

## Supporting information

Task-specific ionic liquids as extractants for the solvent extraction  
of molybdenum (VI) from aqueous solution using different  
commercial ionic liquids as diluents

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**Table S1. Supplementary data corresponding to Figure 2.**

| Ionic liquid  | Initial<br>[Mo(VI)]<br>(g/L) | Initial<br>pH | Equilibrium<br>pH | Equilibrium<br>[Mo(VI)] <sub>aq</sub><br>(g/L) | Equilibrium<br>[Mo(VI)] <sub>org</sub><br>(g/L) | D     | %E   | %E   | U%  |
|---------------|------------------------------|---------------|-------------------|------------------------------------------------|-------------------------------------------------|-------|------|------|-----|
| [TOMA][D2EHP] | 0.94                         | 0.64          | 0.67              | 0.02                                           | 0.92                                            | 46    | 97.9 | 97.9 | 0.1 |
|               | 0.94                         | 0.64          | 0.63              | 0.019                                          | 0.921                                           | 48.5  | 98   |      |     |
|               | 1.01                         | 0.806         | 0.6               | 0.019                                          | 0.991                                           | 52.2  | 98.1 | 97.8 | 0.7 |
|               | 1.01                         | 0.806         | 0.649             | 0.026                                          | 0.984                                           | 37.8  | 97.4 |      |     |
|               | 0.99                         | 0.841         | 0.764             | 0.017                                          | 0.973                                           | 57.2  | 98.3 | 98   | 0.5 |
|               | 0.99                         | 0.841         | 0.697             | 0.022                                          | 0.968                                           | 44    | 97.8 |      |     |
|               | 1.02                         | 0.982         | 0.821             | 0.021                                          | 0.999                                           | 47.6  | 97.9 | 98.1 | 0.3 |
|               | 1.02                         | 0.982         | 0.75              | 0.018                                          | 1,002                                           | 55.7  | 98.2 |      |     |
| [TOMA][BA]    | 1                            | 0.435         | 0.581             | 0.005                                          | 0.995                                           | 199   | 99.5 | 99.5 | 0.1 |
|               | 1                            | 0.435         | 0.631             | 0.006                                          | 0.994                                           | 165.7 | 99.4 |      |     |
|               | 1.02                         | 0.721         | 0.845             | 0.005                                          | 1,015                                           | 203   | 99.5 | 99.5 | 0.1 |
|               | 1.02                         | 0.721         | 0.843             | 0.006                                          | 1,014                                           | 169   | 99.4 |      |     |
|               | 0.92                         | 0.96          | 1,301             | 0.001                                          | 0.919                                           | 919   | 99.9 | 99.9 | 0   |
|               | 0.92                         | 0.96          | 1,233             | 0.001                                          | 0.919                                           | 919   | 99.9 |      |     |
|               | 0.96                         | 1,185         | 1,869             | 0.002                                          | 0.958                                           | 479   | 99.8 | 99.9 | 0.2 |
|               | 0.96                         | 1,185         | 1,955             | 0                                              | 0.96                                            | -     | 100  |      |     |

U = Uncertainty.

**Table S2. Supplementary data corresponding to Figure 3**

| Extractant | Diluent          | Initial<br>pH | Equilibrium<br>pH | Initial<br>[Mo(VI)]<br>(g/L) | Equilibrium<br>[Mo(VI)] <sub>aq</sub><br>(g/L) | Equilibrium<br>[Mo(VI)] <sub>org</sub><br>(g/L) | D    | %E    | %E   | U%  |
|------------|------------------|---------------|-------------------|------------------------------|------------------------------------------------|-------------------------------------------------|------|-------|------|-----|
| 1          | Kerosene         | 0.83          | 1                 | 0.71                         | 0.005                                          | 0.705                                           | 141  | 99.3  | 99.3 | 0   |
|            |                  |               | 0.98              |                              | 0.005                                          | 0.705                                           | 141  | 99.3  |      |     |
| 2          |                  | 1.01          | 1.29              | 0.82                         | 0.001                                          | 0.822                                           | 822  | 99.9  | 99.9 | 0   |
|            |                  |               | 1.31              |                              | 0.001                                          | 0.822                                           | 822  | 99.9  |      |     |
| 3          |                  | 1.08          | 1.11              | 0.78                         | 0.0087                                         | 0.7743                                          | 89   | 98.9  | 98.9 | 0.1 |
|            |                  |               | 1.08              |                              | 0.0093                                         | 0.7737                                          | 83.2 | 98.8  |      |     |
| 4          |                  | 1.07          | 1.34              | 0.92                         | 0.002                                          | 0.914                                           | 457  | 99.8  | 99.8 | 0   |
|            |                  |               | 1.41              |                              | 0.002                                          | 0.914                                           | 457  | 99.8  |      |     |
| 1          | [bmim]<br>[Tf2N] | 0.65          | 0.71              | 0.9                          | 0.65                                           | 0.25                                            | 0.4  | 27.8  | 24.4 | 6.7 |
| 0.68       |                  |               | 0.71              |                              | 0.19                                           | 0.3                                             | 21.1 |       |      |     |
| 2          |                  | 0.62          | 0.7               | 0.9                          | 1                                              | -0.1                                            | -0.1 | -11.1 | 0    | 0   |
|            |                  |               | 0.64              |                              | 1                                              | -0.1                                            | -0.1 | -11.1 |      |     |
| 3          |                  | 0.67          | 0.64              | 0.9                          | 0.69                                           | 0.21                                            | 0.3  | 23.3  | 24.4 | 2.2 |
|            |                  |               | 0.6               |                              | 0.67                                           | 0.23                                            | 0.3  | 25.6  |      |     |
| 4          |                  | 0.66          | 0.48              | 1                            | 0.9                                            | 0.1                                             | 0.1  | 10    | 15.5 | 11  |
|            |                  |               | 0.52              |                              | 0.79                                           | 0.21                                            | 0.3  | 21    |      |     |
| 1          | [omim]<br>[Tf2N] | 0.83          | 0.92              | 0.74                         | 0.09                                           | 0.649                                           | 7.2  | 87.8  | 85.5 | 4.6 |
| 0.95       |                  |               | 0.124             |                              | 0.615                                          | 5                                               | 83.2 |       |      |     |
| 2          |                  | 1.1           | 1.14              | 0.87                         | 0.095                                          | 0.774                                           | 8.1  | 89.1  | 88.7 | 0.8 |
|            |                  |               | 1.06              |                              | 0.102                                          | 0.767                                           | 7.5  | 88.3  |      |     |
| 3          |                  | 1.1           | 0.82              | 0.91                         | 0.164                                          | 0.705                                           | 4.3  | 81.1  | 81.1 | 0.2 |
|            |                  |               | 0.83              |                              | 0.174                                          | 0.74                                            | 4.3  | 81    |      |     |
| 4          |                  | 1.07          | 0.96              | 0.86                         | 0.139                                          | 0.722                                           | 5.2  | 83.9  | 83.3 | 1   |
|            |                  |               | 0.96              |                              | 0.148                                          | 0.713                                           | 4.8  | 82.8  |      |     |

1 [TOMA][D2EHP], 2 [TOMA][BA]. 3 [P6,6,6,14][D2EHP], 4 [P6,6,6,14][BA]

**Table S3. Supplementary data corresponding to Table 1**

| Extractant - Diluent | initial<br>water<br>content<br>(ppm) | Equilibrium<br>Water<br>content (ppm) | Average<br>Initial<br>Water<br>content<br>(ppm) | Average<br>equilibrium<br>water<br>content<br>(ppm) | initial<br>U<br>(ppm) | Equilibrium<br>U<br>(ppm) |
|----------------------|--------------------------------------|---------------------------------------|-------------------------------------------------|-----------------------------------------------------|-----------------------|---------------------------|
| 1 – 2                | 220.7                                | 1677.7                                | 226.9                                           | 1645.6                                              | 7.1                   | 27.5                      |
| 1 – 2                | 224.7                                | 1620.6                                |                                                 |                                                     |                       |                           |
| 1 – 2                | 235.2                                | 1638.5                                |                                                 |                                                     |                       |                           |
| 1 – 3                | 629.1                                | 12591.2                               | 621.0                                           | 12817.3                                             | 7.4                   | 286.3                     |
| 1 – 3                | 620.6                                | 12698.2                               |                                                 |                                                     |                       |                           |
| 1 – 3                | 613.4                                | 13162.5                               |                                                 |                                                     |                       |                           |

1 [TOMA][D2EHP]

2 kerosene

3 [bmim][Tf2N]

**Table S4. Supplementary data corresponding to Figure 6.**

| Initial pH | Equilibrium pH | Initial Extractant concentration (M) | Initial [Mo(VI)] <sub>aq</sub> (g/L) | Equilibrium [Mo(VI)] <sub>aq</sub> (g/L) | U (g/L) |
|------------|----------------|--------------------------------------|--------------------------------------|------------------------------------------|---------|
| 0.68       | 0.69           | 0.006                                | 0.77                                 | 0.42                                     | 0.01    |
|            | 0.69           | 0.006                                |                                      | 0.43                                     |         |
| 0.66       | 0.77           | 0.01                                 | 0.83                                 | 0.15                                     | 0.02    |
|            | 0.72           | 0.01                                 |                                      | 0.17                                     |         |
| 0.64       | 0.72           | 0.012                                | 0.89                                 | 0.2                                      | 0.07    |
|            | 0.75           | 0.012                                |                                      | 0.13                                     |         |
| 0.62       | 0.83           | 0.014                                | 0.87                                 | 0.1                                      | 0       |
|            | 0.77           | 0.014                                |                                      | 0.1                                      |         |

**Table S5. Supplementary data corresponding to Figure 7.**

| Initial pH | Equilibrium pH | Initial Extractant concentration (M) | Initial [Mo(VI)] <sub>aq</sub> (g/L) | Equilibrium [Mo(VI)] <sub>aq</sub> (g/L) | U (g/L) |
|------------|----------------|--------------------------------------|--------------------------------------|------------------------------------------|---------|
| 0.69       | 0.62           | 0.018                                | 1.06                                 | 0.63                                     | 0.009   |
|            | 0.62           | 0.018                                |                                      | 0.62                                     |         |
|            | 0.57           | 0.027                                |                                      | 0.38                                     | 0.002   |
|            | 0.59           | 0.027                                |                                      | 0.38                                     |         |
|            | 0.62           | 0.036                                |                                      | 0.22                                     | 0.01    |
|            | 0.64           | 0.036                                |                                      | 0.21                                     |         |
|            | 0.61           | 0.046                                |                                      | 0.12                                     | 0.023   |
|            | 0.61           | 0.047                                |                                      | 0.1                                      |         |
|            | 0.59           | 0.056                                |                                      | 0.08                                     | 0.002   |
|            | 0.59           | 0.054                                |                                      | 0.07                                     |         |

**Table S6. Supplementary data corresponding to Figure 8.**

| Initial<br>pH | Equilibrium<br>pH | Initial<br>[Mo(VI)] <sub>aq</sub><br>(g/L) | Equilibrium<br>[Mo(VI)] <sub>aq</sub><br>(g/L) | U<br>(g/L) |
|---------------|-------------------|--------------------------------------------|------------------------------------------------|------------|
| 0.85          | 0.86              | 1.08                                       | 1.03                                           | 0.006      |
|               | 0.85              |                                            | 1.03                                           |            |
|               | 0.85              |                                            | 1.01                                           | 0.002      |
|               | 0.85              |                                            | 1                                              |            |
|               | 0.84              |                                            | 1                                              | 0.008      |
|               | 0.87              |                                            | 0.99                                           |            |
|               | 0.87              |                                            | 0.97                                           | 0.006      |
|               | 0.84              |                                            | 0.97                                           |            |
|               | 0.86              |                                            | 0.99                                           | 0.044      |
|               | 0.86              |                                            | 0.95                                           |            |
|               | 0.85              |                                            | 0.95                                           | 0.001      |
|               | 0.84              |                                            | 0.95                                           |            |

**Table S7. Supplementary data corresponding to Figure 9.**

| Extractant - diluent         | Initial<br>[Mo(VI)] <sub>org</sub><br>(g/L) | Equilibrium<br>[Mo(VI)] <sub>aq</sub><br>(g/L) | Equilibrium<br>[Mo(VI)] <sub>org</sub><br>(g/L) | %S   | Average<br>%S | U<br>(%) |
|------------------------------|---------------------------------------------|------------------------------------------------|-------------------------------------------------|------|---------------|----------|
| [TOMA] [D2EHP]-Kerosene      | 1.09                                        | 0.01                                           | 1.08                                            | 0.6  | .9            | 0.5      |
| [TOMA] [D2EHP]-Kerosene      | 1.07                                        | 0.01                                           | 1.06                                            | 1.1  |               |          |
| [TOMA] [D2EHP]-[bmim] [Tf2N] | 0.37                                        | 0.14                                           | 0.23                                            | 37.4 | 52.2          | 28.7     |
| [TOMA] [D2EHP]-[bmim] [Tf2N] | 0.21                                        | 0.14                                           | 0.07                                            | 66.1 |               |          |
| [TOMA] [D2EHP]-[omim] [Tf2N] | 0.30                                        | 0.26                                           | 0.04                                            | 86.7 | 90.7          | 7.9      |
| [TOMA] [D2EHP]-[omim] [Tf2N] | 0.37                                        | 0.35                                           | 0.02                                            | 94.6 |               |          |