



Organic Stable Isotope Analysis with GC-qMS for PBDEs in a molecular view

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PBDEs: Brominated Flame Retardant & Persistent Organic Pollutants

Table 5

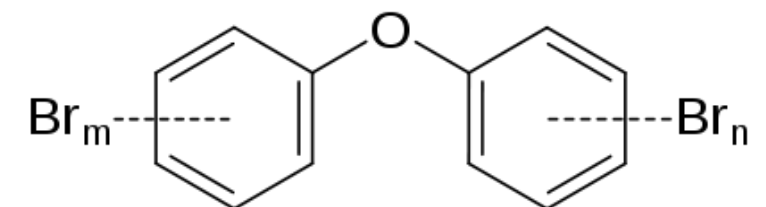
Concentrations of eight PBDE congeners (BDE28, BDE47, BDE99, BDE100, BDE153, BDE154, BDE183, BDE209) in serum samples from the general population in China (ng/g lipid wt).

Types of sites	Electronic-waste recycling sites		Production area	Cities		
	Luqiao (Taizhou)	Wenling (Taizhou)		Tianjin	Hongkong	
Sampling year	2006	2006	2007	2006	2008	
Sample size (n)	27	23	156	115	51 (female)	60 (male)
BDE28	2.3	31.28	29.2	0.38		
BDE47	5.76	44.72	21.4	1.19	2.57	2.59
BDE99	1.96	7.90	23.4	0.95	0.11	0.06
BDE100	0.88	4.12	14.8	0.25	0.06	0.06
BDE153	14.6	26.12	32.5	0.48	0.67	0.63
BDE154	0.96	2.30	41.8	0.15	0.06	0.05
BDE183	3.92	7.26	46.9	0.59	0.30	0.27
BDE209	87.20	210.48	403	36.4	1.32	1.03
\sum PBDEs	117.58	334.18	613	40.39	5.74 ^a	5.25 ^a
Reference	Zhao et al. (2010)	Zhao et al. (2010)	Jin et al. (2009)	Zhu et al. (2009)	Qin et al. (2011a,b)	

^a \sum_{10} PBDEs: Sum of BDE47, 85, 99, 100, 119, 153, 154, 183, 184, 209.

Ni Kun et.al 2013 Int J Hyg Environ Healthntal Health

- Sources of high concentration BDE-47 in Environmental samples
 - Release from e-waste
 - Debromination from high brominated PBDEs



ISOTOPE

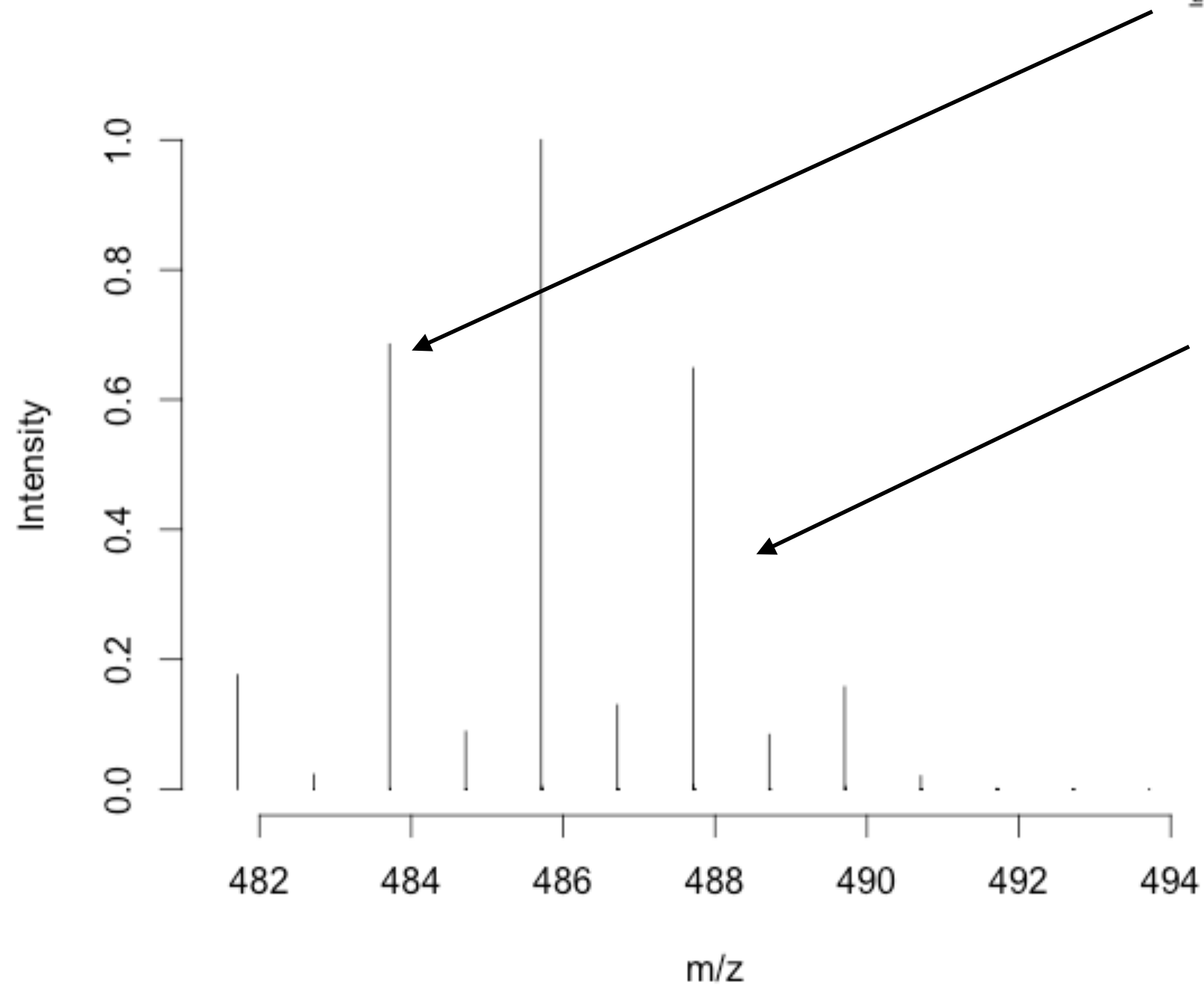
We need **another method** to get the **sources** of PBDEs



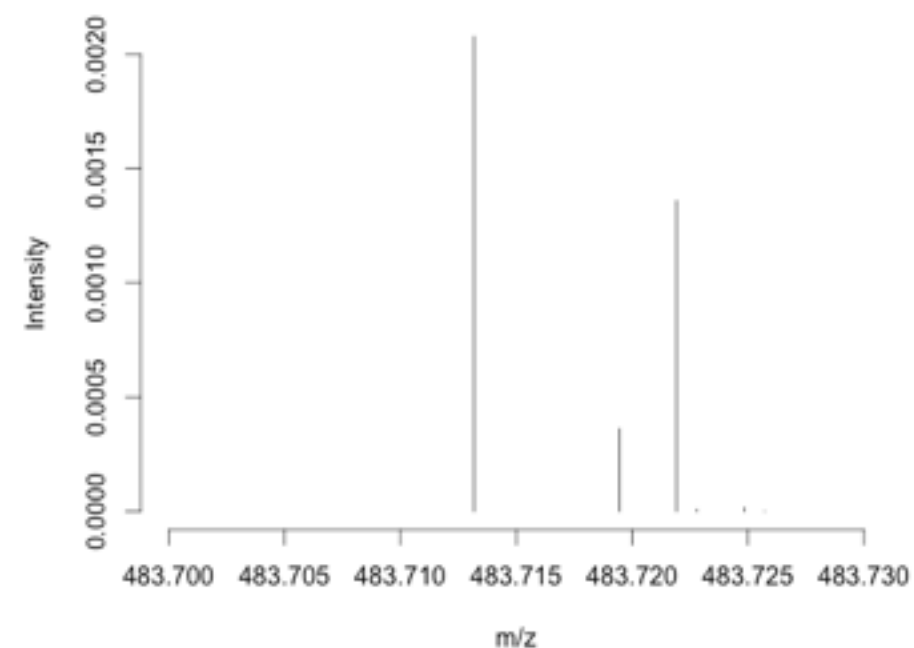
Why molecular?



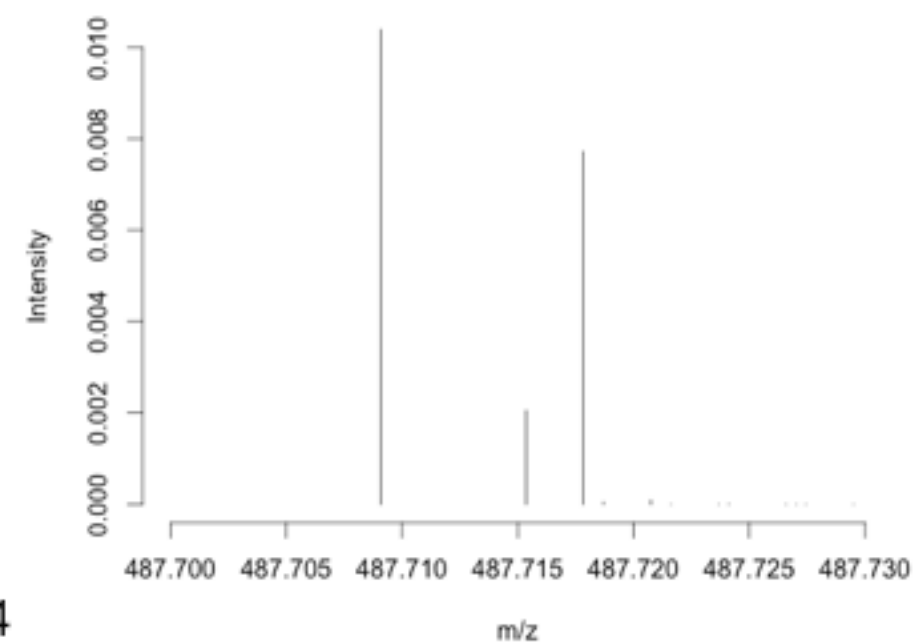
Isotopologue are actually isotopologues



m/z 483.7



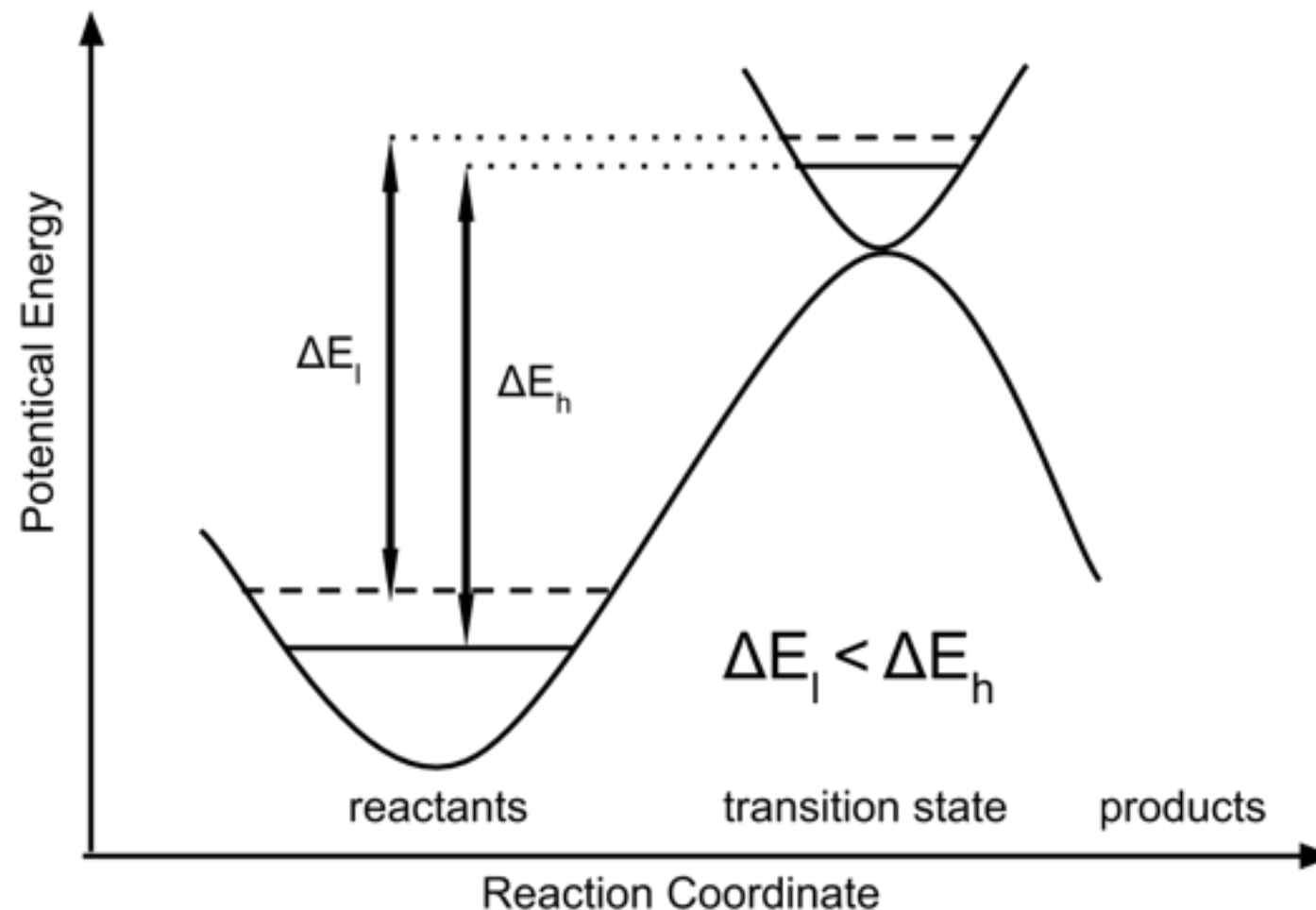
m/z 487.7



Molecular Isotope Ratio

$$\text{Molecular isotope ratio}(R_m) = \frac{\text{Isotopologues}_L}{\text{Isotopologues}_H}$$

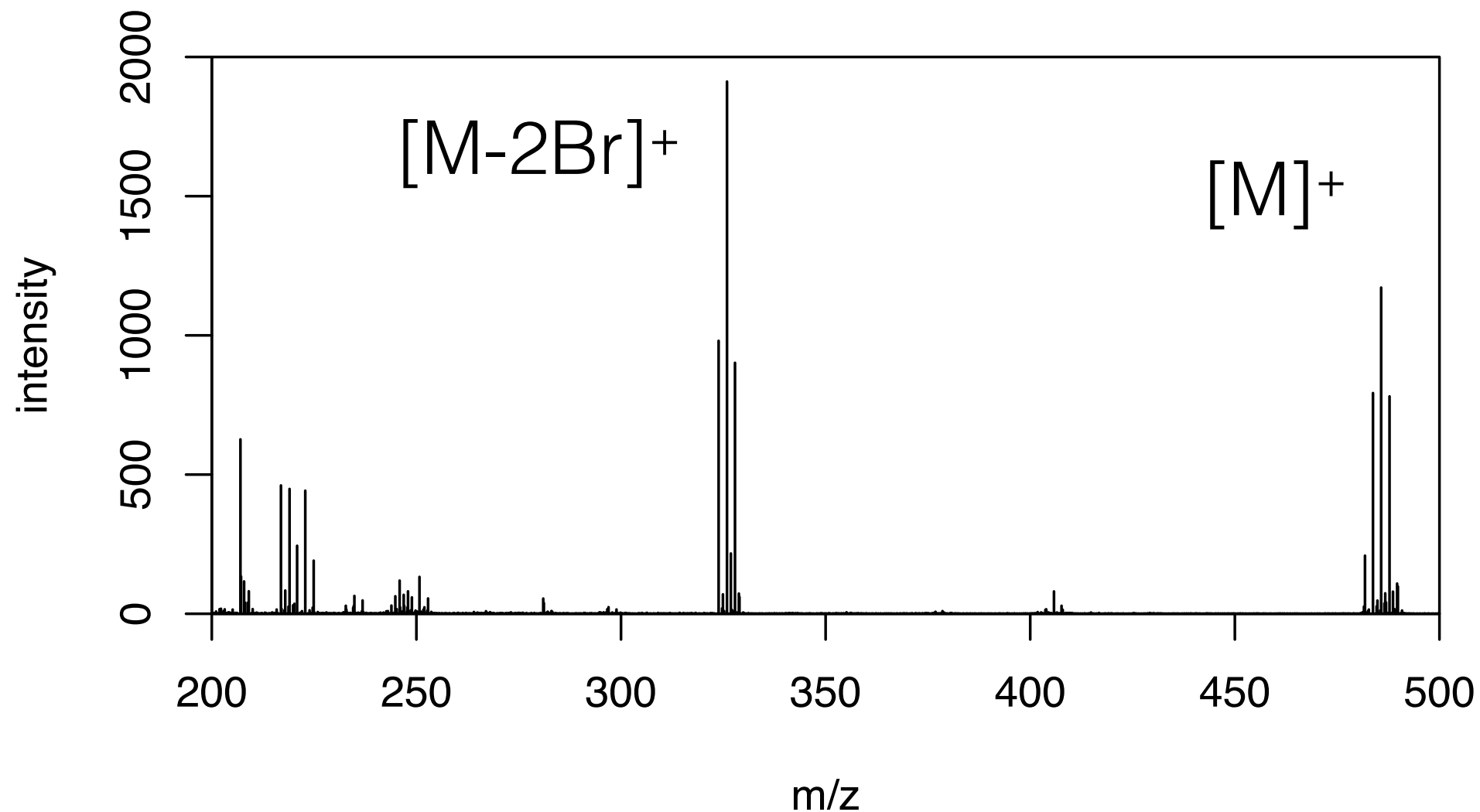
$$\delta_m = \left(\frac{R_m}{R_{ms}} - 1 \right) \times 1000\text{‰}$$



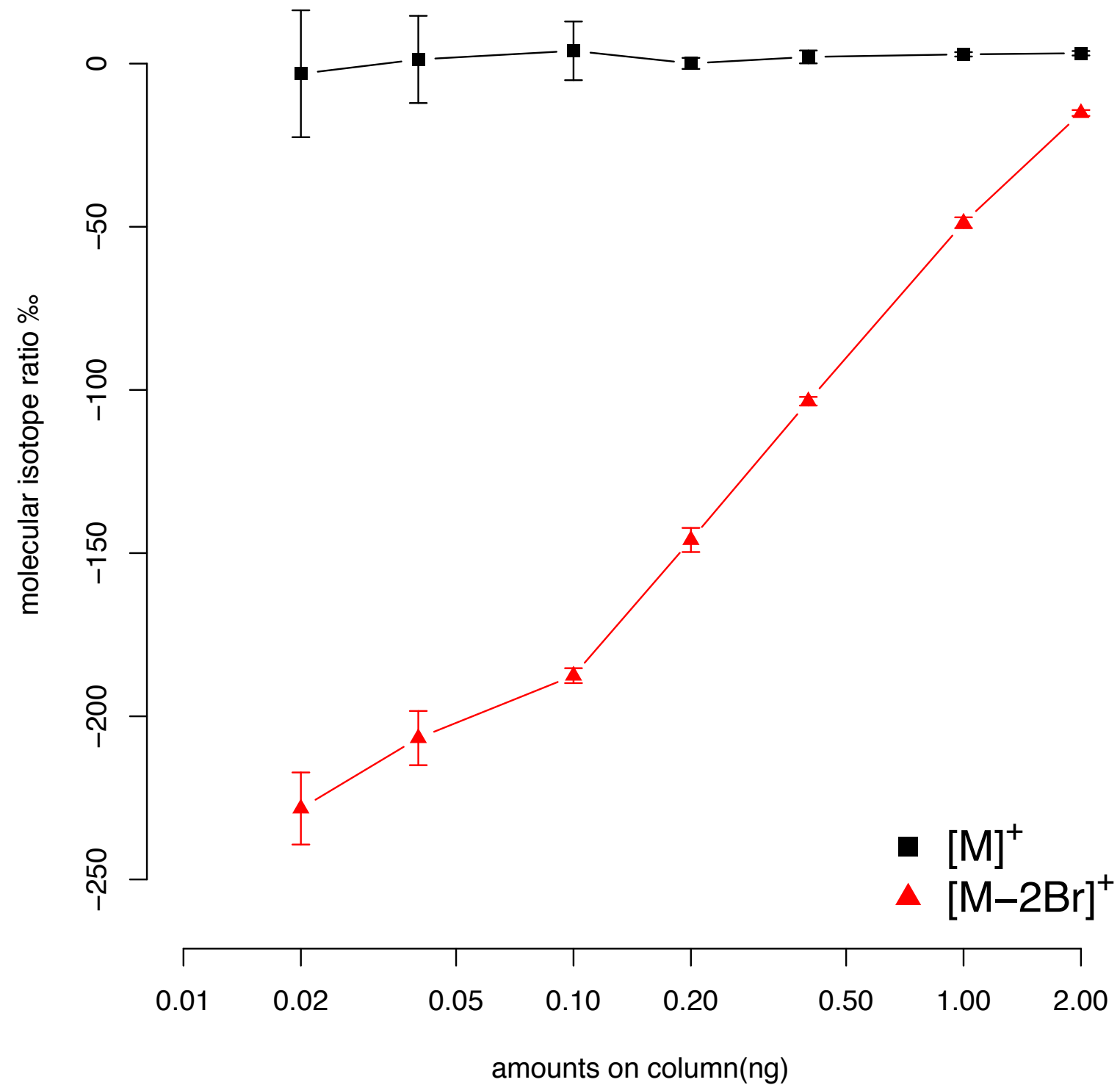
Which pair?

$$R_m = \frac{Isotopolgues A_L}{Isotopolgues A_H} = \frac{Isotopolgues B_L}{Isotopolgues B_H} = \frac{\alpha \cdot Isotopolgues A_L + \beta \cdot Isotopolgues B_L}{\alpha \cdot Isotopolgues A_H + \beta \cdot Isotopolgues B_H}$$

BDE-47



Which pair?



How to make the results comparable?

General web app

<https://yufree.shinyapps.io/MIRtools/>

Molecule Isotop Ratio(MIR)

Import Formula such as C₁₂H₆OBr₄

C₁₂H₆OBr₄

Peaks Width(+/-)

0 0.3 1

Choose CSV File for light molecular isotopologue peak

选择文件 未选择任何文件

SKIP

3

Rows Number

1500

Choose CSV File for heavy molecular isotopologue peak

选择文件 未选择任何文件



环境化学与生态毒理学国家重点实验室
State Key Laboratory of Environmental Chemistry and Ecotoxicology

Description Peaks Molecule Isotop Ratio

This app is developed for molecular isotope studies.

Usage

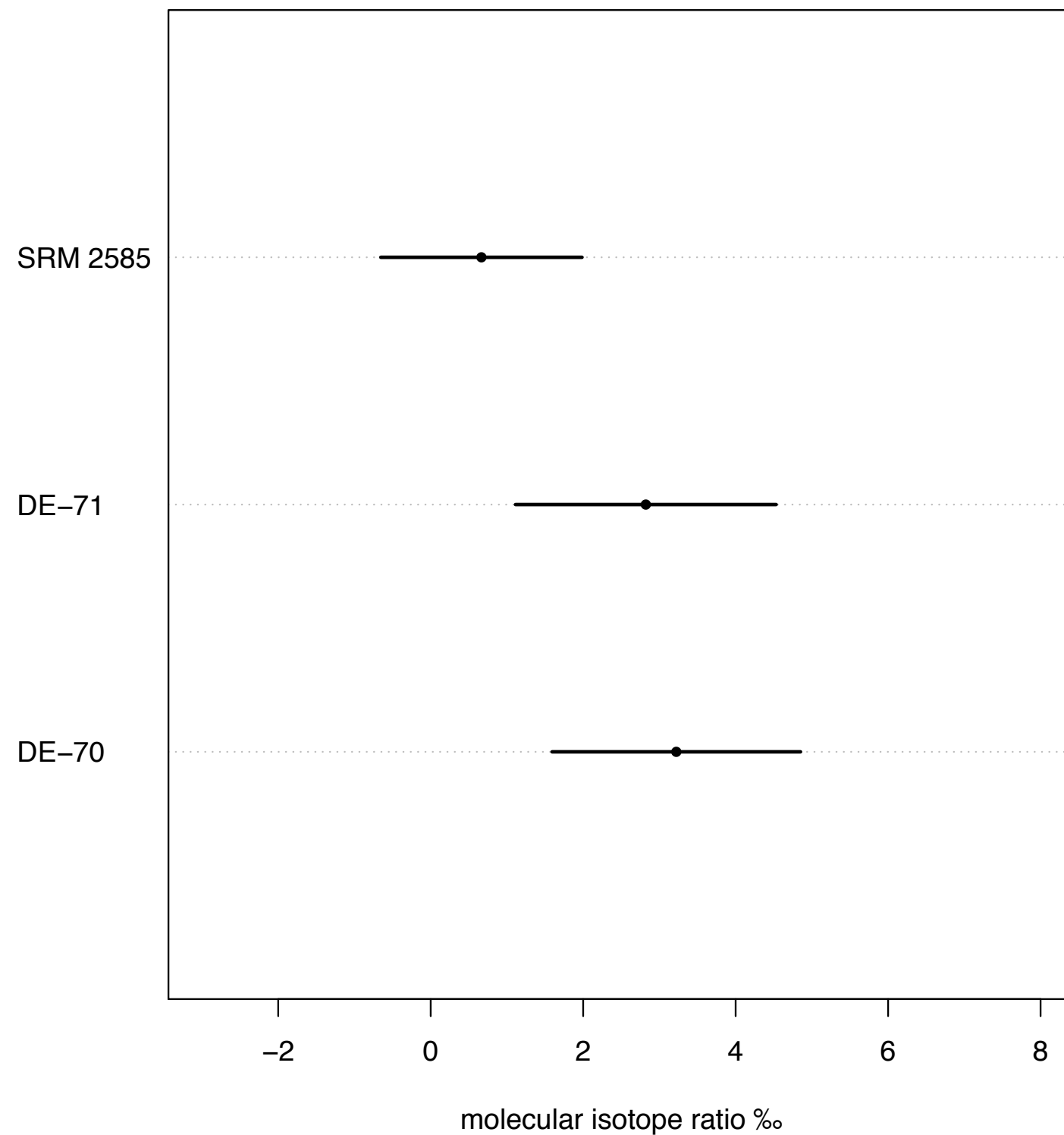
Input the molecular formula and the peak width of isotopologues on your mass spectrum in the side bar. Then in the 'Peaks' tab, you might find the selected peaks for that molecular and a calculated ratio of selected peaks on your mass spectrum. The default molecular is BDE-47

You may upload your data of certain isotopologues in csv format to get the molecular isotope ratio for your experiment in tab 'Molecule Isotop Ratio'. The first column would be time and second column responses. The 'SKIP' means you can skip certain header lines and row numbers means the lines for that isotopologues. When both of the light and heavy isotopologues were in the same file, such parameters will help you to separate them apart.

RT start and RT end mean the scale of your retention time which included the peaks for light and heavy isotopologues.

Points in the moving average smooth box, numbers of points for regression, threshold value for start/stop peaks and points

BDE-47 in SRM



Summary

- GC-qMS could be used to get molecular isotope ratio
- In-source fractionation phenomena for fragmental ions
- BDE-47 in SRM has different MIR compared with technical product DE-70

Thank you for your attention!

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<http://yufree.cn>