

Supplementary Data

Table S1. Concentration and recovery percentages for Mixture A compounds (10 mg/L), injected at different times after preparation

| Concentration (mg/L) | | | | | | | | |
|----------------------|---------|---------|--------------|-----------|--------|------------|--------|-------------|
| Time (hours) | Benzene | Toluene | Ethylbenzene | o- Xylene | Indene | m/p-Xylene | Indane | Naphthalene |
| 1 | 10.74 | 10.65 | 10.51 | 10.25 | 9.97 | 10.88 | 10.48 | 10.52 |
| 2 | 10.56 | 10.52 | 10.44 | 10.20 | 9.93 | 10.58 | 10.34 | 10.39 |
| 6 | 10.81 | 10.75 | 10.62 | 10.59 | 10.27 | 10.45 | 10.44 | 10.47 |
| 12 | 9.12 | 9.56 | 9.60 | 9.59 | 9.53 | 9.69 | 9.91 | 9.98 |
| 24 | 6.55 | 7.62 | 7.96 | 8.02 | 7.65 | 8.25 | 8.63 | 8.80 |
| Recovery (%) | | | | | | | | |
| 1 | 107 | 107 | 105 | 103 | 100 | 109 | 105 | 105 |
| 2 | 106 | 105 | 104 | 102 | 99 | 106 | 103 | 104 |
| 6 | 108 | 107 | 106 | 106 | 103 | 104 | 104 | 105 |
| 12 | 91 | 96 | 96 | 96 | 95 | 97 | 99 | 100 |
| 24 | 66 | 76 | 80 | 80 | 77 | 83 | 86 | 88 |

Table S2. Specific conditions of each detector used in this study

| UV | | | |
|-----------------|----------------|---------------------|--------------------|
| Wavelength (nm) | Bandwidth (nm) | ref Wavelength (nm) | ref Bandwidth (nm) |
| 210 | 1 | 600 | 1 |
| FLD | | | |
| Excitation (nm) | Emission (nm) | Sensitivity | Filter wheel |
| 210 | 260 | 4 | auto |
| 260 | 330 | 2 | auto |
| 280 | 310 | 4 | auto |

For the UV detector, the data collection rate is 50 and the response time is 500 ms.

The FLD detector has a multichannel performance, where the collection data rate and response time can be defined itself. In this study, the standard option with a maximum of 4hz data collection rate and the response time is less than 250 ms was used. When the filter wheel is auto, the detector automatically selects a filter wheel position.

Table S3. T-test P-values at each concentration tested for the compounds in mixture A, in groundwater. Highlighted columns

| Concentration | Mixture A | | | | | | | |
|---------------|-----------|-------|-------|-------|---------|-------|-------|-------|
| | B | T | E | o-X | m/p-X | IA | IE | N |
| 0.5 mg/L | 0.429 | 0.868 | 0.678 | 0.669 | < 0.001 | 0.609 | 0.477 | 0.124 |
| 1 mg/L | 0.076 | 0.220 | 0.009 | 0.038 | 0.002 | 0.189 | 0.189 | 0.110 |
| 2.5 mg/L | 0.116 | 0.238 | 0.159 | 0.150 | 0.002 | 0.017 | 0.078 | 0.380 |
| 5 mg/L | 0.676 | 0.208 | 0.205 | 0.359 | 0.001 | 0.141 | 0.009 | 0.004 |
| 7.5 mg/L | 0.850 | 0.423 | 0.390 | 0.278 | 0.002 | 0.986 | 0.070 | 0.001 |
| 10 mg/L | 0.762 | 0.530 | 0.432 | 0.278 | 0.001 | 0.158 | 0.097 | 0.003 |

represent p-values < 0.05, indicating a significant matrix effect

B; benzene, T; toluene, E; ethylbenzene, X; xylene, IA; indane, IE; indene, N; naphthalene

Table S4. T-test P-values at each concentration tested for the compounds in mixture B, in medium. Highlighted columns

| Concentration | Mixture B | | | |
|---------------|-----------|-------------------|---------|---------|
| | Benzene | Monochlorobenzene | 1,2-DCB | 1,4-DCB |
| 1 mg/L | 0.055 | 0.031 | 0.276 | 0.059 |
| 2.5 mg/L | 0.043 | 0.005 | 0.033 | 0.001 |
| 5 mg/L | 0.007 | 0.020 | 0.062 | 0.017 |
| 7.5 mg/L | 0.007 | 0.027 | 0.067 | 0.016 |
| 12 mg/L | 0.020 | 0.016 | 0.017 | 0.053 |

represent p-values < 0.05, indicating a significant matrix effect

DCB; Dichlorobenzene

Table S5. Intercept, slope and R² values of the linear calibration line from the compounds of mixture A

| Compounds | Mixture A | | | | | | | |
|----------------|-----------|--------|--------|--------|--------|--------|--------|--------|
| | B | T | E | o-X | m/p-X | IA | IE | N |
| Intercept (a) | 12116 | 59006 | 72661 | 62736 | 639601 | 200006 | 231467 | 200006 |
| Slope (b) | 2194 | 8707 | 9974 | 4655 | 81357 | 142190 | 35704 | 106999 |
| R ² | 0.998 | 0.9984 | 0.9988 | 0.9968 | 0.9986 | 0.9993 | 0.9988 | 0.9994 |

B; benzene, T; toluene, E; ethylbenzene, X; xylene, IA; indane, IE; indene, N; naphthalene

Table S6. Intercept, slope and R² values of the linear calibration line from the compounds of mixture B

| Compounds | Mixture B | | | |
|----------------|-----------|-------------------|---------|---------|
| | Benzene | Monochlorobenzene | 1,2-DCB | 1,4-DCB |
| Intercept (a) | 0.8476 | 1.7032 | 1.4351 | 1.3978 |
| Slope (b) | 0.324 | 0.8452 | 0.9298 | 1.1396 |
| R ² | 0.9987 | 0.9971 | 0.9936 | 0.9916 |

DCB; Dichlorobenzene

Table S7. RSD values for each compound in mixture A, at different concentrations for the determination of intermediate precision of the method

| Intermediate Precision | | | | | | | | |
|------------------------|-------|-------|------|------|-------|-------|------|------|
| (%) | | | | | | | | |
| Concentration | B | T | E | o-X | m/p-X | IA | IE | N |
| 0.5 mg/L | 10.91 | 8.19 | 7.30 | 4.34 | 1.11 | 9.15 | 2.09 | 0.25 |
| 1 mg/L | 14.39 | 10.35 | 7.29 | 5.88 | 0.25 | 9.24 | 0.59 | 2.22 |
| 2.5 mg/L | 4.47 | 1.82 | 1.66 | 2.46 | 2.60 | 1.39 | 2.75 | 3.39 |
| 5 mg/L | 1.78 | 3.88 | 2.64 | 2.18 | 0.96 | 13.22 | 2.39 | 3.05 |
| 7.5 mg/L | 4.58 | 3.38 | 1.98 | 1.83 | 3.12 | 0.61 | 1.49 | 2.81 |
| 10 mg/L | 7.78 | 6.14 | 3.55 | 3.14 | 3.53 | 12.64 | 2.86 | 2.74 |

B; benzene, T; toluene, E; ethylbenzene, X; xylene, IA; indane, IE; indene, N; naphthalene

Table S8. RSD values for each compound in mixture B, at different concentrations for the determination of intermediate precision of the method

| Intermediate Precision | | | | |
|------------------------|---------|-------------------|---------|---------|
| (%) | | | | |
| Concentration | Benzene | Monochlorobenzene | 1,2-DCB | 1,4-DCB |
| 1 mg/L | 2.88 | 0.68 | 2.56 | 3.51 |
| 2.5 mg/L | 3.43 | 2.45 | 2.57 | 3.68 |
| 5 mg/L | 3.67 | 4.01 | 1.48 | 3.46 |
| 7.5 mg/L | 1.57 | 1.89 | 2.46 | 3.16 |
| 12 mg/L | 1.60 | 1.58 | 3.00 | 3.65 |

DCB; Dichlorobenzene

Table S9. Recovery values and mean recovery percentages obtained at 10 mg/L for mixture A.

| Recovery (10 mg/L) | | | | | | | | |
|----------------------------|------|-------|-------|-------|-------|-------|-------|-------|
| | B | T | E | o-X | m/p-X | IA | IE | N |
| Sample 1 | 8.70 | 10.31 | 10.05 | 10.09 | 10.19 | 10.18 | 10.31 | 10.64 |
| Sample 2 | 8.88 | 10.89 | 11.24 | 11.63 | 10.98 | 10.85 | 10.89 | 11.36 |
| Recovery (mean) | 88% | 106% | 106% | 109% | 106% | 105% | 106% | 110% |

B; benzene, T; toluene, E; ethylbenzene, X; xylene, IA; indane, IE; indene, N; naphthalene

Table S10. Recovery values and mean recovery percentages obtained at 10 mg/L for mixture B.

| Recovery (10 mg/L) | | | | |
|----------------------------|---------|-------|---------|---------|
| | Benzene | MCB | 1,2-DCB | 1,4-DCB |
| Sample 1 | 8.33 | 10.62 | 9.49 | 9.35 |
| Sample 2 | 8.01 | 10.23 | 9.32 | 9.50 |
| Recovery (mean) | 82% | 104% | 94% | 94% |

MCB; Monochlorobenzene, DCB; Dichlorobenzene