Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Assessment of different isotope dilution strategies and combination with switchable solvent liquid phase microextraction prior to quantification of bisphenol A at trace levels by GC-MS

Süleyman Bodur[1], Sezin Erarpat[1], Dotse Selali Chormey[1], Gamze Dalgıç Bozyiğit[2], Ersoy Öz[3], Nizamettin Özdoğan[4], Sezgin Bakırdere[1,5*]

[1]*Yıldız Technical University, Faculty of Art and Science, Department of Chemistry, 34220 Davutpasa, Esenler, İstanbul, Turkey*

[2]*Yildiz Technical University, Faculty of Civil Engineering, Department of Environmental Engineering, 34220 İstanbul, Turkey*

[3]*Yıldız Technical University, Faculty of Arts and Sciences, Department of Statistics, ,34220, Davutpasa, Esenler, İstanbul, Turkey*

[4]*Bülent Ecevit University, Institute of Science, Department of Environmental Engineering, 67100, Zonguldak, Turkey*

[5]*Turkish Academy of Sciences, Piyade Sokak No: 27, Çankaya, 06690, Ankara, Turkey*

Supplementary Material 4

Mathematical expressions used for the different isotope dilution strategies.

***Corresponding author:** Sezgin Bakırdere, email: bsezgin23@yahoo.com, Phone: +902123834245*

Table S1. Notation and description of symbols.

Symbol	Description
A*	The analyte
A	Sample (containing the analyte)
B	Labelled material
A*B	Blend of A* and B
AB	Blend of A and B
$\mathbf{w_x}$	Mass fraction of standard, sample or labelled solution, x: A*, A or B
$\mathbf{r_x}$	Ratio of isotope amount in the solution (A*B, AB or A*AB) by measuring the mass spectrometer.
$\mathbf{M_x}$	Molecular mass of the analyte or its isotope, x: A*, A, B

***Corresponding author:** *Sezgin Bakırdere, email: bsezgin23@yahoo.com, Phone: +902123834245*

- **ID²MS** [34]

$$w_A = w_{A*} \cdot \frac{(r_A - r_{A*B})}{(r_{A*B} - r_B)} \cdot \frac{(r_B - r_{AB})}{(r_{AB} - r_A)} \cdot \frac{(m_{A*(A*B),\ aq})}{(m_{B(A*B),aq})} \cdot \frac{(m_{B(AB),aq})}{(m_{A(AB),aq})}$$

Eq. (A.1)

- **ID³MS** [34]

$$w_A = \frac{w_{A*-2} \cdot \frac{m_{A*(A*B-2),aq}}{m_{B(A*B-2),aq}} \cdot (r_{AB} - r_{A*B-1}) \cdot (r_A - r_{A*B-2}) + w_{A*-1} \cdot \frac{m_{A*(A*B}}{m_{B(A*B}}}{(r_{AB} - r_A) \cdot (r_{A*B-1} - r_{A*B-2})} \cdot \frac{m_{B(AB),aq}}{m_{A(AB),aq}}$$

Eq. (A.2)

- **ID⁴MS** [34]

$$w_A = -\frac{m_{A*-2} \cdot m_{A*-3} \cdot k_1 + m_{A*-1} \cdot m_{A*-3} \cdot k_2 + m_{A*-1} \cdot m_{A*-2} \cdot k_3}{m_{A*-1} \cdot k_1 + m_{A*-2} \cdot k_2 + m_{A*-2} \cdot k_3}$$

Eq. (A.3)

$$m_{A*-x} = w_{A*-x} \cdot \frac{m_{A*(A*B-x)}}{m_{B(A*B-x)}}$$

Eq. (A.4)

***Corresponding author:** *Sezgin Bakırdere, email: bsezgin23@yahoo.com, Phone: +902123834245*

$$k_1 = (r_{AB} - r_{A*B-1}) \cdot (r_{A*B-2} - r_{A*B-3})$$ Eq. (A.5)

$$k_2 = (r_{AB} - r_{A*B-2}) \cdot (r_{A*B-3} - r_{A*B-1})$$ Eq. (A.6)

$$k_3 = (r_{AB} - r_{A*B-3}) \cdot (r_{A*B-1} - r_{A*B-2})$$ Eq. (A.7)

- **SA-ID²MS** [33]

$$w_A = w_{A*} \cdot \frac{- m_{A*-1} \cdot m_{B-2} \cdot (r_{A*AB-1} - r_{A*}) \cdot (r_B - r_2) - m_{B-1} \cdot m_{A*-2} \cdot (r_B - r_{A}}{m_{A-1} \cdot m_{B-2} \cdot (r_{A*AB-1} - r_A) \cdot (r_B - r_{A*AB-2}) + m_{B-1} \cdot m_{A-2} \cdot (r_B - } \cdot \frac{M_A}{M_{A*}}$$ Eq. (A.8)

- **SA-ID³MS** [33]

$$w_A = w_{A*} \cdot (\frac{- m_{A*-1} \cdot m_{B-2} \cdot m_{B-3} \cdot (r_{A*AB-2} - r_{A*AB-3}) + m_{A*-2} \cdot m_{B-1} \cdot m_{B-3} \cdot (r_{A*AB-1} - r_{A*AB-3})}{+ m_{A-1} \cdot m_{B-2} \cdot m_{B-3} \cdot (r_{A*AB-2} - r_{A*AB-3}) - m_{A-2} \cdot m_{B-1} \cdot m_{B-3} \cdot (r_{A*AB-1} - r_{A*AB-3}) -}$$ Eq. (A.9)

***Corresponding author:** *Sezgin Bakırdere, email: bsezgin23@yahoo.com, Phone: +902123834245*

***Corresponding author:** Sezgin Bakırdere, email: bsezgin23@yahoo.com, Phone: +902123834245*

References

33 E. Pagliano and J. Meija, *Metrologia*, 2016, **53**, 829–834.

34 E. Pagliano, Z. Mester and J. Meija, *Anal. Bioanal. Chem.*, 2013, **405**, 2879–2887.

***Corresponding author:** Sezgin Bakırdere, email: bsezgin23@yahoo.com, Phone: +902123834245*