



Application Note 2003/2

Stir Bar Sorptive Extraction (SBSE) Recovery Calculator: Easy Calculation of Extraction Recoveries for SBSE



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
Keywords
Stir Bar Sorptive Extraction (SBSE), Twister,
Twister calculator, Recovery



Introduction
A spreadsheet is presented for the calculation of extraction recoveries of analytes from water samples with Stir Bar Sorptive Extraction (SBSE) applying the Gerstel Twisters. For a given sample volume and $\log K_{o/w}$ value of the analyte, SBSE recoveries are calculated for four commercial types of Twisters. Note that recoveries are at equilibrium conditions which is a must for application of SBSE (see Application Note 2003/1).



Use and download of the TwisterCalculator
The calculation can be executed directly from this website at URL

http://www.richrom.com/html/ric_apnnotes/SBSEcalculator.htm. The application requires Microsoft Excel® installation on your PC. In case your browser does not support Microsoft Excel implementation, you can download the 'SBSECalculator.xls' file at the same URL pressing the  button. The application procedure is valid for both approaches.

Theoretical Background

The fundamentals and principles of Stir Bar Sorptive Extraction are detailed by E. Baltussen *et al.* [1]. Similar calculations for SBSE extraction recoveries were used in this program. Basically, the SBSE recovery of a compound from a water sample can be calculated from the sample volume, the volume of polydimethylsiloxane (PDMS) phase on the Twister and the analyte's octanol-water distribution coefficient (Ko/w). For the four sets of Twisters commercially available, each with a known amount of PDMS extraction phase, the recovery for a specific solute is calculated from the sample volume (mL) and log Ko/w.

Operation

The four different types of Twisters (Type 1-4) contain volumes of PDMS ranging from 24 to 126 µL and are listed in four different columns (Figure 1). The sample volume and the log Ko/w of the analyte is introduced in the spreadsheet and the SBSE recoveries (%) are automatically calculated for four sampling sets (Set 1-4) that use the four different Twister types (Type 1-4). The values (%) are listed in the four columns and are also visualized in the histogram below. In addition, the

calculated recoveries are situated in the theoretical recovery curves of the four sampling sets. These curves represent the relation of the solute's log Ko/w in function of the SBSE recovery for a given phase ratio (sample volume: PDMS volume) and are shown for the four Twister types and the given sample volume.

As an example, malathion (log Ko/w=2.29) is enriched from a 10 mL water sample. This compound can be recovered from the sample for 31.9% when a Twister of type 1 (1.0 mm long, 0.5 mm df PDMS) is used. For the types 2, 3 and 4, this is 55.1, 47.8 and 71.1%, respectively (Figure 1). This means that if malathion is present in the water in a concentration of 10 µg/L (total amount=100 ng), 31.9 ng is theoretically enriched in Twister type 1. With the other Twisters, this is 55.1, 47.8 and 71.1 ng, respectively.

Octanol-water distribution coefficients (Ko/w)

The log Ko/w-value for a large series of solutes is available in the literature and can also be calculated from its CAS number of chemical structure using the SRC KOWWIN calculator [2] that is available free of charge from the EPA website at URL <http://www.epa.gov/opptintr/exposure/docs/episuite.html>.

References

- [1] E. Baltussen, P. Sandra, F. David and C.A. Cramers, J. Microcolumn Sep., 11 (1999) 737.
- [2] W.M. Meylan, SRC KOWWIN software, SRC-LOGKOW Version 1.66, Syracuse Research Corporation, Syracuse, USA.

Stir Bar Sorptive Extraction Recovery Calculator

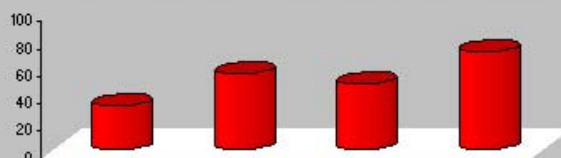
- Available Twister types

	type 1	type 2	type 3	type 3
Length L x film thickness df:	10 mm x 0.5 mm	10 mm x 1.0 mm	20 mm x 0.5 mm	20 mm x 1.0 mm
Twister volume (μL)	24	63	47	126

- Sample Volume (mL) = mL

- Compound log K_{ow} =

RECOVERY (%)	set 1	set 2	set 3	set 4
	31.9	55.1	47.8	71.1



- Locate your results in the SBSE recovery curves

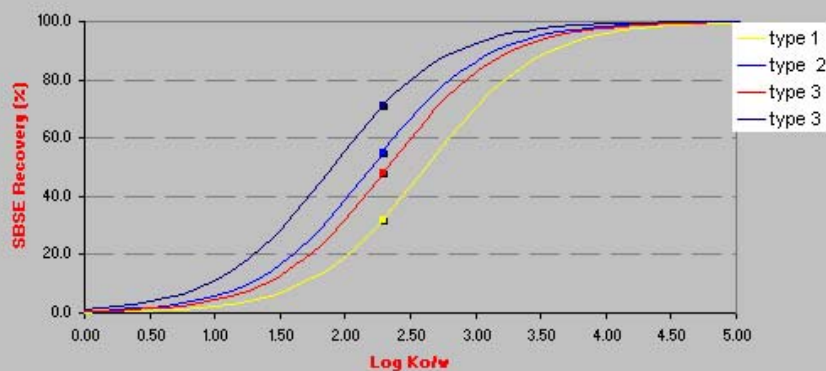


Figure 1. Snapshot of the SBSE Recovery Calculator for the analysis of malathion (log K_{ow}=2.29) in a 10 mL water sample.

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