Solvation dynamics on the diffusion timescale elucidated using energy-represented dynamics theory

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Table S1: Atomic charges on Prodan at the ground (GS) and excited (ES) states. The label of each atom is shown in Fig. S1.

| site name	atomic charge at GS (e)	atomic charge at ES (e)	difference
C1	-0.16703	-0.20922	-0.04219
C2	-0.21334	-0.30112	-0.08778
C3	0.30188	0.30558	0.00370
C4	-0.40712	-0.30964	0.09748
C5	0.20250	0.16139	-0.04111
C6	0.11120	0.20825	0.09705
C7	-0.21616	-0.33364	-0.11748
C8	-0.07123	0.02150	0.09273
C9	-0.01159	-0.05330	-0.04171
C10	-0.23902	-0.25537	-0.01635
C11	0.09300	0.06970	-0.02330
C12	0.09210	0.08956	-0.00254
N	-0.26505	-0.19167	0.07338
C13	0.38845	0.31197	-0.07648
O	-0.44136	-0.45568	-0.01432
C14	0.15965	0.24546	0.08581
C15	-0.14782	-0.19386	-0.04604
H1	0.11247	0.11805	0.00558
H2	0.12682	0.13465	0.00783
H3	0.16547	0.13830	-0.02717
H4	0.11577	0.10156	-0.01421
H5	0.08113	0.08488	0.00375
H6	0.11117	0.10350	-0.00767
H7, H8, H9	0.01343	0.03329	0.01986
H10, H11, H12	0.01296	0.02878	0.01582
H13, H14	-0.02970	-0.04745	-0.01775
H15, H16, H17	0.03278	0.03928	0.00650
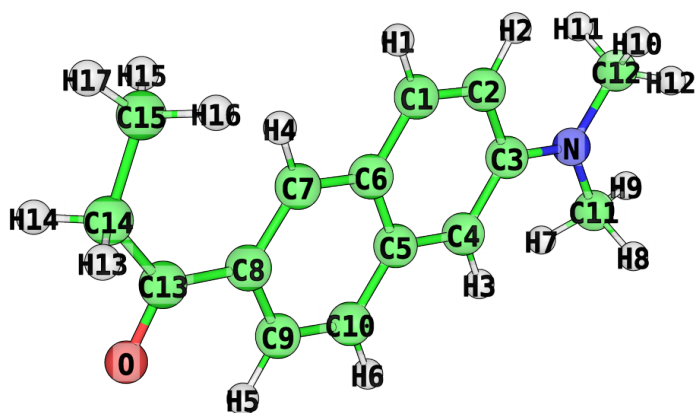
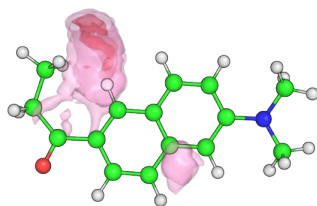Fig. S1: Definitions of the atom labels for Prodan.
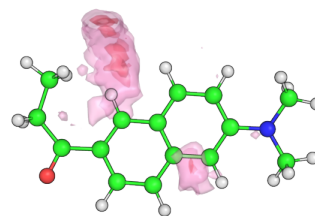
(a) Water
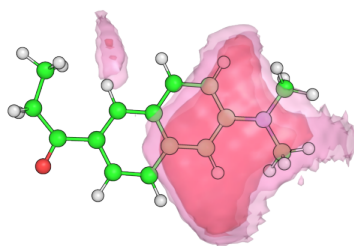
(b) MeOH
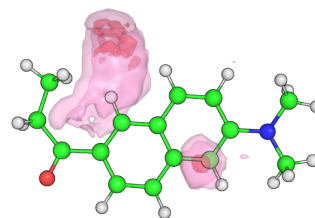
(c) EtOH

(d) PrOH

Fig. S2: Spatial distribution functions (SDFs) of the hydroxyl hydrogens corresponding to the destabilized region ($\varepsilon \geq 1.0$ kcal mol^{-1}) for (a) water, (b) MeOH, (c) EtOH, and (d) PrOH. The isovalues of SDFs for solid and transparent surfaces are 0.1 and 0.05, respectively, relative to the bulk density.
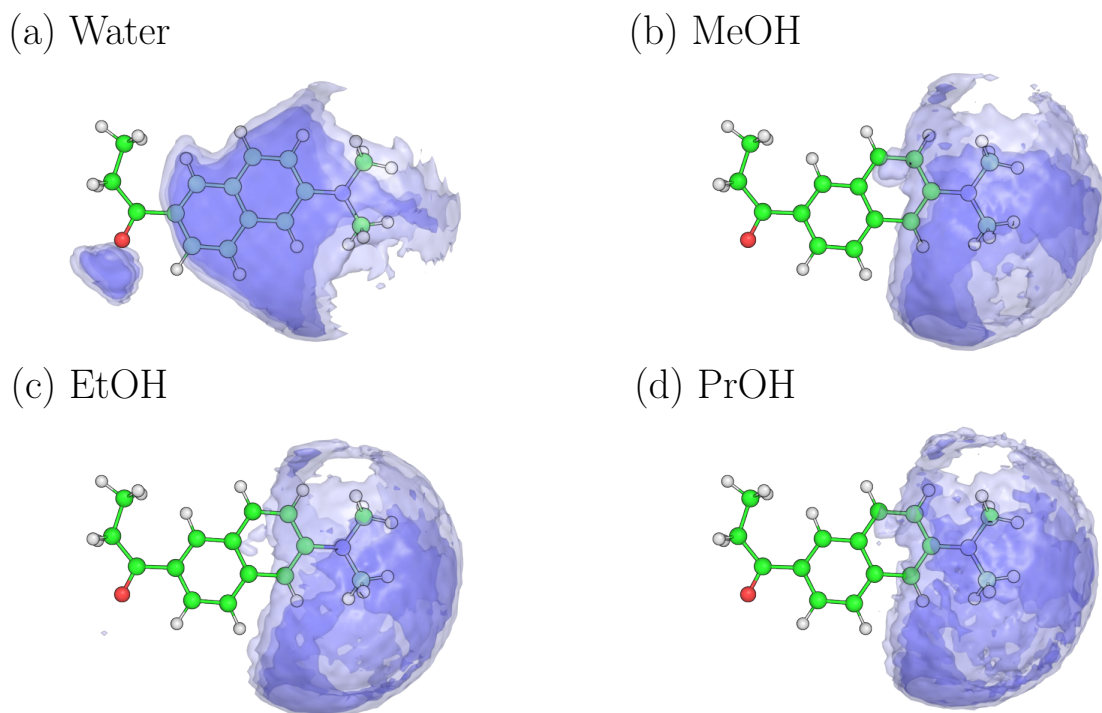
Fig. S3: Spatial distribution functions (SDFs) of the hydroxyl hydrogens corresponding to the stabilized region ($\varepsilon \leq -1.0$ kcal mol^{-1}) for (a) water, (b) MeOH, (c) EtOH, and (d) PrOH, respectively. The isovalues of SDFs for solid and transparent surfaces are 0.1 and 0.05, respectively, relative to the bulk density.
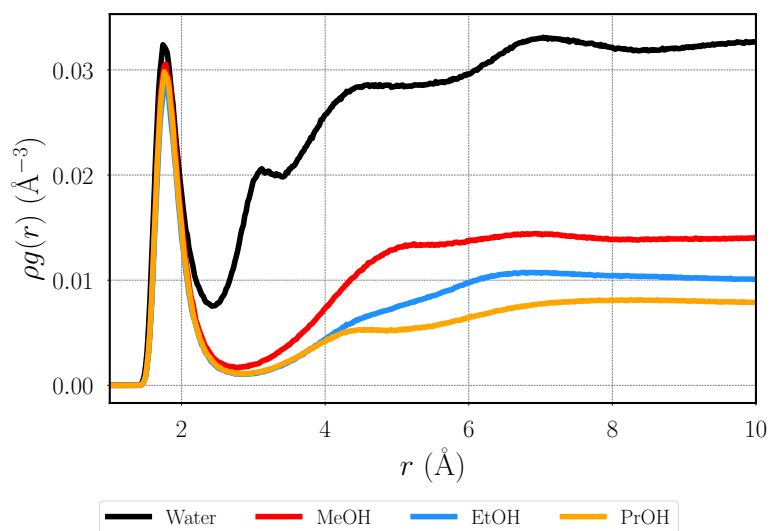

Fig. S4: Radial densities of the hydroxyl hydrogens around the oxygen atom of Prodan, $\rho g\left(r\right)$.