Electronic Supplementary Material (ESI) for Green Chemistry.


# Environmental safety of cholinium-based ionic liquids: assessing structure-ecotoxicity relationships

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**Table S1.** Nomenclature and chemical structure of the choline compounds studied.

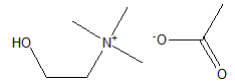
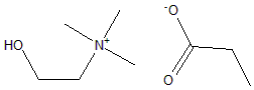
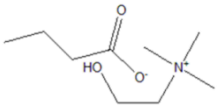
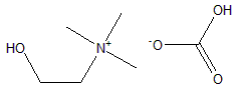
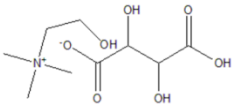
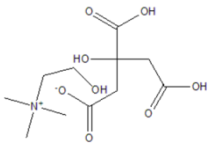
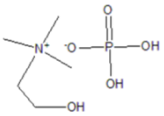
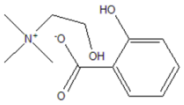
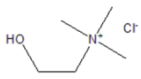
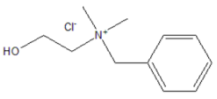
| Abbreviation | Name | Chemical Structure |
|---|---|---|
| **[Chol][Ac]** | Cholinium acetate |  |
| **[Chol][Prop]** | Cholinium propanoate |  |
| **[Chol][But]** | Cholinium butanoate |  |
| **[Chol][Bic]** | Cholinium bicarbonate |  |
| **[Chol][Bit]** | Cholinium bitartrate |  |
| **[Chol][DHCit]** | Cholinium dihydrogenocitrate |  |
| **[Chol][DHPhosp]** | cholinium dihydrogenophosphate |  |
| **[Chol][Sal]** | Cholinium salicylate |  |
| **[Chol]Cl** | Cholinium chloride |  |
| **[BzChol]Cl** | Benzyldimethyl(2-hydro-xyethyl)ammonium chloride |  |

**Table S2.** $EC_{50}$ values (mg $L^{-1}$) estimated following exposure of the four biological models to the tested cholinium-based ILs, with the respective 95% confidence interval (within brackets). $EC_{50}$ values were estimated for *V. fischeri* after 30 min exposure of the organism to the ILs. For *R. subcapitata*, $EC_{50}$ values were estimated based on the yield ($E_yC_{50}$) and growth rate ($E_rC_{50}$). For *L. minor*, $EC_{50}$ values were estimated based on the yield and growth rate considering the number of fronds and dry weight. Data for *V. fischeri* originated in Ventura et al. (2014).

| **Ionic liquid** | $EC_x$ | ***V. fischeri*** | ***R. subcapitata*** | | ***L. minor*** | | | | ***D. magna*** |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | Frond number | | Dry weight | | |
| | | | $\mathbf{E_yC_x}$ | $\mathbf{E_rC_x}$ | $\mathbf{E_yC_x}$ | $\mathbf{E_rC_x}$ | $\mathbf{E_yC_x}$ | $\mathbf{E_rC_x}$ | |
| [Chol][DHCit] | $EC_{50}$ | 37.23 (28.60-45.85) | 87.16 (80.62-93.70) | 155.2 (147.0-163.5) | 1863 (1007-2720) | 5649 (3287- 8011) | --- | --- | 445.0 (417.3-467.0) |
| | $EC_{20}$ | 23.11 (13.69-32.54) | 68.65 (60.66-76.64) | --- | --- | 765.7 (190.7-1341) | --- | --- | 373.6 (322.0-404.1) |
| | $EC_{10}$ | 17.48 (7.810-27.15) | 59.69 (50.08-69.30) | --- | 53.51 (0.000-125.3) | 237.5 (0.000-501.5) | --- | --- | 333.4 (269.4-373.9) |
| [Chol]Cl | $EC_{50}$ | 469.3 (383.8-554.9) | 72.51 (52.14-92.88) | 629.6 (201.2-1058) | 234.2 (154.0-314.5) | 443.8 (263.2- 624.5) | 1185 (415.5-1955) | 5947 (473.4-11420) | 695.4 (642.8-761.3) |
| | $EC_{20}$ | 148.1 (97.10-199.1) | 38.90 (18.46-59.34) | --- | 79.81 (32.87-126.8) | 118.5 (31.23-205.8) | 140.1 (0.000-300.7) | 497.7 (121.9-872.9) | --- |
| | $EC_{10}$ | 75.35 (39.33-111.4) | 27.02 (7.793-46.25) | --- | 42.49 (8.984-75.99) | 54.70 (0.000-109.8) | 40.09 (0.000-108.8) | 116.3 (0.000-271.7) | --- |
| [Chol][Bit] | $EC_{50}$ | 37.90 (32.73-43.08) | 27.26 (24.56-29.97) | 125.3 (111.4-139.1) | 1063 (858.8-1267) | 1632(1417- 1847) | 1197 (802.6-1590) | 5694 (3417-7970) | 410.5 (388.2-434.5) |
| | $EC_{20}$ | 28.74 (24.15-33.33) | 13.19 (10.74-15.64) | --- | 493.2 (327.4-659.0) | 868.6 (670.1-1067) | 332.9 (130.8-535.0) | 1058 (576.1-1540) | 360.8 (326.7-383.6) |
| | $EC_{10}$ | 24.44 (19.27-29.60) | 8.621 (6.391-10.85) | --- | 314.5 (171.0-458.1) | 600.3 (411.7-789.0) | 157.4 (25.22-289.7) | 394.6 (93.42-695.8) | 337.7 (290.5-361.0) |
| [Chol][But] | $EC_{50}$ | 884.1 (670.6-1098) | 87.56 (80.63-94.49) | 163.6 (152.5-174.8) | 150.1 (96.74-203.6) | 404.5 (281.3- 527.7) | 104.0 (61.21-146.7) | 214.6 (68.29-360.8) | 637.3 (605.3-671.7) |
| | $EC_{20}$ | 339.4 (191.5-487.4) | 64.58 (48.56-80.60) | 108.3 (96.29-120.3) | 31.44 (0.192-52.68) | 153.6 (71.26-235.9) | 28.48 (6.266-50.69) | 88.52 (0.000-190.9) | 535.5 (489.0-569.9) |
| | $EC_{10}$ | 193.8 (80.23-307.3) | 53.28 (35.37-71.19) | --- | 12.58(0.991-24.17) | 87.06 (24.00-150.1) | 13.34 (0.000-27.45) | 52.73 (0.000-134.4) | 482.2 (422.0-522.8) |
| [Chol][Prop] | $EC_{50}$ | 487.9 (351.5-624.3) | 50.17 (42.50-57.85) | 152.4 (139.1-165.8) | 149.1 (109.7-188.5) | 237.1 (196.3- 277.8) | 208.0 (128.3-287.7) | 556.4 (395.2-717.7 | 673.2 (639.2-711.4) |
| | $EC_{20}$ | 128.8 (65.30-192.4) | 32.78 (25.21-40.36) | --- | 70.31 (39.05-101.6) | 124.3 (88.03-160.6) | 59.93 (19.64-100.2) | 157.1 (73.33-240.8) | 524.9 (475.8-562.5) |
| | $EC_{10}$ | 59.06(20.28-97.84) | 25.55 (17.62-33.49) | --- | --- | 85.15 (51.74-118.6) | 28.92 (2.734-55.10) | 74.90 (19.60-130.2) | 447.4 (381.1-493.8) |
| [Chol][DHPhosp] | $EC_{50}$ | 572.7 (487.5-657.9) | 131.0 (106.0-156.1) | 420.0(368.1-472.0) | 1097(801.0-1393) | 1718 (1385- 2051) | --- | --- | 675.7 (644.2-710.2) |
| | $EC_{20}$ | 114.1 (79.83-148.3) | 64.03(42.16-85.90) | --- | 514.0 (263.7-764.4) | 744.5 (499.7-989.3) | 1833 (445.4-3221) | --- | 552.7(508.8-586.9) |
| | $EC_{10}$ | 44.34 (25.71-62.97) | 42.10(22.31-61.89) | --- | 329.9 (104.3-555.5) | 456.3 (229.8-682.8) | 1065 (0.000-2572) | 1970 (524.3-3399) | 488.3 (431.3-529.2) |
| [Chol][Bic] | $EC_{50}$ | --- | 232.4 (183.1-281.6) | 1375 (1220-1529) | 483.6 (375.1-592.1) | 658.1(558.5- 757.8) | 2589 (392.7-4785) | --- | 840.3 (791.5-890.9) |
| | $EC_{20}$ | --- | 93.15 (57.09-129.2) | 619.0 (494.5-743.4) | 247.8 (152.0-343.6) | 341.8 (252.0-431.6) | 1174 (486.7-1860) | 2331 (925.6-3737) | 698.1 (621.4-750.8) |
| | $EC_{10}$ | 742.0 (12.47-1471) | 54.53 (25.85-83.21) | --- | 167.5 (79.63-255.3) | 232.9 (149.2-316.6) | --- | 1439 (850.1-2027) | 623.8 (523.3-686.8) |
| [Chol][Ac] | $EC_{50}$ | 673.2 (606.5-739.9) | 124.1 (108.4-139.7) | 835.8 (770.2-901.4) | 680.9 (498.9-862.8) | 1121 (899.0- 1343) | 939.0 (541.9-1336) | 2090 (1405-2775) | 694.6 (663.5-728.2) |
| | $EC_{20}$ | 246.2 (203.0-289.3) | 43.18 (33.09-53.27) | --- | 309.6 (163.5-455.7) | 456.1 (289.1-623.0) | 349.0 (74.68-623.3) | 638.8 (323.1-954.5) | 593.9 (550.2-627.1) |
| | $EC_{10}$ | 136.6 (104.2-168.9) | 23.27 (15.86-30.68) | --- | --- | 269.4 (129.4-409.5) | 195.2 (0.000-410.9) | 319.1 (69.57-568.6) | 541.2 (485.2-580.0) |
| [Chol][Sal] | $EC_{50}$ | 236.1 (137.4-334.8) | 302.0 (181.0-423.0) | --- | 110.1 (93.65-126.5) | 136.9 (120.6- 153.3) | 140.1 (107.8-172.4) | 178.4 (148.5-208.3) | 1086 (830.6-1290) |
| | $EC_{20}$ | 56.18 (12.10-100.3) | 50.00 (23.00; 77.00) | 1274 (126.9-2421) | 68.77 (50.14-87.40) | 88.50 (68.75-108.3) | 78.77 (44.97-112.6) | 114.4 (84.00-144.8) | 585.4 (0.000-838.0) |
| | $EC_{10}$ | 24.23 (0.000-49.94) | 17.00 (2.000; 33.00) | 321.5 (183.7-459.4) | 52.21 (32.83-71.59) | 68.54 (46.90-90.18) | 56.21 (21.41-91.01) | 88.20 (51.73-124.7) | 323.7 (0.000-654.2) |
| [Bzchol]Cl | $EC_{50}$ | 1498 (1280-1716) | 196.2 (164.0-228.3) | 456.2 (431.5-481.0) | 11.86 (9.801-13.93) | 13.88 (11.64-16.11) | 26.30 (13.92-38.69) | 49.20 (26.15-72.25) | 217.5 (209.5-225.9) |
| | $EC_{20}$ | 606.6 (449.8-763.4) | 115.2 (84.97-145.4) | --- | 8.020 (5.661-10.38) | 8.619 (6.274-10.96) | 9.090 (0.517-17.66) | 12.33 (1.261-23.39) | 198.9 (186.7-207.2) |
| | $EC_{10}$ | 357.2 (225.5-488.9) | 84.31 (53.65-11.50) | --- | 6.376 (3.845-8.907) | 6.521 (4.138-8.905) | 4.881 (0.000-11.28) | --- | 189.2 (173.4-198.7) |