

## Supplementary Materials

### Fragmentation pathway of organophosphorus flame retardants by liquid chromatography-orbitrap based high resolution mass spectrometry

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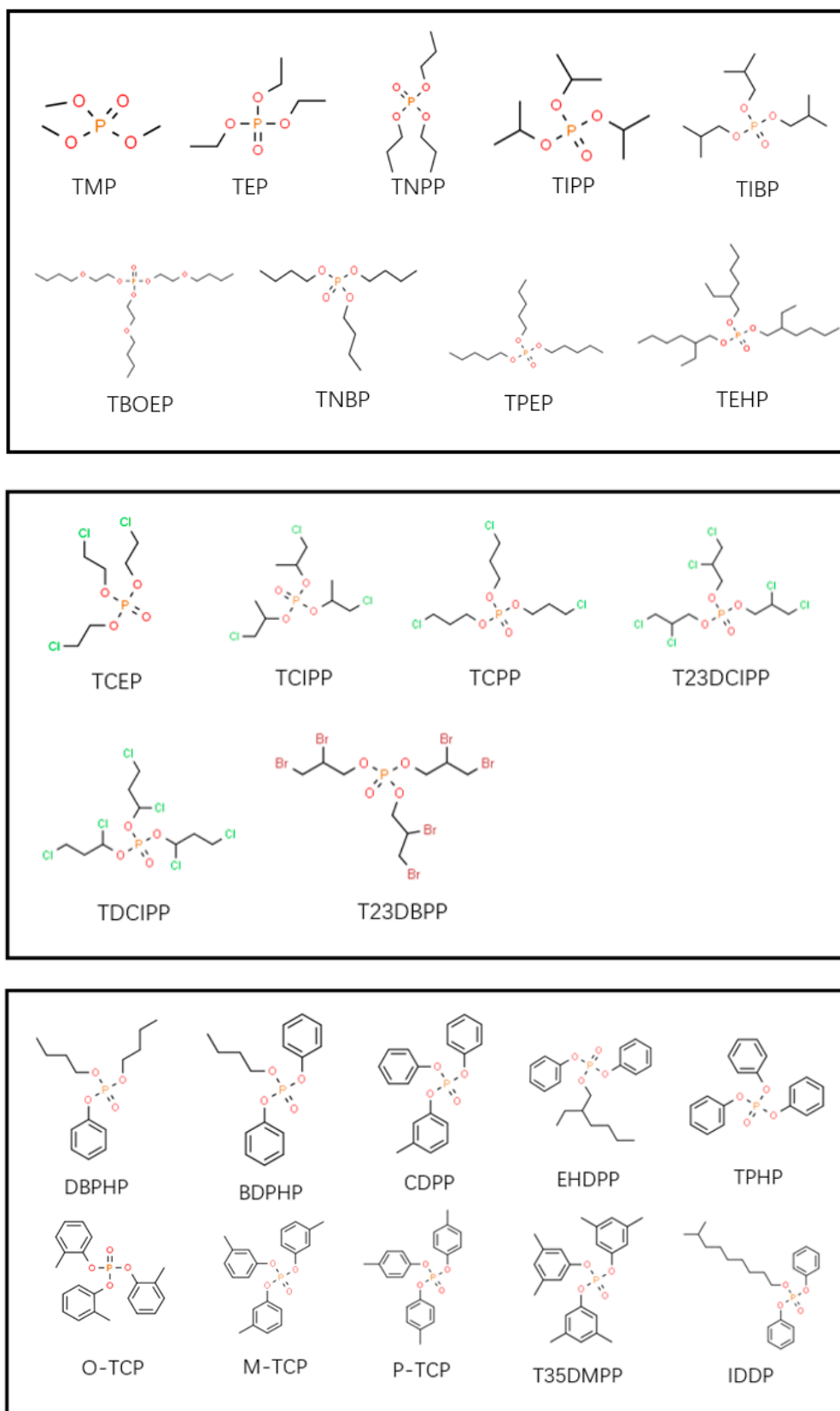
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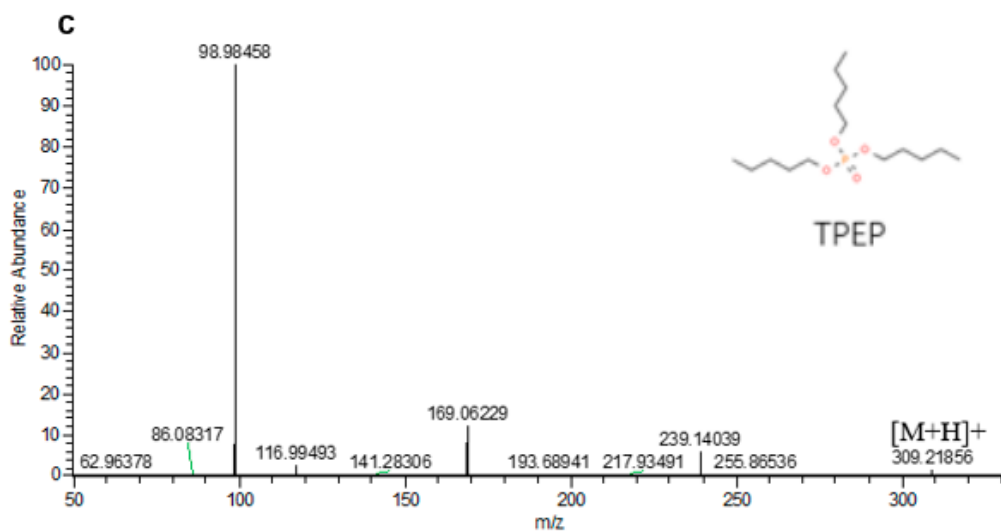
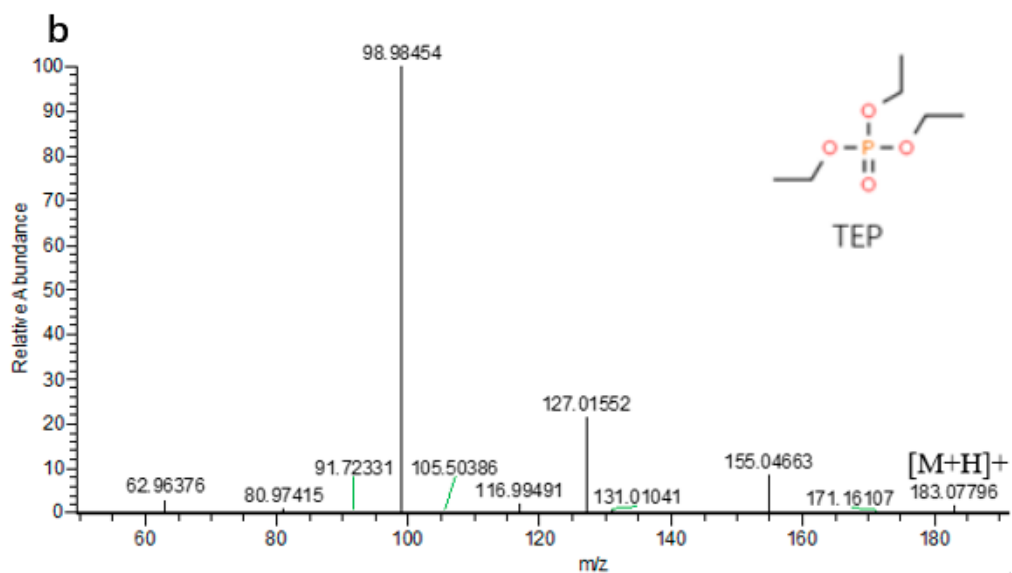
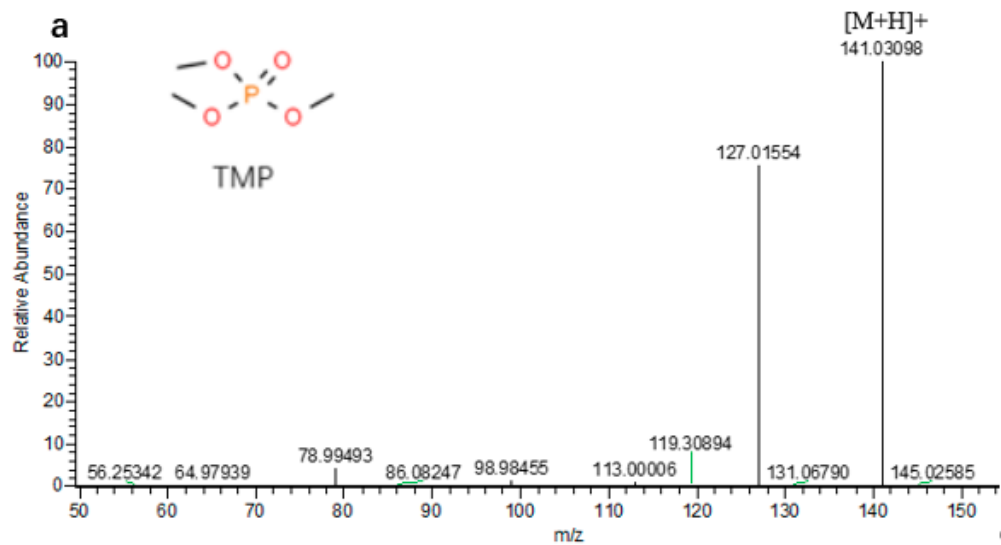
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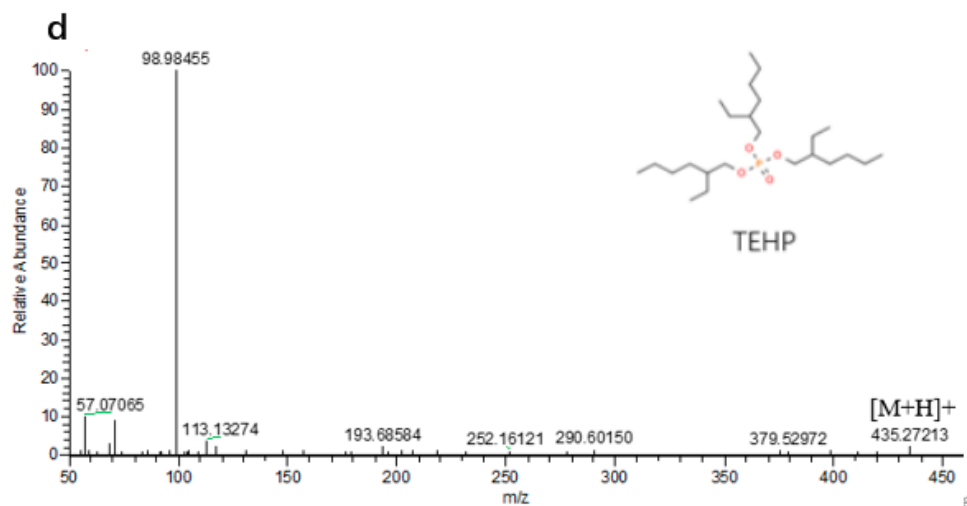
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Figure S1. The structure of 25 OPFRs; Figure (S2-S4). MS<sup>2</sup> spectrums of OPFRs under ESI source; Figure S5. MS<sup>1</sup> spectrums of TDCIPP and T23DBPP; Text S1. Instrument parameter details under EI source; Figure S6. MS<sup>2</sup> spectrums of OPFRs under EI source



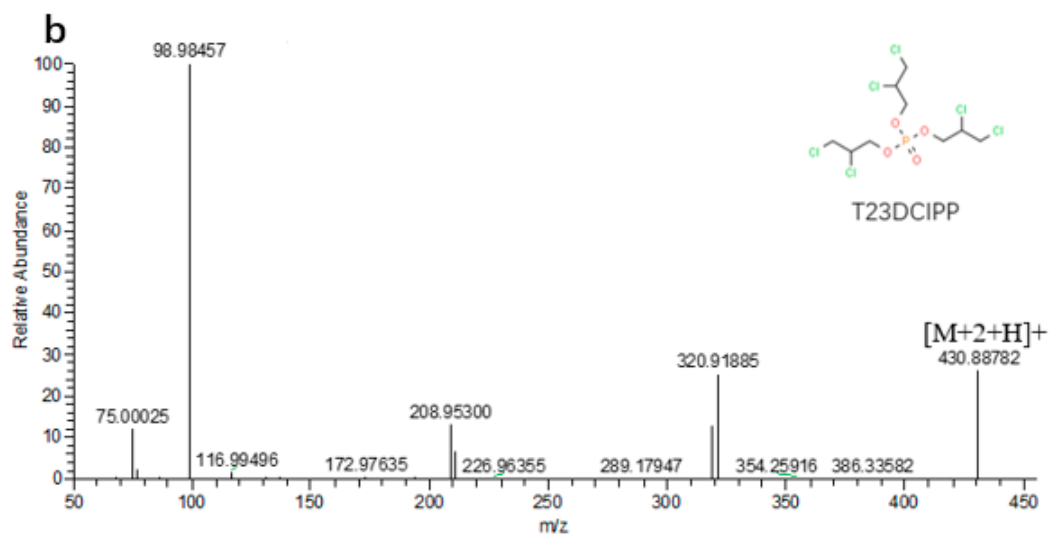
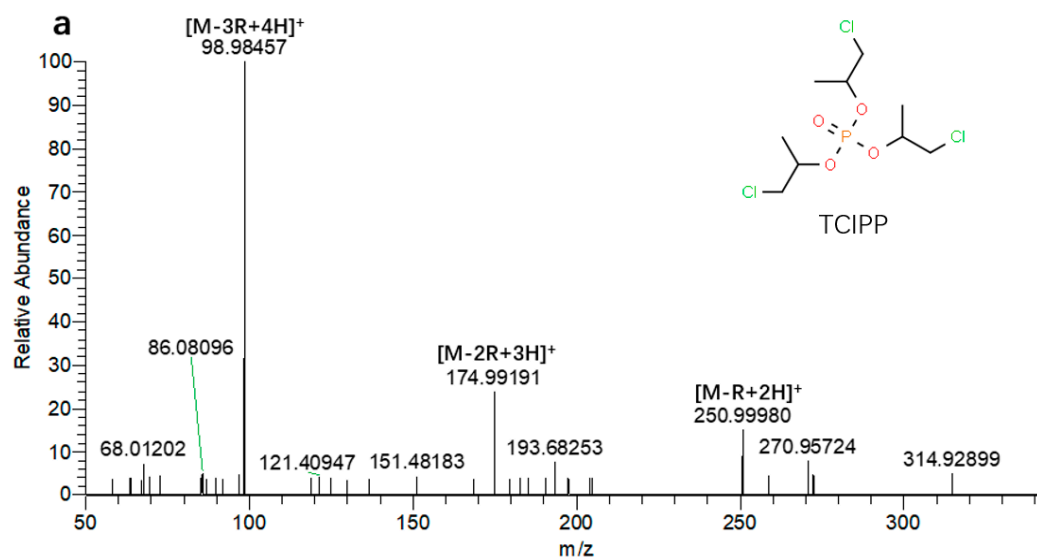
**Figure S1.** The structure of 25 OPFRs

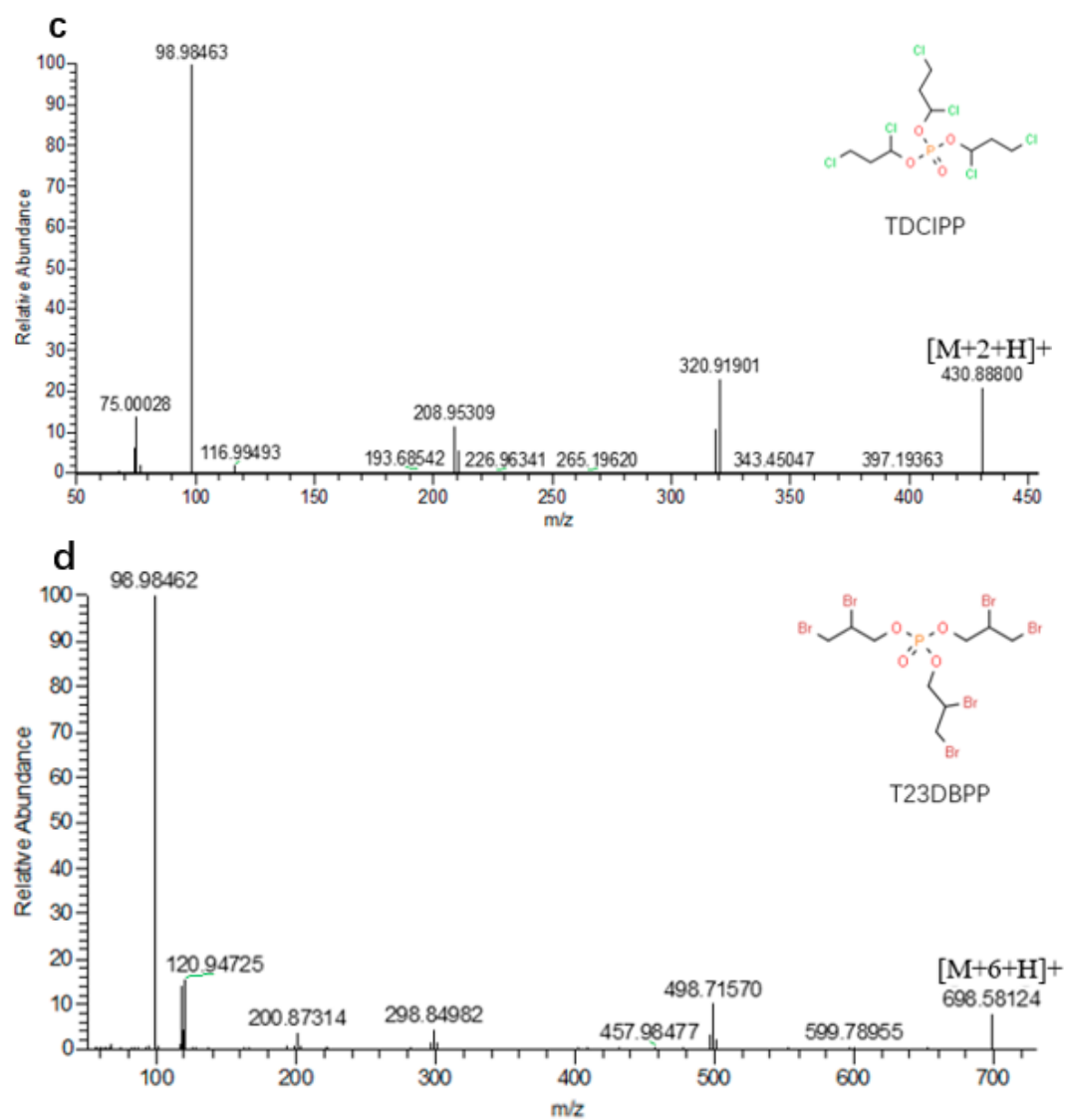




**Figure S2.** MS<sup>2</sup> spectrums of 4 alkyl OPFRs under ESI source

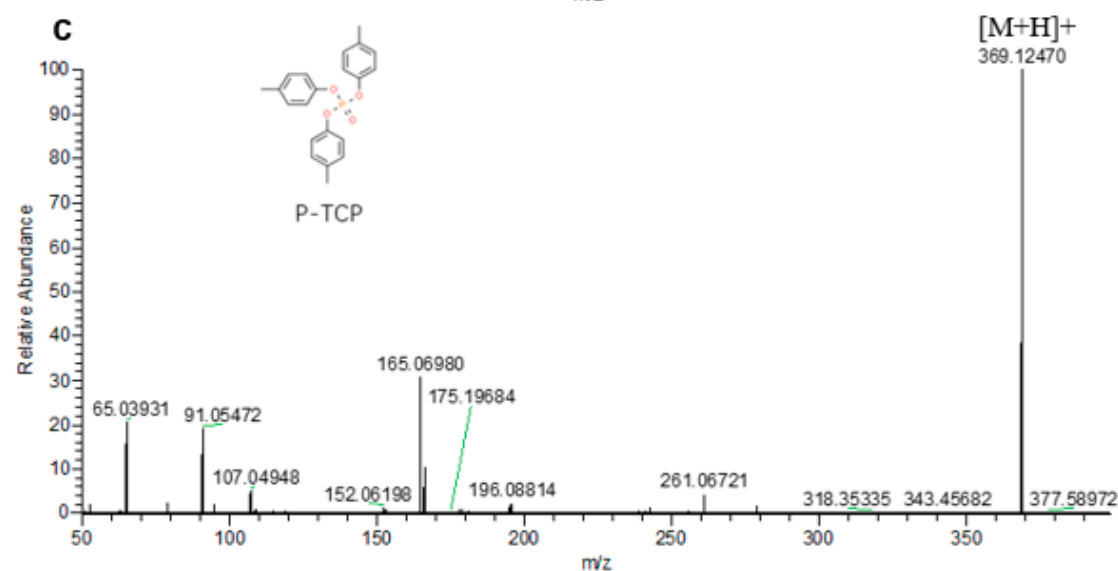
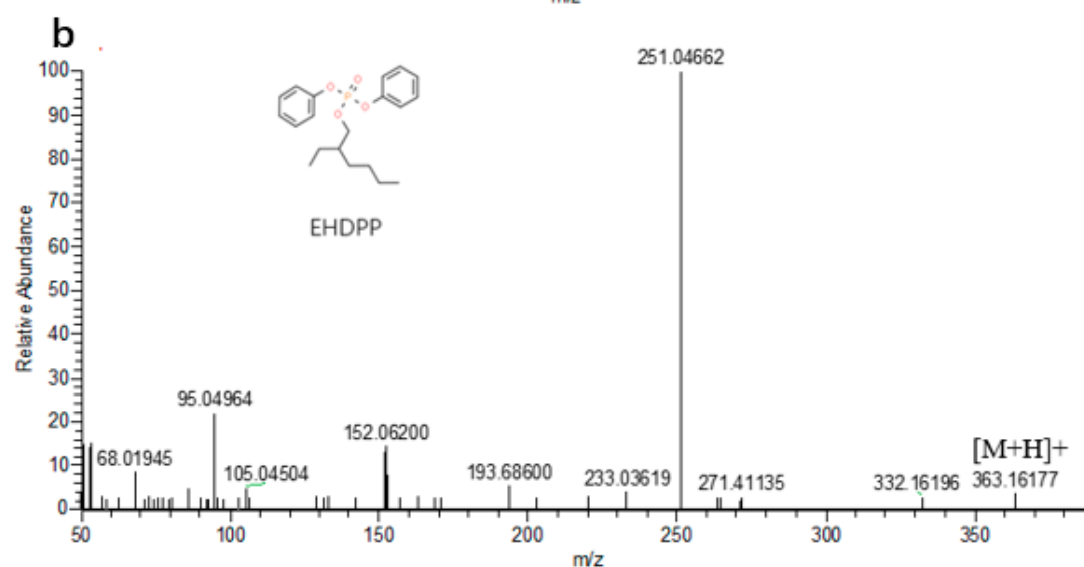
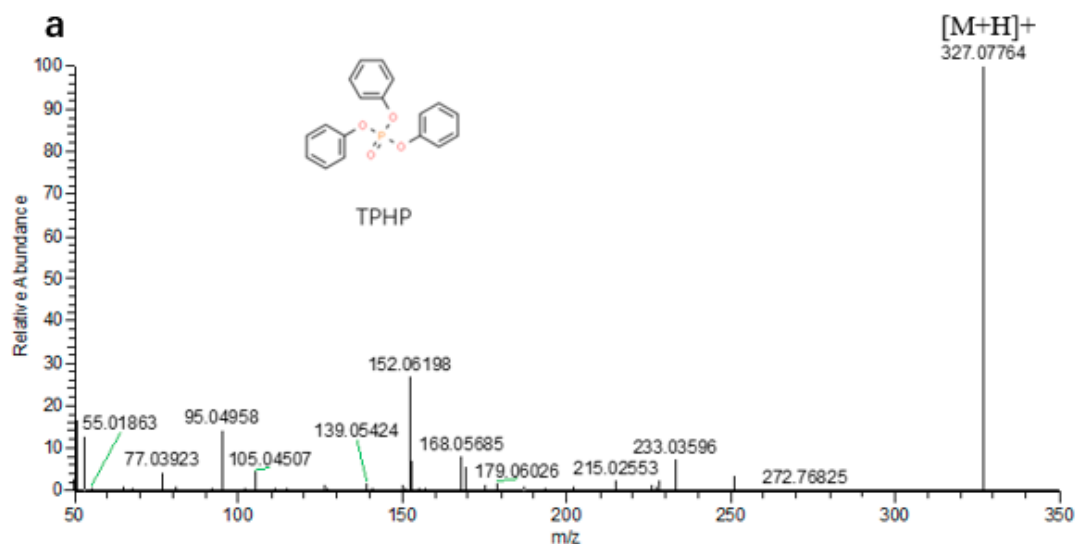
a. TMP; b. TEP; c. TPEP; d. TEHP.

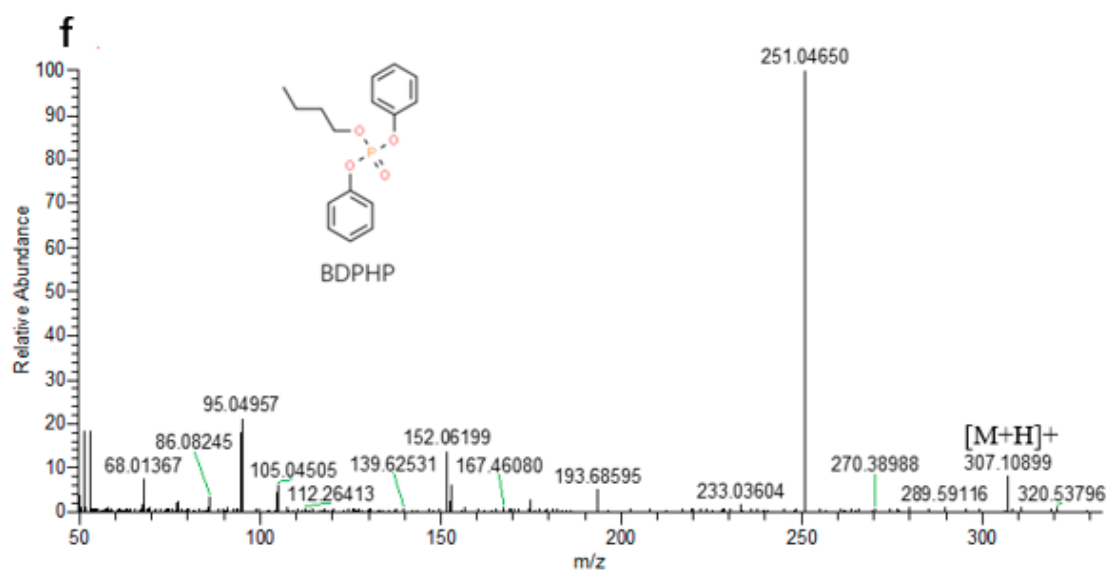
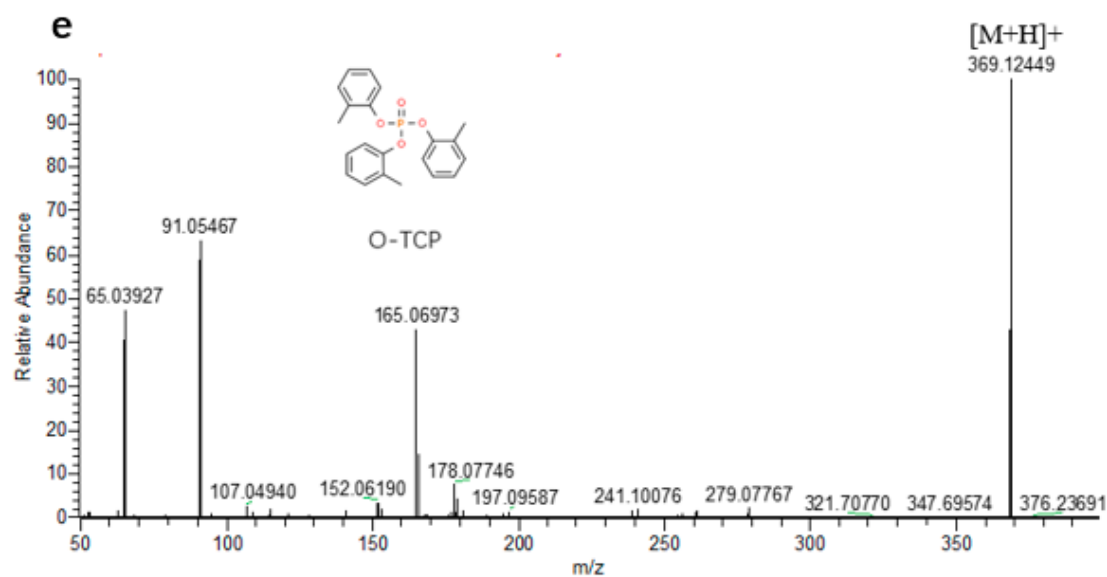
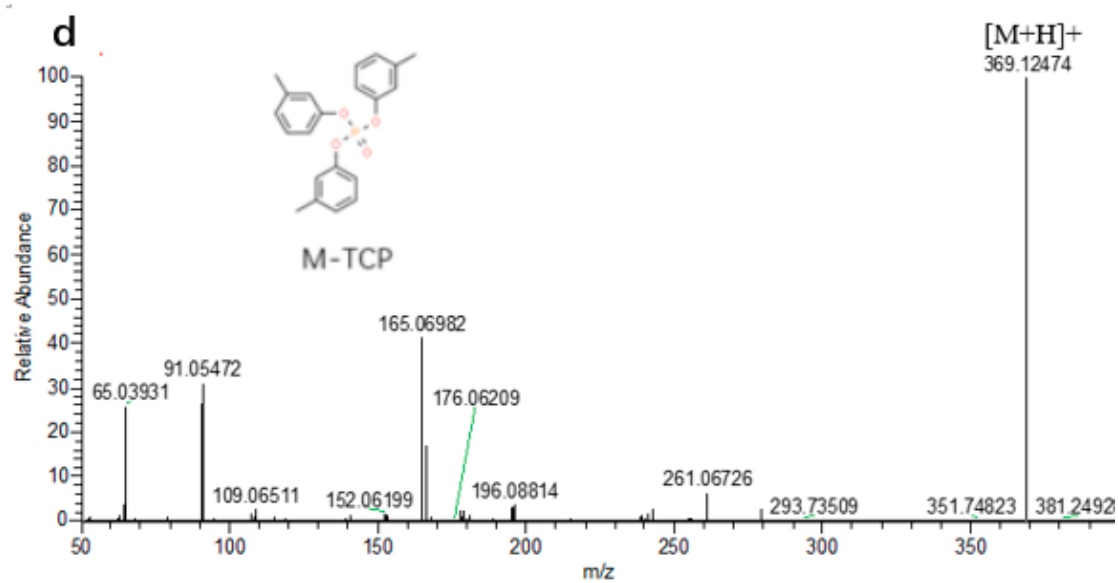


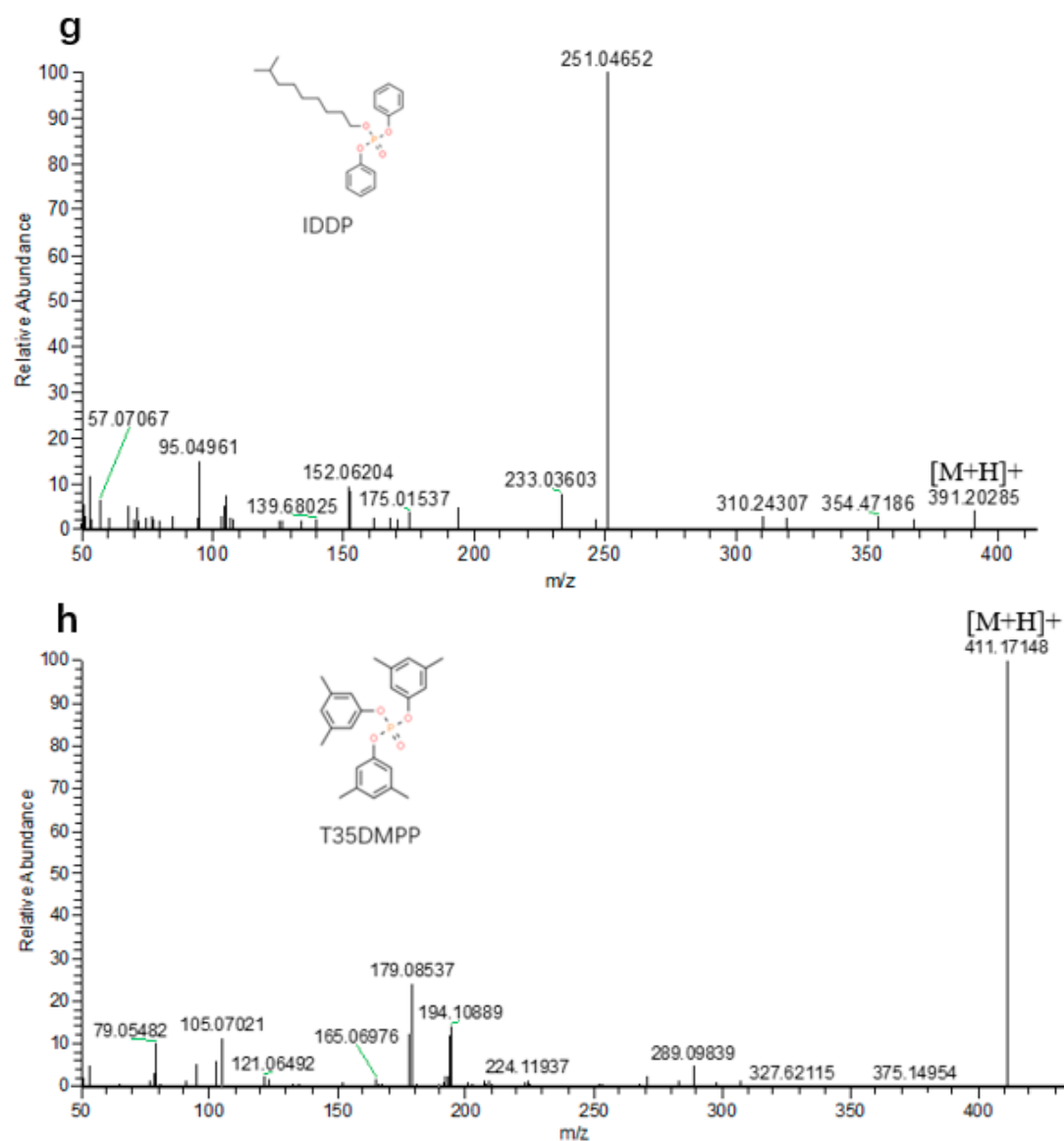


**Figure S3.** MS<sup>2</sup> spectrums of 4 halogenated OPFRs under ESI source

a. TCIPP; b. T23DCIPP; c. TDCIPP; d. T23DBPP.

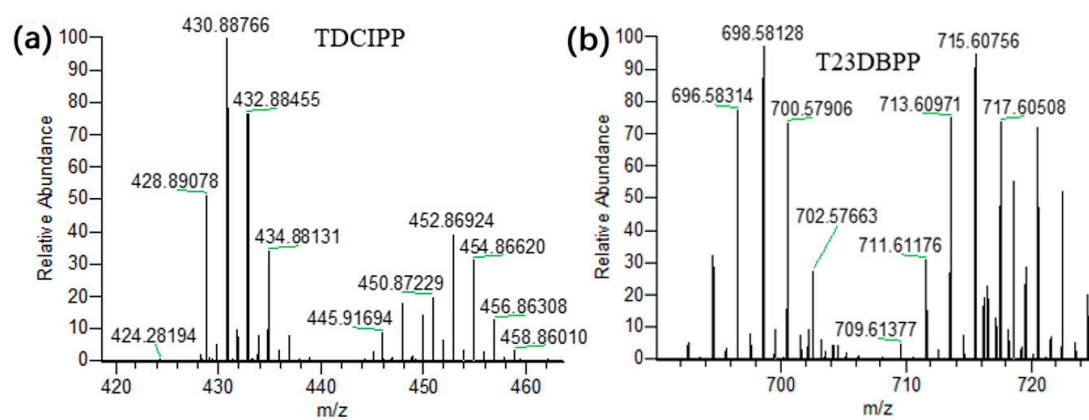






**Figure S4.** MS<sup>2</sup> spectra of 8 aromatic OPFRs under ESI source

a. TPHP; b. EHDPP; c. P-TCP; d. M-TCP; e. O-TCP; f. BDPHP; g. IDDP; h. T35DMPP.



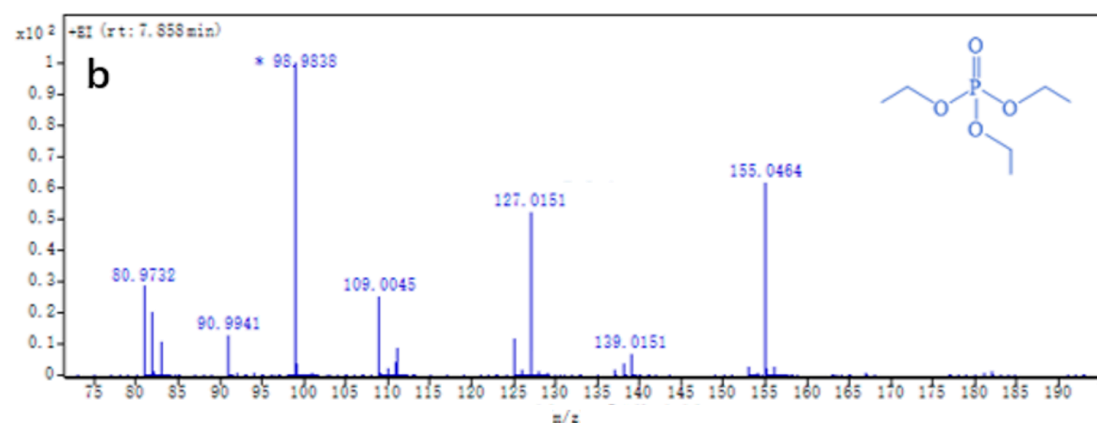
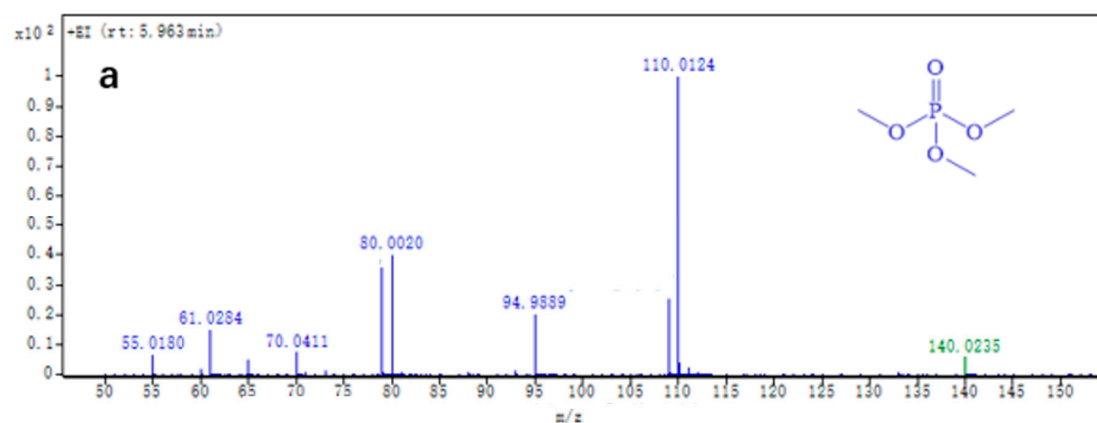
**Figure S5.** MS<sup>1</sup> spectra of TDCIPP and T23DBPP

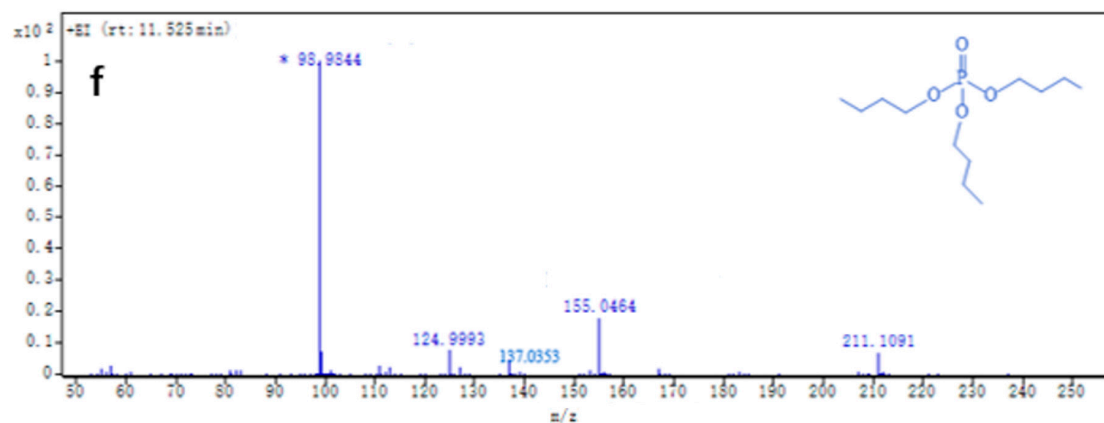
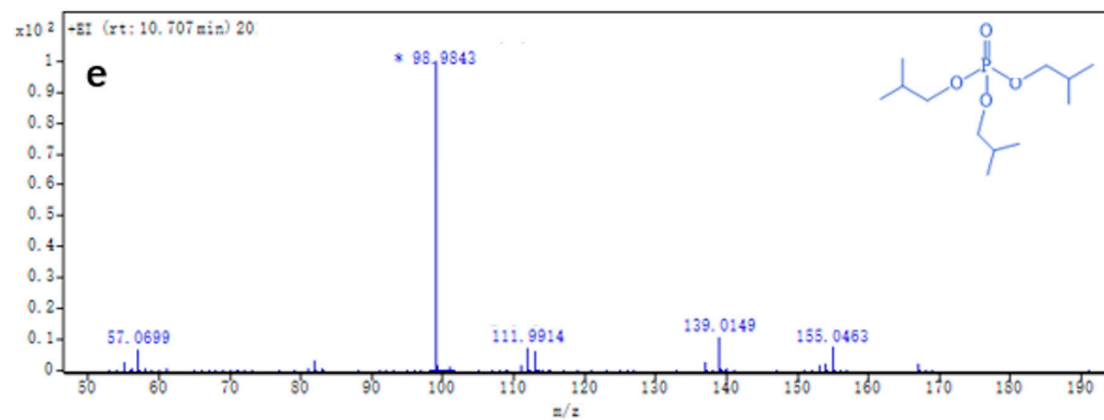
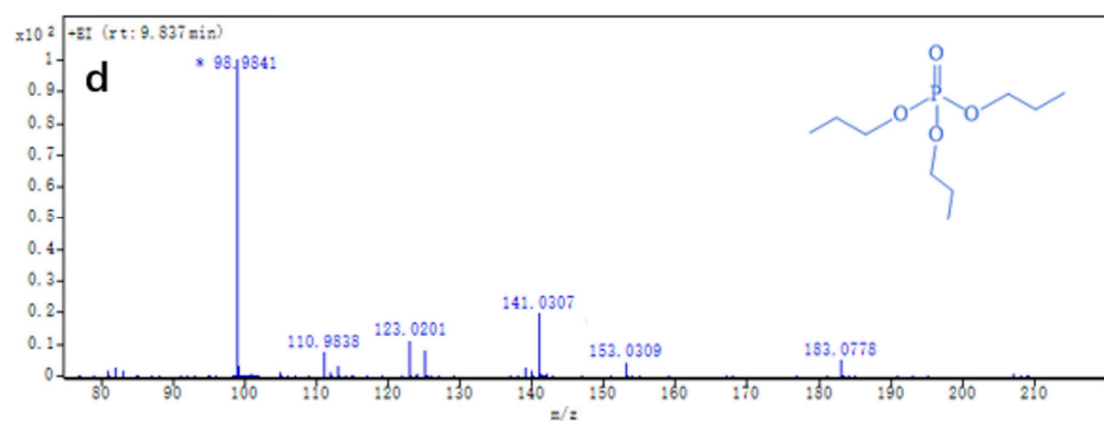
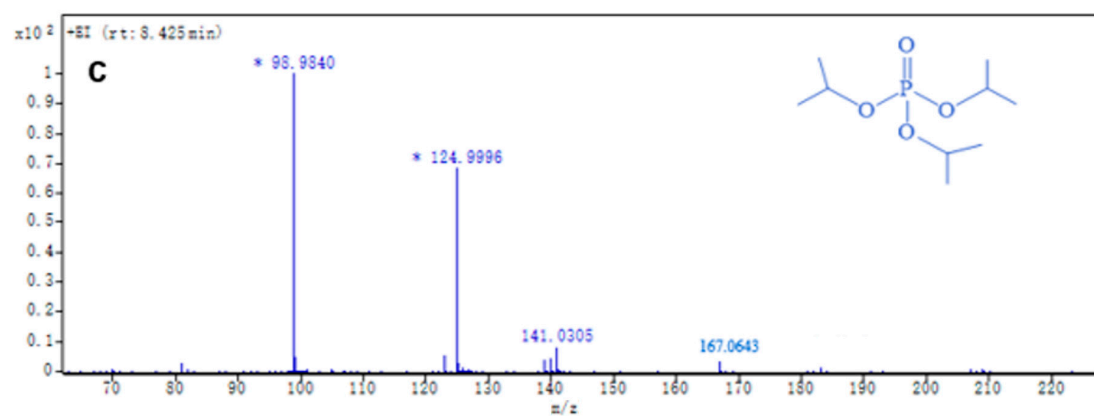
a. TDCIPP; b. T23DBPP

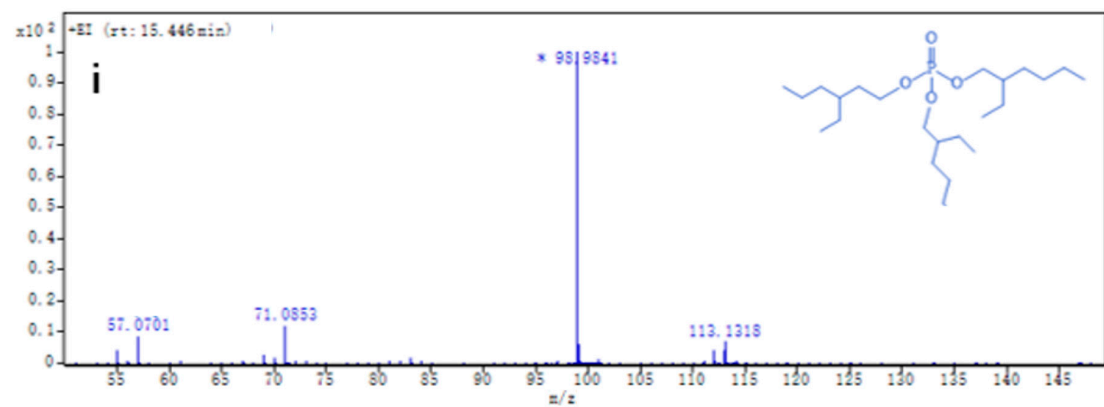
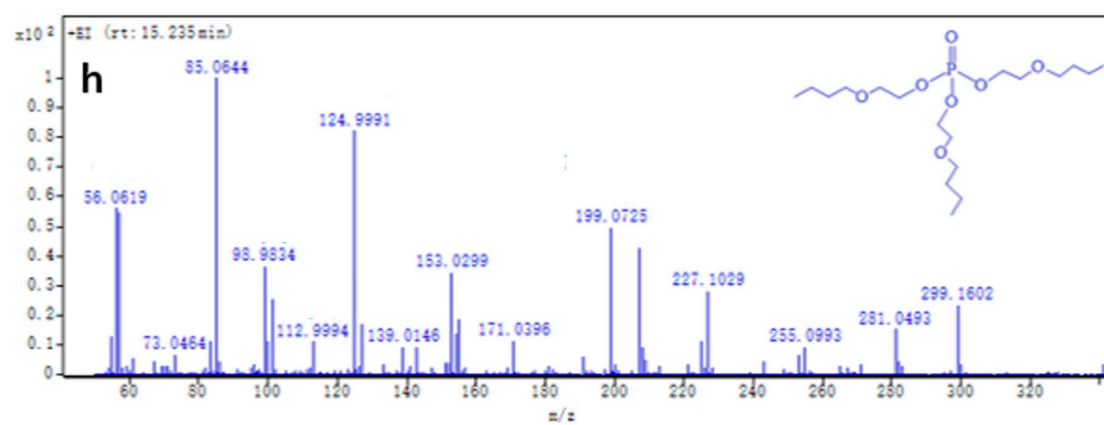
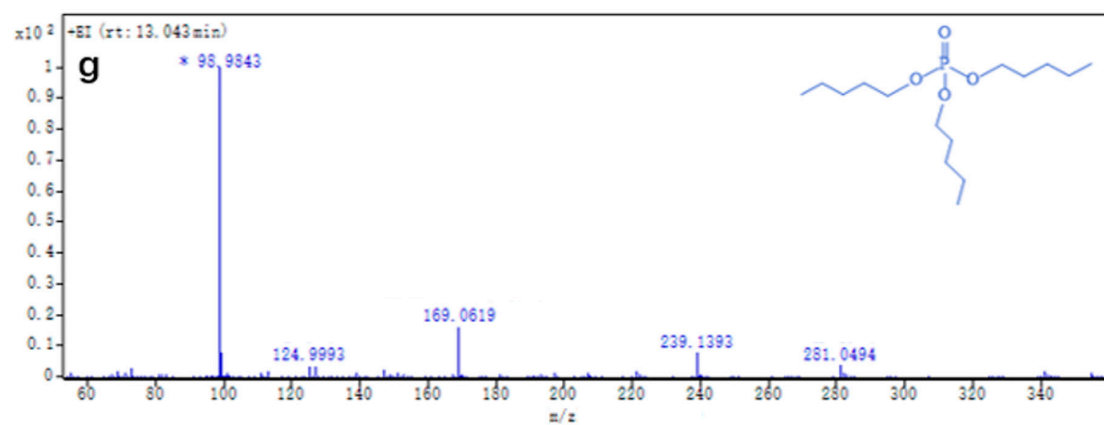


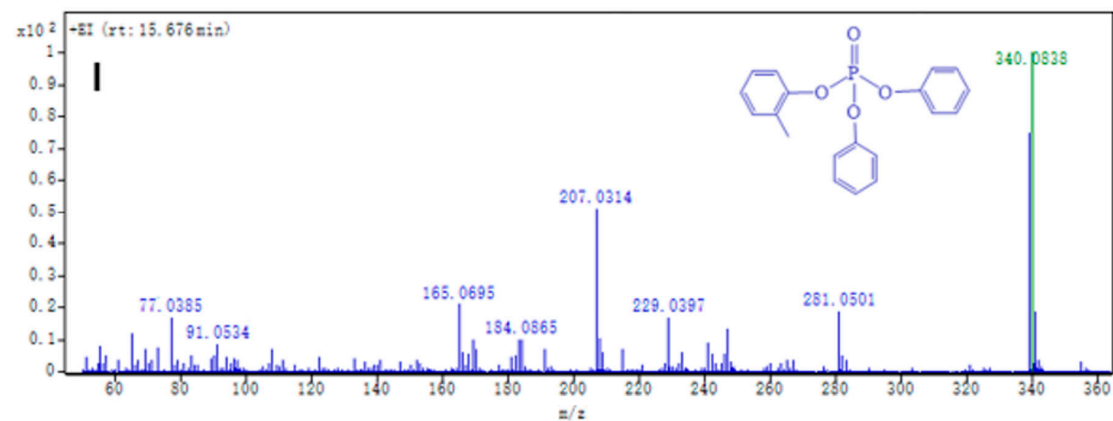
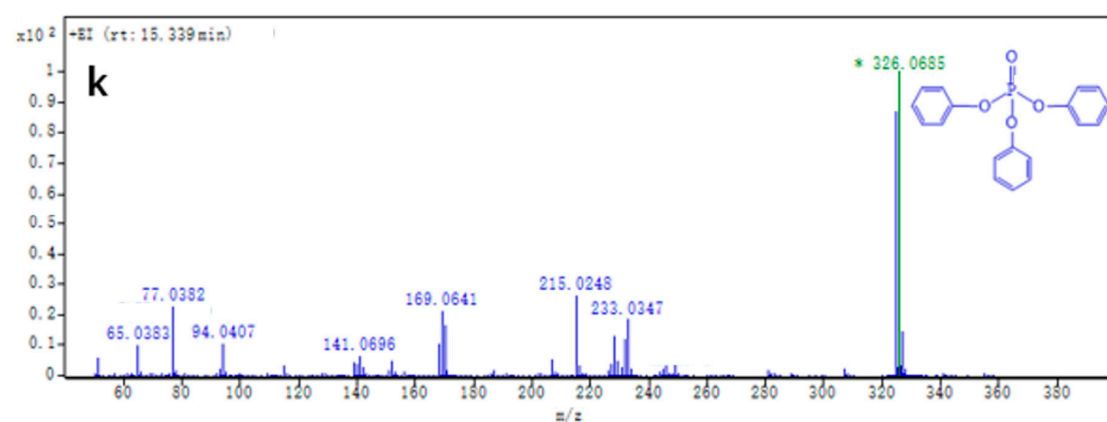
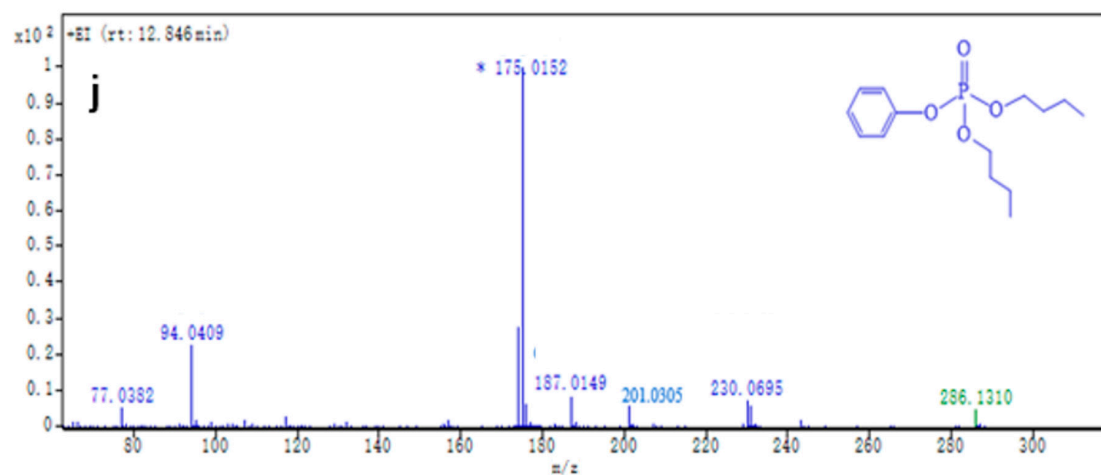
### Text S1. Instrument parameter details under EI source

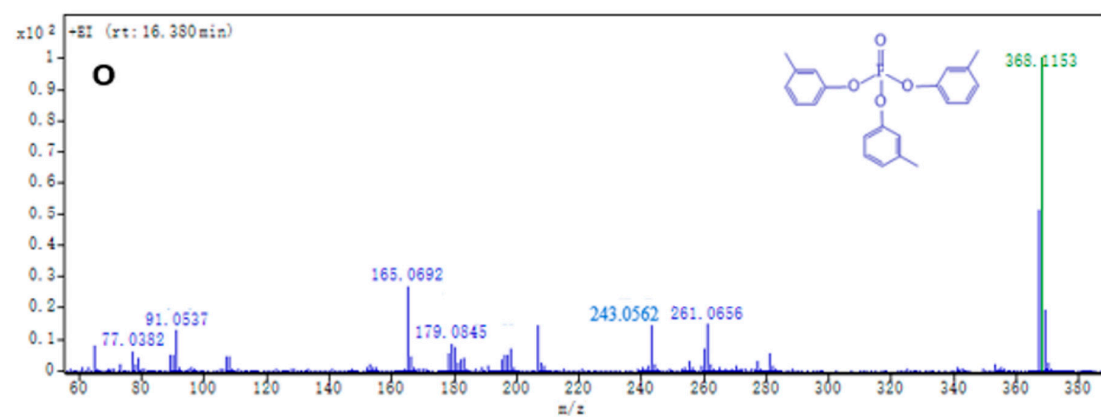
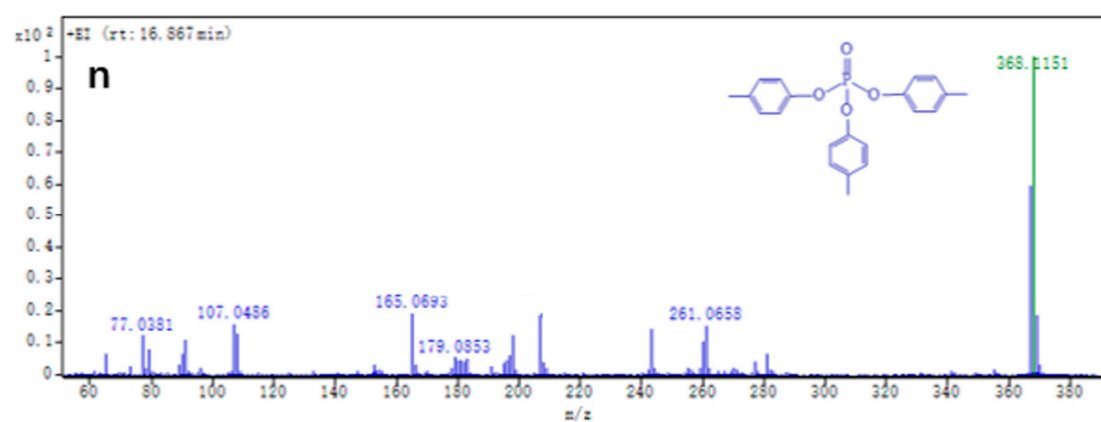
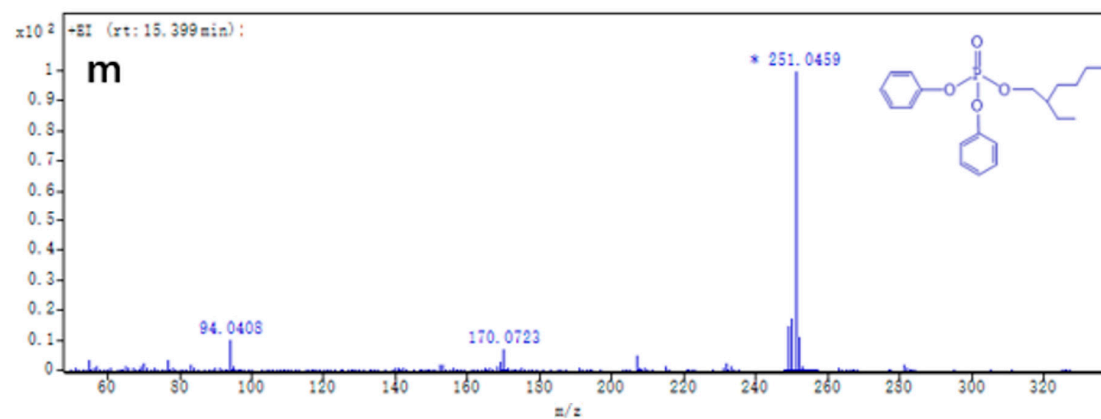
The analysis of OPFR under EI source was performed by a GC-QTOF/MS system consisting of a 7890 B gas chromatography system and a 7200 quadrupole time-of-flight mass spectrometer (Agilent Technologies, Santa Clara, USA). OPFRs were separated on an Agilent DB-5MS-Ultra Inert (30 m × 0.25 mm × 0.25 μm) column. The GC oven temperature was initiated at 50°C and held for 1 min, increased by 20°C /min to 280°C and held for 1 min, then further increased to 300°C by 30°C /min and held for 10 min. The QTOF-MS ion source and quadrupole analyser temperatures were set at 230°C and 150°C, respectively. Mass spectrometric ionization was undertaken in full scan mode with an EI voltage of 50 eV, and TOF for MS was operated at 1 spectrum/s, acquiring the mass range  $m/z$  50–450. [1]

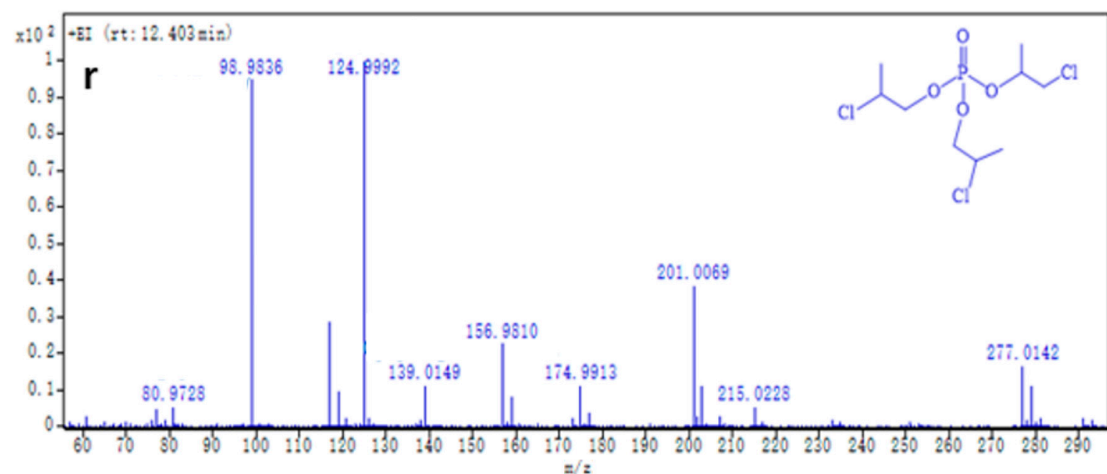
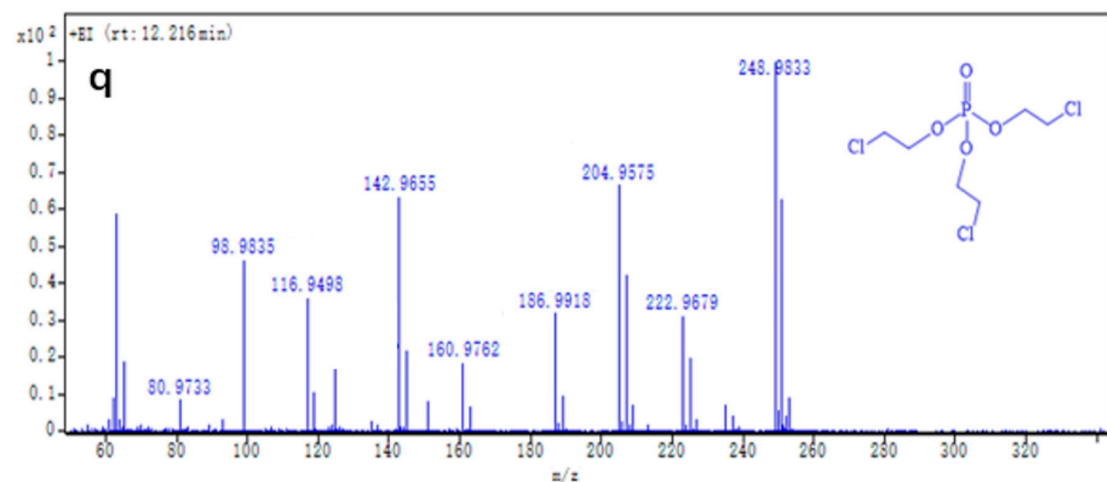
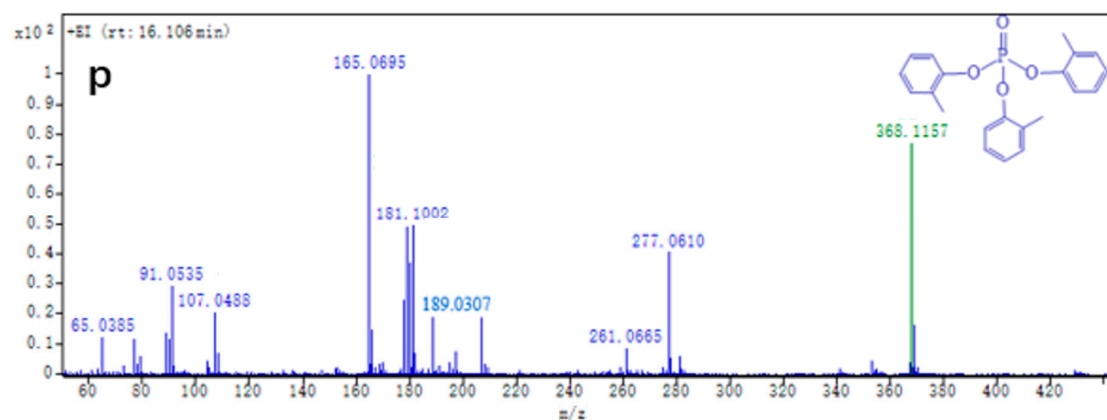


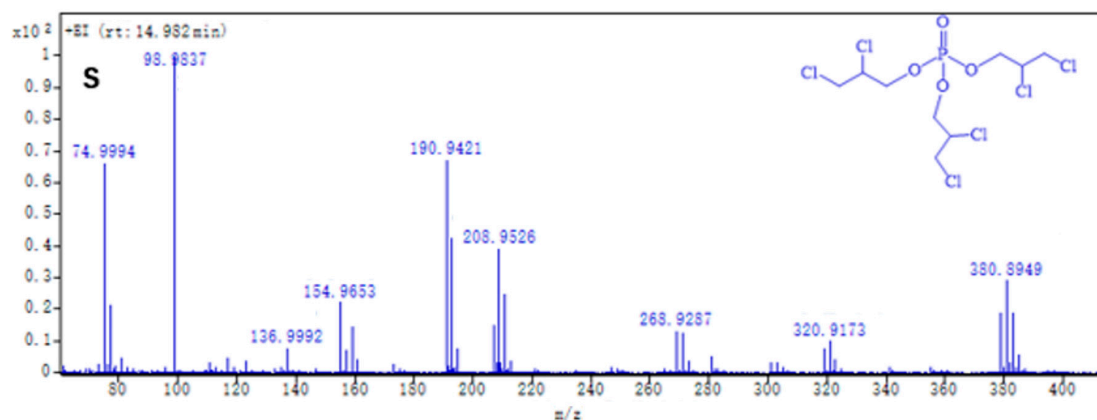












**Figure S6.** MS<sup>2</sup> spectrums of OPFRs under EI source

a. TMP; b. TEP; c. TiPP; d. TnPP; e. TiBP; f. TnBP; g. TPpP; h. TBOEP; i. TEHP; j. dBPhP;  
k. TPHP; l. CDPP; m. EHDPP; n. p-TCP; o. m-TCP; p. o-TCP; q. TCEP; r. TCIPP; s.  
T23DCIPP.

## References

1. Yang, J. S.; Zhang, Q. H.; Su, L. Q. Fragmentation mechanism of organic phosphorus flame retardant by gas chromatography-quadrupole time of flight mass spectrometry. *J. Mass. Spectrom.* 2019, 42, 36-47. [Google Scholar]