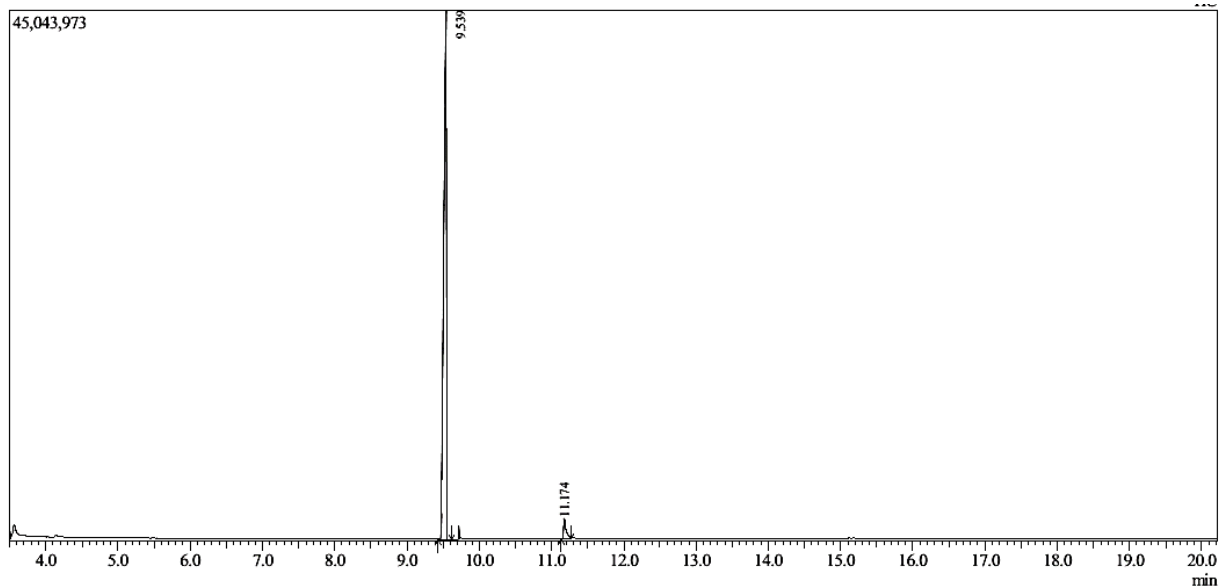
S8. XRD pattern refinement using the Rietveld method of Fe_3O_4 @dop-BPPF-Pd



S9. XRD pattern refinement using the Rietveld method of Fe_3O_4 @dop-BPPF-Rh



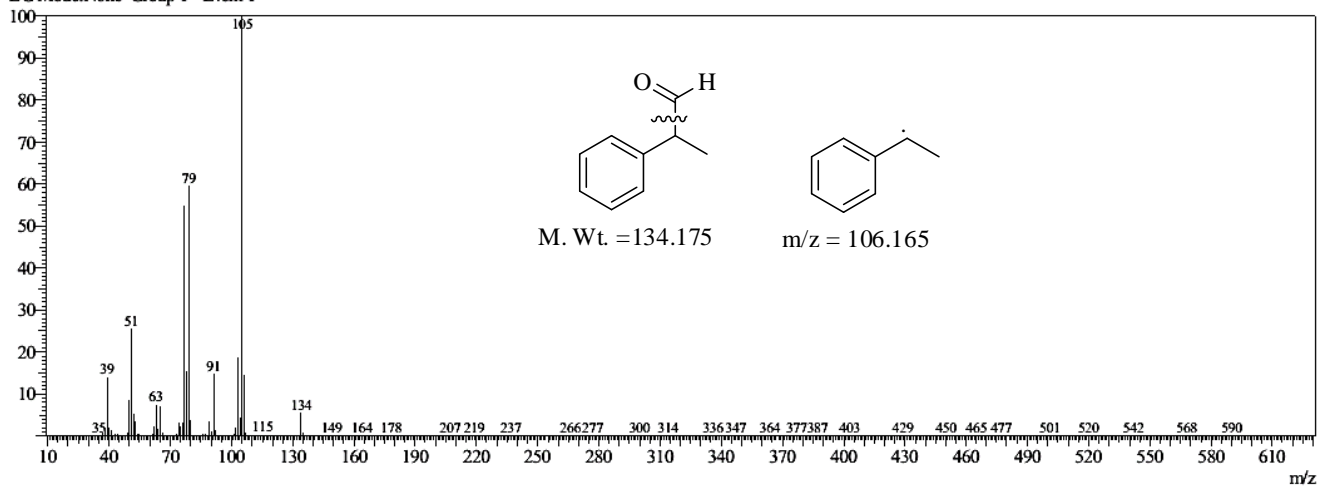
S10: EDX spectra of (a) $\text{Fe}_3\text{O}_4@\text{dop-BPPF-Rh}$ and (b) $\text{Fe}_3\text{O}_4@\text{dop-BPPF-Pd}$



Peak Report TIC										
Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	9.539	9.430	9.615	118818367	96.38	45026016	96.32	2.64	MI	
2	11.174	11.135	11.265	4468029	3.62	1720370	3.68	2.60	MI	
				123286396	100.00	46746386	100.00			

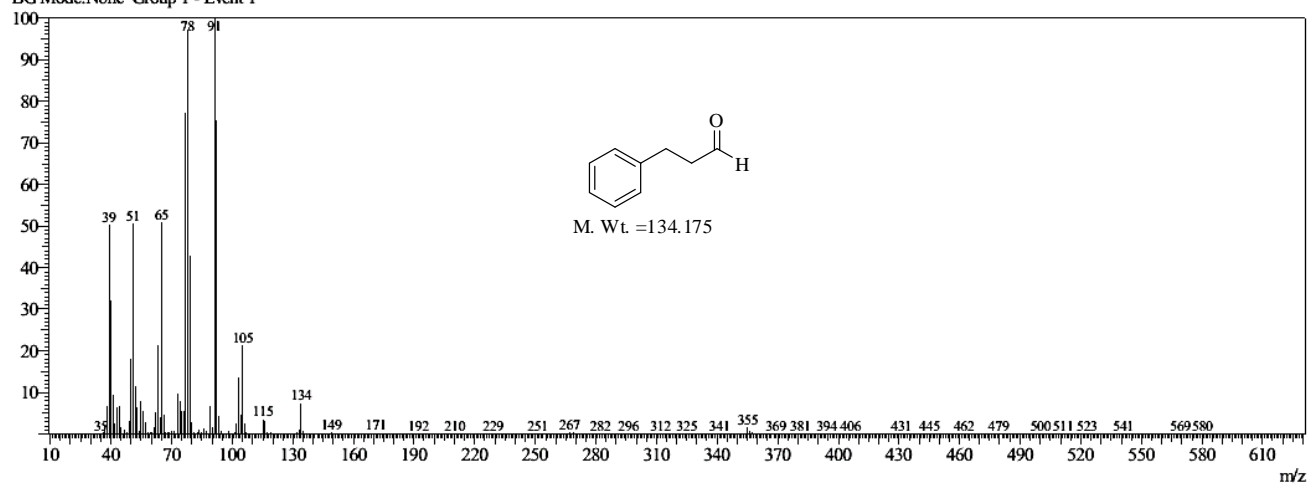
S11: GC spectra of hydroformylated product of styrene in DCM at 45 °C

Line#:1 R.Time:9.515(Scan#:1204)
 MassPeaks:566
 RawMode:Single 9.515(1204) BasePeak:105(8002990)
 BG Mode:None Group 1 - Event 1

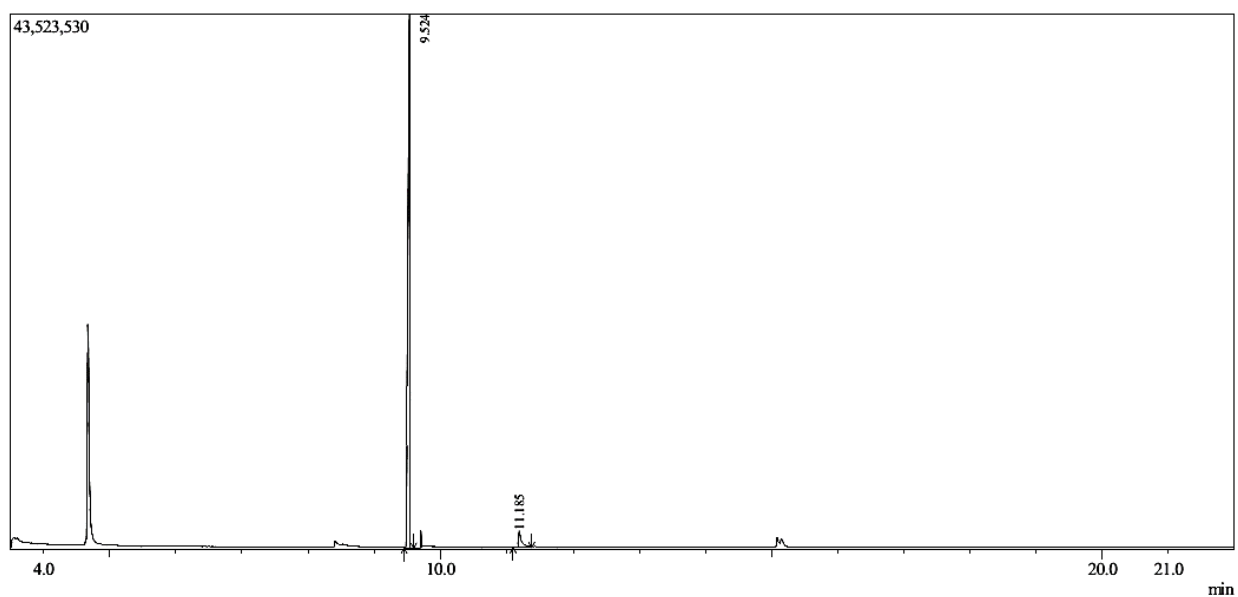


S12: Mass spectra of hydroformylated branched product of styrene

Line#:2 R.Time:11.200(Scan#:1541)
MassPeaks:563
RawMode:Single 11.200(1541) BasePeak:91(104470)
BG Mode:None Group 1 - Event 1

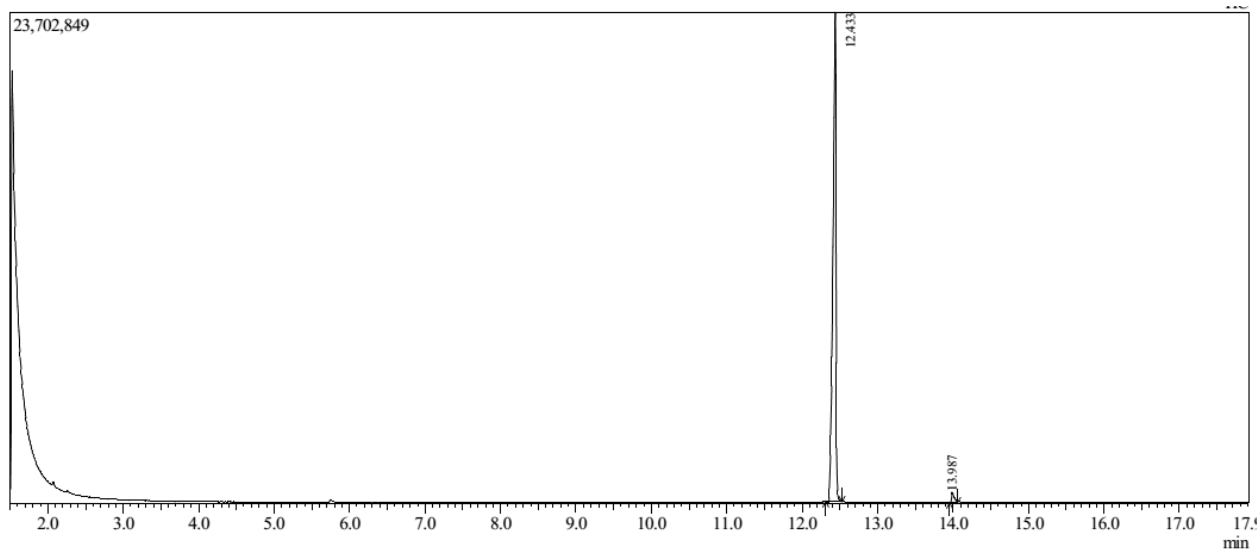


S13: Mass spectra of hydroformylated linear product of styrene



Peak Report TIC										
Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	9.524	9.445	9.590	78577219	94.52	43507808	97.01	1.81	MI	
2	11.185	11.095	11.370	4552580	5.48	1339183	2.99	3.40	MI	
				83129799	100.00	44846991	100.00			

S14: GC spectra of hydroformylated product of styrene in THF at 45 °C



Peak Report TIC										
Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	12.433	12.305	12.525	65543599	98.13	23603131	97.86	2.78	MI	
2	13.987	13.955	14.055	1250366	1.87	517381	2.14	2.42	MI	
				66793965	100.00	24120512	100.00			

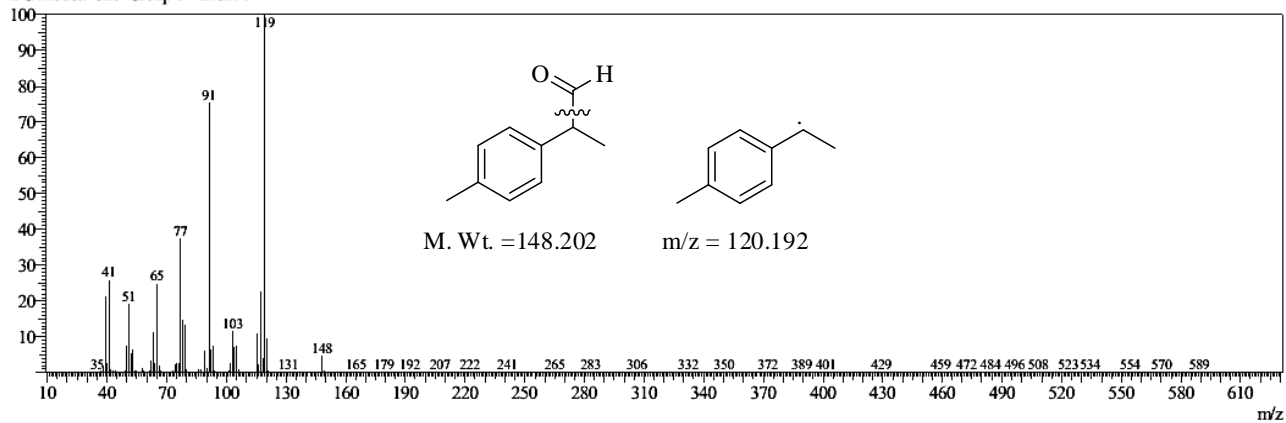
S15: GC spectra of hydroformylated product of 4-methylstyrene in DCM at 45 °C

Line#:1 R.Time:12.435(Scan#:1788)

MassPeaks:560

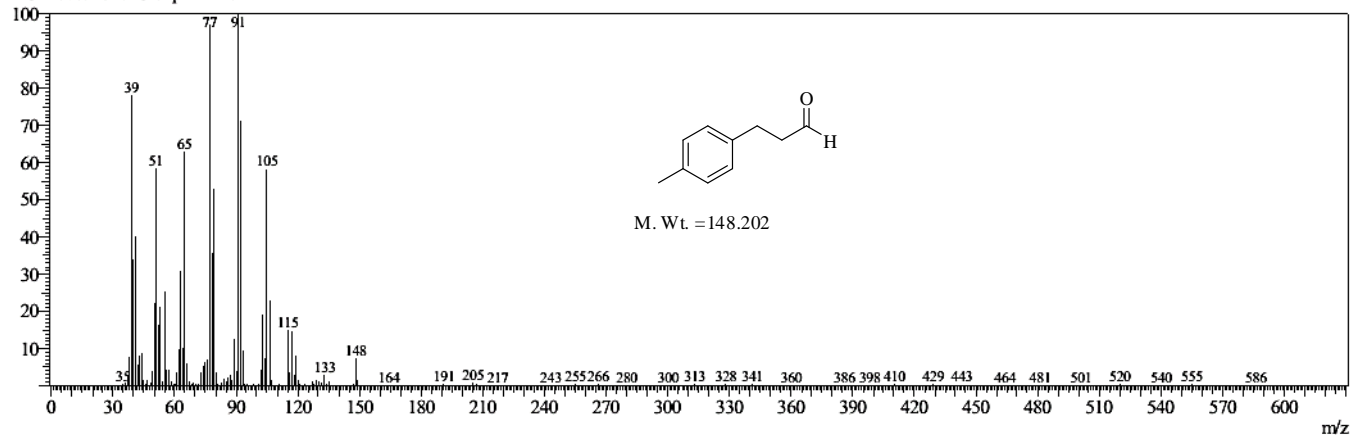
RawMode:Single 12.435(1788) BasePeak:119(5337148)

BG Mode:None Group 1 - Event 1

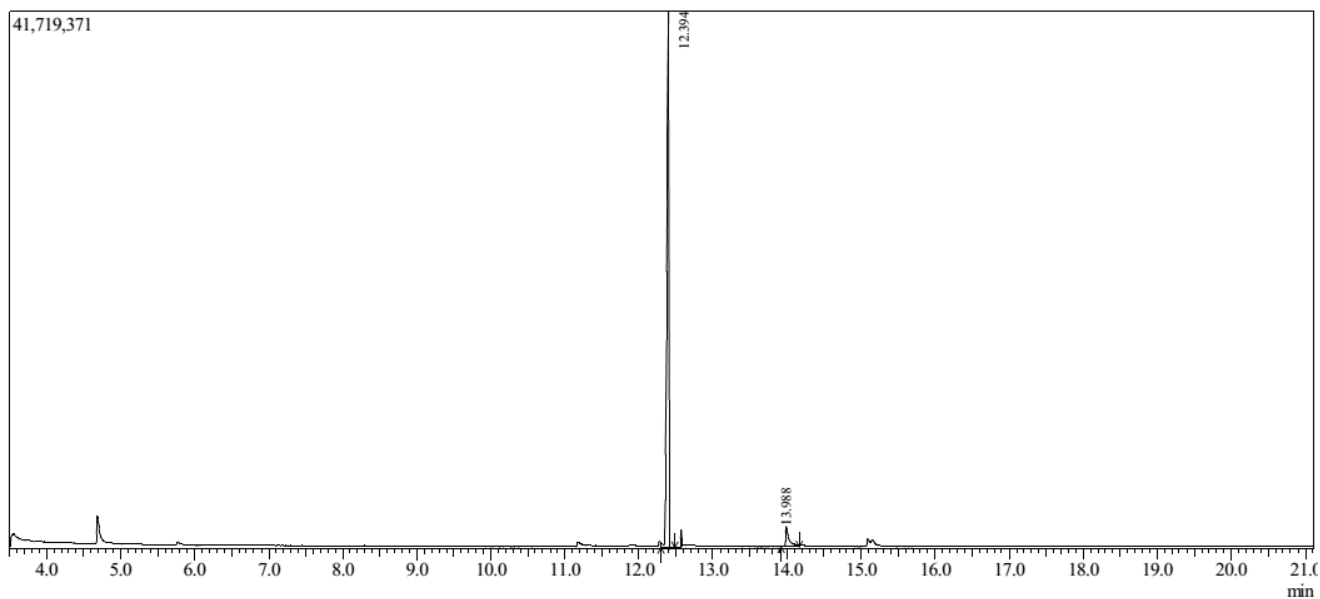


S16: Mass spectra of hydroformylated branched product of 4-methylstyrene

Line#:2 R.Time:14.015(Scan#:2104)
 MassPeaks:564
 RawMode:Single 14.015(2104) BasePeak:91(39290)
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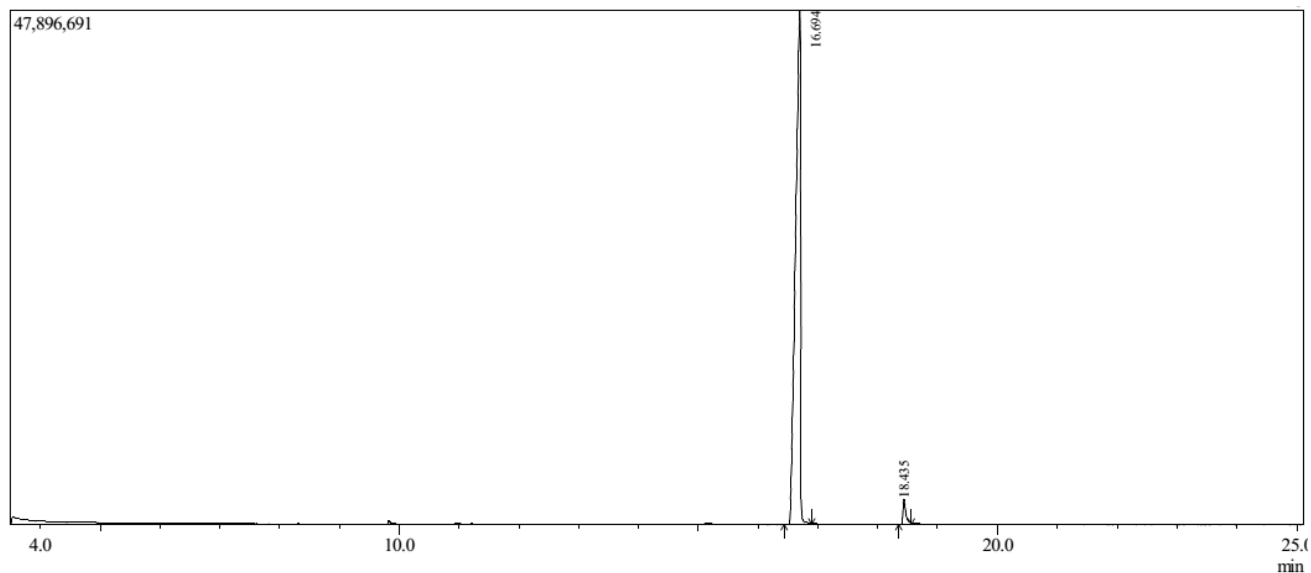


S17: Mass spectra of hydroformylated linear product of 4-methylstyrene



Peak#	R.Time	I.Time	F.Time	Peak Report TIC				A/H	Mark	Name
				Area	Area%	Height	Height%			
1	12.394	12.300	12.480	73988236	93.38	41701803	96.41	1.77	MI	
2	13.988	13.915	14.165	5242049	6.62	1553710	3.59	3.37	MI	
				79230285	100.00	43255513	100.00			

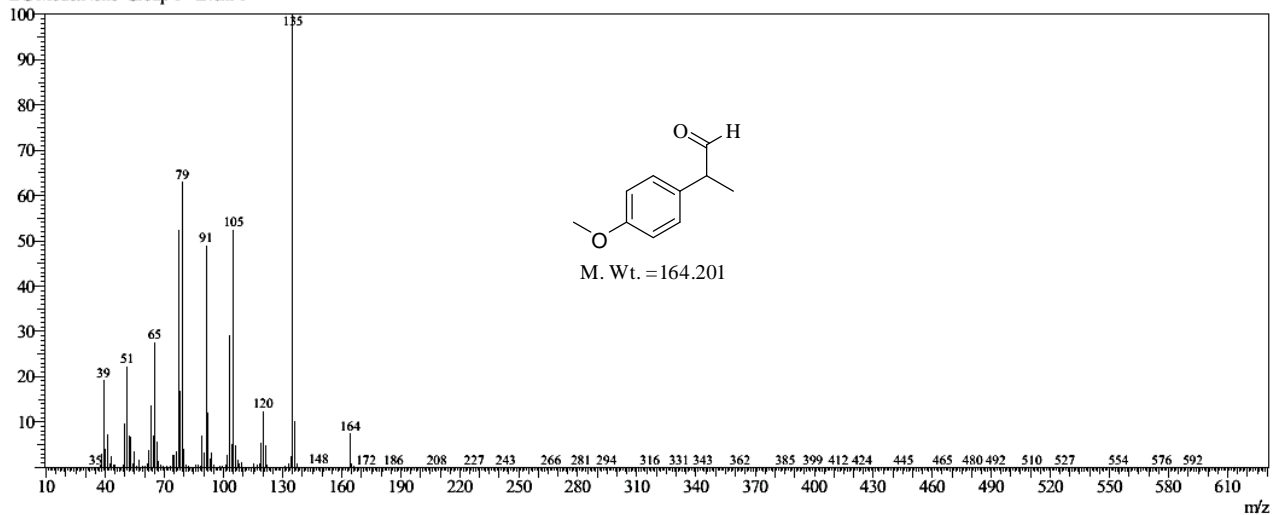
S18: GC spectra of hydroformylated product of 4-methylstyrene in THF at 45 °C



Peak Report TIC										
Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	16.694	16.435	16.895	272905195	97.25	47834968	95.34	5.71	MI	
2	18.435	18.350	18.555	7719051	2.75	2340047	4.66	3.30	MI	
				280624246	100.00	50175015	100.00			

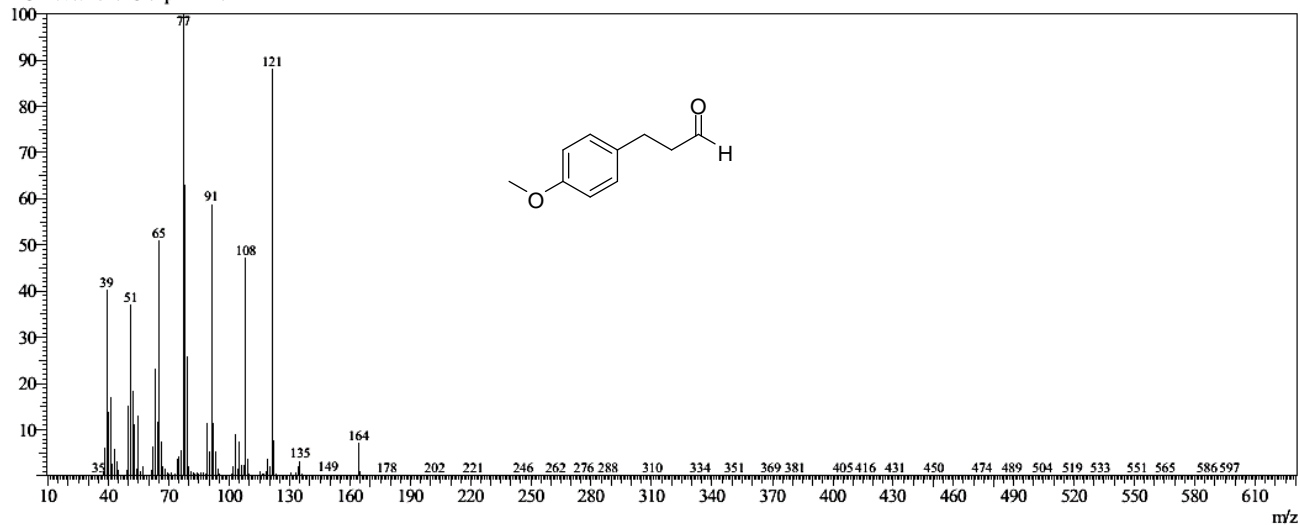
S19: GC spectra of hydroformylated product of 4-vinylanisole in DCM at 45 °C

Line#:1 R.Time:16.635(Scan#:2628)
MassPeaks:566
RawMode:Single 16.635(2628) BasePeak:135(4936366)
BG Mode:None Group 1 - Event 1

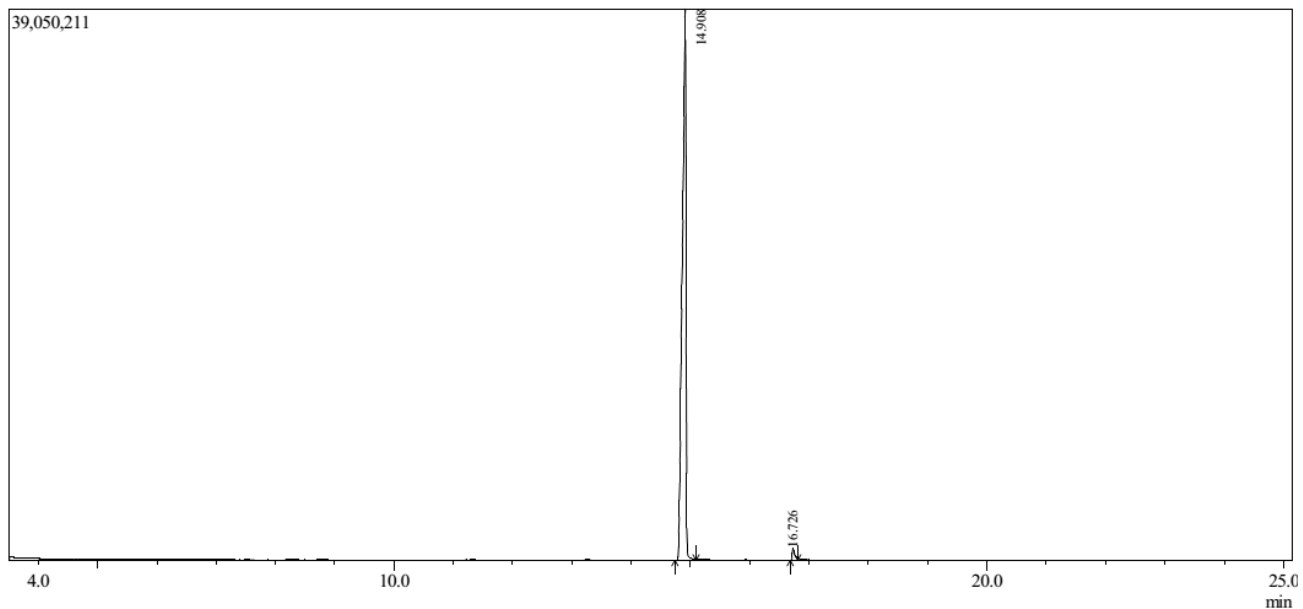


S20: Mass spectra of hydroformylated branched product of 4-vinylanisole

Line#:2 R.Time:18.450(Scan#:2991)
MassPeaks:561
RawMode:Single 18.450(2991) BasePeak:77(236529)
BG Mode:None Group 1 - Event 1



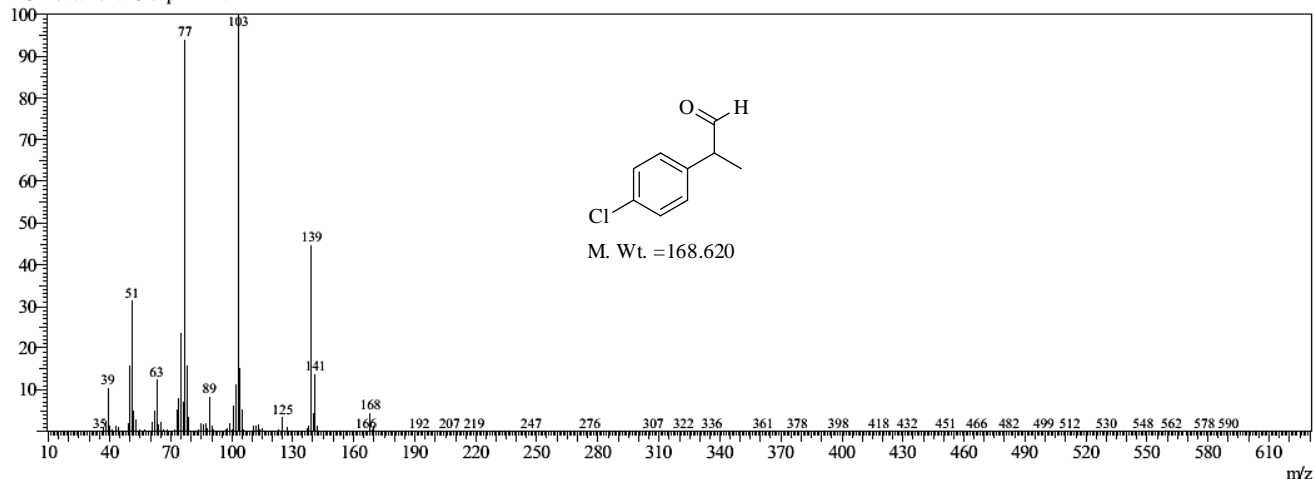
S21: Mass spectra of hydroformylated linear product of 4-vinylanisole



Peak#	R.Time	I.Time	F.Time	Peak Report TIC				A/H	Mark	Name
				Area	Area%	Height	Height%			
1	14.908	14.735	15.095	163683712	98.59	38978682	97.97	4.20	MI	
2	16.726	16.685	16.805	2343331	1.41	807998	2.03	2.90	MI	
				166027043	100.00	39786680	100.00			

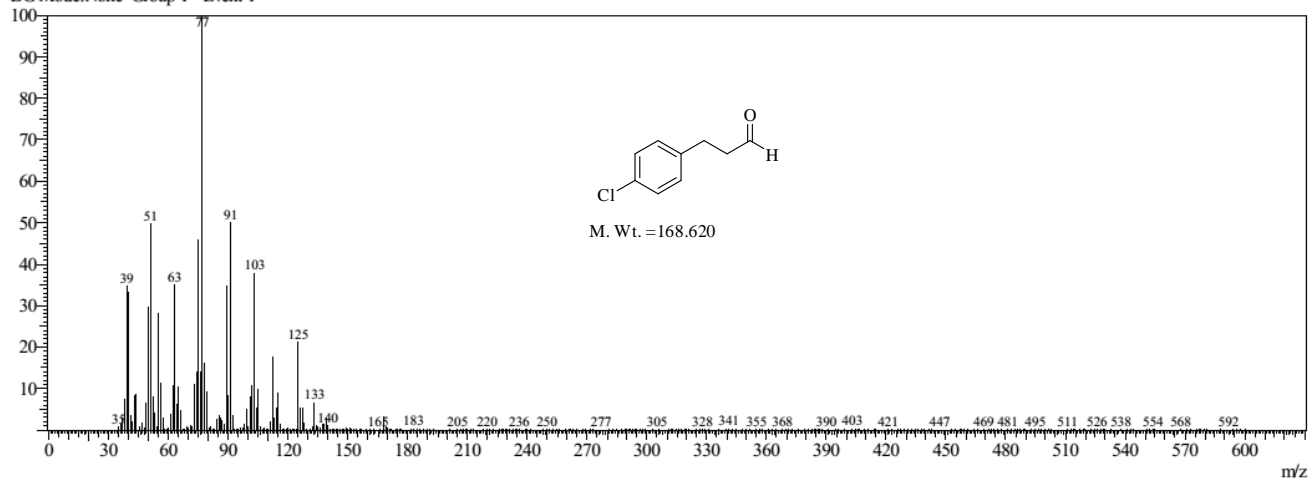
S22: GC spectra of hydroformylated product of 4-chlorostyrene in DCM at 45 °C

Line#:1 R.Time:14.875(Scan#:2276)
MassPeaks:566
RawMode:Single 14.875(2276) BasePeak:103(5180978)
BG Mode:None Group 1 - Event 1

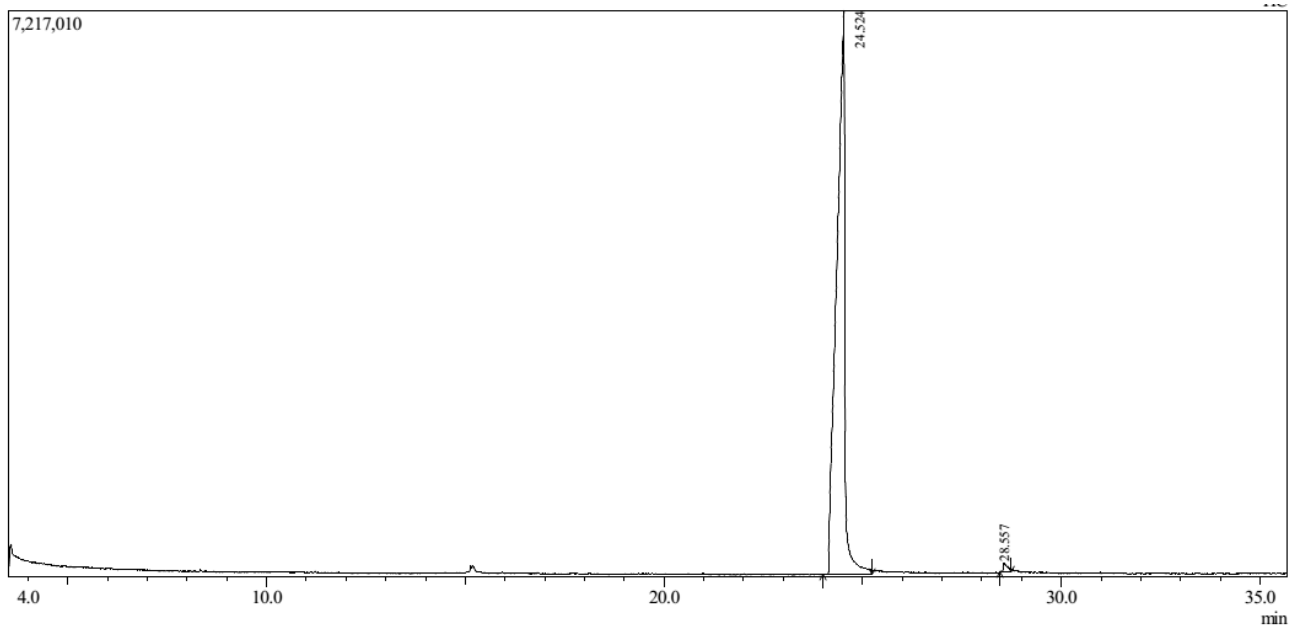


S23: Mass spectra of hydroformylated branched product of 4-chlorostyrene

Line#:2 R.Time:16.755(Scan#:2652)
MassPeaks:564
RawMode:Single 16.755(2652) BasePeak:77(53304)
BG Mode:None Group 1 - Event 1



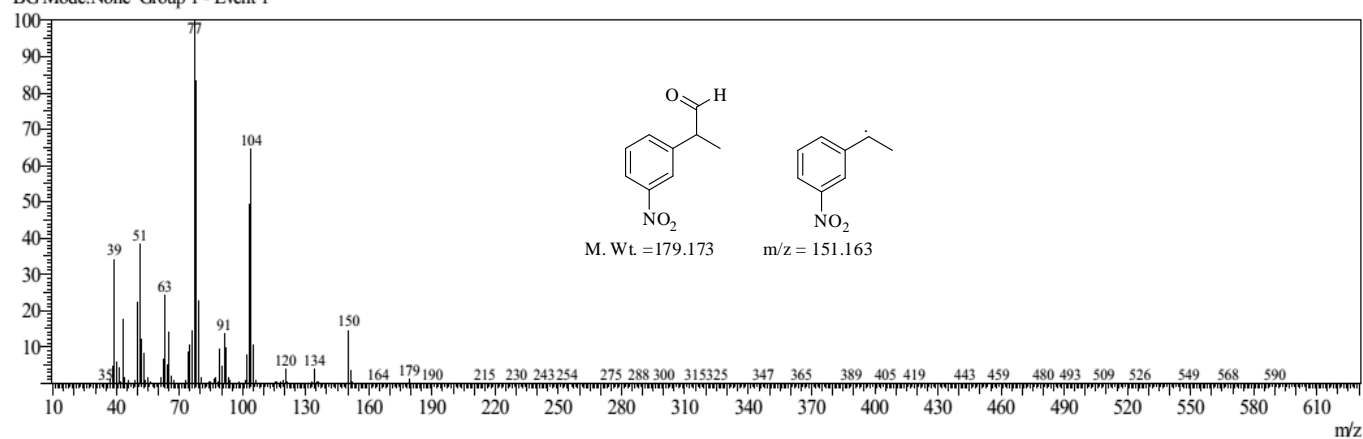
S24: Mass spectra of hydroformylated linear product of 4-chlorostyrene



Peak#	R.Time	I.Time	F.Time	Peak Report TIC				A/H	Mark	Name
				Area	Area%	Height	Height%			
1	24.524	24.005	25.230	103093923	99.23	7172205	98.44	14.37	MI	
2	28.557	28.460	28.740	804413	0.77	113857	1.56	7.07	MI	
				103898336	100.00	7286062	100.00			

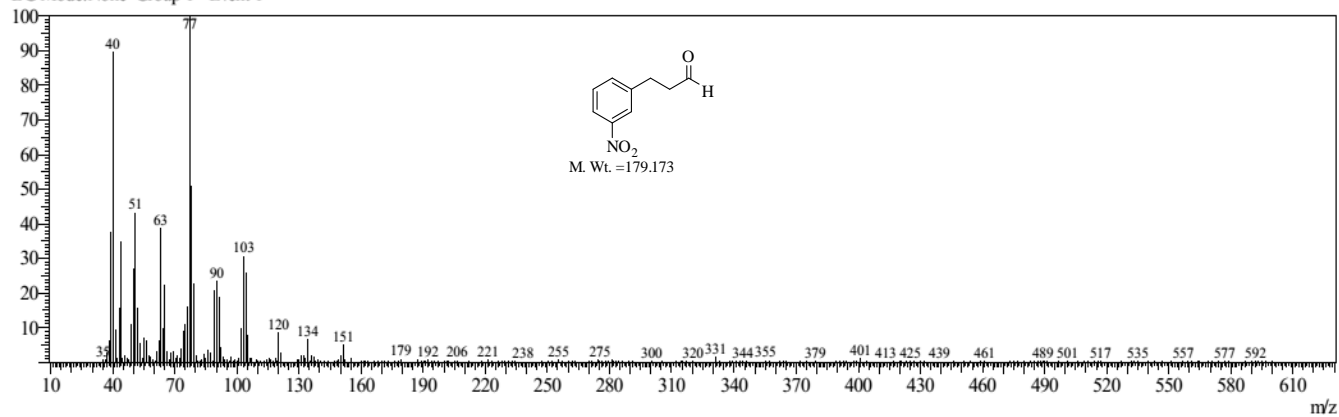
S25: GC spectra of hydroformylated product of 3-nitrostyrene in DCM at 45 °C

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MassPeaks:555
RawMode:Single 24.410(4183) BasePeak:77(763040)
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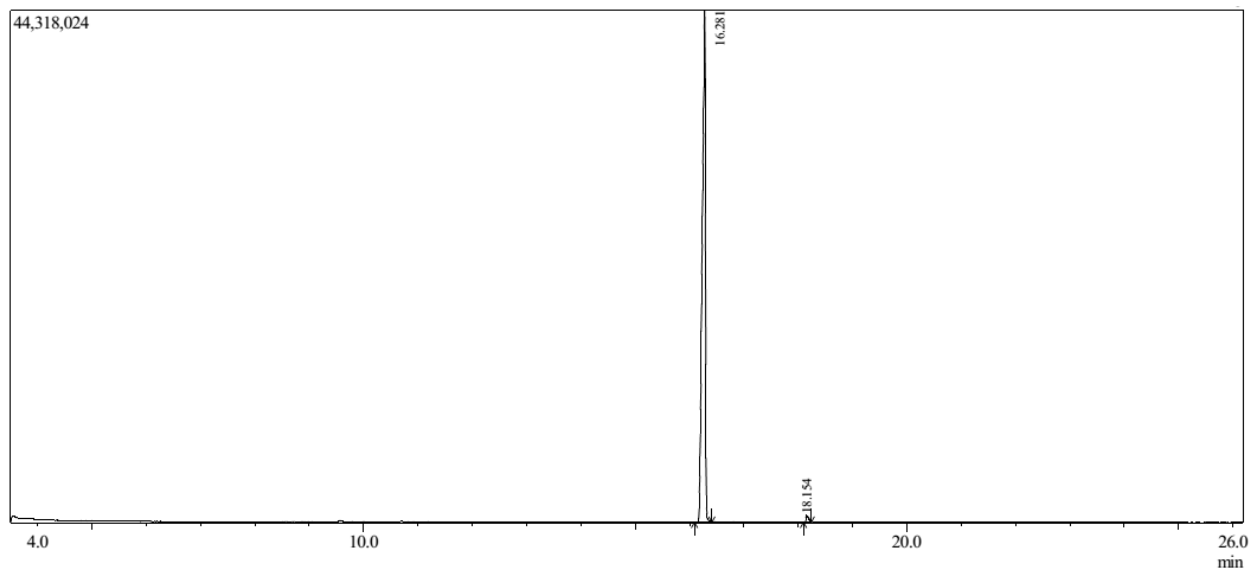


S26: Mass spectra of hydroformylated branched product of 3-nitrostyrene

Line#:2 R.Time:28.595(Scan#:5020)
MassPeaks:550
RawMode:Single 28.595(5020) BasePeak:77(18414)
BG Mode:None Group 1 - Event 1



S27: Mass spectra of hydroformylated linear product of 3-nitrostyrene

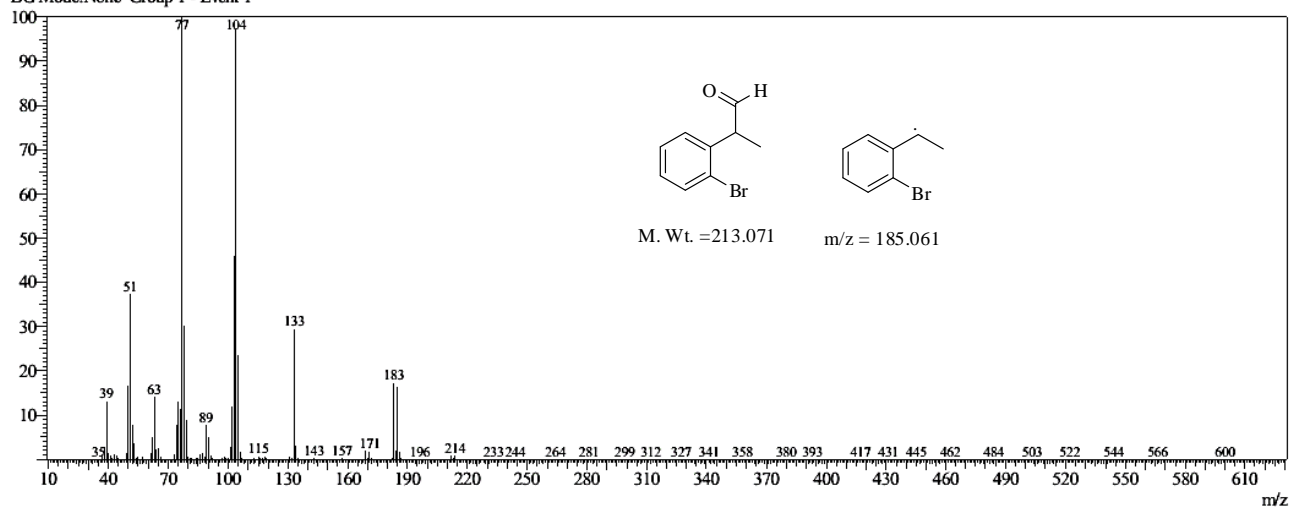


Peak Report TIC

Peak#	R.Time	L.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	16.281	16.090	16.410	178343429	98.91	44257404	98.65	4.03	MI	
2	18.154	18.095	18.240	1972289	1.09	607337	1.35	3.25	MI	
				180315718	100.00	44864741	100.00			

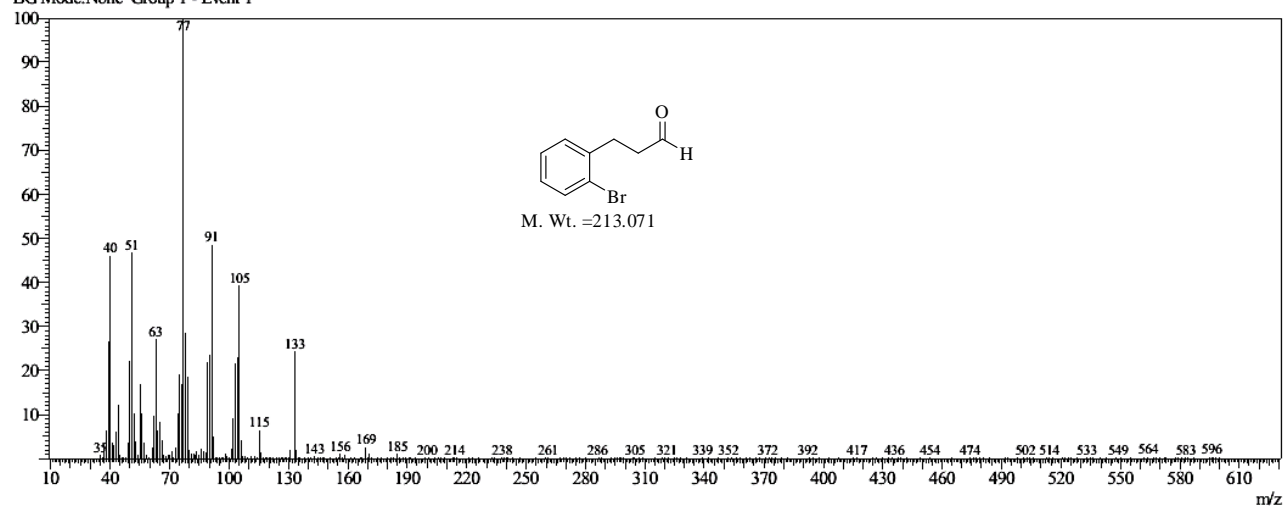
S28: GC spectra of hydroformylated product of 2-bromostyrene in DCM at 45 °C

Line#:1 R.Time:16.255(Scan#:2552)
MassPeaks:558
RawMode:Single 16.255(2552) BasePeak:77(5925094)
BG Mode:None Group 1 - Event 1

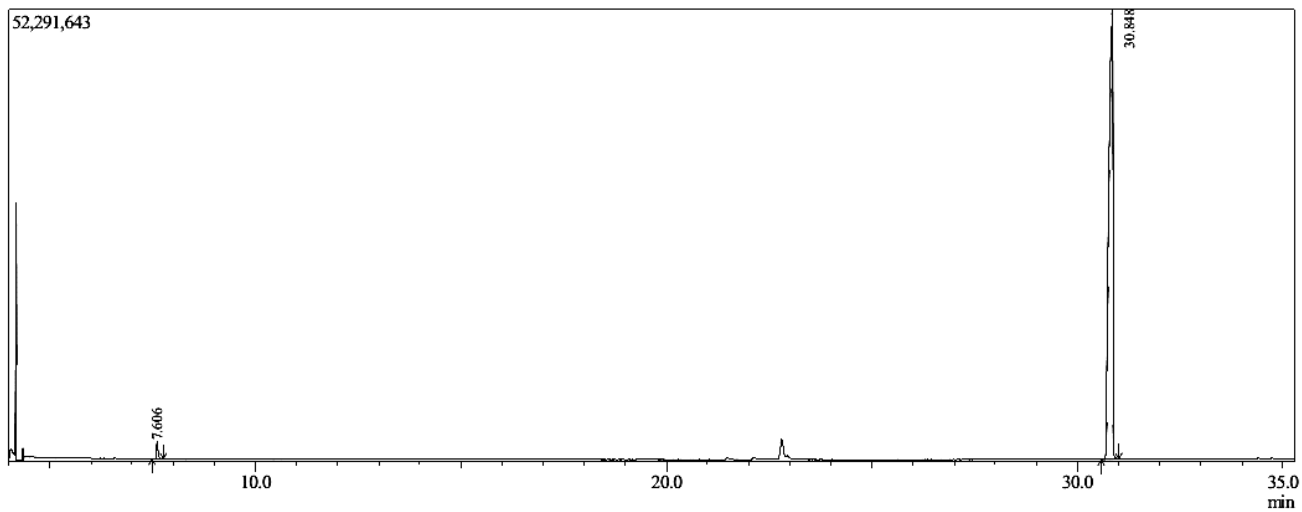


S29: Mass spectra of hydroformylated branched product of 2-bromostyrene

Line#:2 R.Time:18.190(Scan#:2939)
MassPeaks:562
RawMode:Single 18.190(2939) BasePeak:77(48836)
BG Mode:None Group 1 - Event 1

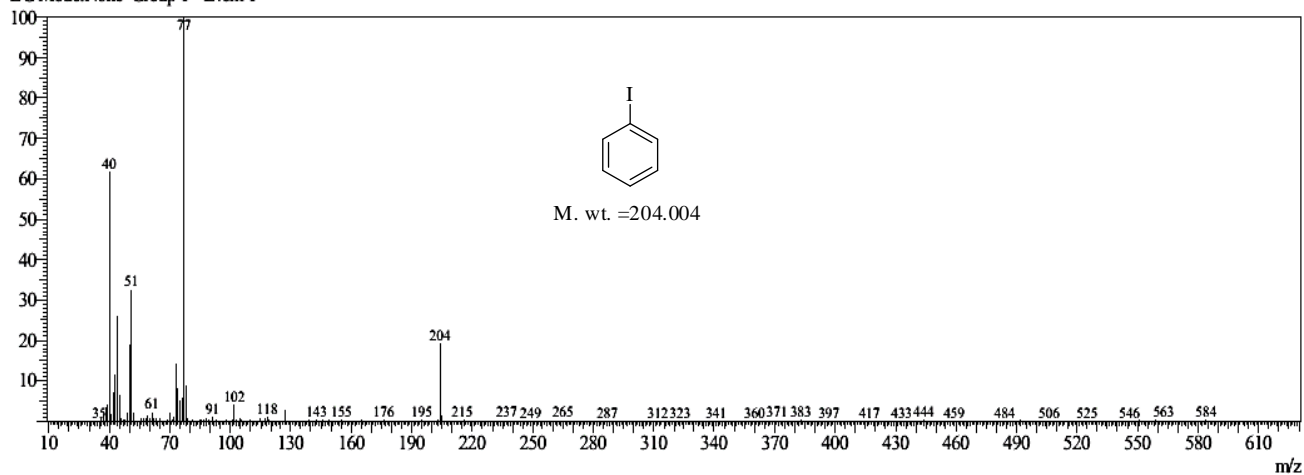


S30: Mass spectra of hydroformylated linear product of 2-bromostyrene



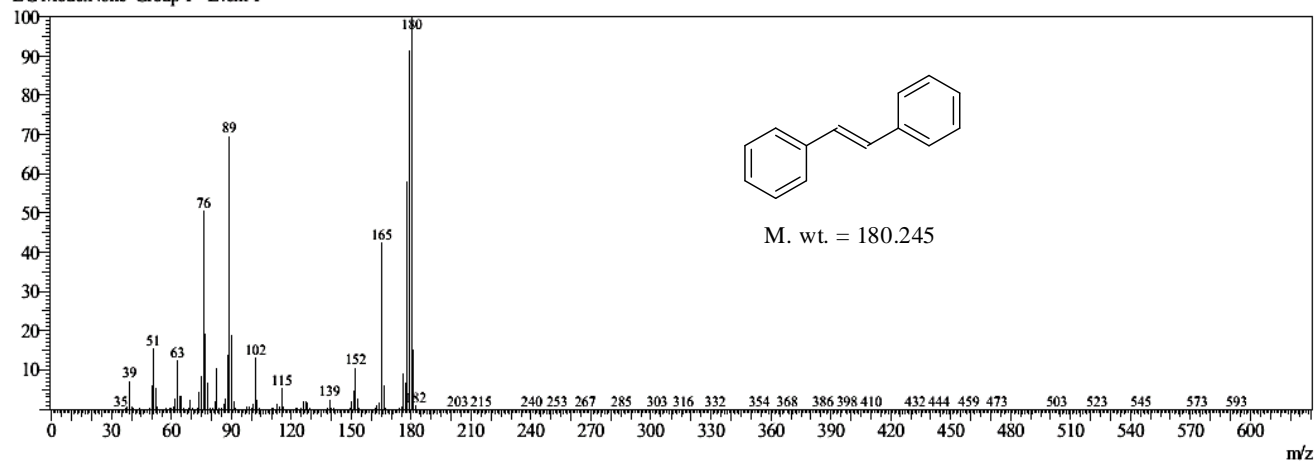
S31: GC spectra of Mizoroki-Heck reaction product of styrene and iodobenzene at 95°C

Line#:2 R.Time:7.585(Scan#:718)
MassPeaks:546
RawMode:Single 7.585(718) BasePeak:77(92893)
BG Mode:None Group 1 - Event 1

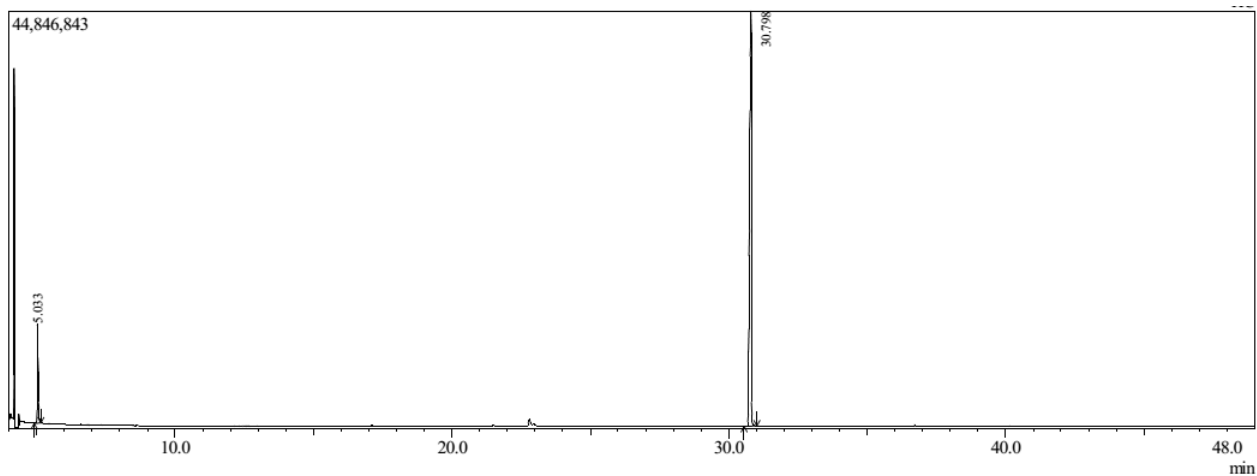


S32: Mass spectra of iodobenzene at $R_t = 7.585$.

Line#:3 R.Time:30.825(Scan#:5366)
MassPeaks:520
RawMode:Single 30.825(5366) BasePeak:180(7433609)
BG Mode:None Group 1 - Event 1

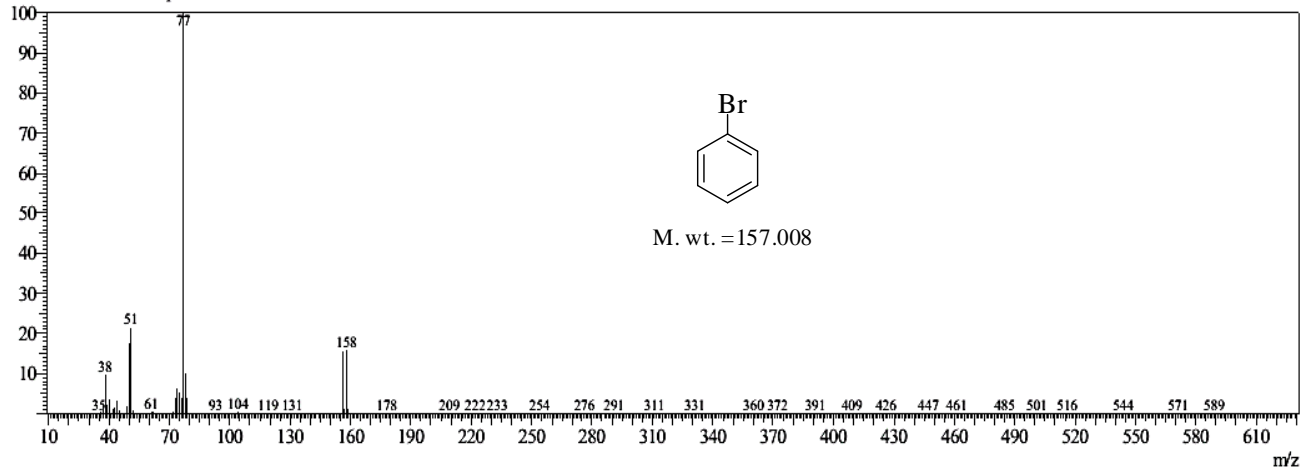


S33: Mass spectra of coupling reaction product of styrene and iodobenzene

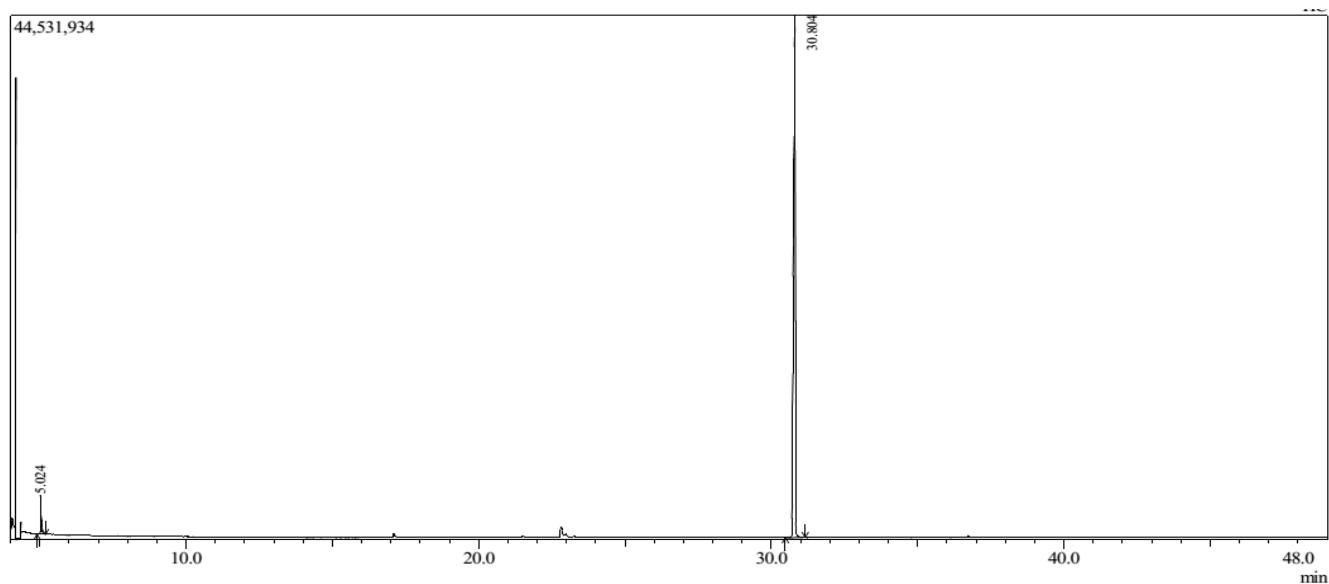


S34: GC spectra of Mizoroki-Heck reaction product of styrene and bromobenzene at 95°C after 1 hour

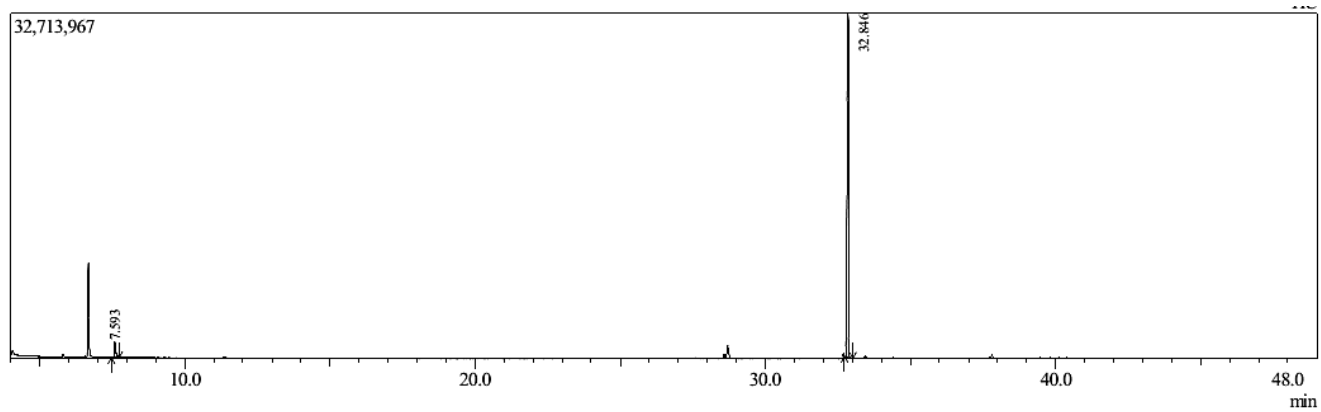
Line#:2 R.Time:5.055(Scan#:212)
 MassPeaks:561
 RawMode:Single 5.055(212) BasePeak:77(2522236)
 BG Mode:None Group 1 - Event 1



S35: Mass spectra of bromobenzene at $R_t = 5.055$.



S36: GC spectra of Mizoroki-Heck reaction product of styrene and bromobenzene at 95°C after 2 hour



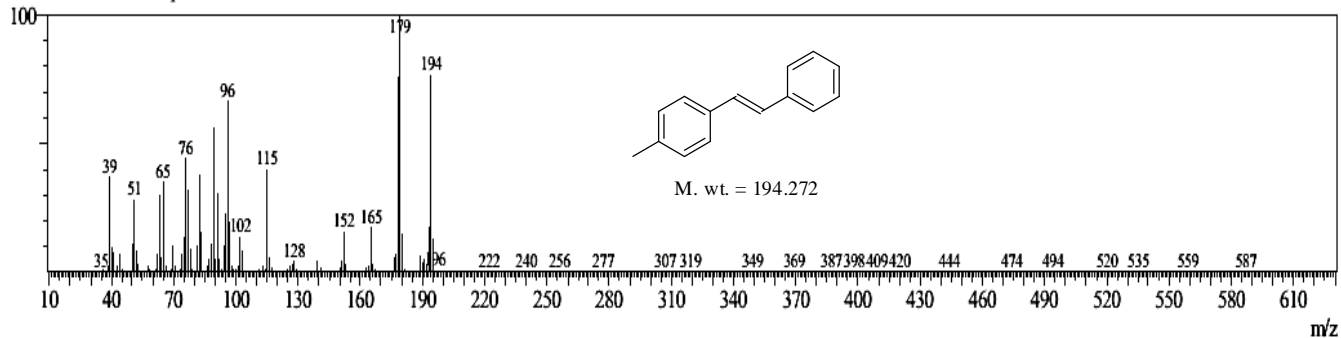
S37: GC spectra of Mizoroki-Heck reaction product of 4-methylstyrene and iodobenzene at 95°C

Line#:3 R.Time:32.870(Scan#:5775)

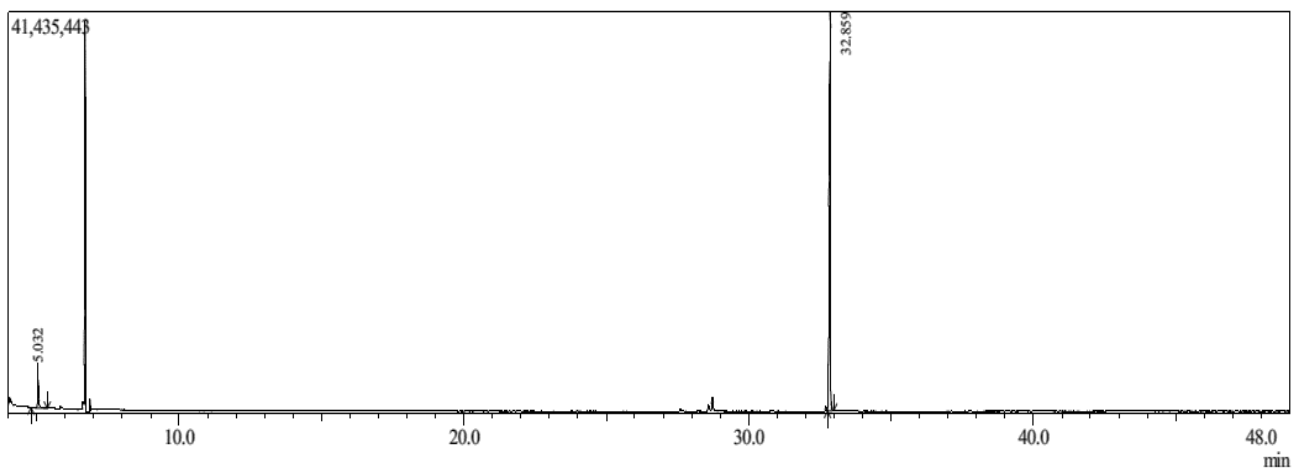
MassPeaks:489

RawMode:Single 32.870(5775) BasePeak:179(182713)

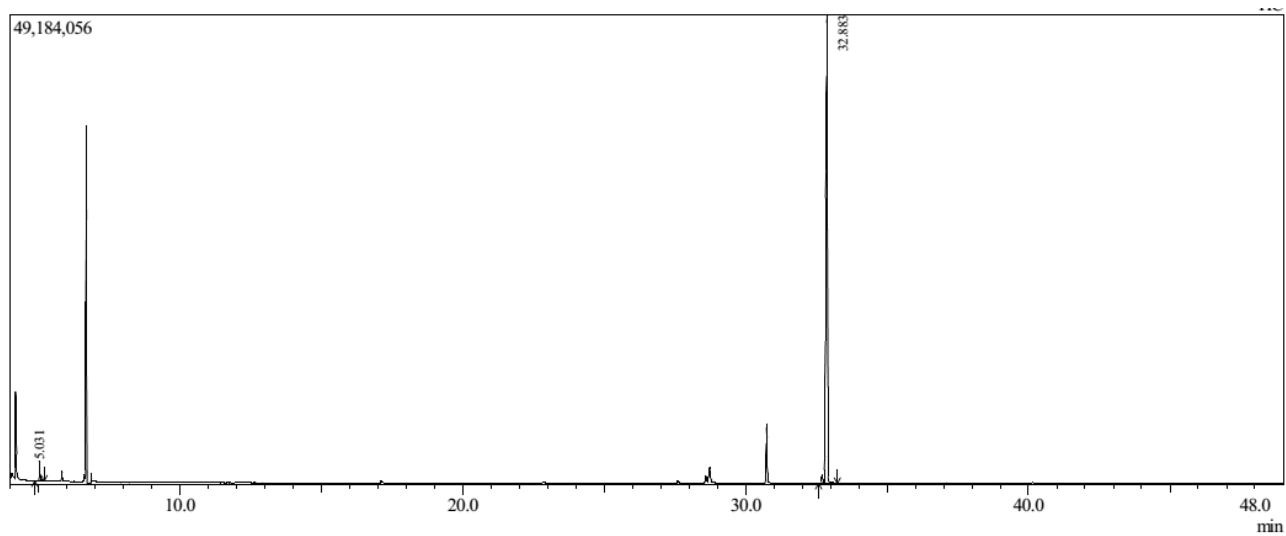
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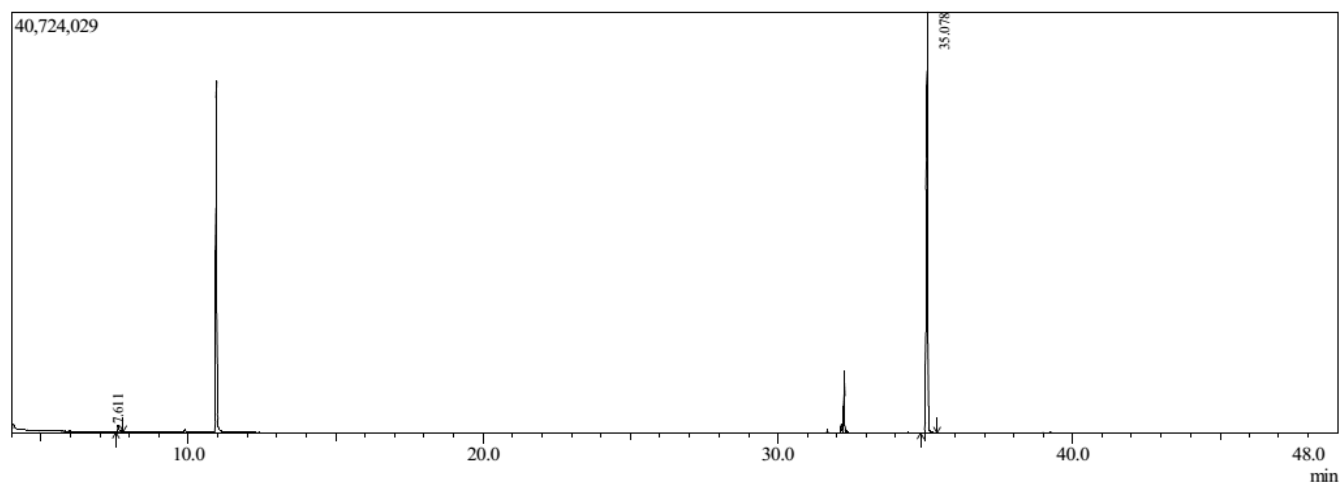
S38: Mass spectra of Mizoroki-Heck coupling reaction product of 4-methylstyrene



S39: GC spectra of Mizoroki-Heck reaction product of 4-methylstyrene and bromobenzene at 95°C after 30 minutes



S40: GC spectra of Mizoroki-Heck reaction product of 4-methylstyrene and bromobenzene at 95°C after 2 hours



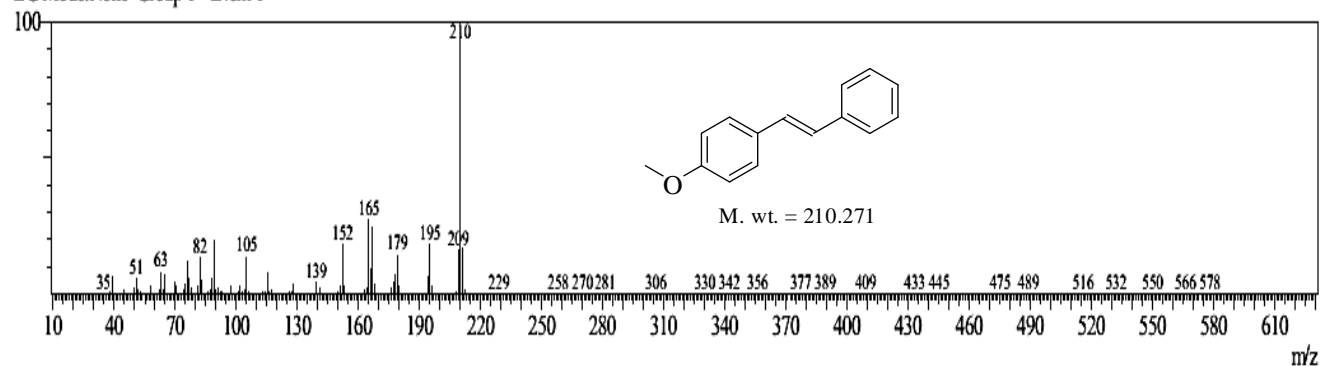
S41: GC spectra of Mizoroki-Heck reaction product of 4-vinylanisole and iodobenzene at 95°C after 30 minutes

Line#3 R.Time:35.050(Scan#:6211)

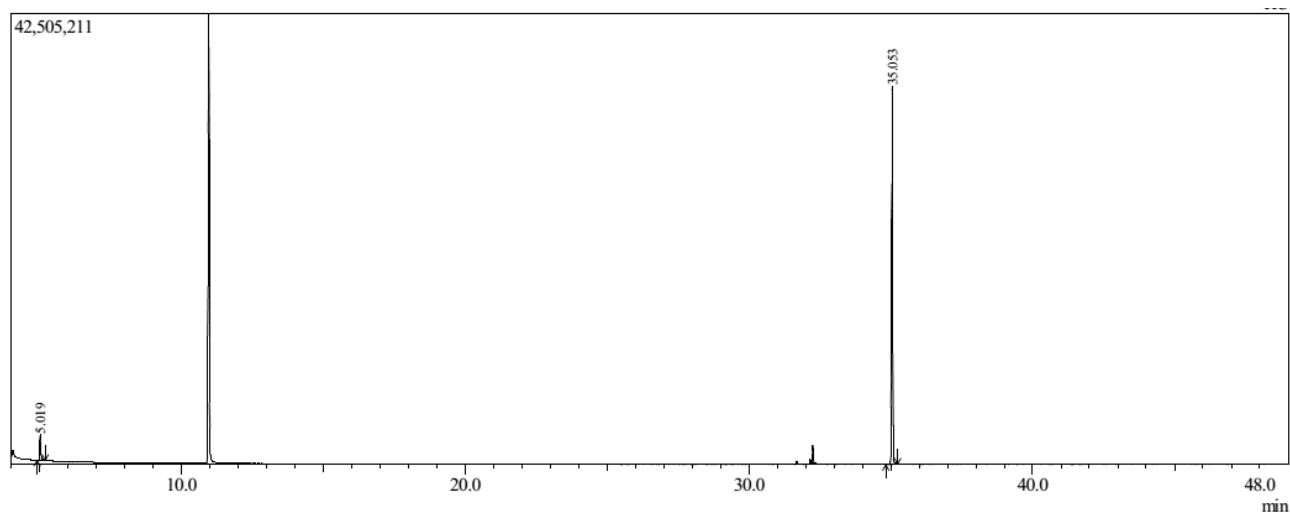
MassPeaks:482

RawMode:Single 35.050(6211) BasePeak:210(7036137)

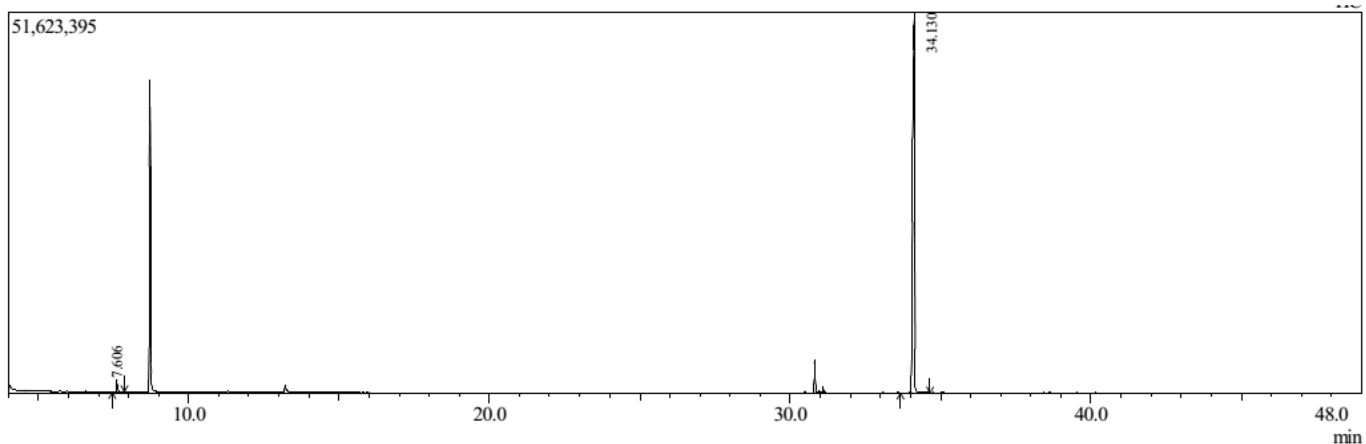
BG Mode:None Group 1 - Event 1



S42: Mass spectra of Mizoroki-Heck coupling reaction product of 4-vinylanisole



S43: GC spectra of Mizoroki-Heck reaction product of 4-vinylanisole and bromobenzene at 95°C after 1 hour



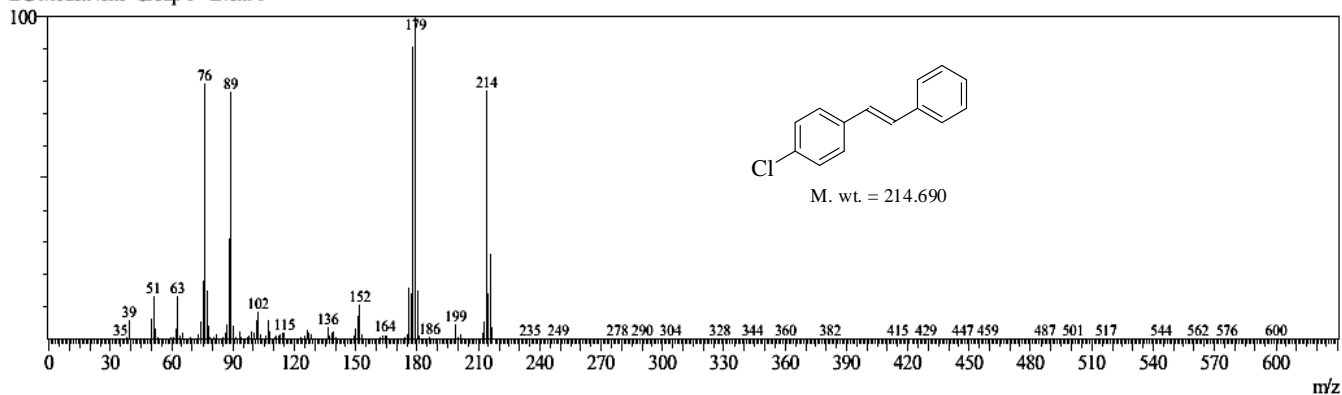
S44: GC spectra of Mizoroki-Heck reaction product of 4-chlorostyrene and iodobenzene at 95°C after 30 minutes

Line#:4 R.Time:34.105(Scan#:6022)

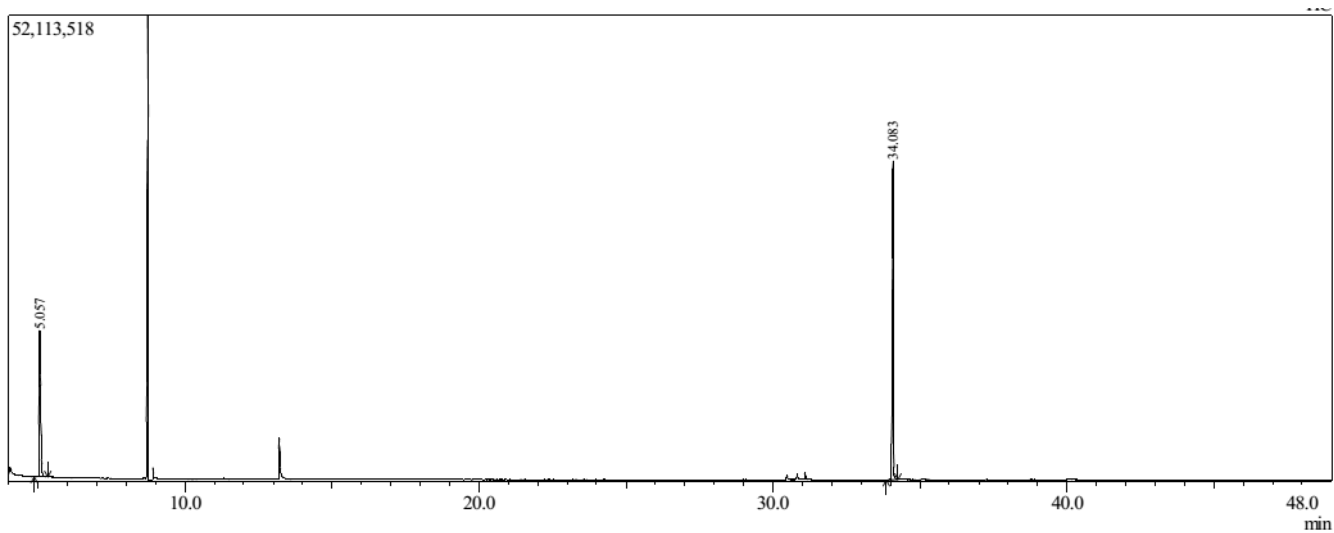
MassPeaks:496

RawMode:Single 34.105(6022) BasePeak:179(6070313)

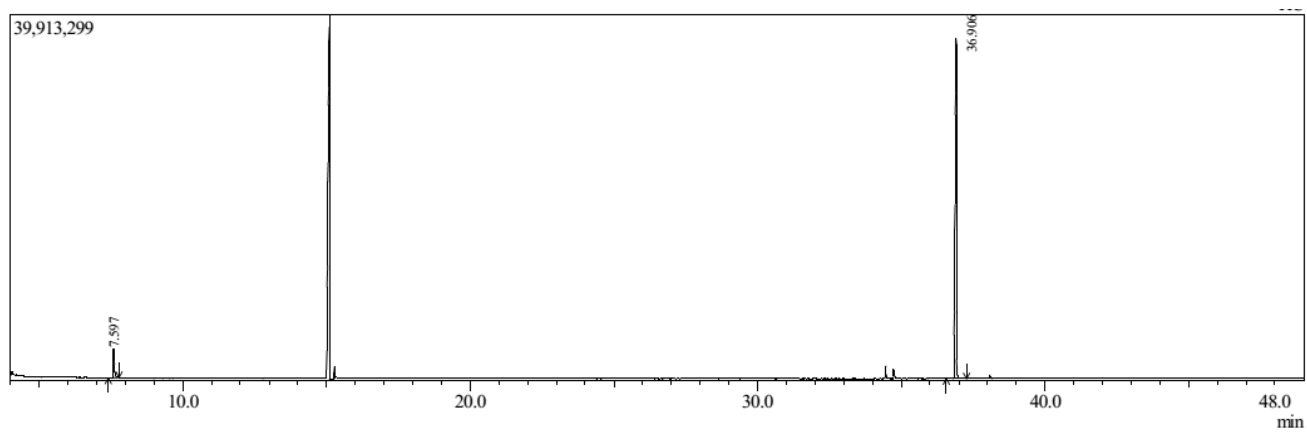
BG Mode:None Group 1 - Event 1



S45: Mass spectra of Mizoroki-Heck coupling reaction product of 4-chlorostyrene

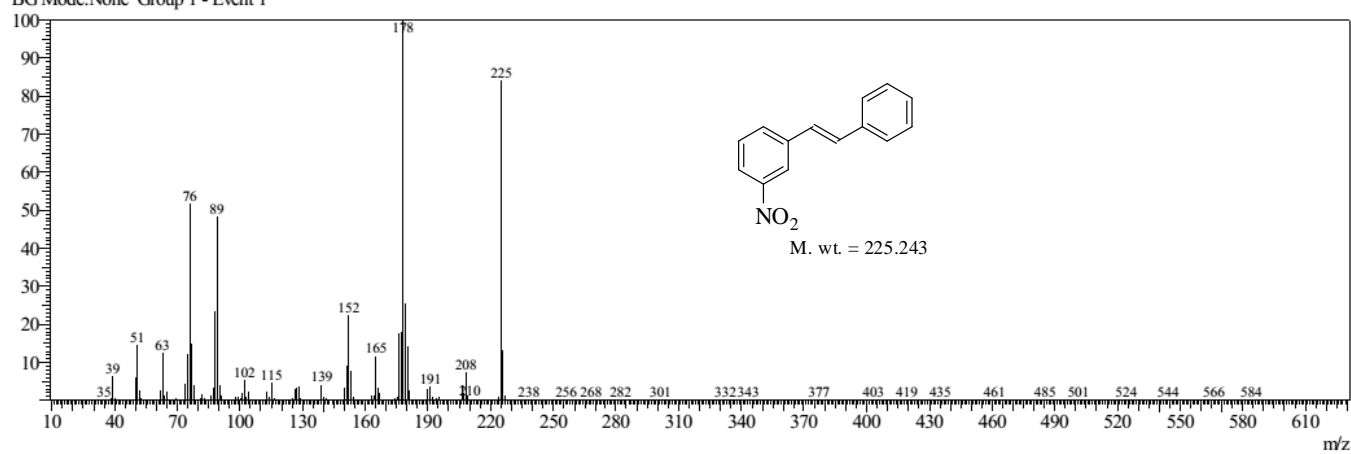


S46: GC spectra of Mizoroki-Heck reaction product of 4-chlorostyrene and bromobenzene at 95°C after 1 hour



S47: GC spectra of Mizoroki-Heck reaction product of 3-nitrostyrene and iodobenzene at 95°C after 30 minutes

Line#:3 R.Time:36.900(Scan#:6581)
MassPeaks:538
RawMode:Single 36.900(6581) BasePeak:178(5630766)
BG Mode:None Group 1 - Event 1



S48: Mass spectra of Mizoroki-Heck coupling reaction product of 3-nitrostyrene

