Enhanced photocatalytic degradation of Amaranth dye on mesoporous anatase TiO_2: evidence of C-N, N=N bond cleavage and identification of new intermediates

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Supplementary Material

Submitted

To

Photochemical & Photobiological Sciences

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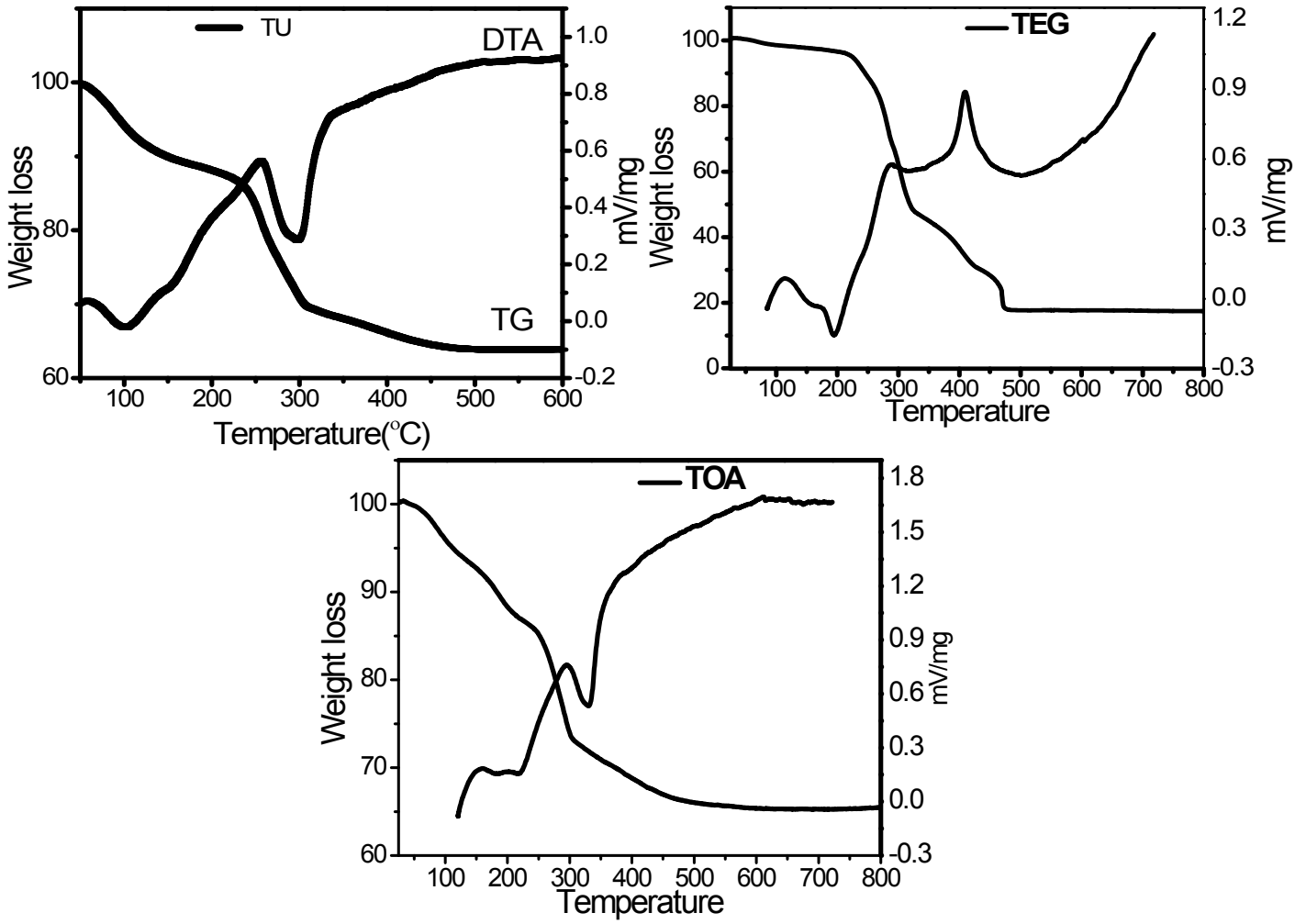
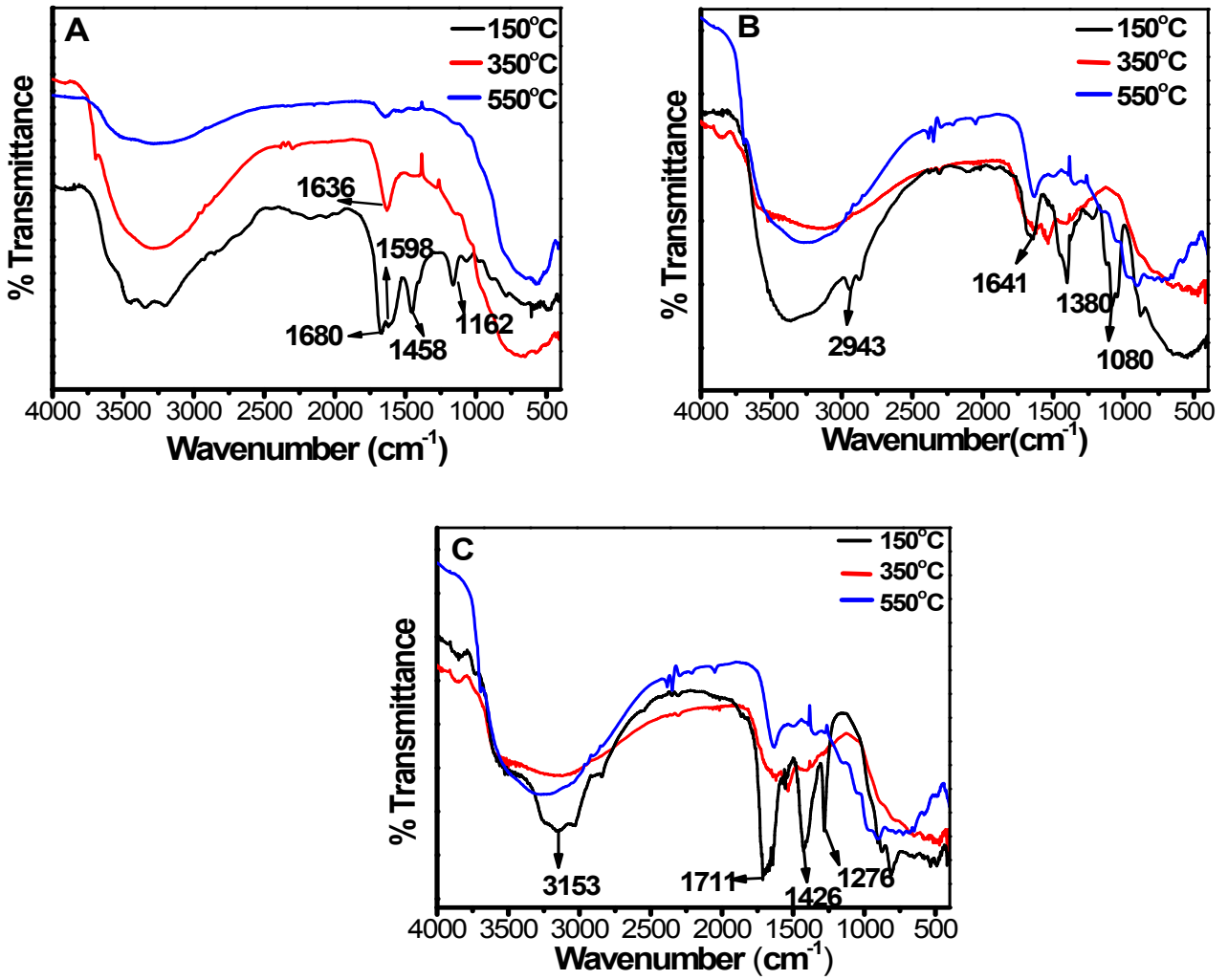
Time (min)	*A (%)	#B (%)
0	90	10
2	90	10
9	10	90
11	10	90
13	90	10
15	90	10

**A= H_2O, 0.1% formic acid + 5% acetonitrile #B = Acetonitrile, 0.1% formic acid, Constant Flow rate =1 mL min^{-1}*

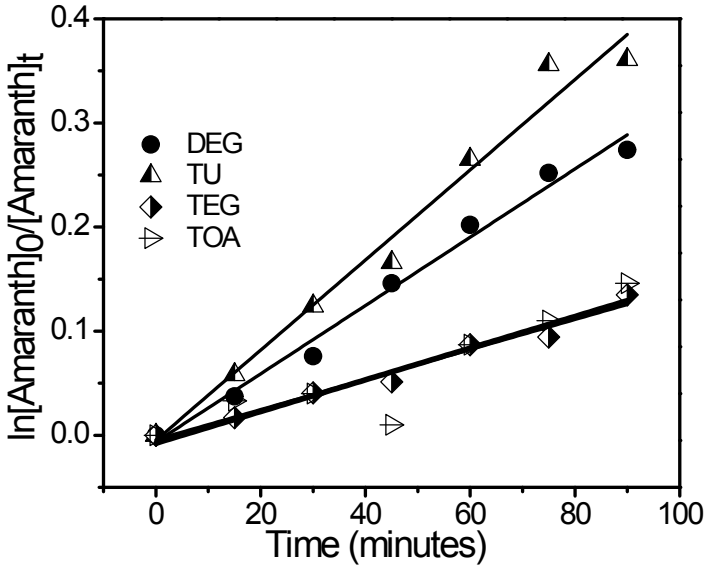
ST 1: Optimised eluent gradient conditions for HPLC separation



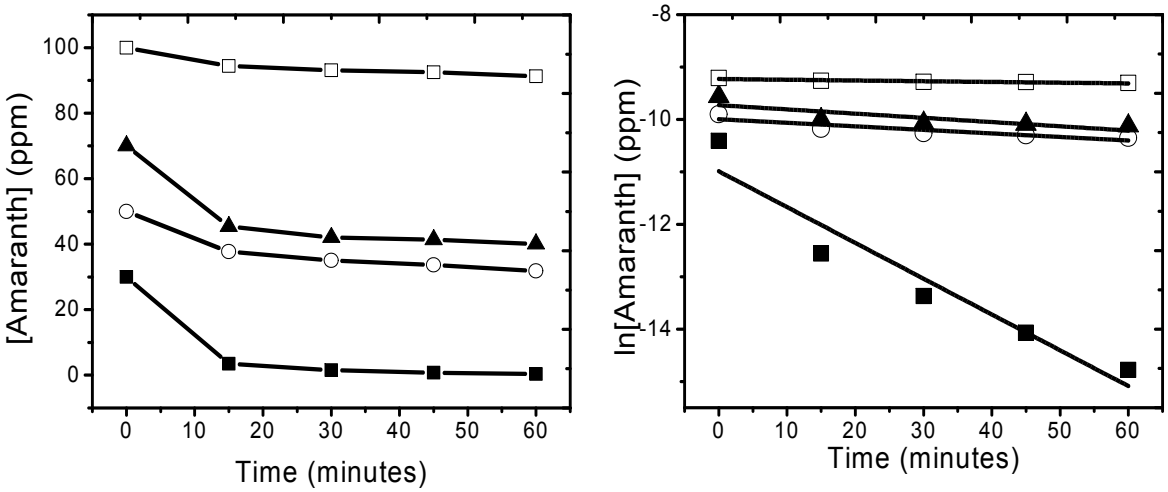
SF1: TG-DTA curves of as-synthesized mixtures of titanium isopropoxide using urea (TU) ethylene glycol (TEG) and oxalic acid (TOA).



SF2: IR spectra of as-synthesized mixtures of titanium isopropoxide using urea (TU), ethylene glycol (TEG) and oxalic acid (TOA).



SF3: Adsorption profile of amaranth over TiO_2 catalyst, Linear fits to the logarithmic ratio of initial concentration of Amaranth at time '0'to concentration at any given time 't'. $[Amaranth]_0$ = 30 ppm, TiO_2 = 50 mg, solution pH = 5.6 at 30˚C.

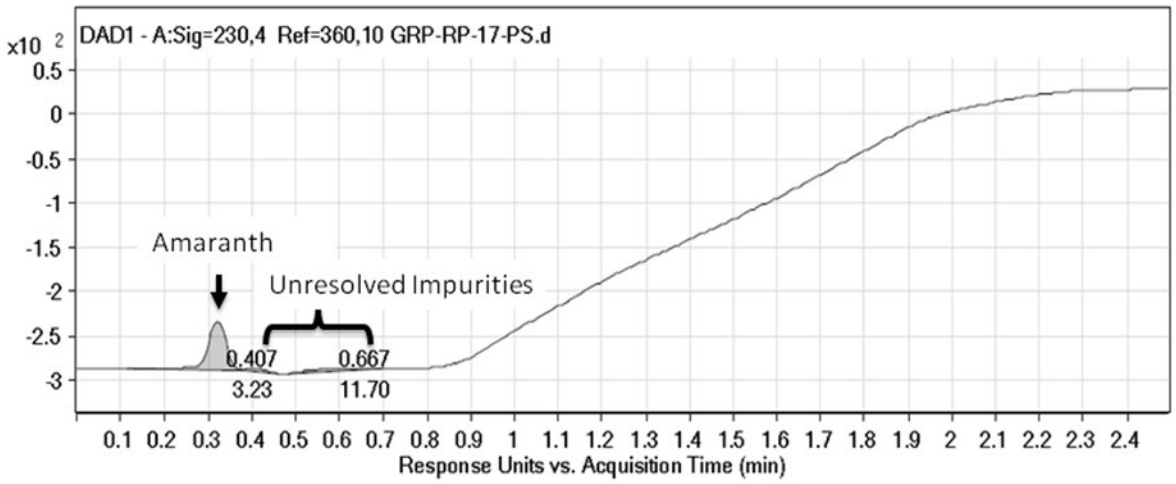


SF4: Kinetic profiles depicting effect of initial dye concentration on degradation rate. Catalyst = TU, Catalyst amount =110 mg, pH=5.6., Temperature = 30^{o}C

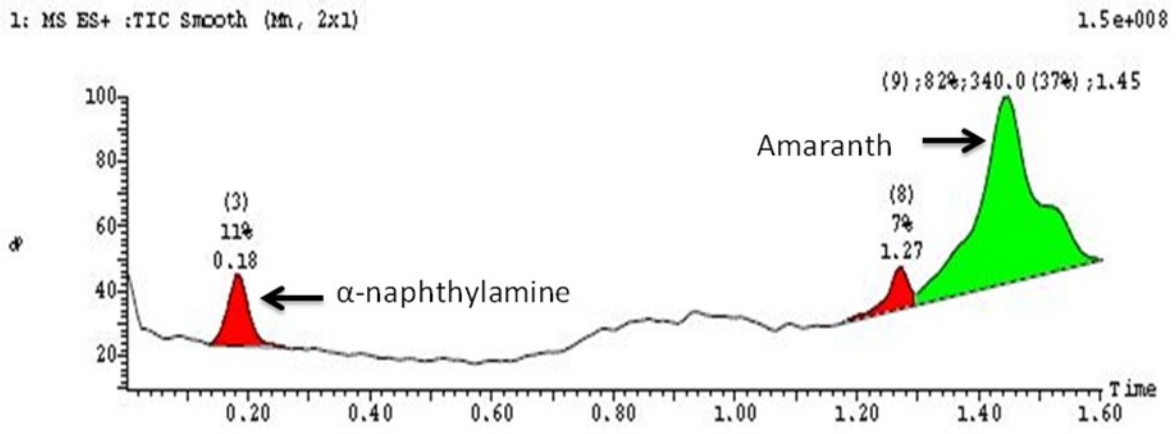
Concentration ppm	% Decolourization	Rate constant min^{-1}
30	82.6	0.051
50	41.7	0.004
70	22.9	0.003
100	13.16	0.001

ST 2: Effect of initial dye concentration on % decolorisation, and rate constant. Catalyst = TU, Catalyst amount =110 mg, pH=5.6., Temperature = 30^{o}C, reaction time = 60 mins

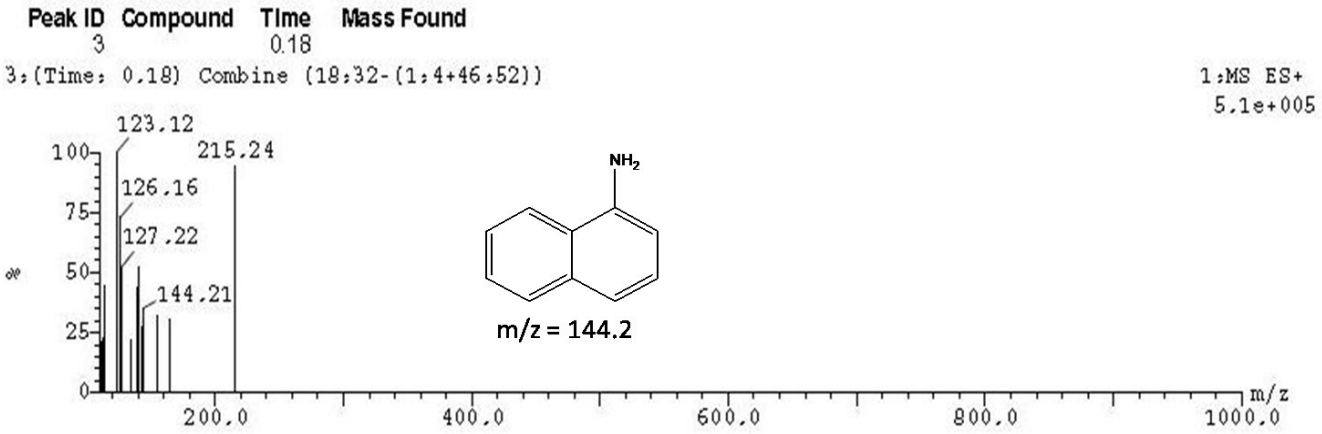
Impurity profile of Amaranth Dye



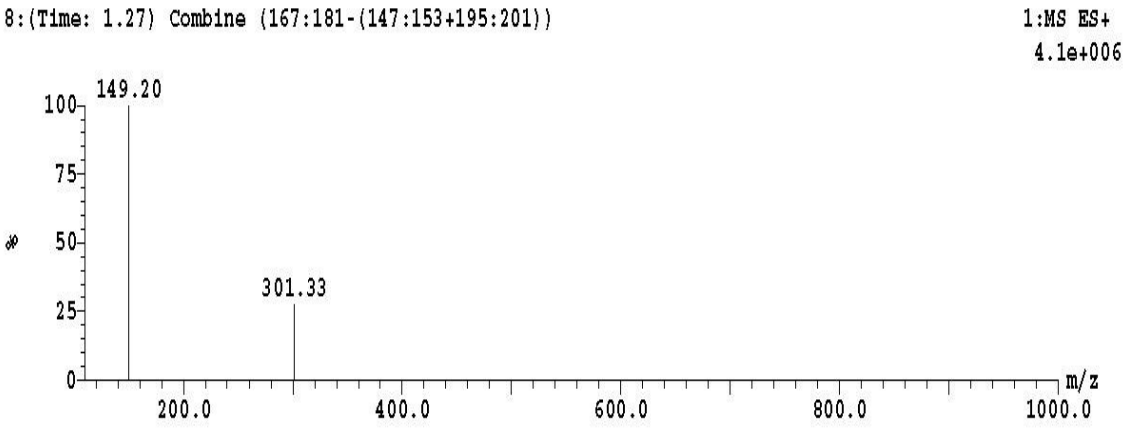
SF5: Liquid Chromatogram of Amaranth dye



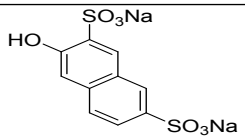
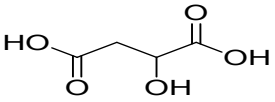
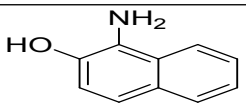
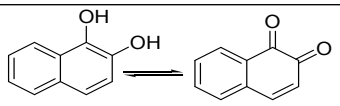
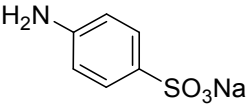
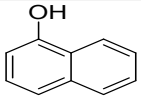
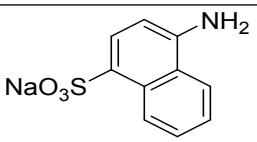
SF6 : Ultra performance liquid Chromatogram of Amaranth dye



SF7: Impurity peak corresponding to m/z value 144

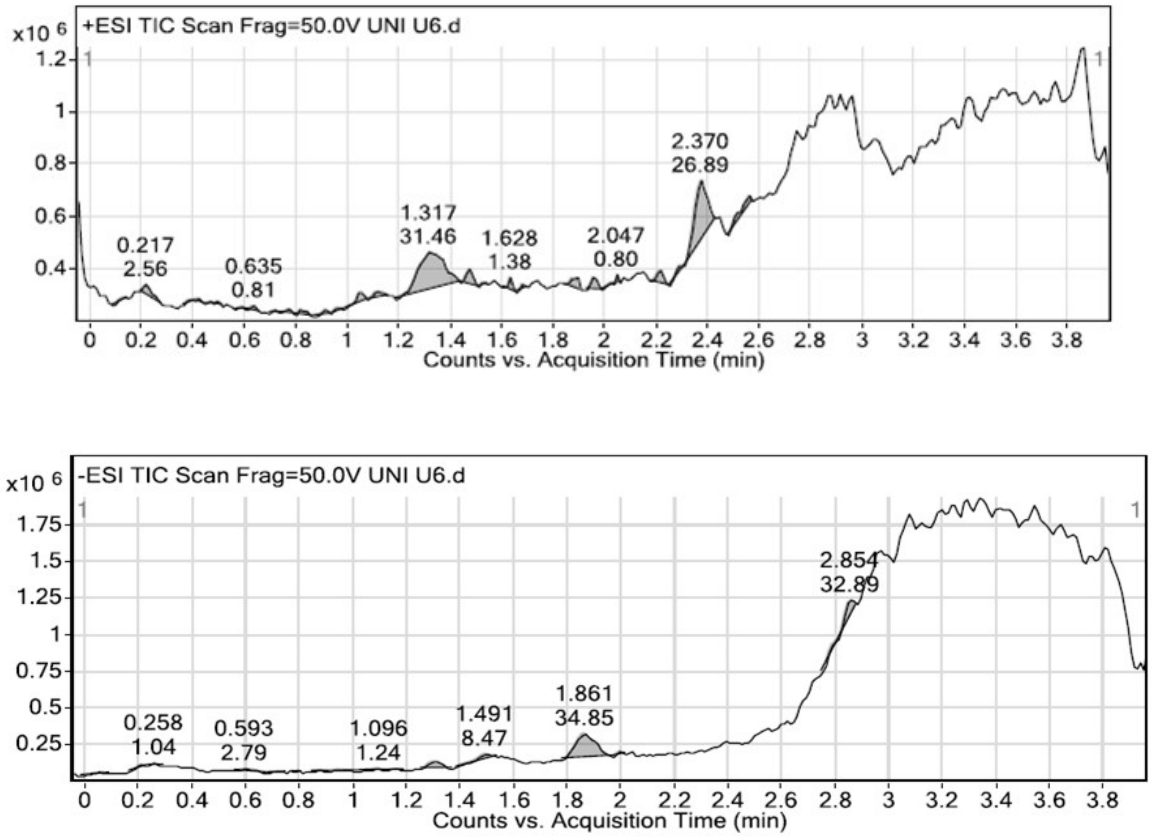


SF 8: Impurity peak corresponding to m/z value 301.33

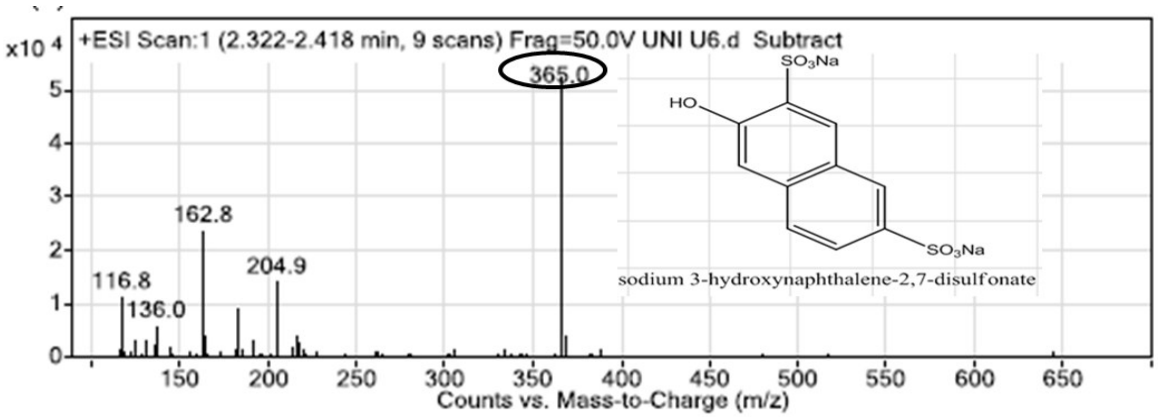
Sr.No.	Mass calculated	Mass obtained	Products
1.	348	$[M+H_2O]$ = 365	
2.	134	[M+H] = 135	
3.	159	$[M+ H_2O+ K]$ =216	
4.	94	[M+Na] = 117	
5	168	[M+Na] = 191	
6	195	[M-Na] = 172	
7	144	$[M+H_2O]$ = 162	
8	245	[M-H]= 244	

ST 3: Various products after photodecolorization of amaranth dye. **[**Amaranth$]_0$ = 30 ppm, TiO_2 = 50 mg, solution pH = 5.6 at 30˚C.

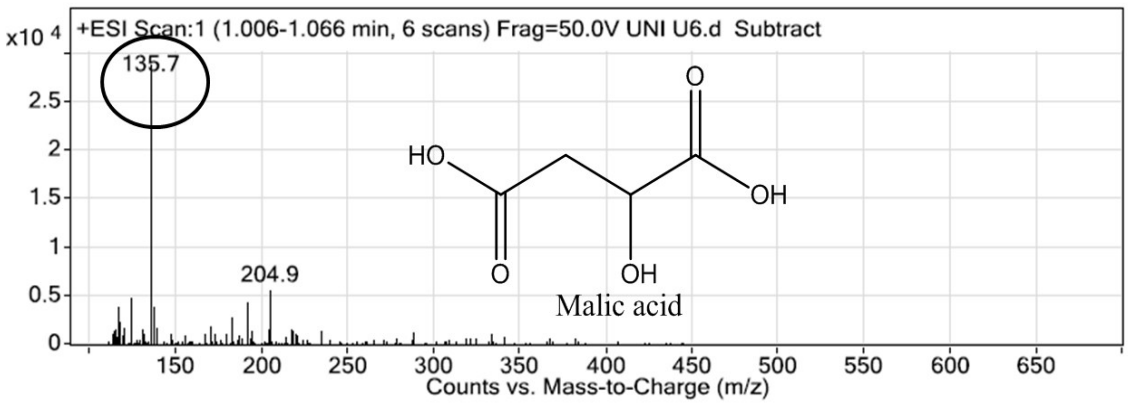
The mass spectrum of various products with corresponding retention time are depicted in the following figure.



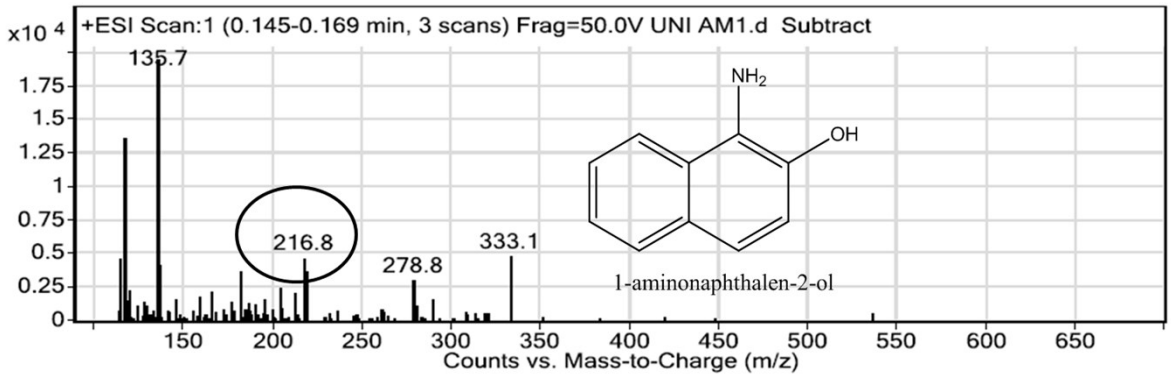
SF 9: The TIC Scan of photocatalytic decolorization of amaranth dye



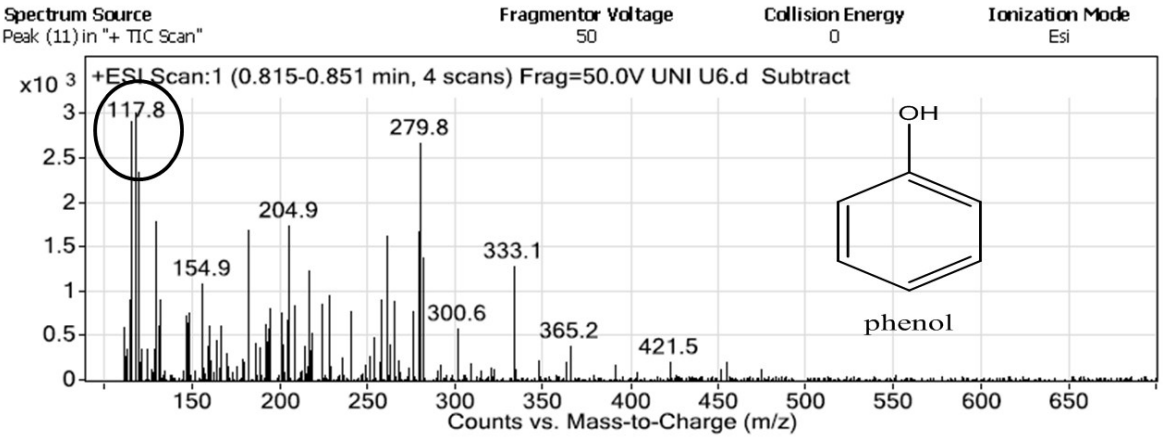
SF 10: Peak corresponding to m/z value 365.



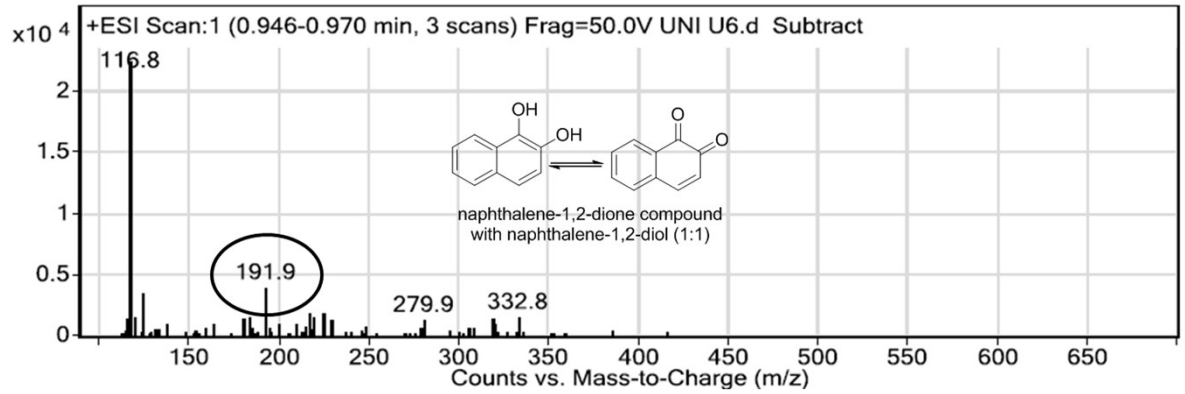
SF 11: Peak corresponding to m/z value 135



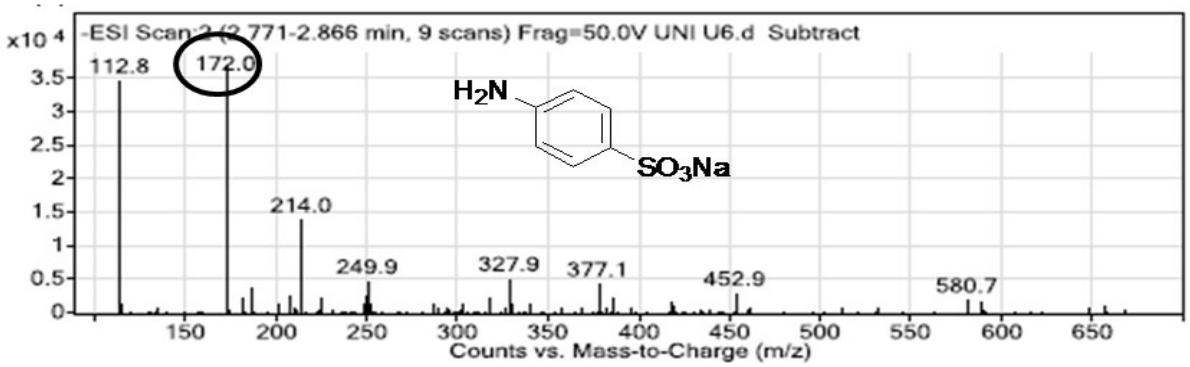
SF 12: Peak corresponding to m/z = 216



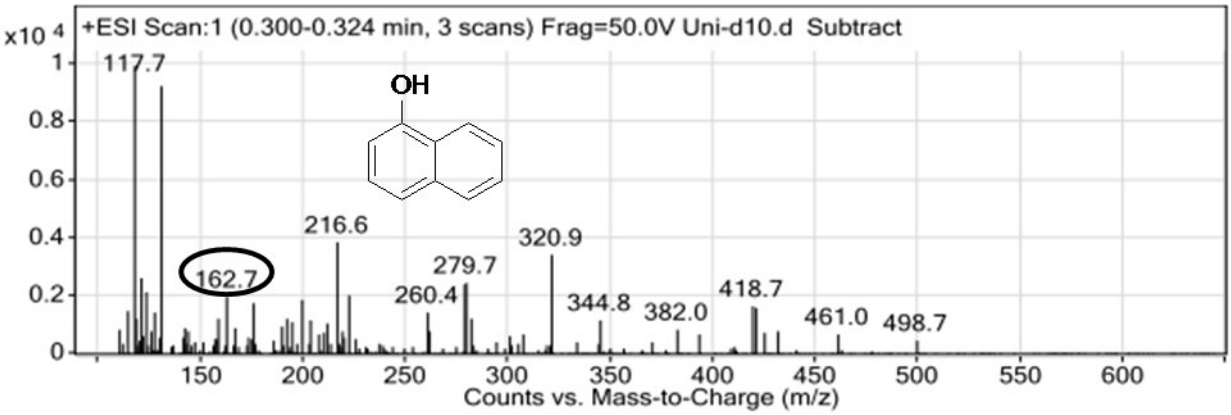
SF 13: Peak corresponding to m/z= 117



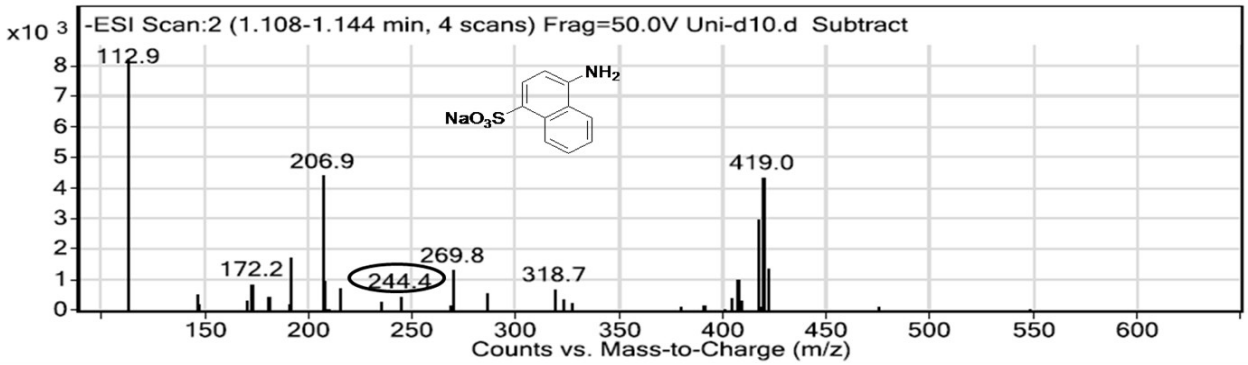
SF 14: Peak corresponding to m/z =191



SF 15: Peak corresponding to m/z = 172



SF 16: Peak corresponding to m/z = 162



SF 17: Peak corresponding to m/z = 244

These are the mass spectra of the various products that are obtained after decolourization of amaranth dye.