

## **Selective oxidative upgrade of waste polystyrene plastics by nitric acid to produce benzoic acid**

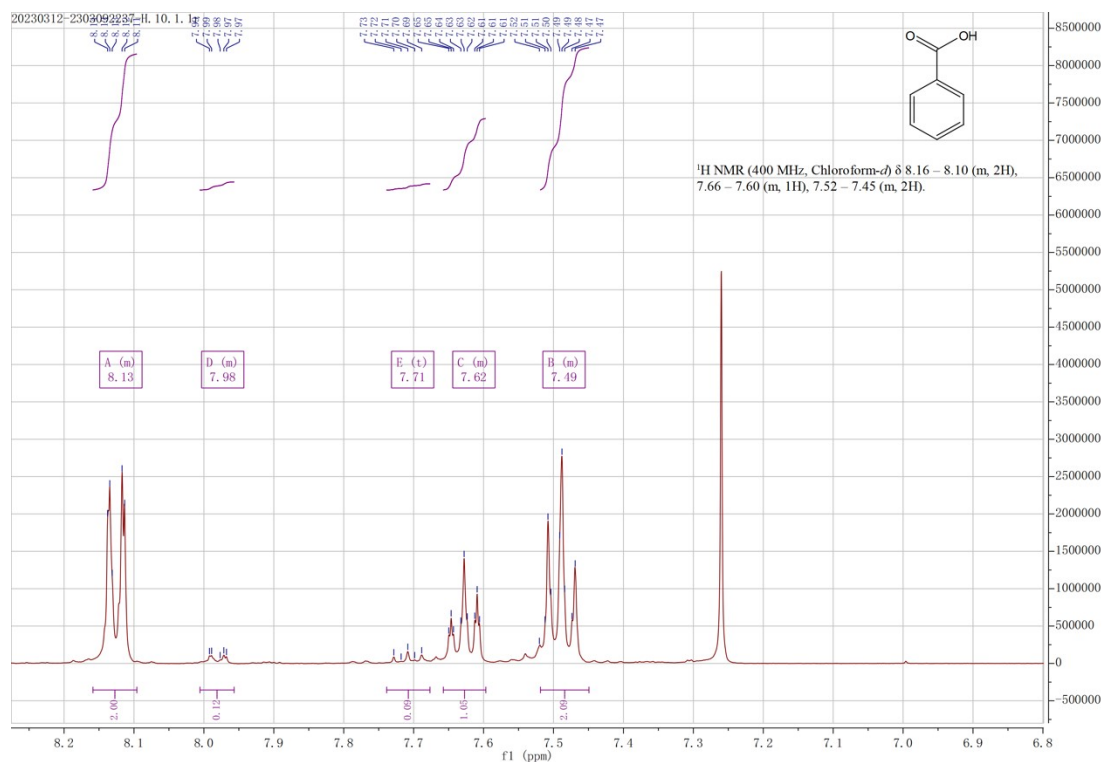
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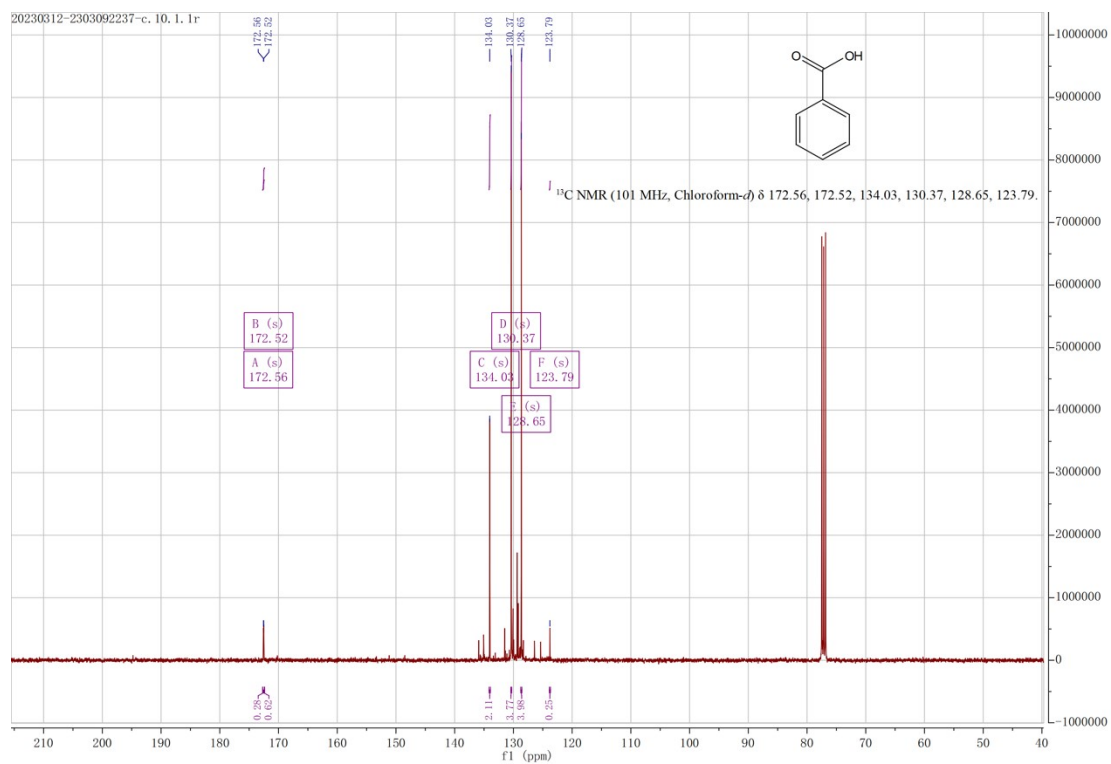
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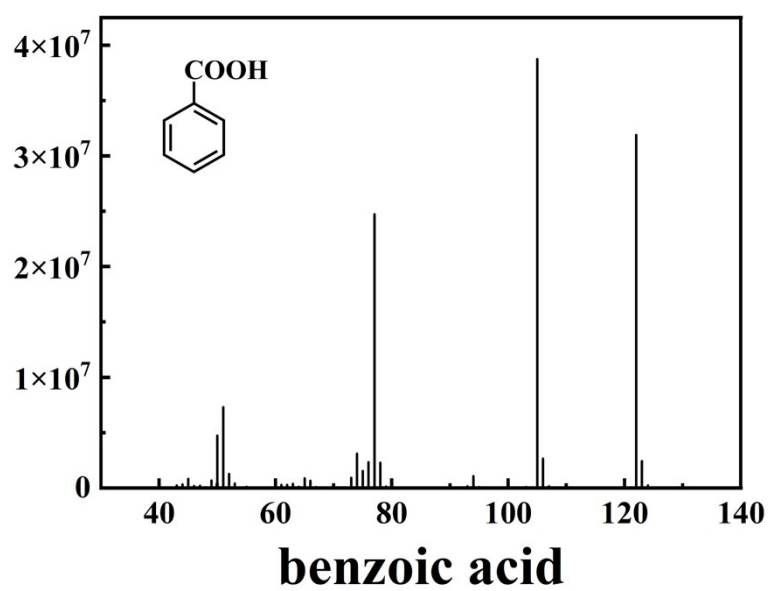
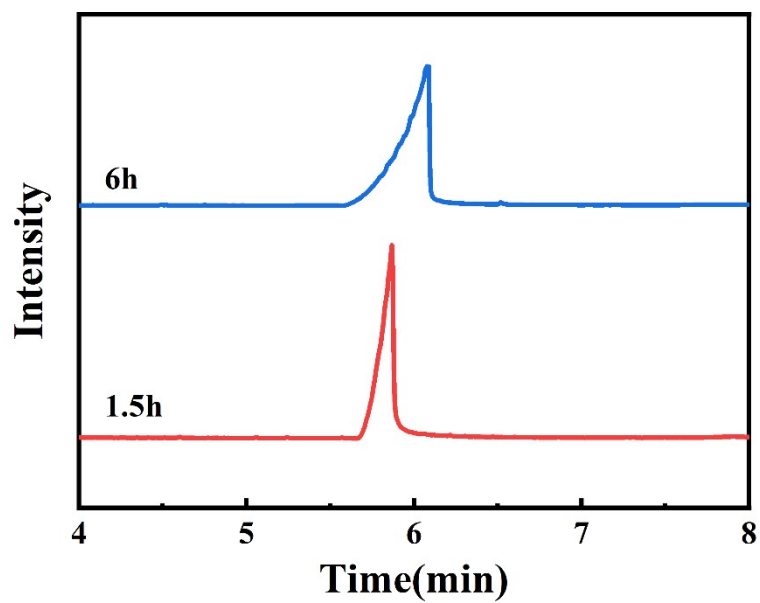
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**Fig. S1** <sup>1</sup>H-NMR spectra of the product (1g PS, 10ml 20% HNO<sub>3</sub>, 180 °C, 3 h).



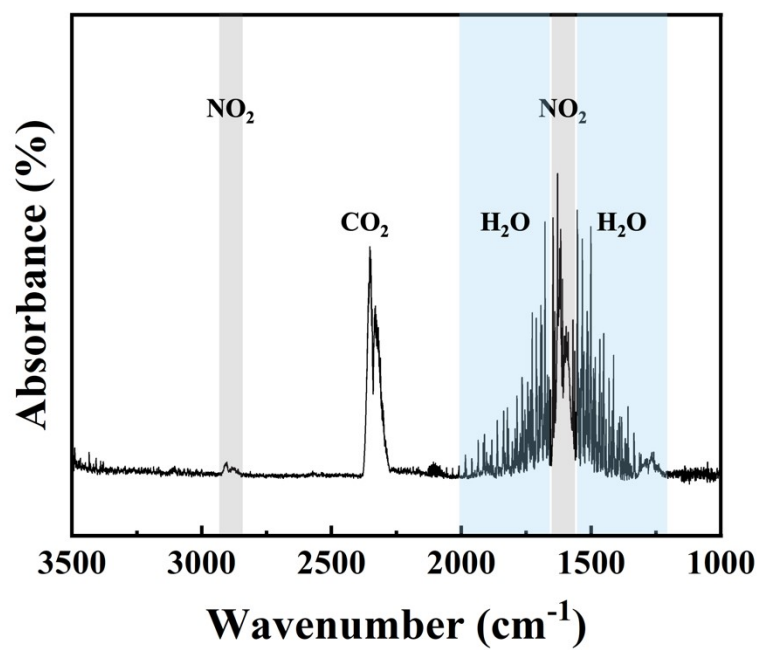
**Fig. S2**  $^{13}\text{C}$ -NMR spectra of the product (1g PS, 10ml 20%  $\text{HNO}_3$ , 180  $^\circ\text{C}$ , 3 h).



**Fig. S3** GC-MS spectra of pure benzoic acid oxidation process (1g benzoic acid, 10ml 20% HNO<sub>3</sub>, 180 °C).



**Fig. S4** Reddish brown gas generated after the reaction.



**Fig. S5** FTIR spectra of the gas collected after the reaction (CO<sub>2</sub> and H<sub>2</sub>O are impurity peaks generated during the detection process).

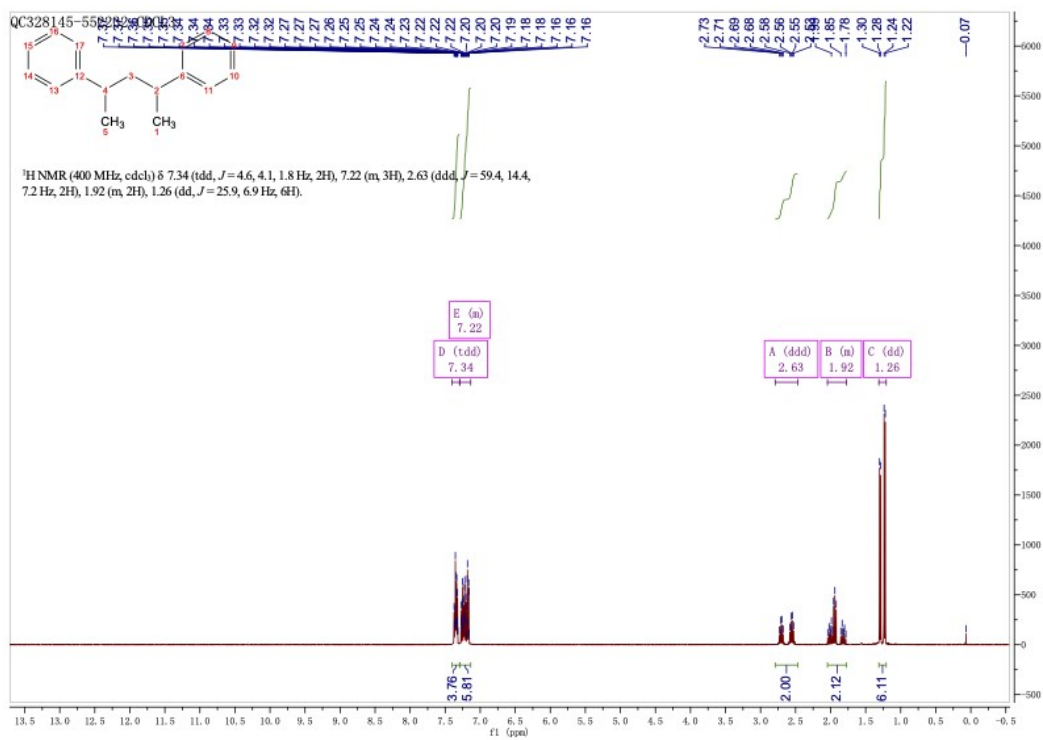
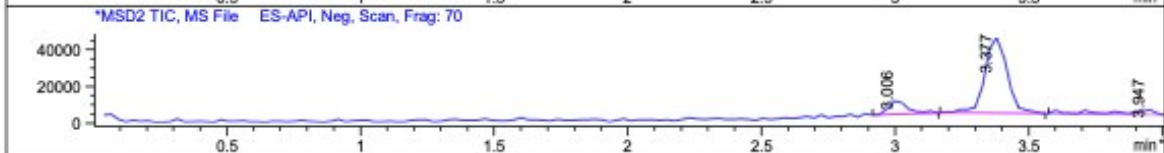
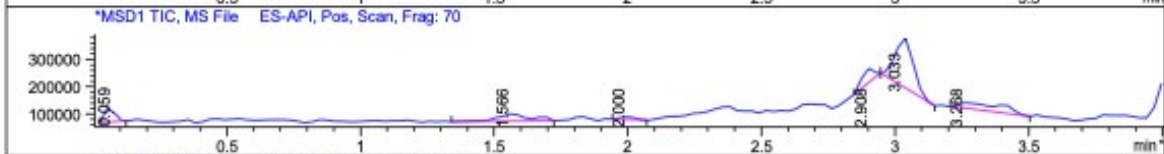
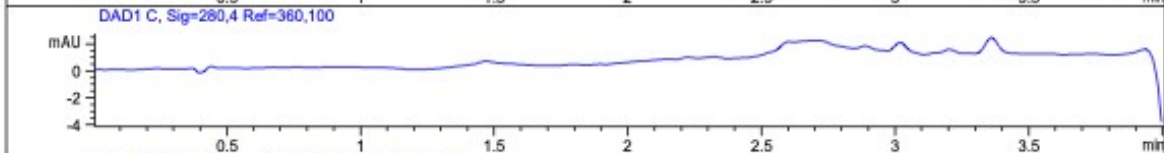
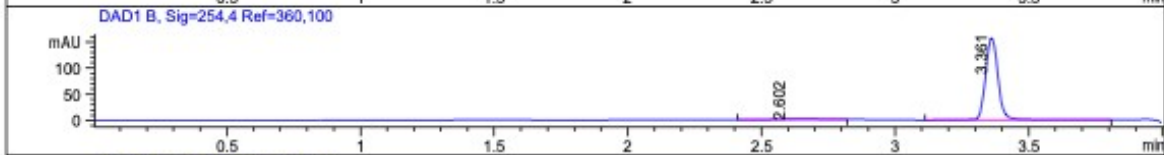
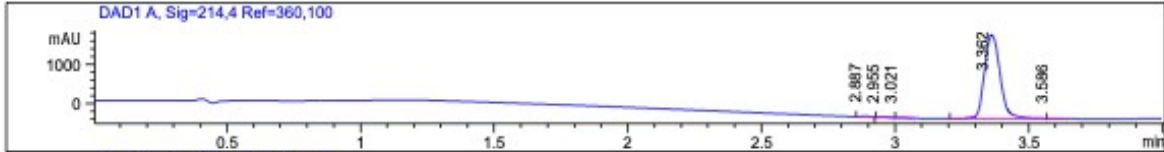


Fig. S6 <sup>1</sup>H-NMR spectra of 2,4-Diphenylpentane.

MS Report from Instrument: LCMS

File ..\02 2023-03-03 09-21-10\OnlineEdited--018.D Tgt Mass (EZ):  
 Injection Date : 3 Mar 23 10:50 am +0800 Seq. Line : 18  
 Sample Name : 20230303-QC396232-661927 Location : 17  
 Acq. Operator : SYSTEM Inj : 1  
 Spec. Reported : MS Integration Inj Volume : 1 ul  
 Acq. Method : D:\Chem32\1\Data\MAFANGYA\02 2023-03-03 09-21-10\20171123--FA02-M.M  
 Analysis Method : D:\Chem32\1\Data\MAFANGYA\02 2023-03-03 09-21-10\20171123--FA02-M.M  
 Sample Info :  
 Method Info :



Integration Results for DAD1 A, Sig=214,4 Ref=360,100

RetTim	Width	Area	Height	Area%	MS (+)	MS (-)
2.89	0.04	32.20	14.23	0.37	247	299
2.96	0.04	22.35	10.05	0.25	247	113
3.02	0.04	20.14	8.11	0.23	301	113
3.36	0.07	8706.95	2154.93	99.06	319	339
3.59	0.05	7.65	2.61	0.09	319	113

Integration Results for DAD1 B, Sig=254,4 Ref=360,100

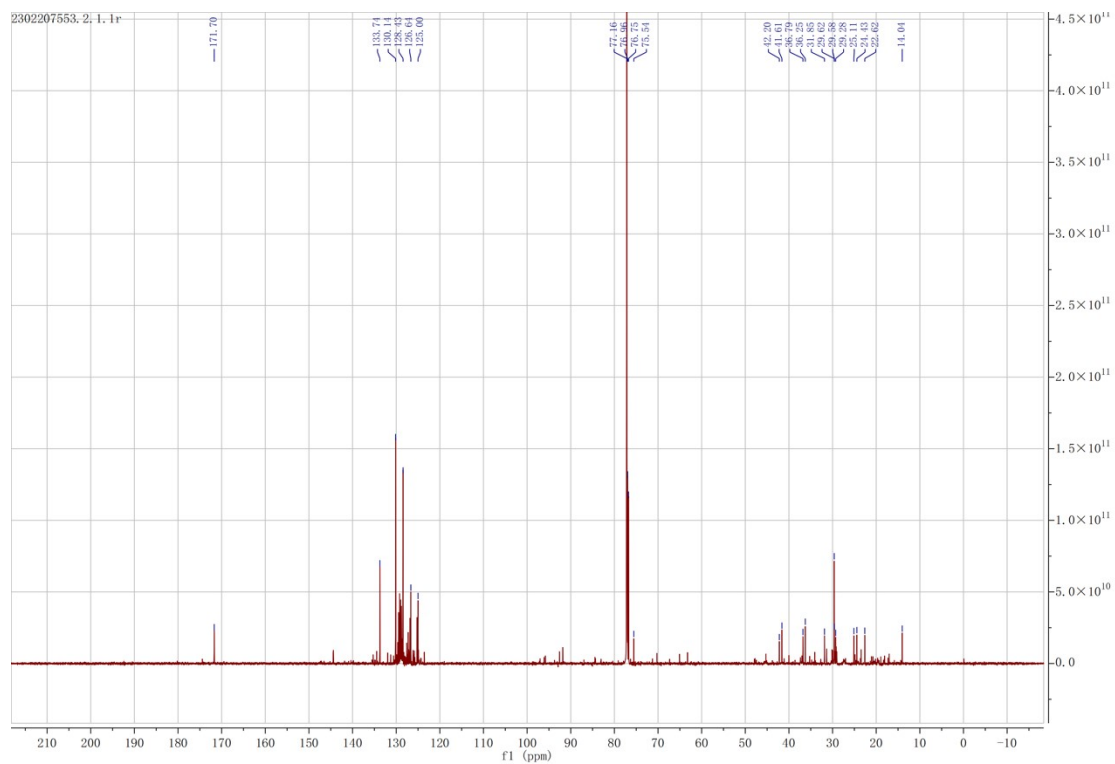
RetTim	Width	Area	Height	Area%	MS (+)	MS (-)
2.60	0.13	15.52	1.50	2.92	117	ND
3.36	0.05	516.65	157.71	97.08	319	113

Integration Results for DAD1 C, Sig=280,4 Ref=360,100

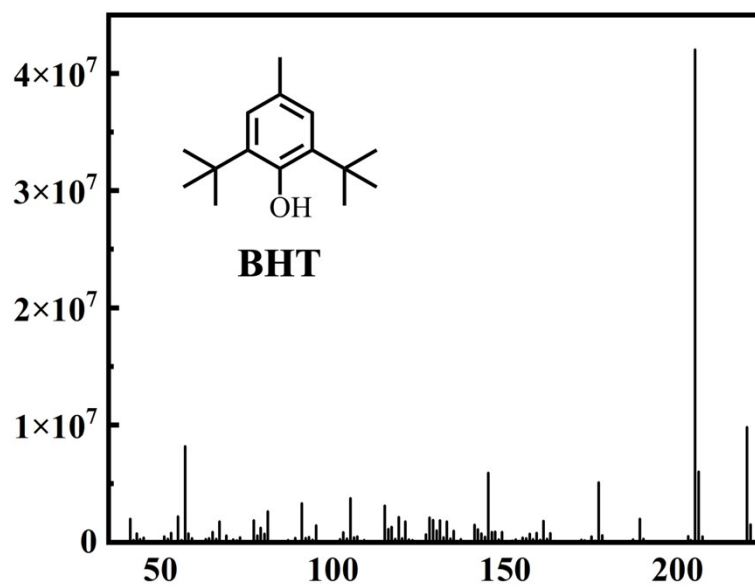
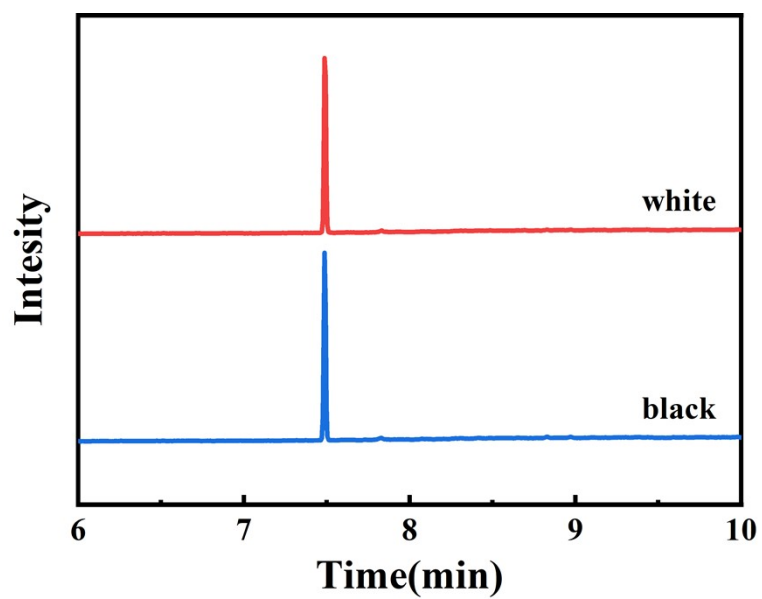
RetTim	Width	Area	Height	Area%	MS (+)	MS (-)

Fig. S7 LC-MS report of 2,4-Diphenylpentane.





**Fig. S8** <sup>13</sup>C-NMR spectra of oxidative upgrade of 2,4-Diphenylpentane (0.1g 2,4-Diphenylpentane, 3ml 20% HNO<sub>3</sub>, 180 °C, 10 min).



**Fig. S9** GC/MS spectra of the solid residue generated after oxidative upgrade of the cup lids.