Table S1 linearity and sensitivity of each metabolite (n=6)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compound |  | Sensitivity | | | | Linearity |
|  | Nominal conc. (ng/ml) | | Found conc.  (ng/ml) | Recovery  (%) | RSD  (%) |  |
| Tetrahydrocannabinol acid | 1.0000 | | 0.9335 | 0.1062 | 93.35 | y = 9.9884x - 4.6402 (R² = 0.9989) |
| Glycocholic acid | 1.0000 | | 1.0340 | 0.1410 | 103.40 | y = 1314.3x - 5.2306 (R² = 0.9997) |
| Glycohyocholic acid | 1.0000 | | 1.0125 | 0.1131 | 101.25 | y = 709.46x - 0.4706 (R² = 0.9973) |
| Tauroursodeoxycholic acid | 1.0000 | | 0.9705 | 0.0956 | 97.05 | y = 1215.6x - 6.3657 (R² = 0.9995) |
| Taurocholic acid | 1.0000 | | 0.9878 | 0.0787 | 98.78 | y = 943.36x + 0.6811 (R² = 0.9953) |
| Cholic acid | 1.0000 | | 0.9828 | 0.1155 | 98.28 | y = 21.447x - 0.7753 (R² = 0.9977) |
| Chenodeoxycholic acid | 1.0000 | | 1.0435 | 0.0789 | 104.35 | y = 141.72x - 1.1172 (R² = 0.9982) |
| Taurochenodeoxycholic acid | 1.0000 | | 0.9735 | 0.0701 | 97.35 | y = 115.7x - 0.5418 (R² = 0.9974) |
| Glycodeoxycholic acid | 1.0000 | | 0.9597 | 0.0991 | 95.97 | y = 412.9x + 0.0881 (R² = 0.9964) |
| Glycoursodeoxycholic acid | 1.0000 | | 0.8878 | 0.0620 | 88.78 | y = 340.37x - 5.5185 (R² = 0.9953) |
| alpha-Muricholic acid | 1.0000 | | 1.0225 | 0.1484 | 102.25 | y = 694.92x - 5.035 (R² = 0.9978) |
| beta-Muricholic acid | 1.0000 | | 0.9949 | 0.0958 | 99.49 | y = 1056.9x - 1.7286 (R² = 0.9989) |
| Glycoehenodeoxycholie acid | 1.0000 | | 1.0111 | 0.1399 | 101.11 | y = 7.0451x - 0.4938 (R² = 0.9973) |
| Taurosulodeoxycholic acid | 1.0000 | | 0.9485 | 0.1153 | 94.85 | y = 21.919x - 11.794 (R² = 0.9960) |
| Trichloroisocyanuric acid | 1.0000 | | 0.9819 | 0.1360 | 98.19 | y = 1230.8x - 2.5833 (R² = 0.9992) |
| Hyodeoxycholic acid | 1.0000 | | 1.0502 | 0.1205 | 105.02 | y = 28.096x + 1.6477 (R² = 0.9935) |
| Lithocholic Acid | 1.0000 | | 0.9962 | 0.0866 | 99.62 | y = 6.0516x + 0.8105 (R² = 0.9951) |
| Deoxycholic acid | 1.0000 | | 1.0120 | 0.1222 | 101.20 | y = 36.022x - 0.4191 (R² = 0.9972) |
| Ursodeoxycholic acid | 1.0000 | | 1.0415 | 0.1022 | 104.15 | y = 61.452x + 0.2593 (R² = 0.9961) |
| 3-keto-Lithocholic Acid | 1.0000 | | 0.9855 | 0.0651 | 98.55 | y = 21.095x - 1.7321 (R² = 0.9989) |
| Adenosine Triphosphate | 1.0000 | | 0.9910 | 0.1082 | 99.10 | y = 4.7788x - 1.4998 (R² = 0.9987) |
| Adenosine diphosphate | 1.0000 | | 1.0033 | 0.1008 | 100.33 | y = 4.4958x - 4.5271 (R² = 0.9991) |
| Adenosine monophosphate | 1.0000 | | 1.0146 | 0.1016 | 101.46 | y = 3.4591x - 4.2754 (R² = 0.9995) |
| Hypoxanthine | 1.0000 | | 0.9990 | 0.1335 | 99.90 | y = 142.34x - 2.2746 (R² = 0.9994) |
| Adenosine | 1.0000 | | 1.0588 | 0.1169 | 105.88 | y = 1.0577x - 1.7273 (R² = 0.9989) |
| Inosine | 1.0000 | | 0.9702 | 0.0590 | 97.02 | y = 26.944x - 1.2393 (R² = 0.9984) |

Table S2 Accuracy and precision (n=6)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compound | Nominal Conc. (ng/ml) | | Mean Conc.(ng/ml) | SD(ng/ml) | Mean Recov.(%) | RSD(%) |
|  | 5.0000 | | 4.9536 | 0.3627 | 99.07 | 8.02 |
| Tetrahydrocannabinol acid | 100.0000 | | 102.0461 | 9.4559 | 102.05 | 10.15 |
|  | 800.0000 | | 846.5166 | 34.0590 | 105.81 | 4.41 |
|  | 5.0000 | | 4.7594 | 0.3985 | 95.19 | 9.17 |
| Glycocholic acid | 100.0000 | | 103.9287 | 9.8137 | 103.93 | 10.34 |
|  | 800.0000 | | 807.5651 | 74.9956 | 100.95 | 10.17 |
|  | 5.0000 | | 4.8901 | 0.2868 | 97.80 | 6.43 |
| Glycohyocholic acid | 100.0000 | | 102.5473 | 9.7887 | 102.55 | 10.46 |
|  | 800.0000 | | 845.3693 | 51.0639 | 105.67 | 6.62 |
|  | 5.0000 | | 4.7950 | 0.4873 | 95.90 | 11.13 |
| Tauroursodeoxycholic acid | 100.0000 | | 101.6726 | 8.2858 | 101.67 | 8.93 |
|  | 800.0000 | | 760.3505 | 71.6003 | 95.04 | 10.32 |
|  | 5.0000 | | 4.9583 | 0.3423 | 99.17 | 7.56 |
| Taurocholic acid | 100.0000 | | 100.7825 | 7.8185 | 100.78 | 8.50 |
|  | 800.0000 | | 785.9571 | 73.9165 | 98.24 | 10.30 |
|  | 5.0000 | | 5.1214 | 0.3605 | 102.43 | 7.71 |
| Cholic acid | 100.0000 | | 105.7997 | 7.8011 | 105.80 | 8.08 |
|  | 800.0000 | | 796.1743 | 56.2650 | 99.52 | 7.74 |
|  | | 5.0000 | 4.7486 | 0.4598 | 94.97 | 10.61 |
| Chenodeoxycholic acid | | 100.0000 | 101.6430 | 6.9921 | 101.64 | 7.54 |
|  | | 800.0000 | 798.9593 | 94.9004 | 99.87 | 13.01 |
|  | | 5.0000 | 5.6175 | 0.2189 | 112.35 | 4.27 |
| Taurochenodeoxycholic acid | | 100.0000 | 110.4290 | 1.9371 | 110.43 | 1.92 |
|  | | 800.0000 | 867.9298 | 43.2977 | 108.49 | 5.46 |
|  | | 5.0000 | 4.7932 | 0.4197 | 95.86 | 9.59 |
| Glycodeoxycholic acid | | 100.0000 | 101.2731 | 8.9119 | 101.27 | 9.64 |
|  | | 800.0000 | 820.2863 | 71.4023 | 102.54 | 9.54 |
|  | | 5.0000 | 4.9622 | 0.4891 | 99.24 | 10.80 |
| Glycoursodeoxycholic acid | | 100.0000 | 100.6173 | 7.2948 | 100.62 | 7.94 |
|  | | 800.0000 | 796.1859 | 66.5185 | 99.52 | 9.15 |
|  | | 5.0000 | 5.7309 | 0.3071 | 114.62 | 5.87 |
| alpha-Muricholic acid | | 100.0000 | 114.4114 | 5.4926 | 114.41 | 5.26 |
|  | | 800.0000 | 885.0517 | 62.4243 | 110.63 | 7.73 |
|  | | 5.0000 | 5.1169 | 0.3491 | 102.34 | 7.47 |
| beta-Muricholic acid | | 100.0000 | 99.4635 | 4.5830 | 99.46 | 5.05 |
|  | | 800.0000 | 794.8170 | 70.2983 | 99.35 | 9.69 |
|  | | 5.0000 | 5.1332 | 0.4458 | 102.66 | 9.51 |
| Glycoehenodeoxycholie acid | | 100.0000 | 105.8906 | 7.1478 | 105.89 | 7.39 |
|  | | 800.0000 | 800.5588 | 52.7601 | 100.07 | 7.22 |
|  | | 5.0000 | 5.0412 | 0.3967 | 100.82 | 8.62 |
| Taurosulodeoxycholic acid | | 100.0000 | 107.7392 | 6.4407 | 107.74 | 6.55 |
|  | | 800.0000 | 737.0192 | 47.4106 | 92.13 | 7.05 |
|  | | 5.0000 | 5.0036 | 0.2973 | 100.07 | 6.51 |
| Trichloroisocyanuric acid | | 100.0000 | 95.5523 | 10.5467 | 95.55 | 12.09 |
|  | | 800.0000 | 811.9914 | 66.6315 | 101.50 | 8.99 |
|  | | 5.0000 | 4.9767 | 0.3547 | 99.53 | 7.81 |
| Hyodeoxycholic acid | | 100.0000 | 98.2119 | 8.3512 | 98.21 | 9.31 |
|  | | 800.0000 | 804.4274 | 53.0640 | 100.55 | 7.23 |
|  | | 5.0000 | 4.9219 | 0.3306 | 98.44 | 7.36 |
| Lithocholic Acid | | 100.0000 | 98.1494 | 7.9448 | 98.15 | 8.87 |
|  | | 800.0000 | 792.2646 | 69.6056 | 99.03 | 9.62 |
|  | | 5.0000 | 4.9035 | 0.3591 | 98.07 | 8.02 |
| Deoxycholic acid | | 100.0000 | 102.8576 | 10.0902 | 102.86 | 10.75 |
|  | | 800.0000 | 806.7084 | 46.1933 | 100.84 | 6.27 |
|  | | 5.0000 | 5.3744 | 0.3418 | 107.49 | 6.97 |
| Ursodeoxycholic acid | | 100.0000 | 102.6265 | 11.9533 | 102.63 | 12.76 |
|  | | 800.0000 | 837.5619 | 35.0913 | 104.70 | 4.59 |
|  | | 5.0000 | 4.7448 | 0.3390 | 94.90 | 7.83 |
| 3-keto-Lithocholic Acid | | 100.0000 | 103.4710 | 7.5906 | 103.47 | 8.04 |
|  | | 800.0000 | 789.3982 | 74.8307 | 98.67 | 10.38 |
|  | | 5.0000 | 4.9782 | 0.3040 | 99.56 | 6.69 |
| Adenosine Triphosphate | | 100.0000 | 94.0295 | 7.1637 | 94.03 | 8.35 |
|  | | 800.0000 | 795.7713 | 58.7066 | 99.47 | 8.08 |
|  | | 5.0000 | 5.2326 | 0.3631 | 104.65 | 7.60 |
| Adenosine diphosphate | | 100.0000 | 101.9245 | 8.7272 | 101.92 | 9.38 |
|  | | 800.0000 | 822.9251 | 67.3985 | 102.87 | 8.97 |
|  | | 5.0000 | 4.9948 | 0.4887 | 99.90 | 10.72 |
| Adenosine monophosphate | | 100.0000 | 99.1976 | 8.0000 | 99.20 | 8.83 |
|  | | 800.0000 | 788.2026 | 51.4441 | 98.53 | 7.15 |
|  | | 5.0000 | 5.3542 | 0.3157 | 107.08 | 6.46 |
| Hypoxanthine | | 100.0000 | 97.3490 | 10.1438 | 97.35 | 11.41 |
|  | | 800.0000 | 781.6017 | 69.5394 | 97.70 | 9.75 |
|  | | 5.0000 | 5.0073 | 0.2800 | 100.15 | 6.13 |
| Adenosine | | 100.0000 | 99.0036 | 5.9177 | 99.00 | 6.55 |
|  | | 800.0000 | 784.2736 | 42.1942 | 98.03 | 5.89 |
|  | | 5.0000 | 5.1716 | 0.4226 | 103.43 | 8.95 |
| Inosine | | 100.0000 | 100.1942 | 6.5198 | 100.19 | 7.13 |
|  | | 800.0000 | 824.4671 | 43.0351 | 103.06 | 5.72 |

Table S3 stability of constant temperature (n=6)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Nominal Conc. (ng/ml) | Mean Conc.(ng/ml) | SD(ng/ml) | Mean Recov.(%) | RSD(%) |
|  | 5.0000 | 5.1627 | 0.3825 | 103.25 | 8.12 |
| Tetrahydrocannabinol acid | 100.0000 | 100.2987 | 8.7062 | 100.30 | 9.51 |
|  | 800.0000 | 818.1225 | 61.9266 | 102.27 | 8.29 |
|  | 5.0000 | 4.9583 | 0.2090 | 99.17 | 4.62 |
| Glycocholic acid | 100.0000 | 106.2422 | 7.1643 | 106.24 | 7.39 |
|  | 800.0000 | 842.8723 | 74.3557 | 105.36 | 9.66 |
|  | 5.0000 | 4.6597 | 0.3766 | 93.19 | 8.85 |
| Glycohyocholic acid | 100.0000 | 101.3053 | 9.6420 | 101.31 | 10.43 |
|  | 800.0000 | 805.5112 | 77.5994 | 100.69 | 10.55 |
|  | 5.0000 | 4.9717 | 0.3900 | 99.43 | 8.59 |
| Tauroursodeoxycholic acid | 100.0000 | 100.9118 | 6.0989 | 100.91 | 6.62 |
|  | 800.0000 | 794.6246 | 64.7719 | 99.33 | 8.93 |
|  | 5.0000 | 4.5872 | 0.2031 | 91.74 | 4.85 |
| Taurocholic acid | 100.0000 | 97.3840 | 10.4110 | 97.38 | 11.71 |
|  | 800.0000 | 815.9301 | 84.6765 | 101.99 | 11.37 |
|  | 5.0000 | 5.2319 | 0.3571 | 104.64 | 7.48 |
| Cholic acid | 100.0000 | 95.6256 | 4.9512 | 95.63 | 5.67 |
|  | 800.0000 | 792.8678 | 57.7495 | 99.11 | 7.98 |
|  | 5.0000 | 4.7395 | 0.3149 | 94.79 | 7.28 |
| Chenodeoxycholic acid | 100.0000 | 102.6188 | 6.3945 | 102.62 | 6.83 |
|  | 800.0000 | 760.4875 | 56.2816 | 95.06 | 8.11 |
|  | 5.0000 | 5.7466 | 0.2300 | 114.93 | 4.38 |
| Taurochenodeoxycholic acid | 100.0000 | 108.1398 | 4.5627 | 108.14 | 4.62 |
|  | 800.0000 | 842.5817 | 31.3655 | 105.32 | 4.08 |
|  | 5.0000 | 4.9037 | 0.3131 | 98.07 | 6.99 |
| Glycodeoxycholic acid | 100.0000 | 106.1717 | 7.9215 | 106.17 | 8.17 |
|  | 800.0000 | 788.8688 | 72.3853 | 98.61 | 10.05 |
|  | 5.0000 | 4.7251 | 0.4258 | 94.50 | 9.87 |
| Glycoursodeoxycholic acid | 100.0000 | 101.7750 | 5.2239 | 101.77 | 5.62 |
|  | 800.0000 | 769.2818 | 83.2410 | 96.16 | 11.85 |
|  | 5.0000 | 4.9545 | 0.3025 | 99.09 | 6.69 |
| alpha-Muricholic acid | 100.0000 | 85.0068 | 36.8141 | 85.01 | 47.44 |
|  | 800.0000 | 783.6370 | 63.6475 | 97.95 | 8.90 |
|  | 5.0000 | 5.2799 | 0.2774 | 105.60 | 5.76 |
| beta-Muricholic acid | 100.0000 | 99.8989 | 8.9063 | 99.90 | 9.77 |
|  | 800.0000 | 793.4020 | 41.4183 | 99.18 | 5.72 |
|  | 5.0000 | 5.0100 | 0.3143 | 100.20 | 6.87 |
| Glycoehenodeoxycholie acid | 100.0000 | 100.0848 | 8.3949 | 100.08 | 9.19 |
|  | 800.0000 | 777.3027 | 63.0358 | 97.16 | 8.88 |
|  | 5.0000 | 5.0185 | 0.3096 | 100.37 | 6.76 |
| Taurosulodeoxycholic acid | 100.0000 | 104.8219 | 2.4241 | 104.82 | 2.53 |
|  | 800.0000 | 719.9350 | 18.1953 | 89.99 | 2.77 |
|  | 5.0000 | 4.8594 | 0.2512 | 97.19 | 5.66 |
| Trichloroisocyanuric acid | 100.0000 | 96.5215 | 5.7732 | 94.65 | 8.36 |
|  | 800.0000 | 798.6750 | 60.4536 | 99.83 | 8.29 |
|  | 5.0000 | 5.0800 | 0.3298 | 101.60 | 7.11 |
| Hyodeoxycholic acid | 100.0000 | 106.8696 | 5.9870 | 106.87 | 6.14 |
|  | 800.0000 | 765.7356 | 49.0836 | 93.69 | 5.44 |
|  | 5.0000 | 4.2561 | 0.3387 | 85.12 | 8.72 |
| Lithocholic Acid | 100.0000 | 95.1831 | 2.9960 | 95.18 | 3.45 |
|  | 800.0000 | 749.5497 | 37.2349 | 95.72 | 7.02 |
|  | 5.0000 | 4.9266 | 0.2953 | 98.53 | 6.57 |
| Deoxycholic acid | 100.0000 | 91.8274 | 5.3157 | 91.83 | 6.34 |
|  | 800.0000 | 815.6808 | 37.3642 | 101.96 | 5.02 |
|  | 5.0000 | 4.9957 | 0.4900 | 99.91 | 10.74 |
| Ursodeoxycholic acid | 100.0000 | 94.3250 | 5.2851 | 94.33 | 6.14 |
|  | 800.0000 | 830.5895 | 74.5243 | 103.82 | 9.83 |
|  | 5.0000 | 5.1164 | 0.3828 | 102.33 | 8.20 |
| 3-keto-Lithocholic Acid | 100.0000 | 99.2235 | 7.2799 | 99.22 | 8.04 |
|  | 800.0000 | 801.4738 | 72.1070 | 100.18 | 9.86 |
|  | 5.0000 | 4.9120 | 0.4048 | 98.24 | 9.03 |
| Adenosine Triphosphate | 100.0000 | 98.1368 | 9.8237 | 98.14 | 10.97 |
|  | 800.0000 | 769.0219 | 51.8680 | 96.13 | 7.39 |
|  | 5.0000 | 4.9300 | 0.4279 | 98.60 | 9.51 |
| Adenosine diphosphate | 100.0000 | 97.9824 | 10.3345 | 97.98 | 11.55 |
|  | 800.0000 | 875.4423 | 39.4711 | 109.43 | 4.94 |
|  | 5.0000 | 4.9144 | 0.5281 | 98.29 | 11.77 |
| Adenosine monophosphate | 100.0000 | 98.6299 | 8.6292 | 98.63 | 9.58 |
|  | 800.0000 | 775.8805 | 55.3721 | 96.99 | 7.82 |
|  | 5.0000 | 5.1736 | 0.5129 | 103.47 | 10.86 |
| Hypoxanthine | 100.0000 | 100.3717 | 9.6217 | 100.37 | 10.50 |
|  | 800.0000 | 800.7672 | 65.3468 | 100.10 | 8.94 |
|  | 5.0000 | 4.7750 | 0.3533 | 95.50 | 8.10 |
| Adenosine | 100.0000 | 104.8246 | 7.0793 | 104.82 | 7.40 |
|  | 800.0000 | 832.8428 | 57.0786 | 104.11 | 7.51 |
|  | 5.0000 | 5.2270 | 0.3951 | 104.54 | 8.28 |
| Inosine | 100.0000 | 100.2560 | 9.2398 | 100.26 | 10.10 |
|  | 800.0000 | 760.3766 | 65.5924 | 95.05 | 9.45 |

Table S4 stability of bench-top (n=6)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Nominal Conc. (ng/ml) | Mean Conc.(ng/ml) | SD(ng/ml) | Mean Recov.(%) | RSD(%) |
|  | 5.0000 | 4.9175 | 0.2218 | 98.35 | 4.94 |
| Tetrahydrocannabinol acid | 100.0000 | 105.1729 | 7.5451 | 105.17 | 7.86 |
|  | 800.0000 | 803.2401 | 75.0061 | 102.27 | 8.29 |
|  | 5.0000 | 5.0345 | 0.4437 | 100.69 | 9.66 |
| Glycocholic acid | 100.0000 | 107.4235 | 4.3665 | 107.42 | 4.45 |
|  | 800.0000 | 807.2112 | 64.8399 | 105.36 | 9.66 |
|  | 5.0000 | 4.9025 | 0.2421 | 98.05 | 5.41 |
| Glycohyocholic acid | 100.0000 | 103.1188 | 8.6173 | 103.12 | 9.15 |
|  | 800.0000 | 785.2669 | 50.3485 | 100.69 | 10.55 |
|  | 5.0000 | 4.9865 | 0.1450 | 99.73 | 3.19 |
| Tauroursodeoxycholic acid | 100.0000 | 101.8917 | 7.0151 | 101.89 | 7.54 |
|  | 800.0000 | 819.4795 | 25.7417 | 99.33 | 8.93 |
|  | 5.0000 | 4.6793 | 0.4384 | 93.59 | 10.26 |
| Taurocholic acid | 100.0000 | 93.3111 | 6.3626 | 93.31 | 7.47 |
|  | 800.0000 | 823.5762 | 33.3346 | 101.99 | 11.37 |
|  | 5.0000 | 5.0334 | 0.5650 | 100.67 | 12.30 |
| Cholic acid | 100.0000 | 97.0951 | 5.1888 | 97.10 | 5.85 |
|  | 800.0000 | 795.6282 | 82.2447 | 99.11 | 7.98 |
|  | 5.0000 | 5.1981 | 0.3828 | 103.96 | 8.07 |
| Chenodeoxycholic acid | 100.0000 | 103.5292 | 8.8026 | 103.53 | 9.31 |
|  | 800.0000 | 782.2942 | 39.5640 | 95.06 | 8.11 |
|  | 5.0000 | 5.2724 | 0.3812 | 105.45 | 7.92 |
| Taurochenodeoxycholic acid | 100.0000 | 108.9488 | 4.5375 | 108.95 | 4.56 |
|  | 800.0000 | 846.8404 | 34.9536 | 105.32 | 4.08 |
|  | 5.0000 | 4.8610 | 0.4206 | 97.22 | 9.48 |
| Glycodeoxycholic acid | 100.0000 | 106.2825 | 6.2571 | 106.28 | 6.45 |
|  | 800.0000 | 745.7884 | 36.4817 | 98.61 | 10.05 |
|  | 5.0000 | 4.9156 | 0.4090 | 98.31 | 9.11 |
| Glycoursodeoxycholic acid | 100.0000 | 104.2289 | 8.3959 | 104.23 | 8.82 |
|  | 800.0000 | 807.4907 | 70.0525 | 96.16 | 11.85 |
|  | 5.0000 | 4.9742 | 0.2524 | 99.48 | 5.56 |
| alpha-Muricholic acid | 100.0000 | 103.7063 | 8.3461 | 103.71 | 8.82 |
|  | 800.0000 | 751.8692 | 37.8548 | 97.95 | 8.90 |
|  | 5.0000 | 5.2274 | 0.3866 | 104.55 | 8.10 |
| beta-Muricholic acid | 100.0000 | 97.5645 | 6.2330 | 97.56 | 7.00 |
|  | 800.0000 | 791.9312 | 72.5905 | 99.18 | 5.72 |
|  | 5.0000 | 5.0451 | 0.5131 | 100.90 | 11.14 |
| Glycoehenodeoxycholie acid | 100.0000 | 104.5702 | 8.0144 | 104.57 | 8.40 |
|  | 800.0000 | 766.3402 | 72.6328 | 97.16 | 8.88 |
|  | 5.0000 | 4.7659 | 0.2779 | 95.32 | 6.39 |
| Taurosulodeoxycholic acid | 100.0000 | 104.4529 | 4.7613 | 104.45 | 4.99 |
|  | 800.0000 | 720.5960 | 54.1245 | 89.99 | 2.77 |
|  | 5.0000 | 5.1157 | 0.4219 | 102.31 | 9.03 |
| Trichloroisocyanuric acid | 100.0000 | 97.4228 | 5.3665 | 97.42 | 6.03 |
|  | 800.0000 | 784.3823 | 41.5190 | 99.83 | 8.29 |
|  | 5.0000 | 5.1735 | 0.4601 | 103.47 | 9.74 |
| Hyodeoxycholic acid | 100.0000 | 100.7793 | 5.3682 | 100.78 | 5.84 |
|  | 800.0000 | 750.0851 | 51.4876 | 95.72 | 7.02 |
|  | 5.0000 | 4.9118 | 0.4831 | 98.24 | 10.77 |
| Lithocholic Acid | 100.0000 | 102.2989 | 6.7367 | 102.30 | 7.21 |
|  | 800.0000 | 731.7893 | 46.4317 | 93.69 | 5.44 |
|  | 5.0000 | 5.0031 | 0.4833 | 100.06 | 10.58 |
| Deoxycholic acid | 100.0000 | 96.0897 | 6.3806 | 96.09 | 7.27 |
|  | 800.0000 | 825.7309 | 59.0834 | 101.96 | 5.02 |
|  | 5.0000 | 4.8812 | 0.5320 | 97.62 | 11.94 |
| Ursodeoxycholic acid | 100.0000 | 98.1810 | 6.4117 | 98.18 | 7.15 |
|  | 800.0000 | 805.6864 | 96.6640 | 103.82 | 9.83 |
|  | 5.0000 | 5.2838 | 0.3719 | 105.68 | 7.71 |
| 3-keto-Lithocholic Acid | 100.0000 | 99.5914 | 8.7770 | 99.59 | 9.65 |
|  | 800.0000 | 748.3757 | 62.2715 | 100.18 | 9.86 |
|  | 5.0000 | 5.0578 | 0.4553 | 101.16 | 9.86 |
| Adenosine Triphosphate | 100.0000 | 95.7172 | 8.1913 | 95.72 | 9.37 |
|  | 800.0000 | 786.4107 | 41.8093 | 96.13 | 7.39 |
|  | 5.0000 | 4.7233 | 0.3444 | 94.47 | 7.99 |
| Adenosine diphosphate | 100.0000 | 105.3988 | 8.9285 | 105.40 | 9.28 |
|  | 800.0000 | 842.8571 | 59.6020 | 109.43 | 4.94 |
|  | 5.0000 | 4.8924 | 0.4593 | 97.85 | 10.28 |
| Adenosine monophosphate | 100.0000 | 102.0079 | 10.1807 | 102.01 | 10.93 |
|  | 800.0000 | 777.6139 | 60.5505 | 96.99 | 7.82 |
|  | 5.0000 | 5.3200 | 0.5290 | 106.40 | 10.89 |
| Hypoxanthine | 100.0000 | 101.6274 | 10.0640 | 101.63 | 10.85 |
|  | 800.0000 | 811.7114 | 45.6428 | 100.10 | 8.94 |
|  | 5.0000 | 4.9650 | 0.5705 | 99.30 | 12.59 |
| Adenosine | 100.0000 | 108.3259 | 5.7510 | 108.33 | 5.82 |
|  | 800.0000 | 782.0940 | 35.0338 | 104.11 | 7.51 |
|  | 5.0000 | 5.1057 | 0.4225 | 102.11 | 9.06 |
| Inosine | 100.0000 | 101.2388 | 6.8992 | 101.24 | 7.47 |
|  | 800.0000 | 763.1284 | 69.1318 | 95.05 | 9.45 |

Table S5 stability of freeze-thaw (n=6)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Nominal Conc. (ng/ml) | Mean Conc.(ng/ml) | SD(ng/ml) | Mean Recov.(%) | RSD(%) |
|  | 5.0000 | 4.8467 | 0.3593 | 96.93 | 8.12 |
| Tetrahydrocannabinol acid | 100.0000 | 101.7171 | 5.8946 | 101.72 | 6.35 |
|  | 800.0000 | 812.3086 | 68.8035 | 101.54 | 9.28 |
|  | 5.0000 | 5.3225 | 0.3142 | 106.45 | 6.47 |
| Glycocholic acid | 100.0000 | 103.6674 | 6.8408 | 103.67 | 7.23 |
|  | 800.0000 | 830.1557 | 60.1580 | 103.77 | 7.94 |
|  | 5.0000 | 4.6285 | 0.2760 | 92.57 | 6.53 |
| Glycohyocholic acid | 100.0000 | 98.6908 | 11.0127 | 98.69 | 12.22 |
|  | 800.0000 | 815.7360 | 48.1999 | 101.97 | 6.47 |
|  | 5.0000 | 4.5794 | 0.3283 | 91.59 | 7.85 |
| Tauroursodeoxycholic acid | 100.0000 | 96.7125 | 8.0646 | 96.71 | 9.13 |
|  | 800.0000 | 817.2518 | 71.3894 | 102.16 | 9.57 |
|  | 5.0000 | 4.6750 | 0.2419 | 93.50 | 5.67 |
| Taurocholic acid | 100.0000 | 93.3093 | 5.8145 | 93.31 | 6.83 |
|  | 800.0000 | 833.1660 | 85.9582 | 104.15 | 11.30 |
|  | 5.0000 | 5.2649 | 0.3736 | 105.30 | 7.77 |
| Cholic acid | 100.0000 | 95.9197 | 9.6524 | 95.92 | 11.02 |
|  | 800.0000 | 806.8368 | 33.4389 | 100.85 | 4.54 |
|  | 5.0000 | 5.1459 | 0.3542 | 102.92 | 7.54 |
| Chenodeoxycholic acid | 100.0000 | 106.4678 | 8.8320 | 106.47 | 9.09 |
|  | 800.0000 | 774.7504 | 72.8703 | 96.84 | 10.30 |
|  | 5.0000 | 5.5245 | 0.1723 | 110.49 | 3.42 |
| Taurochenodeoxycholic acid | 100.0000 | 103.3974 | 4.0546 | 103.40 | 4.30 |
|  | 800.0000 | 877.6079 | 28.5856 | 109.70 | 3.57 |
|  | 5.0000 | 4.8358 | 0.3848 | 96.72 | 8.72 |
| Glycodeoxycholic acid | 100.0000 | 109.0846 | 5.5063 | 109.08 | 5.53 |
|  | 800.0000 | 770.0321 | 97.9486 | 96.25 | 13.93 |
|  | 5.0000 | 5.0045 | 0.4387 | 100.09 | 9.60 |
| Glycoursodeoxycholic acid | 100.0000 | 99.4769 | 8.7548 | 99.48 | 9.64 |
|  | 800.0000 | 803.9520 | 46.0523 | 100.49 | 6.27 |
|  | 5.0000 | 5.1056 | 0.5122 | 102.11 | 10.99 |
| alpha-Muricholic acid | 100.0000 | 98.0000 | 7.3199 | 98.00 | 8.18 |
|  | 800.0000 | 771.8937 | 54.2600 | 96.49 | 7.70 |
|  | 5.0000 | 5.1903 | 0.5127 | 103.81 | 10.82 |
| beta-Muricholic acid | 100.0000 | 97.9798 | 8.7150 | 97.98 | 9.74 |
|  | 800.0000 | 800.7005 | 52.0932 | 100.09 | 7.13 |
|  | 5.0000 | 4.9323 | 0.3365 | 98.65 | 7.47 |
| Glycoehenodeoxycholie acid | 100.0000 | 101.6204 | 6.4326 | 101.62 | 6.93 |
|  | 800.0000 | 804.5176 | 48.0642 | 100.56 | 6.54 |
|  | 5.0000 | 5.0629 | 0.2122 | 101.26 | 4.59 |
| Taurosulodeoxycholic acid | 100.0000 | 105.5102 | 5.4338 | 105.51 | 5.64 |
|  | 800.0000 | 738.8935 | 29.5881 | 92.36 | 4.39 |
|  | 5.0000 | 4.7852 | 0.3019 | 95.70 | 6.91 |
| Trichloroisocyanuric acid | 100.0000 | 95.2877 | 7.0593 | 95.29 | 8.12 |
|  | 800.0000 | 813.4193 | 61.7771 | 101.68 | 8.32 |
|  | 5.0000 | 4.8900 | 0.4040 | 97.80 | 9.05 |
| Hyodeoxycholic acid | 100.0000 | 103.4078 | 9.9559 | 103.41 | 10.55 |
|  | 800.0000 | 778.0824 | 57.3776 | 97.26 | 8.08 |
|  | 5.0000 | 4.7530 | 0.2793 | 95.06 | 6.44 |
| Lithocholic Acid | 100.0000 | 97.6744 | 5.6656 | 97.67 | 6.35 |
|  | 800.0000 | 777.7546 | 36.1664 | 97.22 | 5.09 |
|  | 5.0000 | 4.9394 | 0.2850 | 98.79 | 6.32 |
| Deoxycholic acid | 100.0000 | 93.4697 | 6.2744 | 93.47 | 7.35 |
|  | 800.0000 | 798.8125 | 62.9999 | 99.85 | 8.64 |
|  | 5.0000 | 4.8384 | 0.1842 | 96.77 | 4.17 |
| Ursodeoxycholic acid | 100.0000 | 98.5090 | 7.1374 | 98.51 | 7.94 |
|  | 800.0000 | 820.2495 | 50.3965 | 102.53 | 6.73 |
|  | 5.0000 | 5.1375 | 0.2924 | 102.75 | 6.24 |
| 3-keto-Lithocholic Acid | 100.0000 | 101.7642 | 5.7620 | 101.76 | 6.20 |
|  | 800.0000 | 815.0353 | 111.6079 | 101.88 | 15.00 |
|  | 5.0000 | 4.9233 | 0.3539 | 98.47 | 7.87 |
| Adenosine Triphosphate | 100.0000 | 98.0791 | 7.1951 | 98.08 | 8.04 |
|  | 800.0000 | 799.4965 | 62.1842 | 99.94 | 8.52 |
|  | 5.0000 | 5.2983 | 0.3448 | 105.97 | 7.13 |
| Adenosine diphosphate | 100.0000 | 97.1779 | 9.5649 | 97.18 | 10.78 |
|  | 800.0000 | 877.3675 | 28.3153 | 109.67 | 3.54 |
|  | 5.0000 | 5.0969 | 0.4853 | 101.94 | 10.43 |
| Adenosine monophosphate | 100.0000 | 99.2930 | 6.9446 | 99.29 | 7.66 |
|  | 800.0000 | 786.9548 | 67.0271 | 98.37 | 9.33 |
|  | 5.0000 | 5.1122 | 0.4216 | 102.24 | 9.03 |
| Hypoxanthine | 100.0000 | 98.1004 | 6.3397 | 98.10 | 7.08 |
|  | 800.0000 | 814.3396 | 95.1472 | 101.79 | 12.80 |
|  | 5.0000 | 4.8781 | 0.4363 | 97.56 | 9.80 |
| Adenosine | 100.0000 | 100.7479 | 6.6551 | 100.75 | 7.24 |
|  | 800.0000 | 824.6035 | 46.1358 | 103.08 | 6.13 |
|  | 5.0000 | 5.2048 | 0.4066 | 104.10 | 8.56 |
| Inosine | 100.0000 | 98.6161 | 9.6653 | 98.62 | 10.74 |
|  | 800.0000 | 769.7896 | 62.1376 | 96.22 | 8.84 |

Table S6 stability of long-term storage (n=6)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Nominal Conc. (ng/ml) | Mean Conc.(ng/ml) | SD(ng/ml) | Mean Recov.(%) | RSD(%) |
|  | 5.0000 | 4.9590 | 0.4307 | 99.18 | 9.52 |
| Tetrahydrocannabinol acid | 100.0000 | 98.6970 | 7.2082 | 98.70 | 8.00 |
|  | 800.0000 | 808.5454 | 70.8991 | 101.07 | 9.61 |
|  | 5.0000 | 4.9772 | 0.2253 | 99.54 | 4.96 |
| Glycocholic acid | 100.0000 | 103.5074 | 7.7529 | 103.51 | 8.21 |
|  | 800.0000 | 811.4128 | 51.5766 | 101.43 | 6.96 |
|  | 5.0000 | 4.6708 | 0.3833 | 93.42 | 8.99 |
| Glycohyocholic acid | 100.0000 | 98.5696 | 8.1922 | 98.57 | 9.10 |
|  | 800.0000 | 799.0786 | 46.6449 | 99.88 | 6.39 |
|  | 5.0000 | 4.7397 | 0.3839 | 94.79 | 8.87 |
| Tauroursodeoxycholic acid | 100.0000 | 98.6196 | 6.6605 | 98.62 | 7.40 |
|  | 800.0000 | 783.6845 | 52.0296 | 97.96 | 7.27 |
|  | 5.0000 | 4.5924 | 0.1782 | 91.85 | 4.25 |
| Taurocholic acid | 100.0000 | 98.3555 | 10.3303 | 98.36 | 11.51 |
|  | 800.0000 | 785.5610 | 56.2411 | 98.20 | 7.84 |
|  | 5.0000 | 5.0801 | 0.3210 | 101.60 | 6.92 |
| Cholic acid | 100.0000 | 94.3688 | 5.0475 | 94.37 | 5.86 |
|  | 800.0000 | 755.9731 | 52.1055 | 94.50 | 7.55 |
|  | 5.0000 | 5.1385 | 0.3992 | 102.77 | 8.51 |
| Chenodeoxycholic acid | 100.0000 | 101.8574 | 8.6090 | 101.86 | 9.26 |
|  | 800.0000 | 778.3338 | 58.9934 | 97.29 | 8.30 |
|  | 5.0000 | 5.1034 | 0.3294 | 102.07 | 7.07 |
| Taurochenodeoxycholic acid | 100.0000 | 108.3837 | 3.8280 | 108.38 | 3.87 |
|  | 800.0000 | 870.1824 | 32.2555 | 108.77 | 4.06 |
|  | 5.0000 | 4.9403 | 0.3547 | 98.81 | 7.87 |
| Glycodeoxycholic acid | 100.0000 | 105.4750 | 4.6930 | 105.47 | 4.87 |
|  | 800.0000 | 803.1240 | 60.4148 | 100.39 | 8.24 |
|  | 5.0000 | 5.1215 | 0.4499 | 102.43 | 9.62 |
| Glycoursodeoxycholic acid | 100.0000 | 98.9020 | 7.4143 | 98.90 | 8.21 |
|  | 800.0000 | 861.2738 | 39.8950 | 107.66 | 5.07 |
|  | 5.0000 | 4.8794 | 0.2747 | 97.59 | 6.17 |
| alpha-Muricholic acid | 100.0000 | 99.7911 | 9.5589 | 99.79 | 10.49 |
|  | 800.0000 | 780.7197 | 52.2843 | 97.59 | 7.34 |
|  | 5.0000 | 4.9931 | 0.5455 | 99.86 | 11.97 |
| beta-Muricholic acid | 100.0000 | 102.2500 | 5.4586 | 102.25 | 5.85 |
|  | 800.0000 | 742.1369 | 51.6669 | 92.77 | 7.63 |
|  | 5.0000 | 4.8954 | 0.4784 | 97.91 | 10.71 |
| Glycoehenodeoxycholie acid | 100.0000 | 101.2478 | 7.7987 | 101.25 | 8.44 |
|  | 800.0000 | 792.1782 | 68.4423 | 99.02 | 9.46 |
|  | 5.0000 | 4.8661 | 0.2941 | 97.32 | 6.62 |
| Taurosulodeoxycholic acid | 100.0000 | 104.3950 | 6.2816 | 104.39 | 6.59 |
|  | 800.0000 | 735.7106 | 47.2372 | 91.96 | 7.03 |
|  | 5.0000 | 4.8148 | 0.2879 | 96.30 | 6.55 |
| Trichloroisocyanuric acid | 100.0000 | 99.5418 | 8.9674 | 99.54 | 9.87 |
|  | 800.0000 | 780.1260 | 65.2344 | 97.52 | 9.16 |
|  | 5.0000 | 4.8983 | 0.4165 | 97.97 | 9.31 |
| Hyodeoxycholic acid | 100.0000 | 101.6483 | 9.1452 | 101.65 | 9.86 |
|  | 800.0000 | 761.7421 | 60.7230 | 95.22 | 8.73 |
|  | 5.0000 | 4.5476 | 0.1757 | 90.95 | 4.23 |
| Lithocholic Acid | 100.0000 | 98.7001 | 6.6127 | 98.70 | 7.34 |
|  | 800.0000 | 738.6906 | 47.2554 | 92.34 | 7.01 |
|  | 5.0000 | 4.8355 | 0.3342 | 96.71 | 7.57 |
| Deoxycholic acid | 100.0000 | 91.7802 | 7.1161 | 91.78 | 8.49 |
|  | 800.0000 | 804.9923 | 52.2146 | 100.62 | 7.11 |
|  | 5.0000 | 4.8326 | 0.1957 | 97.85 | 6.37 |
| Ursodeoxycholic acid | 100.0000 | 92.8791 | 2.9722 | 96.65 | 4.44 |
|  | 800.0000 | 811.1967 | 78.7148 | 92.88 | 3.51 |
|  | 5.0000 | 4.8925 | 0.2846 | 101.40 | 10.63 |
| 3-keto-Lithocholic Acid | 100.0000 | 96.6345 | 7.1544 | 97.85 | 6.37 |
|  | 800.0000 | 779.4355 | 99.1934 | 96.63 | 8.11 |
|  | 5.0000 | 4.7467 | 0.3595 | 97.43 | 13.94 |
| Adenosine Triphosphate | 100.0000 | 102.0113 | 5.5944 | 94.93 | 8.30 |
|  | 800.0000 | 782.0876 | 58.0942 | 102.01 | 6.01 |
|  | 5.0000 | 5.1763 | 0.4424 | 97.76 | 8.14 |
| Adenosine diphosphate | 100.0000 | 98.4561 | 7.3236 | 103.53 | 9.36 |
|  | 800.0000 | 861.0312 | 32.9029 | 98.46 | 8.15 |
|  | 5.0000 | 4.9078 | 0.4665 | 107.63 | 4.19 |
| Adenosine monophosphate | 100.0000 | 100.6506 | 8.3965 | 100.65 | 9.14 |
|  | 800.0000 | 760.5149 | 44.5609 | 95.06 | 6.42 |
|  | 5.0000 | 4.9414 | 0.2442 | 98.83 | 5.41 |
| Hypoxanthine | 100.0000 | 101.8549 | 9.2301 | 101.85 | 9.93 |
|  | 800.0000 | 820.4421 | 58.6580 | 102.56 | 7.83 |
|  | 5.0000 | 4.8712 | 0.4530 | 97.42 | 10.19 |
| Adenosine | 100.0000 | 101.0291 | 4.8805 | 101.03 | 5.29 |
|  | 800.0000 | 796.4947 | 69.8171 | 99.56 | 9.60 |
|  | 5.0000 | 5.1567 | 0.3941 | 103.13 | 8.37 |
| Inosine | 100.0000 | 97.9843 | 8.4685 | 97.98 | 9.47 |
|  | 800.0000 | 798.8543 | 76.5032 | 99.86 | 10.49 |

Table S7 matrix effect of the serum (n=6)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Nominal Conc. (ng/ml) | Mean Conc.(ng/ml) | SD(ng/ml) | Mean Recov.(%) | RSD(%) |
|  | 5.0000 | 4.7226 | 0.3527 | 94.45 | 8.18 |
| Tetrahydrocannabinol acid | 100.0000 | 103.6410 | 7.5774 | 103.64 | 8.01 |
|  | 800.0000 | 795.0882 | 73.1633 | 99.39 | 10.08 |
|  | 5.0000 | 5.0092 | 0.3805 | 100.18 | 8.32 |
| Glycocholic acid | 100.0000 | 108.9400 | 2.8856 | 108.94 | 2.90 |
|  | 800.0000 | 839.0804 | 63.2108 | 104.89 | 8.25 |
|  | 5.0000 | 4.7283 | 0.3760 | 94.57 | 8.71 |
| Glycohyocholic acid | 100.0000 | 100.3688 | 8.7473 | 100.37 | 9.55 |
|  | 800.0000 | 795.3982 | 45.9853 | 99.42 | 6.33 |
|  | 5.0000 | 4.7843 | 0.4159 | 95.69 | 9.52 |
| Tauroursodeoxycholic acid | 100.0000 | 103.5776 | 2.8937 | 103.58 | 3.06 |
|  | 800.0000 | 831.0592 | 29.5537 | 103.88 | 3.90 |
|  | 5.0000 | 4.5641 | 0.3119 | 91.28 | 7.49 |
| Taurocholic acid | 100.0000 | 98.4096 | 5.4923 | 98.41 | 6.11 |
|  | 800.0000 | 804.1250 | 62.9869 | 100.52 | 8.58 |
|  | 5.0000 | 5.0369 | 0.5035 | 100.74 | 10.95 |
| Cholic acid | 100.0000 | 101.1904 | 6.7578 | 101.19 | 7.32 |
|  | 800.0000 | 806.0611 | 35.6584 | 100.76 | 4.85 |
|  | 5.0000 | 4.7900 | 0.3902 | 95.80 | 8.92 |
| Chenodeoxycholic acid | 100.0000 | 103.0049 | 7.9994 | 103.00 | 8.51 |
|  | 800.0000 | 768.5393 | 36.7953 | 96.07 | 5.24 |
|  | 5.0000 | 4.6553 | 0.4361 | 93.11 | 10.26 |
| Taurochenodeoxycholic acid | 100.0000 | 111.6099 | 1.6273 | 111.61 | 1.60 |
|  | 800.0000 | 852.0588 | 40.8944 | 106.51 | 5.26 |
|  | 5.0000 | 4.8394 | 0.4240 | 96.79 | 9.60 |
| Glycodeoxycholic acid | 100.0000 | 108.3319 | 4.5103 | 108.33 | 4.56 |
|  | 800.0000 | 785.3669 | 68.9310 | 98.17 | 9.61 |
|  | 5.0000 | 4.7059 | 0.4106 | 94.12 | 9.56 |
| Glycoursodeoxycholic acid | 100.0000 | 108.9101 | 4.2186 | 108.91 | 4.24 |
|  | 800.0000 | 768.5872 | 54.4622 | 96.07 | 7.76 |
|  | 5.0000 | 4.8549 | 0.2503 | 97.10 | 5.65 |
| alpha-Muricholic acid | 100.0000 | 101.9646 | 8.3795 | 101.96 | 9.00 |
|  | 800.0000 | 781.4942 | 75.0854 | 97.69 | 10.52 |
|  | 5.0000 | 5.0981 | 0.3796 | 101.96 | 8.16 |
| beta-Muricholic acid | 100.0000 | 101.3103 | 6.9795 | 101.31 | 7.55 |
|  | 800.0000 | 786.6783 | 55.6891 | 98.33 | 7.75 |
|  | 5.0000 | 4.9393 | 0.3118 | 98.79 | 6.92 |
| Glycoehenodeoxycholie acid | 100.0000 | 104.6467 | 5.6356 | 104.65 | 5.90 |
|  | 800.0000 | 777.7999 | 73.5835 | 97.22 | 10.36 |
|  | 5.0000 | 5.1472 | 0.4889 | 102.94 | 10.40 |
| Taurosulodeoxycholic acid | 100.0000 | 110.2644 | 3.6811 | 110.26 | 3.66 |
|  | 800.0000 | 714.7411 | 46.6810 | 89.34 | 7.15 |
|  | 5.0000 | 4.8238 | 0.4206 | 96.48 | 9.55 |
| Trichloroisocyanuric acid | 100.0000 | 98.7538 | 4.4438 | 98.75 | 4.93 |
|  | 800.0000 | 784.4378 | 59.8376 | 98.05 | 8.36 |
|  | 5.0000 | 4.8098 | 0.3555 | 96.20 | 8.10 |
| Hyodeoxycholic acid | 100.0000 | 110.7862 | 4.1599 | 110.79 | 4.11 |
|  | 800.0000 | 768.4429 | 84.3609 | 96.06 | 12.03 |
|  | 5.0000 | 4.3092 | 0.0661 | 86.18 | 1.68 |
| Lithocholic Acid | 100.0000 | 102.6622 | 3.9579 | 102.66 | 4.22 |
|  | 800.0000 | 769.4637 | 36.2212 | 96.18 | 5.16 |
|  | 5.0000 | 4.8464 | 0.3066 | 96.93 | 6.93 |
| Deoxycholic acid | 100.0000 | 99.1004 | 7.5978 | 99.10 | 8.40 |
|  | 800.0000 | 804.7804 | 60.7073 | 100.60 | 8.26 |
|  | 5.0000 | 4.9189 | 0.3896 | 98.38 | 8.68 |
| Ursodeoxycholic acid | 100.0000 | 97.3498 | 4.3364 | 97.35 | 4.88 |
|  | 800.0000 | 792.3081 | 72.5636 | 99.04 | 10.03 |
|  | 5.0000 | 4.8017 | 0.2342 | 96.03 | 5.34 |
| 3-keto-Lithocholic Acid | 100.0000 | 104.0832 | 9.0596 | 104.08 | 9.53 |
|  | 800.0000 | 791.9539 | 70.9785 | 98.99 | 9.82 |
|  | 5.0000 | 4.7779 | 0.2706 | 95.56 | 6.21 |
| Adenosine Triphosphate | 100.0000 | 99.4533 | 8.8917 | 99.45 | 9.79 |
|  | 800.0000 | 762.6744 | 79.4117 | 95.33 | 11.41 |
|  | 5.0000 | 4.7764 | 0.3474 | 95.53 | 7.97 |
| Adenosine diphosphate | 100.0000 | 94.4861 | 6.0496 | 94.49 | 7.01 |
|  | 800.0000 | 853.2629 | 49.7671 | 106.66 | 6.39 |
|  | 5.0000 | 4.8614 | 0.4134 | 97.23 | 9.31 |
| Adenosine monophosphate | 100.0000 | 100.8927 | 7.7020 | 100.89 | 8.36 |
|  | 800.0000 | 765.3946 | 61.7749 | 95.67 | 8.84 |
|  | 5.0000 | 5.0260 | 0.4530 | 100.52 | 9.87 |
| Hypoxanthine | 100.0000 | 100.1333 | 6.2776 | 100.13 | 6.87 |
|  | 800.0000 | 800.6955 | 43.8016 | 100.09 | 5.99 |
|  | 5.0000 | 4.9059 | 0.4064 | 98.12 | 9.07 |
| Adenosine | 100.0000 | 109.6781 | 2.8075 | 109.68 | 2.80 |
|  | 800.0000 | 812.9394 | 75.4104 | 101.62 | 10.16 |
|  | 5.0000 | 5.0737 | 0.3960 | 101.47 | 8.55 |
| Inosine | 100.0000 | 102.5498 | 4.1523 | 102.55 | 4.44 |
|  | 800.0000 | 752.1174 | 35.5770 | 94.01 | 5.18 |

Table S8 matrix effect of the solvent (n=6)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Nominal Conc. (ng/ml) | Mean Conc.(ng/ml) | SD(ng/ml) | Mean Recov.(%) | RSD(%) |
|  | 5.0000 | 5.2407 | 0.2359 | 104.81 | 4.93 |
| Tetrahydrocannabinol acid | 100.0000 | 99.3769 | 8.7669 | 99.38 | 9.66 |
|  | 800.0000 | 784.3880 | 65.9390 | 98.05 | 9.21 |
|  | 5.0000 | 4.7014 | 0.2956 | 94.03 | 6.89 |
| Glycocholic acid | 100.0000 | 105.1918 | 4.6726 | 105.19 | 4.87 |
|  | 800.0000 | 812.1185 | 57.8922 | 101.51 | 7.81 |
|  | 5.0000 | 4.7744 | 0.2274 | 95.49 | 5.22 |
| Glycohyocholic acid | 100.0000 | 98.7525 | 8.4181 | 98.75 | 9.34 |
|  | 800.0000 | 801.6938 | 74.7553 | 100.21 | 10.21 |
|  | 5.0000 | 4.7730 | 0.2839 | 95.46 | 6.52 |
| Tauroursodeoxycholic acid | 100.0000 | 102.0728 | 9.2883 | 102.07 | 9.97 |
|  | 800.0000 | 805.0588 | 59.1526 | 100.63 | 8.05 |
|  | 5.0000 | 4.4291 | 0.1681 | 88.58 | 4.16 |
| Taurocholic acid | 100.0000 | 98.7944 | 6.8610 | 98.79 | 7.61 |
|  | 800.0000 | 788.9179 | 52.1620 | 98.61 | 7.24 |
|  | 5.0000 | 5.1464 | 0.3045 | 102.93 | 6.48 |
| Cholic acid | 100.0000 | 98.4136 | 8.7355 | 98.41 | 9.72 |
|  | 800.0000 | 758.2921 | 57.7879 | 94.79 | 8.35 |
|  | 5.0000 | 5.0946 | 0.3009 | 101.89 | 6.47 |
| Chenodeoxycholic acid | 100.0000 | 101.5644 | 9.4656 | 101.56 | 10.21 |
|  | 800.0000 | 744.5939 | 39.8821 | 93.07 | 5.87 |
|  | 5.0000 | 5.4476 | 0.1997 | 108.95 | 4.02 |
| Taurochenodeoxycholic acid | 100.0000 | 113.1528 | 8.1580 | 113.15 | 7.90 |
|  | 800.0000 | 897.3199 | 11.1698 | 112.16 | 1.36 |
|  | 5.0000 | 4.8625 | 0.2636 | 97.25 | 5.94 |
| Glycodeoxycholic acid | 100.0000 | 99.7745 | 4.3093 | 99.77 | 4.73 |
|  | 800.0000 | 809.6763 | 49.0250 | 101.21 | 6.63 |
|  | 5.0000 | 4.9753 | 0.3985 | 99.51 | 8.77 |
| Glycoursodeoxycholic acid | 100.0000 | 102.8360 | 6.1317 | 102.84 | 6.53 |
|  | 800.0000 | 799.8524 | 60.0502 | 99.98 | 8.22 |
|  | 5.0000 | 5.0751 | 0.2840 | 101.50 | 6.13 |
| alpha-Muricholic acid | 100.0000 | 99.1428 | 8.3131 | 99.14 | 9.19 |
|  | 800.0000 | 786.6327 | 80.1018 | 98.33 | 11.15 |
|  | 5.0000 | 4.8731 | 0.2435 | 97.46 | 5.47 |
| beta-Muricholic acid | 100.0000 | 100.2433 | 9.0019 | 100.24 | 9.84 |
|  | 800.0000 | 812.2350 | 68.0438 | 101.53 | 9.18 |
|  | 5.0000 | 5.1258 | 0.2993 | 102.52 | 6.40 |
| Glycoehenodeoxycholie acid | 100.0000 | 100.6228 | 9.0681 | 100.62 | 9.87 |
|  | 800.0000 | 774.0565 | 69.2086 | 96.76 | 9.79 |
|  | 5.0000 | 5.0181 | 0.2190 | 100.36 | 4.78 |
| Taurosulodeoxycholic acid | 100.0000 | 100.1492 | 6.4070 | 100.15 | 7.01 |
|  | 800.0000 | 740.0702 | 39.7215 | 92.51 | 5.88 |
|  | 5.0000 | 4.7617 | 0.2760 | 95.23 | 6.35 |
| Trichloroisocyanuric acid | 100.0000 | 99.0505 | 5.8100 | 99.05 | 6.43 |
|  | 800.0000 | 804.5497 | 50.2738 | 100.57 | 6.85 |
|  | 5.0000 | 4.9669 | 0.3596 | 99.34 | 7.93 |
| Hyodeoxycholic acid | 100.0000 | 104.6919 | 5.7906 | 104.69 | 6.06 |
|  | 800.0000 | 810.9373 | 59.2553 | 101.37 | 8.00 |
|  | 5.0000 | 4.5336 | 0.1972 | 90.67 | 4.77 |
| Lithocholic Acid | 100.0000 | 95.9766 | 7.6584 | 95.98 | 8.74 |
|  | 800.0000 | 729.1707 | 22.2377 | 91.15 | 3.34 |
|  | 5.0000 | 4.8840 | 0.2976 | 97.68 | 6.68 |
| Deoxycholic acid | 100.0000 | 99.5286 | 5.4027 | 99.53 | 5.95 |
|  | 800.0000 | 816.9222 | 75.1103 | 102.12 | 10.07 |
|  | 5.0000 | 4.8960 | 0.4870 | 97.92 | 10.90 |
| Ursodeoxycholic acid | 100.0000 | 97.4048 | 6.6799 | 97.40 | 7.51 |
|  | 800.0000 | 839.7746 | 61.8402 | 104.97 | 8.07 |
|  | 5.0000 | 5.1444 | 0.2967 | 102.89 | 6.32 |
| 3-keto-Lithocholic Acid | 100.0000 | 98.7942 | 7.6912 | 98.79 | 8.53 |
|  | 800.0000 | 811.1039 | 75.0804 | 101.39 | 10.14 |
|  | 5.0000 | 4.9338 | 0.4884 | 98.68 | 10.84 |
| Adenosine Triphosphate | 100.0000 | 102.8637 | 8.9352 | 102.86 | 9.52 |
|  | 800.0000 | 757.5916 | 28.8281 | 94.70 | 4.17 |
|  | 5.0000 | 4.9680 | 0.4047 | 99.36 | 8.92 |
| Adenosine diphosphate | 100.0000 | 95.9089 | 9.1291 | 95.91 | 10.43 |
|  | 800.0000 | 869.1789 | 81.2151 | 108.65 | 10.24 |
|  | 5.0000 | 4.7596 | 0.4710 | 95.19 | 10.84 |
| Adenosine monophosphate | 100.0000 | 106.7242 | 3.7830 | 106.72 | 3.88 |
|  | 800.0000 | 769.3508 | 74.7882 | 96.17 | 10.65 |
|  | 5.0000 | 5.0407 | 0.5166 | 100.81 | 11.23 |
| Hypoxanthine | 100.0000 | 101.1086 | 12.8274 | 101.11 | 13.90 |
|  | 800.0000 | 794.2138 | 84.6997 | 99.28 | 11.68 |
|  | 5.0000 | 4.9002 | 0.2289 | 98.00 | 5.12 |
| Adenosine | 100.0000 | 105.1754 | 7.0377 | 105.18 | 7.33 |
|  | 800.0000 | 798.3733 | 50.8950 | 99.80 | 6.98 |
|  | 5.0000 | 5.0000 | 0.1603 | 100.00 | 3.51 |
| Inosine | 100.0000 | 106.1099 | 4.2721 | 106.11 | 4.41 |
|  | 800.0000 | 740.1853 | 52.9487 | 92.52 | 7.84 |