Quantitative Determination and Fingerprint of Phenolic Compounds with Anti-inflammatory Activities for the Quality Control of Mangosteen Extract

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**Figure S1.** The UV spectrum of α-mangostin



**Figure S2.** The HPLC chromatogram of α-mangostin



**Figure S3.** The 1H NMR spectrum of α-mangostin

**Table S1.** The evaluation of different methods of extraction

|  |  |
| --- | --- |
| Methods of extraction | Peak area |
| Catechin | Epicatechin | Procyanidin B2 |
| Ultrasound | 125.7 | 1505.9 | 628.6 |
| Reflux | 23.4 | 449.4 | 161 |
| Maceration | 15.9 | 100.7 | 44.5 |

**Table S2.** The evaluation of different solvents of extraction

|  |  |
| --- | --- |
| Solvents of extraction | Peak area |
| Catechin | Epicatechin | Procyanidin B2 |
| Methanol | 125.7 | 1505.9 | 628.6 |
| Ethyl acetate | 86.6 | 592 | 254.1 |

**Table S3.** The evaluation of different extraction time

|  |  |
| --- | --- |
| Time of extraction | Peak area |
| Catechin | Epicatechin | Procyanidin B2 |
| 0.5 h | 95.5 | 1226.7 | 522.2 |
| 1.0 h | 125.7 | 1505.9 | 628.6 |
| 1.5 h | 115.5 | 1474.3 | 659.3 |

**Table S4.** The linear relationship of catechin

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Amount (ng) | 50 | 100 | 150 | 200 | 250 |
| Peak area | 94.2 | 194.5 | 285.4 | 383.4 | 491.3 |

**Table S5.** The linear relationship of epicatechin

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Amount (ng) | 250 | 500 | 750 | 1000 | 1250 |
| Peak area | 453.9 | 939.2 | 1517.8 | 2076.7 | 2604.2 |

**Table S6.** The linear relationship of procyanidin B2

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Amount (ng) | 250 | 500 | 750 | 1000 | 1250 |
| Peak area | 220.3 | 425.2 | 657.5 | 861.7 | 1068.4 |

**Table S7.** The result of precision

|  |  |  |
| --- | --- | --- |
| Compounds | Average peak area | RSD |
| Catechin | 2957.6±66.72 | 2.26% |
| Epicatechin | 2472.2±46.46 | 1.88% |
| Procyanidin B2 | 1031.1±21.39 | 2.07% |

**Table S8.** The result of stability

|  |  |  |
| --- | --- | --- |
| Compounds | Average peak area | RSD |
| Catechin | 107.28±2.13 | 1.99% |
| Epicatechin | 1643.88±28.45 | 2.84% |
| Procyanidin B2 | 741.54±21.07 | 1.73% |

**Table S9.** The result of repeatability

|  |  |  |
| --- | --- | --- |
| Compounds | Average amount | RSD |
| Catechin | 0.006±0.0001% | 1.99% |
| Epicatechin | 0.081±0.0012% | 1.45% |
| Procyanidin B2 | 0.086±0.0026% | 2.96% |

**Table S10.** The result of recovery

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compounds | Pre-spike (mg) | Spiked (mg) | Post-spike (mg) | Recovery | Average recovery | RSD |
| Catechin | 0.29 | 0.25 | 0.53 | 96.6% | 99.3% | 2.8% |
| 0.28 | 0.25 | 0.52 | 96.1% |
| 0.28 | 0.25 | 0.53 | 100.9% |
| 0.28 | 0.25 | 0.53 | 98.9% |
| 0.29 | 0.25 | 0.55 | 103.4% |
| 0.29 | 0.25 | 0.54 | 99.8% |
| Epicatechin | 4.10 | 3.50 | 7.48 | 96.5% | 99.5% | 2.7% |
| 4.11 | 3.50 | 7.56 | 98.5% |
| 3.99 | 3.50 | 7.62 | 103.6% |
| 4.02 | 3.50 | 7.48 | 98.9% |
| 3.97 | 3.50 | 7.53 | 101.8% |
| 4.04 | 3.50 | 7.46 | 97.9% |
| Procyanidin B2 | 4.11 | 3.50 | 7.55 | 98.3% | 99.8% | 2.7% |
| 4.35 | 3.50 | 7.77 | 97.6% |
| 4.31 | 3.50 | 7.91 | 102.9% |
| 4.31 | 3.50 | 7.79 | 99.5% |
| 4.45 | 3.50 | 7.85 | 97.1% |
| 4.46 | 3.50 | 8.08 | 103.3% |

**Table S11.** The results of quantitative determination of catechin, epicatechin, and procyanidin B2

|  |  |
| --- | --- |
| Batches | Content |
| Catechin | Epicatechin | Procyanidin B2 |
| 2090526 | 0.007% | 0.074% | 0.073% |
| 2100624 | 0.006% | 0.082% | 0.082% |

**Table S12.** The result of precision (relative retention time of common peaks)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Number of common peaks | 1 | 2 | 3 | 4 (S) | 5 | RSD |
| 1 | 0.3377 | 0.3372 | 0.3371 | 0.3373 | 0.3373 | 0.07% |
| 2 | 0.4839 | 0.4904 | 0.4899 | 0.4901 | 0.4896 | 0.56% |
| 3 | 0.5497 | 0.5499 | 0.5497 | 0.5500 | 0.5500 | 0.03% |
| 4 (S) | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | / |
| 5 | 1.5130 | 1.5113 | 1.5109 | 1.5119 | 1.5120 | 0.05% |
| 6 | 1.6050 | 1.6035 | 1.6030 | 1.6042 | 1.6045 | 0.05% |
| 7 | 1.8623 | 1.8607 | 1.8601 | 1.8615 | 1.8621 | 0.05% |

S: reference substance (α-mangostin)

**Table S13.** The result of precision (peak area ratio of common peaks)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Number of common peaks | 1 | 2 | 3 | 4 (S) | 5 | RSD |
| 1 | 0.0168 | 0.0175 | 0.0174 | 0.0174 | 0.0173 | 1.61% |
| 2 | 0.1154 | 0.1173 | 0.1140 | 0.1138 | 0.1116 | 1.84% |
| 3 | 0.0253 | 0.0271 | 0.0266 | 0.0266 | 0.0266 | 2.55% |
| 4 (S) | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | / |
| 5 | 0.0073 | 0.0078 | 0.0078 | 0.0077 | 0.0077 | 2.71% |
| 6 | 0.0202 | 0.0208 | 0.0208 | 0.0207 | 0.0206 | 1.21% |
| 7 | 0.0039 | 0.0040 | 0.0041 | 0.0041 | 0.0040 | 2.08% |

S: reference substance (α-mangostin)

**Table S14.** The result of stability (relative retention time of common peaks)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Number of common peaks | 1 | 2 | 3 | 4 (S) | 5 | RSD |
| 1 | 0.3375 | 0.3371 | 0.3373 | 0.3366 | 0.3371 | 0.10% |
| 2 | 0.4894 | 0.4888 | 0.4899 | 0.4896 | 0.4916 | 0.21% |
| 3 | 0.5504 | 0.5497 | 0.5495 | 0.5474 | 0.5479 | 0.23% |
| 4 (S) | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | / |
| 5 | 1.5139 | 1.5115 | 1.5220 | 1.5147 | 1.5150 | 0.26% |
| 6 | 1.6066 | 1.6040 | 1.6161 | 1.6068 | 1.6068 | 0.29% |
| 7 | 1.8647 | 1.8619 | 1.8778 | 1.8656 | 1.8652 | 0.33% |

S: reference substance (α-mangostin)

**Table S15.** The result of stability (peak area ratio of common peaks)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Number of common peaks | 1 | 2 | 3 | 4 (S) | 5 | RSD |
| 1 | 0.0144 | 0.0143 | 0.0148 | 0.0149 | 0.0149 | 1.94% |
| 2 | 0.1174 | 0.1120 | 0.1147 | 0.1129 | 0.1121 | 2.00% |
| 3 | 0.0181 | 0.0183 | 0.0186 | 0.0180 | 0.0185 | 1.41% |
| 4 (S) | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | / |
| 5 | 0.0077 | 0.0077 | 0.0077 | 0.0080 | 0.0080 | 1.81% |
| 6 | 0.0208 | 0.0207 | 0.0199 | 0.0195 | 0.0200 | 2.63% |
| 7 | 0.0030 | 0.0031 | 0.0030 | 0.0032 | 0.0030 | 2.92% |

S: reference substance (α-mangostin)

**Table S16.** The result of reproducibility (relative retention time of common peaks)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Number of common peaks | 1 | 2 | 3 | 4 (S) | 5 | RSD |
| 1 | 0.3376 | 0.3372 | 0.3372 | 0.3370 | 0.3372 | 0.07% |
| 2 | 0.4867 | 0.4896 | 0.499 | 0.4899 | 0.4906 | 0.31% |
| 3 | 0.5501 | 0.5498 | 0.5496 | 0.5487 | 0.5490 | 0.10% |
| 4 (S) | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | / |
| 5 | 1.5135 | 1.5114 | 1.5165 | 1.5133 | 1.5135 | 0.12% |
| 6 | 1.6058 | 1.6038 | 1.6096 | 1.6055 | 1.6057 | 0.13% |
| 7 | 1.8635 | 1.8613 | 1.8690 | 1.8636 | 1.8637 | 0.15% |

S: reference substance (α-mangostin)

**Table S17.** The result of reproducibility (peak area ratio of common peaks)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Number of common peaks | 1 | 2 | 3 | 4 (S) | 5 | RSD |
| 1 | 0.0156 | 0.0159 | 0.0161 | 0.0161 | 0.0161 | 1.43% |
| 2 | 0.1164 | 0.1146 | 0.1143 | 0.1134 | 0.1118 | 1.47% |
| 3 | 0.0217 | 0.0227 | 0.0226 | 0.0223 | 0.0226 | 1.77% |
| 4 (S) | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | / |
| 5 | 0.0075 | 0.0078 | 0.0078 | 0.0078 | 0.0078 | 1.77% |
| 6 | 0.0205 | 0.0207 | 0.0204 | 0.0201 | 0.0203 | 1.13% |
| 7 | 0.0035 | 0.0035 | 0.0036 | 0.0037 | 0.0035 | 2.08% |

S: reference substance (α-mangostin)