Data Article

A dataset of 112 ligands for the preconcentration of mercury, uranium, lanthanum and other pollutants and heavy metals in water

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A B S T R A C T

This dataset manuscript describes the preparation procedure and lists the preconcentration efficiency of 112 ligands, immobilized on solid-state polymer membranes, for pollutants/elements monitoring in tap water and in environmentally relevant water matrices. Specifically, the energy dispersive X-ray fluorescence (EDXRF) spectra are presented, along with the preconcentration efficiency of each ligand in tap water. The main materials required for membrane preparation include the membrane matrix, a plasticizer, an ionophore, a catalyst (used only when producing anion-selective membranes), and a complexing agent, i.e. ligand. These are simply mixed, applied on a desired surface, here on a BoPET (biaxially-oriented polyethylene terephthalate) film (Mylar®), and left to dry and solidify, producing anion- or cation-selective membranes. Once the membranes are produced, they can be used even by non-specialised personnel directly on the field, which could be of particular importance for low and middle income countries (LMIC) and for remote or insular areas. The membranes can be functionalised with different ligands, suggesting that they can be used for identifying a vast array of different pollutants/elements in water matrices. Here a dataset of 112 ligands, immobilized on anion-selective membranes, are presented in terms of calcium (Ca), iron (Fe), nickel (Ni), zinc (Zn), antimony (Sb), lanthanum (La), uranium (U), copper (Cu), and gold (Au) preconcentration in tap water. Strontium (Sr) was also attempted to be measured, however, quantifiable results were not obtained.

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Furthermore, data for mercury (Hg) preconcentration, in cation-selective membranes, are also given. The enclosed data show that the most promising ligand for Hg, Ca, Fe, Ni, Zn, Sr, La, U, Cu, and Au preconcentration were 4-(2-Pyridylazo)resorcinol, Eriochrome Black T, di-Ammonium hydrogen citrate, 1,5-Diphenylcarbazide, dithizone, 1,1'-Carbonyldiimidazole, Bis(cyclopentadienyl)titanium dichloride, sodium dibenzylthiocarbamate, calconcarbonsaure, and dibenzoylmethane, respectively. Interpretation of the data can be found in our previous work [1]. Overall, the main intention of this dataset manuscript is to communicate and promote the adoption of the proposed method by researchers and the water industry alike. This could further advance the method and encourage the assessment of additional ligands or/and pollutants/elements, including heavy metals which are typically found in water.

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### Specifications Table

| Subject                  | Analytical Chemistry, Environmental Chemistry, Environmental Engineering |
|--------------------------|--------------------------------------------------------------------------|
| Specific subject area    | Environmental monitoring and assessment of water                          |
| Type of data             | Table:                                                                   |
|                          | The preconcentration efficiencies, in counts/300s, for 112 ligands and for the Ca, Fe, Ni, Zn, Sr, La, U, Cu, and Au |
|                          | Image:                                                                   |
|                          | Photographs of the membrane preparations steps.                          |
|                          | Graph:                                                                   |
|                          | The EDXRF spectra for Hg preconcentration in tap water using i) 4-(2-Pyridylazo)resorcinol (PAR), ii) thiourea, iii) dithizone, and iv) calconcarbonsaure (CCS) functionalised membranes. |
| How data were acquired   | The data were acquired by Energy dispersive X-ray fluorescence (EDXRF) spectrometry |
|                          | Instruments: Pictures were taken using a compact digital camera.          |
|                          | The spectra were obtained by an EDXRF spectrometer                       |
|                          | Model AMETEK SPECTRO XEPOS unit                                          |
|                          | The spectra were processed with X-Lab Pro 4.0 software, using the TurboQuant screening method. |
| Data format              | The raw EDXRF spectra were collected using the secondary/molybdenum mode at 40 kV and 0.9 mA, with helium gas flushing, and 300 s irradiation duration. |
| Parameters for data collection | The processed spectra in shown in, Tables in .docx, diagrams in .xls format |
| Description of data collection | The images of the membrane preparations steps in .jpg format |
|                          | Pictures were taken at the laboratory showing the membrane preparation procedure. The EDXRF spectra were collected by an AMETEK SPECTRO XEPOS unit, using the secondary/molybdenum mode at 40 kV and 0.9 mA, with helium gas flushing, and 300 s irradiation duration. |
| Data source location     | Laboratory of Analytical and Environmental Chemistry/Technical University of Crete/University Campus/Chania/Greece |
| Data accessibility       | With the article                                                         |
| Related research article | N. Kallithrakas-Kontos, S. Foteinis, E. M. Vazgiouraki, A. G. Karydas, J. Osán, E. Chatzisymeon, Solid-state polymer membranes for simple, sensitive, and low-cost monitoring of mercury in water, Science of The Total Environment, 697, 2019, 134099, https://doi.org/10.1016/j.scitotenv.2019.134099 |
1. Data description

The effectiveness of solid-state polymer membranes for mercury preconcentration in water was examined in a recent work of our group [1]. In this data article the EDXRF spectra (Fig. 1) along with the raw EDXRF data for Hg preconcentration in water are given. In addition, the raw EDXRF data regarding the screening of 112 ligands, immobilized on anion-selective solid-state membranes, for calcium (Ca), iron (Fe), nickel (Ni), zinc (Zn), strontium (Sr), lanthanum (La), uranium (U), copper (Cu), and gold (Au) preconcentration in tap water are enclosed (multimedia component 1-112). Table 1 lists the quantitative values of the data.

The dataset regarding the membrane preparation procedure, i.e. the enclosed pictures and description, can be put forward by other researchers and the water industry alike to test, further improve, and apply the method to address real-world problems. The membranes are easily reproducible, cost-effective, and easy to use even by non-specialised personnel. Therefore, the dataset regarding the membrane preparation procedure also can encourage the application of the method in low and middle-income countries (LMIC), where the identification and monitoring of clean water resources is a matter of emerging concern [2].

More importantly, the raw and processed EDXRF datasets covering 112 ligands, which were screened in terms of targeted pollutants/elements identification and quantification in tap water, can provide context with the literature and promote further research to furnish the proposed method, both in terms of efficiency and practicality.

Finally, the data can be put forward by other researchers to examine additional ligands and/or pollutants/elements, thus complementing the enclosed dataset.

Fig. 1. The preconcentration efficiency for Hg(II) in tap water and for four different membranes functionalised with a) resorcinol (PAR), b) dithizone, c) thiourea, and d) CCS. Around 12,643 channels correspond to 1 keV.
| Ligand                                                                 | Ca   | Fe   | Ni   | Zn   | Sr   | Au  | U    | La   | Cu   |
|------------------------------------------------------------------------|------|------|------|------|------|-----|------|------|------|
| 1. Amarillo de titan (Titan yellow)                                     | 14   | 324  | 0    | 42   | 0    | 119 | 31   | 40   | 127  |
| 2. Methyl orange 0.1%                                                  | 32   | 385  | 118  | 111  | 69   | 136 | 40   | 70   | 91   |
| 3. Alizarin Red S                                                      | 2259 | 156  | 100  | 3246 | 116  | 128 | 0    | 99   | 3153 |
| 4. Bromophenol blue                                                    | 0    | 242  | 0    | 0    | 0    | 313 | 0    | 0    | 0    |
| 5. Azul blue de bromothymol 0.04%                                      | 0    | 187  | 104  | 0    | 0    | 43  | 0    | 0    | 0    |
| 6. Bromocresol green                                                   | 0    | 95   | 0    | 50   | 0    | 133 | 0    | 0    | 77   |
| 7. Eriochrome cyanine R                                                | 0    | 4    | 0    | 873  | 0    | 90  | 0    | 0    | 2163 |
| 8. Hydroxynaphthol blue                                               | 0    | 0    | 0    | 271  | 0    | 64  | 0    | 0    | 1803 |
| 9. Bromothymol blue                                                    | 6    | 0    | 94   | 0    | 117  | 135 | 0    | 44   | 0    |
| 10. Eriochrome Black T                                                | 12662| 235  | 0    | 4132 | 0    | 175 | 378  | 78   | 5402 |
| 11. 1-(2-Pyridylazo)-2-naphthol                                        | 381  | 289  | 265  | 13357| 103  | 217 | 0    | 0    | 1713 |
| 12. 1-(3-Dimethylaminopropyl)-3-ethy carbodiimide, polymer-bound       | 78   | 139  | 263  | 0    | 0    | 126 | 303  | 0    | 5333 |
| 13. 1-Butyl-3-methylimidazolium hexafluorophosphate                     | 61   | 831  | 344  | 362  | 0    | 86  | 0    | 188  |      |
| 14. 1,10-Phenanthroline monohydrate                                    | 0    | 1102 | 572  | 317  | 0    | 10  | 0    | 185  |      |
| 15. D(-)-Fructose                                                      | 109  | 299  | 163  | 52   | 0    | 52  | 0    | 26   | 12   |
| 16. 1,10-Phenanthroline 1/40 M Ferroin solution                        | 0    | 222  | 211  | 0    | 0    | 159 | 0    | 0    | 35   |
| 17. 1,1'-Carbonyldiimidazole                                           | 93   | 176  | 100  | 269  | 148  | 98  | 0    | 0    | 97   |
| 18. 1,5-Diphenylcarbazide                                              | 31   | 170  | 1226 | 0    | 0    | 117 | 0    | 0    | 7    |
| 19. 1,6-Diaminohexane-N,N,N',N'-tetraacetic acid                       | 404  | 356  | 160  | 0    | 35   | 22  | 0    | 42   | 0    |
| 20. 1-Benzimidazole                                                    | 132  | 162  | 145  | 0    | 64   | 108 | 44   | 104  | 19   |
| 21. 1-Butyl-3-methylimidazolium tetrafluoroborate                      | 53   | 675  | 38   | 283  | 0    | 139 | 0    | 35   | 271  |
| 22. 1-Hexanesulfonic acid sodium salt                                  | 29   | 750  | 403  | 0    | 0    | 100 | 0    | 65   | 0    |
| 23. 1-Nitroso-2-naphthol                                              | 159  | 1157 | 103  | 879  | 0    | 61  | 0    | 26   | 776  |
| 24. 2-Aminobenzothiazole                                              | 0    | 508  | 36   | 287  | 0    | 45  | 0    | 64   | 143  |
| 25. 2-Aminothiazole                                                   | 0    | 2250 | 402  | 119  | 0    | 161 | 0    | 0    | 167  |
| 26. 2-Mercaptopyrimidine                                               | 338  | 942  | 41   | 702  | 81   | 256 | 0    | 34   | 825  |
| 27. 2-(5-Bromo-2-pyridylazo)-5-(diethylamino)phenol                    | 0    | 111  | 0    | 17   | 0    | 141 | 0    | 36   | 156  |
| 28. 2,4,6-Tris(2-pyridyl)-s-triazine                                   | 86   | 371  | 90   | 172  | 0    | 88  | 0    | 20   | 39   |
| 29. 2-Hydroxybiphenyl 98%                                              | 11   | 655  | 461  | 100  | 0    | 154 | 0    | 35   | 100  |
| 30. 2-Mercaptobenzimidazole                                           | 0    | 64   | 0    | 1759 | 0    | 67  | 0    | 35   | 1391 |
| 31. 2-Mercaptobenzothiazole                                           | 0    | 426  | 293  | 246  | 0    | 96  | 0    | 0    | 593  |
| 32. 3-(2-Pyridyl)-5,6-diphenyl-1,2,4-triazine.-p,p'-disulfonic acid    | 169  | 515  | 40   | 703  | 140  | 0   | 0    | 29   | 242  |
| 33. 3'-Diaminobenzidine tetrahydrochloride hydrate                     | 0    | 2364 | 986  | 0    | 0    | 230 | 0    | 43   | 661  |
| 34. 3,5-Diaminobenzoic acid 98%                                        | 4    | 2328 | 857  | 117  | 53   | 65  | 0    | 25   | 498  |
| 35. 4- Aminosalicylic acid                                            | 0    | 13   | 107  | 0    | 0    | 218 | 241  | 36   | 511  |
| 36. 4-(4-Nitophenylazo)-1-naphthol                                    | 0    | 258  | 77   | 161  | 0    | 123 | 0    | 27   | 101  |
| 37. 4- Nitrocatechol                                                  | 622  | 2246 | 677  | 311  | 0    | 210 | 0    | 37   | 1949 |
| Compound                                      | 4-(2-Pyridylazo)resorcinol | 4-(2-Thiazolylazo)resorcinol | 4-Chlorophenol | 4-Chlorophenyl sulfoxide | 5-Amino-1,3,4-thiadiazole-2-thiol | 5-Sulfoisaliclyc acid | 5-(4-Dimethylaminobenzyldiene)-rhodanine | 3-(2-Pyridyl)-5,6-diphenyl-1,2,4-triazine | 8-Hydroxyquinoline | a-Benzoin oxime | Cupric acetylacetonate | Ammonium hexacyanoferrate(II) hydrate | Ammonium pyrrolidinedithiocarbamate | Antipyrine 98% | Barbituric acid | Bis(cyclopentadienyl)titanium dichloride | Bis(cyclopentadienyl)zirconium dichloride | Bismuthiol I | N,N-Diethyl-p-phenylenediamine sulfate salt | Calconcarbonsaure | Cibacron Blue F3G-A | Cytidine, cell culture | Dibenzoylemethane | Dimethylglyoxime | 4-Methylcatechol | Diphenylcarbazone | Dithiooxamide | Dithione | Epichlorohydrin | HEDTA | Hippuric acid 98% | Hydrazine sulfate | Mercury ionophore I | Michler's Ketone | Murexide | N-Benzoyl-N-phenylhydroxylamine | N.N.N',N'-Tetramethyl-1,8-naphthalenediamine | N-Hydroxysulfosuccinimide sodium salt | Nicotinic acid | Nitroso-R-salt |
|-----------------------------------------------|-----------------------------|-------------------------------|----------------|-------------------------|---------------------------------|-----------------------|-----------------------------------------------|-------------------------------------------------|--------------------------------|----------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------|---------------------------------|-----------------------------------------------|-----------------------------------------------|--------------------------------|-----------------------------------------------|---------------------------------------------|----------------------------------------------|---------------------------------|-------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|---------------|-----------------------------|------------------------------------------------|--------------------------------|-----------------------------|
| 38.                                           | 22                          | 498                           | 364            | 4085                    | 0                               | 210                   | 341                           | 0                                               | 439                              |                |                                |                                                                                  |                                                            |                                                                                           |    | 57.                                           | 251                          | 463                          | 351                          | 6276                    | 30                             | 224                   | 1073                          | 207                              | 5899                           |                                                                  |                                |                                             | 58.                                           | 739                          | 840                          | 258                          | 255                        | 65                            | 266                   | 35                            | 622                              | 3553                           |                                                                  |                                |                                             | 59.                                           | 292                          | 315                          | 240                          | 0                            | 136                           | 0                     | 37                            | 147                              | 12590                          |                                                                  |                                |                                             | 60.                                           | 158                          | 2431                         | 952                          | 90                         | 0                              | 174                   | 67                             | 80                                | 231                             |                                                                  |                                |                                             | 61.                                           | 309                          | 1085                         | 219                          | 658                       | 108                           | 211                   | 66                             | 97                               | 12590                          |                                                                  |                                |                                             | 62.                                           | 0                            | 428                          | 310                          | 34                         | 0                              | 40                     | 0                              | 27                                | 10                               |                                                                  |                                |                                             | 63.                                           | 0                            | 163                          | 38                           | 1059                      | 0                              | 108                   | 175                           | 0                                  | 1340                           |                                                                  |                                |                                             | 64.                                           | 136                          | 366                          | 388                          | 9                          | 0                               | 169                   | 0                              | 33                                | 6                                |                                                                  |                                |                                             | 65.                                           | 0                            | 232                          | 198                          | 654                        | 0                              | 86                     | 0                              | 70                                | 899                             |                                                                  |                                |                                             | 66.                                           | 0                            | 264                          | 346                          | 270                        | 18809                  | 0                              | 192                   | 46                             | 89                                | 10609                          |                                                                  |                                |                                             | 67.                                           | 0                            | 693                          | 465                          | 203                        | 0                             | 91                     | 0                              | 59                                | 59                              |                                                                  |                                |                                             | 68.                                           | 0                            | 509                          | 563                          | 173                        | 268                        | 99                        | 162                    | 0                             | 53                     | 472                            |                                                                  |                                |                                             | 69.                                           | 0                            | 199                          | 97                           | 0                          | 109                       | 75                         | 46                       | 12                     |                                                                  |                                |                                             | 70.                                           | 135                          | 443                          | 290                          | 374                        | 0                             | 167                   | 116                           | 63                                | 109                             |                                                                  |                                |                                             | 71.                                           | 0                            | 1006                         | 63                            | 12                        | 88                      | 51                         | 0                             | 36                     | 40                                |                                                                  |                                |                                             | 72.                                           | 0                            | 248                          | 383                          | 5                          | 0                             | 121                   | 0                              | 0                               | 0                                |                                                                  |                                |                                             | 73.                                           | 197                          | 0                            | 0                            | 0                          | 0                             | 91                     | 0                              | 38                                | 0                                |                                                                  |                                |                                             | 74.                                           | 0                            | 19                            | 375                          | 0                          | 0                             | 65                     | 0                              | 35                                | 25                                |                                                                  |                                |                                             | 75.                                           | 0                            | 153                          | 108                          | 401                        | 0                             | 290                   | 0                             | 35                                | 763                             |                                                                  |                                |                                             | 76.                                           | 0                            | 340                          | 138                          | 70                         | 0                             | 198                   | 0                              | 57                                | 53                              |                                                                  |                                |                                             | 77.                                           | 0                            | 130                          | 83                           | 20                         | 0                             | 152                   | 0                              | 41                                | 20                              |                                                                  |                                |                                             | 78.                                           | 0                            | 554                          | 135                          | 124                        | 0                             | 173                   | 0                              | 0                               | 141                             |                                                                  |                                |                                             | 79.                                           | 194                          | 1240                         | 107                          | 167                        | 90                        | 208                    | 0                             | 38                                | 146                             |                                                                  |                                |                                             | 80.                                           | 0                            | 298                          | 0                            | 0                          | 106                        | 0                         | 106                            | 0                                | 257                             |                                                                  |                                |                                             | 5.                                             | 5                            | 10                           | 27                           | 4                          | 0                             | 4                     | 0                              | 0                                | 0                                |                                                                  |                                |                                             | (continued on next page)                                                   |  

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| Ligand                                           | Ca       | Fe       | Ni       | Zn       | Sr       | Au       | U        | La       | Cu       |
|------------------------------------------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 81. o-Dianisidine                                | 0        | 132      | 29       | 27       | 62       | 159      | 43       | 35       | 159      |
| 82. Orotic acid                                 | 99       | 150      | 126      | 245      | 0        | 85       | 0        | 48       | 138      |
| 83. Sodium oxalate                              | 0        | 184      | 0        | 104      | 95       | 181      | 70       | 44       | 93       |
| 84. Phenyl acetate 99%                          | 7        | 572      | 128      | 161      | 0        | 99       | 0        | 66       | 84       |
| 85. 2,6-Pyridinedicarboxylic acid               | 92       | 0        | 934      | 0        | 0        | 48       | 0        | 34       |          |
| 86. Quinaldic acid 98%                          | 248      | 278      | 391      | 0        | 0        | 0        | 0        | 30       | 0        |
| 87. Rhodizonic acid disodium salt               | 40       | 558      | 857      | 706      | 114      | 108      | 0        | 46       | 608      |
| 88. Sodium cyanide                              | 53       | 376      | 43       | 0        | 0        | 120      | 0        | 63       | 13       |
| 89. Sodium dibenzylthiocarbamate                | 32       | 661      | 149      | 1291     | 0        | 722      | 0        | 33       | 9976     |
| 90. Sodium diethylthiocarbamate trihydrate      | 34       | 430      | 105      | 106      | 0        | 56       | 82       | 45       | 497      |
| 91. syn-2-Pyrindineldaloxime                    | 39       | 266      | 98       | 44       | 0        | 93       | 0        | 57       | 23       |
| 92. Thymine                                     | 0        | 416      | 0        | 80       | 88       | 85       | 0        | 0        | 0        |
| 93. Titrplex II (ethylenedinitrilotetraacetic acid) | 25   | 0        | 0        | 0        | 80       | 47       | 47       | 62       | 0        |
| 94. Triethylenetetramine-N,N,N',N'-hexaacetic acid | 45   | 431      | 654      | 0        | 64       | 13       | 0        | 42       | 0        |
| 95. Trioctyolphosphine oxide                     | 0        | 179      | 778      | 0        | 0        | 191      | 62       | 34       | 50       |
| 96. Xylenol orange, sodium salt                 | 0        | 337      | 226      | 32       | 69       | 83       | 52       | 25       | 0        |
| 97. N,N,N',N'-Tetraacetic acid                  | 0        | 78       | 0        | 0        | 39       | 54       | 43       | 0        |          |
| 98. N-Allyliothiurea                             | 0        | 395      | 0        | 143      | 0        | 416      | 107      | 41       | 403      |
| 99. Menthol                                     | 77       | 405      | 227      | 110      | 0        | 62       | 0        | 25       | 59       |
| 100. Cupferron                                  | 7        | 650      | 260      | 126      | 109      | 119      | 0        | 25       | 173      |
| 101. Thiourea                                   | 0        | 307      | 441      | 0        | 0        | 286      | 0        | 126      | 203      |
| 102. Starch                                     | 65       | 310      | 128      | 153      | 0        | 134      | 0        | 32       | 73       |
| 103. Toluene-3,4-dithiol                        | 33       | 422      | 50       | 2774     | 0        | 119      | 0        | 0        | 2003     |
| 104. 1,1'-Carbonyl-di-(1,2,4-triazole)           | 32       | 950      | 200      | 23       | 0        | 42       | 0        | 45       | 23       |
| 105. L-carnosine                                | 163      | 542      | 0        | 245      | 0        | 118      | 0        | 95       | 205      |
| 106. Uracil                                     | 74       | 353      | 277      | 138      | 0        | 97       | 0        | 66       | 108      |
| 107. 1,8,9-Anthracenetriol                      | 60       | 74       | 47       | 407      | 0        | 137      | 164      | 45       | 3063      |
| 108. 3,3'-Diaminobenzidine                      | 0        | 0        | 0        | 0        | 0        | 72       | 0        | 1108     |          |
| 109. o-Phenanthroline                           | 0        | 0        | 0        | 0        | 0        | 84       | 0        | 0        |          |
| 110. Citric acid                                | 0        | 0        | 15       | 0        | 0        | 76       | 0        | 0        |          |
| 111. Arsenazo III                               | 446      | 190      | 108      | 10232    | 109      | 314      | 158      | 62       | 1391     |
| 112. Ferrocene                                  | 0        | 899      | 59       | 0        | 0        | 210      | 0        | 100      | 98       |
results for the 112 ligands, while the ten most promising ligands for the preconcentration of the targeted elements is shown in Figs. 2–4 and listed in Tables 2–10. The quantitative data used to generate Figs. 2–4 are also enclosed (Figs. 1–3.xlsx). To provide context, the blank spectrum of the Mylar® film alone (Mylar blank), as well as the spectrum of the membrane before being immersed in the water matrix (EVA blank) are also given in the enclosed dataset. Finally, in Figs. 5–7 photographs of experimental procedure and instrumentation, which has been previously described [1], are shown.

Specifically, the data regarding the Hg(II) preconcentration were obtained using cation-selective polymer-based membranes. The EDXRF spectra for the cation-selective membranes, using polyvinyl chloride (PVC) as the membrane matrix, and for four examined ligands, i.e. i) 4-(2-Pyridylazo)resorcinol (PAR), ii) thiourea, iii) dithizone, and iv) calconcarbonsaure (CCS) are shown in Fig. 1. As mentioned above, the raw data of the EDXRF spectra are also enclosed in this dataset manuscript. As shown in Fig. 1, resorcinol (PAR) appears to be the most promising ligand, judging from the Hg peak in the corresponding spectrum (Fig. 1a), for aqueous Hg(II) preconcentration, by and large, followed by dithizone and thiourea. On the other hand, CCS had a very low preconcentration efficiency, suggesting its limited potential for mercury preconcentration in water matrices. However, as will be discussed below, CCS was found particularly promising for U preconcentration in water.

In addition, the membranes were also screened using 112 different ligands were immobilized on the solid-state membranes and were screened regarding their preconcentration efficiency for the

![Fig. 2. Graphic presentation of the data for the ten most promising ligands, from higher to lower score, for a) Ca, b) Fe, c) Ni, and d) Zn preconcentration in tap water.](image-url)
Fig. 3. Graphic presentation of the data for the ten most promising ligands, from higher to lower score, for a) Sr, b) La, c) Au, and d) U preconcentration in tap water.

Cu preconcentration

Fig. 4. Graphic presentation of the data for the ten most promising ligands, from higher to lower score, for Cu preconcentration in tap water.
### Table 2
The ten most promising ligands for the calcium (Ca) preconcentration in the solid-state membranes.

| Ligand                                      | Counts/300s |
|---------------------------------------------|-------------|
| Eriochrome Black T                          | 12662       |
| Alizarin red S                              | 2259        |
| Cibacron Blue F3G-A                         | 739         |
| 4-Nitrocatechol                             | 622         |
| Fluorescein sodium                          | 509         |
| Arsenazo III                                | 446         |
| Barbituric acid                             | 430         |
| 1,6-Diaminohexane-N,N,N',N'-tetraacetic acid| 404         |
| 1-(2-Pyridylazo)-2-naphthol                 | 381         |
| 2-Mercaptopyrindimide                       | 338         |

### Table 3
The ten most promising ligands for the iron (Fe) preconcentration in the solid-state membranes.

| Ligand                                      | Counts/300s |
|---------------------------------------------|-------------|
| di-Ammonium hydrogen citrate                | 2431        |
| 2,4,6-Tris(2-pyridyl)-s-triazine             | 2401        |
| 2-Mercaptobenzimidazole                     | 2364        |
| 3,5-Diaminobenzoic acid 98%                 | 2328        |
| 2-Aminothiazole                             | 2250        |
| 4-Nitrocatechol                             | 2246        |
| Nicotinic Acid                              | 1240        |
| 1-Nitroso-2-naphthol                        | 1157        |
| 1,10-Phenanthroline monohydrate             | 1102        |
| Dibenzoylmethane                            | 1085        |

### Table 4
The ten most promising ligands for the nickel (Ni) preconcentration in the solid-state membranes.

| Ligand                                      | Counts/300s |
|---------------------------------------------|-------------|
| 1,5-Diphenylcarbazide                       | 1226        |
| 3,3'-Diaminobenzidine tetrahydrochloride hydrate| 986        |
| di-Ammonium hydrogen citrate                | 952         |
| 2,6-Pyridinedicarboxylic acid               | 934         |
| 3,5-Diaminobenzoic acid 98%                 | 857         |
| Rhodizonic acid disodium salt               | 857         |
| Triocetylphosphine oxide                    | 778         |
| 4-Nitrocatechol                             | 677         |
| 5-Sulfosalicylic acid                       | 659         |
| 1,10-Phenanthroline monohydrate             | 572         |

### Table 5
The ten most promising ligands for the zinc (Zn) preconcentration in the solid-state membranes.

| Ligand                                      | Counts/300s |
|---------------------------------------------|-------------|
| Dithizone                                   | 18809       |
| 1-(2-Pyridylazo)-2-naphthol                 | 13357       |
| Arsenazo III                                | 10232       |
| Calconcarbonsaure                           | 6267        |
| Eriochrome Black T                          | 4132        |
| 4-(2-Pyridylazo)resorcinol                  | 4085        |
| Bis(cyclopentadienyl)titanium dichloride    | 3353        |
| Alizarin red S                              | 3246        |
| Toluene-3,4-dithiol                         | 2774        |
| Bismuthiol I                                | 2182        |
Table 6
The ten most promising ligands for strontium (Sr) preconcentration in the solid-state membranes.

| Ligand                                                                 | Counts/300s |
|------------------------------------------------------------------------|-------------|
| 1,1’-Carbonyl-diimidazol                                               | 148         |
| 3-(2-Pyridyl)-5,6-diphenyl-1,2,4-triazine-p,p’-disulfonic acid          | 140         |
| Alizarin Red S                                                         | 116         |
| Rhodizonic acid disodium salt                                          | 114         |
| Cupferron                                                              | 109         |
| Arsenazo III                                                           | 109         |
| Dibenzoylmethane                                                       | 108         |
| 1-(2-Pyridylazo)-2-naphthol                                            | 103         |
| Barbituric acid                                                        | 99          |
| Fluorescein sodium                                                     | 99          |

Table 7
The ten most promising ligands for the lanthanum (La) preconcentration in the solid-state membranes.

| Ligand                                                                 | Counts/300s |
|------------------------------------------------------------------------|-------------|
| Bis(cyclopentadienyl)titanium dichloride                                | 391         |
| Calconcarbonsaure                                                      | 207         |
| Thiourea                                                               | 126         |
| 1-Benzylimidazole                                                      | 104         |
| Ferrocene                                                              | 100         |
| Alizarin Red S                                                         | 99          |
| Dibenzoylmethane                                                       | 97          |
| L-carnosine                                                            | 95          |
| Dithizone                                                              | 89          |
| Cupric acetylacetonate                                                 | 84          |

Table 8
The ten most promising ligands for the gold (Au) preconcentration in the solid-state membranes.

| Ligand                                                                 | Counts/300s |
|------------------------------------------------------------------------|-------------|
| Sodium dibenzylthiocarbamate                                           | 722         |
| N-Allylthiourea                                                        | 416         |
| Barbituric acid                                                        | 337         |
| Arsenazo III                                                           | 314         |
| Bromophenol blue                                                       | 313         |
| Cupric acetylacetonate                                                 | 292         |
| Murexide                                                               | 286         |
| Thiourea                                                               | 290         |
| Cibacron Blue F3G-A                                                   | 266         |
| 5-(4-Dimethylaminobenzylidene)-rhodanine                                | 263         |

Table 9
The ten most promising ligands for the uranium (U) preconcentration in the solid-state membranes.

| Ligand                                                                 | Counts/300s |
|------------------------------------------------------------------------|-------------|
| Calconcarbonsaure (CCS)                                                | 1073        |
| Eriochrome Black T                                                     | 378         |
| 4-(2-Pyridylazo)resorcinol                                             | 341         |
| 1-(3-Dimethylaminopropyl)-3-ethylcarbodiimide, polymer-bound           | 303         |
| 4- Aminosalicylic acid                                                | 241         |
| 4-Methy Catechol                                                       | 175         |
| 1,8,9-Anthracenetriol                                                  | 164         |
| Arsenazo III                                                           | 158         |
| Bis(cyclopentadienyl)zirconium dichloride                              | 124         |
| HEDTA                                                                  | 116         |
determination of 9 different pollutants/elements, i.e. Ca, Fe, Ni, Zn, Sr, La, U, Cu, and Au. The quantitative results of the EDXR measurements, along with the name of each examined ligand, are given in Table 1. It should be noted that the membranes were also screened in terms of antimony (Sb) preconcentration in water, however no quantifiable results were obtained and thus Sb is not included in Table 1. Specifically, during the screening process the efficiency of both anion- and cation-selective membranes was examined and it was identified that the vast majority of the examined pollutants/elements were preferably complexing with the ligand that was immobilized on anion-selective membranes. For this reason the 112 ligands were screened using anion-selective membranes, with the membrane matrix being ethylene vinyl acetate (EVA). To this end, 1 L of tap water was spiked with 20 μg L⁻¹ Au, 20 μg L⁻¹ La, 50 μg L⁻¹ U, 50 μg L⁻¹ Sb, and 100 μg L⁻¹ Sr. Then, each membrane was immersed in the spiked tap water and left for 24 h to reach equilibrium. In this screening process the water matrix (tap water) was not spiked with Hg(II), since the Hg(II) spectrum could overlap and largely interfere with that of Au, thus making Au quantification difficult. Furthermore, Ca, Fe, Ni, Zn, and Cu are naturally present in tap water and in many instances (i.e. in many of the examined ligands) these elements were preconcentrated on the membranes and thus were able to be quantified, as shown in Table 1. Finally, as mentioned above the raw EDXRF spectra, which include also the non-quantifiable Sb concentrations, are enclosed in this dataset manuscript. In the context of this work, the quantification of La, U, Au was achieved using the Lz lines, while for Ca, Fe, Ni, Zn, Sr, Sb, and Cu the Kα lines were used. However, as already mentioned Sb did not yield quantifiable results and hence is not included in Table 1.

From Table 1 it is possible to identify the most promising functionalised membranes for each examined element, i.e. the most promising ligands since in practise only the ligand is diversified between membranes. Specifically, in the electronically available Tables 2–10 the ten most promising membranes/ligands for Ca, Fe, Ni, Zn, Sr, La, U, Cu, and Au preconcentration in tap water, along with the achieved efficiency (in counts per 300 s), are given. Furthermore, in Fig. 2 the ten most promising ligands for Ca, Fe, Ni, and Zn preconcentration are shown, in Fig. 3 the ten most promising ligands for Sr,
La, Au, and U, and in Fig. 4 the ten most promising ligands for Cu preconcentration in tap water are shown.

As observed in Fig. 2 the most promising ligand, by and large, for Ca preconcentration is Eriochrome Black T. For Fe preconcentration in water six ligands appear to yield very good scores, with di-Ammonium hydrogen citrate having the higher score, while the best ligands for Ni and Zn preconcentration are 1,5-Diphenylcarbazide and dithizone, respectively. From Fig. 3 it can be inferred that for Sr preconcentration 1,1′-Carboxyldiimidazole is the most promising ligand, closely followed by 3-(2-Pyridyl)-5,6-diphenyl-1,2,4-triazine-p,p′-disulfonic acid. For La and Au preconcentration in water the most promising ligands are bis(cyclopentadienyl)titanium dichloride...

Fig. 6. a) the membrane solution, b) the double open ended XRF sample cup along with the Mylar® film, c) the solidified membrane, and d) the immersed membrane in the water matrix.

Fig. 7. a) the AMETEK SPECTRO XEPOS unit used for the EDXRF measurements, and b) the 12 position autosampler.
and sodium dibenzyldithiocarbamate, respectively, while for U the most promising ligand is, by and large, Calconcarbonsaure (CSS). Finally, from Fig. 4 it is inferred that dibenzoylmethane, closely followed by 5-(4-Dimethylaminobenzylidene)rhodanine, are the most promising ligands for Cu preconcentration in tap water, while dithizone and sodium dibenzyldithiocarbamate were also found promising.

2. Experimental design, materials and methods

A main strength of the solid-state polymer membranes lies in the fact that they are fairly simple to produced and used, as is described below. Specifically, in order to produce the membranes, a solution containing the following reagents needs to be prepared. First a polymer, such as EVA or PVC, is used as the membrane matrix. This will be mixed with a plasticizer, here dibutyl phthalate (DBP); an ionophore, here DTNB (5,5'-Dithiobis-(2-nitrobenzoic acid), popularly known as Ellman’s reagent); a catalyst, which is only used when producing anion-selective membranes (here the Aliquat® 336 was used); and finally a complexing agent, which is the ligand that was used to functionalise each membrane. The abovementioned chemical reagents are in solid form. For this reasons they were added into small cylindrical bottles, diluted with tetrahydrofuran (THF) and simply shaken for homogenisation (Fig. 5). The reagents concentration for the anion-selective membranes, which were used for the screening of the 112 ligands, was 9.4 g THF, 0.081 g EVA, 0.054 g Aliquat® 336, 0.02 g DTNB, 0.094 g DBP, and 0.015 g ligand. If a cation-selective membrane needs to be prepared then the catalyst, i.e. Aliquat® 336, should be omitted, i.e. not added to the abovementioned mixture. If the membranes are expected to be produced on a more comprehensive scale, mixing could be achieved using more elaborate techniques.

Once the membrane solution is homogenised, through shaking or mixing, this is simply applied on the desired surface, in this case a 2.5 μm thickness Mylar® film that is firmly place in a 32 mm double open ended XRF sample cup. In this work, this was achieved by placing 10 μL of the membrane solution, using a single-channel pipette, directly on the center of the Mylar® film. A spot is created, which was then slowly spread uniformly across the film surface using the pipette tip. Emphasis was given to ensure that the liquid form of the membrane will be spread uniformly on the Mylar® surface, and, to the extent possible, without touching the plastic edges of the XRF sample cups (Fig. 6a-c). The reason is that the part that is attached to the plastic edges of the sample cup will not be quantified during the EDXRF analysis. Given the large number of membranes that were examined in this work, in general, the liquid form of each membranes was spread relatively uniformly covering all of the Mylar® film surface, while a miniscule amount could be also deposited at the plastic edges of the XRF cups. However, this does not affected the analysis, since this is a comparative study and the same procedure was followed in all the examined membranes. A higher amount of the membrane could be also applied to the Mylar® film, which could make the uniformly application of the liquid form of the membrane easier. Finally, for solvent evaporation and membrane solidification the applied membrane solution is left to dry at room temperature for 24 h (an IR lamp can be used to reduce the drying duration). It should be noted that if the total reflection X-ray fluorescence (TXRF) technique is planned to be used, instead of the EDXRF technique, the membrane solution can be directly applied on the center of the quartz reflector, instead of the Mylar® film, and then left to solidified.

The solidified membrane is then ready to be used. In the context of this work, the prepared membranes were immersed in 1 L of tap water spiked with 20 μg L-1 Au, 20 μg L-1 La, 50 μg L-1 U, 50 μg L-1 Sb, and 100 μg L-1 Sr, as mentioned above. The membranes were left to rest for 24 h inside the water matrix, in order for the pollutants/elements contained in the water matrix to reach equilibrium on the membrane surface (Fig. 6d). The water matrix can be kept under continuous stirring, which enhances ion mobility and binding on the membrane surface thus lowering detection limits, or left unstirred. Here the water matrix was left unstirred. The reason is twofold. First, the main objective of this study was to compare the different membranes/ligands in terms of pollutants/elements pre-concentration efficiency and not identify the detection limits of each examine ligand. Second, the unstirred water matrix requires a simpler configuration, compared to continuous stirring, and is also easier to be use directly on the field and even by non-specialised personnel.
Finally, after 24 h of equilibrium inside the water matrix, the membrane is retrieved, washed with ultrapure water, and left to dry, before being measured by means of an EDXRF unit. Here, the membranes were assessed by an AMETEK SPECTRO XEPOS unit (Fig. 7 a), using the secondary/molybdenum mode at 40 kV and 0.9 mA, with helium gas flushing and 300 s irradiation duration. The unit is equipped with a 12 position autosampler (Fig. 7 b), equip with trays for different sample diameters (here the 32mm diameter was used). This allows for multiple samples, up to 12, to be measured. The spectra were then processed and quantified by means of the X-Lab Pro 4.0 software and using the TurboQuant method. The above suggest that the proposed method can provide robust results using relatively low irradiation times (i.e. 300 s). Furthermore, due to its simplicity and ability to be applied in unstirred water matrices, this method could be promising for the application of the method in low and middle income countries (LMIC), where the identification and monitoring of fresh water resources is a matter of emerging concern. The method could also achieve very low detection limits, even lower than μg·L⁻¹ by means of EDXRF, as was highlighted in our previous work [1]. Overall, the presented data suggests that the proposed solid-state membranes can be a promising method for pollutants monitoring and assessment in water matrices of environmental concern. Furthermore, future works of our group will focus on identifying the sensitivity and the detection limit of the most promising membranes/ligands for each of the examined element.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2020.105236.

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