

Supplementary Information for:

Molecular Insights on the Two Fluorescence Lifetimes Displayed by Warfarin from Fluorescence Anisotropy and Molecular Dynamics Studies

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MD Production Phase Data

TABLE S1: MD Production Phase Data

| Solvent ^a | xyz (Å) | ρ (g/cm ³) | T (K) | P (bar) | Energies (kcal/mol) | | |
|----------------------|--------------------|-----------------------------|-------------|-----------|---------------------|-----------------|----------------|
| | | | | | KIN | POT | TOT |
| Water | 32.2 × 32.4 × 32.7 | 0.988 ± 0.004 | 298.0 ± 5.1 | 0.9 ± 308 | 2010.2 ± 34.5 | -10738.1 ± 50.3 | -8727.9 ± 62.4 |
| ACN | 31.1 × 32.0 × 38.9 | 0.732 ± 0.003 | 298.1 ± 5.3 | 0.8 ± 196 | 1850.3 ± 33.1 | -7893.5 ± 34.6 | -6043.3 ± 48.7 |
| EtOH | 29.4 × 36.8 × 33.5 | 0.793 ± 0.004 | 298.1 ± 4.7 | 0.9 ± 250 | 2336.8 ± 36.9 | -2125.4 ± 45.5 | 211.4 ± 58.9 |
| 2-PrOH | 31.5 × 31.5 × 31.1 | 0.802 ± 0.005 | 298.2 ± 5.1 | 1.0 ± 278 | 2044.9 ± 34.8 | -3204.7 ± 43.6 | -1159.8 ± 56.3 |
| CHCl ₃ | 39.3 × 39.4 × 39.4 | 1.467 ± 0.005 | 298.0 ± 5.0 | 1.0 ± 141 | 2027.7 ± 34.2 | -2440.4 ± 36.9 | -412.7 ± 50.8 |

^a Number of solvent molecules were: 1115 (TIP3P-WAT), 410 (ACN), 371 (EtOH), 243 (2-PrOH) and 450 (CHCl₃)

MD Hydrogen Bond Analysis

TABLE S2: Molecular Dynamics Data from Warfarin Solvation Simulations

| Solvent | N _{shell} (r) | | | Occupied (%) | | | |
|-------------------|------------------------|-------------|-------------|--------------|--------------------|--------------------|-------|
| | -OH | C=O | C=O (SC) | -OH | C=O | C=O (SC) | Intra |
| Water | 0.99 | 2.1 | 2.1 | 79 | 60+58 ^a | 54+59 ^a | 2.6 |
| ACN | 0.25 | <i>n.a.</i> | <i>n.a.</i> | 9.5 | <i>n.a.</i> | <i>n.a.</i> | 66 |
| EtOH | 0.75 | 1.3 | 0.88 | 48 | 75 | 49 | 22 |
| 2-PrOH | 0.81 | 1.1 | 0.99 | 55 | 48 | 59 | 14 |
| AcOH | 0.99 | 0.87 | 0.98 | 63 | 72 | 72 | 0.01 |
| CHCl ₃ | <i>n.a.</i> | <i>n.a.</i> | <i>n.a.</i> | <i>n.a.</i> | <i>n.a.</i> | <i>n.a.</i> | 85 |

^a Analysis was performed on both water hydrogens, H1 and H2, and interactions formed to the C=O functionality on warfarin.

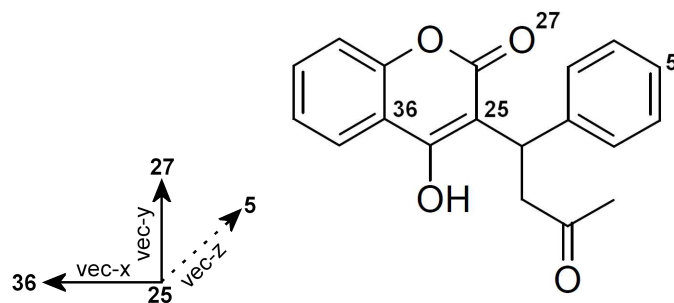


Figure S1. Vectors analysed on the warfarin molecule in the rotational time-correlation studies: In the X-direction $\mathbf{r}_{|a25-a36|}$, in the Y-direction $\mathbf{r}_{|a25-a27|}$ and in the Z-direction $\mathbf{r}_{|a25-a5|}$.