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  |