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)	South coastal area of Laizhou Bay	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.

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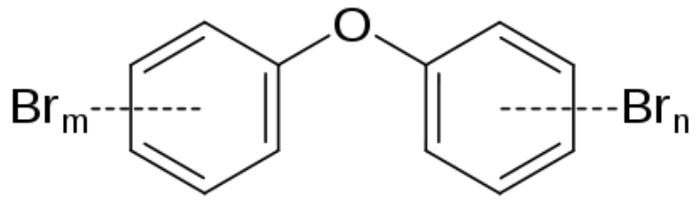
- Sources of high concentration BDE-47 in Environmental samples
  - Release from e-waste
  - Debromination from high brominated PBDEs



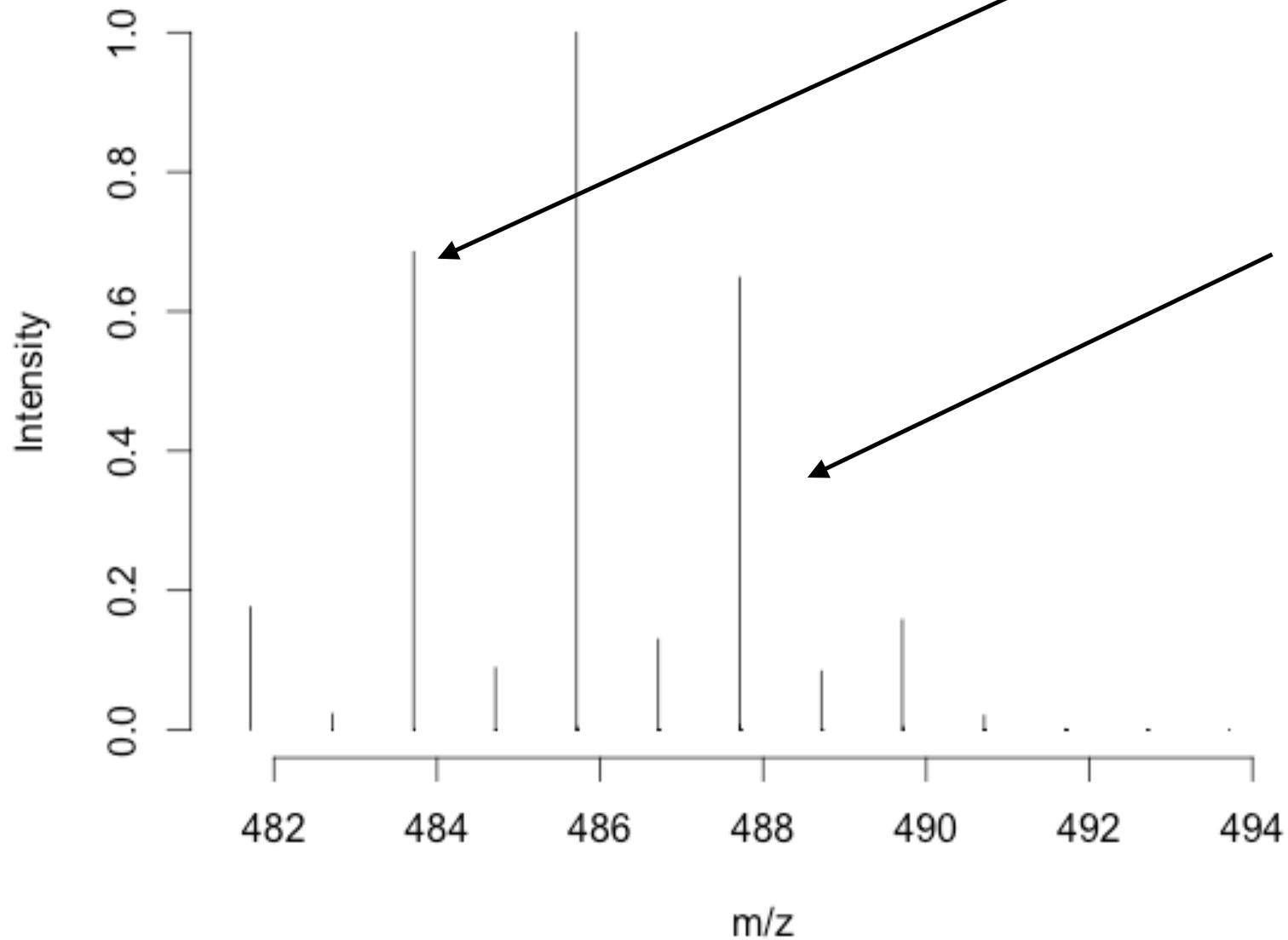
ISOTOPE

We need another method to get the sources of PBDEs

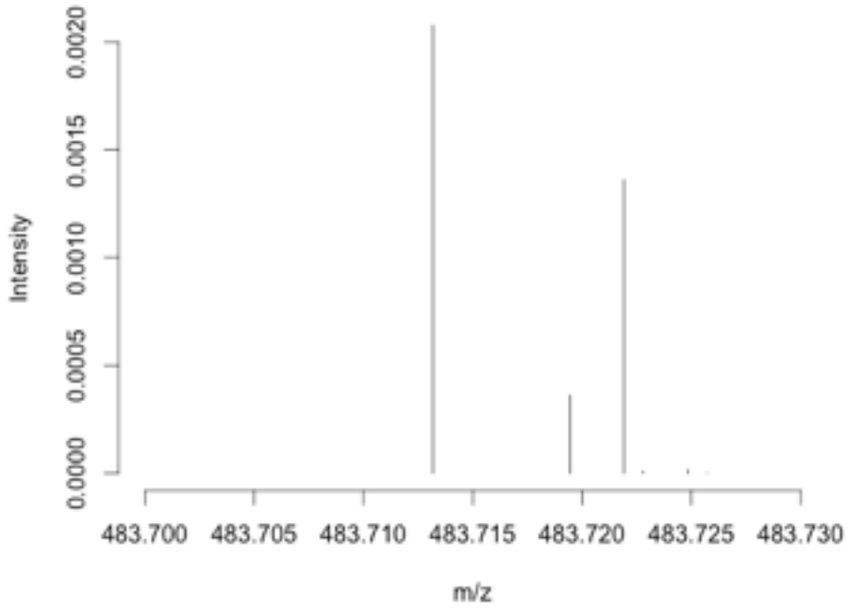
Δ

Why molecular?

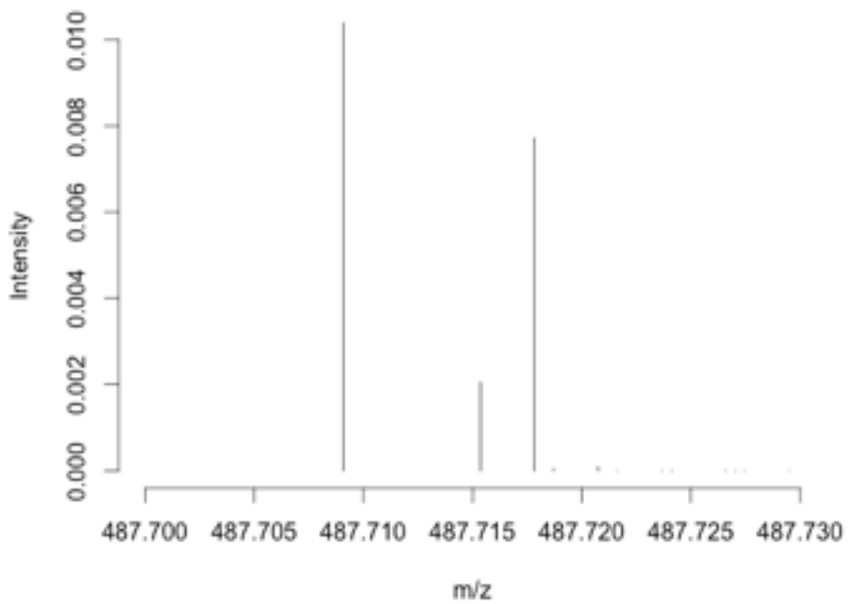
Isotopolugue are actually isotopolugues



m/z 483.7



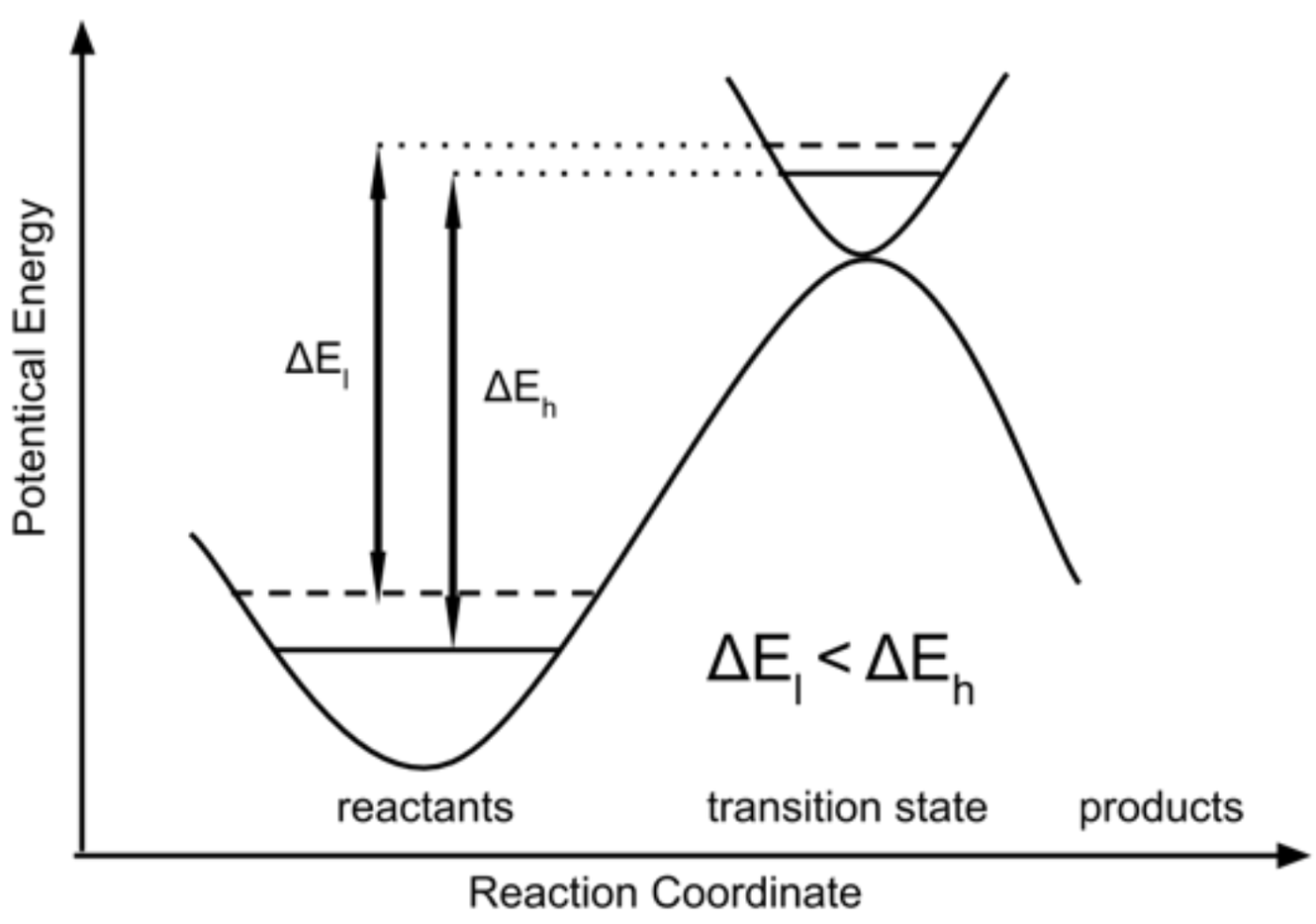
m/z 487.7



Molecular Isotope Ratio

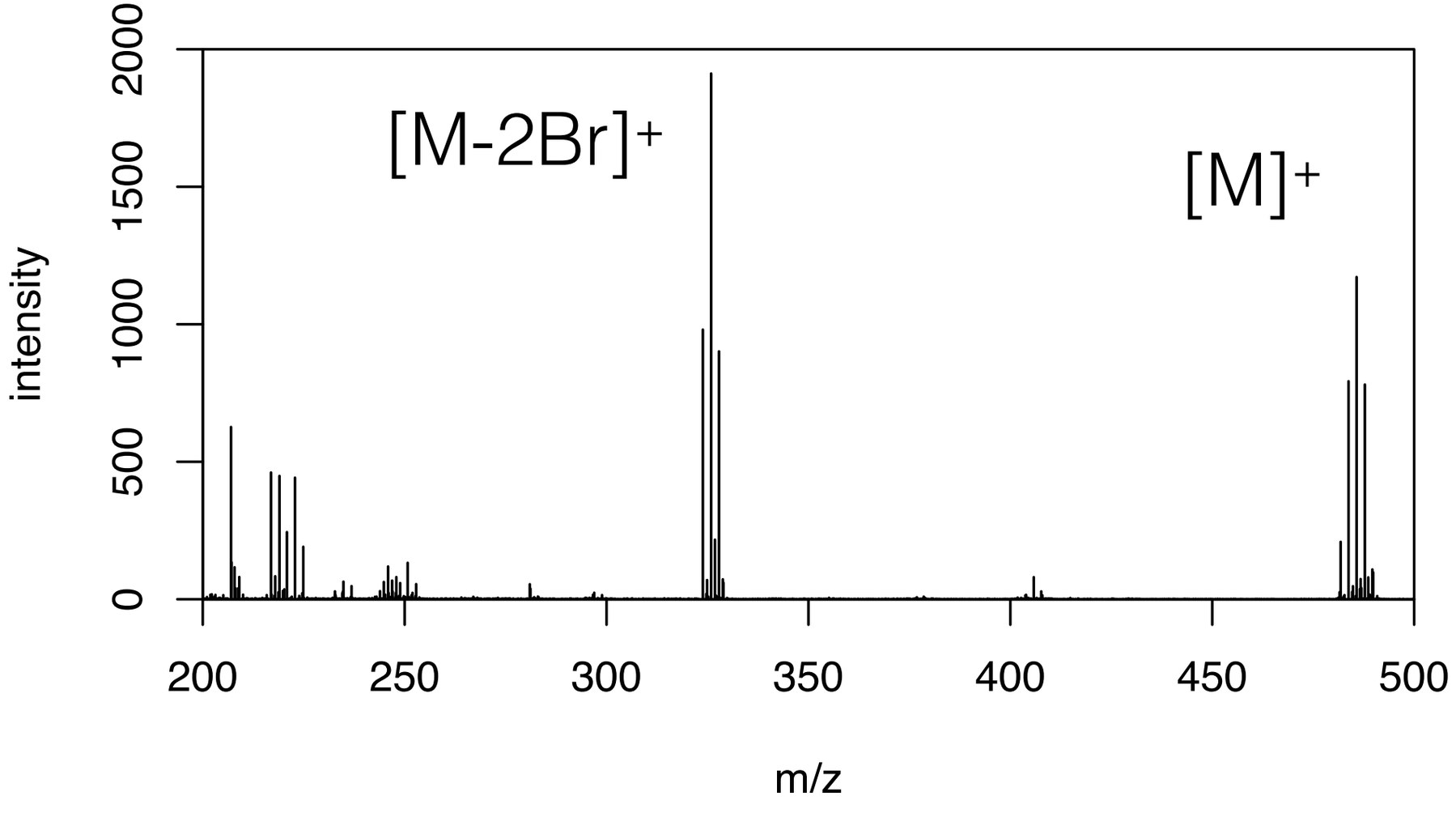
$$Molecular\ isotope\ ratio(R_m) = \frac{Isotopologues_L}{Isotopologues_H}$$

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

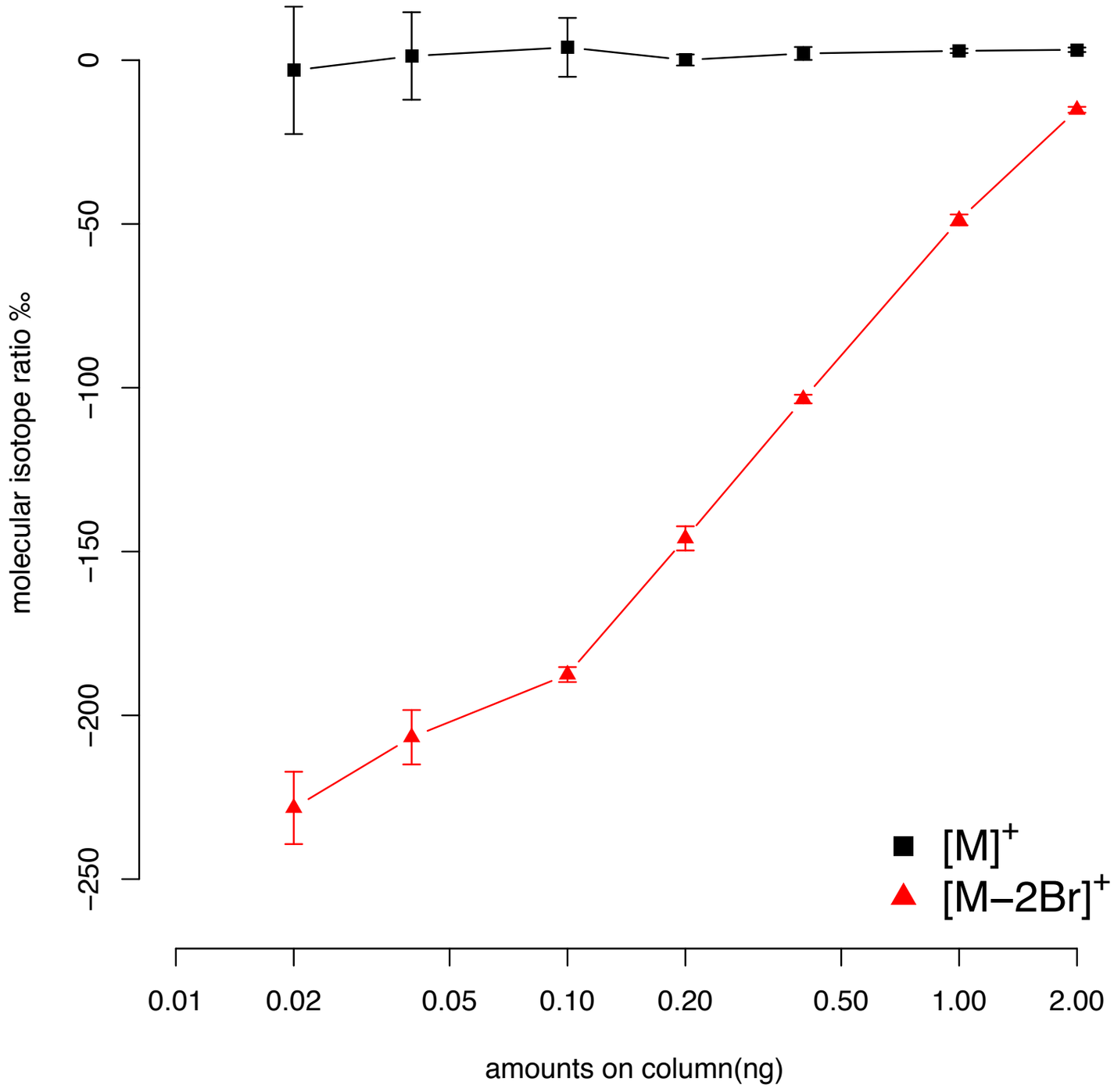


Which pair?

$$R_m = \frac{IsotopolguesA_L}{IsotopolguesA_H} = \frac{IsotopolguesB_L}{IsotopolguesB_H} = \frac{\alpha \cdot IsotopolguesA_L + \beta \cdot IsotopolguesB_L}{\alpha \cdot IsotopolguesA_H + \beta \cdot IsotopolguesB_H}$$



Which pair?

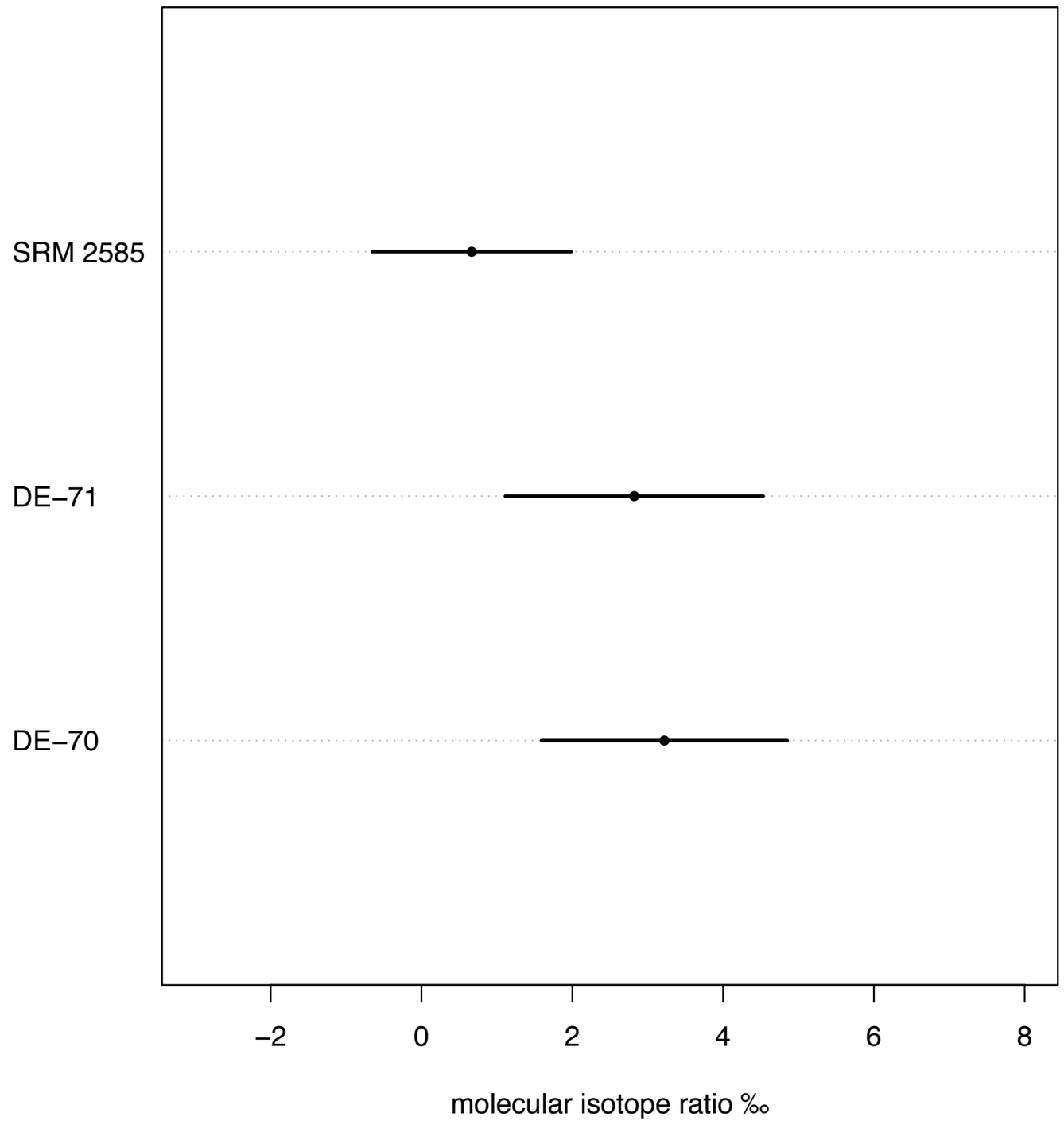

molecular isotope ratio ‰
0
−50
−100
−150
−200
−250
0.01
0.02
0.05
0.10
0.20
0.50
1.00
2.00
amounts on column(ng)
[M]+
[M−2Br]+

How to make the results comparable?

General web app

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

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