Supplemental Information for Raw Data

**A simple spectrophotometric evaluation method for the hydrophobic anticancer drug paclitaxel**

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Raw data related to Figure 2

Correlation between PTX concentration and absorbance using 40% methanol as solvent

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | 0.313 (μg/mL) | 0.625 (μg/mL) | 1.25 (μg/mL) | 2.5 (μg/mL) |
| 1 | 0.036 | 0.079 | 0.166 | 0.346 |
| 2 | 0.062 | 0.132 | 0.167 | 0.363 |
| 3 | 0.036 | 0.079 | 0.163 | 0.359 |
| AVG | 0.044667 | 0.096667 | 0.165333 | 0.356 |
| STD | 0.015011 | 0.0306 | 0.002082 | 0.008888 |

Correlation between PTX concentration and absorbance using 50% methanol as solvent

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | 0.313 (μg/mL) | 0.625 (μg/mL) | 1.25 (μg/mL) | 2.5 (μg/mL) |
| 1 | 0.033 | 0.066 | 0.130 | 0.266 |
| 2 | 0.034 | 0.067 | 0.133 | 0.271 |
| 3 | 0.034 | 0.066 | 0.134 | 0.271 |
| AVG | 0.033667 | 0.066333 | 0.132333 | 0.269333 |
| STD | 0.000577 | 0.000577 | 0.002082 | 0.002887 |

Correlation between PTX concentration and absorbance using 60% methanol as solvent

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | 0.313 (μg/mL) | 0.625 (μg/mL) | 1.25 (μg/mL) | 2.5 (μg/mL) |
| 1 | 0.032 | 0.065 | 0.130 | 0.263 |
| 2 | 0.034 | 0.067 | 0.135 | 0.274 |
| 3 | 0.034 | 0.066 | 0.132 | 0.271 |
| AVG | 0.033333 | 0.066 | 0.132333 | 0.269333 |
| STD | 0.001155 | 0.001 | 0.002517 | 0.005686 |

Correlation between PTX concentration and absorbance using 70% methanol as solvent

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | 0.313 (μg/mL) | 0.625 (μg/mL) | 1.25 (μg/mL) | 2.5 (μg/mL) |
| 1 | 0.032 | 0.060 | 0.110 | 0.216 |
| 2 | 0.034 | 0.060 | 0.112 | 0.217 |
| 3 | 0.038 | 0.063 | 0.121 | 0.229 |
| AVG | 0.034667 | 0.061 | 0.114333 | 0.220667 |
| STD | 0.003055 | 0.001732 | 0.005859 | 0.007234 |

Correlation between PTX concentration and absorbance using 80% methanol as solvent

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | 0.313 (μg/mL) | 0.625 (μg/mL) | 1.25 (μg/mL) | 2.5 (μg/mL) |
| 1 | 0.088 | 0.115 | 0.162 | 0.237 |
| 2 | 0.090 | 0.111 | 0.164 | 0.242 |
| 3 | 0.093 | 0.115 | 0.161 | 0.240 |
| AVG | 0.090333 | 0.113667 | 0.162333 | 0.239667 |
| STD | 0.002517 | 0.002309 | 0.001528 | 0.002517 |

Correlation between PTX concentration and absorbance using 90% methanol as solvent

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | 0.313 (μg/mL) | 0.625 (μg/mL) | 1.25 (μg/mL) | 2.5 (μg/mL) |
| 1 | 0.119 | 0.143 | 0.172 | 0.236 |
| 2 | 0.124 | 0.141 | 0.170 | 0.233 |
| 3 | 0.123 | 0.134 | 0.166 | 0.232 |
| AVG | 0.122 | 0.139333 | 0.169333 | 0.233667 |
| STD | 0.002646 | 0.004726 | 0.003055 | 0.002082 |

Correlation between PTX concentration and absorbance using 100% methanol as solvent

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | 0.313 (μg/mL) | 0.625 (μg/mL) | 1.25 (μg/mL) | 2.5 (μg/mL) |
| 1 | 0.116 | 0.144 | 0.192 | 0.279 |
| 2 | 0.123 | 0.143 | 0.190 | 0.274 |
| 3 | 0.122 | 0.157 | 0.202 | 0.274 |
| AVG | 0.120333 | 0.148 | 0.194667 | 0.275667 |
| STD | 0.003786 | 0.00781 | 0.006429 | 0.002887 |

Raw data related to Figure 3 and Table 1

Concentrations of the PTX-saturated saline obtained using HPLC

|  |  |
| --- | --- |
|  | Concentration (μg/mL) |
| 1 | 0.685398 |
| 2 | 0.739070 |
| 3 | 0.770013 |
| AVG | 0.731494 |
| STD | 0.042813 |

Absorbance of the PTX-saturated saline obtained using spectroscopy

|  |  |
| --- | --- |
|  | Absorbance |
| 1 | 0.058 |
| 2 | 0.074 |
| 3 | 0.058 |
| 4 | 0.062 |
| 5 | 0.065 |
| AVG | 0.0634 |
| STD | 0.006618 |

Quantitative concentrations (μg/mL) of the PTX-saturated saline calculated using each calibration curve

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | 40% | 50% | 60% | 70% | 80% |
| 1 | 0.419 | 0.607 | 0.612 | 0.683 | 0.036 |
| 2 | 0.176 | 0.594 | 0.589 | 0.667 | 0.031 |
| 3 | 0.518 | 0.594 | 0.600 | 0.610 | N/A |
| AVG | 0.371 | 0.598333 | 0.600333 | 0.653333 | 0.0335 |
| STD | 0.17598 | 0.007506 | 0.011504 | 0.038371 | 0.003536 |

Accuracy (relative error) of the quantitative concentrations obtained using spectroscopy, which was defined as the deviation from the HPLC results

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | 40% | 50% | 60% | 70% | 80% |
| 1 | -0.42681 | -0.16963 | -0.16279 | -0.06566 | -0.95075 |
| 2 | -0.75923 | -0.18741 | -0.19425 | -0.08755 | -0.95759 |
| 3 | -0.29138 | -0.18741 | -0.17921 | -0.16553 | N/A |
| AVG | -0.49248 | -0.18149 | -0.17875 | -0.10625 | -0.95417 |
| STD | 0.240739 | 0.010268 | 0.015737 | 0.052491 | 0.004837 |

Raw data related to Figure 4

Absorbance at each dilution with PTX

|  |  |  |
| --- | --- | --- |
| Dilution ratio | Dilution magnification | Absorbance |
| 0.125 | 8 | 1.873 |
| 0.0625 | 16 | 0.920 |
| 0.03125 | 32 | 0.428 |
| 0.015625 | 64 | 0.202 |
| 0.007813 | 128 | 0.091 |
| 0.003906 | 256 | 0.045 |
| 0.001953 | 512 | 0.020 |
| 0.000977 | 1024 | 0.010 |

Absorbance at each dilution without PTX

|  |  |  |
| --- | --- | --- |
| Dilution ratio | Dilution magnification | Absorbance |
| 0.125 | 8 | 1.348 |
| 0.0625 | 16 | 0.688 |
| 0.03125 | 32 | 0.343 |
| 0.015625 | 64 | 0.176 |
| 0.007813 | 128 | 0.086 |
| 0.003906 | 256 | 0.041 |
| 0.001953 | 512 | 0.020 |
| 0.000977 | 1024 | 0.010 |

Absorbance derived from PTX which was calculated from the above difference, and concentration of the PTX in each dilution compared to that obtained using HPLC, which was calculated using the differential absorbance obtained above and a calibration curve prepared using 65.8% methanol

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Dilution ratio | Dilution magnification | Absorbance | Concentration (μg/mL) (Spectroscopy) | Concentration (μg/mL)  (HPLC) |
| 0.125 | 8 | 0.525 | 10.73663 | 6.43462 |
| 0.0625 | 16 | 0.232 | 4.707819 | 3.17152 |
| 0.03125 | 32 | 0.085 | 1.683128 | 1.51453 |
| 0.015625 | 64 | 0.026 | 0.469136 | 0.716337 |
| 0.007813 | 128 | 0.005 | 0.037037 | 0.315126 |
| 0.003906 | 256 | 0.004 | 0.016461 | 0.136420 |
| 0.001953 | 512 | 0 | N/A | 0.0525180 |
| 0.000977 | 1024 | 0 | N/A | 0.0202840 |

Raw data related to Figure 5

Absorbance of the commercially available PTX formulation which was further diluted 32-fold with saline after mixing (100-fold dilution with saline)

|  |  |
| --- | --- |
|  | Absorbance |
| 1 | 0.365 |
| 2 | 0.358 |
| 3 | 0.396 |
| 4 | 0.359 |
| 5 | 0.384 |
| AVG | 0.3724 |
| STD | 0.016832 |

Absorbance of the reference solution without PTX

|  |  |
| --- | --- |
|  | Absorbance |
| 1 | 0.312 |
| 2 | 0.311 |
| 3 | 0.309 |
| 4 | 0.312 |
| 5 | 0.293 |
| AVG | 0.3074 |
| STD | 0.008142 |

Absorbance of the PTX calculated from the above difference and concentration of the PTX calculated using the differential absorbance obtained above and a calibration curve prepared using 65.8% methanol

|  |  |  |
| --- | --- | --- |
|  | Absorbance | Concentration (μg/mL) |
| 1 | 0.058 | 1.127572 |
| 2 | 0.051 | 0.983539 |
| 3 | 0.089 | 1.765432 |
| 4 | 0.052 | 1.004115 |
| 5 | 0.077 | 1.518519 |
| AVG | 0.0654 | 1.279835 |
| STD | 0.016832 | 0.346328 |

Concentration of the commercially available PTX formulation obtained using HPLC

|  |  |
| --- | --- |
|  | Concentration (μg/mL) |
| 1 | 1.08856 |
| 2 | 1.15334 |
| 3 | 1.16808 |
| 4 | 1.14637 |
| 5 | 1.13973 |
| AVG | 1.139216 |
| STD | 0.030208 |