

Supplementary information

**Pinacolyl methylphosphonate acid toxic effects and
bioaccumulation obviously in zebrafish following soman
exposure to water environment**

Xing-Xing Zong, Niannian Cao, Qian Jing, Xuejun Chen, Tong Shi, Ruihua Zhang,
Jingjing Shi, Chen Wang*, Liqin Li*

State Key Laboratory of NBC Protection for Civilian, Beijing, 102205, PR China

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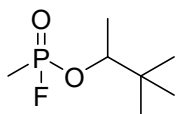
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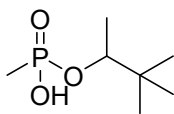
Table S2. Intra-and inter-day precisions and accuracies of PMPA in whole zebrafish and tissue.

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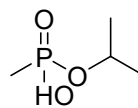
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Soman, Pinacolyl
methylphosphonofluoridate



PMPA, Pinacolyl
methylphosphonate



IMPA, Isopropyl
methylphosphonate

Figure S1. The structures of soman, PMPA, IMPA.

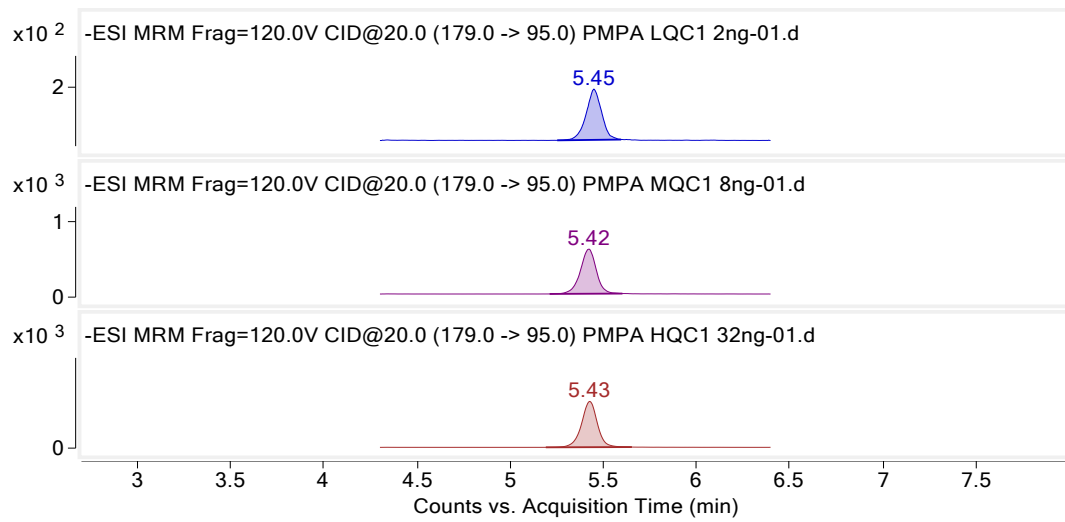


Figure S2. The TIC of QCs sample at three different levels.

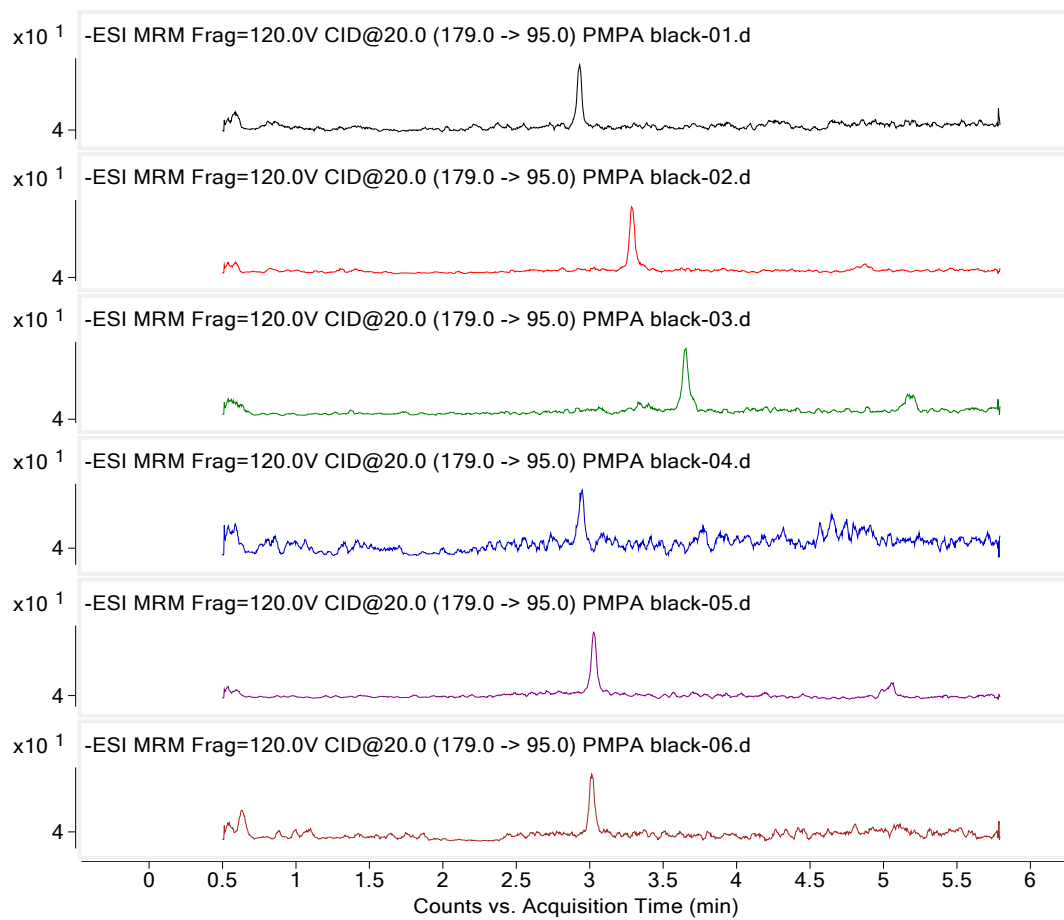


Figure S3. Mass chromatogram from the MRM transition for the blank matrix of whole zebrafish.

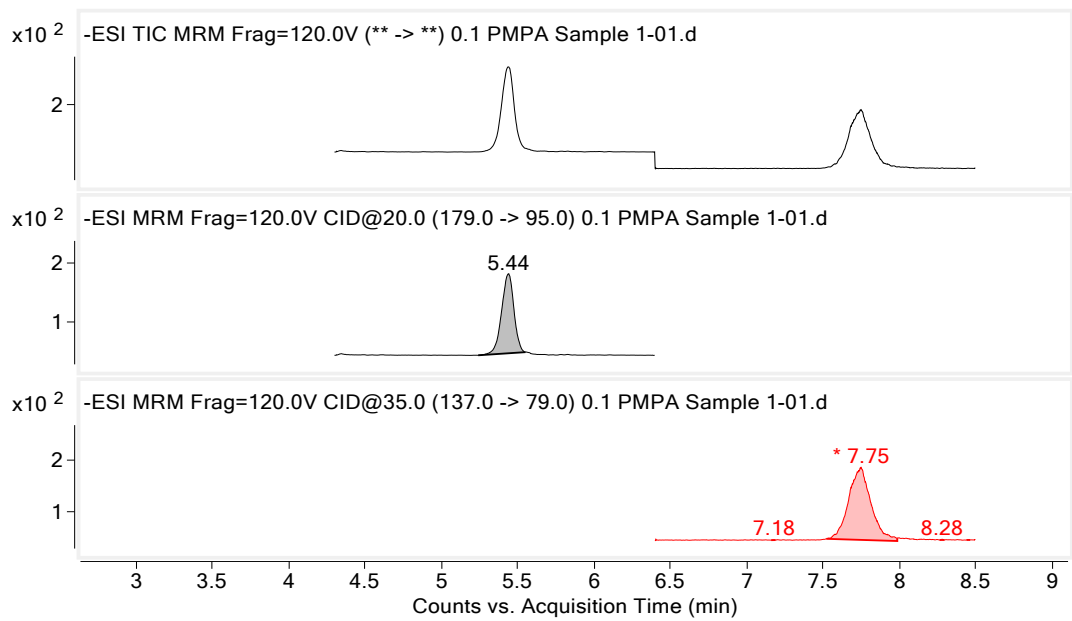


Figure S4. Mass chromatogram from the MRM transition for test sample of whole zebrafish.

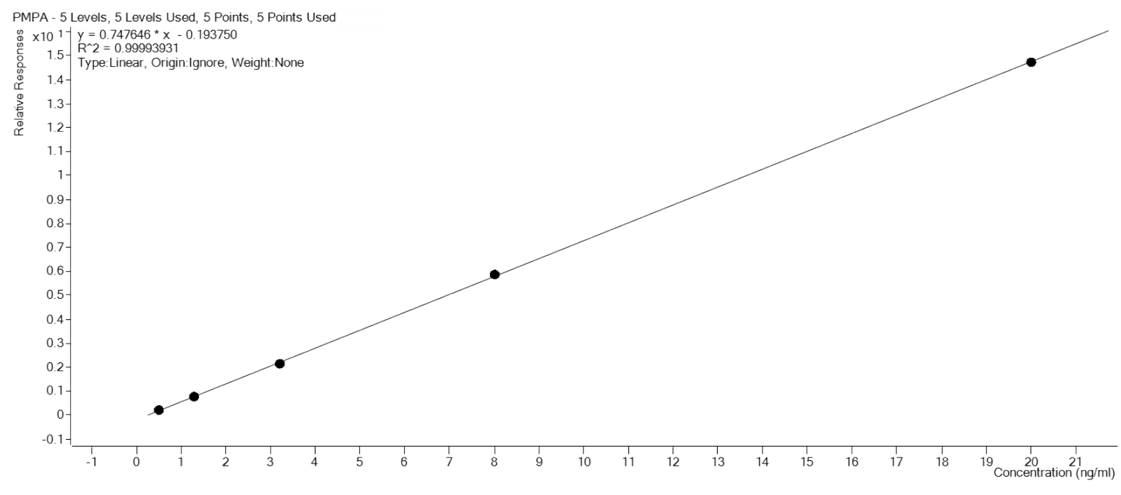


Figure S5. Calibration curve for test sample of whole zebrafish.

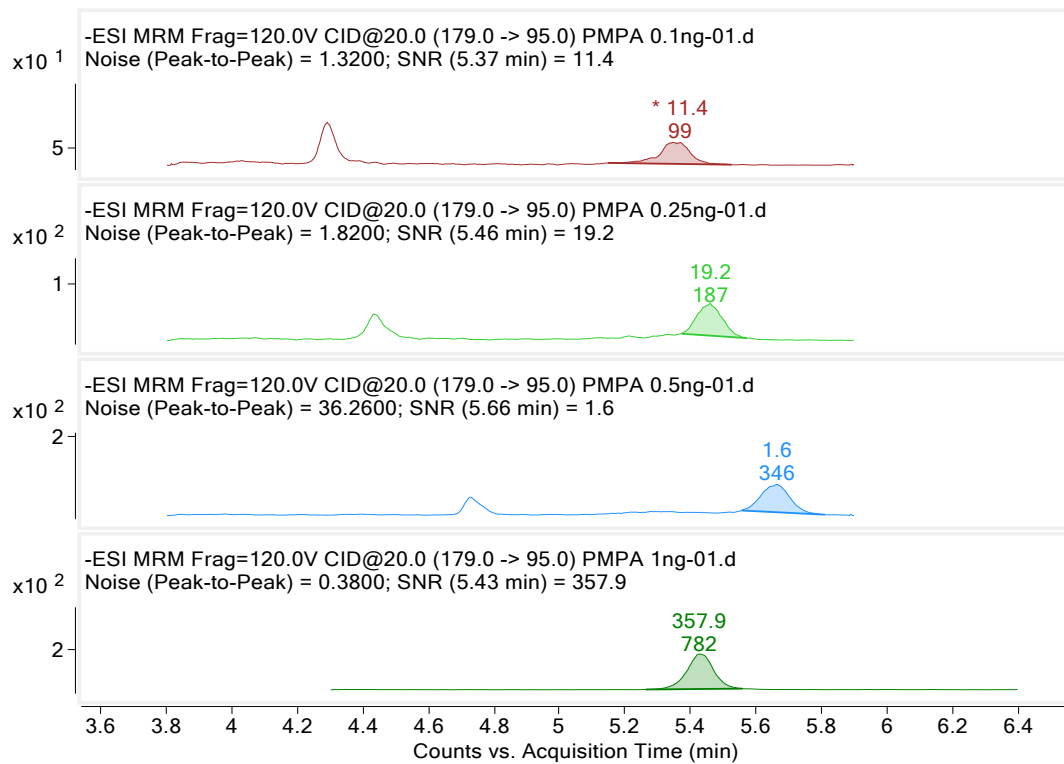


Figure S6. Mass chromatogram from the MRM transition for whole zebrafish sample at 0.1, 0.25, 0.5, 1.0 ng/mL.

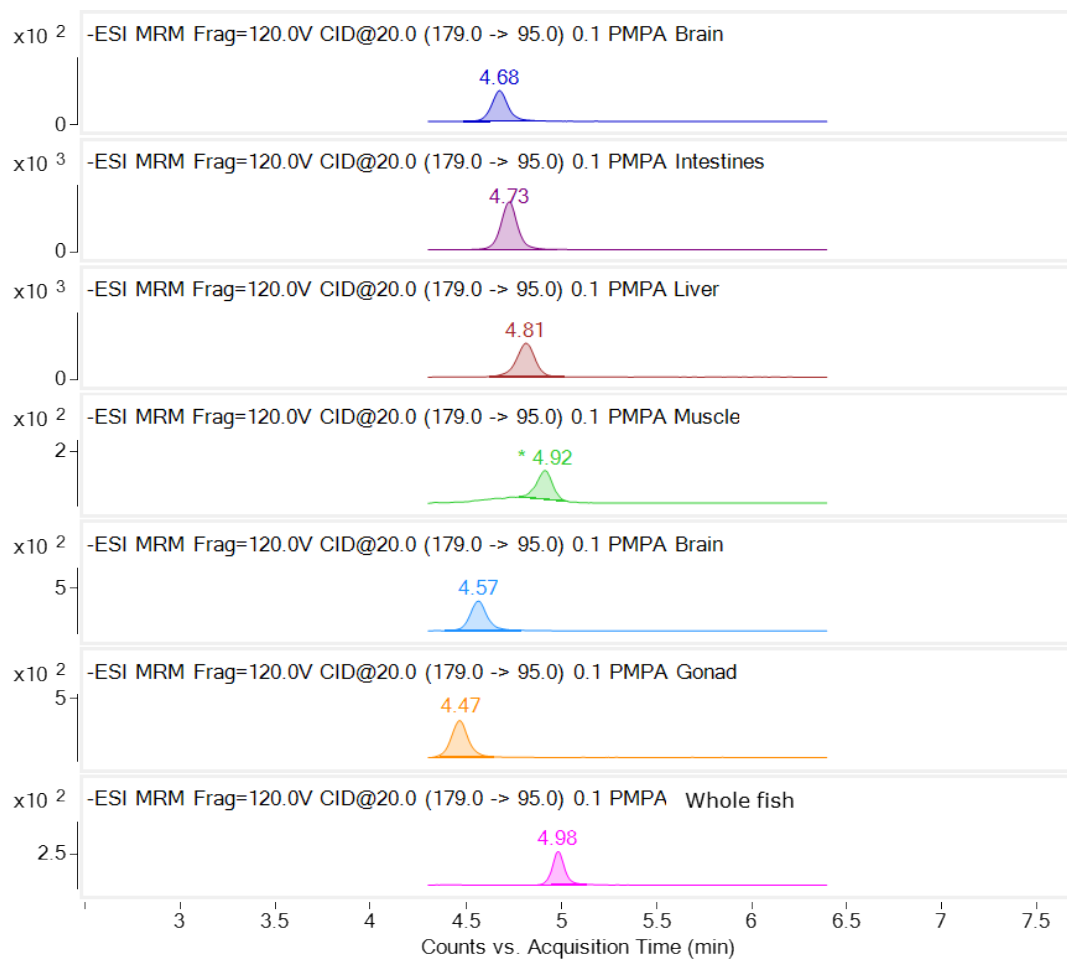


Figure S7. Mass chromatogram from the MRM transition for test sample of whole zebrafish and tissue.

Table S1. The parameters of characteristic transitions, fragmentor voltages, and collision energy for PMPA and IMPA.

Analytes	Transitions	Precursor ion (m/z)	Product ion (m/z)	Fragmentor (V)	Collision Energy (V)	Retention time (min)
PMPA	Target	179.0	95.0	120	20	5.2
	Qualifier	179.0	79.0	120	45	
IMPA	Target	137.0	95.0	120	20	7.5
	Qualifier	137.0	79.0	120	45	

Table S2. Intra-and inter-day precisions and accuracies of PMPA in whole zebrafish and tissue.

Sample	Precision						Accuracy					
	Intra-day (RSD %)			Inter-day (RSD %)			Intra-day (RE %)			Inter-day (RE %)		
	Low	Medium	High	Low	Medium	High	Low	Medium	High	Low	Medium	High
Whole fish	6.2	5.5	4.7	7.6	4.4	2.8	-2.4	1.7	-2.8	-2.9	-3.7	3.0
Muscle	7.8	8.4	5.8	7.1	6.8	4.3	6.2	5.5	5.9	-4.2	6.1	2.8
Liver	8.5	7.2	6.9	10.6	5.1	5.5	11.2	5.7	8.5	12.9	10.7	-6.2
Gonad	10.3	8.7	7.7	7.9	8.3	5.9	7.6	-8.1	8.7	-6.7	7.9	-7.5
Intestine	11.5	10.6	9.3	7.7	8.8	5.3	-12.6	10.5	6.1	8.4	-9.1	7.7
Brain	8.1	7.4	6.6	9.9	8.0	4.6	-3.3	4.4	2.2	5.5	-6.3	3.8

Table S3. Extraction recoveries and matrix effects of PMPA in whole zebrafish and tissue.

Sample	Extraction recovery (%)			Matrix effect (%)		
	Low	Medium	High	Low	Medium	High
Whole fish	112.2	107.2	106.1	88.5	77.3	89.2
Muscle	87.3	115.5	98.26	79.1	83.9	82.6
Liver	96.2	93.1	101.0	85.1	87.9	82.2
Gonad	92.4	95.7	108.3	86.6	79.5	82.4
Intestine	96.7	98.0	105.9	82.6	81.5	79.3
Brain	113.1	109.1	97.8	77.8	86.6	86.8

Table S4. Stabilities of PMPA at three freeze-thaw cycles; long-term storage; and short-term storage in whole zebrafish and tissue.

Sample	Freeze-thaw cycle stability (RE%)			Long-term stability (RE%)			Short-term stability (RE%)		
	Low	Medium	High	Low	Medium	High	Low	Medium	High
Whole fish	-7.64	-2.45	1.88	-3.92	1.38	4.30	-5.35	1.12	-5.21
Muscle	-7.23	2.24	3.24	-2.98	-4.99	-3.48	-2.60	-4.55	-6.99
Liver	-2.52	-6.61	-6.53	2.16	1.83	1.73	3.84	-5.75	1.95
Gonad	1.69	-5.64	-5.43	-4.77	-2.69	-6.85	-7.16	-3.87	1.50
Intestine	-12.68	-8.04	-9.25	-10.85	-8.86	-7.27	-14.41	-4.62	-7.57
Brain	-2.57	2.90	-2.87	2.72	-5.73	-7.82	-4.48	-2.44	1.45