

Local Molecular Reactivity of the Colored Dansylglycine in
Water and Dioxane Studied through Conceptual DFT
Supplementary Information

Table S1: Calculated bond lengths (in Å) of the dansylglycine molecule with the MN12SX density functional using water as a solvent simulated with the SMD solvation model

Bond	Distance	Bond	Distance	Bond	Distance	Bond	Distance
R(1-2)	1.475	R(7-20)	1.466	R(12-22)	1.091	R(18-30)	1.102
R(1-3)	1.480	R(7-28)	1.041	R(13-16)	1.376	R(18-31)	1.103
R(1-7)	1.710	R(8-9)	1.428	R(13-23)	1.097	R(19-32)	1.103
R(1-10)	1.691	R(8-10)	1.439	R(14-16)	1.411	R(19-33)	1.102
R(4-21)	1.362	R(8-12)	1.426	R(14-24)	1.100	R(19-34)	1.102
R(4-37)	1.016	R(9-11)	1.448	R(15-17)	1.413	R(20-21)	1.513
R(5-21)	1.221	R(9-13)	1.427	R(15-25)	1.092	R(20-35)	1.133
R(6-11)	1.452	R(10-14)	1.386	R(16-26)	1.093	R(20-36)	1.125
R(6-18)	1.493	R(11-15)	1.384	R(17-27)	1.095		
R(6-19)	1.497	R(12-17)	1.376	R(18-29)	1.104		

Table S2: Calculated bond angles (in $^{\circ}$) of the dansylglycine molecule with the MN12SX density functional using water as a solvent simulated with the SMD solvation model

Bond	Angle	Bond	Angle	Bond	Angle	Bond	Angle
A(2-1-3)	112.7	A(6-11-9)	117.6	A(8-9-13)	118.8	A(16-13-23)	119.2
A(2-1-7)	105.0	A(6-11-15)	122.6	A(10-8-12)	121.9	A(13-16-14)	120.2
A(2-1-10)	112.0	A(18-6-19)	110.0	A(8-10-14)	120.0	A(13-16-26)	120.8
A(3-1-7)	107.3	A(6-18-29)	108.8	A(8-12-17)	120.5	A(16-14-24)	117.5
A(3-1-10)	110.9	A(6-18-30)	115.4	A(8-12-22)	121.4	A(14-16-26)	119.0
A(7-1-10)	108.6	A(6-18-31)	110.2	A(11-9-13)	122.1	A(17-15-25)	118.1
A(1-7-20)	118.0	A(6-19-32)	109.2	A(9-11-15)	119.7	A(15-17-27)	118.7
A(1-7-28)	117.5	A(6-19-33)	114.1	A(9-13-16)	121.2	A(29-18-30)	107.2
A(1-10-8)	119.2	A(6-19-34)	111.2	A(9-13-23)	119.6	A(29-18-31)	106.8
A(1-10-14)	120.8	A(20-7-28)	112.2	A(10-14-16)	120.8	A(30-18-31)	108.1
A(21-4-37)	113.6	A(7-20-21)	115.7	A(10-14-24)	121.7	A(32-19-33)	107.6
A(4-21-5)	120.1	A(7-20-35)	109.0	A(11-15-17)	120.5	A(32-19-34)	107.0
A(4-21-20)	112.9	A(7-20-36)	111.7	A(11-15-25)	121.4	A(33-19-34)	107.4
A(5-21-20)	127.0	A(9-8-10)	119.0	A(17-12-22)	118.1	A(21-20-35)	107.1
A(11-6-18)	113.9	A(9-8-12)	119.1	A(12-17-15)	121.0	A(21-20-36)	109.2
A(11-6-19)	111.2	A(8-9-11)	119.1	A(12-17-27)	120.3	A(35-20-36)	103.2

Table S3: Calculated bond lengths (in Å) of the dansylglycine molecule with the MN12SX density functional using dioxane as a solvent simulated with the SMD solvation model

Bond	Distance	Bond	Distance	Bond	Distance	Bond	Distance
R(1-2)	1.455	R(7-20)	1.466	R(12-22)	1.098	R(18-30)	1.101
R(1-3)	1.452	R(7-28)	1.034	R(13-16)	1.376	R(18-31)	1.104
R(1-7)	1.734	R(8-9)	1.428	R(13-23)	1.097	R(19-32)	1.104
R(1-10)	1.719	R(8-10)	1.431	R(14-16)	1.413	R(19-33)	1.102
R(4-21)	1.369	R(8-12)	1.429	R(14-24)	1.100	R(19-34)	1.102
R(4-37)	1.000	R(9-11)	1.448	R(15-17)	1.418	R(20-21)	1.520
R(5-21)	1.208	R(9-13)	1.426	R(15-25)	1.089	R(20-35)	1.124
R(6-11)	1.450	R(10-14)	1.383	R(16-26)	1.090	R(20-36)	1.121
R(6-18)	1.490	R(11-15)	1.381	R(17-27)	1.093		
R(6-19)	1.494	R(12-17)	1.372	R(18-29)	1.104		

Table S4: Calculated bond angles (in $^{\circ}$) of the dansylglycine molecule with the MN12SX density functional using dioxane as a solvent simulated with the SMD solvation model

Bond	Angle	Bond	Angle	Bond	Angle	Bond	Angle
A(2-1-3)	118.4	A(6-11-9)	116.6	A(8-9-13)	119.3	A(16-13-23)	120.0
A(2-1-7)	103.9	A(6-11-15)	123.3	A(10-8-12)	122.8	A(13-16-14)	119.8
A(2-1-10)	109.8	A(18-6-19)	111.0	A(8-10-14)	120.3	A(13-16-26)	120.9
A(3-1-7)	107.8	A(6-18-29)	108.4	A(8-12-17)	120.8	A(16-14-24)	118.2
A(3-1-10)	112.5	A(6-18-30)	115.3	A(8-12-22)	120.2	A(14-16-26)	119.2
A(7-1-10)	102.9	A(6-18-31)	109.9	A(11-9-13)	121.6	A(17-15-25)	118.3
A(1-7-20)	118.6	A(6-19-32)	108.7	A(9-11-15)	120.0	A(15-17-27)	118.5
A(1-7-28)	116.5	A(6-19-33)	114.1	A(9-13-16)	120.9	A(29-18-30)	107.8
A(1-10-8)	123.1	A(6-19-34)	110.8	A(9-13-23)	119.1	A(29-18-31)	106.8
A(1-10-14)	116.6	A(20-7-28)	111.5	A(10-14-16)	121.0	A(30-18-31)	108.3
A(21-4-37)	112.9	A(7-20-21)	115.3	A(10-14-24)	120.8	A(32-19-33)	108.1
A(4-21-5)	120.6	A(7-20-35)	109.0	A(11-15-17)	120.1	A(32-19-34)	107.3
A(4-21-20)	111.3	A(7-20-36)	110.9	A(11-15-25)	121.5	A(33-19-34)	107.6
A(5-21-20)	128.1	A(9-8-10)	118.5	A(17-12-22)	119.0	A(21-20-35)	107.5
A(11-6-18)	114.4	A(9-8-12)	118.7	A(12-17-15)	121.1	A(21-20-36)	108.5
A(11-6-19)	112.0	A(8-9-11)	119.1	A(12-17-27)	120.4	A(35-20-36)	105.0