

Solubility determination, dissolution properties and solid transformation of resmetirom (form A) in heptane and seven alcohols

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Table S1 Parameters and *ARD%* of the modified Apelblat equation for the solubility of form A in six solvents.

| Solvent | Apelblat | | | <i>ARD%</i> |
|--------------------|----------|----------|----------|-------------|
| | <i>A</i> | <i>B</i> | <i>C</i> | |
| Propanol | 9.666 | -3107.3 | 0.040 | 0.146 |
| Isopropyl alcohol | 8.456 | -2803.4 | 0.056 | 0.194 |
| Butanol | 7.510 | -2555.1 | 0.026 | 0.116 |
| Isobutyl alcohol | 8.261 | -2328.7 | -0.279 | 0.222 |
| 3-Methyl-1-butanol | 8.026 | -2250.7 | -0.324 | 0.123 |
| Heptane | 5.067 | -2089.5 | -0.001 | 0.312 |

Table S2 Parameters and *ARD%* of the λh equation and the Wilson model for the solubility of form A in six solvents.

| Solvent | λh | | | Wilson | | |
|--------------------|---------------|---------|-------------|-----------------------|-----------------------|-------------|
| | $10^2\lambda$ | 10^5h | <i>ARD%</i> | $10^{-4}\lambda_{12}$ | $10^{-4}\lambda_{21}$ | <i>ARD%</i> |
| Propanol | 10.403 | 2.974 | 0.223 | 2.492 | 16.231 | 0.313 |
| Isopropyl alcohol | 5.567 | 4.996 | 0.157 | 2.512 | 16.038 | 0.906 |
| Butanol | 2.637 | 9.518 | 0.241 | 7.64 | 0.688 | 1.699 |
| Isobutyl alcohol | 1.163 | 18.619 | 0.305 | 7.759 | 0.689 | 2.161 |
| 3-Methyl-1-butanol | 0.775 | 26.629 | 0.353 | 7.377 | 0.732 | 2.815 |
| Heptane | 0.386 | 51.666 | 0.336 | 7.895 | 0.805 | 5.535 |

Table S3 Parameters and *ARD%* of the modified Apelblat equation and λh equation for the solubility of form A in propanol + heptane.

| ω | Apelblat | | | ARD% | λh | | ARD% |
|----------|----------|---------|--------|-------|---------------|------------|-------|
| | A | B | C | | $10^2\lambda$ | $10^{-5}h$ | |
| 0.2 | 3.361 | -2174.4 | 0.398 | 0.558 | 0.762 | 2.917 | 0.527 |
| 0.4 | 8.082 | -2548.5 | -0.160 | 0.527 | 1.476 | 1.655 | 1.000 |
| 0.6 | 7.345 | -2678.3 | 0.096 | 0.412 | 2.854 | 0.933 | 0.414 |
| 0.8 | 8.522 | -2892.3 | 0.065 | 0.491 | 5.453 | 0.528 | 0.326 |

Table S4 Parameters and *ARD%* of the J-A-V model for the solubility of resmetirom (form A) in mixed solvents.

| Propanol + Heptane | |
|--------------------|--------|
| A_1 | 3.028 |
| A_2 | -1.850 |
| B_1 | -3119 |
| B_2 | -2089 |
| J_0 | 4.342 |
| J_1 | 0.160 |
| J_2 | -0.164 |
| <i>ARD%</i> | 0.465 |