

Electronic Supplementary Information  
for the Paper

## Optimisation of an HPLC Selected Reaction Monitoring Electrospray Tandem Mass Spectrometry Method for the Detection of 50 Arsenic Species

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### Contents:

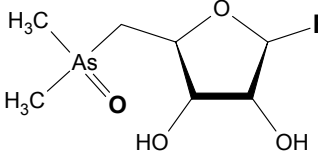
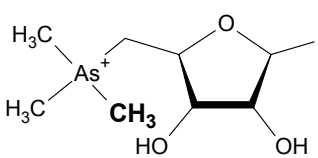
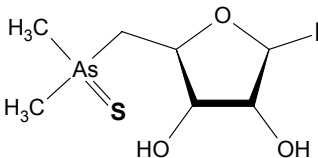
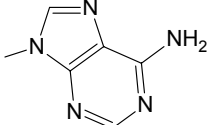
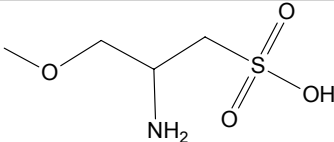
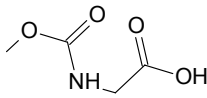
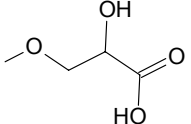
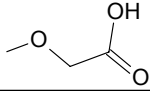
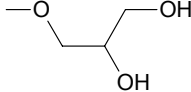
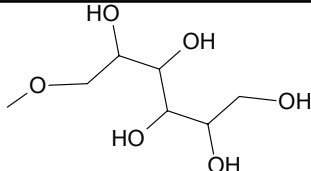
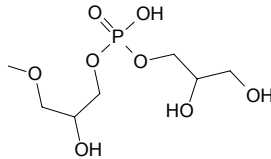
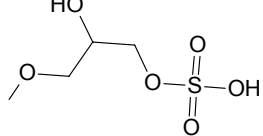
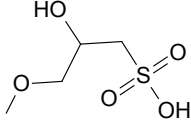
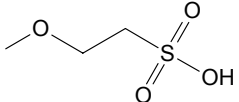
- Structures and names of the investigated arsenic species S2-3

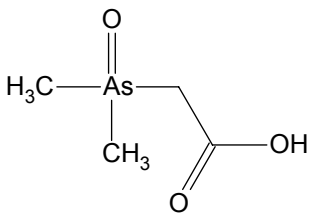
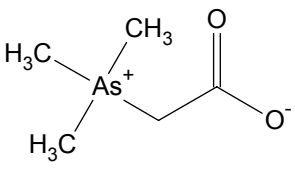
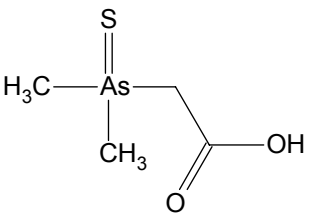
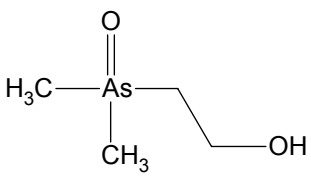
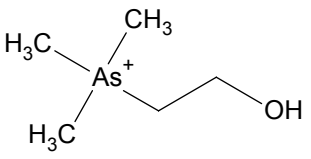
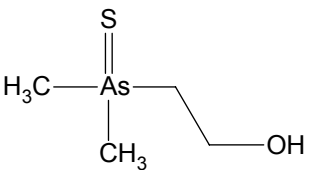
The abbreviations for the arsenosugars are composed of 4 parts

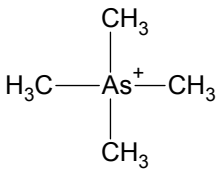
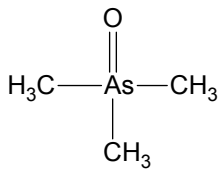
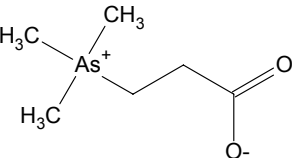
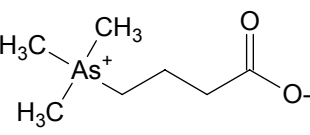
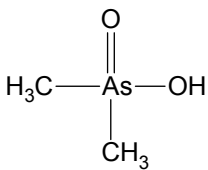
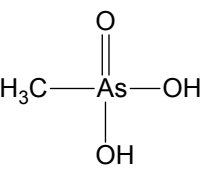
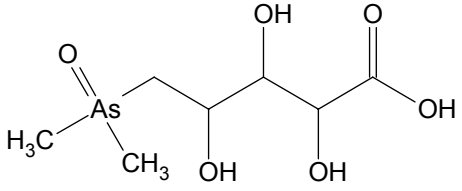
[Nischwitz, V., Pergantis, S.A., *Anal. Chem.*, 2005, **77**, 5551-5563]:

1. The number of methyl-groups bound to the arsenic atom: **DM** for Dimethyl,  
**TM** for Trimethyl
2. Only for the thio-arsenosugars: **Thio**
3. The common core for all  $\beta$ -ribofuranosides: **AsSugar**
4. The characteristic functional group in the aglycone: e.g. **Glycol**

- Collision induced dissociation (CID) breakdown curves for 14 arsenic species S4-8

| R               | DMAsSugar-   | TMAsSugar-   | DMThioAsSugar-  |
|-----------------|--|--|---|
|                 |     |    |  |
| Adenine         |    |  |   |
| Amino-Sulfonate |    |  |   |
| Carbamate       |     |  |   |
| Carboxyl        |     |  |   |
| Carboxyl-2      |    |  |   |
| Glycol          |   |  |   |
| Hydroxy         | -OH  |  |   |
| Mannitol        |  |  |   |
| Methoxy         | -O-CH <sub>3</sub>   |  |   |
| Phosphate       |  |  |   |
| Sulfate         |  |  |   |
| Sulfonate       |   |  |   |
| Sulfonate-2     | (proposed structure in analogy to Carboxyl-2)  |  |   |

|                       | DMArsinoyl-  | TMArsonio-  | DMThioArsinoyl-   |
|-----------------------|--|---|---|
| acetic acid (acetate) |  <p>Dimethylarsinoyl-acetic acid (DMAA)</p> |  <p>Arsenobetaine (AsB)</p> |  <p>Dimethylthioarsinoyl-acetic acid</p> |
| ethanol               |  <p>Dimethylarsinoyl-ethanol (DMAE)</p>     |  <p>Arsenocholine (AsC)</p> |  <p>Dimethylthioarsinoyl-ethanol</p>     |

|  |   |  |   |
|--|---|--|---|
| Tetramethylarsonium ion (TMA)  |  | Trimethylarsine oxide (TMAO)   |  |
| Trimethylarsonio-propionate (AsB-2)  |  | Trimethylarsonio-butyrate (AsB-3)  |  |
| Dimethylarsinic acid (DMA)   |  | Monomethylarsonic acid (MMA)   |  |
| 5-Dimethylarsinoyl-2,3,4-trihydroxypentanoic acid (DMArsinoylTrihydroxypentanoic acid) |   |  |   |

