**Supporting Information**

**A multi-scenario risk assessment strategy applied to mixtures of chemicals of emerging concern in the River Aconcagua basin in Central Chile**

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SI Figure.

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| Figure S1. Frequency of detected and quantified CECs in the River Aconcagua basin. Chemicals were coloured according to their chemical classes (see legend). |

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| Figure S2. Mixture risk assessment estimates and risk drivers for sites RQsum<0.1 (RQExpo1-ToxG-MST and RQExpo1-ToxI-MST) in the River Aconcagua basin. Colours represent the source of the toxicity data, grey means empirical sources and orange QSAR modelling. |

SI Tables

Table S1. Sampling site information. Geographic coordinates in decimal degree (WGS84).

|  |  |  |  |
| --- | --- | --- | --- |
| Site ID | Type | Latitude (N) | Longitude (E) |
| RS1 | “Reference” | -32.854358 | -70.390044 |
| RS2 | “Reference” | -32.509769 | -70.452537 |
| RS3 | “Reference” | -33.003752 | -71.126355 |
| T1 | Tributary | -32.765909 | -70.613844 |
| T2 | Tributary | -32.695661 | -71.212179 |
| T3 | Tributary | -32.938952 | -71.329491 |
| R1 | Main river | -32.852416 | -70.502894 |
| R2 | Main river | -32.762305 | -70.839624 |
| R3 | Main river | -32.916946 | -71.425322 |

Table S2. RQSTU estimates for the different exposures and hazard scenarios (Figure 4 and Table 1 for details). Sites at risk are highlighted.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ToxA (US EPA ECOTOX Database only) | | | | | | | | | | | | |
|  | Expo 1 (ZERO) | | | | Expo 2 (MDL) | | | | Expo 3 (KM) | | | |
| Sites | Algae | Macro-invertebrates | Fish | MST | Algae | Macro-invertebrate | Fish | MST | Algae | Macro-invertebrate | Fish | MST |
| RS1 | 0.0012 | 0.0029 | 0.0008 | 0.0044 | 0.0041 | 0.0128 | 0.0232 | 0.0383 | 0.0012 | 0.0030 | 0.0040 | 0.0077 |
| RS2 | 0.0001 | 0.0001 | 0.0001 | 0.0009 | 0.0032 | 0.0106 | 0.0227 | 0.0353 | 0.0001 | 0.0008 | 0.0001 | 0.0010 |
| RS3 | 0.0001 | 0.0001 | 0.0001 | 0.0002 | 0.0031 | 0.0101 | 0.0226 | 0.0347 | 0.0001 | 0.0002 | 0.0001 | 0.0003 |
| T1 | 0.0088 | **0.2878** | **0.2654** | **0.5305** | 0.0114 | **0.2908** | **0.2796** | **0.5500** | 0.0090 | **0.2735** | **0.2687** | **0.5179** |
| T2 | 0.0002 | 0.0043 | 0.0598 | 0.0641 | 0.0032 | 0.0124 | 0.0693 | 0.0837 | 0.0002 | 0.0023 | 0.0696 | 0.0722 |
| T3 | 0.0096 | **0.1421** | 0.0376 | **0.1725** | 0.0127 | **0.1437** | 0.0578 | **0.1969** | 0.0102 | **0.1480** | **0.1651** | **0.2999** |
| R1 | 0.0275 | 0.0010 | 0.0544 | 0.0827 | 0.0280 | 0.0108 | 0.0751 | **0.1126** | 0.0039 | 0.0010 | 0.0546 | 0.0596 |
| R2 | 0.0002 | 0.0023 | 0.0334 | 0.0356 | 0.0033 | 0.0115 | 0.0549 | 0.0683 | 0.0003 | 0.0022 | 0.0364 | 0.0387 |
| R3 | 0.0059 | 0.0578 | **0.6259** | **0.6811** | 0.0088 | 0.0645 | **0.6359** | **0.6999** | 0.0063 | 0.0580 | **0.7043** | **0.7565** |
| ToxB (QSAR VEGA only) | | | | | | | | | | | | |
| RS1 | 0.0007 | 0.0079 | 0.0020 | 0.0091 | 0.0025 | 0.0116 | 0.0057 | 0.0166 | 0.0007 | 0.0079 | 0.0022 | 0.0093 |
| RS2 | 0.0004 | 0.0069 | 0.0017 | 0.0077 | 0.0023 | 0.0108 | 0.0054 | 0.0154 | 0.0004 | 0.0069 | 0.0018 | 0.0078 |
| RS3 | 0.0006 | 0.0065 | 0.0018 | 0.0077 | 0.0023 | 0.0102 | 0.0047 | 0.0146 | 0.0006 | 0.0065 | 0.0018 | 0.0078 |
| T1 | 0.0185 | 0.0549 | 0.0471 | **0.1042** | 0.0191 | 0.0582 | 0.0488 | **0.1091** | 0.0186 | 0.0550 | 0.0473 | **0.1046** |
| T2 | 0.0052 | 0.0096 | 0.0156 | 0.0228 | 0.0067 | 0.0100 | 0.0178 | 0.0258 | 0.0052 | 0.0096 | 0.0158 | 0.0230 |
| T3 | 0.0059 | 0.0122 | 0.0330 | 0.0428 | 0.0074 | 0.0156 | 0.0351 | 0.0487 | 0.0060 | 0.0122 | 0.0332 | 0.0433 |
| R1 | 0.0042 | 0.0025 | 0.0174 | 0.0179 | 0.0057 | 0.0072 | 0.0198 | 0.0251 | 0.0043 | 0.0026 | 0.0175 | 0.0182 |
| R2 | 0.0015 | 0.0056 | 0.0111 | 0.0157 | 0.0032 | 0.0066 | 0.0144 | 0.0201 | 0.0016 | 0.0057 | 0.0113 | 0.0160 |
| R3 | 0.0150 | 0.0136 | **0.1445** | **0.1538** | 0.0166 | 0.0170 | **0.1466** | **0.1597** | 0.0151 | 0.0137 | **0.1447** | **0.1542** |
| ToxC (QSAR ECOSAR only) | | | | | | | | | | | | |
| RS1 | 0.0003 | 0.0008 | 0.0007 | 0.0010 | 0.0075 | 0.0257 | 0.0073 | 0.0365 | 0.0003 | 0.0009 | 0.0007 | 0.0011 |
| RS2 | 0.0001 | 0.0004 | 0.0004 | 0.0005 | 0.0074 | 0.0254 | 0.0072 | 0.0361 | 0.0001 | 0.0004 | 0.0004 | 0.0005 |
| RS3 | 0.0002 | 0.0006 | 0.0005 | 0.0007 | 0.0074 | 0.0255 | 0.0071 | 0.0362 | 0.0002 | 0.0007 | 0.0005 | 0.0008 |
| T1 | 0.0232 | **2.2479** | **0.1000** | **2.3016** | 0.0284 | **2.2489** | **0.1009** | **2.3078** | 0.0233 | **2.2479** | **0.1000** | **2.3018** |
| T2 | 0.0013 | 0.0079 | 0.0048 | 0.0084 | 0.0084 | 0.0324 | 0.0112 | 0.0435 | 0.0013 | 0.0080 | 0.0049 | 0.0087 |
| T3 | 0.0552 | **0.2784** | 0.0069 | **0.3323** | 0.0573 | **0.2805** | 0.0131 | **0.3399** | 0.0551 | **0.2754** | 0.0049 | **0.3294** |
| R1 | 0.0014 | 0.0044 | 0.0046 | 0.0055 | 0.0084 | 0.0286 | 0.0106 | 0.0401 | 0.0015 | 0.0045 | 0.0047 | 0.0058 |
| R2 | 0.0002 | 0.0006 | 0.0005 | 0.0007 | 0.0074 | 0.0254 | 0.0072 | 0.0361 | 0.0002 | 0.0006 | 0.0006 | 0.0009 |
| R3 | 0.0016 | 0.0046 | 0.0039 | 0.0060 | 0.0088 | 0.0291 | 0.0103 | 0.0410 | 0.0016 | 0.0031 | 0.0028 | 0.0046 |
| ToxD (US EPA ECOTOX Database amended QSAR VEGA) | | | | | | | | | | | | |
| RS1 | 0.0018 | 0.0040 | 0.0027 | 0.0065 | 0.0058 | 0.0143 | 0.0267 | 0.0425 | 0.0019 | 0.0042 | 0.0060 | 0.0102 |
| RS2 | 0.0006 | 0.0019 | 0.0016 | 0.0027 | 0.0047 | 0.0124 | 0.0260 | 0.0394 | 0.0006 | 0.0020 | 0.0018 | 0.0032 |
| RS3 | 0.0006 | 0.0005 | 0.0014 | 0.0015 | 0.0048 | 0.0111 | 0.0257 | 0.0383 | 0.0006 | 0.0006 | 0.0016 | 0.0019 |
| T1 | 0.0129 | **0.2903** | **0.2731** | **0.5375** | 0.0161 | **0.2937** | **0.2887** | **0.5585** | 0.0132 | **0.2762** | **0.2767** | **0.5252** |
| T2 | 0.0054 | 0.0089 | 0.0717 | 0.0783 | 0.0092 | 0.0173 | 0.0824 | 0.0993 | 0.0054 | 0.0071 | 0.0820 | 0.0870 |
| T3 | 0.0148 | **0.1469** | 0.0674 | **0.2053** | 0.0188 | **0.1489** | 0.0888 | **0.2311** | 0.0155 | **0.1529** | **0.1949** | **0.3319** |
| R1 | 0.0316 | 0.0035 | 0.0609 | 0.0896 | 0.0328 | 0.0137 | 0.0826 | **0.1207** | 0.0080 | 0.0037 | 0.0614 | 0.0670 |
| R2 | 0.0017 | 0.0035 | 0.0442 | 0.0467 | 0.0056 | 0.0133 | 0.0671 | 0.0811 | 0.0018 | 0.0035 | 0.0475 | 0.0502 |
| R3 | 0.0204 | 0.0653 | **0.7692** | **0.8269** | 0.0243 | 0.0725 | **0.7803** | **0.8470** | 0.0210 | 0.0657 | **0.8479** | **0.9022** |
| ToxE (US EPA ECOTOX Database amended QSAR VEGA \*100 deviation factor) | | | | | | | | | | | | |
| RS1 | 0.0012 | 0.0030 | 0.0009 | 0.0044 | 0.0041 | 0.0128 | 0.0232 | 0.0384 | 0.0013 | 0.0030 | 0.0040 | 0.0077 |
| RS2 | 0.0001 | 0.0008 | 0.0001 | 0.0009 | 0.0032 | 0.0107 | 0.0228 | 0.0353 | 0.0001 | 0.0008 | 0.0001 | 0.0010 |
| RS3 | 0.0003 | 0.0001 | 0.0001 | 0.0002 | 0.0031 | 0.0101 | 0.0227 | 0.0347 | 0.0001 | 0.0002 | 0.0001 | 0.0003 |
| T1 | 0.0088 | **0.2878** | **0.2655** | **0.5306** | 0.0114 | **0.2908** | **0.2797** | **0.5501** | 0.0090 | **0.2736** | **0.2688** | **0.5180** |
| T2 | 0.0002 | 0.0043 | 0.0599 | 0.0642 | 0.0033 | 0.0125 | 0.0694 | 0.0839 | 0.0003 | 0.0023 | 0.0698 | 0.0724 |
| T3 | 0.0097 | **0.1421** | 0.0379 | **0.1729** | 0.0128 | **0.1437** | 0.0581 | **0.1972** | 0.0102 | **0.1480** | **0.1654** | **0.3003** |
| R1 | 0.0276 | 0.0010 | 0.0544 | 0.0828 | 0.0280 | 0.0108 | 0.0752 | **0.1127** | 0.0040 | 0.0010 | 0.0547 | 0.0597 |
| R2 | 0.0002 | 0.0024 | 0.0335 | 0.0358 | 0.0033 | 0.0115 | 0.0550 | 0.0684 | 0.0003 | 0.0022 | 0.0365 | 0.0388 |
| R3 | 0.0060 | 0.0579 | **0.6274** | **0.6826** | 0.0090 | 0.0646 | **0.6373** | **0.7013** | 0.0064 | 0.0581 | **0.7058** | **0.7580** |
| ToxF (US EPA ECOTOX Database amended QSAR VEGA /100 deviation factor) | | | | | | | | | | | | |
| RS1 | 0.0668 | **0.1099** | **0.1831** | **0.2302** | **0.1742** | **0.1656** | **0.3754** | **0.4950** | 0.0681 | **0.1114** | **0.1904** | **0.2395** |
| RS2 | 0.0449 | **0.1137** | **0.1552** | **0.1952** | **0.1547** | **0.1856** | **0.3522** | **0.4808** | 0.0458 | **0.1145** | **0.1575** | **0.2007** |
| RS3 | 0.0603 | 0.0347 | **0.1335** | **0.1397** | **0.1688** | **0.1120** | **0.3342** | **0.4311** | 0.0611 | 0.0357 | **0.1364** | **0.1456** |
| T1 | **0.4271** | **0.5405** | **1.0358** | **1.6323** | **0.4805** | **0.5826** | **1.1840** | **1.8088** | **0.4302** | **0.5295** | **1.0478** | **1.6272** |
| T2 | **0.5177** | **0.4696** | **1.2512** | **1.5183** | **0.6020** | **0.5009** | **1.3848** | **1.7111** | **0.5191** | **0.4698** | **1.2651** | **1.5281** |
| T3 | **0.5320** | **0.6217** | **3.0178** | **3.4655** | **0.6207** | **0.6642** | **3.1594** | **3.6672** | **0.5357** | **0.6305** | **3.1155** | **3.4937** |
| R1 | **0.4334** | **0.2530** | **0.7103** | **0.8812** | **0.5067** | **0.3045** | **0.8255** | **1.0639** | **0.4114** | **0.2550** | **0.7157** | **0.8720** |
| R2 | **0.1508** | **0.1197** | **1.1169** | **1.1462** | **0.2426** | **0.1878** | **1.2724** | **1.3847** | **0.1528** | **0.1222** | **1.1262** | **1.1584** |
| R3 | **1.4647** | **0.8113** | **14.9551** | **15.3103** | **1.5532** | **0.8572** | **15.0711** | **15.4924** | **1.4693** | **0.8142** | **15.0197** | **15.3309** |
| ToxG (US EPA ECOTOX Database amended QSAR ECOSAR) | | | | | | | | | | | | |
| RS1 | 0.0015 | 0.0038 | 0.0015 | 0.0052 | 0.0053 | 0.0155 | 0.0249 | 0.0403 | 0.0015 | 0.0040 | 0.0017 | 0.0056 |
| RS2 | 0.0003 | 0.0013 | 0.0005 | 0.0014 | 0.0043 | 0.0131 | 0.0243 | 0.0370 | 0.0003 | 0.0014 | 0.0005 | 0.0016 |
| RS3 | 0.0002 | 0.0008 | 0.0006 | 0.0010 | 0.0042 | 0.0127 | 0.0243 | 0.0366 | 0.0003 | 0.0010 | 0.0007 | 0.0012 |
| T1 | 0.0117 | **0.2930** | **0.2710** | **0.5341** | 0.0146 | **0.2970** | **0.2859** | **0.5544** | 0.0119 | **0.2932** | **0.2715** | **0.5351** |
| T2 | 0.0015 | 0.0122 | 0.0622 | 0.0672 | 0.0054 | 0.0219 | 0.0727 | 0.0879 | 0.0016 | 0.0124 | 0.0624 | 0.0677 |
| T3 | 0.0109 | **0.1481** | 0.0419 | **0.1793** | 0.0147 | **0.1513** | 0.0630 | **0.2045** | 0.0110 | **0.1482** | 0.0424 | **0.1803** |
| R1 | 0.0286 | 0.0055 | 0.0579 | 0.0863 | 0.0298 | 0.0165 | 0.0792 | **0.1167** | 0.0286 | 0.0057 | 0.0582 | 0.0869 |
| R2 | 0.0005 | 0.0030 | 0.0340 | 0.0364 | 0.0043 | 0.0140 | 0.0565 | 0.0701 | 0.0005 | 0.0032 | 0.0341 | 0.0368 |
| R3 | 0.0069 | 0.0621 | **0.6298** | **0.6861** | 0.0107 | 0.0704 | **0.6405** | **0.7057** | 0.0070 | 0.0623 | **0.6300** | **0.6869** |
| ToxH (US EPA ECOTOX Database amended QSAR ECOSAR \*100 deviation factor) | | | | | | | | | | | | |
| RS1 | 0.0012 | 0.0030 | 0.0008 | 0.0044 | 0.0041 | 0.0128 | 0.0232 | 0.0384 | 0.0012 | 0.0030 | 0.0040 | 0.0077 |
| RS2 | 0.0001 | 0.0008 | 0.0001 | 0.0009 | 0.0032 | 0.0107 | 0.0228 | 0.0353 | 0.0001 | 0.0008 | 0.0001 | 0.0010 |
| RS3 | 0.0002 | 0.0001 | 0.0001 | 0.0002 | 0.0031 | 0.0101 | 0.0226 | 0.0347 | 0.0001 | 0.0002 | 0.0001 | 0.0003 |
| T1 | 0.0088 | **0.2878** | **0.2655** | **0.5305** | 0.0114 | **0.2908** | **0.2797** | **0.5501** | 0.0090 | **0.2736** | **0.2688** | **0.5179** |
| T2 | 0.0002 | 0.0044 | 0.0598 | 0.0641 | 0.0032 | 0.0125 | 0.0693 | 0.0838 | 0.0002 | 0.0024 | 0.0697 | 0.0723 |
| T3 | 0.0096 | **0.1421** | 0.0376 | **0.1726** | 0.0127 | **0.1437** | 0.0578 | **0.1969** | 0.0102 | **0.1480** | **0.1651** | **0.3000** |
| R1 | 0.0275 | 0.0010 | 0.0544 | 0.0827 | 0.0280 | 0.0108 | 0.0752 | **0.1126** | 0.0039 | 0.0011 | 0.0546 | 0.0596 |
| R2 | 0.0002 | 0.0023 | 0.0334 | 0.0357 | 0.0033 | 0.0116 | 0.0549 | 0.0683 | 0.0003 | 0.0022 | 0.0364 | 0.0387 |
| R3 | 0.0059 | 0.0579 | **0.6260** | **0.6812** | 0.0088 | 0.0646 | **0.6359** | **0.6999** | 0.0063 | 0.0581 | **0.7044** | **0.7565** |
| ToxI (US EPA ECOTOX Database amended QSAR ECOSAR /100 deviation factor) | | | | | | | | | | | | |
| RS1 | 0.02743 | 0.0861 | 0.0683 | **0.1054** | **0.1127** | **0.2870** | **0.1926** | **0.3591** | 0.0281 | 0.0891 | 0.0709 | 0.1105 |
| RS2 | 0.01316 | 0.0458 | 0.0362 | 0.0489 | **0.1044** | **0.2566** | **0.1731** | **0.3160** | 0.0135 | 0.0476 | 0.0377 | 0.0517 |
| RS3 | 0.02175 | 0.0660 | 0.0489 | 0.0746 | **0.1076** | **0.2697** | **0.1770** | **0.3331** | 0.0221 | 0.0679 | 0.0501 | 0.0771 |
| T1 | **0.30323** | **0.7962** | **0.8177** | **1.2815** | **0.3249** | **0.8675** | **0.8919** | **1.3915** | **0.3046** | **0.8003** | **0.8225** | **1.2904** |
| T2 | **0.12656** | **0.7913** | **0.3060** | **0.8938** | **0.2111** | **0.9584** | **0.4122** | **1.0999** | **0.1278** | **0.7957** | **0.3092** | **0.9006** |
| T3 | **0.11576** | **0.4342** | **0.3559** | **0.6081** | **0.1933** | **0.5963** | **0.4574** | **0.8108** | **0.1176** | **0.4413** | **0.3616** | **0.6212** |
| R1 | **0.1068** | **0.4435** | **0.4030** | **0.5587** | **0.1754** | **0.5744** | **0.4705** | **0.7263** | **0.1079** | **0.4466** | **0.4047** | **0.5637** |
| R2 | 0.0183 | 0.0599 | 0.0895 | **0.1056** | **0.1006** | **0.2571** | **0.2070** | **0.3508** | 0.0191 | 0.0636 | 0.0925 | **0.1121** |
| R3 | 0.0981 | **0.3070** | **0.9470** | **1.0715** | **0.1811** | **0.4723** | **1.0369** | **1.26765** | **0.1003** | **0.3141** | **0.9513** | **1.0822** |

Table S3. *Potential* absolute risk drivers. *Potential* absolute risk drivers are chemicals that are not actual absolute risk drivers (Table 4) but could become one if their QSAR-based hazard estimate is underestimated by a factor of 100 (details in main text). Chemicals are listed in descending order of their mean RQExpo1-ToxI-MST. Experimental and QSAR ECOSAR concentrations in µM. N = number of sites where the respective chemicals were *potential* absolute risk driver.

| Chemical Name | CAS Number | Class | minRQ | meanRQ | maxRQ | N | Algae  ECOTOX | Macroinv.  ECOTOX | Fish  ECOTOX | Algae  ECOSAR | Macroinv.  ECOSAR | Fish  ECOSAR |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Chlorfenapyr | 122453-73-0 | Insecticide | 0.0923 | 0.3418 | 0.5372 | 2 |  |  | 0.003 | 0.076 | 0.008 | 0.019 |
| Telmisartan | 144701-48-4 | Antihypertensive | 0.1708 | 0.2387 | 0.3065 | 2 |  |  |  | 0.084 | 0.004 | 0.006 |
| Octocrylene | 6197-30-4 | UV filter | 0.2022 | 0.2022 | 0.2022 | 1 |  |  | 0.015 | 0.049 | 0.040 | 0.006 |
| Benzyl 2-naphthyl ether | 613-62-7 | Thermal coating | 0.1544 | 0.1544 | 0.1544 | 1 |  |  |  | 1.499 | 0.282 | 0.244 |
| Boscalid | 188425-85-6 | Fungicide | 0.1525 | 0.1525 | 0.1525 | 1 | 1.924 | 0.060 |  | 2.982 | 1.904 | 0.200 |
| TDAO | 3332-27-2 | Surfactant | 0.1309 | 0.1309 | 0.1309 | 1 |  |  |  | 0.035 | 0.025 | 0.021 |
| Allethrin | 584-79-2 | Insecticide | 0.0357 | 0.0901 | 0.1300 | 3 |  |  |  | 0.309 | 0.015 | 0.013 |
| N,N-Dimethyldodecylamine | 112-18-5 | Surfactant | 0.0723 | 0.0814 | 0.0904 | 2 | 0.075 |  |  | 0.031 | 0.022 | 0.018 |
| Lauryl diethanolamide | 120-40-1 | Surfactant | 0.0568 | 0.0568 | 0.0568 | 1 |  |  |  | 9.009 | 11.110 | 1.096 |
| Desethylterbutylazine | 30125-63-4 | Herbicide | 0.0405 | 0.0532 | 0.0658 | 2 |  |  |  | 5.147 | 1.105 | 3.869 |
| 1,3-Diphenylguanidine | 102-06-7 | Rubber additive | 0.0301 | 0.0498 | 0.0998 | 6 |  |  |  | 1.578 | 0.596 | 2.105 |
| Myclobutanil | 88671-89-0 | Fungicide | 0.0447 | 0.0447 | 0.0447 | 1 | 1.939 | 0.012 |  | 1.934 | 0.998 | 0.320 |
| DDAO | 1643-20-5 | Surfactant | 0.0426 | 0.0426 | 0.0426 | 1 |  |  |  | 0.160 | 0.089 | 0.131 |
| N-Methyldodecylamine | 7311-30-0 | Surfactant | 0.0373 | 0.0373 | 0.0373 | 1 |  |  |  | 0.043 | 0.029 | 0.026 |
| Benzyl benzoate | 120-51-4 | Antimicrobial | 0.0307 | 0.0331 | 0.0356 | 2 |  |  |  | 3.938 | 5.420 | 1.110 |
| Thiabendazole | 148-79-8 | Fungicide | 0.0308 | 0.0308 | 0.0308 | 1 |  | 0.208 |  | 2.278 | 1.128 | 0.709 |
| Celecoxib | 169590-42-5 | NSAID | 0.0250 | 0.0250 | 0.0250 | 1 |  |  | 0.204 | 1.658 | 0.801 | 0.277 |
| DEHT | 66753-06-8 | Herbicide | 0.0215 | 0.0215 | 0.0215 | 1 |  |  |  | 19.246 | 2.489 | 6.782 |
| Diphenyl glycol | 104-66-5 | Thermal coating | 0.0206 | 0.0206 | 0.0207 | 2 |  |  |  | 7.412 | 2.039 | 2.332 |

TDAO = N,N-Dimethyltetradecylamine-N-oxide

DDAO = Lauramine oxide

DEHT = Terbutylazine-desethyl-2-hydroxy

NSAID = Non-steroidal anti-inflammatory drug

Table S4. Relative risk drivers are chemical which contribute 20% or more of the final RQ-sum (i.e., 20% of the total RQMST). Chemicals organised meanRelTU descending, based on RQExpo1-ToxG-MST. Experimental concentrations in µM. N = number of sites where the respective chemicals were relative risk drivers.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Chemical Name | CAS Number | Class | minRelTU | meanRelTU | maxRelTU | N | Algae  ECOTOX | Macroinv.  ECOTOX | Fish  ECOTOX |
| Trenbolone | 10161-33-8 | Anabolic steroid | 0.6794 | 0.7884 | 0.8974 | 2 |  |  | 0.0003 |
| Daidzein | 486-66-8 | Phytoestrogen | 0.3742 | 0.6172 | 0.9020 | 3 |  |  | 0.0039 |
| Terbuthylazine | 5915-41-3 | Herbicide | 0.2069 | 0.4425 | 0.5662 | 3 | 0.0529 | 0.0089 | 3.5697 |
| 1,3-Diphenylguanidine | 102-06-7 | Rubber additive | 0.3138 | 0.3138 | 0.3138 | 1 |  |  |  |
| Clarithromycin | 81103-11-9 | Antibiotic | 0.3042 | 0.3042 | 0.3042 | 1 | 0.0005 |  |  |
| Chlorpyrifos | 2921-88-2 | Insecticide | 0.2213 | 0.2213 | 0.2213 | 1 | 0.2488 | 0.0018 | 0.0126 |
| Chlorfenapyr | 122453-73-0 | Insecticide | 0.2102 | 0.2102 | 0.2102 | 1 |  |  | 0.0033 |
| Methomyl | 16752-77-5 | Insecticide | 0.2047 | 0.2047 | 0.2047 | 1 | 440.7491 | 0.0180 | 0.1838 |

Table S5. *Potential* relative risk drivers in the River Aconcagua basin. N = sites where the respective chemicals were *potential* relative risk driver, based on based on RQExpo1-ToxI-MST. No empirical data could be retrieved from ECOTOX for any of these chemicals.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Chemical Name | CAS Number | Class | minRelTU | meanRelTU | maxRelTU | N | RQMSTRelTU |
| Didecyldimethylammonium | 20256-56-8 | Disinfectant | 0.1800 | 0.1800 | 0.1800 | 1 | 0.2346 |
| Diphenyl glycol | 104-66-5 | Thermal coating | 0.1274 | 0.1538 | 0.1802 | 2 | 0.3548 |
| Benzothiazole | 95-16-9 | Rubber additive (transformation product) | 0.1028 | 0.1028 | 0.1028 | 1 | 0.2865 |
| 1,3-Diphenylguanidine | 102-06-7 | Rubber additive | 0.0628 | 0.0628 | 0.0628 | 1 | 0.3138 |
| Telmisartan | 144701-48-4 | Antihypertensive | 0.0171 | 0.0171 | 0.0171 | 1 | 0.3585 |
| Benzyl-2-naphthyl ether | 613-62-7 | Thermal coating | 0.0179 | 0.0179 | 0.0179 | 1 | 0.2647 |