Supporting Information: A Comprehensive Solute-Medium Interaction Model for Anisotropic NMR Data Prediction

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Supplementary Theory and Method

The Order Transfer Equation for the Polymeric Gel Medium

In paper 1, the order transfer equation (OTE) in the gel medium was derived by analogy to the OTE of the liquid crystal (LC) medium through the definition of an excluded volume, *i.e.*, the sample volume that is inaccessible to the solute due to the hard-body repulsion by the medium. However, when soft interactions between the solute and medium are considered, the excluded volume is no longer the only contributor to order transfer. Despite this difference, a formally identical OTE can still be obtained for the gel medium via a more direct derivation, as shown below.

A simple model system for the gel-based alignment medium contains a solute molecule, a giant gel polymer molecule, and the solvent molecules. The polymer is considered a fixed scaffold with no internal or external motions (the effects of internal motions can be partially accounted for by increasing the number of paraboloid structures as shown in paper 1). The solvent molecules are treated as polarizable continuum. Therefore, the solute is the only dynamic component in the system, which contrasts with the LC system in which both the solute and the mesogen have positional and orientational dynamics. The orientational distribution function (ODF) of the solute is then given by:

$$f_s(\boldsymbol{a}) = \frac{\int d\boldsymbol{r}\, exp[-\beta\, \Delta G(\boldsymbol{a},\boldsymbol{r})]}{\int d\boldsymbol{a} \int d\boldsymbol{r}\, exp[-\beta\, \Delta G(\boldsymbol{a},\boldsymbol{r})]} \qquad S(1)$$

Here, $f_s(\boldsymbol{a})$ is the solute ODF which is the probability density of the solute adopting a laboratory-frame orientation $\boldsymbol{a}$. Vector $\boldsymbol{r}$ is a three-dimensional (3-D) vector which describes the position of the solute in the laboratory frame. $\Delta G(\boldsymbol{a},\boldsymbol{r})$ is the Gibbs free energy of the system as a function of the solute's orientation and position.

Prior to surface decomposition, the gel's *vdW* surface is represented by the MEB-excluded surface (MEB-ES) as described in paper 1, and the MEB-ES is subject to surface decomposition. Applying the polar sampling scheme as described in paper 1 to the decomposed medium surface, the following approximation is obtained:

$$\int d\boldsymbol{r}\, exp[-\beta\, \Delta G(\boldsymbol{a},\boldsymbol{r})] \approx \sum_{i=1}^{n} SP_i \int d\boldsymbol{a_i}\; f_i(\boldsymbol{a_i}) \int_0^{r_{max}} dr\; w_i(r)\, exp[-\beta \Delta G_i(\boldsymbol{a}, r, \boldsymbol{a_i})] + V_{iso} \qquad S(2)$$

The sigma summation is over n paraboloid structures. $\boldsymbol{a_i}$ is the laboratory-frame orientation of paraboloid i. $f_i(\boldsymbol{a_i})$ is the ODF representing the orientational histogram of all paraboloids in the same group having structure i. Different from the 3-D vector $\boldsymbol{r}$ on the left side of Eq S(2), the scalar variable r on the right side of Eq S(2) is the distance from the solute's MEB center to the paraboloid surface along the normal vector of the paraboloid surface, which is referred to as the relative position between the solute and the paraboloid in the main text. S is the area of the closed MEB-accessible surface (MEB-AS) of the medium, and P_i is the fraction of S that is attributed to paraboloid structure i ($\sum_i P_i = 1$). r_{max} is the maximal distance within which the solute and medium can effectively interact, set to $r_{max} = r_{MEB} + 2R_s$ in model B. V_{iso} is the sample volume within which $\Delta G(\boldsymbol{a},\boldsymbol{r})$ is zero, *i.e.*, there is no solute-medium interaction at any $\boldsymbol{a}$, which corresponds to solute

positions whose distances to any paraboloid are more than r_{max}. Realizing $\Delta G_i(\boldsymbol{a}, r, \boldsymbol{a_i})$ only depends on the relative orientation between the solute and the paraboloid, the first term on the right side of Eq S(2) can be transformed from the laboratory-frame to the solute frame, leading to:

$$\int d\boldsymbol{r}\, exp[-\beta\, \Delta G(\boldsymbol{a}, \boldsymbol{r})] \approx \sum_{i=1}^{n} SP_i \int d\boldsymbol{\Omega}\, f_i(\hat{R}\boldsymbol{a}) \int_0^{r_{max}} dr\, w_i(r)\, exp[-\beta \Delta G_i(\boldsymbol{\Omega}, r)] + V_{iso} \qquad S(3)$$

Here, $\boldsymbol{\Omega}$ is the relative orientation between the paraboloid frame and the solute frame. $\hat{R}$ is the rotation matrix for the transformation between the solute and paraboloid axis frames such that $\hat{R}\boldsymbol{a}$ gives the laboratory-frame orientation of the paraboloid. Plugging S(3) into S(1), expanding both $f_s(\boldsymbol{a})$ and $f_i(\hat{R}\boldsymbol{a})$ into power series, and equating the coefficients of the 2nd order terms, leads to the OTE as shown in Eq (1) of the main text, also shown below:

$$\sqrt{\frac{4\pi}{5}}\langle Y_2^m\rangle_S \approx \sum_{m'=-2}^{2} \sum_{i=1}^{n} \sqrt{\frac{4\pi}{5}}\langle Y_2^{m'}\rangle_i \left\{ \frac{SP_i}{8\pi^2 V_a^r} \int d\boldsymbol{\Omega}\, D^2_{m'm}(\hat{R}) \int_0^{r_{max}} dr\, w_i(r)\, exp[-\beta \Delta G_i(\boldsymbol{\Omega}, r)] \right\} \qquad S(4)$$

The volumetric parameter V_a^r is the denominator in Eq S(1):

$$V_a^r = \int d\boldsymbol{a} \int d\boldsymbol{r}\, exp[-\beta\, \Delta G(\boldsymbol{a}, \boldsymbol{r})] \qquad S(5)$$

If only hard-body interaction is considered, $exp[-\beta\, \Delta G(\boldsymbol{a}, \boldsymbol{r})]$ is either zero or 1, so V_a^r corresponds to the average volume in the sample that is accessible to the solute when all solute orientations are considered. When soft interactions are considered, V_a^r no longer represents the exact accessible volume. V_a^r does not require explicit calculation but can be absorbed into the alignment amplitude during the model optimization process.

Algorithm for Pseudoatomic Representation of the Medium Paraboloid

Following the convention in paper 1, the paraboloid is described by:

$$y = -\frac{1}{2}(k_x x^2 + k_z z^2) \qquad S(6)$$

First, evenly spaced grid points $(x[i], -\frac{1}{2}(k_x x^2[i] + k_z z^2[j]), z[j])$ are created on the 3D surface. The indices *i* and *j* are positive or negative integers or zero. The two arrays $x[i]$ and $z[j]$ can be generated independently by the same method as shown below. The first point is chosen on the origin $(0, 0, 0)$, *i.e.*, $x[0] = 0$ and $z[0] = 0$. Due to the symmetry $x[-i] = -x[i]$ and $z[-j] = -z[j]$, only positive *i* and *j* need be considered. In this work, $x[1]$ and $z[1]$ are both set to $d = 1.8$ Å. Then, on the parabolic cross-section by any given $z[j]$, the distance between the two neighboring points $(x[1], -\frac{1}{2}(k_x x^2[1] + k_z z^2[j]), z[j])$ and $(x[0], -\frac{1}{2}(k_x x^2[0] + k_z z^2[j]), z[j])$, labeled as $L_x(1,0)$, is $\sqrt{d^2 + \frac{1}{4}k_x^2 d^4}$. Likewise, on the parabolic cross-section by any given $x[i]$, the distance between the two neighboring points $(x[i], -\frac{1}{2}(k_x x^2[i] + k_z z^2[0]), z[0])$ and $(x[i], -\frac{1}{2}(k_x x^2[i] + k_z z^2[1]), z[1])$, labeled as $L_z(1,0)$, is $\sqrt{d^2 + \frac{1}{4}k_z^2 d^4}$. The other grid points are generated recursively such that:

$$\begin{cases} L_x(i, i+1) = \sqrt{d^2 + \frac{1}{4}k_x^2 d^4} \\ L_z(j, j+1) = \sqrt{d^2 + \frac{1}{4}k_z^2 d^4} \end{cases} \qquad S(7)$$

for any *i* and *j*.

Defining the increment $\Delta_{x,i+1} = x[i+1] - x[i]$, the following quartic equation can be used to solve for $\Delta_{x,i+1}$ that satisfies the first equation in Eq S(7):

$$\frac{k_x^2}{4}\Delta_{x,i+1}^4 + k_x^2\, x[i]\, \Delta_{x,i+1}^3 + (k_x^2\, x^2[i] + 1)\, \Delta_{x,i+1}^2 - \left(d^2 + \frac{1}{4}k_x^2\, d^4\right) = 0 \qquad S(8)$$

, in which $\Delta_{x,i+1}$ takes the only real root.

Similarly, the $z[j]$ array can be expanded from $z[1]$ recursively using the following equation:

$$\frac{k_z^2}{4}\Delta_{z,i+1}^4 + k_z^2\, z[i]\, \Delta_{z,i+1}^3 + (k_z^2\, z^2[i] + 1)\, \Delta_{z,i+1}^2 - \left(d^2 + \frac{1}{4}k_z^2\, d^4\right) = 0 \qquad S(9)$$

Applying Eq S(8) and S(9) creates equally spaced grid points on the paraboloid surface. As mentioned in the main text, only the paraboloid region surrounding the origin can interact with the solute, so only the points with $(x[i], z[j])$ satisfying the following conditions are considered:

$$\begin{cases} x^2[i] + z^2[j] \le (r_{MEB} + 2.5R_s)^2 \\ \frac{1}{2}(k_x x^2[i] + k_z z^2[j]) \le r_{MEB} \end{cases} \qquad S(10)$$

Next, a pseudoatom is installed for each grid point. Because the pseudoatom has a finite *vdW* radius of $r_p = 1.2$Å, the pseudoatomic center is placed below the paraboloid surface on its normal vector with a distance r_p to the surface point $\left(x[i], -\frac{1}{2}(k_x x^2[i] + k_z z^2[j]), z[j]\right)$. By this construction, all pseudoatoms are beneath the paraboloid surface and tangent to it, touching only at the grid points.

The center position (x_p, y_p, z_p) of the pseudoatom that is tangent at $\left(x[i], -\frac{1}{2}(k_x x^2[i] + k_z z^2[j]), z[j]\right)$ is calculated by:

$$\begin{cases} x_p = x[i] - \dfrac{k_x\, x[i]\, r_p}{\sqrt{1 + k_x^2 x^2[i] + k_z^2 z^2[j]}} \\ y_p = -\dfrac{1}{2}(k_x x^2[i] + k_z z^2[j]) - \dfrac{r_p}{\sqrt{1 + k_x^2 x^2[i] + k_z^2 z^2[j]}} \\ z_p = z[j] - \dfrac{k_z\, z[j]\, r_p}{\sqrt{1 + k_x^2 x^2[i] + k_z^2 z^2[j]}} \end{cases} \qquad S(11)$$

Supplementary Figures

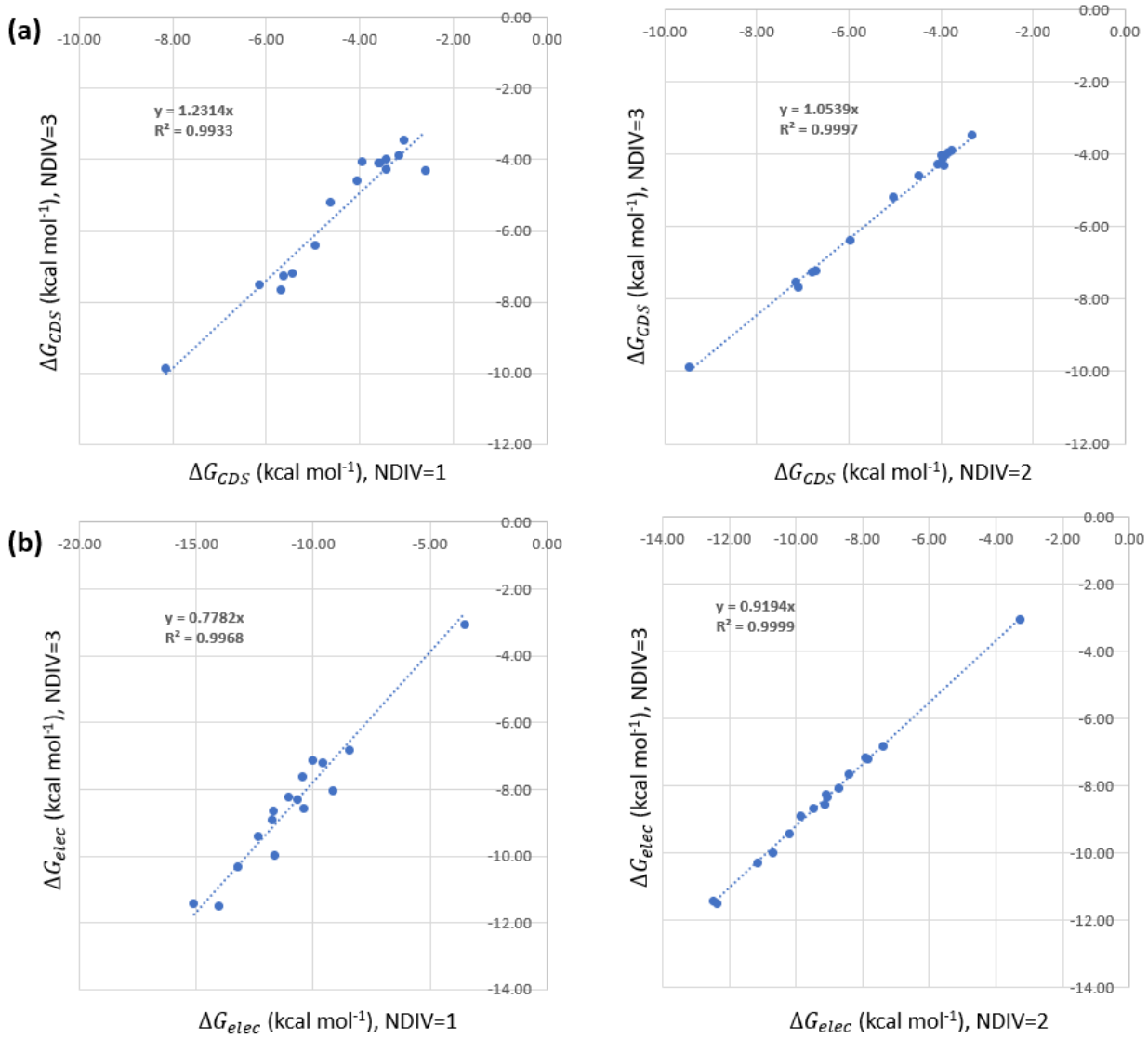


Figure S1. Effects of surface tessellation level (NDIV) on the calculated ΔG_{CDS} (a) and ΔG_{elec} (b) in chloroform by the SMD. Calculations were performed for sixteen compounds in the PMMA database, corresponding to the sixteen dots in each panel. ΔG_{elec} is calculated based on CM5 partial charges. NDIV=3 is used as the reference, and NDIV=1 and 2 are tested. Clearly, NDIV=1 vs 3 shows significant scatter indicating insufficient digitization by 1, whereas NDIV=2 vs 3 yields good linearity with a slope close to 1, for both ΔG_{CDS} and ΔG_{elec}. Note that increasing NDIV by one increases the computational time by four-fold. Therefore, NDIV=2 was chosen in this work.

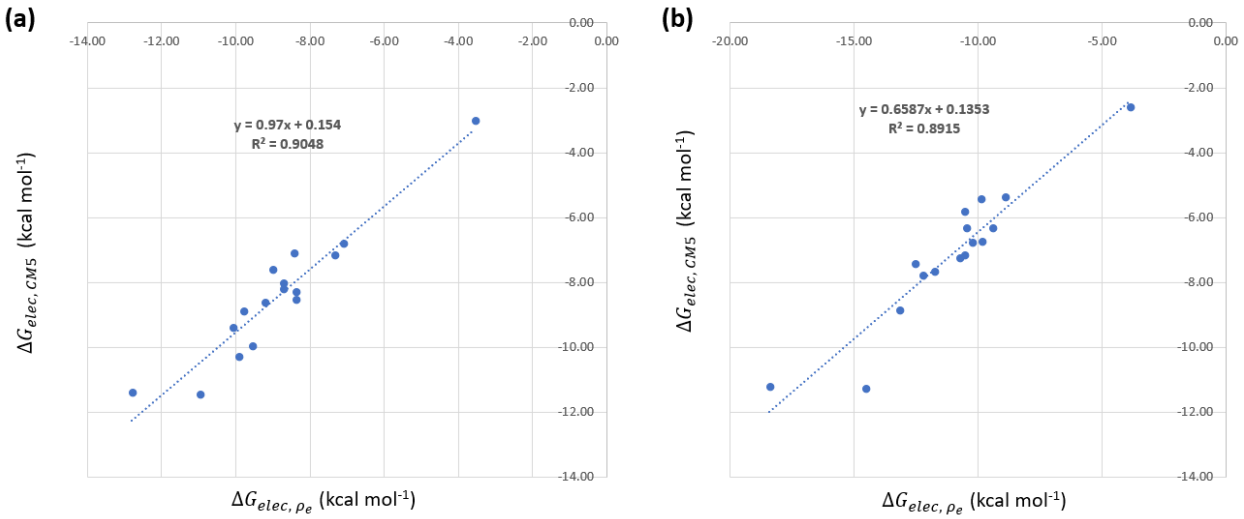


Figure S2. Comparison of ΔG_{elec} calculated using CM5 partial charges ($\Delta G_{elec,\,CM5}$) and electron density ρ_e ($\Delta G_{elec,\,\rho_e}$) for sixteen compounds in chloroform (a) and DMSO (b). $\Delta G_{elec,\,CM5}$ is calculated by adding up the electrostatic free energies (inside the parentheses of Eq (3)) of all electrostatic tesserae. $\Delta G_{elec,\,\rho_e}$ is obtained by: $G_{SMD} - G_{vacuo} - \Delta G_{CDS}$, where G_{SMD} and G_{vacuo} are the single-point DFT (B3LYP-GD2/6-311G**) energies in solution (SMD) and in vacuo, respectively, and ΔG_{CDS} is the CDS component of the solvation free energy. Panel (a) shows that $\Delta G_{elec,\,CM5}$ and $\Delta G_{elec,\,\rho_e}$ agree well in chloroform with differences within 1 kcal mol^{-1}, whereas panel (b) shows that in DMSO $\Delta G_{elec,\,CM5}$ systematically under-estimates the magnitude of ΔG_{elec} due to point charge approximation, albeit displaying a linear correlation.

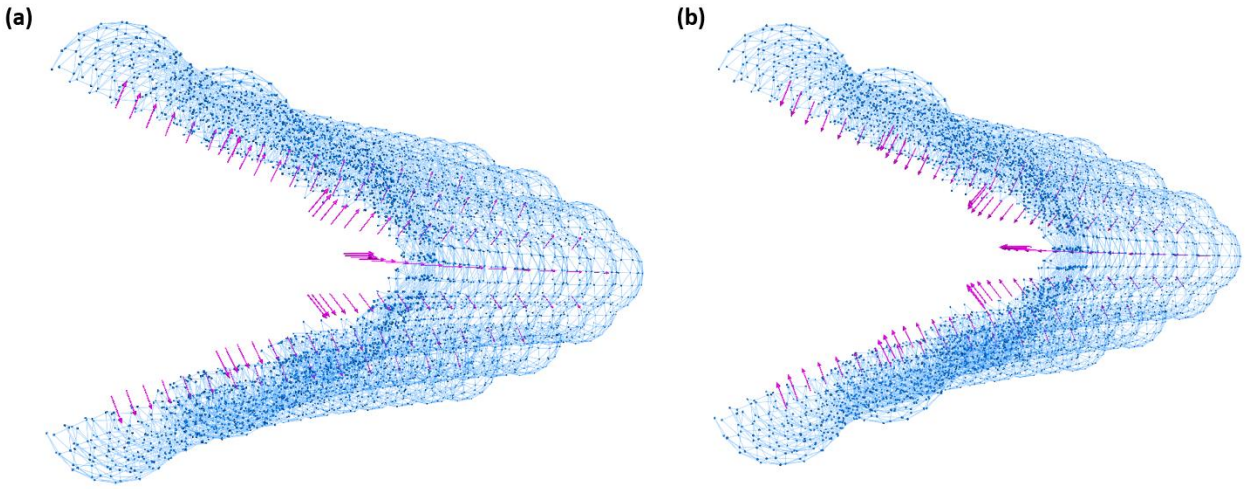


Figure S3. The vectorial direction of pseudoatomic point dipoles in the medium model. The point dipole $m\overrightarrow{n_p}$ is located at the center of each pseudoatom. The magnitude of a point dipole is controlled by m, which is a fitting variable and is the same for all pseudoatoms. The point dipole aligns along the normal vector of the medium surface, pointing either outwards (positive charges on the surface and negative charges in the center) if $m > 0$ as shown in (a), or inwards if $m < 0$ as shown in (b).

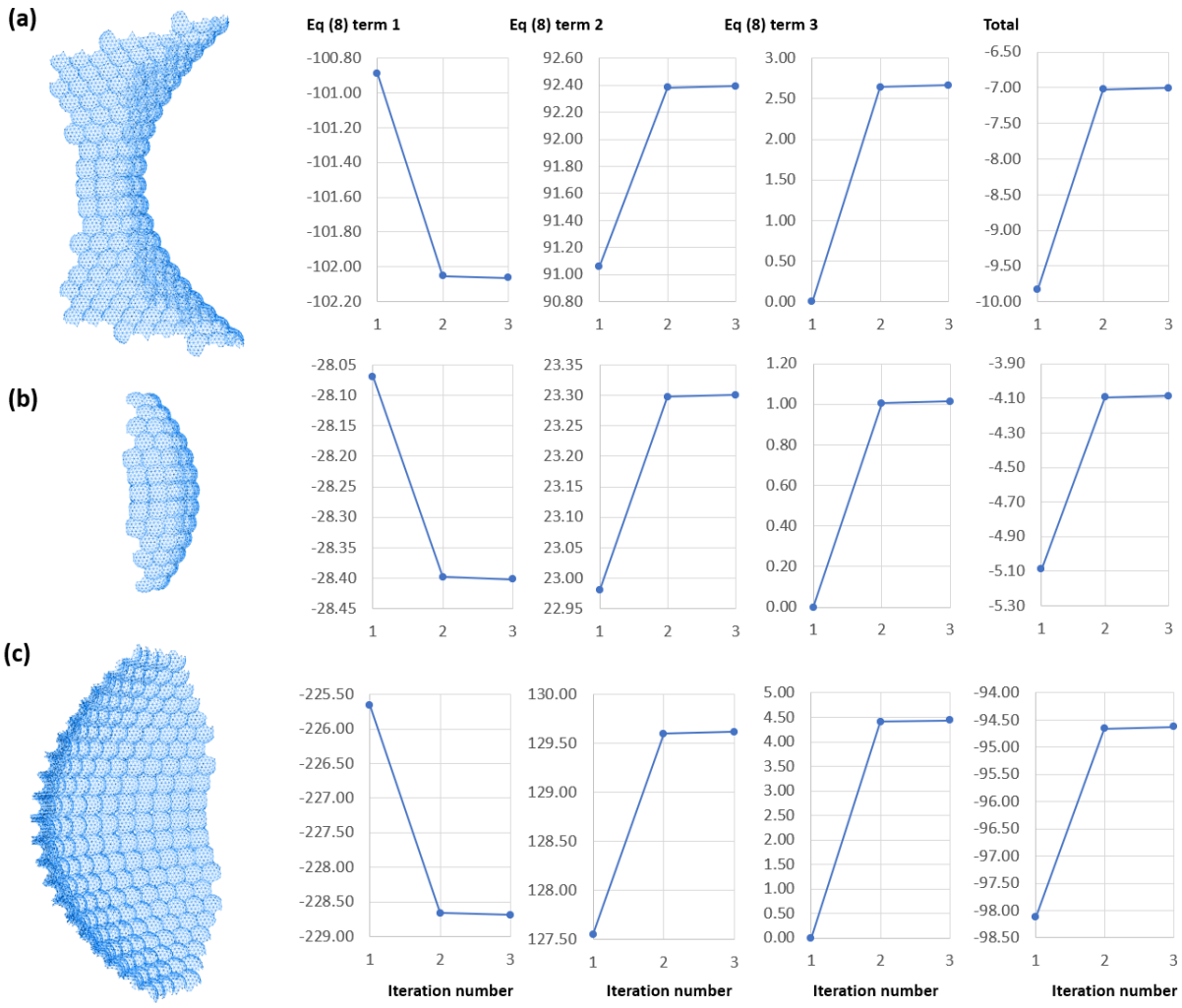
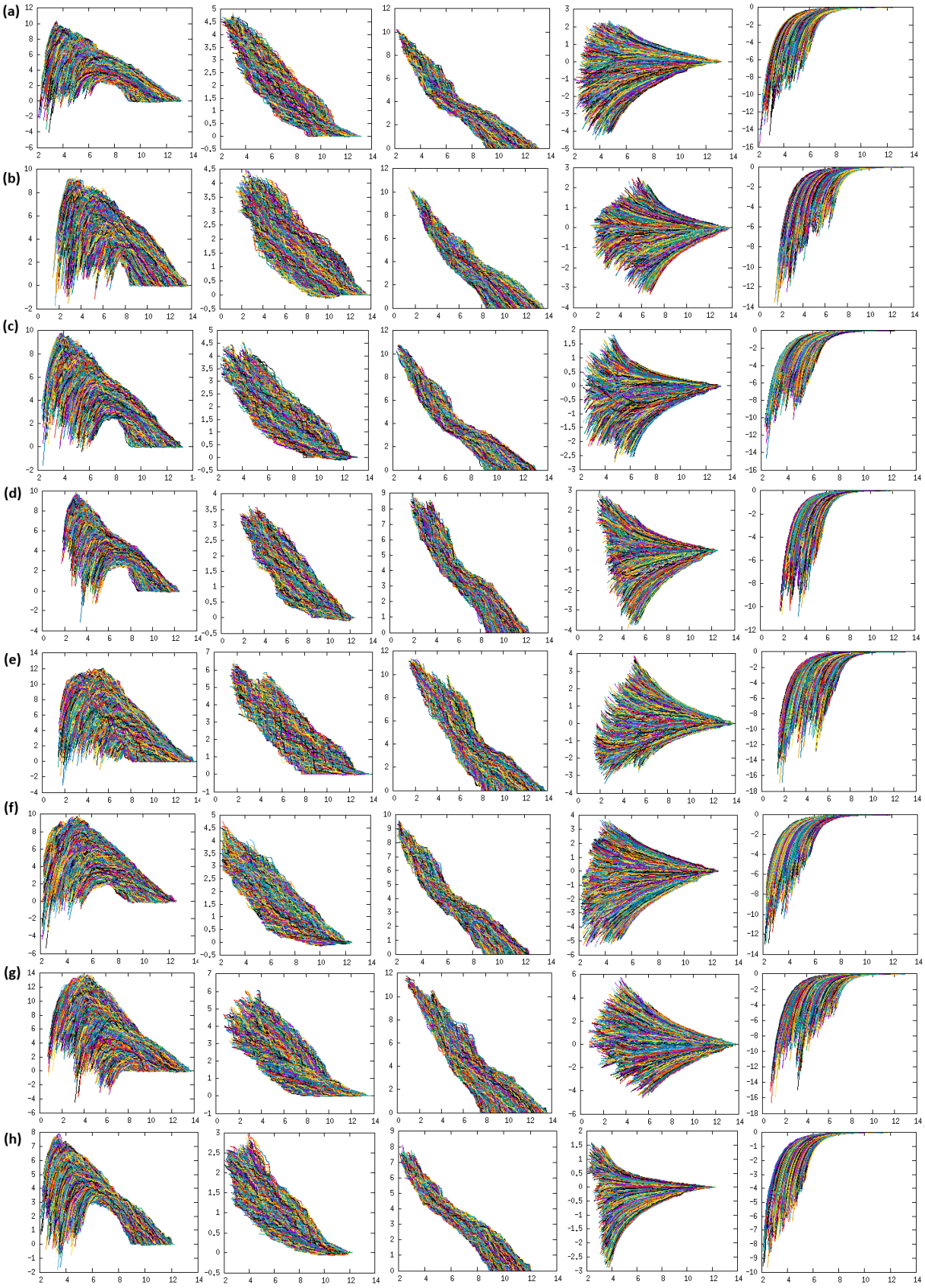


Figure S4. Convergence of SCF calculation for the electrostatic component of the medium solvation free energy $\Delta G_{elec,\,m}$ (Eq (8)) by the PCM. (a) A saddle-like medium structure with $k_x = 0.5$, $k_z = -0.1$. (b) A hump-like medium structure with $k_x = 0.5$, $k_z = 0.1$. (c) A basin-like medium structure with $k_x = -0.1$, $k_z = -0.1$. The pseudoatomic representation of each medium structure is shown on the left, followed by the convergence plots for the first (interaction between point dipoles and surface polarization charges), second (self-interaction of surface polarization charges), and third (change in self-interaction of point dipoles) energy terms in Eq (8), and finally the electrostatic free energy of solvation $\Delta G_{elec,\,m}$. In all cases, SCF calculation converges after 3 iterations. Also note that a concave medium surface (negative curvature) requires considering a larger pseudoatomic surface than a convex surface, because it can have a more extensive interaction with the solute. For example, (c) has two negative curvatures making it more capable of interacting with the solute, therefore demanding a more extensive surface model. In contrast, for (b) only a small surface region needs to be considered because any surface beyond the displayed region is unable to interact with the solute. The size of the pseudoatomic model is determined as described in the main text. Other parameters used for the calculations are: $m = 0.1$ $[e]$ Å, $\alpha_m = 0.02$ Å^3, $r_{MEB} = 5.9$ Å (strychine), $\varepsilon_r = 46.7$ $(DMSO)$.


(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)

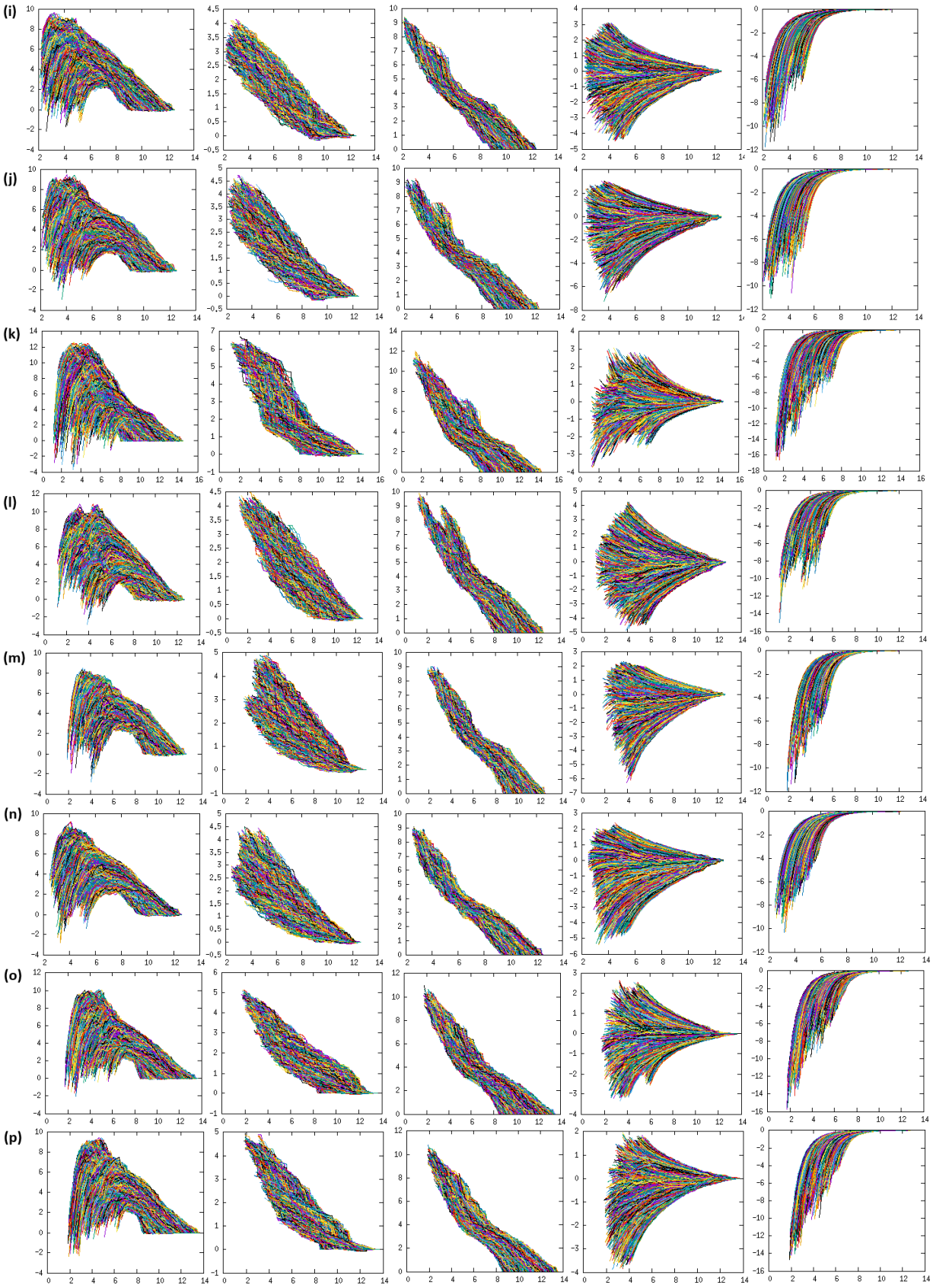

(i)
(j)
(k)
(l)
(m)
(n)
(o)
(p)

Figure S5. PES projections on the r-energy plane generated from optimized P1B FP's for PMMA/chloroform. (a)-(p) for compounds **1**-**16**, respectively. Column 1: the total Gibbs free energy of the system: $\Delta G(\boldsymbol{\Omega}, r)$; column 2: desolvation free energy of solute: $\Delta\Delta G_{sol,s}$; column 3: desolvation free energy of medium: $\Delta\Delta G_{sol,m}$; column 4: solute-medium electrostatic interaction energy: $\Delta\Delta G_{elec,s/m} + \Delta\Delta G_{elec,m/m}$; column 5: solute-medium dispersion interaction: $\Delta\Delta G_{disp,s/m}$. The X-axis is the solute-medium distance r in Å. The Y-axis is the energy in kcal mol^{-1}.

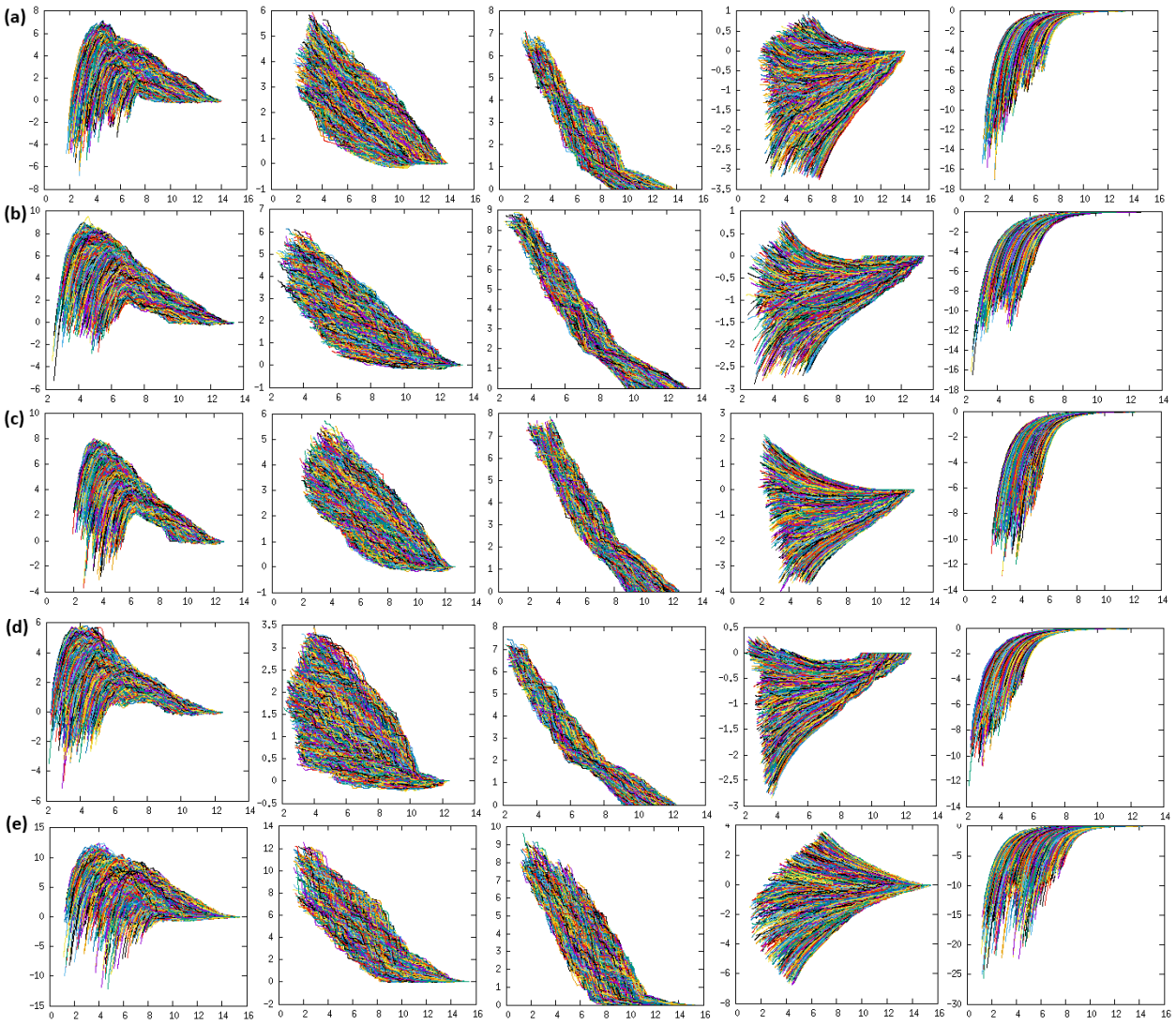


Figure S6. PES projections on the r-energy plane generated from optimized P1B FP's for poly-HEMA/DMSO. (a)-(e) for compounds **2**, **3**, **4**, **8**, and **17**, respectively. Column 1: the total Gibbs free energy of the system: $\Delta G(\boldsymbol{\Omega}, r)$; column 2: desolvation free energy of solute: $\Delta\Delta G_{sol,s}$; column 3: desolvation free energy of medium: $\Delta\Delta G_{sol,m}$; column 4: solute-medium electrostatic interaction energy: $\Delta\Delta G_{elec,s/m} + \Delta\Delta G_{elec,m/m}$; column 5: solute-medium dispersion interaction: $\Delta\Delta G_{disp,s/m}$. The X-axis is the solute-medium distance r in Å. The Y-axis is the energy in kcal mol^{-1}.

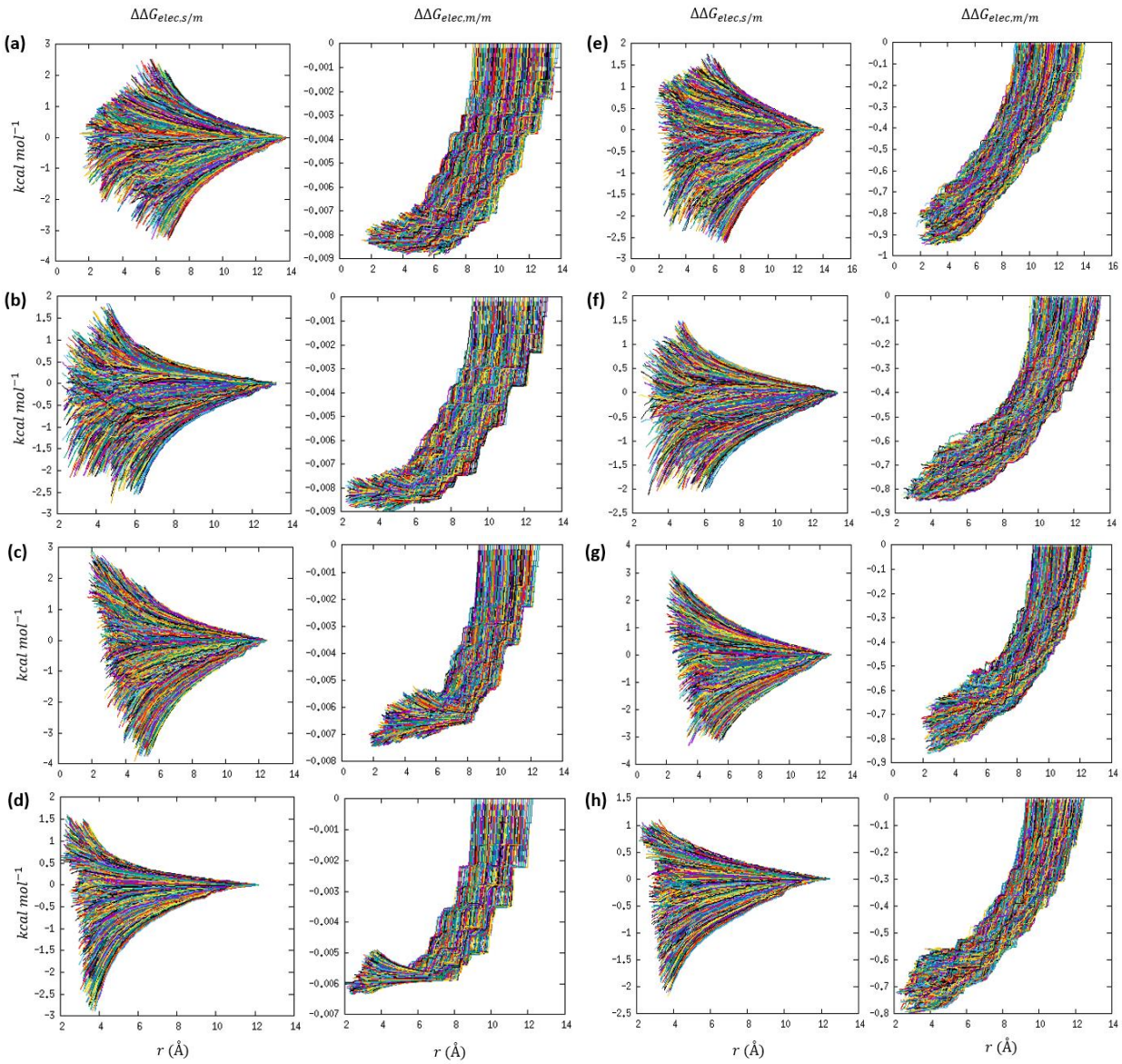


Figure S7. 2-D r-energy PES of Coulomb interaction $\Delta\Delta G_{elec,s/m}$ and medium self-interaction $\Delta\Delta G_{elec,m/m}$. (a)-(d): $\Delta\Delta G_{elec,s/m}$ (left) and $\Delta\Delta G_{elec,m/m}$ (right) for compounds **2**, **3**, **4**, and **8**, respectively, in PMMA/chloroform. (e)-(h): $\Delta\Delta G_{elec,s/m}$ (left) and $\Delta\Delta G_{elec,m/m}$ (right) for compounds **2**, **3**, **4**, and **8**, respectively, in poly-HEMA/DMSO. Notice that $\Delta\Delta G_{elec,s/m}$ has a similar distribution of positive and negative energies for the same compound in the two different alignment medium, whereas $\Delta\Delta G_{elec,m/m}$ drops to substantially more negative values at short solute-medium distances in poly-HEMA/DMSO than PMMA/chloroform.

Solute Geometry and Predetermined Model Parameters

Table S1. Solute parameters for the sixteen compounds measured in PMMA/chloroform

		X	Y	Z	Coulomb *R* (Å)	Bondi *R* (Å)	Grimme D2 *R* (Å)	CM5 *pQ* ([e])	γ (cal mol^{-1} Å^{-2})	C_6^m (J nm^6 mol^{-1})
strychnine (**1**)	C1	2.359	0.439	0.172	1.85	1.7	1.452	0.091	-80.92	1.75
	C2	2.013	-0.913	0.023	1.85	1.7	1.452	-0.017	-83.44	1.75
	C3	2.989	-1.845	-0.316	1.85	1.7	1.452	-0.099	-28.04	1.75
	C4	4.307	-1.417	-0.512	1.85	1.7	1.452	-0.114	-27.88	1.75
	C5	4.636	-0.069	-0.353	1.85	1.7	1.452	-0.103	-27.90	1.75
	C6	3.671	0.882	-0.005	1.85	1.7	1.452	-0.109	-27.92	1.75
	C7	0.553	-1.128	0.365	1.85	1.7	1.452	0.007	-124.32	1.75
	N8	1.209	1.198	0.488	1.89	1.6	1.397	-0.274	2.62	1.23
	C9	1.082	2.563	0.314	1.85	1.7	1.452	0.260	-18.04	1.75
	O10	2.038	3.317	0.194	2.02	1.5	1.342	-0.358	-2.42	0.7
	C11	0.001	0.336	0.415	1.85	1.7	1.452	0.027	-64.26	1.75
	C12	-0.359	3.075	0.317	1.85	1.7	1.452	-0.145	-16.78	1.75
	C13	-1.42	2.204	-0.412	1.85	1.7	1.452	0.021	-16.11	1.75
	C14	-0.814	0.836	-0.793	1.85	1.7	1.452	-0.080	-71.04	1.75
	O15	-2.523	2.142	0.488	2.02	1.5	1.342	-0.270	2.69	0.7
	C16	-3.714	1.536	-0.023	1.85	1.7	1.452	-0.053	36.14	1.75
	C17	-3.717	0.035	0.139	1.85	1.7	1.452	-0.120	-25.58	1.75
	C18	-2.821	-0.767	-0.448	1.85	1.7	1.452	-0.017	-80.21	1.75
	C19	-2.721	-2.251	-0.155	1.85	1.7	1.452	-0.057	-13.05	1.75
	C20	-1.739	-0.243	-1.393	1.85	1.7	1.452	-0.072	-71.69	1.75
	C21	-0.82	-1.405	-1.817	1.85	1.7	1.452	-0.149	-17.33	1.75
	C22	-0.269	-2.079	-0.558	1.85	1.7	1.452	0.015	-64.62	1.75
	C23	0.366	-1.839	1.73	1.85	1.7	1.452	-0.147	-16.90	1.75
	C24	-1.099	-2.281	1.703	1.85	1.7	1.452	-0.063	-12.24	1.75
	N25	-1.368	-2.619	0.293	1.89	1.6	1.397	-0.366	-31.50	1.23
	H26	2.734	-2.896	-0.426	1.20	1.2	1.001	0.104	-35.49	0.14
	H27	5.075	-2.137	-0.781	1.20	1.2	1.001	0.100	-35.50	0.14
	H28	5.663	0.255	-0.502	1.20	1.2	1.001	0.102	-35.49	0.14
	H29	3.914	1.928	0.114	1.20	1.2	1.001	0.101	-35.61	0.14
	H30	-0.601	0.479	1.319	1.20	1.2	1.001	0.109	-35.34	0.14
	H31	-0.327	4.093	-0.077	1.20	1.2	1.001	0.106	-35.40	0.14
	H32	-0.687	3.148	1.362	1.20	1.2	1.001	0.113	-35.29	0.14
	H33	-1.749	2.707	-1.336	1.20	1.2	1.001	0.099	-35.21	0.14
	H34	-0.086	1.061	-1.587	1.20	1.2	1.001	0.103	-35.24	0.14
	H35	-3.853	1.827	-1.078	1.20	1.2	1.001	0.097	-35.19	0.14
	H36	-4.534	1.982	0.549	1.20	1.2	1.001	0.106	-35.35	0.14
	H37	-4.459	-0.393	0.812	1.20	1.2	1.001	0.093	-35.45	0.14
	H38	-2.974	-2.843	-1.045	1.20	1.2	1.001	0.099	-35.28	0.14
	H39	-3.433	-2.546	0.623	1.20	1.2	1.001	0.108	-35.34	0.14
	H40	-2.223	0.187	-2.284	1.20	1.2	1.001	0.100	-35.22	0.14

	H41	0.01	-1.034	-2.429	1.20	1.2	1.001	0.095	-35.33	0.14
	H42	-1.358	-2.137	-2.43	1.20	1.2	1.001	0.095	-35.33	0.14
	H43	0.389	-2.909	-0.854	1.20	1.2	1.001	0.095	-35.25	0.14
	H44	0.606	-1.192	2.58	1.20	1.2	1.001	0.095	-35.35	0.14
	H45	1.032	-2.708	1.774	1.20	1.2	1.001	0.092	-35.33	0.14
	H46	-1.287	-3.144	2.354	1.20	1.2	1.001	0.092	-35.30	0.14
	H47	-1.751	-1.462	2.05	1.20	1.2	1.001	0.086	-35.20	0.14
estrone (**2**)	C1	-0.369	-1.771	-0.084	1.85	1.7	1.452	-0.153	-16.37	1.75
	C2	0.279	-0.436	-0.526	1.85	1.7	1.452	-0.073	-70.74	1.75
	C3	-0.465	0.795	0.06	1.85	1.7	1.452	-0.079	-71.57	1.75
	C4	-1.945	0.683	-0.309	1.85	1.7	1.452	-0.077	-71.28	1.75
	C5	-2.596	-0.607	0.251	1.85	1.7	1.452	-0.015	-125.46	1.75
	C6	-1.89	-1.83	-0.345	1.85	1.7	1.452	-0.152	-17.08	1.75
	C7	1.787	-0.36	-0.267	1.85	1.7	1.452	-0.031	-82.08	1.75
	C8	2.421	0.874	-0.004	1.85	1.7	1.452	-0.015	-82.75	1.75
	C9	1.636	2.17	0.114	1.85	1.7	1.452	-0.148	-18.31	1.75
	C10	0.212	2.077	-0.437	1.85	1.7	1.452	-0.154	-17.75	1.75
	C11	2.595	-1.503	-0.34	1.85	1.7	1.452	-0.105	-27.94	1.75
	C12	3.974	-1.454	-0.153	1.85	1.7	1.452	-0.131	-28.10	1.75
	C13	4.587	-0.227	0.111	1.85	1.7	1.452	0.072	-28.05	1.75
	C14	3.805	0.925	0.181	1.85	1.7	1.452	-0.123	-28.03	1.75
	C15	-2.952	1.799	0.038	1.85	1.7	1.452	-0.155	-16.54	1.75
	C16	-4.316	1.123	-0.234	1.85	1.7	1.452	-0.153	-16.58	1.75
	C17	-4.058	-0.395	-0.156	1.85	1.7	1.452	0.189	-17.22	1.75
	O18	-4.876	-1.261	-0.381	2.024	1.52	1.342	-0.331	-2.55	0.7
	C19	-2.616	-0.685	1.801	1.85	1.7	1.452	-0.226	38.02	1.75
	H20	-0.368	0.773	1.156	1.2	1.2	1.001	0.089	-35.24	0.14
	H21	0.137	-0.372	-1.619	1.2	1.2	1.001	0.087	-35.17	0.14
	H22	-1.983	0.58	-1.408	1.2	1.2	1.001	0.090	-35.17	0.14
	O23	5.935	-0.094	0.305	2.024	1.52	1.342	-0.401	1.05	0.7
	H24	-3.103	0.182	2.259	1.2	1.2	1.001	0.087	-35.35	0.14
	H25	-3.172	-1.576	2.107	1.2	1.2	1.001	0.087	-35.36	0.14
	H26	-1.61	-0.755	2.221	1.2	1.2	1.001	0.090	-35.39	0.14
	H27	-0.158	-1.939	0.979	1.2	1.2	1.001	0.082	-35.31	0.14
	H28	0.096	-2.606	-0.617	1.2	1.2	1.001	0.088	-35.36	0.14
	H29	-2.074	-1.854	-1.427	1.2	1.2	1.001	0.084	-35.29	0.14
	H30	-2.309	-2.758	0.059	1.2	1.2	1.001	0.087	-35.34	0.14
	H31	2.188	2.978	-0.382	1.2	1.2	1.001	0.091	-35.31	0.14
	H32	1.588	2.452	1.176	1.2	1.2	1.001	0.089	-35.25	0.14
	H33	0.229	2.075	-1.536	1.2	1.2	1.001	0.083	-35.27	0.14
	H34	-0.357	2.963	-0.133	1.2	1.2	1.001	0.087	-35.33	0.14
	H35	-2.807	2.698	-0.567	1.2	1.2	1.001	0.087	-35.38	0.14
	H36	-2.862	2.1	1.088	1.2	1.2	1.001	0.085	-35.33	0.14
	H37	-4.689	1.344	-1.241	1.2	1.2	1.001	0.103	-35.32	0.14
	H38	-5.113	1.408	0.46	1.2	1.2	1.001	0.102	-35.35	0.14

	H39	2.146	-2.468	-0.551	1.2	1.2	1.001	0.100	-35.53	0.14
	H40	4.568	-2.363	-0.216	1.2	1.2	1.001	0.103	-35.48	0.14
	H41	4.297	1.873	0.383	1.2	1.2	1.001	0.103	-35.49	0.14
	H42	6.35	-0.963	0.224	1.2	1.2	1.001	0.358	-19.96	0.14
retrorsine (**3**)	C1	-2.234	-0.125	-1.162	1.85	1.7	1.452	0.025	-16.96	1.75
	C2	-3.684	0.344	-0.978	1.85	1.7	1.452	-0.152	-17.39	1.75
	C3	-4.12	-0.378	0.305	1.85	1.7	1.452	-0.059	-12.54	1.75
	N4	-3.438	-1.675	0.239	1.89	1.55	1.397	-0.364	-32.41	1.23
	C5	-2.344	-1.613	-0.762	1.85	1.7	1.452	0.018	-66.52	1.75
	C6	-2.928	-2.238	1.494	1.85	1.7	1.452	-0.051	-13.94	1.75
	C7	-1.53	-2.672	1.155	1.85	1.7	1.452	-0.079	-25.93	1.75
	C8	-1.188	-2.321	-0.088	1.85	1.7	1.452	-0.024	-81.74	1.75
	O9	-1.345	0.537	-0.228	2.024	1.52	1.342	-0.190	0.71	0.7
	C10	-1.05	1.841	-0.478	1.85	1.7	1.452	0.262	35.65	1.75
	C11	-0.062	2.37	0.516	1.85	1.7	1.452	-0.028	-81.41	1.75
	O12	-1.534	2.463	-1.405	2.024	1.52	1.342	-0.329	-2.50	0.7
	C13	-0.142	3.636	0.965	1.85	1.7	1.452	-0.068	-25.81	1.75
	C14	-1.146	4.696	0.626	1.85	1.7	1.452	-0.228	35.69	1.75
	C15	1.03	1.418	0.955	1.85	1.7	1.452	-0.154	-17.35	1.75
	C16	2.024	1.102	-0.2	1.85	1.7	1.452	-0.078	-70.24	1.75
	C17	0.089	-2.691	-0.775	1.85	1.7	1.452	-0.034	35.59	1.75
	O18	1.043	-1.586	-0.853	2.024	1.52	1.342	-0.188	-0.15	0.7
	C19	1.797	-1.384	0.232	1.85	1.7	1.452	0.264	37.35	1.75
	C20	2.79	-0.222	0.066	1.85	1.7	1.452	0.077	-70.80	1.75
	O21	1.727	-2.032	1.261	2.024	1.52	1.342	-0.318	-2.49	0.7
	C22	2.973	2.288	-0.426	1.85	1.7	1.452	-0.235	37.27	1.75
	O23	3.544	-0.145	1.273	2.024	1.52	1.342	-0.432	2.69	0.7
	C24	3.785	-0.595	-1.052	1.85	1.7	1.452	-0.063	37.57	1.75
	O25	4.413	-1.829	-0.754	2.024	1.52	1.342	-0.462	2.69	0.7
	H26	-2.628	-2.153	-1.683	1.2	1.2	1.001	0.099	-35.16	0.14
	H27	-1.92	4.342	-0.052	1.2	1.2	1.001	0.088	-35.47	0.14
	H28	-1.607	5.086	1.542	1.2	1.2	1.001	0.092	-35.30	0.14
	H29	-0.644	5.546	0.147	1.2	1.2	1.001	0.095	-35.30	0.14
	H30	3.684	2.37	0.401	1.2	1.2	1.001	0.083	-35.37	0.14
	H31	3.538	2.197	-1.358	1.2	1.2	1.001	0.085	-35.37	0.14
	H32	2.401	3.219	-0.483	1.2	1.2	1.001	0.082	-35.36	0.14
	H33	-4.271	-0.008	-1.833	1.2	1.2	1.001	0.100	-35.34	0.14
	H34	-3.772	1.429	-0.932	1.2	1.2	1.001	0.097	-35.44	0.14
	H35	-5.209	-0.495	0.364	1.2	1.2	1.001	0.092	-35.31	0.14
	H36	-3.803	0.197	1.192	1.2	1.2	1.001	0.086	-35.18	0.14
	H37	-3.54	-3.083	1.848	1.2	1.2	1.001	0.093	-35.22	0.14
	H38	-2.928	-1.494	2.31	1.2	1.2	1.001	0.096	-35.17	0.14
	H39	0.569	0.497	1.322	1.2	1.2	1.001	0.090	-35.37	0.14
	H40	1.586	1.851	1.792	1.2	1.2	1.001	0.095	-35.36	0.14
	H41	-0.082	-2.955	-1.822	1.2	1.2	1.001	0.120	-35.38	0.14

	H42	0.576	-3.523	-0.264	1.2	1.2	1.001	0.117	-35.42	0.14
	H43	4.521	0.212	-1.154	1.2	1.2	1.001	0.101	-35.31	0.14
	H44	3.263	-0.716	-2.005	1.2	1.2	1.001	0.108	-35.38	0.14
	H45	-1.853	0.035	-2.173	1.2	1.2	1.001	0.111	-35.40	0.14
	H46	1.442	0.937	-1.115	1.2	1.2	1.001	0.094	-35.31	0.14
	H47	-0.89	-3.211	1.846	1.2	1.2	1.001	0.111	-35.52	0.14
	H48	0.614	3.934	1.692	1.2	1.2	1.001	0.103	-35.43	0.14
	H49	3.113	-0.766	1.888	1.2	1.2	1.001	0.323	-19.90	0.14
	H50	4.758	-1.72	0.146	1.2	1.2	1.001	0.326	-19.94	0.14
aquatolide (**4**)	C1	-1.65	-0.308	-1.242	1.85	1.7	1.452	0.027	-14.54	1.75
	C2	-1.996	-1.149	0.044	1.85	1.7	1.452	-0.008	-123.61	1.75
	C3	-0.724	-0.722	0.823	1.85	1.7	1.452	-0.058	-69.38	1.75
	C4	-0.45	0.774	0.303	1.85	1.7	1.452	-0.005	-122.58	1.75
	O5	-2.279	0.994	-1.123	2.024	1.52	1.342	-0.207	0.99	0.7
	C6	-1.65	1.626	-0.087	1.85	1.7	1.452	0.253	36.69	1.75
	O7	-2.002	2.695	0.346	2.024	1.52	1.342	-0.335	-2.62	0.7
	C8	0.429	-1.145	-0.141	1.85	1.7	1.452	-0.078	-70.89	1.75
	C9	-0.139	-0.014	-1.013	1.85	1.7	1.452	-0.079	-72.45	1.75
	C10	0.625	1.553	1.06	1.85	1.7	1.452	-0.149	-17.81	1.75
	C11	1.718	2.165	0.177	1.85	1.7	1.452	-0.144	-18.71	1.75
	C12	1.857	-1.02	0.399	1.85	1.7	1.452	0.190	-18.68	1.75
	C13	2.866	-0.112	-0.26	1.85	1.7	1.452	-0.030	-81.00	1.75
	C14	2.764	1.224	-0.364	1.85	1.7	1.452	-0.087	-25.51	1.75
	O15	2.213	-1.796	1.273	2.024	1.52	1.342	-0.321	-2.44	0.7
	C16	4.099	-0.853	-0.732	1.85	1.7	1.452	-0.225	36.32	1.75
	H17	0.381	-2.167	-0.527	1.2	1.2	1.001	0.108	-35.37	0.14
	H18	0.406	0.434	-1.845	1.2	1.2	1.001	0.099	-35.42	0.14
	H19	-1.957	-0.734	-2.197	1.2	1.2	1.001	0.120	-35.44	0.14
	C20	-2.098	-2.655	-0.265	1.85	1.7	1.452	-0.228	37.50	1.75
	C21	-3.293	-0.729	0.758	1.85	1.7	1.452	-0.233	37.42	1.75
	H22	-0.674	-0.945	1.891	1.2	1.2	1.001	0.104	-35.40	0.14
	H23	3.853	-1.602	-1.495	1.2	1.2	1.001	0.088	-35.30	0.14
	H24	4.549	-1.392	0.108	1.2	1.2	1.001	0.091	-35.35	0.14
	H25	4.838	-0.166	-1.152	1.2	1.2	1.001	0.092	-35.38	0.14
	H26	-1.999	-3.248	0.651	1.2	1.2	1.001	0.089	-35.33	0.14
	H27	-1.348	-3.011	-0.975	1.2	1.2	1.001	0.088	-35.39	0.14
	H28	-3.078	-2.875	-0.699	1.2	1.2	1.001	0.088	-35.36	0.14
	H29	-3.485	-1.421	1.585	1.2	1.2	1.001	0.088	-35.34	0.14
	H30	-4.149	-0.772	0.078	1.2	1.2	1.001	0.088	-35.36	0.14
	H31	-3.255	0.279	1.177	1.2	1.2	1.001	0.086	-35.39	0.14
	H32	0.106	2.358	1.591	1.2	1.2	1.001	0.097	-35.34	0.14
	H33	1.09	0.927	1.829	1.2	1.2	1.001	0.095	-35.34	0.14
	H34	1.26	2.72	-0.656	1.2	1.2	1.001	0.097	-35.24	0.14
	H35	2.25	2.931	0.758	1.2	1.2	1.001	0.100	-35.27	0.14
	H36	3.598	1.734	-0.849	1.2	1.2	1.001	0.100	-35.41	0.14

caulamidine A (**5**)	C1	-4.021	1.026	1.527	1.85	1.7	1.452	-0.099	-27.92	1.75
	C2	-2.729	0.675	1.109	1.85	1.7	1.452	0.082	-81.37	1.75
	C3	-2.528	0.27	-0.227	1.85	1.7	1.452	-0.015	-83.58	1.75
	C4	-3.604	0.21	-1.11	1.85	1.7	1.452	-0.105	-28.16	1.75
	C5	-4.88	0.556	-0.667	1.85	1.7	1.452	-0.005	-28.10	1.75
	C6	-5.099	0.967	0.648	1.85	1.7	1.452	-0.108	-28.17	1.75
	N7	-1.679	0.761	2.029	1.89	1.55	1.397	-0.389	28.69	1.23
	C8	-0.556	0.161	1.783	1.85	1.7	1.452	0.258	-192.45	1.75
	C9	-1.11	-0.02	-0.638	1.85	1.7	1.452	-0.143	-18.17	1.75
	C10	1.199	-0.796	0.128	1.85	1.7	1.452	0.010	-125.10	1.75
	C11	-0.313	-0.675	0.515	1.85	1.7	1.452	0.014	-123.26	1.75
	C12	1.377	-1.864	-0.964	1.85	1.7	1.452	0.252	-193.22	1.75
	N13	0.817	-3.101	-0.798	1.89	1.55	1.397	-0.305	-18.85	1.23
	C14	-0.567	-3.135	-0.291	1.85	1.7	1.452	-0.039	-12.22	1.75
	C15	-0.849	-2.113	0.814	1.85	1.7	1.452	-0.144	-16.24	1.75
	N16	2.105	-1.506	-1.978	1.89	1.55	1.397	-0.393	28.65	1.23
	C17	1.108	-4.099	-1.823	1.85	1.7	1.452	-0.118	41.63	1.75
	CL18	-6.236	0.471	-1.789	2.38	1.75	1.639	-0.090	-35.15	5.07
	C19	2.429	-0.151	-1.763	1.85	1.7	1.452	0.080	-81.04	1.75
	C20	1.864	0.372	-0.58	1.85	1.7	1.452	-0.020	-83.13	1.75
	C21	2.005	1.713	-0.255	1.85	1.7	1.452	-0.095	-28.11	1.75
	C22	2.747	2.522	-1.127	1.85	1.7	1.452	-0.002	-27.88	1.75
	C23	3.33	2.012	-2.286	1.85	1.7	1.452	-0.099	-27.99	1.75
	C24	3.17	0.662	-2.615	1.85	1.7	1.452	-0.095	-28.07	1.75
	CL25	2.94	4.231	-0.742	2.38	1.75	1.639	-0.086	-35.15	5.07
	C26	1.967	-1.212	1.41	1.85	1.7	1.452	-0.021	-17.21	1.75
	N27	0.409	0.151	2.764	1.89	1.55	1.397	-0.291	-19.30	1.23
	C28	1.811	-0.17	2.509	1.85	1.7	1.452	-0.046	-13.51	1.75
	C29	0.158	0.89	3.999	1.85	1.7	1.452	-0.119	41.70	1.75
	CL30	3.745	-1.483	1.142	2.38	1.75	1.639	-0.092	-35.15	5.07
	H31	1.604	-2.181	1.747	1.2	1.2	1.001	0.112	-35.47	0.14
	H32	2.173	-4.074	-2.055	1.2	1.2	1.001	0.108	-35.43	0.14
	H33	0.837	-5.086	-1.441	1.2	1.2	1.001	0.107	-35.39	0.14
	H34	0.552	-3.908	-2.752	1.2	1.2	1.001	0.097	-35.26	0.14
	H35	-0.895	0.803	4.259	1.2	1.2	1.001	0.105	-35.47	0.14
	H36	0.78	0.469	4.794	1.2	1.2	1.001	0.107	-35.37	0.14
	H37	0.394	1.957	3.892	1.2	1.2	1.001	0.100	-35.29	0.14
	H38	-0.617	0.921	-0.908	1.2	1.2	1.001	0.098	-35.32	0.14
	H39	-1.074	-0.651	-1.533	1.2	1.2	1.001	0.103	-35.33	0.14
	H40	-0.761	-4.141	0.094	1.2	1.2	1.001	0.114	-35.35	0.14
	H41	-1.261	-2.982	-1.133	1.2	1.2	1.001	0.101	-35.22	0.14
	H42	-0.436	-2.469	1.761	1.2	1.2	1.001	0.098	-35.39	0.14
	H43	-1.933	-2.059	0.955	1.2	1.2	1.001	0.102	-35.35	0.14
	H44	2.243	-0.565	3.433	1.2	1.2	1.001	0.116	-35.37	0.14
	H45	2.387	0.728	2.245	1.2	1.2	1.001	0.101	-35.27	0.14

	H46	-4.162	1.342	2.556	1.2	1.2	1.001	0.106	-35.52	0.14
	H47	-3.453	-0.098	-2.14	1.2	1.2	1.001	0.107	-35.52	0.14
	H48	-6.097	1.234	0.976	1.2	1.2	1.001	0.107	-35.55	0.14
	H49	1.55	2.151	0.627	1.2	1.2	1.001	0.110	-35.53	0.14
	H50	3.899	2.671	-2.933	1.2	1.2	1.001	0.109	-35.53	0.14
	H51	3.605	0.254	-3.52	1.2	1.2	1.001	0.112	-35.55	0.14
10-epi-8-deoxycumambrin B (**6**)	C1	1.901	0.224	-0.444	1.85	1.7	1.452	-0.068	-67.77	1.75
	C2	0.498	0.935	-0.608	1.85	1.7	1.452	-0.072	-70.07	1.75
	C3	-0.644	0.259	0.163	1.85	1.7	1.452	0.022	-16.92	1.75
	C4	-1.191	-1.017	-0.517	1.85	1.7	1.452	-0.076	-73.15	1.75
	C5	-0.397	-2.292	-0.252	1.85	1.7	1.452	-0.151	-17.80	1.75
	C6	1.064	-2.232	-0.722	1.85	1.7	1.452	-0.156	-16.49	1.75
	C7	1.997	-1.251	0.041	1.85	1.7	1.452	0.084	-69.95	1.75
	C8	2.758	1.197	0.422	1.85	1.7	1.452	-0.158	-17.77	1.75
	C9	2.01	2.495	0.338	1.85	1.7	1.452	-0.117	-25.93	1.75
	C10	0.792	2.382	-0.207	1.85	1.7	1.452	-0.025	-80.72	1.75
	O11	-1.808	1.143	0.236	2.024	1.52	1.342	-0.194	0.81	0.7
	C12	-2.966	0.425	0.235	1.85	1.7	1.452	0.249	35.63	1.75
	C13	-2.634	-1.001	-0.079	1.85	1.7	1.452	-0.023	-81.99	1.75
	O14	-4.045	0.927	0.446	2.024	1.52	1.342	-0.345	-2.59	0.7
	C15	-3.522	-1.989	0.05	1.85	1.7	1.452	-0.152	30.06	1.75
	O16	1.672	-1.259	1.448	2.024	1.52	1.342	-0.428	2.69	0.7
	C17	3.451	-1.73	-0.136	1.85	1.7	1.452	-0.234	37.51	1.75
	C18	-0.158	3.514	-0.477	1.85	1.7	1.452	-0.233	35.83	1.75
	H19	2.335	0.216	-1.451	1.2	1.2	1.001	0.094	-35.31	0.14
	H20	0.2	0.919	-1.667	1.2	1.2	1.001	0.091	-35.25	0.14
	H21	-0.341	0.052	1.193	1.2	1.2	1.001	0.107	-35.37	0.14
	H22	-1.18	-0.822	-1.603	1.2	1.2	1.001	0.102	-35.19	0.14
	H23	-0.886	-3.124	-0.774	1.2	1.2	1.001	0.091	-35.30	0.14
	H24	-0.433	-2.525	0.818	1.2	1.2	1.001	0.086	-35.33	0.14
	H25	1.484	-3.241	-0.62	1.2	1.2	1.001	0.087	-35.29	0.14
	H26	1.106	-1.997	-1.795	1.2	1.2	1.001	0.089	-35.26	0.14
	H27	3.781	1.286	0.036	1.2	1.2	1.001	0.084	-35.31	0.14
	H28	2.837	0.841	1.457	1.2	1.2	1.001	0.084	-35.30	0.14
	H29	2.431	3.435	0.688	1.2	1.2	1.001	0.094	-35.48	0.14
	H30	-3.272	-3.023	-0.168	1.2	1.2	1.001	0.107	-35.51	0.14
	H31	-4.532	-1.769	0.383	1.2	1.2	1.001	0.107	-35.51	0.14
	H32	1.943	-2.105	1.829	1.2	1.2	1.001	0.337	-19.96	0.14
	H33	4.153	-1.073	0.384	1.2	1.2	1.001	0.088	-35.38	0.14
	H34	3.569	-2.743	0.269	1.2	1.2	1.001	0.086	-35.30	0.14
	H35	3.728	-1.767	-1.195	1.2	1.2	1.001	0.089	-35.34	0.14
	H36	0.319	4.474	-0.255	1.2	1.2	1.001	0.085	-35.35	0.14
	H37	-0.466	3.523	-1.531	1.2	1.2	1.001	0.085	-35.29	0.14

	H38	-1.074	3.43	0.114	1.2	1.2	1.001	0.086	-35.37	0.14
mefloquine (**7**)	C1	0.753	-3.311	-0.69	1.85	1.7	1.452	-0.081	-28.13	1.75
	C2	2.054	-2.992	-0.238	1.85	1.7	1.452	-0.073	-28.05	1.75
	C3	2.413	-1.683	-0.009	1.85	1.7	1.452	-0.025	-83.07	1.75
	C4	1.47	-0.629	-0.223	1.85	1.7	1.452	0.120	-81.96	1.75
	C5	0.144	-0.956	-0.664	1.85	1.7	1.452	0.002	-84.63	1.75
	C6	-0.178	-2.322	-0.896	1.85	1.7	1.452	-0.076	-27.83	1.75
	N7	1.874	0.647	0	1.89	1.55	1.397	-0.339	28.96	1.23
	C8	1.003	1.609	-0.212	1.85	1.7	1.452	0.118	-81.51	1.75
	C9	-0.325	1.41	-0.642	1.85	1.7	1.452	-0.084	-28.07	1.75
	C10	-0.773	0.123	-0.858	1.85	1.7	1.452	0.025	-82.87	1.75
	C11	-2.209	-0.109	-1.286	1.85	1.7	1.452	0.023	-17.09	1.75
	C12	-3.123	-0.648	-0.143	1.85	1.7	1.452	0.011	-65.54	1.75
	C13	-3.128	0.265	1.092	1.85	1.7	1.452	-0.157	-17.34	1.75
	C14	-4.215	-0.138	2.099	1.85	1.7	1.452	-0.153	-17.48	1.75
	C15	-5.586	-0.204	1.417	1.85	1.7	1.452	-0.154	-17.83	1.75
	C16	-5.527	-1.14	0.211	1.85	1.7	1.452	-0.058	-12.58	1.75
	N17	-4.477	-0.704	-0.723	1.89	1.55	1.397	-0.495	1.54	1.23
	O18	-2.753	1.096	-1.787	2.024	1.52	1.342	-0.442	2.68	0.7
	H19	-2.762	-1.647	0.161	1.2	1.2	1.001	0.092	-35.16	0.14
	C20	3.812	-1.358	0.467	1.85	1.7	1.452	0.335	36.28	1.75
	F21	4.548	-2.49	0.614	1.73	1.47	1.287	-0.134	0.00	0.75
	F22	3.807	-0.74	1.663	1.73	1.47	1.287	-0.138	0.00	0.75
	F23	4.474	-0.573	-0.403	1.73	1.47	1.287	-0.137	0.00	0.75
	C24	1.531	3.016	0.027	1.85	1.7	1.452	0.339	36.65	1.75
	F25	0.538	3.932	-0.048	1.73	1.47	1.287	-0.129	0.00	0.75
	F26	2.458	3.349	-0.891	1.73	1.47	1.287	-0.134	0.00	0.75
	F27	2.098	3.129	1.24	1.73	1.47	1.287	-0.131	0.00	0.75
	H28	-3.298	1.295	0.759	1.2	1.2	1.001	0.088	-35.33	0.14
	H29	-2.141	0.238	1.564	1.2	1.2	1.001	0.086	-35.36	0.14
	H30	-4.23	0.569	2.935	1.2	1.2	1.001	0.087	-35.34	0.14
	H31	-3.975	-1.123	2.525	1.2	1.2	1.001	0.081	-35.26	0.14
	H32	-5.882	0.797	1.079	1.2	1.2	1.001	0.085	-35.30	0.14
	H33	-6.355	-0.554	2.115	1.2	1.2	1.001	0.089	-35.33	0.14
	H34	-6.48	-1.139	-0.33	1.2	1.2	1.001	0.101	-35.33	0.14
	H35	-5.354	-2.172	0.567	1.2	1.2	1.001	0.083	-35.15	0.14
	H36	-2.208	-0.873	-2.086	1.2	1.2	1.001	0.105	-35.13	0.14
	H37	0.495	-4.349	-0.876	1.2	1.2	1.001	0.116	-35.52	0.14
	H38	2.778	-3.781	-0.076	1.2	1.2	1.001	0.115	-35.56	0.14
	H39	-1.167	-2.589	-1.251	1.2	1.2	1.001	0.114	-35.54	0.14
	H40	-0.989	2.246	-0.807	1.2	1.2	1.001	0.113	-35.61	0.14
	H41	-4.467	-1.336	-1.522	1.2	1.2	1.001	0.301	0.00	0.14
	H42	-3.716	0.98	-1.691	1.2	1.2	1.001	0.312	-19.90	0.14
menthol (**8**)	C1	1.607	1.036	-0.141	1.85	1.7	1.452	-0.161	-17.27	1.75
	C2	0.112	1.146	0.191	1.85	1.7	1.452	0.006	-16.96	1.75

	C3	-0.68	-0.065	-0.349	1.85	1.7	1.452	-0.085	-70.46	1.75
	C4	-0.047	-1.372	0.171	1.85	1.7	1.452	-0.156	-17.03	1.75
	C5	1.446	-1.474	-0.174	1.85	1.7	1.452	-0.157	-17.28	1.75
	C6	2.242	-0.272	0.359	1.85	1.7	1.452	-0.081	-71.95	1.75
	C7	3.728	-0.357	-0.006	1.85	1.7	1.452	-0.234	37.13	1.75
	O8	-0.418	2.392	-0.268	2.024	1.52	1.342	-0.456	2.69	0.7
	C9	-2.208	0.056	-0.1	1.85	1.7	1.452	-0.084	-71.08	1.75
	C10	-3.008	-0.921	-0.975	1.85	1.7	1.452	-0.237	37.29	1.75
	C11	-2.613	-0.086	1.376	1.85	1.7	1.452	-0.237	37.33	1.75
	H12	3.865	-0.352	-1.094	1.2	1.2	1.001	0.078	-35.31	0.14
	H13	4.289	0.49	0.403	1.2	1.2	1.001	0.080	-35.34	0.14
	H14	4.18	-1.277	0.381	1.2	1.2	1.001	0.080	-35.33	0.14
	H15	-2.814	-1.966	-0.704	1.2	1.2	1.001	0.077	-35.31	0.14
	H16	-4.084	-0.752	-0.862	1.2	1.2	1.001	0.079	-35.34	0.14
	H17	-2.762	-0.803	-2.037	1.2	1.2	1.001	0.077	-35.32	0.14
	H18	-2.076	0.618	2.019	1.2	1.2	1.001	0.081	-35.36	0.14
	H19	-3.682	0.116	1.496	1.2	1.2	1.001	0.079	-35.35	0.14
	H20	-2.428	-1.097	1.754	1.2	1.2	1.001	0.078	-35.34	0.14
	H21	2.126	1.906	0.277	1.2	1.2	1.001	0.084	-35.33	0.14
	H22	1.726	1.094	-1.235	1.2	1.2	1.001	0.082	-35.21	0.14
	H23	-0.582	-2.238	-0.236	1.2	1.2	1.001	0.084	-35.32	0.14
	H24	-0.161	-1.426	1.262	1.2	1.2	1.001	0.082	-35.28	0.14
	H25	1.567	-1.527	-1.267	1.2	1.2	1.001	0.079	-35.23	0.14
	H26	1.861	-2.407	0.228	1.2	1.2	1.001	0.082	-35.30	0.14
	H27	-0.001	1.19	1.281	1.2	1.2	1.001	0.100	-35.31	0.14
	H28	-0.541	-0.054	-1.445	1.2	1.2	1.001	0.084	-35.16	0.14
	H29	2.162	-0.282	1.458	1.2	1.2	1.001	0.084	-35.21	0.14
	H30	-2.474	1.074	-0.412	1.2	1.2	1.001	0.082	-35.30	0.14
	H31	-0.305	2.414	-1.229	1.2	1.2	1.001	0.330	-19.95	0.14
ludartin (**9**)	C1	-1.246	-0.435	0.136	1.85	1.7	1.452	-0.031	-82.72	1.75
	C2	-1.127	0.862	0.866	1.85	1.7	1.452	-0.141	-19.88	1.75
	C3	0.215	1.56	0.725	1.85	1.7	1.452	-0.142	-19.24	1.75
	C4	0.587	1.125	-1.737	1.85	1.7	1.452	0.029	-17.32	1.75
	C5	-0.716	0.485	-2.192	1.85	1.7	1.452	-0.069	-73.73	1.75
	C6	-1.1	-0.591	-1.192	1.85	1.7	1.452	-0.030	-80.97	1.75
	H7	-1.31	0.687	1.962	1.2	1.2	1.001	0.088	-34.77	0.14
	H8	-1.944	1.548	0.507	1.2	1.2	1.001	0.089	-34.76	0.14
	H9	-1.529	1.263	-2.241	1.2	1.2	1.001	0.101	-34.74	0.14
	C10	-1.308	-1.909	-1.887	1.85	1.7	1.452	-0.144	-19.77	1.75
	C11	0.336	2.191	-0.64	1.85	1.7	1.452	-0.071	-74.05	1.75
	H12	1.05	0.834	0.901	1.2	1.2	1.001	0.088	-34.86	0.14
	H13	0.293	2.359	1.509	1.2	1.2	1.001	0.088	-34.82	0.14
	O14	1.291	1.822	-2.796	2.024	1.52	1.342	-0.191	1.94	0.7
	H15	1.296	0.33	-1.372	1.2	1.2	1.001	0.104	-34.75	0.14
	C16	1.445	3.174	-0.865	1.85	1.7	1.452	-0.020	-83.07	1.75

	H17	-0.628	2.734	-0.872	1.2	1.2	1.001	0.105	-34.66	0.14
	C18	1.891	2.955	-2.263	1.85	1.7	1.452	0.248	35.08	1.75
	O19	2.644	3.569	-3.009	2.024	1.52	1.342	-0.347	-2.40	0.7
	C20	1.936	4.091	-0.037	1.85	1.7	1.452	-0.135	29.92	1.75
	C21	-0.658	-0.219	-3.546	1.85	1.7	1.452	0.067	-75.94	1.75
	H22	1.565	4.214	0.99	1.2	1.2	1.001	0.111	-35.27	0.14
	H23	2.743	4.774	-0.343	1.2	1.2	1.001	0.110	-35.24	0.14
	C24	-1.05	-1.656	-3.354	1.85	1.7	1.452	-0.005	-19.88	1.75
	H25	-2.354	-2.276	-1.727	1.2	1.2	1.001	0.094	-34.87	0.14
	H26	-0.593	-2.682	-1.504	1.2	1.2	1.001	0.094	-34.86	0.14
	C27	0.188	0.29	-4.655	1.85	1.7	1.452	-0.223	35.12	1.75
	O28	-1.962	-0.712	-3.94	2.024	1.52	1.342	-0.280	2.69	0.7
	H29	-0.759	-2.495	-4.002	1.2	1.2	1.001	0.113	-35.26	0.14
	C30	-1.612	-1.573	1.021	1.85	1.7	1.452	-0.219	35.22	1.75
	H31	-2.616	-1.385	1.481	1.2	1.2	1.001	0.087	-34.86	0.14
	H32	-0.862	-1.669	1.846	1.2	1.2	1.001	0.085	-34.88	0.14
	H33	-1.656	-2.546	0.477	1.2	1.2	1.001	0.084	-34.95	0.14
	H34	1.269	0.142	-4.41	1.2	1.2	1.001	0.089	-34.90	0.14
	H35	0.009	1.383	-4.807	1.2	1.2	1.001	0.088	-34.91	0.14
	H36	-0.052	-0.25	-5.604	1.2	1.2	1.001	0.087	-34.91	0.14
parthenolide (**10**)	C1	-3.326	-0.214	-0.87	1.85	1.7	1.452	-0.151	-18.18	1.75
	C2	-2.688	-1.621	-0.806	1.85	1.7	1.452	-0.148	-17.79	1.75
	C3	-1.526	-1.642	0.165	1.85	1.7	1.452	0.069	-76.58	1.75
	C4	-0.195	-1.352	-0.398	1.85	1.7	1.452	-0.009	-21.34	1.75
	C5	-1.88	1.775	-0.166	1.85	1.7	1.452	-0.026	-81.26	1.75
	C6	-2.257	0.832	-1.04	1.85	1.7	1.452	-0.113	-25.71	1.75
	C7	0.907	-0.651	0.345	1.85	1.7	1.452	0.028	-17.99	1.75
	C8	1.257	0.742	-0.245	1.85	1.7	1.452	-0.069	-71.92	1.75
	C9	0.592	1.975	0.401	1.85	1.7	1.452	-0.144	-16.70	1.75
	C10	-0.604	2.557	-0.381	1.85	1.7	1.452	-0.151	-18.05	1.75
	O11	2.105	-1.457	0.2	2.024	1.52	1.342	-0.197	0.13	0.7
	C12	3.194	-0.694	-0.001	1.85	1.7	1.452	0.248	35.38	1.75
	C13	2.766	0.725	-0.165	1.85	1.7	1.452	-0.024	-82.24	1.75
	O14	-0.554	-2.677	-0.018	2.024	1.52	1.342	-0.271	2.69	0.7
	O15	4.309	-1.156	-0.035	2.024	1.52	1.342	-0.348	-2.60	0.7
	C16	3.657	1.711	-0.227	1.85	1.7	1.452	-0.149	29.94	1.75
	C17	-1.865	-1.365	1.61	1.85	1.7	1.452	-0.229	36.15	1.75
	C18	-2.609	2.13	1.105	1.85	1.7	1.452	-0.229	36.05	1.75
	H19	-4.03	-0.192	-1.71	1.2	1.2	1.001	0.090	-35.32	0.14
	H20	-3.909	-0.035	0.038	1.2	1.2	1.001	0.091	-35.37	0.14
	H21	-2.318	-1.911	-1.796	1.2	1.2	1.001	0.095	-35.33	0.14
	H22	-3.441	-2.358	-0.504	1.2	1.2	1.001	0.093	-35.32	0.14
	H23	-0.128	-1.225	-1.481	1.2	1.2	1.001	0.111	-35.39	0.14
	H24	-1.649	0.721	-1.942	1.2	1.2	1.001	0.089	-35.37	0.14
	H25	0.702	-0.581	1.417	1.2	1.2	1.001	0.117	-35.37	0.14

	H26	0.991	0.718	-1.313	1.2	1.2	1.001	0.107	-35.23	0.14
	H27	0.293	1.733	1.429	1.2	1.2	1.001	0.091	-35.30	0.14
	H28	1.35	2.76	0.486	1.2	1.2	1.001	0.091	-35.35	0.14
	H29	-0.347	2.587	-1.447	1.2	1.2	1.001	0.090	-35.31	0.14
	H30	-0.752	3.594	-0.055	1.2	1.2	1.001	0.088	-35.31	0.14
	H31	3.367	2.751	-0.343	1.2	1.2	1.001	0.109	-35.51	0.14
	H32	4.717	1.482	-0.163	1.2	1.2	1.001	0.109	-35.50	0.14
	H33	-2.164	-0.324	1.756	1.2	1.2	1.001	0.091	-35.38	0.14
	H34	-2.702	-2.004	1.913	1.2	1.2	1.001	0.093	-35.33	0.14
	H35	-1.019	-1.587	2.262	1.2	1.2	1.001	0.095	-35.42	0.14
	H36	-3.479	1.501	1.302	1.2	1.2	1.001	0.089	-35.41	0.14
	H37	-1.941	2.074	1.973	1.2	1.2	1.001	0.088	-35.31	0.14
	H38	-2.955	3.169	1.045	1.2	1.2	1.001	0.089	-35.31	0.14
yohimbine (**11**)	C1	-4.535	2.169	0.361	1.85	1.7	1.452	-0.116	-28.26	1.75
	C2	-3.658	1.087	0.282	1.85	1.7	1.452	0.080	-82.57	1.75
	C3	-4.086	-0.209	-0.108	1.85	1.7	1.452	-0.039	-85.63	1.75
	C4	-5.438	-0.409	-0.424	1.85	1.7	1.452	-0.111	-28.05	1.75
	C5	-6.315	0.664	-0.346	1.85	1.7	1.452	-0.126	-27.91	1.75
	C6	-5.868	1.94	0.043	1.85	1.7	1.452	-0.121	-27.87	1.75
	C7	-2.928	-1.056	-0.071	1.85	1.7	1.452	-0.054	-84.07	1.75
	C8	-1.875	-0.274	0.315	1.85	1.7	1.452	0.086	-80.58	1.75
	N9	-2.306	1.017	0.533	1.89	1.55	1.397	-0.411	28.57	1.23
	C10	-0.471	-0.747	0.508	1.85	1.7	1.452	0.025	-69.46	1.75
	N11	-0.34	-2.071	-0.096	1.89	1.55	1.397	-0.362	-33.60	1.23
	C12	-1.429	-2.968	0.271	1.85	1.7	1.452	-0.054	-13.49	1.75
	C13	-2.751	-2.512	-0.343	1.85	1.7	1.452	-0.148	-19.59	1.75
	C14	0.574	0.198	-0.093	1.85	1.7	1.452	-0.152	-17.92	1.75
	C15	1.983	-0.345	0.132	1.85	1.7	1.452	-0.076	-72.21	1.75
	C16	2.084	-1.78	-0.4	1.85	1.7	1.452	-0.080	-72.94	1.75
	C17	0.968	-2.635	0.188	1.85	1.7	1.452	-0.054	-13.98	1.75
	C18	3.084	0.521	-0.51	1.85	1.7	1.452	-0.080	-72.45	1.75
	C19	4.484	-0.065	-0.208	1.85	1.7	1.452	0.013	-17.39	1.75
	C20	4.57	-1.497	-0.718	1.85	1.7	1.452	-0.154	-18.37	1.75
	C21	3.466	-2.372	-0.132	1.85	1.7	1.452	-0.155	-18.16	1.75
	H22	-0.269	-0.813	1.603	1.2	1.2	1.001	0.090	-34.96	0.14
	H23	2.176	-0.373	1.215	1.2	1.2	1.001	0.093	-35.24	0.14
	H24	1.918	-1.743	-1.489	1.2	1.2	1.001	0.089	-35.21	0.14
	O25	4.761	-0.088	1.175	2.024	1.52	1.342	-0.458	2.65	0.7
	C26	3.017	1.948	-0.032	1.85	1.7	1.452	0.267	36.00	1.75
	O27	2.528	2.784	-0.953	2.024	1.52	1.342	-0.204	-0.16	0.7
	O28	3.372	2.323	1.072	2.024	1.52	1.342	-0.328	-2.48	0.7
	C29	2.446	4.159	-0.565	1.85	1.7	1.452	-0.113	91.88	1.75
	H30	-4.193	3.156	0.662	1.2	1.2	1.001	0.102	-35.49	0.14
	H31	-5.794	-1.391	-0.726	1.2	1.2	1.001	0.098	-35.49	0.14
	H32	-7.364	0.52	-0.588	1.2	1.2	1.001	0.094	-35.51	0.14

	H33	-6.577	2.761	0.095	1.2	1.2	1.001	0.095	-35.51	0.14
	H34	-1.731	1.786	0.831	1.2	1.2	1.001	0.347	0.00	0.14
	H35	-1.538	-3.034	1.372	1.2	1.2	1.001	0.079	-35.09	0.14
	H36	-1.173	-3.97	-0.089	1.2	1.2	1.001	0.102	-35.34	0.14
	H37	-2.745	-2.713	-1.423	1.2	1.2	1.001	0.086	-35.28	0.14
	H38	-3.572	-3.097	0.089	1.2	1.2	1.001	0.092	-35.31	0.14
	H39	0.477	1.189	0.37	1.2	1.2	1.001	0.091	-35.29	0.14
	H40	0.369	0.314	-1.164	1.2	1.2	1.001	0.090	-35.31	0.14
	H41	1.011	-3.639	-0.25	1.2	1.2	1.001	0.102	-35.32	0.14
	H42	1.133	-2.752	1.281	1.2	1.2	1.001	0.080	-35.03	0.14
	H43	2.938	0.527	-1.597	1.2	1.2	1.001	0.108	-35.31	0.14
	H44	5.235	0.55	-0.733	1.2	1.2	1.001	0.092	-35.18	0.14
	H45	5.557	-1.895	-0.459	1.2	1.2	1.001	0.091	-35.34	0.14
	H46	4.503	-1.484	-1.815	1.2	1.2	1.001	0.088	-35.27	0.14
	H47	3.527	-3.383	-0.554	1.2	1.2	1.001	0.085	-35.30	0.14
	H48	3.62	-2.465	0.95	1.2	1.2	1.001	0.085	-35.31	0.14
	H49	4.516	0.778	1.537	1.2	1.2	1.001	0.310	-19.94	0.14
	H50	3.44	4.547	-0.327	1.2	1.2	1.001	0.110	-35.38	0.14
	H51	2.025	4.68	-1.423	1.2	1.2	1.001	0.116	-35.46	0.14
	H52	1.803	4.272	0.311	1.2	1.2	1.001	0.108	-35.39	0.14
santonin (**12**)	C1	3.423	-0.388	-0.552	1.85	1.7	1.452	-0.108	-27.12	1.75
	C2	2.859	0.967	-0.431	1.85	1.7	1.452	0.155	-21.53	1.75
	C3	1.43	1.099	0.003	1.85	1.7	1.452	-0.022	-81.13	1.75
	C4	0.716	-0.014	0.296	1.85	1.7	1.452	0.009	-79.63	1.75
	C5	1.302	-1.436	0.281	1.85	1.7	1.452	0.004	-125.08	1.75
	C6	2.714	-1.475	-0.233	1.85	1.7	1.452	-0.057	-25.90	1.75
	C7	-0.753	-0.067	0.637	1.85	1.7	1.452	0.027	-18.28	1.75
	C8	-1.53	-0.894	-0.405	1.85	1.7	1.452	-0.077	-72.48	1.75
	C9	-1.068	-2.345	-0.369	1.85	1.7	1.452	-0.147	-17.70	1.75
	C10	0.448	-2.381	-0.638	1.85	1.7	1.452	-0.142	-15.51	1.75
	O11	-1.474	1.179	0.703	2.024	1.52	1.342	-0.192	1.26	0.7
	C12	-2.784	0.964	0.352	1.85	1.7	1.452	0.262	37.25	1.75
	C13	-2.972	-0.499	-0.074	1.85	1.7	1.452	-0.071	-72.55	1.75
	C14	1.356	-2.015	1.729	1.85	1.7	1.452	-0.222	38.41	1.75
	O15	3.547	1.951	-0.693	2.024	1.52	1.342	-0.340	-2.36	0.7
	C16	0.92	2.523	0.046	1.85	1.7	1.452	-0.238	36.29	1.75
	O17	-3.606	1.84	0.388	2.024	1.52	1.342	-0.334	-2.66	0.7
	C18	-4.02	-0.659	-1.173	1.85	1.7	1.452	-0.224	36.88	1.75
	H19	4.449	-0.445	-0.905	1.2	1.2	1.001	0.108	-35.50	0.14
	H20	3.157	-2.468	-0.314	1.2	1.2	1.001	0.112	-35.43	0.14
	H21	-0.873	-0.544	1.622	1.2	1.2	1.001	0.114	-35.23	0.14
	H22	-1.286	-0.474	-1.393	1.2	1.2	1.001	0.101	-35.23	0.14
	H23	-1.585	-2.945	-1.128	1.2	1.2	1.001	0.096	-35.31	0.14
	H24	-1.307	-2.795	0.604	1.2	1.2	1.001	0.090	-35.28	0.14
	H25	0.623	-2.084	-1.68	1.2	1.2	1.001	0.089	-35.30	0.14

	H26	0.831	-3.404	-0.534	1.2	1.2	1.001	0.094	-35.30	0.14
	H27	-3.299	-1.045	0.827	1.2	1.2	1.001	0.113	-35.19	0.14
	H28	1.916	-1.344	2.388	1.2	1.2	1.001	0.088	-35.35	0.14
	H29	0.362	-2.167	2.159	1.2	1.2	1.001	0.090	-35.37	0.14
	H30	1.862	-2.987	1.722	1.2	1.2	1.001	0.091	-35.33	0.14
	H31	1.775	3.199	0	1.2	1.2	1.001	0.084	-35.42	0.14
	H32	0.274	2.742	-0.812	1.2	1.2	1.001	0.089	-35.32	0.14
	H33	0.336	2.723	0.945	1.2	1.2	1.001	0.088	-35.43	0.14
	H34	-4.967	-0.209	-0.861	1.2	1.2	1.001	0.091	-35.36	0.14
	H35	-3.7	-0.158	-2.094	1.2	1.2	1.001	0.089	-35.32	0.14
	H36	-4.193	-1.716	-1.4	1.2	1.2	1.001	0.089	-35.35	0.14
sesquiterpenoid-13 (**13**)	C1	-3.551	1.209	0.105	1.85	1.7	1.452	-0.152	-17.51	1.75
	C2	-3.55	-0.32	0.036	1.85	1.7	1.452	-0.156	-17.41	1.75
	C3	-2.273	-0.868	-0.626	1.85	1.7	1.452	-0.074	-69.80	1.75
	C4	-0.952	-0.374	0.078	1.85	1.7	1.452	0.002	-123.38	1.75
	C5	-1.024	1.144	0.261	1.85	1.7	1.452	0.028	-80.00	1.75
	C6	-2.298	1.716	0.837	1.85	1.7	1.452	-0.145	-18.37	1.75
	C7	0.252	-0.737	-0.831	1.85	1.7	1.452	-0.149	-17.26	1.75
	C8	1.543	0.002	-0.514	1.85	1.7	1.452	0.062	-74.65	1.75
	C9	1.335	1.505	-0.499	1.85	1.7	1.452	0.164	-20.78	1.75
	C10	0.011	1.958	-0.041	1.85	1.7	1.452	-0.121	-26.71	1.75
	C11	-2.365	-2.395	-0.779	1.85	1.7	1.452	-0.233	37.34	1.75
	C12	2.71	-0.604	0.222	1.85	1.7	1.452	0.079	-74.80	1.75
	O13	2.706	-0.463	-1.21	2.024	1.52	1.342	-0.260	2.69	0.7
	C14	3.712	0.268	0.955	1.85	1.7	1.452	-0.234	36.45	1.75
	C15	2.669	-2.034	0.729	1.85	1.7	1.452	-0.227	36.48	1.75
	O16	2.209	2.305	-0.814	2.024	1.52	1.342	-0.328	-2.39	0.7
	C17	-0.771	-1.024	1.476	1.85	1.7	1.452	-0.230	38.03	1.75
	H18	-4.451	1.576	0.612	1.2	1.2	1.001	0.088	-35.32	0.14
	H19	-3.569	1.623	-0.913	1.2	1.2	1.001	0.084	-35.27	0.14
	H20	-4.419	-0.671	-0.534	1.2	1.2	1.001	0.087	-35.31	0.14
	H21	-3.66	-0.738	1.047	1.2	1.2	1.001	0.083	-35.26	0.14
	H22	-2.239	-0.441	-1.64	1.2	1.2	1.001	0.088	-35.24	0.14
	H23	-2.249	2.81	0.826	1.2	1.2	1.001	0.095	-35.34	0.14
	H24	-2.368	1.418	1.894	1.2	1.2	1.001	0.097	-35.24	0.14
	H25	0.427	-1.814	-0.813	1.2	1.2	1.001	0.098	-35.41	0.14
	H26	-0.003	-0.484	-1.869	1.2	1.2	1.001	0.095	-35.28	0.14
	H27	-0.079	3.035	0.081	1.2	1.2	1.001	0.102	-35.48	0.14
	H28	-2.477	-2.895	0.19	1.2	1.2	1.001	0.081	-35.32	0.14
	H29	-3.243	-2.653	-1.38	1.2	1.2	1.001	0.084	-35.35	0.14
	H30	-1.493	-2.823	-1.282	1.2	1.2	1.001	0.084	-35.36	0.14
	H31	4.703	-0.195	0.893	1.2	1.2	1.001	0.091	-35.33	0.14
	H32	3.768	1.265	0.521	1.2	1.2	1.001	0.090	-35.46	0.14
	H33	3.446	0.347	2.016	1.2	1.2	1.001	0.089	-35.31	0.14

	H34	2.391	-2.064	1.788	1.2	1.2	1.001	0.092	-35.34	0.14
	H35	3.671	-2.47	0.635	1.2	1.2	1.001	0.093	-35.31	0.14
	H36	1.981	-2.665	0.166	1.2	1.2	1.001	0.093	-35.43	0.14
	H37	-0.65	-2.108	1.389	1.2	1.2	1.001	0.088	-35.36	0.14
	H38	0.118	-0.626	1.972	1.2	1.2	1.001	0.084	-35.38	0.14
	H39	-1.626	-0.836	2.131	1.2	1.2	1.001	0.086	-35.37	0.14
artemisinin (**14**)	C1	1.45	-5.6	-1.805	1.85	1.7	1.452	0.121	37.97	1.75
	O2	1.057	-4.218	-1.87	2.024	1.52	1.342	-0.207	0.28	0.7
	C3	1.949	-3.26	-2.196	1.85	1.7	1.452	0.260	36.48	1.75
	C4	2.983	-3.629	-3.244	1.85	1.7	1.452	-0.079	-72.76	1.75
	C5	3.575	-5.035	-3.039	1.85	1.7	1.452	-0.076	-71.77	1.75
	C6	2.427	-6.051	-2.922	1.85	1.7	1.452	0.076	-70.29	1.75
	C7	4.554	-5.137	-1.862	1.85	1.7	1.452	-0.154	-17.91	1.75
	C8	5.099	-6.554	-1.725	1.85	1.7	1.452	-0.156	-17.92	1.75
	C9	3.986	-7.597	-1.562	1.85	1.7	1.452	-0.081	-71.30	1.75
	C10	2.949	-7.501	-2.715	1.85	1.7	1.452	-0.079	-69.64	1.75
	C11	1.811	-8.534	-2.522	1.85	1.7	1.452	-0.158	-16.72	1.75
	C12	0.512	-8.273	-3.299	1.85	1.7	1.452	-0.160	-16.95	1.75
	C13	-0.084	-6.869	-3.059	1.85	1.7	1.452	0.168	-17.40	1.75
	O14	0.266	-6.408	-1.753	2.024	1.52	1.342	-0.235	2.69	0.7
	C15	-1.607	-6.914	-3.14	1.85	1.7	1.452	-0.224	36.83	1.75
	O16	1.833	-2.124	-1.744	2.024	1.52	1.342	-0.340	-2.37	0.7
	C17	4.061	-2.546	-3.35	1.85	1.7	1.452	-0.230	37.09	1.75
	C18	4.617	-8.991	-1.459	1.85	1.7	1.452	-0.233	37.18	1.75
	O19	0.347	-5.93	-4.054	2.024	1.52	1.342	-0.145	1.09	0.7
	O20	1.79	-6.073	-4.224	2.024	1.52	1.342	-0.140	1.09	0.7
	H21	1.917	-5.717	-0.821	1.2	1.2	1.001	0.134	-35.34	0.14
	H22	2.441	-3.616	-4.2	1.2	1.2	1.001	0.115	-35.27	0.14
	H23	4.144	-5.268	-3.953	1.2	1.2	1.001	0.105	-35.22	0.14
	H24	5.404	-4.463	-2.014	1.2	1.2	1.001	0.094	-35.34	0.14
	H25	4.076	-4.831	-0.925	1.2	1.2	1.001	0.090	-35.33	0.14
	H26	5.705	-6.793	-2.608	1.2	1.2	1.001	0.085	-35.30	0.14
	H27	5.774	-6.593	-0.862	1.2	1.2	1.001	0.088	-35.32	0.14
	H28	3.477	-7.4	-0.609	1.2	1.2	1.001	0.090	-35.28	0.14
	H29	3.46	-7.789	-3.647	1.2	1.2	1.001	0.098	-35.23	0.14
	H30	2.178	-9.528	-2.805	1.2	1.2	1.001	0.092	-35.31	0.14
	H31	1.56	-8.604	-1.455	1.2	1.2	1.001	0.084	-35.28	0.14
	H32	-0.202	-9.037	-2.966	1.2	1.2	1.001	0.098	-35.30	0.14
	H33	0.674	-8.443	-4.37	1.2	1.2	1.001	0.096	-35.32	0.14
	H34	-1.943	-7.255	-4.125	1.2	1.2	1.001	0.099	-35.34	0.14
	H35	-2.031	-7.566	-2.369	1.2	1.2	1.001	0.103	-35.34	0.14
	H36	-2.028	-5.914	-2.983	1.2	1.2	1.001	0.095	-35.32	0.14
	H37	3.622	-1.6	-3.687	1.2	1.2	1.001	0.086	-35.33	0.14
	H38	4.54	-2.35	-2.385	1.2	1.2	1.001	0.085	-35.34	0.14
	H39	4.833	-2.829	-4.074	1.2	1.2	1.001	0.086	-35.33	0.14

	H40	5.387	-9.011	-0.68	1.2	1.2	1.001	0.083	-35.33	0.14
	H41	3.873	-9.749	-1.194	1.2	1.2	1.001	0.081	-35.35	0.14
	H42	5.084	-9.286	-2.404	1.2	1.2	1.001	0.082	-35.35	0.14
19-OH-eburnamonine (**15**)	O1	-0.886	-3.193	0.044	2.024	1.52	1.342	-0.333	-2.49	0.7
	C2	-0.339	-2.131	-0.19	1.85	1.7	1.452	0.278	-17.46	1.75
	N3	-1.044	-0.933	-0.276	1.89	1.55	1.397	-0.244	15.76	1.23
	C4	-2.42	-0.698	-0.081	1.85	1.7	1.452	0.085	-80.68	1.75
	C5	-3.462	-1.594	0.149	1.85	1.7	1.452	-0.103	-28.13	1.75
	C6	-4.739	-1.055	0.306	1.85	1.7	1.452	-0.108	-27.78	1.75
	C7	-4.965	0.329	0.236	1.85	1.7	1.452	-0.110	-27.85	1.75
	C8	-3.917	1.217	0.006	1.85	1.7	1.452	-0.103	-27.97	1.75
	C9	-2.623	0.706	-0.156	1.85	1.7	1.452	-0.025	-85.09	1.75
	C10	-0.424	0.308	-0.467	1.85	1.7	1.452	0.082	-79.53	1.75
	C11	-1.33	1.317	-0.401	1.85	1.7	1.452	-0.034	-83.39	1.75
	C12	-0.899	2.753	-0.486	1.85	1.7	1.452	-0.145	-17.80	1.75
	C13	0.621	2.843	-0.814	1.85	1.7	1.452	-0.051	-10.80	1.75
	N14	1.463	1.808	-0.179	1.89	1.55	1.397	-0.338	-31.34	1.23
	C15	1.049	0.468	-0.671	1.85	1.7	1.452	0.023	-66.75	1.75
	C16	1.871	-0.7	-0.061	1.85	1.7	1.452	-0.004	-122.94	1.75
	C17	1.903	-0.562	1.48	1.85	1.7	1.452	-0.153	-16.79	1.75
	C18	2.321	0.84	1.948	1.85	1.7	1.452	-0.157	-17.61	1.75
	C19	1.447	1.913	1.297	1.85	1.7	1.452	-0.060	-11.94	1.75
	C20	3.29	-0.683	-0.729	1.85	1.7	1.452	0.012	-16.21	1.75
	O21	3.965	0.556	-0.565	2.024	1.52	1.342	-0.463	2.69	0.7
	C22	1.16	-2.019	-0.466	1.85	1.7	1.452	-0.139	-16.92	1.75
	H23	1.255	0.47	-1.754	1.2	1.2	1.001	0.114	-35.20	0.14
	C24	4.253	-1.766	-0.249	1.85	1.7	1.452	-0.236	36.87	1.75
	H25	-3.273	-2.657	0.205	1.2	1.2	1.001	0.105	-35.60	0.14
	H26	-5.576	-1.724	0.487	1.2	1.2	1.001	0.101	-35.50	0.14
	H27	-5.973	0.712	0.362	1.2	1.2	1.001	0.100	-35.52	0.14
	H28	-4.099	2.286	-0.048	1.2	1.2	1.001	0.103	-35.51	0.14
	H29	-1.456	3.297	-1.26	1.2	1.2	1.001	0.097	-35.29	0.14
	H30	-1.123	3.266	0.459	1.2	1.2	1.001	0.091	-35.28	0.14
	H31	0.762	2.749	-1.897	1.2	1.2	1.001	0.103	-35.32	0.14
	H32	1.009	3.824	-0.522	1.2	1.2	1.001	0.105	-35.35	0.14
	H33	0.901	-0.78	1.872	1.2	1.2	1.001	0.087	-35.29	0.14
	H34	2.566	-1.322	1.905	1.2	1.2	1.001	0.091	-35.35	0.14
	H35	2.214	0.914	3.036	1.2	1.2	1.001	0.090	-35.33	0.14
	H36	3.37	1.016	1.702	1.2	1.2	1.001	0.086	-35.40	0.14
	H37	0.423	1.831	1.696	1.2	1.2	1.001	0.087	-35.21	0.14
	H38	1.815	2.913	1.551	1.2	1.2	1.001	0.103	-35.34	0.14
	H39	3.104	-0.858	-1.807	1.2	1.2	1.001	0.086	-35.10	0.14
	H40	3.297	1.27	-0.617	1.2	1.2	1.001	0.293	-19.87	0.14
	H41	1.284	-2.185	-1.546	1.2	1.2	1.001	0.112	-35.26	0.14

	H42	1.613	-2.878	0.033	1.2	1.2	1.001	0.110	-35.40	0.14
	H43	3.87	-2.773	-0.434	1.2	1.2	1.001	0.087	-35.38	0.14
	H44	4.472	-1.66	0.817	1.2	1.2	1.001	0.086	-35.37	0.14
	H45	5.196	-1.656	-0.791	1.2	1.2	1.001	0.089	-35.38	0.14
eburnamonine (**16**)	C1	0.096	-2.109	-0.224	1.85	1.7	1.452	0.276	-17.56	1.75
	C2	2.209	-0.733	-0.061	1.85	1.7	1.452	0.084	-80.74	1.75
	C3	0.251	0.328	-0.505	1.85	1.7	1.452	0.082	-79.24	1.75
	C4	2.452	0.664	-0.129	1.85	1.7	1.452	-0.026	-85.14	1.75
	C5	4.507	-1.153	0.394	1.85	1.7	1.452	-0.110	-27.75	1.75
	C6	4.771	0.225	0.331	1.85	1.7	1.452	-0.112	-27.85	1.75
	C7	3.754	1.14	0.071	1.85	1.7	1.452	-0.105	-27.97	1.75
	C8	3.22	-1.656	0.199	1.85	1.7	1.452	-0.104	-28.11	1.75
	C9	1.184	1.31	-0.41	1.85	1.7	1.452	-0.036	-83.40	1.75
	C10	-1.214	0.534	-0.746	1.85	1.7	1.452	0.023	-67.18	1.75
	C11	-0.711	2.886	-0.876	1.85	1.7	1.452	-0.054	-11.14	1.75
	C12	-1.646	1.994	1.196	1.85	1.7	1.452	-0.061	-12.63	1.75
	C13	-1.388	-1.953	-0.548	1.85	1.7	1.452	-0.141	-17.02	1.75
	C14	-2.07	-0.617	-0.153	1.85	1.7	1.452	0.000	-123.82	1.75
	C15	-3.482	-0.548	-0.795	1.85	1.7	1.452	-0.153	-16.70	1.75
	C16	-2.121	-0.469	1.386	1.85	1.7	1.452	-0.154	-16.93	1.75
	C17	-2.566	0.937	1.806	1.85	1.7	1.452	-0.153	-17.77	1.75
	C18	0.798	2.758	-0.506	1.85	1.7	1.452	-0.147	-17.73	1.75
	C19	-4.537	-1.516	-0.248	1.85	1.7	1.452	-0.235	37.14	1.75
	N20	-1.597	1.88	-0.269	1.89	1.55	1.397	-0.358	-31.78	1.23
	N21	0.834	-0.931	-0.297	1.89	1.55	1.397	-0.245	15.79	1.23
	O22	0.608	-3.185	0.032	2.024	1.52	1.342	-0.336	-2.48	0.7
	H23	5.319	-1.844	0.599	1.2	1.2	1.001	0.100	-35.51	0.14
	H24	5.785	0.581	0.487	1.2	1.2	1.001	0.099	-35.51	0.14
	H25	3.966	2.204	0.023	1.2	1.2	1.001	0.103	-35.51	0.14
	H26	3.001	-2.715	0.25	1.2	1.2	1.001	0.104	-35.57	0.14
	H27	-1.396	0.535	-1.833	1.2	1.2	1.001	0.110	-35.21	0.14
	H28	-1.078	3.88	-0.598	1.2	1.2	1.001	0.101	-35.34	0.14
	H29	-0.819	2.796	-1.964	1.2	1.2	1.001	0.099	-35.31	0.14
	H30	-2.012	3.001	1.431	1.2	1.2	1.001	0.099	-35.31	0.14
	H31	-0.648	1.897	1.66	1.2	1.2	1.001	0.082	-35.16	0.14
	H32	-1.48	-2.097	-1.634	1.2	1.2	1.001	0.110	-35.26	0.14
	H33	-1.885	-2.806	-0.08	1.2	1.2	1.001	0.107	-35.39	0.14
	H34	-3.363	-0.727	-1.872	1.2	1.2	1.001	0.084	-35.28	0.14
	H35	-3.849	0.48	-0.708	1.2	1.2	1.001	0.084	-35.34	0.14
	H36	-2.779	-1.233	1.813	1.2	1.2	1.001	0.089	-35.34	0.14
	H37	-1.123	-0.66	1.802	1.2	1.2	1.001	0.086	-35.29	0.14
	H38	-2.541	1.027	2.898	1.2	1.2	1.001	0.090	-35.33	0.14
	H39	-3.6	1.123	1.494	1.2	1.2	1.001	0.087	-35.33	0.14
	H40	1.008	3.263	0.447	1.2	1.2	1.001	0.089	-35.27	0.14
	H41	1.393	3.287	-1.261	1.2	1.2	1.001	0.094	-35.30	0.14

H42	-5.461	-1.431	-0.829	1.2	1.2	1.001	0.083	-35.35	0.14
H43	-4.791	-1.303	0.795	1.2	1.2	1.001	0.081	-35.35	0.14
H44	-4.213	-2.56	-0.305	1.2	1.2	1.001	0.081	-35.35	0.14

Table S2. Solute parameters for the five compounds measured in poly-HEMA/DMSO

		X	Y	Z	Coulomb *R* (Å)	Bondi *R* (Å)	Grimme D2 *R* (Å)	CM5 *pQ* ([e])	γ (cal mol^{-1} Å^{-2})	C_6^m (J nm^6 mol^{-1})
estrone (**2**)	C1	-0.369	-1.771	-0.084	1.85	1.7	1.452	-0.153	5.17	1.75
	C2	0.279	-0.436	-0.526	1.85	1.7	1.452	-0.073	-48.12	1.75
	C3	-0.465	0.795	0.06	1.85	1.7	1.452	-0.079	-48.93	1.75
	C4	-1.945	0.683	-0.309	1.85	1.7	1.452	-0.076	-48.64	1.75
	C5	-2.596	-0.607	0.251	1.85	1.7	1.452	-0.015	-101.74	1.75
	C6	-1.89	-1.83	-0.345	1.85	1.7	1.452	-0.152	4.47	1.75
	C7	1.787	-0.36	-0.267	1.85	1.7	1.452	-0.034	-59.22	1.75
	C8	2.421	0.874	-0.004	1.85	1.7	1.452	-0.018	-59.89	1.75
	C9	1.636	2.17	0.114	1.85	1.7	1.452	-0.148	3.27	1.75
	C10	0.212	2.077	-0.437	1.85	1.7	1.452	-0.153	3.82	1.75
	C11	2.595	-1.503	-0.34	1.85	1.7	1.452	-0.108	-6.17	1.75
	C12	3.974	-1.454	-0.153	1.85	1.7	1.452	-0.133	-6.33	1.75
	C13	4.587	-0.227	0.111	1.85	1.7	1.452	0.068	-6.28	1.75
	C14	3.805	0.925	0.181	1.85	1.7	1.452	-0.128	-6.26	1.75
	C15	-2.952	1.799	0.038	1.85	1.7	1.452	-0.155	5.00	1.75
	C16	-4.316	1.123	-0.234	1.85	1.7	1.452	-0.153	4.96	1.75
	C17	-4.058	-0.395	-0.156	1.85	1.7	1.452	0.190	4.34	1.75
	O18	-4.876	-1.261	-0.381	2.024	1.52	1.342	-0.334	-77.47	0.7
	C19	-2.616	-0.685	1.801	1.85	1.7	1.452	-0.227	58.47	1.75
	H20	-0.368	0.773	1.156	1.2	1.2	1.001	0.090	-34.54	0.14
	H21	0.137	-0.372	-1.619	1.2	1.2	1.001	0.089	-34.47	0.14
	H22	-1.983	0.58	-1.408	1.2	1.2	1.001	0.091	-34.46	0.14
	O23	5.935	-0.094	0.305	2.024	1.52	1.342	-0.400	-67.81	0.7
	H24	-3.103	0.182	2.259	1.2	1.2	1.001	0.089	-34.64	0.14
	H25	-3.172	-1.576	2.107	1.2	1.2	1.001	0.086	-34.66	0.14
	H26	-1.61	-0.755	2.221	1.2	1.2	1.001	0.091	-34.68	0.14
	H27	-0.158	-1.939	0.979	1.2	1.2	1.001	0.082	-34.61	0.14
	H28	0.096	-2.606	-0.617	1.2	1.2	1.001	0.089	-34.65	0.14
	H29	-2.074	-1.854	-1.427	1.2	1.2	1.001	0.084	-34.59	0.14
	H30	-2.309	-2.758	0.059	1.2	1.2	1.001	0.085	-34.63	0.14
	H31	2.188	2.978	-0.382	1.2	1.2	1.001	0.092	-34.60	0.14
	H32	1.588	2.452	1.176	1.2	1.2	1.001	0.090	-34.55	0.14
	H33	0.229	2.075	-1.536	1.2	1.2	1.001	0.083	-34.56	0.14
	H34	-0.357	2.963	-0.133	1.2	1.2	1.001	0.088	-34.62	0.14
	H35	-2.807	2.698	-0.567	1.2	1.2	1.001	0.088	-34.67	0.14
	H36	-2.862	2.1	1.088	1.2	1.2	1.001	0.087	-34.62	0.14
	H37	-4.689	1.344	-1.241	1.2	1.2	1.001	0.103	-34.61	0.14
	H38	-5.113	1.408	0.46	1.2	1.2	1.001	0.102	-34.65	0.14
	H39	2.146	-2.468	-0.551	1.2	1.2	1.001	0.103	-34.82	0.14
	H40	4.568	-2.363	-0.216	1.2	1.2	1.001	0.107	-34.77	0.14
	H41	4.297	1.873	0.383	1.2	1.2	1.001	0.104	-34.78	0.14

	H42	6.35	-0.963	0.224	1.2	1.2	1.001	0.358	-19.57	0.14
retrorsine (**3**)	C1	-2.234	-0.125	-1.162	1.85	1.7	1.452	0.026	4.59	1.75
	C2	-3.684	0.344	-0.978	1.85	1.7	1.452	-0.152	4.17	1.75
	C3	-4.12	-0.378	0.305	1.85	1.7	1.452	-0.060	-0.25	1.75
	N4	-3.438	-1.675	0.239	1.89	1.55	1.397	-0.368	46.22	1.23
	C5	-2.344	-1.613	-0.762	1.85	1.7	1.452	0.019	-52.94	1.75
	C6	-2.928	-2.238	1.494	1.85	1.7	1.452	-0.052	-1.63	1.75
	C7	-1.53	-2.672	1.155	1.85	1.7	1.452	-0.081	-4.20	1.75
	C8	-1.188	-2.321	-0.088	1.85	1.7	1.452	-0.023	-58.90	1.75
	O9	-1.345	0.537	-0.228	2.024	1.52	1.342	-0.190	-68.74	0.7
	C10	-1.05	1.841	-0.478	1.85	1.7	1.452	0.261	56.15	1.75
	C11	-0.062	2.37	0.516	1.85	1.7	1.452	-0.030	-58.58	1.75
	O12	-1.534	2.463	-1.405	2.024	1.52	1.342	-0.329	-77.34	0.7
	C13	-0.142	3.636	0.965	1.85	1.7	1.452	-0.068	-4.08	1.75
	C14	-1.146	4.696	0.626	1.85	1.7	1.452	-0.229	56.18	1.75
	C15	1.03	1.418	0.955	1.85	1.7	1.452	-0.155	4.20	1.75
	C16	2.024	1.102	-0.2	1.85	1.7	1.452	-0.078	-47.62	1.75
	C17	0.089	-2.691	-0.775	1.85	1.7	1.452	-0.034	56.09	1.75
	O18	1.043	-1.586	-0.853	2.024	1.52	1.342	-0.187	-71.04	0.7
	C19	1.797	-1.384	0.232	1.85	1.7	1.452	0.263	57.81	1.75
	C20	2.79	-0.222	0.066	1.85	1.7	1.452	0.077	-48.17	1.75
	O21	1.727	-2.032	1.261	2.024	1.52	1.342	-0.318	-77.30	0.7
	C22	2.973	2.288	-0.426	1.85	1.7	1.452	-0.236	57.73	1.75
	O23	3.544	-0.145	1.273	2.024	1.52	1.342	-0.432	-63.42	0.7
	C24	3.785	-0.595	-1.052	1.85	1.7	1.452	-0.063	58.03	1.75
	O25	4.413	-1.829	-0.754	2.024	1.52	1.342	-0.462	-63.43	0.7
	H26	-2.628	-2.153	-1.683	1.2	1.2	1.001	0.102	-34.46	0.14
	H27	-1.92	4.342	-0.052	1.2	1.2	1.001	0.087	-34.76	0.14
	H28	-1.607	5.086	1.542	1.2	1.2	1.001	0.093	-34.60	0.14
	H29	-0.644	5.546	0.147	1.2	1.2	1.001	0.096	-34.60	0.14
	H30	3.684	2.37	0.401	1.2	1.2	1.001	0.083	-34.66	0.14
	H31	3.538	2.197	-1.358	1.2	1.2	1.001	0.087	-34.66	0.14
	H32	2.401	3.219	-0.483	1.2	1.2	1.001	0.081	-34.65	0.14
	H33	-4.271	-0.008	-1.833	1.2	1.2	1.001	0.101	-34.63	0.14
	H34	-3.772	1.429	-0.932	1.2	1.2	1.001	0.096	-34.74	0.14
	H35	-5.209	-0.495	0.364	1.2	1.2	1.001	0.092	-34.60	0.14
	H36	-3.803	0.197	1.192	1.2	1.2	1.001	0.087	-34.48	0.14
	H37	-3.54	-3.083	1.848	1.2	1.2	1.001	0.093	-34.51	0.14
	H38	-2.928	-1.494	2.31	1.2	1.2	1.001	0.098	-34.47	0.14
	H39	0.569	0.497	1.322	1.2	1.2	1.001	0.088	-34.67	0.14
	H40	1.586	1.851	1.792	1.2	1.2	1.001	0.096	-34.65	0.14
	H41	-0.082	-2.955	-1.822	1.2	1.2	1.001	0.123	-34.67	0.14
	H42	0.576	-3.523	-0.264	1.2	1.2	1.001	0.117	-34.71	0.14
	H43	4.521	0.212	-1.154	1.2	1.2	1.001	0.102	-34.60	0.14
	H44	3.263	-0.716	-2.005	1.2	1.2	1.001	0.110	-34.67	0.14

	H45	-1.853	0.035	-2.173	1.2	1.2	1.001	0.113	-34.69	0.14
	H46	1.442	0.937	-1.115	1.2	1.2	1.001	0.095	-34.60	0.14
	H47	-0.89	-3.211	1.846	1.2	1.2	1.001	0.111	-34.81	0.14
	H48	0.614	3.934	1.692	1.2	1.2	1.001	0.106	-34.72	0.14
	H49	3.113	-0.766	1.888	1.2	1.2	1.001	0.321	-19.50	0.14
	H50	4.758	-1.72	0.146	1.2	1.2	1.001	0.324	-19.54	0.14
aquatolide (**4**)	C1	-1.65	-0.308	-1.242	1.85	1.7	1.452	0.028	6.96	1.75
	C2	-1.996	-1.149	0.044	1.85	1.7	1.452	-0.007	-99.93	1.75
	C3	-0.724	-0.722	0.823	1.85	1.7	1.452	-0.058	-46.79	1.75
	C4	-0.45	0.774	0.303	1.85	1.7	1.452	-0.006	-98.92	1.75
	O5	-2.279	0.994	-1.123	2.024	1.52	1.342	-0.209	-67.98	0.7
	C6	-1.65	1.626	-0.087	1.85	1.7	1.452	0.252	57.16	1.75
	O7	-2.002	2.695	0.346	2.024	1.52	1.342	-0.338	-77.66	0.7
	C8	0.429	-1.145	-0.141	1.85	1.7	1.452	-0.077	-48.26	1.75
	C9	-0.139	-0.014	-1.013	1.85	1.7	1.452	-0.077	-49.79	1.75
	C10	0.625	1.553	1.06	1.85	1.7	1.452	-0.150	3.75	1.75
	C11	1.718	2.165	0.177	1.85	1.7	1.452	-0.144	2.88	1.75
	C12	1.857	-1.02	0.399	1.85	1.7	1.452	0.190	2.90	1.75
	C13	2.866	-0.112	-0.26	1.85	1.7	1.452	-0.032	-58.17	1.75
	C14	2.764	1.224	-0.364	1.85	1.7	1.452	-0.088	-3.79	1.75
	O15	2.213	-1.796	1.273	2.024	1.52	1.342	-0.323	-77.18	0.7
	C16	4.099	-0.853	-0.732	1.85	1.7	1.452	-0.226	56.80	1.75
	H17	0.381	-2.167	-0.527	1.2	1.2	1.001	0.110	-34.66	0.14
	H18	0.406	0.434	-1.845	1.2	1.2	1.001	0.101	-34.71	0.14
	H19	-1.957	-0.734	-2.197	1.2	1.2	1.001	0.123	-34.73	0.14
	C20	-2.098	-2.655	-0.265	1.85	1.7	1.452	-0.228	57.96	1.75
	C21	-3.293	-0.729	0.758	1.85	1.7	1.452	-0.234	57.88	1.75
	H22	-0.674	-0.945	1.891	1.2	1.2	1.001	0.104	-34.69	0.14
	H23	3.853	-1.602	-1.495	1.2	1.2	1.001	0.089	-34.60	0.14
	H24	4.549	-1.392	0.108	1.2	1.2	1.001	0.089	-34.64	0.14
	H25	4.838	-0.166	-1.152	1.2	1.2	1.001	0.093	-34.68	0.14
	H26	-1.999	-3.248	0.651	1.2	1.2	1.001	0.088	-34.63	0.14
	H27	-1.348	-3.011	-0.975	1.2	1.2	1.001	0.090	-34.68	0.14
	H28	-3.078	-2.875	-0.699	1.2	1.2	1.001	0.089	-34.65	0.14
	H29	-3.485	-1.421	1.585	1.2	1.2	1.001	0.088	-34.63	0.14
	H30	-4.149	-0.772	0.078	1.2	1.2	1.001	0.087	-34.65	0.14
	H31	-3.255	0.279	1.177	1.2	1.2	1.001	0.084	-34.69	0.14
	H32	0.106	2.358	1.591	1.2	1.2	1.001	0.095	-34.63	0.14
	H33	1.09	0.927	1.829	1.2	1.2	1.001	0.094	-34.63	0.14
	H34	1.26	2.72	-0.656	1.2	1.2	1.001	0.098	-34.53	0.14
	H35	2.25	2.931	0.758	1.2	1.2	1.001	0.100	-34.57	0.14
	H36	3.598	1.734	-0.849	1.2	1.2	1.001	0.102	-34.71	0.14
menthol (**8**)	C1	1.607	1.036	-0.141	1.85	1.7	1.452	-0.161	4.28	1.75
	C2	0.112	1.146	0.191	1.85	1.7	1.452	0.006	4.59	1.75
	C3	-0.68	-0.065	-0.349	1.85	1.7	1.452	-0.084	-47.84	1.75

	C4	-0.047	-1.372	0.171	1.85	1.7	1.452	-0.156	4.52	1.75
	C5	1.446	-1.474	-0.174	1.85	1.7	1.452	-0.157	4.28	1.75
	C6	2.242	-0.272	0.359	1.85	1.7	1.452	-0.081	-49.30	1.75
	C7	3.728	-0.357	-0.006	1.85	1.7	1.452	-0.235	57.60	1.75
	O8	-0.418	2.392	-0.268	2.024	1.52	1.342	-0.456	-63.42	0.7
	C9	-2.208	0.056	-0.1	1.85	1.7	1.452	-0.084	-48.44	1.75
	C10	-3.008	-0.921	-0.975	1.85	1.7	1.452	-0.238	57.76	1.75
	C11	-2.613	-0.086	1.376	1.85	1.7	1.452	-0.238	57.80	1.75
	H12	3.865	-0.352	-1.094	1.2	1.2	1.001	0.078	-34.61	0.14
	H13	4.289	0.49	0.403	1.2	1.2	1.001	0.080	-34.63	0.14
	H14	4.18	-1.277	0.381	1.2	1.2	1.001	0.080	-34.63	0.14
	H15	-2.814	-1.966	-0.704	1.2	1.2	1.001	0.078	-34.60	0.14
	H16	-4.084	-0.752	-0.862	1.2	1.2	1.001	0.078	-34.64	0.14
	H17	-2.762	-0.803	-2.037	1.2	1.2	1.001	0.078	-34.61	0.14
	H18	-2.076	0.618	2.019	1.2	1.2	1.001	0.080	-34.65	0.14
	H19	-3.682	0.116	1.496	1.2	1.2	1.001	0.079	-34.65	0.14
	H20	-2.428	-1.097	1.754	1.2	1.2	1.001	0.078	-34.64	0.14
	H21	2.126	1.906	0.277	1.2	1.2	1.001	0.083	-34.62	0.14
	H22	1.726	1.094	-1.235	1.2	1.2	1.001	0.084	-34.51	0.14
	H23	-0.582	-2.238	-0.236	1.2	1.2	1.001	0.084	-34.61	0.14
	H24	-0.161	-1.426	1.262	1.2	1.2	1.001	0.083	-34.58	0.14
	H25	1.567	-1.527	-1.267	1.2	1.2	1.001	0.079	-34.53	0.14
	H26	1.861	-2.407	0.228	1.2	1.2	1.001	0.082	-34.59	0.14
	H27	-0.001	1.19	1.281	1.2	1.2	1.001	0.101	-34.61	0.14
	H28	-0.541	-0.054	-1.445	1.2	1.2	1.001	0.086	-34.46	0.14
	H29	2.162	-0.282	1.458	1.2	1.2	1.001	0.085	-34.51	0.14
	H30	-2.474	1.074	-0.412	1.2	1.2	1.001	0.080	-34.59	0.14
	H31	-0.305	2.414	-1.229	1.2	1.2	1.001	0.328	-19.55	0.14
cryptospirolepine (**17**)	C1	-5.222	1.325	-0.959	1.85	1.7	1.452	-0.110	-6.06	1.75
	C2	-3.851	1.005	-0.912	1.85	1.7	1.452	-0.039	-61.83	1.75
	C3	-2.911	2.001	-1.319	1.85	1.7	1.452	0.084	-69.58	1.75
	C4	-3.309	3.261	-1.779	1.85	1.7	1.452	-0.113	-6.39	1.75
	C5	-4.669	3.534	-1.828	1.85	1.7	1.452	-0.118	-6.09	1.75
	C6	-5.616	2.576	-1.416	1.85	1.7	1.452	-0.128	-6.06	1.75
	C7	-3.064	-0.133	-0.493	1.85	1.7	1.452	0.067	-68.47	1.75
	C8	-1.742	0.21	-0.626	1.85	1.7	1.452	0.071	-67.42	1.75
	N9	-1.646	1.49	-1.148	1.89	1.55	1.397	-0.406	46.22	1.23
	N10	-3.457	-1.37	0.019	1.89	1.55	1.397	-0.287	46.22	1.23
	C11	-2.479	-2.174	0.603	1.85	1.7	1.452	0.098	-68.19	1.75
	C12	-1.098	-1.857	0.508	1.85	1.7	1.452	-0.027	-58.93	1.75
	C13	-0.582	-0.679	-0.33	1.85	1.7	1.452	0.113	-104.95	1.75
	C14	-2.855	-3.318	1.339	1.85	1.7	1.452	-0.116	-5.98	1.75
	C15	-1.905	-4.128	1.947	1.85	1.7	1.452	-0.106	-6.47	1.75
	C16	-0.547	-3.817	1.855	1.85	1.7	1.452	-0.125	-6.40	1.75

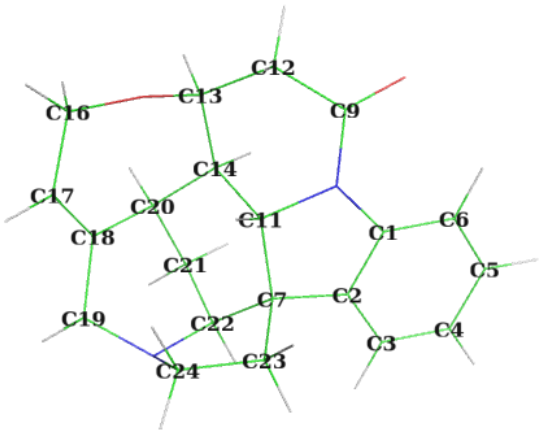
C17	-0.166	-2.687	1.139	1.85	1.7	1.452	-0.104	-6.32	1.75
C18	-0.015	-1.265	-1.699	1.85	1.7	1.452	0.137	3.27	1.75
C19	1.388	-1.164	-2.017	1.85	1.7	1.452	-0.160	-5.28	1.75
C20	2.28	-0.503	-1.202	1.85	1.7	1.452	0.003	-62.63	1.75
C21	1.796	0.118	-0.023	1.85	1.7	1.452	0.080	-69.98	1.75
N22	0.478	0.075	0.388	1.89	1.55	1.397	-0.252	46.22	1.23
C23	3.723	-0.36	-1.383	1.85	1.7	1.452	-0.022	-61.14	1.75
C24	4.504	0.403	-0.457	1.85	1.7	1.452	0.108	-67.73	1.75
N25	3.913	1.046	0.63	1.89	1.55	1.397	-0.251	46.22	1.23
C26	2.563	0.842	0.875	1.85	1.7	1.452	0.097	-68.71	1.75
C27	4.383	-0.973	-2.467	1.85	1.7	1.452	-0.090	-6.23	1.75
C28	5.748	-0.861	-2.657	1.85	1.7	1.452	-0.108	-6.51	1.75
C29	6.507	-0.125	-1.738	1.85	1.7	1.452	-0.090	-6.44	1.75
C30	5.9	0.492	-0.657	1.85	1.7	1.452	-0.104	-6.04	1.75
C31	-4.782	-1.901	-0.263	1.85	1.7	1.452	-0.110	52.38	1.75
C32	4.673	1.996	1.433	1.85	1.7	1.452	-0.102	52.58	1.75
C33	0.39	0.751	1.596	1.85	1.7	1.452	0.096	-68.58	1.75
C34	1.687	1.25	1.947	1.85	1.7	1.452	-0.030	-61.70	1.75
C35	1.836	1.933	3.172	1.85	1.7	1.452	-0.098	-6.07	1.75
C36	0.729	2.128	3.984	1.85	1.7	1.452	-0.117	-6.15	1.75
C37	-0.54	1.649	3.606	1.85	1.7	1.452	-0.101	-6.12	1.75
C38	-0.724	0.953	2.42	1.85	1.7	1.452	-0.110	-6.38	1.75
O39	-0.837	-1.811	-2.427	2.294	1.52	1.342	-0.366	-77.03	0.7
H40	-5.202	-1.374	-1.119	1.2	1.2	1.001	0.113	-34.74	0.14
H41	-4.713	-2.96	-0.53	1.2	1.2	1.001	0.108	-34.65	0.14
H42	-5.472	-1.801	0.587	1.2	1.2	1.001	0.101	-34.56	0.14
H43	5.324	2.593	0.79	1.2	1.2	1.001	0.118	-34.68	0.14
H44	3.982	2.679	1.921	1.2	1.2	1.001	0.119	-34.78	0.14
H45	5.287	1.501	2.195	1.2	1.2	1.001	0.113	-34.61	0.14
H46	-5.973	0.615	-0.631	1.2	1.2	1.001	0.105	-34.83	0.14
H47	-2.575	4	-2.085	1.2	1.2	1.001	0.111	-34.81	0.14
H48	-5.007	4.503	-2.184	1.2	1.2	1.001	0.101	-34.80	0.14
H49	-6.673	2.822	-1.452	1.2	1.2	1.001	0.098	-34.80	0.14
H50	-3.905	-3.557	1.454	1.2	1.2	1.001	0.108	-34.85	0.14
H51	-2.231	-4.999	2.508	1.2	1.2	1.001	0.106	-34.80	0.14
H52	0.201	-4.443	2.331	1.2	1.2	1.001	0.101	-34.81	0.14
H53	0.888	-2.437	1.058	1.2	1.2	1.001	0.103	-34.80	0.14
H54	1.685	-1.643	-2.943	1.2	1.2	1.001	0.099	-34.84	0.14
H55	3.793	-1.555	-3.167	1.2	1.2	1.001	0.112	-34.82	0.14
H56	6.225	-1.347	-3.502	1.2	1.2	1.001	0.109	-34.81	0.14
H57	7.583	-0.042	-1.86	1.2	1.2	1.001	0.113	-34.80	0.14
H58	6.517	1.028	0.053	1.2	1.2	1.001	0.115	-34.86	0.14
H59	2.804	2.287	3.505	1.2	1.2	1.001	0.111	-34.85	0.14
H60	0.845	2.652	4.928	1.2	1.2	1.001	0.104	-34.80	0.14
H61	-1.391	1.816	4.26	1.2	1.2	1.001	0.107	-34.80	0.14

H62	-1.697	0.571	2.139	1.2	1.2	1.001	0.104	-34.86	0.14
H63	-0.785	1.999	-1.263	1.2	1.2	1.001	0.356	0.00	0.14

Experimental vs Predicted RDC/RCSA Values

Table S3. strychnine (**1**) in PMMA/chloroform[1]

strychnine (**1**)

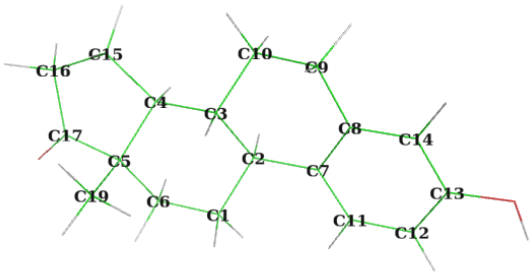


	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C6	-17.7	-12.5	-15.7	-15.3	-17.9
C3	-17.3	-12.4	-15.5	-15.1	-17.6
C13	17.5	18.8	18.5	18.8	16.7
C14	5.2	2.4	3.2	8.0	3.9
C11	9.0	9.2	11.9	15.6	6.0
C17	0.5	-2.6	-3.1	1.8	0.7
C20	15.3	17.5	17.7	16.5	17.2
C22	-10.6	-12.4	-11.9	-14.5	-12.6
C4	-10.4	-13.9	-13.0	-15.9	-11.1
C5	-8.3	-16.4	-16.6	-16.4	-5.0
C19*	5.1	8.5	9.8	12.2	4.7
C21*	-3.3	-2.1	-2.2	-0.6	-1.8
C12*	2.7	7.1	6.5	9.1	2.0
C16*	7.6	9.1	10.7	11.7	7.6
C24*	-5.7	-5.0	-6.3	-5.7	-6.5
C23*	-4.3	-0.1	0.4	-1.6	-3.7
	RCSA (Hz @ 150 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C3	10.5	10.3	11.4	11.7	9.6
C4	9.2	10.5	10.7	11.7	8.4
C6	9.1	9.9	10.8	11.3	8.7
C1	6.6	7.8	7.9	8.8	6.2
C2	7.7	9.2	9.7	10.0	6.5
C7	-0.1	-0.7	-0.8	-0.7	-0.2
C22	0.2	-0.5	-0.4	-0.1	-0.2
C9	6.2	6.5	7.0	8.2	4.8
C12	-1.0	-2.0	-1.9	-2.2	-0.9
C14	0.2	0.1	0.1	0.3	0.3
C20	0.4	0.7	0.8	0.9	0.6
C11	-1.8	-2.1	-2.4	-2.5	-1.8
C23	1.4	0.9	0.9	1.3	1.1
C24	2.8	3.1	3.5	3.7	2.6
C17	3.2	2.8	3.7	1.9	3.1
C16	-0.5	-1.6	-1.7	-2.1	-0.3
C18	5.5	5.2	6.4	4.9	5.7
C5	8.9	11.5	12.0	12.4	7.5
C19	0.0	-0.8	-0.8	-1.1	-0.1
C21	-1.1	-1.2	-1.3	-1.3	-1.1

* methylene RDC is reported as the average of the two $^{1}D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Table S4. estrone (2) in PMMA/chloroform[2]

estrone (**2**)



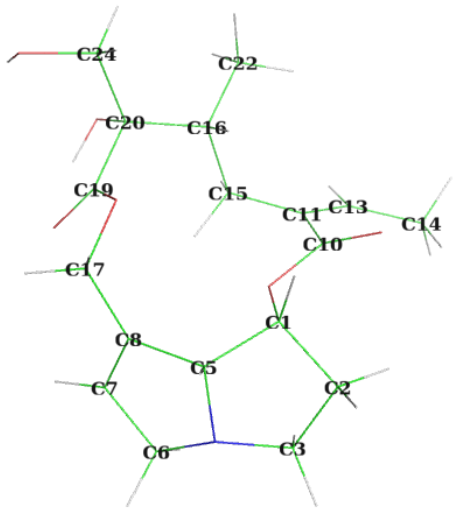
	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C11	-16.2	-8.4	-14.8	-7.0	-11.9
C12	-6.7	-9.7	-6.2	-10.2	-4.0
C14	-16.3	-8.6	-14.7	-7.2	-12.2
C2	12.0	19.8	15.2	19.5	17.9
C3	13.5	20.6	15.5	20.1	18.1
C4	14.0	20.2	14.7	19.8	17.5
C19	-3.8	-6.3	-4.8	-6.0	-5.1
C9*	2.2	9.6	4.7	8.8	3.2
C16*	10.0	8.8	9.7	8.0	8.8
C1*	3.8	8.4	6.1	8.0	8.9
C15*	4.1	11.0	5.6	10.4	6.7
C10*	3.6	7.2	5.5	6.5	7.4
C6*	0.9	8.9	4.0	8.5	4.0
	RCSA (Hz @ 150 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C17	4.7	6.6	5.2	6.1	4.4
C13	1.1	6.9	4.3	6.3	4.5
C8	6.0	8.1	6.3	7.7	5.6
C7	5.3	8.2	5.7	7.6	5.6
C11	7.7	7.1	6.9	6.5	6.0
C14	4.4	5.3	5.3	4.9	4.7
C12	3.1	5.3	3.9	5.1	3.3
C4	-1.3	-1.1	-0.7	-1.0	-0.8
C5	0.0	-0.4	0.2	-0.4	0.0
C3	-0.5	-0.1	0.0	-0.1	0.1
C16	-1.6	-1.2	-1.2	-1.1	-1.0
C6	-0.8	0.0	-0.1	-0.1	0.0
C9	-0.4	-1.0	-0.5	-1.0	-0.5
C10	-0.7	0.0	-0.3	0.0	-0.4
C1	-0.7	-0.5	-0.4	-0.5	-0.6
C15	-0.5	-1.0	-0.4	-0.9	-0.5
C19	0.1	1.1	0.6	1.0	0.5
C2	-0.1	0.3	0.4	0.2	0.4

* methylene RDC is reported as the average of the two $^1D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Note that a mixed solvent system of 95% $CDCl_3$ and 5% DMSO-d_6 (v/v) was used to prevent self-association of estrone.

Table S5. retrorsine (**3**) in PMMA/chloroform[2]

retrorsine (**3**)



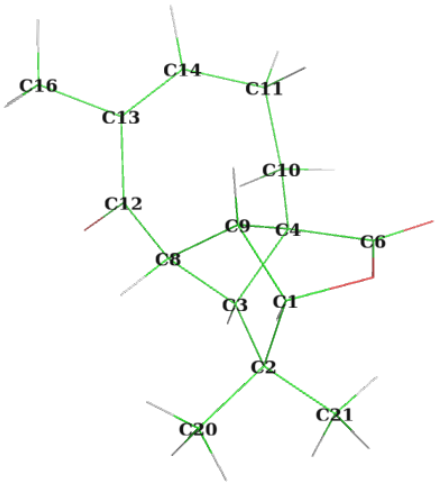
	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C13	-0.2	13.0	0.6	13.9	10.3
C5	26.2	37.3	31.1	37.5	34.0
C1	46.5	49.8	45.2	49.5	49.4
C16	16.2	36.4	26.3	37.7	34.1
C14	8.9	9.5	5.1	8.8	8.0
C22	6.2	6.1	8.9	7.2	7.5
C24*	2.6	9.9	-0.4	8.8	6.3
C6*	7.9	4.2	1.2	2.3	1.1
C17*	16.0	23.2	25.6	24.1	23.2
C3*	-7.1	-2.1	-8.5	-1.7	-2.7
C15*	5.5	8.2	0.1	6.3	4.0
C2*	0.5	1.5	1.8	1.0	-0.8
	RCSA (Hz @ 125 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C19	1.7	-2.8	1.2	-2.5	-1.5
C10	2.9	3.0	5.0	3.8	4.5
C7	7.9	6.9	4.4	6.0	5.0
C13	7.7	3.1	3.5	2.5	3.0
C11	6.2	3.3	3.2	2.6	2.9
C8	7.0	5.6	2.9	4.5	3.6
C20	-1.2	-1.2	-0.9	-1.0	-1.0
C5	-2.3	-2.8	-2.3	-2.7	-2.3
C1	-2.6	-2.2	-2.5	-2.2	-2.3
C24	-1.2	-2.5	-1.0	-2.4	-2.1
C6	1.5	2.1	2.5	2.3	2.3
C17	-2.2	-3.9	-4.6	-4.2	-4.2
C3	-1.8	-2.8	-0.7	-2.7	-2.4
C15	-1.3	-1.7	-1.2	-1.5	-1.4
C16	-1.5	-1.7	-0.9	-1.5	-1.4
C2	-1.8	-1.8	-1.1	-1.7	-1.4
C14	-0.9	-1.4	-0.8	-1.3	-1.0
C22	0.5	-0.3	-0.8	-0.4	-0.4

* methylene RDC is reported as the average of the two $^1D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Note that a mixed solvent system of 95% $CDCl_3$ and 5% DMSO-d_6 (v/v) was used to prevent self-association of retrorsine.

Table S6. aquatolide (**4**) in PMMA/chloroform[2]

aquatolide (**4**)



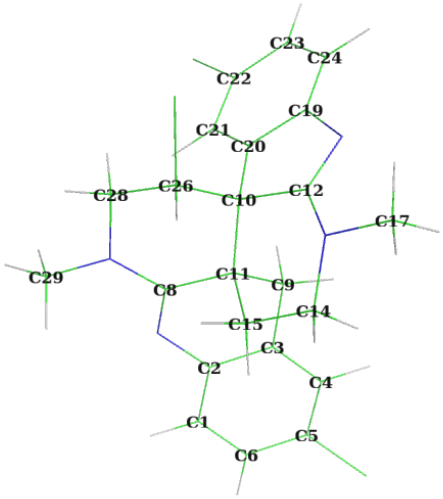
	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C14	-8.3	-7.1	-8.0	-6.1	-7.3
C1	11.0	9.6	8.8	9.1	8.2
C9	0.7	1.0	0.7	2.7	1.2
C8	-0.8	-1.8	0.6	-2.9	-2.5
C3	10.7	12.2	11.3	13.2	12.0
C35	-1.2	0.6	0.1	-0.9	-1.7
C11[#]	5.2	8.3	7.3	8.1	8.3
C11[#]	0.1	2.0	1.6	1.8	1.3
C20	1.2	0.8	0.1	1.2	1.1
C21	0.9	2.0	1.8	1.6	1.3
C10[*]	3.8	2.2	3.4	2.3	3.2
C11[*]	2.5	4.4	3.7	3.6	3.3
	RCSA (Hz @ 150 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C12	2.1	1.1	2.1	1.2	1.5
C6	-1.3	-1.5	-0.8	-1.2	-1.1
C13	3.0	3.5	3.2	3.1	2.9
C14	3.0	3.3	3.1	2.9	2.9
C1	-0.4	-0.4	-0.2	-0.5	-0.3
C4	0.0	-0.4	-0.5	-0.4	-0.4
C3	0.6	0.5	0.4	0.4	0.4
C2	0.2	-0.1	0.0	-0.1	0.0
C11	0.1	-0.2	-0.2	-0.2	-0.2
C20	-0.1	-0.3	-0.1	-0.3	-0.3
C21	-0.3	-0.6	-0.5	-0.5	-0.5

[*] methylene RDC is reported as the average of the two $^1D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

[#] both $^1D_{CH}$'s for the methylene group are reported when the F2-coupled HSQC is used for RDC measurement. The diastereotopic methylene protons is stereospecifically assigned by doing SVD fitting for both possibilities and keeping the better fit. Note that RDC's measured from different experiments on the same NMR sample can be directly combined for data analysis, so methylene RDCs may have reported values for both the average by the F1-coupled HSQC and the two separate RDC's from the F2-coupled HSQC.

Table S7. caulamidine A (**5**) in PMMA/chloroform[2]

caulamidine A (**5**)

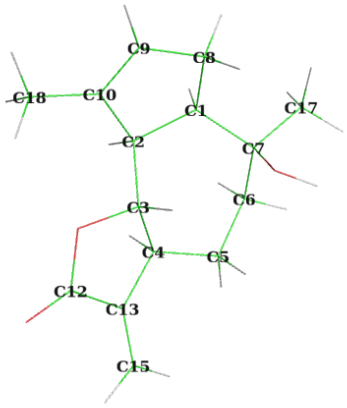


	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C23	29.9	15.8	7.1	22.9	22.5
C6	-7.3	-15.2	-22.4	-11.6	-12.0
C4	-34.5	-36.1	-34.4	-35.8	-35.6
C1	-39.0	-36.1	-34.1	-36.0	-35.9
C21	-40.0	-43.0	-44.6	-41.4	-37.7
C24	-37.6	-42.8	-44.5	-41.0	-37.7
C26	25.1	26.9	25.3	28.5	32.2
C29	16.5	11.6	10.2	12.2	11.4
C17	18.5	10.8	9.0	11.8	10.2
C28*	25.0	20.2	19.0	21.2	19.9
	RCSA (Hz @ 150 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C12	15.8	5.4	3.5	6.2	4.8
C8	13.1	6.6	4.5	7.9	9.2
C19	12.5	4.2	2.8	4.7	2.3
C2	6.7	5.5	4.4	6.1	9.1
C20	2.4	2.5	3.9	1.2	-0.6
C23	0.5	1.9	3.5	0.2	-1.3
C6	7.6	8.6	9.7	8.1	9.5
C22	10.7	1.4	-0.2	2.2	0.2
C5	1.9	0.8	-0.6	1.6	4.2
C4	12.5	11.5	10.9	11.4	12.7
C1	12.5	11.7	11.4	11.7	13.1
C3	8.6	9.4	10.1	9.0	10.8
C21	12.5	10.1	10.7	9.3	7.2
C24	12.8	9.9	10.5	9.1	7.0
C10	0.5	0.7	0.7	0.6	0.7
C26	0.0	-1.5	-2.0	-1.2	-2.0
C28	-3.6	-3.2	-3.7	-2.9	-2.8
C14	-3.1	-2.6	-3.1	-2.3	-2.5
C11	-0.8	-0.3	-0.1	-0.4	-0.3
C17	-6.8	-4.2	-3.6	-4.6	-3.8
C29	-5.3	-4.2	-4.0	-4.3	-3.9
C9	2.1	0.6	0.1	0.9	0.5
C15	-1.4	-0.7	-0.5	-0.9	-0.5

* methylene RDC is reported as the average of the two $^{1}D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Table S8. 10-epi-8-deoxycumambrin B (6) in PMMA/chloroform[3]

10-epi-8-deoxycumambrin B (**6**)



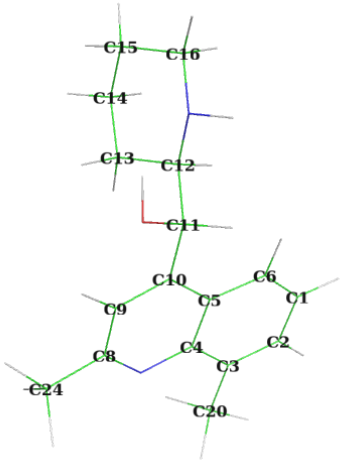
	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C1	8.0	25.3	22.5	22.3	24.9
C9	-13.0	-12.5	-12.9	-14.4	-10.6
C2	29.3	30.3	30.4	31.2	32.0
C3	34.2	29.8	31.2	32.8	32.0
C4	27.2	32.6	32.6	33.8	34.7
C18	-0.8	4.6	3.4	1.1	2.6
C17	5.8	5.0	5.2	5.5	6.6
C15*	-14.0	-15.6	-15.6	-12.7	-13.5
C8*	4.4	9.7	8.5	5.8	5.3

* methylene RDC is reported as the average of the two $^1D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Note that because the original RDC data were collected in a compressed PMMA gel, their signs are inverted here to be consistent with a stretched gel model.

Table S9. mefloquine (7) in PMMA/chloroform[1]

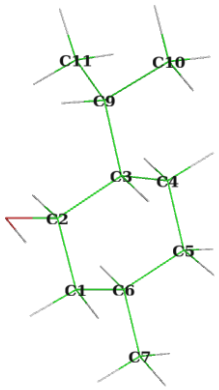
mefloquine (**7**)



	RCSA (Hz @ 150 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C10	42.5	41.8	40.5	40.6	39.4
C8	24.8	31.0	24.5	17.6	15.5
C4	38.2	38.8	36.2	31.2	31.9
C3	26.6	31.4	30.6	35.5	31.3
C2	43.5	39.7	40.6	35.2	41.4
C1	29.4	36.6	29.0	23.9	21.5
C6	31.1	35.2	29.4	35.8	26.3
C5	39.0	42.2	38.4	36.1	33.7
C20	-0.4	-1.1	-1.0	1.2	-0.4
C24	-0.8	-0.9	-2.0	-2.1	-3.7
C9	43.2	39.8	41.4	35.6	39.9
C11	-0.6	0.3	-0.1	1.2	-2.0
C12	-1.6	-2.9	-3.7	-4.5	-0.6
C16	2.6	1.9	-0.1	0.6	5.6
C15	1.4	0.5	0.7	1.0	1.8
C13	-1.0	-0.7	-1.2	-1.4	-0.2
C14	0.0	-1.2	-1.5	-1.6	-0.8

Table S10. menthol (**8**) in PMMA/chloroform[1]

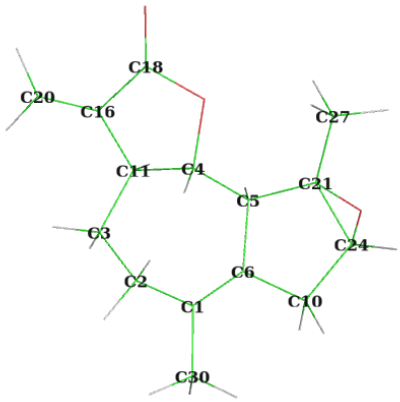
menthol (**8**)



	RCSA (Hz @ 150 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C2	-0.1	-0.3	-0.4	-0.3	-0.4
C3	-0.2	-0.2	-0.4	-0.3	-0.3
C1	-2.4	-1.5	-1.6	-1.7	-1.8
C5	-0.8	-0.9	-1.0	-0.9	-0.9
C6	-0.4	-0.8	-0.8	-0.7	-0.7
C9	-0.8	-0.5	-0.5	-0.5	-0.5
C4	-1.3	-0.9	-1.0	-1.0	-1.0
C7	-3.1	-2.7	-2.9	-2.8	-2.9
C10	0.6	0.2	0.5	0.4	0.5
C11	1.0	1.4	1.2	1.3	1.2

Table S11. ludartin (**9**) in PMMA/chloroform[4]

ludartin (**9**)

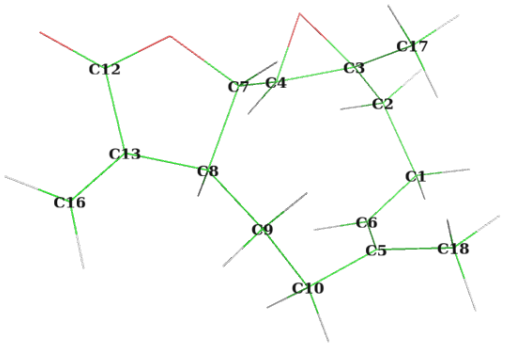


	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C10[#]	-27.0	-1.5	5.5	-1.0	-0.7
C10[#]	85.0	80.9	73.9	82.3	85.1
C24	7.0	-10.6	-15.4	-11.8	-17.6
C5	98.0	82.8	77.1	83.9	84.8
C4	97.0	79.1	71.6	80.6	83.2
C11	81.0	91.1	91.2	90.1	93.2
C2[#]	89.0	87.5	83.3	87.7	90.9
C2[#]	-34.0	-42.7	-34.8	-43.2	-38.0
C20[#]	-34.0	-44.9	-44.8	-40.7	-42.1
C20[#]	-38.0	-44.3	-34.0	-45.9	-42.8

[#] both $^{1}D_{CH}$'s for the methylene group are reported when the F2-coupled HSQC is used for RDC measurement. The diastereotopic methylene protons is stereospecifically assigned by doing SVD fitting for both possibilities and keeping the better fit.

Table S12. parthenolide (**10**) in PMMA/chloroform[2]

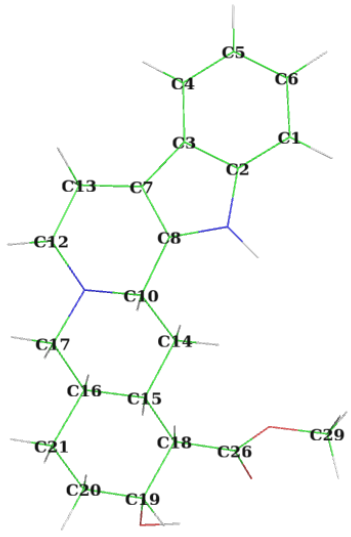
parthenolide (**10**)



	RCSA (Hz @ 150 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C12	15.8	7.7	12.4	8.0	9.0
C13	13.8	17.2	16.3	16.4	15.4
C5	3.0	-1.1	3.1	1.1	5.0
C6	0.3	-3.3	-1.1	-1.6	1.3
C16	23.6	22.9	22.8	23.2	23.4
C7	-4.8	-5.5	-5.6	-5.2	-5.0
C4	7.1	4.9	5.9	5.1	5.8
C3	9.9	5.0	6.1	6.4	8.2
C8	0.5	-0.5	-0.3	-0.4	-0.3
C10	-1.5	-1.0	-1.2	-1.4	-1.9
C2	2.4	1.8	2.8	1.5	1.6
C9	-1.1	-2.5	-2.7	-2.3	-2.3
C1	-4.6	-2.7	-3.0	-2.9	-3.0
C17	5.4	3.8	4.6	4.0	4.3
C18	2.6	0.2	0.4	0.8	1.2

Table S13. yohimbine (**11**) in PMMA/chloroform[5]

yohimbine (**11**)



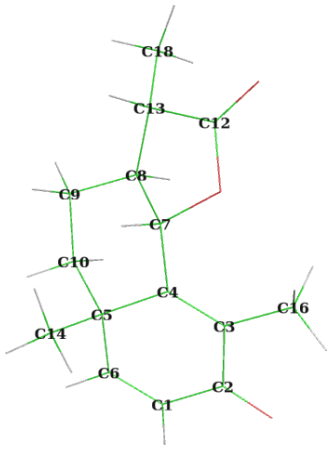
	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C10	29.5	30.0	30.0	29.5	27.8
C4	-6.4	-16.5	-20.8	-13.1	-12.2
C5	-20.6	-13.8	-15.5	-12.1	-13.4
C6	-10.1	-20.3	-13.2	-20.9	-22.0
C1	-9.4	-16.7	-20.8	-13.2	-12.4
C15	30.5	31.3	31.1	30.9	29.4
C18	32.2	32.5	32.0	31.9	30.8
C19	-4.2	0.8	-3.6	-0.9	2.1
C16	30.3	31.8	31.5	31.2	29.8
C12*	7.6	8.8	9.5	8.3	9.2
C14*	10.4	9.2	9.4	9.9	9.5
C20*	9.8	9.3	11.5	8.8	7.0
C21*	7.9	9.1	9.0	9.7	9.5
C17*	9.3	8.6	8.5	9.3	9.1

* methylene RDC is reported as the average of the two $^{1}D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Note that because the original RDC data were collected in a compressed PMMA gel, their signs are inverted here to be consistent with a stretched gel model.

Table S14. santonin (12) in PMMA/chloroform[6]

santonin (**12**)

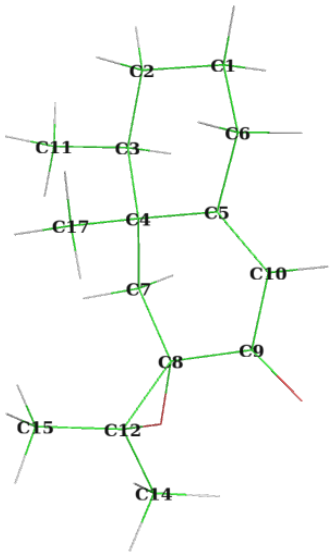


	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C1	-28.3	-27.8	-28.5	-27.4	-32.7
C6	1.6	-22.8	-17.0	-21.5	-13.8
C7	36.5	39.3	38.6	39.7	34.4
C8	38.8	37.9	36.3	39.6	34.3
C13	32.2	29.8	30.8	30.0	25.7
C16	-3.8	5.9	4.0	5.8	3.4
C14	-10.7	-12.5	-11.9	-12.6	-10.9
C18	4.8	-3.7	-2.3	-2.5	-1.2
C9*	20.4	23.9	20.6	25.1	24.2
C10*	20.1	12.6	14.5	13.5	14.0

* methylene RDC is reported as the average of the two $^1D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.
Note that because the original RDC data were collected in a compressed PMMA gel, their signs are inverted here to be consistent with a stretched gel model.

Table S15. sesquiterpenoid-13 (13) in PMMA/chloroform[7]

sesquiterpenoid-13 (**13**)

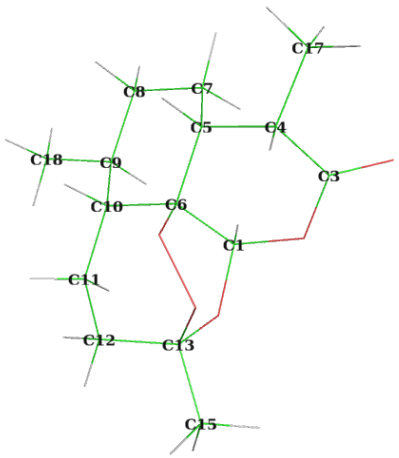


	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C3	12.0	12.3	12.3	11.9	12.1
C10	-2.4	-2.2	-0.3	-3.5	-3.3
C11	0.5	0.5	0.1	0.9	0.8
C17	-3.4	-3.1	-3.1	-3.0	-3.0
C6*	5.6	5.8	6.6	5.0	5.3
C1*	2.7	3.9	4.0	4.0	3.8
C2*	2.8	3.5	2.6	3.7	3.8
C7*	4.6	4.1	4.9	3.5	3.3
C14/15[†]	0.2	-0.2	-0.2	-0.2	-0.1

* methylene RDC is reported as the average of the two $^1D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.
[†] the average of the two methyl RDC's from the isopropyl group is reported without stereospecific assignment.
Note that because the original RDC data were collected in a compressed PMMA gel, their signs are inverted here to be consistent with a stretched gel model.

Table S16. artemisinin (**14**) in PMMA/chloroform[8]

artemisinin (**14**)

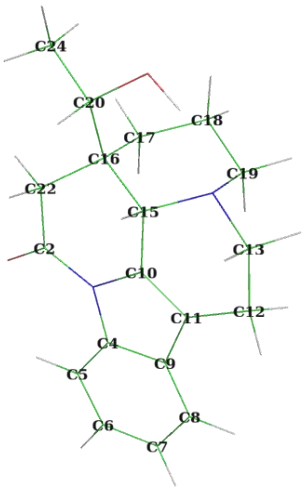


	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C10	23.8	22.0	23.4	20.4	20.8
C9	21.4	23.3	24.4	21.4	21.5
C5	20.8	21.0	22.5	19.6	20.0
C4	10.3	11.3	12.1	9.1	8.0
C1	12.0	13.2	14.1	11.2	10.7
C15	2.4	4.0	3.0	3.5	3.5
C18	3.9	4.3	3.9	3.1	1.8
C17	4.7	3.5	4.8	3.8	5.0
C12*	7.6	10.1	7.9	7.8	5.8
C11*	8.5	9.4	9.4	9.1	10.3
C8*	12.5	12.3	14.0	11.1	11.0
C7*	2.4	5.8	4.7	4.5	2.7

* methylene RDC is reported as the average of the two $^1D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.
Note that because the original RDC data were collected in a compressed PMMA gel, their signs are inverted here to be consistent with a stretched gel model.

Table S17. 19-OH-eburnamonine (**15**) in PMMA/chloroform[9]

19-OH-eburnamonine (**15**)

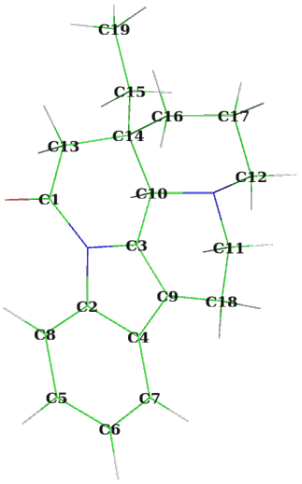


	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C8	-20.8	-16.3	-23.2	-17.3	-16.3
C7	-19.8	-23.9	-18.9	-24.5	-23.8
C6	-10.6	-17.0	-15.1	-15.1	-14.5
C5	-20.4	-16.6	-23.6	-17.6	-16.6
C15	21.6	30.7	33.3	33.8	35.6
C20	38.6	35.5	35.8	34.9	33.5
C24	5.4	4.0	5.2	4.9	5.5
C13*	14.0	13.4	12.7	14.0	14.6
C12*	12.9	15.9	15.0	15.1	14.5
C19*	-6.0	-13.0	-11.3	-12.0	-10.8
C18*	7.9	6.6	11.2	8.7	9.8
C17*	-16.4	-14.3	-13.1	-14.3	-14.3
C22*	8.2	12.9	10.8	12.8	12.6

* methylene RDC is reported as the average of the two $^1D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.
Note that because the original RDC data were collected in a compressed PMMA gel, their signs are inverted here to be consistent with a stretched gel model.

Table S18. eburnamonine (**16**) in PMMA/chloroform[5]

eburnamonine (**16**)



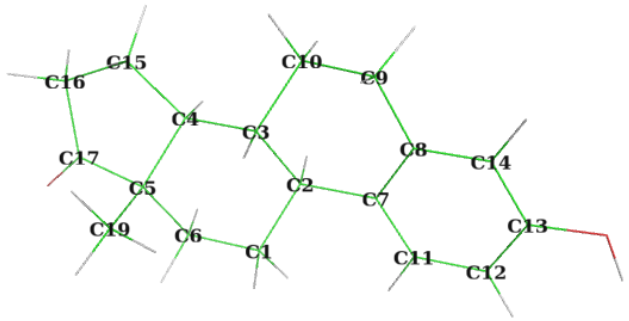
	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C8	-16.7	-12.2	-17.4	-12.8	-14.2
C5	-10.9	-12.2	-13.3	-10.4	-10.9
C6	-16.7	-19.5	-15.2	-18.3	-15.2
C7	-14.5	-12.0	-17.2	-12.6	-14.0
C10	26.8	24.0	26.1	25.2	28.3
C13*	8.9	9.8	9.2	9.2	8.8
C12*	-9.6	-9.3	-9.5	-8.0	-6.8
C11*	11.4	10.6	9.6	10.5	10.6
C18*	11.9	11.9	12.5	10.8	10.6
C17*	8.0	5.8	8.6	7.2	9.6
C16*	-11.7	-11.0	-10.0	-10.4	-9.9

* methylene RDC is reported as the average of the two $^{1}D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Note that because the original RDC data were collected in a compressed PMMA gel, their signs are inverted here to be consistent with a stretched gel model.

Table S19. Estrone (**2**) in poly-HEMA/DMSO

estrone (**2**)



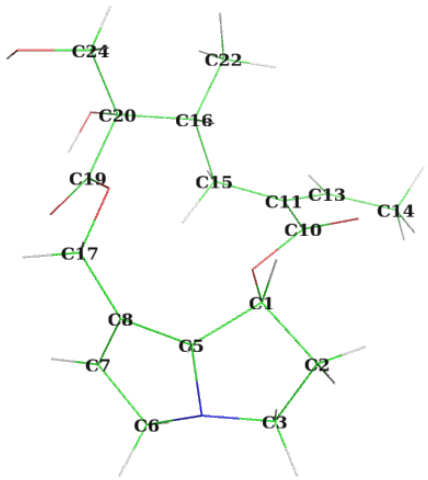
	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C11	1.0	-5.0	-1.4	-1.0	-7.4
C12	10.1	-12.8	-9.9	27.2	20.0
C14	3.1	-6.2	-2.8	-6.3	-11.8
C2	30.7	33.2	37.1	31.7	32.0
C3	35.6	34.2	37.0	34.0	34.1
C4	35.6	34.0	35.8	36.2	35.2
C19	-11.4	-10.2	-9.6	-10.8	-11.2
C9*	14.6	16.4	8.3	17.7	18.9
C16*	10.3	10.8	8.0	9.6	12.0
C10*	24.0	13.2	12.5	35.0	31.3
C6*	13.3	17.0	14.0	18.5	19.0
	RCSA (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C17	9.3	9.4	6.0	6.9	8.4
C13	19.4	12.2	9.5	19.3	18.9
C8	9.7	12.2	9.2	8.2	10.2
C7	18.9	13.8	10.6	19.7	19.9
C11	8.8	9.7	6.5	9.9	11.9
C14	6.1	7.3	5.5	7.4	8.8
C12	5.3	7.9	5.9	2.3	4.0
C4	-3.3	-2.0	-1.9	-2.9	-2.8
C5	-1.9	-1.1	-1.0	-1.9	-1.6
C2	1.6	0.4	0.3	1.5	1.4
C3	-0.1	-0.2	0.1	-0.5	-0.5
C16	0.5	-1.4	-0.9	0.2	-0.4
C6	1.7	0.1	-0.3	1.5	1.2
C9	-1.6	-1.9	-1.6	-2.5	-2.4
C10	0.4	0.0	-0.3	-0.4	-0.3
C1	-1.1	-1.0	-1.2	-2.1	-1.8
C15	-2.2	-1.9	-1.5	-2.4	-2.4
C19	2.1	1.8	1.3	1.7	1.9

* methylene RDC is reported as the average of the two $^1D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Data were collected at 298 K on a 600 MHz spectrometer with *ca*. 5 mg estrone dissolved in 330 μL DMSO-d_6 soaked in a 60 % poly-HEMA gel of 0.05 % cross-linking ratio stretched in a two-stage NMR tube with 4.2 mm inner diameter at the wider section and 3.0 mm inner diameter at the narrower section.[10]

Table S20. retrorsine (**3**) in poly-HEMA/DMSO

retrorsine (**3**)



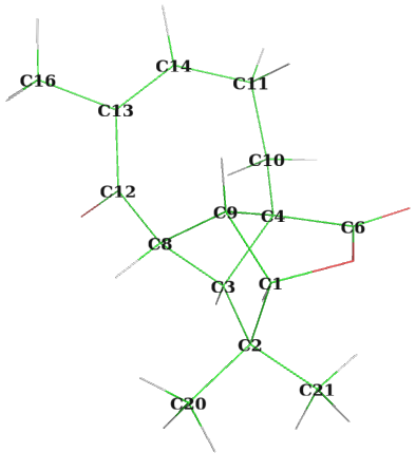
	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C7	-25.9	6.3	0.5	-26.8	-26.0
C13	10.9	12.7	6.8	3.3	2.2
C1	14.1	40.8	41.8	18.3	19.1
C5	19.2	33.6	27.8	16.5	16.4
C16	8.3	33.2	25.3	3.5	3.3
C22	-7.0	6.2	3.6	-6.0	-5.0
C17*	-7.1	21.3	17.0	-5.8	-5.2
C15*	18.5	6.1	7.8	14.9	12.8
C2*	3.9	2.4	0.7	2.6	1.8
C3*	8.3	-1.5	-3.2	4.6	4.4
C6*	17.3	2.5	5.6	16.9	15.7
	RCSA (Hz @ 150 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C19	-7.4	-2.8	-2.4	-4.8	-4.1
C10	-8.6	3.4	2.2	-5.6	-4.6
C7	12.6	6.6	7.6	10.8	10.0
C13	5.8	2.1	4.8	6.7	6.7
C11	7.0	2.4	4.8	7.5	7.4
C8	14.3	5.0	6.7	11.6	10.7
C20	0.4	-1.0	-1.5	-1.2	-1.1
C5	-2.1	-3.1	-2.6	-1.7	-1.5
C1	0.4	-2.1	-2.3	0.0	-0.1
C24	-1.8	-2.4	-2.5	-2.7	-2.6
C6	-2.6	2.5	1.6	-2.7	-2.5
C17	2.1	-4.3	-3.3	2.3	2.0
C3	-4.8	-2.6	-2.7	-3.4	-3.2
C15	-1.2	-1.6	-1.7	-1.5	-1.4
C16	-1.8	-1.5	-1.8	-2.0	-1.8
C2	-2.1	-1.9	-1.7	-1.7	-1.5
C14	-1.2	-1.4	-1.4	-1.8	-1.7
C22	1.4	-0.4	-0.1	1.3	1.2

* methylene RDC is reported as the average of the two $^1D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Data were collected at 298 K on a 600 MHz spectrometer with *ca*. 5 mg retrorsine dissolved in 330 μL DMSO-d_6 soaked in a 60 % poly-HEMA gel of 0.05 % cross-linking ratio stretched in a two-stage NMR tube with 4.2 mm inner diameter at the wider section and 3.0 mm inner diameter at the narrower section.[10]

Table S21. aquatolide (**4**) in poly-HEMA/DMSO[11]

aquatolide (**4**)

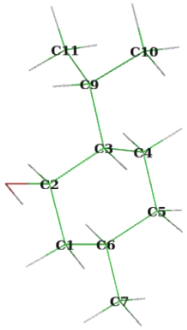


	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C14	-2.6	-9.6	-3.5	-2.1	-4.3
C1	22.2	13.8	10.8	20.0	20.8
C9	13.5	3.7	14.6	8.4	8.8
C8	-5.4	-0.9	-2.8	-6.6	-3.4
C3	23.1	18.9	25.0	21.9	24.2
C16	2.9	3.0	3.9	4.7	5.6
C20	2.9	0.7	1.0	2.7	1.7
C21	1.8	2.9	2.9	3.0	4.2
C10*	0.6	3.6	3.1	-3.6	-2.1
C11*	3.2	5.6	3.4	6.6	7.8
	RCSA (Hz @ 125 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C12	4.0	2.1	2.0	0.2	0.8
C13	2.5	4.0	3.1	4.1	4.9
C14	2.7	3.6	2.1	3.1	3.8
C1	-1.6	-0.4	-0.5	-1.4	-1.2
C4	-1.2	-0.7	-0.9	-0.3	-0.6
C3	-1.0	0.6	0.6	0.6	0.7
C8	0.6	-0.6	-0.9	-0.1	-0.3
C9	-1.6	-1.4	-1.8	-1.3	-1.6
C2	0.3	-0.1	0.0	-0.5	-0.5
C11	0.0	-0.3	-0.4	0.0	-0.2
C20	0.7	-0.2	-0.2	-0.6	-0.4
C21	0.1	-0.7	-0.8	-0.7	-0.9
C10	-0.6	-0.3	-0.4	0.1	0.0
C16	-0.5	-0.8	-0.8	-1.2	-1.4

* methylene RDC is reported as the average of the two $^{1}D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Table S22. menthol (**8**) in poly-HEMA/DMSO[12]

menthol (**8**)

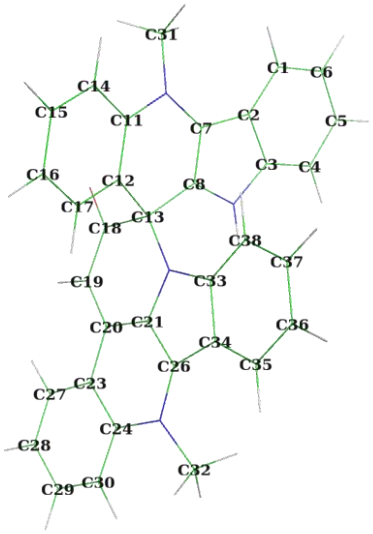


	RCSA (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C2	7.7	5.9	5.9	5.8	5.8
C3	7.7	5.7	5.7	5.9	5.9
C6	8.5	5.9	5.9	5.9	5.8
C9	4.6	2.0	2.3	3.5	4.4
C6	3.2	2.1	2.5	2.5	2.5
C4*	2.6	2.9	3.7	3.6	3.2
C5*	5.1	3.6	3.5	3.8	4.1
C1*	3.6	2.9	3.7	3.6	3.2

* methylene RDC is reported as the average of the two $^{1}D_{CH}$'s when the F1-coupled HSQC is used for RDC measurement.

Table S23. cryptospirolepine (**17**) in poly-HEMA/DMSO[11]

cryptospirolepine (**17**)



	RDC (Hz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C1	17.0	-10.5	15.9	2.0	14.2
C6	2.5	-30.7	-2.3	3.8	-1.0
C17	24.5	-32.6	17.8	13.3	17.7
C19	3.3	11.7	5.2	-2.7	3.0
C35	26.5	-24.1	20.4	27.8	22.2
C4	15.0	-9.3	15.4	2.3	13.8
C15	-6.1	12.0	-4.2	-14.4	-5.4
C38	26.4	-25.1	21.3	26.9	22.8
C36	8.6	16.0	11.4	13.1	11.0
C37	3.9	-16.5	5.7	-10.2	2.9
C27	20.8	1.3	19.7	29.2	21.1
C30	18.9	0.3	19.8	30.1	21.4
C16	-23.6	-2.8	-23.9	-6.9	-20.8
C14	20.3	-32.9	17.6	12.0	17.3
C28	1.5	4.9	1.9	-8.2	-0.5
C29	17.5	-34.3	12.6	8.8	12.5
C5	-23.8	13.4	-29.0	-20.2	-27.5
	RCSA (Hz @ 125 MHz)	P1A (Hz)	P2A (Hz)	P1B (Hz)	P2B (Hz)
C18	-7.0	3.6	-4.9	-1.8	-4.3
C11	4.2	3.7	3.4	2.0	2.9
C33	-7.8	2.4	-6.5	-5.7	-6.2
C24	-7.5	3.7	-5.2	-4.1	-4.9

C20	-9.1	6.7	-6.0	-3.5	-5.5
C3	1.0	6.5	1.4	0.9	1.1
C29	-10.8	9.4	-7.2	-6.0	-7.0
C15	3.6	1.6	2.4	3.5	2.3
C17	-1.0	7.9	-0.6	-0.6	-0.9
C37	-8.1	6.8	-6.6	-3.2	-6.0
C27	-10.5	3.5	-7.9	-8.3	-7.8
C12	2.6	3.0	2.2	3.8	2.3
C26	-5.7	3.7	-4.0	-2.4	-3.7
C35	-10.8	5.8	-7.9	-8.2	-8.0
C28	-7.3	3.0	-5.2	-3.2	-4.7
C5	6.5	1.6	6.2	5.0	5.8
C7	4.0	0.4	3.7	3.0	3.5
C21	-6.6	4.6	-4.5	-2.9	-4.2
C36	-8.6	1.3	-7.1	-6.5	-6.9
C1	-1.1	6.1	-0.3	1.3	-0.3
C16	6.3	3.6	5.0	2.0	4.3
C6	1.2	8.4	1.9	1.1	1.6
C34	-7.5	5.6	-5.7	-3.6	-5.3
C8	3.6	0.1	4.0	3.8	3.9
C2	4.9	2.4	3.7	3.6	3.5
C23	-9.7	6.3	-6.7	-6.1	-6.5
C30	-10.4	4.7	-7.1	-7.9	-7.2
C14	-0.4	6.5	-0.7	0.3	-0.8
C4	0.3	3.6	0.7	1.9	0.7
C38	-10.0	7.2	-7.6	-6.3	-7.4
C19	-3.9	1.8	-3.1	-1.6	-2.8

Supplementary References

1. N. Nath, M. Schmidt, R. R. Gil, R. T. Williamson, G. E. Martin, A. Navarro-Vázquez, C. Griesinger and Y. Z. Liu, *J Am Chem Soc*, 2016, **138**, 9548-9556.
2. Y. Z. Liu, I. E. Ndukwe, M. Reibarkh, G. E. Martin and R. T. Williamson, *Phys Chem Chem Phys*, 2022, **24**, 20164-20182.
3. C. Gayathri, N. V. Tsarevsky and R. R. Gil, *Chem-Eur J*, 2010, **16**, 3622-3626.
4. R. R. Gil, C. Gayathri, N. V. Tsarevsky and K. Matyjaszewski, *J Org Chem*, 2008, **73**, 840-848.
5. E. Troche-Pesqueira, C. Anklin, R. R. Gil and A. Navarro-Vázquez, *Angew Chem Int Edit*, 2017, **56**, 3660-3664.
6. F. Hallwass, R. R. Teles, E. Hellemann, C. Griesinger, R. R. Gil and A. Navarro-Vázquez, *Magn Reson Chem*, 2018, **56**, 321-328.
7. S. J. Castro, M. E. García, J. M. Padrón, A. Navarro-Vázquez, R. R. Gil and V. E. Nicotra, *J Nat Prod*, 2018, **81**, 2329-2337.
8. A. Navarro-Vázquez, R. R. Gil and K. Blinov, *J Nat Prod*, 2018, **81**, 203-210.
9. P. Trigo-Mourino, R. Sifuentes, A. Navarro-Vázquez, C. Gayathri, H. Maruenda and R. R. Gil, *Nat Prod Commun*, 2012, **7**, 735-738.
10. Y. Z. Liu and J. H. Prestegard, *J Biomol Nmr*, 2010, **47**, 249-258.
11. Y. Liu, J. Saurí, E. Mevers, M. W. Peczuh, H. Hiemstra, J. Clardy, G. E. Martin and R. T. Williamson, *Science*, 2017, **356**.
12. L. F. Gil-Silva, R. Santamaría-Fernández, A. Navarro-Vázquez and R. R. Gil, *Chem-Eur J*, 2016, **22**, 472-476.