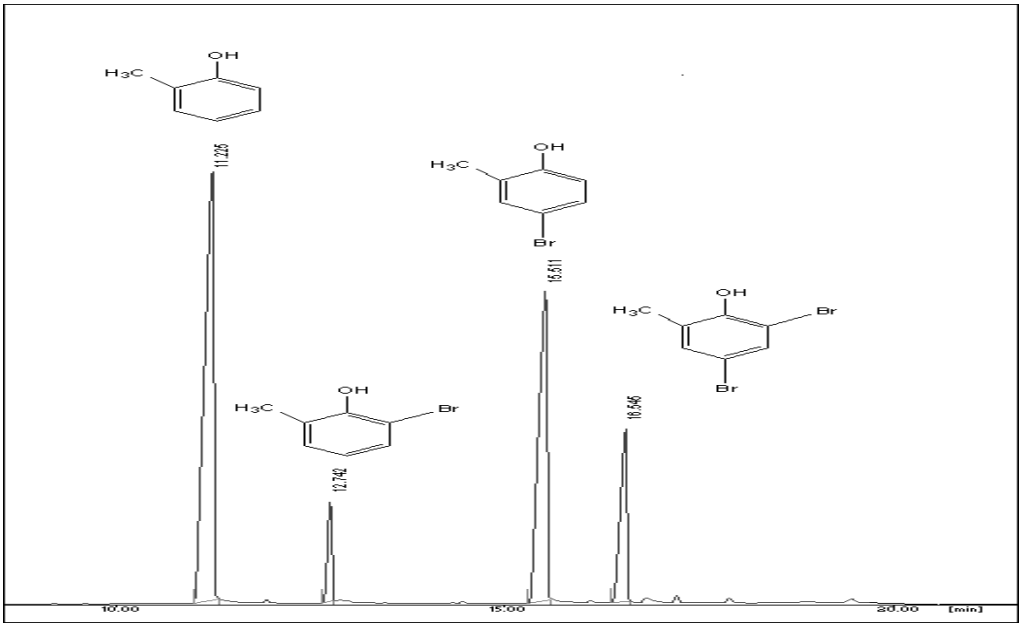

Fig.S1: Retention time of the corresponding brominated products including the substrate o-cresol in the gas chromatogram with catalyst 1. (Done in Agilent 6890N GC System)

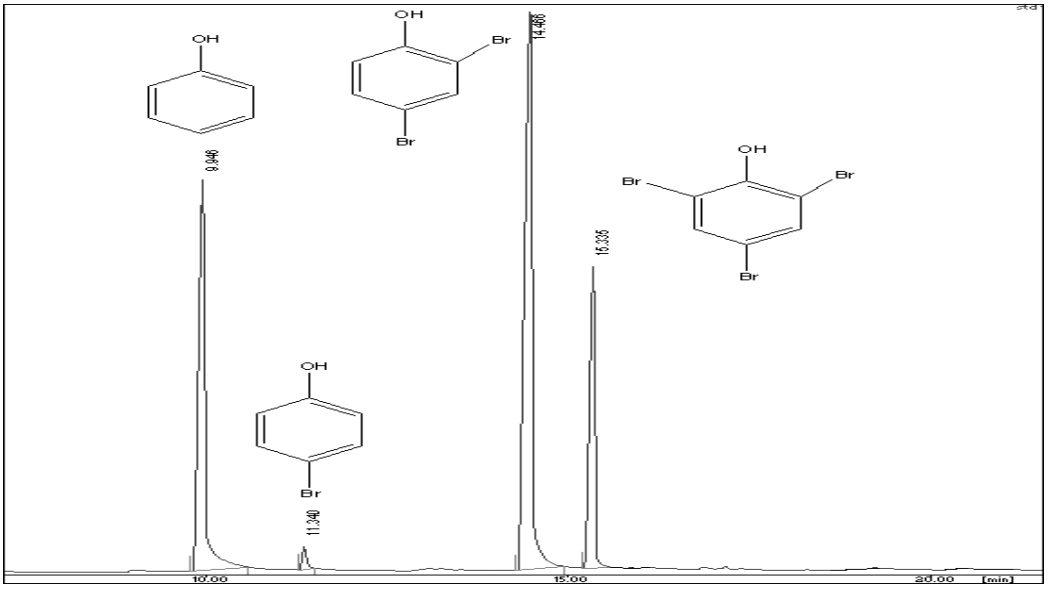

Fig.S2: Retention time of the corresponding brominated products including the substrate phenol in the gas chromatogram with catalyst 1. (Done in Agilent 6890N GC System)

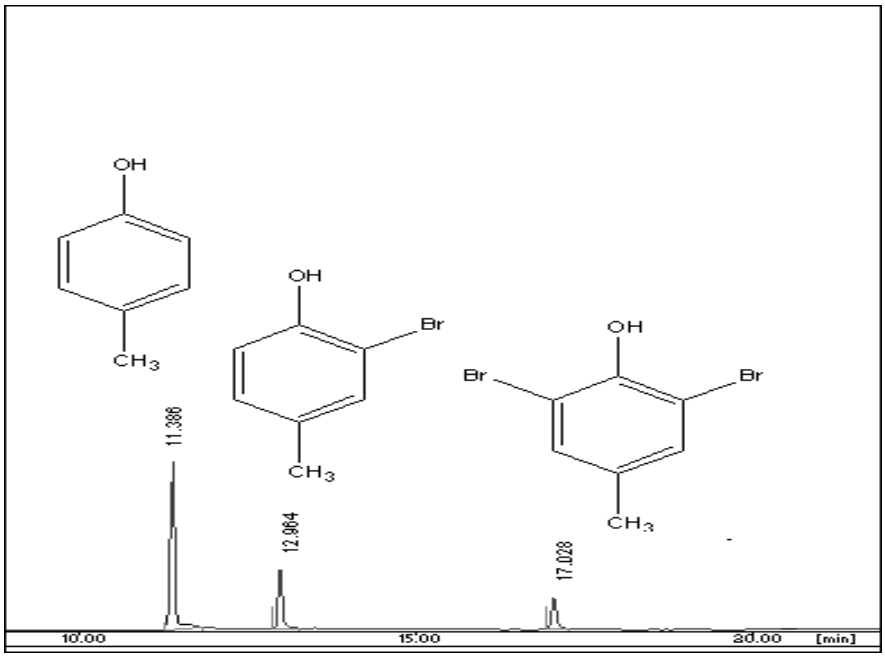

Fig.S3: Retention time of the corresponding brominated products including the substrate p-cresol in the gas chromatogram with catalyst 1. (Done in Agilent 6890N GC System)

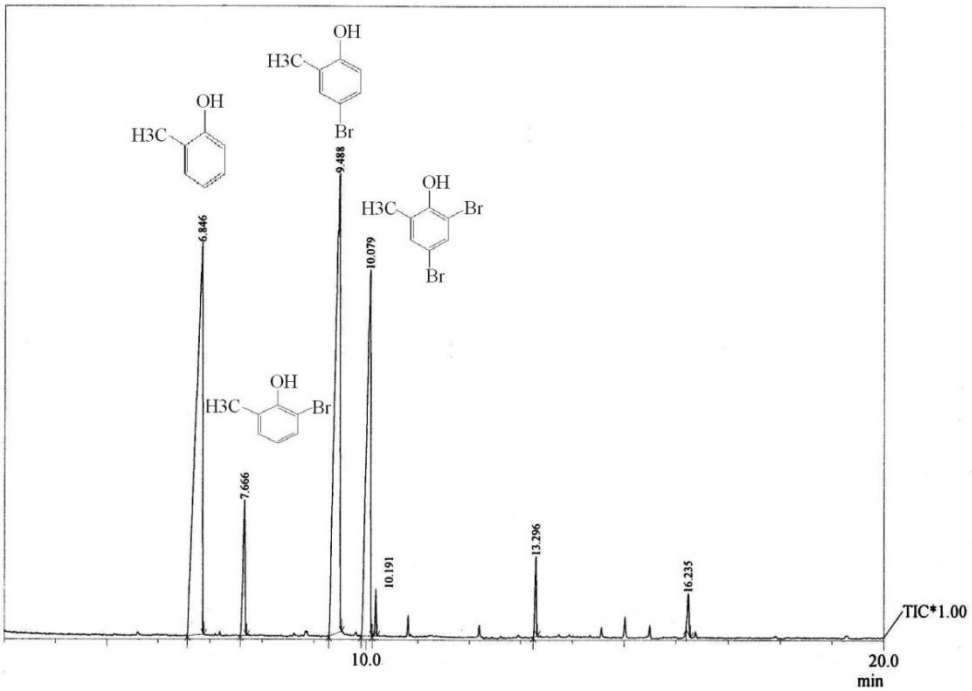

Fig.S4: Retention time of the corresponding brominated products including the substrate o-cresol in the gas chromatogram with catalyst 2. (Done in SHIMADZU-QP-5050A GC-MS)

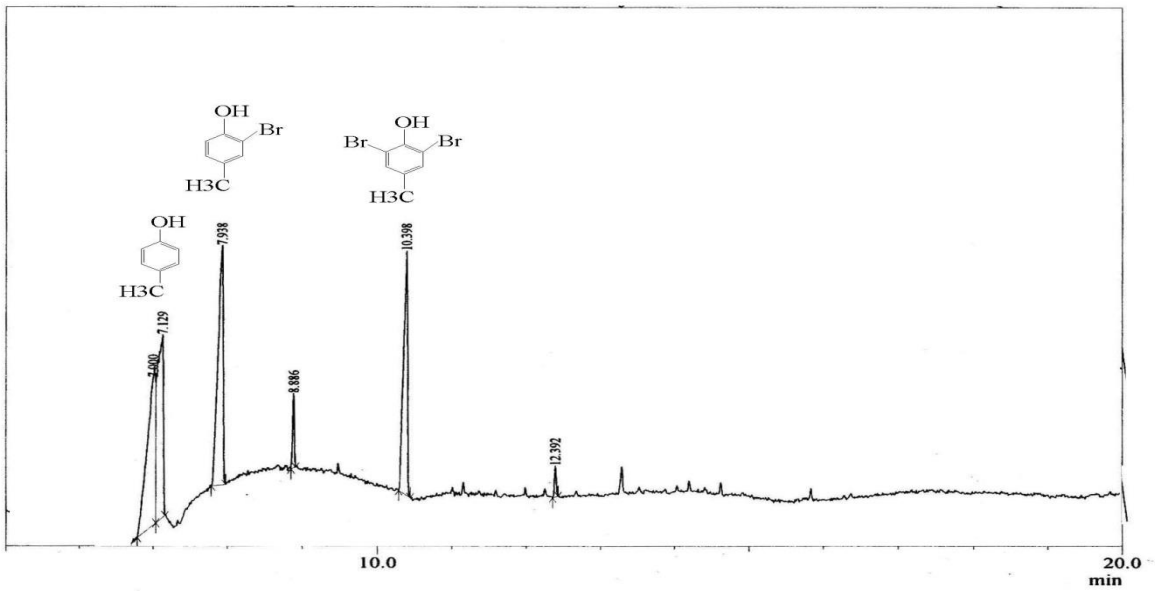

Fig.S5: Retention time of the corresponding brominated products including the substrate p-cresol in the gas chromatogram with catalyst 2. (Done in SHIMADZU-QP-5050A GC-MS)

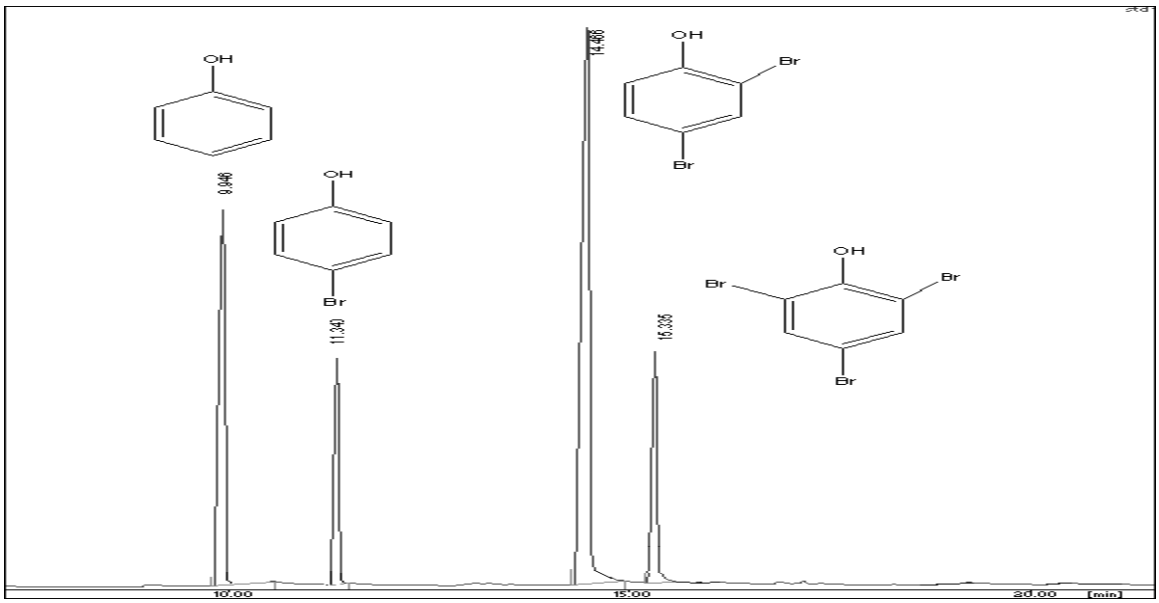

Fig.S6: Retention time of the corresponding brominated products including the substrate phenol in the gas chromatogram with catalyst 2. (Done in Agilent 6890N GC System)

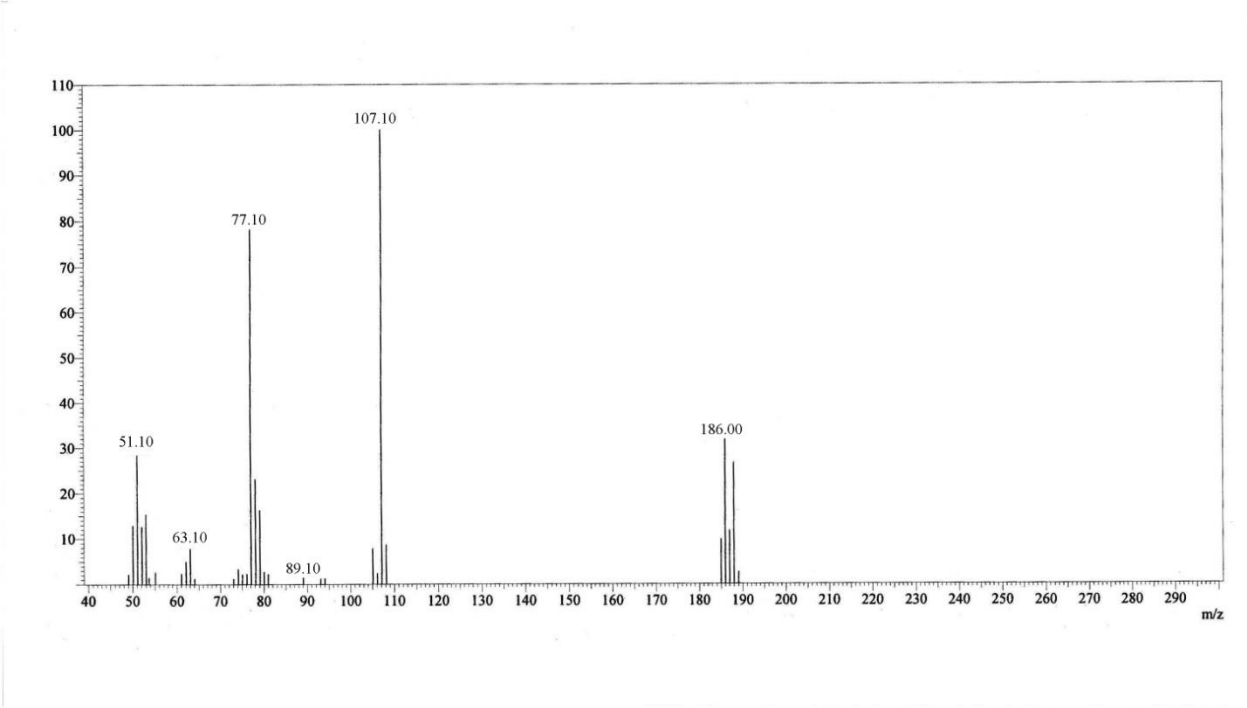

Fig.S7: Mass spectram of 2-bromo para-cresol

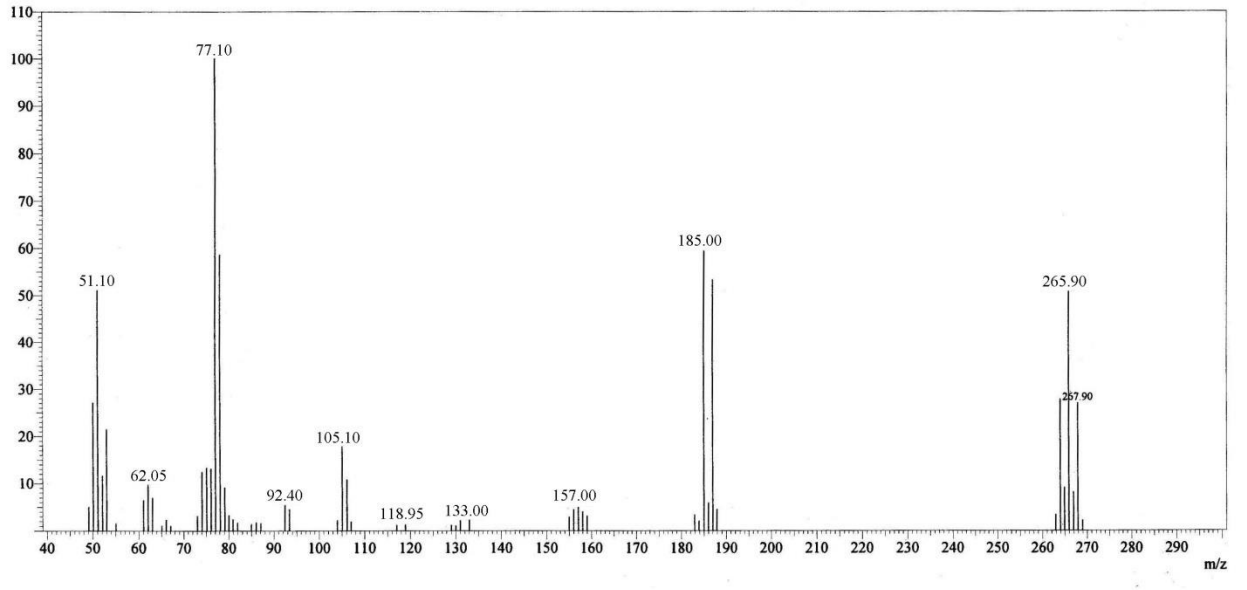

Fig.S8: Mass spectram of 2,6- dibromo para-cresol

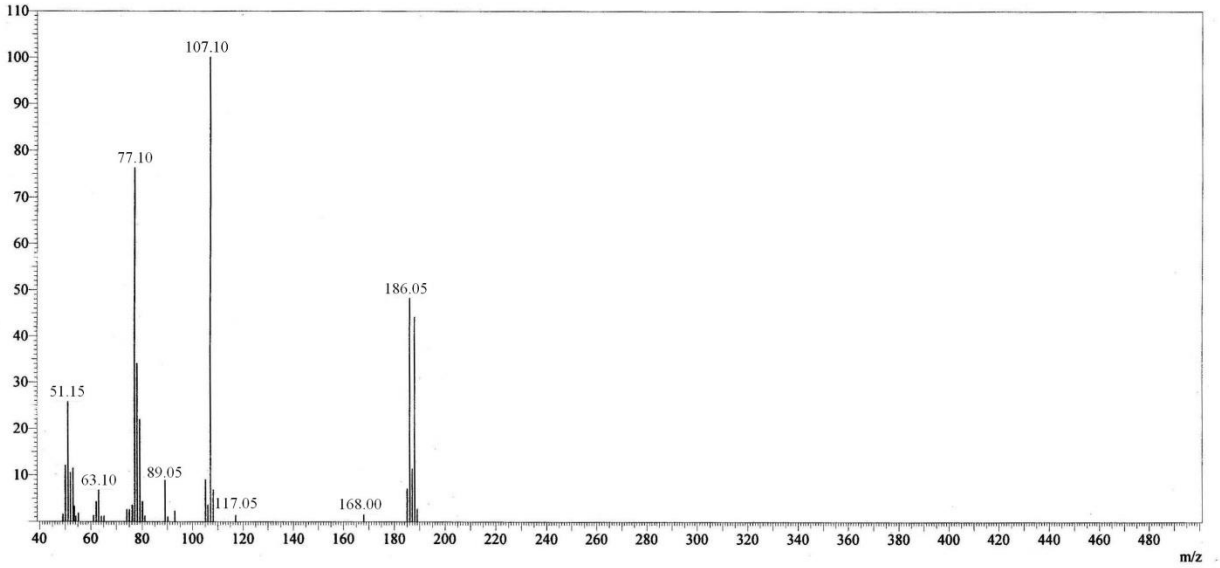

Fig.S9: Mass spectram of 2- bromo ortho-cresol

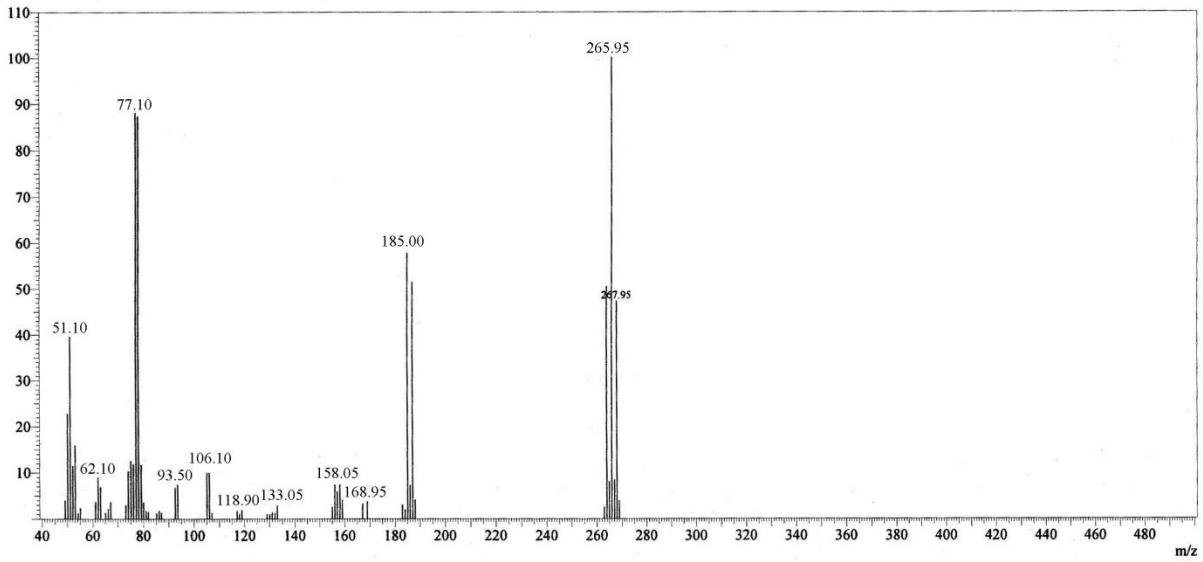

Fig.S10: Mass spectram of 2,4 -dibromo ortho-cresol

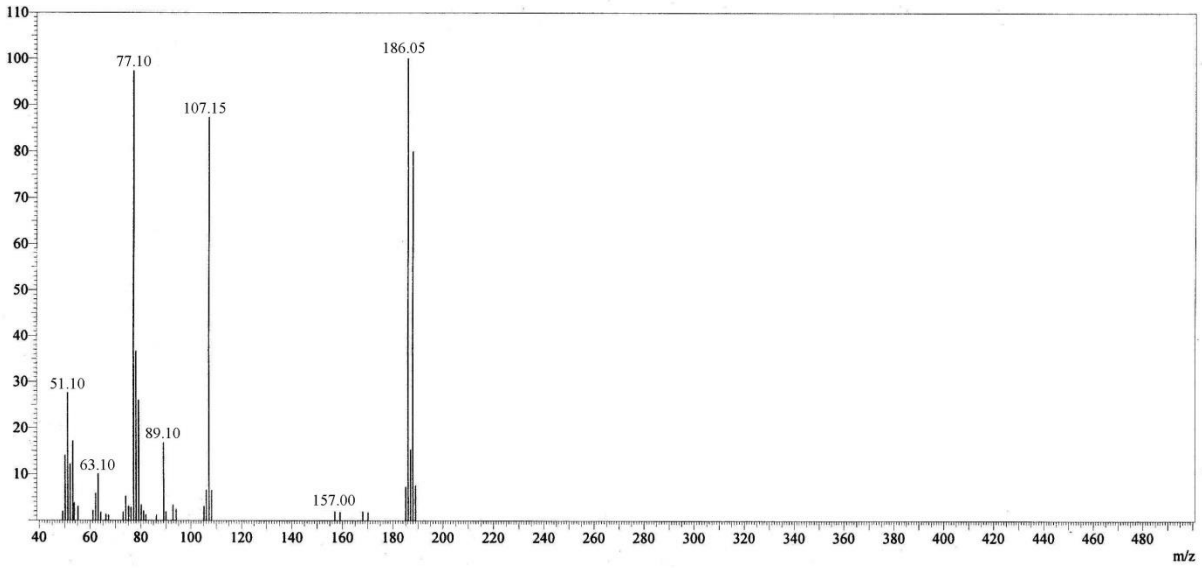

Fig.S11: Mass spectram of 4- bromo ortho-cresol

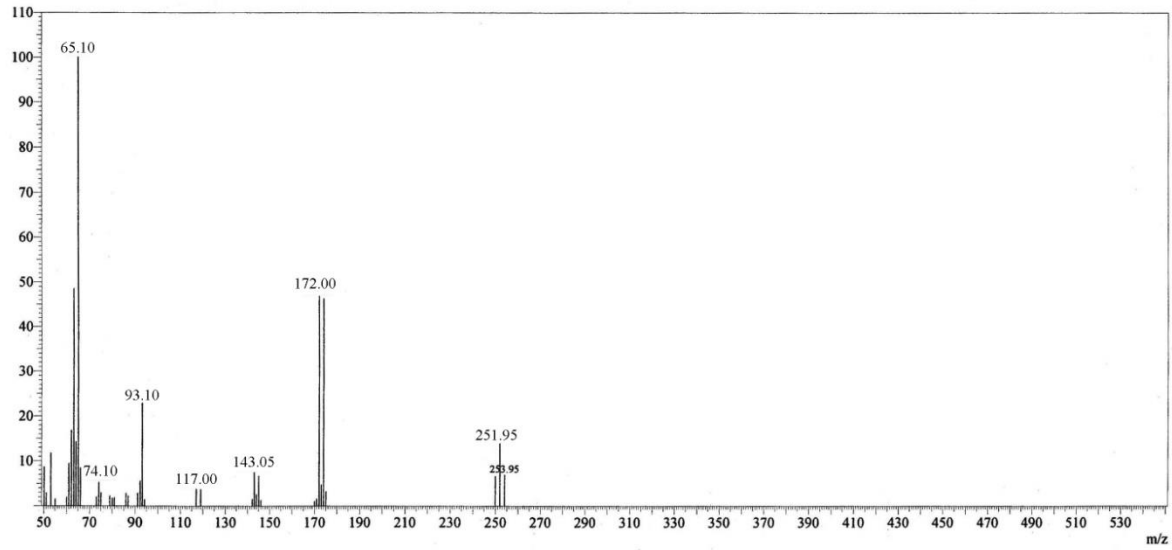

Fig.S12: Mass spectram of 4- bromo phenol

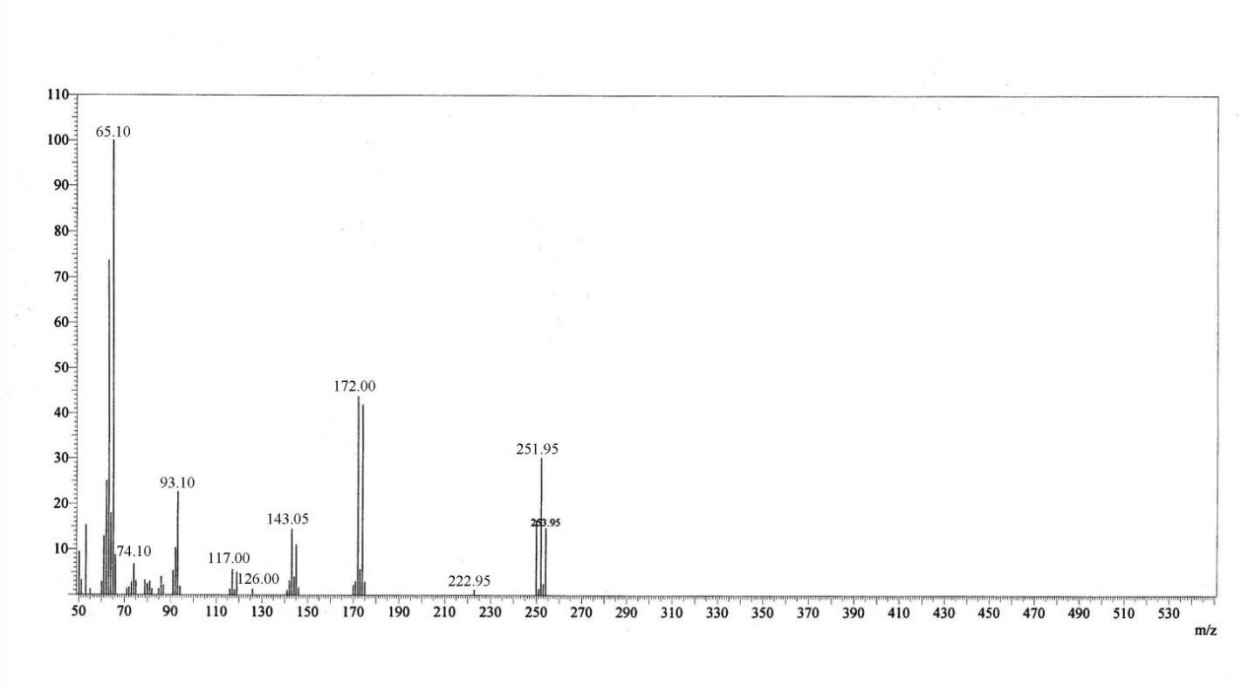

Fig.S13: Mass spectram of 2,4 -dibromophenol

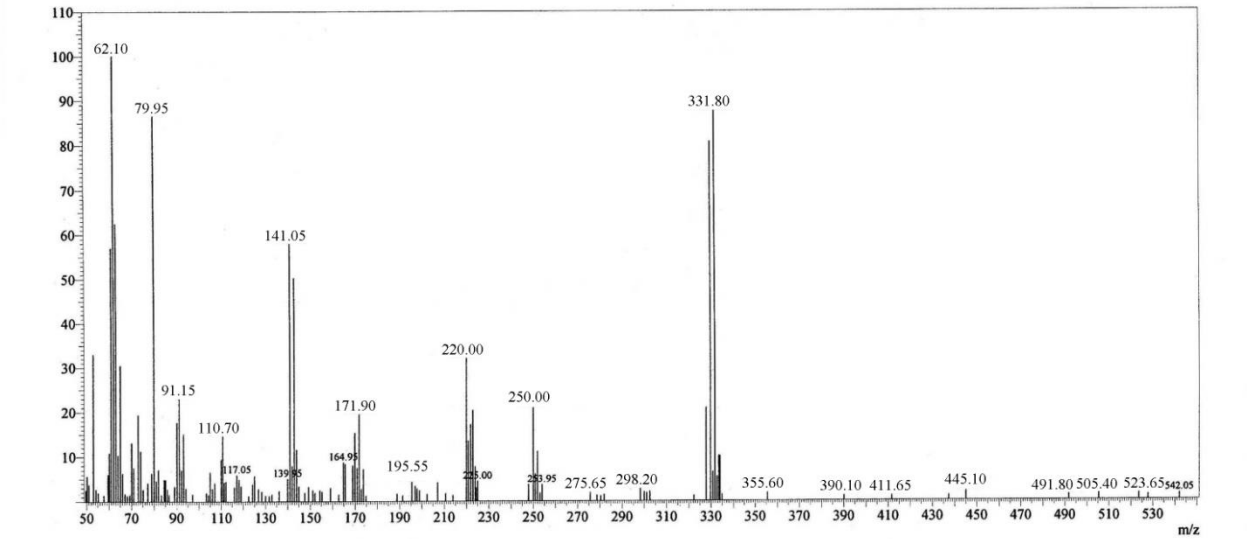

Fig.S14: Mass spectram of 2,4,6-tribromophenol

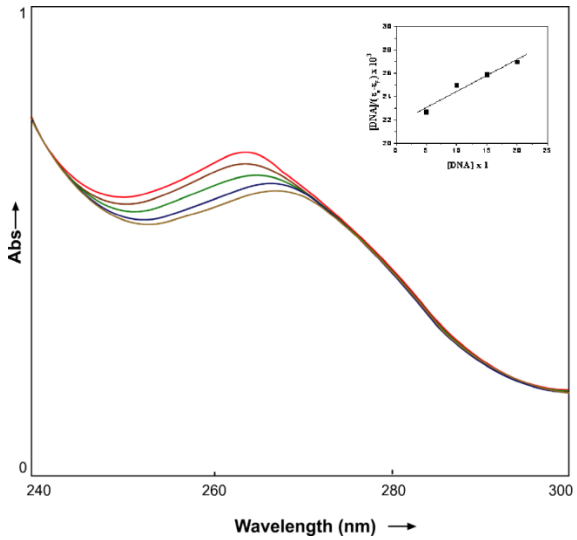

Fig. S15: Absorption spectra of the complex 1 in the presence of increasing amounts of CT DNA. A fixed concentration of complex (10^{-4} M) was treated with increasing amounts of DNA over a range of (0.2–1.0)x10^{-4} M. Inset: plot of [DNA] / ($\varepsilon_a - \varepsilon_f$)×$10^3$ M/M^{-1} cm^{-1} vs. [DNA]×1.0 M.

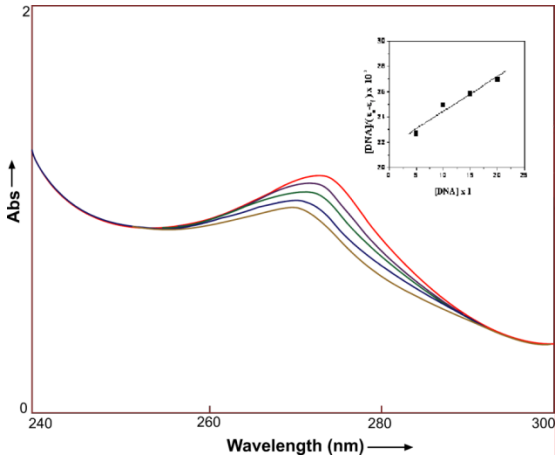

Fig. S16: Absorption spectra of the complex 2 in the presence of increasing amounts of CT DNA. A fixed concentration of complex (10^{-4} M) was treated with increasing amounts of DNA over a range of (0.2–1.0)x10^{-4} M. Inset: plot of [DNA]/($\varepsilon_a - \varepsilon_f$)×$10^3$ M/M^{-1} cm^{-1} vs.[DNA]×1.0 M.

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
N1 -- H1 .. O2$^{(i)}$	0.75(2)	2.10(2)	2.840(2)	170(2)
C3 -- H3 .. O7	0.94(2)	2.48(3)	2.830(2)	102.1(19)
C7 -- H7 .. O2$^{(iv)}$	1.00(2)	2.54(2)	3.473(2)	155.0(17)
C11 - H11 .. O5$^{(ii)}$	0.95(2)	2.57(2)	3.227(3)	126.6(17)

Symmetry Codes: (i) x,1-y,-1/2+z (ii) x,2-y,1/2+z

Table S1: Hydrogen Bonds (Angstrom, Deg) for 1.

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
C3 -- H3 .. O4$^{(iii)}$	0.93(3)	2.51(3)	3.331(3)	148(3)
C11 -- H11.. O2$^{(iv)}$	0.93(3)	2.53(2)	3.329(3)	144(19)
C18 -- H18 .. O5$^{(v)}$	0.93(3)	2.39(3)	3.316(3)	172(2)

Symmetry Codes: (iii) 3/2-x,1/2+y,1/2-z (iv) x,-1+y,z (v) -x,2-y,-z

Table S2: Hydrogen Bonds (Angstrom, Deg) for 2.

[VO(PyDC)(BHA)] (**1**)		[VO(PyDC)(BPHA)] (**2**)	
Bond Distances:			
V(1) – O(6)	1.8497(12)	V(1) – O(6)	1.8634(13)
V(1) - O(3)	1.9411(14)	V(1) – O(3)	1.9320(14)
V(1) - O(4)	1.9693(14)	V(1) – O(4)	1.9557(14)
Bond Angles:			
O(1) – V(1) – O(3)	98.48(7)	O(1) - V(1) - O(3)	99.19(8)
O(3) – V(1) – O(6)	103.49(6)	O(3) - V(1) - O(6)	93.33(6)
O(3) – V(1) – O(4)	149.99(6)	O(3) - V(1) - O(4)	150.86(7)
O(3) – V(1) – N(2)	75.96(6)	O(3) - V(1) - N(2)	75.71(6)
O(3) – V(1) – O(7)	85.27(6)	O(3) - V(1) - O(7)	91.00(6)
O(4) – V(1) – O(6)	101.07(6)	O(4) - V(1) - O(6)	111.57(6)
O(4) – V(1) – N(2)	75.47(5)	O(4) - V(1) - N(2)	75.59(7)
O(4) – V(1) – O(7)	84.34(5)	O(4) - V(1) - O(7)	81.34(6)
O(6) – V(1) – O(7)	75.68(5)	O(6) - V(1) - O(7)	75.48(6)
O(6) – V(1) – N(2)	162.76(6)	O(6) - V(1) - N(2)	156.99(7)
O(7) – V(1) – N(2)	87.13(5)	O(7) - V(1) - N(2)	84.41(6)

Table S3: Bond Distances (Å) and Bond Angles (^{O}) of Complex 1 and 2.