Supplementary Information

Figure S1. Chemical structure of the DACM probe. The atoms are numbered in concert with Table S1, which gives the atom types and charges used in the simulation.

Figure S2. Chemical structure of the eosin probe. The atoms are numbered in concert with Table S2, which gives the atom types and charges used in the simulation.

Figure S3. Histograms showing the distributions of κ values for all of the eight probe orientation families.

Figure S4. Histograms showing the distributions of R_{DA} values for all of the eight probe orientation families.

Figure S5. 2D histograms showing the distribution of the DACM (upper) and eosin (lower) transition dipole orientations throughout the trajectory. Protein motion was removed prior to creation of the histogram. Structures were sampled every 200 fs throughout the 37 ns trajectory, so 185,000 total structures are accounted for in each figure. Binsize is 6° for both the polar (θ) angle and the azimuthal (ϕ) angle. Note that the dark blue color present over most of both plots represents exactly zero population.

Table S1: Atom types and charges for the DACM probe used in the simulation. Atom numbers are defined in Fig. S1.

Atom Number	Atom Type	Charge
1	OA	-0.335
2	CA	0.707
3	CA	-0.05
4	CA	0.009
5	CA	-0.071
6	CA	0.231
7	CA	-0.237
7a	HA	0.177
8	CA	-0.153
9	CA	0.115
9a	HA	0.181
10	CA	-0.02
10a	HA	0.089
11	O	-0.554
12	N	-0.029
13	C	0.45
14	CT	0.04
14a	HC	0.014
15	CT	0.04
15a	HC	0.014
15b	HC	0.014
16	C	0.45
17	CT	-0.191
17a	HC	0.084
17b	HC	0.084
17c	HC	0.084
18	NH	-0.315
19	CT	-0.091
19a	H1	0.068
19b	H1	0.068
19c	H1	0.068
20	O	-0.527
21	O	-0.527
22	CT	-0.091
22a	H1	0.068
22b	H1	0.068
22c	H1	0.068

Table S2: Atom types and charges for the eosin probe used in the simulation. Atom numbers are defined in Fig. S2.

Atom Number	Atom Type	Charge
1	OA	0.023
2	CA	0.071
3	CA	-0.279
4	CA	0.56
5	CA	-0.142
6	CA	-0.115
6a	HA	0.118
7	CA	-0.01
8	CA	0.308
9	CA	-0.01
10	CA	0.071
11	CA	-0.279
12	CA	0.56
13	CA	-0.142
14	CA	-0.115
14a	HA	0.118
15	Br	-0.142
16	O	-0.568
17	Br	-0.182
18	CA	-0.084
19	CA	0.059
20	CA	-0.093
20a	HA	0.072
21	CA	-0.213
21a	HA	0.106
22	CA	-0.084
22a	HA	0.093
23	CA	-0.176
23a	HA	0.058
24	Br	-0.142
25	O	-0.568
26	Br	-0.182
27	C	0.549
28	O	-0.62
29	O	-0.62

Figure S1 VanBeek et al.

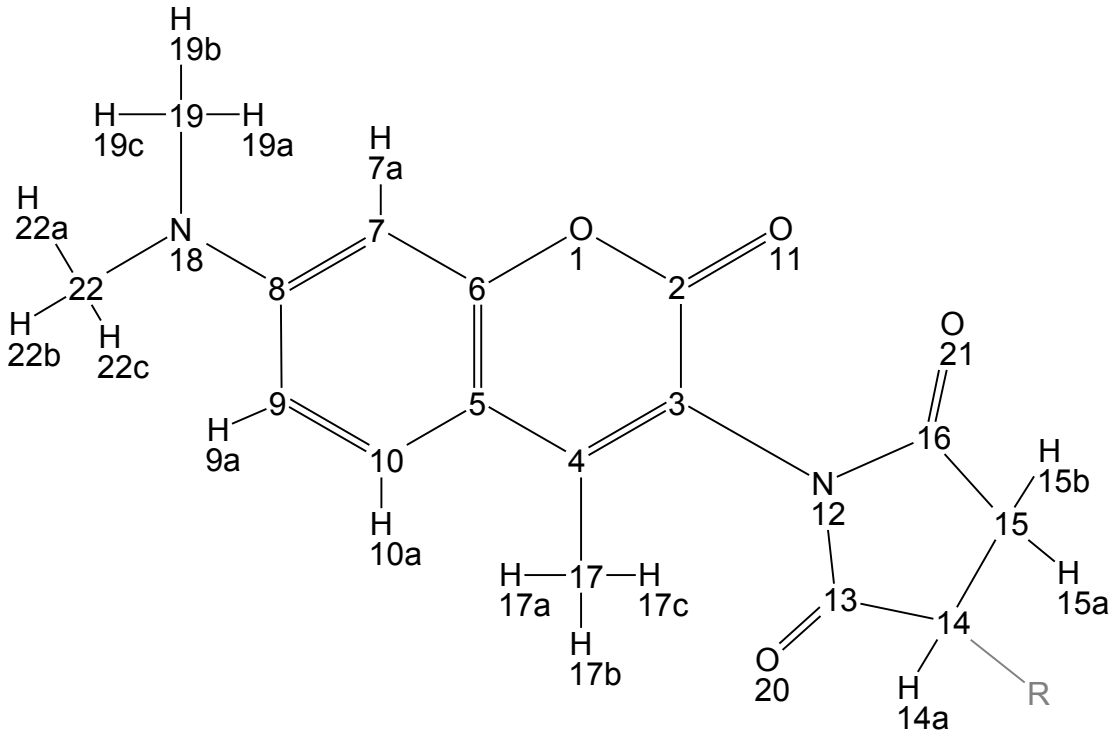

Figure S2 VanBeek et al.

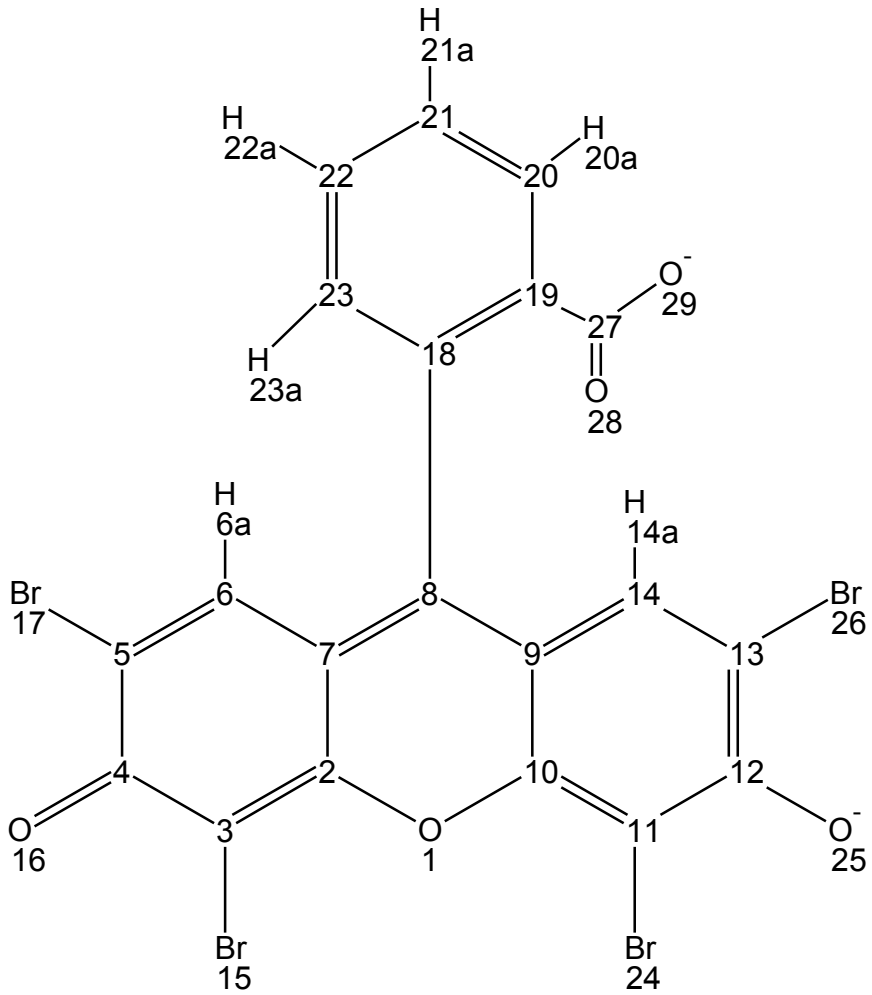

Figure S3 VanBeek et al.

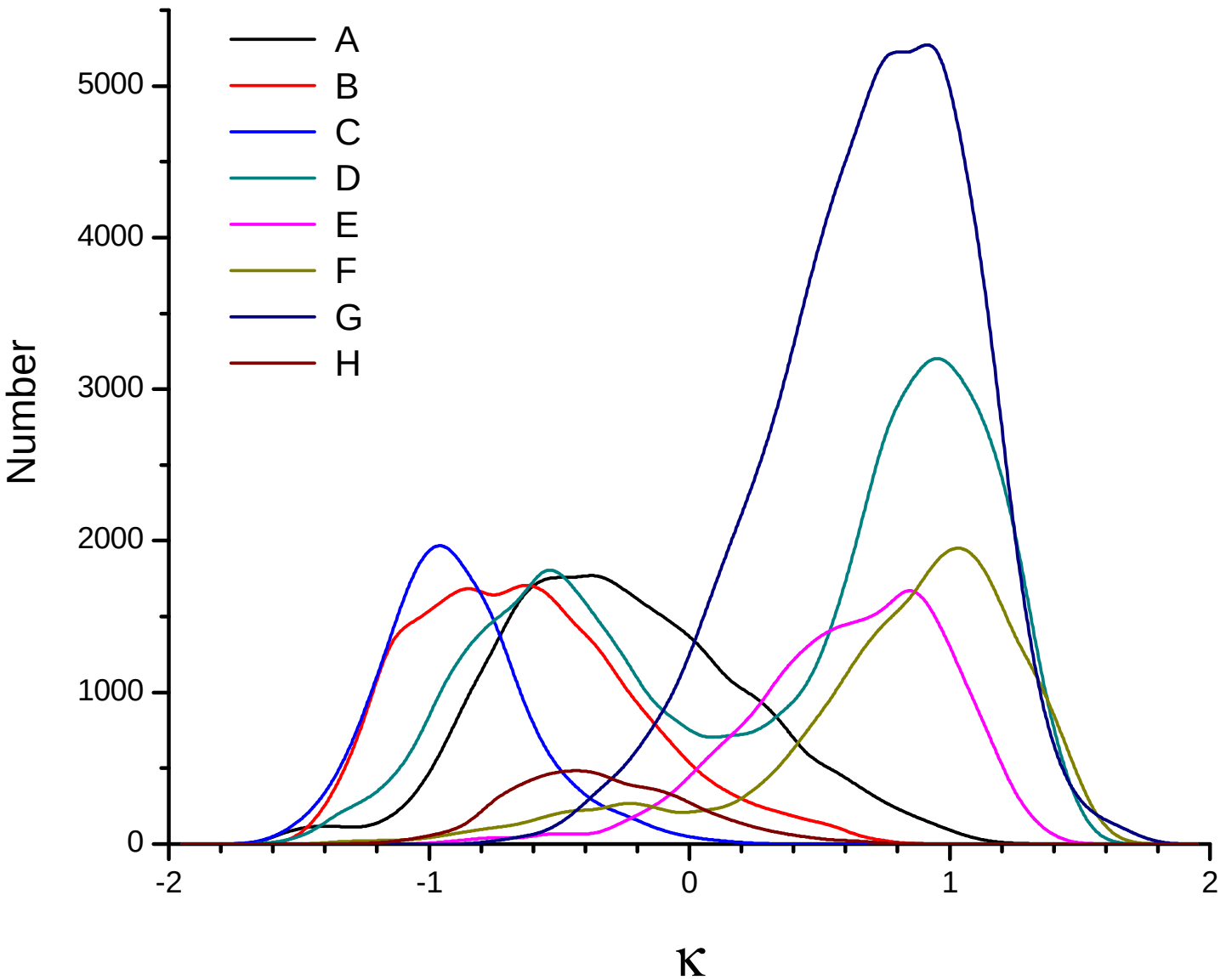

Figure S4 VanBeek et al.

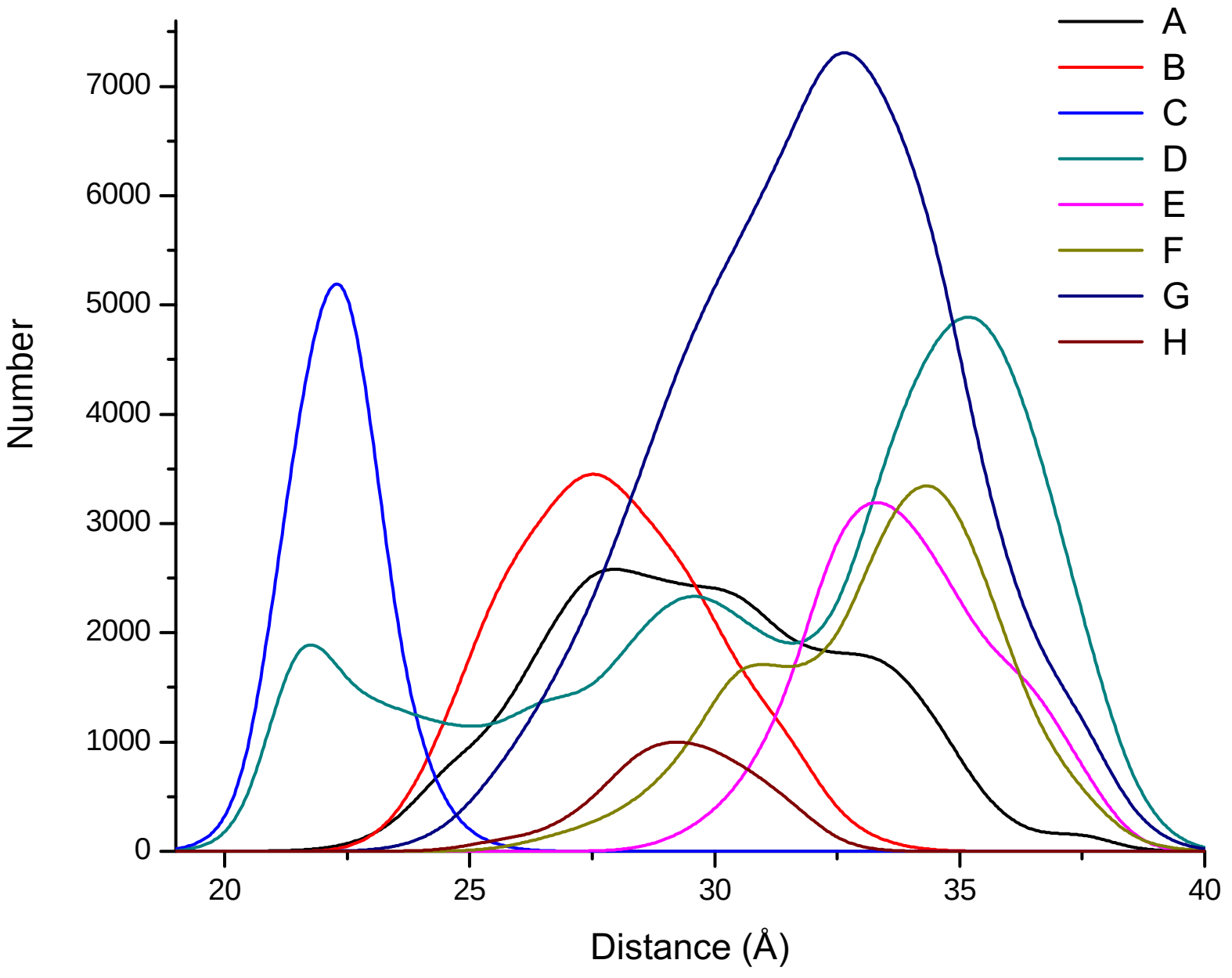

Figure S5 VanBeek et al.