Supporting Information

Photosensitive peptidomimetic for light controlled reversible DNA compaction

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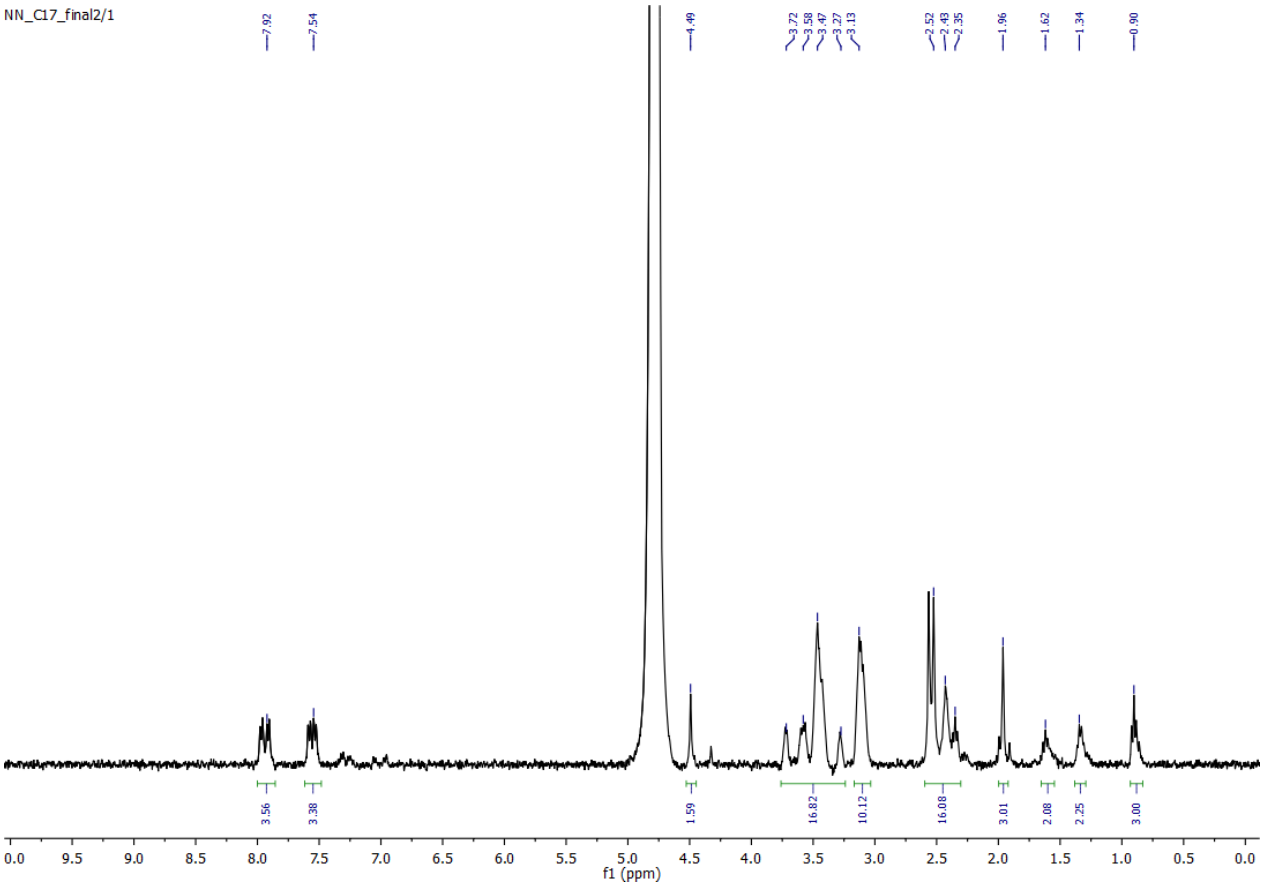


Figure S1. The ^{1}H NMR, data of the final product, Azo-PM. ^{1}H NMR (400 MHz, D_2O): δ = 7.94 (m 4H, Ar*H*), 7.56 (m, 4H, Ar*H*), 4.49 (s, 2H, Ar-CH_2-), 3.77 – 3,01 (m, 26H, -NH-CH_2), 2.63 – 2.24 (m, 16H, C(O)-CH_2), 2.00 – 1.89 (m, 3H, -C(O)CH_3), 1.65 – 1.51 (m, 2H, -CH_2-CH_2-CH_3), 1.34 (m, 2H, -CH_2-CH_2-CH_3), 0.89 (m, 3H, -CH_2-CH_3).

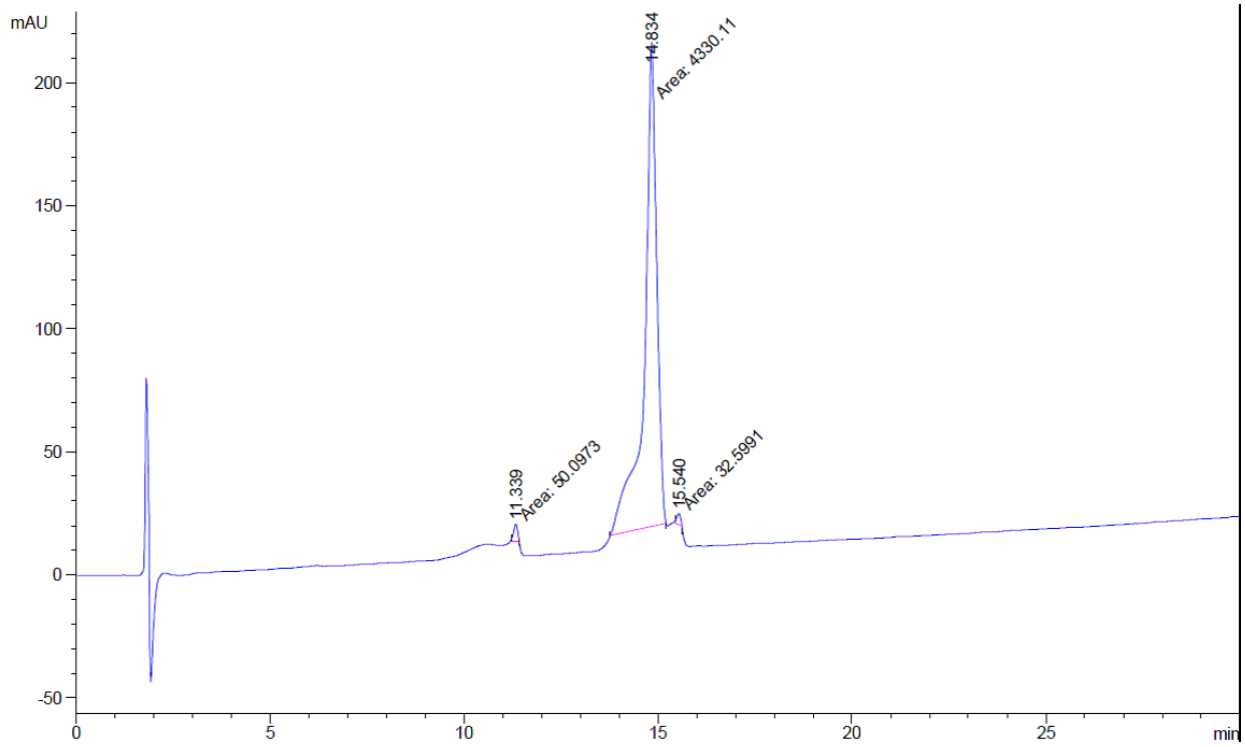


Figure S2. The RP-HPLC data of the final product, Azo-PM. RP-HPLC (5% to 30% MeCN in H_2O in 30 min): t_R = 14.8 min.

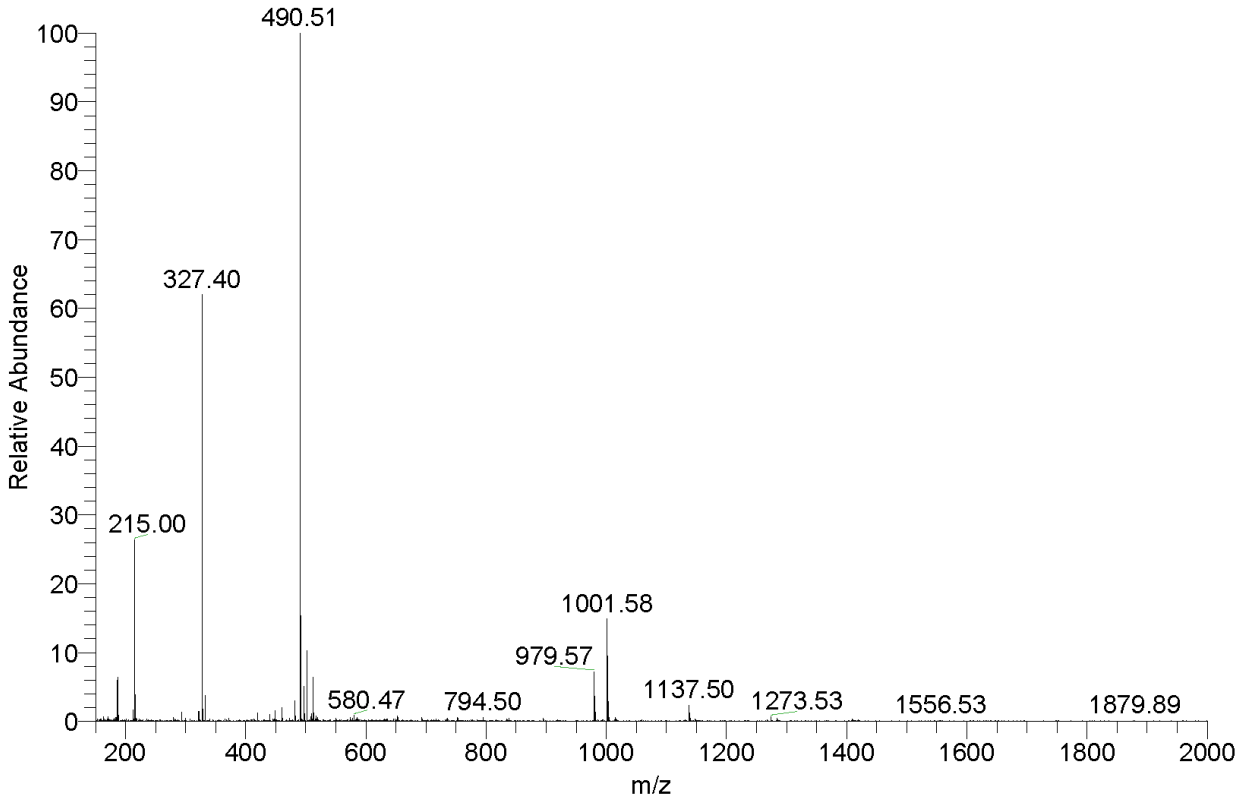
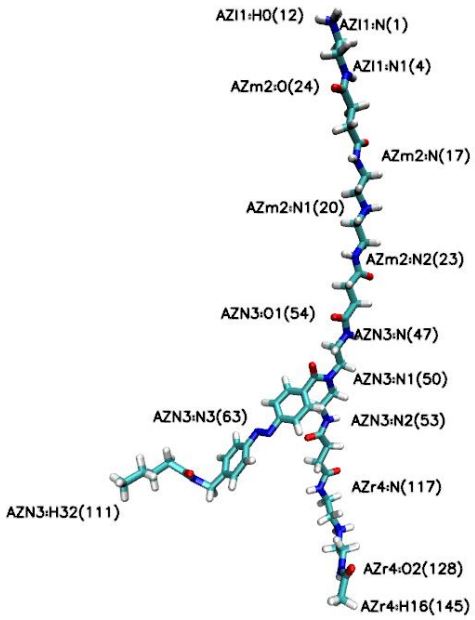


Figure S3. The ESI-MS data of the final product, Azo-PM. ESI-MS calcd.for $C_{47}H_{74}N_{14}O_9$ $[M+H]^+$ 979.58; found 979.57, $[M+2H]^{2+}$ 490.29; found 490.51, $[M+3H]^{3+}$ 327.20; found 327.40, $[M+Na]^+$ 1001.57; found 1001.58.

Figure S4. Four tables, the molecular structure of the Azo-PM molecule in *cis* and *trans*-form, protonated and unprotonated are reported according to the format of a mol2 file. The last column contains the partial charges obtained after the ensemble averaging procedure (see computational methods in the main text). The first four columns are atom index, atom name, x-coordinate, y-coordinate, **and** z-coordinate.

Figure below shows some selected atom labels on the structure of protonated Azo-PM in its trans state, to facilitate navigating the tables. The residue names Azl, AZm, AZN and AZrcorrespond to the segments L, M, N and R in Scheme 2, main text. In parentheses, the atom index is given. Note that for the unprotonated species the indexing shifts by 1 each time a protonation site is encountered along the structure (going from top to bottom).



Reduced protonated cis

1	N	29.94	40.02	28.15	AZl	-0.4968
2	C	29.14	40.64	29.23	AZl	0.109
3	C1	29.14	39.85	30.55	AZl	-0.1613
4	N1	28.3	40.61	31.51	AZl	-0.3476
5	H	29.68	39.03	28.04	AZl	0.3667
6	H1	29.58	40.35	27.24	AZl	0.3667
7	H2	29.47	41.68	29.29	AZl	0.1071
8	H3	28.09	40.72	28.94	AZl	0.1071
9	H4	28.63	38.91	30.37	AZl	0.1509
10	H5	30.17	39.77	30.89	AZl	0.1509
11	H6	27.67	41.35	31.24	AZl	0.2806
12	H0	30.96	40.02	28.15	AZl	0.3667
13	C	28.33	40.34	32.83	AZm	0.57
14	C1	27.4	41.21	33.69	AZm	-0.137
15	C2	27.42	40.92	35.19	AZm	-0.1945

16	C3	26.49	41.81	35.99	AZm	0.6975
17	N	26.48	41.58	37.34	AZm	-0.6311
18	C4	25.48	42.17	38.3	AZm	0.0479
19	C5	25.93	41.89	39.72	AZm	-0.1394
20	N1	25.02	42.43	40.74	AZm	-0.1723
21	C6	25.56	42.08	42.12	AZm	-0.1468
22	C7	24.74	42.57	43.38	AZm	-0.0413
23	N2	25.34	42.19	44.67	AZm	-0.3432
24	O	29.02	39.49	33.28	AZm	-0.5601
25	O1	25.83	42.7	35.42	AZm	-0.5682
26	H	27.62	42.27	33.58	AZm	0.0842
27	H1	26.41	40.96	33.31	AZm	0.0842
28	H2	28.4	40.98	35.69	AZm	0.0926
29	H3	27.16	39.89	35.42	AZm	0.0926
30	H4	26.9	40.72	37.66	AZm	0.3366
31	H5	25.32	43.24	38.1	AZm	0.1119
32	H6	24.49	41.75	38.12	AZm	0.1119
33	H7	25.98	40.8	39.82	AZm	0.1439
34	H8	26.85	42.45	39.88	AZm	0.1439
35	H9	24.81	43.43	40.59	AZm	0.3156
36	H10	26.57	42.51	42.1	AZm	0.1412
37	H11	25.67	41.01	42.19	AZm	0.1412
38	H12	23.76	42.07	43.35	AZm	0.1176
39	H13	24.63	43.65	43.41	AZm	0.1176
40	H14	26.21	41.67	44.74	AZm	0.2679
41	H0	24.06	42.1	40.51	AZm	0.3156
42	C	24.76	42.53	45.84	AZn	0.4964
43	C1	25.47	42.09	47.05	AZn	-0.1118
44	C2	24.83	42.46	48.44	AZn	-0.1201
45	O	23.69	43.17	45.88	AZn	-0.5373
46	C3	25.66	41.95	49.63	AZn	0.6785
47	N	25.01	42.03	50.88	AZn	-0.6275
48	C4	25.68	41.81	52.12	AZn	0.1466
49	C5	24.81	41.95	53.44	AZn	-0.1721
50	N1	25.57	41.71	54.69	AZn	-0.2058
51	C6	24.87	41.89	55.93	AZn	-0.0901
52	C7	25.82	41.7	57.13	AZn	0.0936
53	N2	25.2	41.87	58.45	AZn	-0.5617
54	O1	26.85	41.61	49.72	AZn	-0.589
55	C8	26.94	41.4	54.72	AZn	0.6197
56	O2	27.59	41.4	55.77	AZn	-0.5919
57	C9	27.65	41.21	53.43	AZn	-0.1068
58	C10	28.45	42.3	52.91	AZn	-0.0908
59	C11	27.52	40.04	52.66	AZn	-0.0908
60	C12	28.12	39.96	51.45	AZn	-0.3978
61	C13	29.01	42.25	51.6	AZn	-0.3978

62	C14	28.88	41	50.93	AZn	0.6088
63	N3	29.13	40.88	49.52	AZn	-0.3058
64	N4	30.3	41	49.07	AZn	-0.301
65	C15	31.56	40.98	49.82	AZn	0.5395
66	C16	31.77	40.05	50.8	AZn	-0.3555
67	C17	32.5	41.89	49.43	AZn	-0.3555
68	C18	33.68	41.97	50.14	AZn	-0.1802
69	C19	33.92	41.16	51.23	AZn	0.0704
70	C20	32.97	40.16	51.58	AZn	-0.1802
71	C21	35.18	41.16	52.07	AZn	-0.0148
72	N5	35.03	41.47	53.47	AZn	-0.6044
73	C22	35.04	42.77	53.94	AZn	0.746
74	C23	35.02	42.84	55.43	AZn	-0.2768
75	C24	36.48	42.72	55.98	AZn	0.026
76	C25	36.59	42.45	57.46	AZn	0.0599
77	O3	35.07	43.73	53.2	AZn	-0.6015
78	C26	38	41.92	57.88	AZn	-0.2266
79	H	26.54	42.33	47	AZn	0.0625
80	H1	25.46	40.99	46.96	AZn	0.0625
81	H2	23.8	42.15	48.59	AZn	0.0658
82	H3	24.7	43.54	48.56	AZn	0.0658
83	H4	24.08	42.44	50.97	AZn	0.318
84	H5	26.48	42.56	52.22	AZn	0.0583
85	H6	26.21	40.86	52.11	AZn	0.0583
86	H7	23.87	41.41	53.46	AZn	0.1039
87	H8	24.59	43.01	53.46	AZn	0.1039
88	H9	24.05	41.17	56.03	AZn	0.0979
89	H10	24.37	42.87	55.98	AZn	0.0979
90	H11	26.23	40.7	57.11	AZn	0.0686
91	H12	26.61	42.46	57.04	AZn	0.0686
92	H13	24.59	42.65	58.66	AZn	0.3186
93	H14	28.5	43.24	53.45	AZn	0.1596
94	H15	26.76	39.34	53	AZn	0.1596
95	H16	27.96	39.09	50.81	AZn	0.2245
96	H17	29.36	43.12	51.07	AZn	0.2245
97	H18	30.92	39.36	50.88	AZn	0.2185
98	H19	32.26	42.41	48.52	AZn	0.2185
99	H20	34.35	42.82	49.94	AZn	0.1726
100	H21	33.14	39.52	52.43	AZn	0.1726
101	H22	35.59	40.16	51.97	AZn	0.1021
102	H23	35.89	41.82	51.56	AZn	0.1021
103	H24	35.25	40.83	54.22	AZn	0.3283
104	H25	34.3	42.07	55.74	AZn	0.0736
105	H26	34.64	43.79	55.82	AZn	0.0736
106	H27	37.04	43.65	55.81	AZn	0.0203
107	H28	36.85	41.87	55.38	AZn	0.0203

108	H29	36.43	43.34	58.07	AZn	0.0084
109	H30	35.91	41.71	57.86	AZn	0.0084
110	H31	38.02	41.62	58.93	AZn	0.0567
111	H32	38.68	42.75	57.7	AZn	0.0567
112	H33	38.31	41.15	57.17	AZn	0.0567
113	C	25.42	40.99	59.44	AZr	0.6434
114	C1	24.72	41.29	60.71	AZr	-0.1381
115	C2	25.01	40.22	61.84	AZr	-0.1905
116	C3	24.33	40.5	63.14	AZr	0.6827
117	N	24.52	39.65	64.18	AZr	-0.6388
118	C4	23.71	39.74	65.39	AZr	0.0715
119	C5	22.91	38.45	65.59	AZr	-0.1591
120	N1	21.96	38.34	66.86	AZr	-0.1512
121	O	26.15	39.99	59.29	AZr	-0.5902
122	O1	23.6	41.46	63.32	AZr	-0.5593
123	C6	21.59	36.97	67.29	AZr	-0.1552
124	C7	20.98	36.11	66.22	AZr	0.0264
125	N2	20.65	34.77	66.75	AZr	-0.6607
126	C8	20.08	33.75	66.03	AZr	0.8118
127	C9	19.93	32.41	66.83	AZr	-0.4498
128	O2	19.75	33.83	64.88	AZr	-0.595
129	H	25.12	42.19	61.17	AZr	0.0788
130	H1	23.67	41.5	60.5	AZr	0.0788
131	H2	26.09	40.25	62.05	AZr	0.087
132	H3	24.8	39.17	61.63	AZr	0.087
133	H4	25.23	38.94	64.11	AZr	0.3398
134	H5	23	40.57	65.33	AZr	0.1036
135	H6	24.36	39.87	66.26	AZr	0.1036
136	H7	23.53	37.56	65.7	AZr	0.1443
137	H8	22.18	38.3	64.8	AZr	0.1443
138	H9	22.38	38.75	67.71	AZr	0.3067
139	H10	22.55	36.49	67.48	AZr	0.1479
140	H11	21.07	36.97	68.25	AZr	0.1479
141	H12	20.07	36.55	65.8	AZr	0.1165
142	H13	21.69	36.14	65.38	AZr	0.1165
143	H14	20.68	34.71	67.76	AZr	0.3407
144	H15	20.25	32.6	67.86	AZr	0.134
145	H16	18.85	32.26	66.87	AZr	0.134
146	H17	20.47	31.59	66.36	AZr	0.134
147	H0	21.16	38.98	66.75	AZr	0.3067

Reduced protonated trans

1	N	28.99	28.19	27.45	AZl	-0.4968
2	C	28.19	28.82	28.53	AZl	0.109

3	C1	28.19	28.02	29.85	AZl	-0.1613
4	N1	27.36	28.78	30.8	AZl	-0.3476
5	H	28.74	27.2	27.33	AZl	0.3667
6	H1	28.64	28.53	26.54	AZl	0.3667
7	H2	28.53	29.86	28.58	AZl	0.1071
8	H3	27.14	28.89	28.23	AZl	0.1071
9	H4	27.69	27.08	29.66	AZl	0.1509
10	H5	29.23	27.94	30.19	AZl	0.1509
11	H6	26.73	29.52	30.54	AZl	0.2806
12	H0	30.02	28.19	27.45	AZl	0.3667
13	C	27.38	28.51	32.12	AZm	0.57
14	C1	26.46	29.38	32.99	AZm	-0.137
15	C2	26.48	29.09	34.48	AZm	-0.1945
16	C3	25.55	29.98	35.29	AZm	0.6975
17	N	25.54	29.75	36.63	AZm	-0.6311
18	C4	24.54	30.35	37.59	AZm	0.0479
19	C5	24.98	30.06	39.02	AZm	-0.1394
20	N1	24.08	30.6	40.04	AZm	-0.1723
21	C6	24.62	30.26	41.42	AZm	-0.1468
22	C7	23.8	30.74	42.67	AZm	-0.0413
23	N2	24.4	30.36	43.97	AZm	-0.3432
24	O	28.08	27.66	32.58	AZm	-0.5601
25	O1	24.88	30.87	34.72	AZm	-0.5682
26	H	26.67	30.45	32.87	AZm	0.0842
27	H1	25.47	29.13	32.6	AZm	0.0842
28	H2	27.45	29.15	34.98	AZm	0.0926
29	H3	26.22	28.06	34.72	AZm	0.0926
30	H4	25.95	28.89	36.96	AZm	0.3366
31	H5	24.38	31.41	37.4	AZm	0.1119
32	H6	23.54	29.93	37.41	AZm	0.1119
33	H7	25.03	28.98	39.11	AZm	0.1439
34	H8	25.91	30.62	39.17	AZm	0.1439
35	H9	23.86	31.6	39.88	AZm	0.3156
36	H10	25.62	30.68	41.39	AZm	0.1412
37	H11	24.72	29.18	41.49	AZm	0.1412
38	H12	22.82	30.24	42.65	AZm	0.1176
39	H13	23.68	31.82	42.71	AZm	0.1176
40	H14	25.27	29.84	44.03	AZm	0.2679
41	H0	23.12	30.28	39.81	AZm	0.3156
42	C	23.81	30.7	45.13	AZN	0.4868
43	C1	24.55	30.24	46.38	AZN	-0.1045
44	C2	23.76	30.71	47.61	AZN	-0.1495
45	O	22.79	31.32	45.18	AZN	-0.536
46	C3	24.42	30.3	48.93	AZN	0.7113
47	N	24	30.87	50.08	AZN	-0.644
48	C4	24.69	30.8	51.33	AZN	0.1218

49	C5	24.07	31.52	52.55	AZN	-0.1462
50	N1	24.87	31.39	53.83	AZN	-0.2144
51	C6	24.27	32.17	54.98	AZN	-0.0688
52	C7	25.06	32.12	56.22	AZN	0.1197
53	N2	24.31	32.8	57.3	AZN	-0.5637
54	O1	25.35	29.53	49.05	AZN	-0.5993
55	C8	26.05	30.69	53.89	AZN	0.6414
56	O2	26.43	29.97	52.99	AZN	-0.5916
57	C9	26.73	30.74	55.2	AZN	-0.1923
58	C10	27.94	31.45	55.3	AZN	-0.0553
59	C11	26.28	29.92	56.26	AZN	-0.0553
60	C12	27.08	29.83	57.41	AZN	-0.2439
61	C13	28.76	31.38	56.46	AZN	-0.2439
62	C14	28.25	30.59	57.5	AZN	0.3916
63	N3	28.95	30.52	58.8	AZN	-0.2321
64	N4	29.88	31.32	58.9	AZN	-0.1986
65	C15	30.59	31.28	60.21	AZN	0.3268
66	C16	31.37	32.42	60.46	AZN	-0.1999
67	C17	30.45	30.3	61.17	AZN	-0.1999
68	C18	31.13	30.39	62.43	AZN	-0.1747
69	C19	31.93	31.48	62.65	AZN	0.0128
70	C20	32.07	32.47	61.64	AZN	-0.1747
71	C21	32.87	31.52	63.89	AZN	-0.0035
72	N5	34.25	31.65	63.46	AZN	-0.6007
73	C22	34.95	30.72	62.82	AZN	0.7477
74	C23	36.38	31.08	62.31	AZN	-0.271
75	C24	37.44	30.53	63.25	AZN	0.0257
76	C25	37.83	29.06	62.83	AZN	0.079
77	O3	34.42	29.65	62.61	AZN	-0.6072
78	C26	38.97	28.47	63.71	AZN	-0.2524
79	H	25.53	30.74	46.43	AZN	0.0612
80	H1	24.64	29.16	46.44	AZN	0.0612
81	H2	22.74	30.35	47.48	AZN	0.0723
82	H3	23.77	31.79	47.62	AZN	0.0723
83	H4	23.17	31.45	50.12	AZN	0.3257
84	H5	25.59	31.43	51.19	AZN	0.0648
85	H6	24.9	29.78	51.66	AZN	0.0648
86	H7	23.11	31.04	52.77	AZN	0.1003
87	H8	23.91	32.55	52.24	AZN	0.1003
88	H9	23.26	31.79	55.18	AZN	0.0882
89	H10	24.15	33.2	54.62	AZN	0.0882
90	H11	25.21	31.06	56.46	AZN	0.0599
91	H12	26.05	32.56	56.05	AZN	0.0599
92	H13	23.47	33.31	57.09	AZN	0.3215
93	H14	28.33	31.98	54.43	AZN	0.1513
94	H15	25.27	29.5	56.15	AZN	0.1513

95	H16	26.7	29.18	58.2	AZN	0.1418
96	H17	29.68	31.92	56.58	AZN	0.1418
97	H18	31.64	33.16	59.71	AZN	0.1394
98	H19	29.93	29.39	60.89	AZN	0.1394
99	H20	31.13	29.59	63.16	AZN	0.1695
100	H21	32.69	33.35	61.8	AZN	0.1695
101	H22	32.6	32.33	64.58	AZN	0.104
102	H23	32.77	30.65	64.55	AZN	0.104
103	H24	34.61	32.58	63.61	AZN	0.3263
104	H25	36.43	32.18	62.21	AZN	0.0712
105	H26	36.67	30.71	61.33	AZN	0.0712
106	H27	37.07	30.61	64.27	AZN	0.0179
107	H28	38.26	31.23	63.26	AZN	0.0179
108	H29	36.91	28.49	62.92	AZN	0.0053
109	H30	38.21	29.01	61.8	AZN	0.0053
110	H31	38.99	27.41	63.43	AZN	0.0637
111	H32	38.75	28.6	64.78	AZN	0.0637
112	H33	39.9	28.99	63.49	AZN	0.0637
113	C	24.71	32.74	58.58	AZr	0.6434
114	C1	23.85	33.46	59.54	AZr	-0.1381
115	C2	24.38	33.36	61.04	AZr	-0.1905
116	C3	23.53	34.07	62.03	AZr	0.6827
117	N	23.9	34.06	63.34	AZr	-0.6388
118	C4	23.01	34.56	64.38	AZr	0.0715
119	C5	22.66	33.42	65.36	AZr	-0.1591
120	N1	21.7	33.74	66.57	AZr	-0.1512
121	O	25.74	32.12	58.92	AZr	-0.5902
122	O1	22.52	34.69	61.74	AZr	-0.5593
123	C6	21.76	32.82	67.73	AZr	-0.1552
124	C7	21.55	31.36	67.39	AZr	0.0264
125	N2	21.63	30.52	68.6	AZr	-0.6607
126	C8	21.49	29.16	68.64	AZr	0.8118
127	C9	21.71	28.53	70.05	AZr	-0.4498
128	O2	21.25	28.48	67.68	AZr	-0.595
129	H	23.9	34.53	59.38	AZr	0.0788
130	H1	22.81	33.17	59.37	AZr	0.0788
131	H2	25.36	33.84	61.07	AZr	0.087
132	H3	24.53	32.37	61.47	AZr	0.087
133	H4	24.81	33.71	63.59	AZr	0.3398
134	H5	22.07	34.93	63.96	AZr	0.1036
135	H6	23.5	35.34	64.96	AZr	0.1036
136	H7	23.53	32.99	65.87	AZr	0.1443
137	H8	22.09	32.64	64.86	AZr	0.1443
138	H9	21.89	34.66	67	AZr	0.3067
139	H10	22.8	32.86	68.04	AZr	0.1479
140	H11	21.18	33.18	68.58	AZr	0.1479

141	H12	20.59	31.18	66.9	AZr	0.1165
142	H13	22.28	31.15	66.6	AZr	0.1165
143	H14	21.6	31.05	69.47	AZr	0.3407
144	H15	21.87	29.35	70.77	AZr	0.134
145	H16	20.74	28.1	70.29	AZr	0.134
146	H17	22.53	27.81	70.06	AZr	0.134
147	H0	20.74	33.92	66.23	AZr	0.3067

Reduced unprotonated cis

1	N	48.56	30.72	35.45	AZL	-0.9864
2	C	49.29	30.72	36.72	AZL	0.3807
3	C1	48.96	29.48	37.56	AZL	-0.1769
4	N1	49.73	29.51	38.86	AZL	-0.4455
5	H	47.56	30.72	35.62	AZL	0.3646
6	H1	48.7	29.79	35.05	AZL	0.3646
7	H2	50.38	30.72	36.58	AZL	-0.0098
8	H3	49.09	31.62	37.29	AZL	-0.0098
9	H4	47.92	29.46	37.89	AZL	0.1124
10	H5	49.14	28.56	36.99	AZL	0.1124
11	H6	50.59	30.02	38.95	AZL	0.2937
12	C	49.29	28.85	39.95	AZM	0.6115
13	C1	50.18	28.98	41.19	AZM	-0.1848
14	C2	49.44	28.5	42.55	AZM	-0.1373
15	C3	50.35	28.65	43.69	AZM	0.6687
16	N	49.73	28.75	44.87	AZM	-0.5237
17	C4	50.4	28.7	46.16	AZM	-0.1513
18	C5	49.47	28.84	47.45	AZM	0.1172
19	N1	50.32	28.76	48.7	AZM	-0.6478
20	C6	49.49	28.9	49.93	AZM	0.1015
21	C7	50.45	28.78	51.16	AZM	-0.1528
22	N2	49.75	28.9	52.35	AZM	-0.4682
23	O	48.26	28.21	39.94	AZM	-0.5674
24	O1	51.54	28.84	43.63	AZM	-0.589
25	H	50.97	28.24	41.01	AZM	0.0766
26	H1	50.67	29.95	41.22	AZM	0.0766
27	H2	49.17	27.45	42.49	AZM	0.0659
28	H3	48.52	29.08	42.55	AZM	0.0659
29	H4	48.73	28.72	44.86	AZM	0.2902
30	H5	51.01	27.78	46.17	AZM	0.1262
31	H6	50.99	29.61	46.23	AZM	0.1262
32	H7	48.95	29.81	47.41	AZM	0.0487
33	H8	48.72	28.05	47.43	AZM	0.0487
34	H9	50.65	27.83	48.88	AZM	0.3666
35	H10	48.7	28.14	49.98	AZM	0.0523

36	H11	48.97	29.85	49.97	AZM	0.0523
37	H12	51.29	29.47	51.08	AZM	0.1242
38	H13	50.73	27.73	51.17	AZM	0.1242
39	H14	48.76	29.03	52.31	AZM	0.2788
40	C	50.38	28.83	53.54	AZn	0.4964
41	C1	49.5	28.97	54.72	AZn	-0.1118
42	C2	50.19	28.89	56.14	AZn	-0.1201
43	O	51.6	28.66	53.63	AZn	-0.5373
44	C3	49.18	29.05	57.3	AZn	0.6785
45	N	49.77	29.25	58.56	AZn	-0.6275
46	C4	49.02	29.19	59.78	AZn	0.1466
47	C5	49.83	29.43	61.12	AZn	-0.1721
48	N1	48.99	29.36	62.35	AZn	-0.2058
49	C6	49.66	29.48	63.61	AZn	-0.0901
50	C7	48.67	29.29	64.78	AZn	0.0936
51	N2	49.26	29.39	66.11	AZn	-0.5617
52	O1	47.95	28.89	57.34	AZn	-0.589
53	C8	47.61	29.1	62.33	AZn	0.6197
54	O2	46.98	28.86	63.36	AZn	-0.5919
55	C9	46.93	28.98	61.01	AZn	-0.1068
56	C10	46.64	27.66	60.5	AZn	-0.0908
57	C11	46.62	30.1	60.22	AZn	-0.0908
58	C12	46.07	29.93	58.99	AZn	-0.3978
59	C13	46.16	27.47	59.17	AZn	-0.3978
60	C14	45.81	28.66	58.48	AZn	0.6088
61	N3	45.58	28.67	57.06	AZn	-0.3058
62	N4	44.57	28.09	56.58	AZn	-0.301
63	C15	43.38	27.61	57.29	AZn	0.5395
64	C16	42.79	28.39	58.25	AZn	-0.3555
65	C17	42.88	26.4	56.9	AZn	-0.3555
66	C18	41.81	25.87	57.57	AZn	-0.1802
67	C19	41.23	26.53	58.64	AZn	0.0704
68	C20	41.7	27.83	58.99	AZn	-0.1802
69	C21	40.05	26.04	59.44	AZn	-0.0148
70	N5	40.26	25.84	60.85	AZn	-0.6044
71	C22	40.74	24.64	61.35	AZn	0.746
72	C23	40.74	24.6	62.84	AZn	-0.2768
73	C24	39.32	24.14	63.34	AZn	0.026
74	C25	39.06	24.36	64.82	AZn	0.0599
75	O3	41.12	23.73	60.64	AZn	-0.6015
76	C26	37.55	24.29	65.18	AZn	-0.2266
77	H	48.62	28.33	54.65	AZn	0.0625
78	H1	49.08	29.98	54.61	AZn	0.0625
79	H2	51.01	29.59	56.31	AZn	0.0658
80	H3	50.73	27.96	56.29	AZn	0.0658
81	H4	50.78	29.23	58.69	AZn	0.318

82	H5	48.58	28.19	59.87	AZn	0.0583
83	H6	48.16	29.86	59.73	AZn	0.0583
84	H7	50.48	30.3	61.16	AZn	0.1039
85	H8	50.45	28.53	61.17	AZn	0.1039
86	H9	50.13	30.46	63.71	AZn	0.0979
87	H10	50.5	28.78	63.69	AZn	0.0979
88	H11	47.9	30.05	64.72	AZn	0.0686
89	H12	48.25	28.28	64.69	AZn	0.0686
90	H13	50.12	28.92	66.37	AZn	0.3186
91	H14	46.95	26.78	61.06	AZn	0.1596
92	H15	47.02	31.05	60.57	AZn	0.1596
93	H16	45.9	30.78	58.33	AZn	0.2245
94	H17	46.19	26.52	58.65	AZn	0.2245
95	H18	43.29	29.36	58.33	AZn	0.2185
96	H19	43.34	26.01	56	AZn	0.2185
97	H20	41.54	24.83	57.38	AZn	0.1726
98	H21	41.26	28.36	59.82	AZn	0.1726
99	H22	39.27	26.8	59.3	AZn	0.1021
100	H23	39.67	25.15	58.93	AZn	0.1021
101	H24	39.77	26.34	61.58	AZn	0.3283
102	H25	41.08	25.59	63.15	AZn	0.0736
103	H26	41.44	23.88	63.27	AZn	0.0736
104	H27	39.18	23.07	63.18	AZn	0.0203
105	H28	38.67	24.76	62.72	AZn	0.0203
106	H29	39.54	23.61	65.46	AZn	0.0084
107	H30	39.38	25.32	65.22	AZn	0.0084
108	H31	37.38	24.58	66.22	AZn	0.0567
109	H32	37.26	23.26	65	AZn	0.0567
110	H33	36.98	24.88	64.45	AZn	0.0567
111	C	48.68	30.13	67.08	AZR	0.5913
112	C1	49.4	30.14	68.39	AZR	-0.1671
113	C2	48.68	30.97	69.36	AZR	-0.1396
114	C3	49.33	31.04	70.7	AZR	0.6829
115	N	48.66	31.77	71.64	AZR	-0.5674
116	C4	48.94	31.87	73.07	AZR	-0.1322
117	C5	47.67	32.38	73.84	AZR	0.1201
118	N1	48.02	32.46	75.29	AZR	-0.6489
119	O	47.64	30.74	66.89	AZR	-0.5626
120	O1	50.36	30.46	70.97	AZR	-0.5892
121	C6	46.85	32.51	76.17	AZR	0.1054
122	C7	47.42	32.95	77.49	AZR	-0.117
123	N2	46.4	33.08	78.58	AZR	-0.5836
124	C8	46.56	33.45	79.86	AZR	0.8163
125	C9	45.33	33.34	80.64	AZR	-0.4497
126	O2	47.65	33.7	80.31	AZR	-0.6332
127	H	49.57	29.11	68.72	AZR	0.0761

128	H1	50.38	30.54	68.15	AZR	0.0761
129	H2	47.64	30.66	69.45	AZR	0.0638
130	H3	48.65	31.98	68.92	AZR	0.0638
131	H4	47.79	32.14	71.3	AZR	0.3074
132	H5	49.79	32.52	73.25	AZR	0.1236
133	H6	49.17	30.91	73.53	AZR	0.1236
134	H7	46.85	31.7	73.62	AZR	0.0468
135	H8	47.28	33.34	73.47	AZR	0.0468
136	H9	48.6	33.27	75.5	AZR	0.3505
137	H10	46.03	33.17	75.88	AZR	0.0519
138	H11	46.48	31.48	76.2	AZR	0.0519
139	H12	48.19	32.25	77.82	AZR	0.1155
140	H13	47.91	33.93	77.41	AZR	0.1155
141	H14	45.48	32.82	78.27	AZR	0.3033
142	H15	44.44	33.67	80.12	AZR	0.1193
143	H16	45.29	32.32	81.04	AZR	0.1193
144	H17	45.45	34.03	81.49	AZR	0.1193

Reduced unprotonated trans

1	N	43.31	31.12	34.41	AZL	-0.9864
2	C	44.05	31.12	35.68	AZL	0.3807
3	C1	43.72	29.88	36.52	AZL	-0.1769
4	N1	44.49	29.91	37.83	AZL	-0.4455
5	H	42.31	31.12	34.59	AZL	0.3646
6	H1	43.45	30.2	34.01	AZL	0.3646
7	H2	45.14	31.12	35.55	AZL	-0.0098
8	H3	43.84	32.03	36.26	AZL	-0.0098
9	H4	42.67	29.87	36.86	AZL	0.1124
10	H5	43.9	28.97	35.96	AZL	0.1124
11	H6	45.35	30.42	37.91	AZL	0.2937
12	C	44.05	29.26	38.91	AZM	0.6115
13	C1	44.94	29.38	40.16	AZM	-0.1848
14	C2	44.19	28.91	41.52	AZM	-0.1373
15	C3	45.1	29.05	42.66	AZM	0.6687
16	N	44.49	29.16	43.84	AZM	-0.5237
17	C4	45.16	29.1	45.13	AZM	-0.1513
18	C5	44.22	29.25	46.42	AZM	0.1172
19	N1	45.07	29.17	47.67	AZM	-0.6478
20	C6	44.24	29.3	48.9	AZM	0.1015
21	C7	45.21	29.19	50.13	AZM	-0.1528
22	N2	44.51	29.3	51.32	AZM	-0.4682
23	O	43.01	28.61	38.91	AZM	-0.5674
24	O1	46.29	29.24	42.6	AZM	-0.589
25	H	45.72	28.65	39.98	AZM	0.0766

26	H1	45.42	30.35	40.19	AZM	0.0766
27	H2	43.92	27.85	41.46	AZM	0.0659
28	H3	43.27	29.49	41.52	AZM	0.0659
29	H4	43.48	29.12	43.83	AZM	0.2902
30	H5	45.76	28.19	45.13	AZM	0.1262
31	H6	45.74	30.02	45.2	AZM	0.1262
32	H7	43.7	30.22	46.38	AZM	0.0487
33	H8	43.47	28.46	46.4	AZM	0.0487
34	H9	45.41	28.23	47.85	AZM	0.3666
35	H10	43.45	28.55	48.95	AZM	0.0523
36	H11	43.72	30.26	48.94	AZM	0.0523
37	H12	46.04	29.88	50.05	AZM	0.1242
38	H13	45.48	28.13	50.14	AZM	0.1242
39	H14	43.51	29.44	51.27	AZM	0.2788
40	C	45.13	29.23	52.51	AZN	0.4868
41	C1	44.23	29.38	53.72	AZN	-0.1045
42	C2	45.09	29.28	54.98	AZN	-0.1495
43	O	46.31	29.07	52.6	AZN	-0.536
44	C3	44.28	29.41	56.28	AZN	0.7113
45	N	44.85	29.06	57.46	AZN	-0.644
46	C4	44.14	28.86	58.68	AZN	0.1218
47	C5	44.96	28.46	59.93	AZN	-0.1462
48	N1	44.13	28.28	61.18	AZN	-0.2144
49	C6	44.94	27.82	62.37	AZN	-0.0688
50	C7	44.15	27.56	63.59	AZN	0.1197
51	N2	45.07	27.25	64.7	AZN	-0.5637
52	O1	43.12	29.75	56.35	AZN	-0.5993
53	C8	42.76	28.46	61.2	AZN	0.6414
54	O2	42.16	28.97	60.27	AZN	-0.5916
55	C9	42.11	28.16	62.49	AZN	-0.1923
56	C10	41.28	27.03	62.57	AZN	-0.0553
57	C11	42.16	29.11	63.54	AZN	-0.0553
58	C12	41.35	28.88	64.66	AZN	-0.2439
59	C13	40.45	26.78	63.7	AZN	-0.2439
60	C14	40.57	27.72	64.74	AZN	0.3916
61	N3	39.86	27.53	66.02	AZN	-0.2321
62	N4	39.31	26.43	66.11	AZN	-0.1986
63	C15	38.6	26.19	67.4	AZN	0.3268
64	C16	38.32	24.84	67.65	AZN	-0.1999
65	C17	38.31	27.16	68.33	AZN	-0.1999
66	C18	37.67	26.83	69.58	AZN	-0.1747
67	C19	37.36	25.51	69.8	AZN	0.0128
68	C20	37.65	24.53	68.81	AZN	-0.1747
69	C21	36.46	25.11	71.02	AZN	-0.0035
70	N5	35.27	24.44	70.55	AZN	-0.6007
71	C22	34.28	25.01	69.86	AZN	0.7477

72	C23	33.13	24.11	69.32	AZN	-0.271
73	C24	31.9	24.22	70.22	AZN	0.0257
74	C25	30.98	25.41	69.75	AZN	0.079
75	O3	34.35	26.21	69.65	AZN	-0.6072
76	C26	29.67	25.51	70.59	AZN	-0.2524
77	H	43.52	28.54	53.75	AZN	0.0612
78	H1	43.71	30.34	53.75	AZN	0.0612
79	H2	45.9	30.01	54.88	AZN	0.0723
80	H3	45.51	28.27	55.02	AZN	0.0723
81	H4	45.84	28.85	57.53	AZN	0.3257
82	H5	43.57	27.94	58.53	AZN	0.0648
83	H6	43.53	29.73	58.98	AZN	0.0648
84	H7	45.64	29.28	60.17	AZN	0.1003
85	H8	45.52	27.58	59.65	AZN	0.1003
86	H9	45.71	28.56	62.59	AZN	0.0882
87	H10	45.47	26.91	62.04	AZN	0.0882
88	H11	43.59	28.48	63.79	AZN	0.0599
89	H12	43.41	26.77	63.4	AZN	0.0599
90	H13	46.05	27.1	64.53	AZN	0.3215
91	H14	41.15	26.38	61.7	AZN	0.1513
92	H15	42.92	29.88	63.45	AZN	0.1513
93	H16	41.42	29.64	65.45	AZN	0.1418
94	H17	39.81	25.92	63.81	AZN	0.1418
95	H18	38.4	24.05	66.91	AZN	0.1394
96	H19	38.44	28.19	68.05	AZN	0.1394
97	H20	37.33	27.57	70.29	AZN	0.1695
98	H21	37.43	23.48	68.97	AZN	0.1695
99	H22	37.01	24.49	71.73	AZN	0.104
100	H23	36.19	25.96	71.65	AZN	0.104
101	H24	35.3	23.45	70.71	AZN	0.3263
102	H25	33.51	23.08	69.25	AZN	0.0712
103	H26	32.74	24.33	68.33	AZN	0.0712
104	H27	32.24	24.3	71.25	AZN	0.0179
105	H28	31.43	23.24	70.22	AZN	0.0179
106	H29	31.59	26.29	69.86	AZN	0.0053
107	H30	30.65	25.29	68.71	AZN	0.0053
108	H31	29.24	26.47	70.29	AZN	0.0637
109	H32	29.88	25.49	71.67	AZN	0.0637
110	H33	29.03	24.66	70.36	AZN	0.0637
111	C	44.63	27.16	65.97	AZR	0.5913
112	C1	45.68	26.84	66.98	AZR	-0.1671
113	C2	45.09	26.76	68.33	AZR	-0.1396
114	C3	46.06	26.45	69.4	AZR	0.6829
115	N	45.54	26.33	70.66	AZR	-0.5674
116	C4	46.2	25.86	71.87	AZR	-0.1322
117	C5	45.13	25.4	72.93	AZR	0.1201

118	N1	45.87	24.93	74.15	AZR	-0.6489
119	O	43.46	27.32	66.26	AZR	-0.5626
120	O1	47.24	26.28	69.2	AZR	-0.5892
121	C6	45.06	24.09	75.03	AZR	0.1054
122	C7	45.85	24.06	76.31	AZR	-0.117
123	N2	45.22	23.25	77.4	AZR	-0.5836
124	C8	45.65	23.01	78.65	AZR	0.8163
125	C9	44.79	22.08	79.38	AZR	-0.4497
126	O2	46.71	23.43	79.03	AZR	-0.6332
127	H	46.22	25.94	66.69	AZR	0.0761
128	H1	46.39	27.65	66.9	AZR	0.0761
129	H2	44.26	26.06	68.35	AZR	0.0638
130	H3	44.65	27.75	68.51	AZR	0.0638
131	H4	44.54	26.44	70.67	AZR	0.3074
132	H5	46.85	26.62	72.28	AZR	0.1236
133	H6	46.82	24.97	71.7	AZR	0.1236
134	H7	44.51	24.63	72.47	AZR	0.0468
135	H8	44.4	26.17	73.19	AZR	0.0468
136	H9	46.24	25.7	74.69	AZR	0.3505
137	H10	44.04	24.43	75.24	AZR	0.0519
138	H11	45.02	23.12	74.54	AZR	0.0519
139	H12	46.85	23.65	76.12	AZR	0.1155
140	H13	46.01	25.06	76.72	AZR	0.1155
141	H14	44.36	22.82	77.1	AZR	0.3033
142	H15	43.73	22.23	79.22	AZR	0.1193
143	H16	45.16	21.07	79.16	AZR	0.1193
144	H17	44.97	22.27	80.44	AZR	0.1193

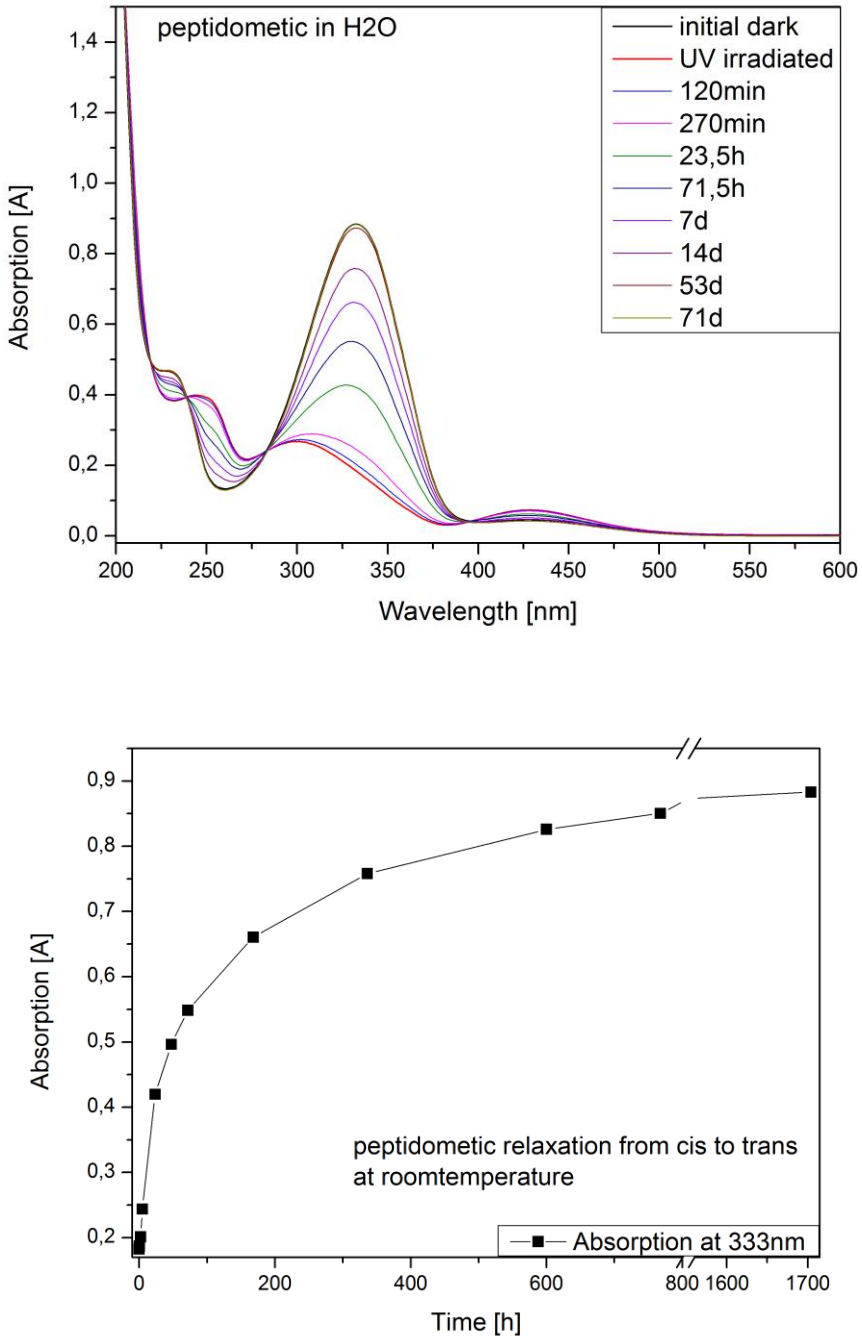


Figure S5. Thermal relaxation kinetic from *cis*- to *trans*-somer of the azobenzene containing peptidometic. The relaxation curve can be fitted with an exponential decay second order, with relaxation times τ_1= 18(± 2) h and τ_2= 270(± 18) h.

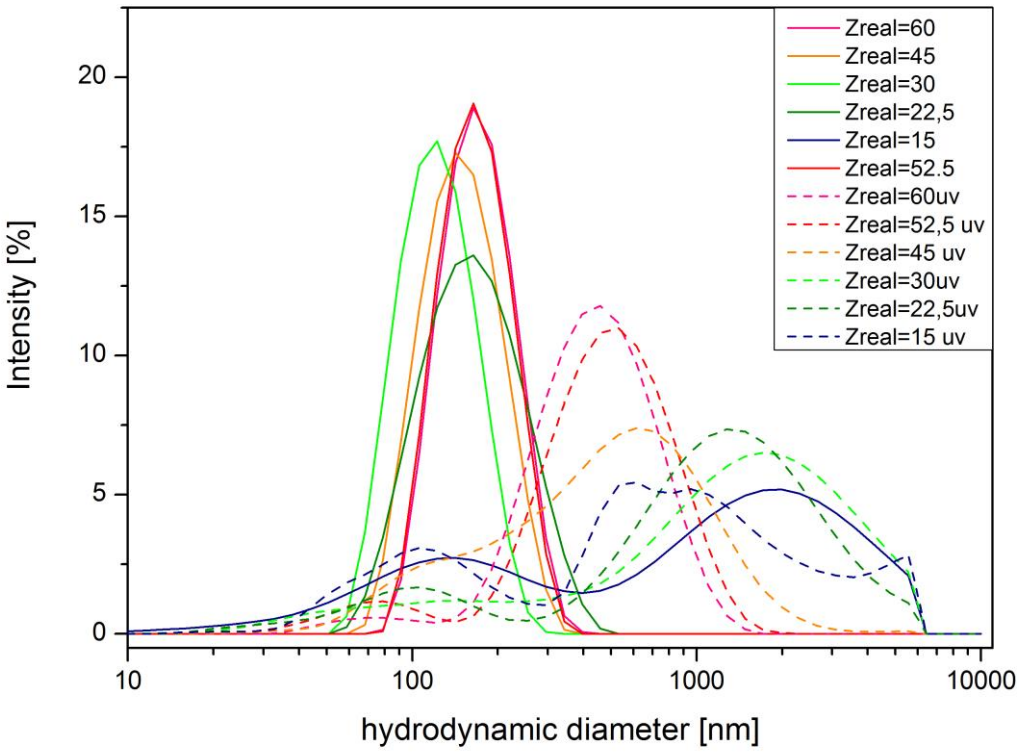


Figure S6. DLS data of DNA-PM complexes with varying Z values (15 to 60), in dark state (solid lines), irradiated with UV light (dashed lines).

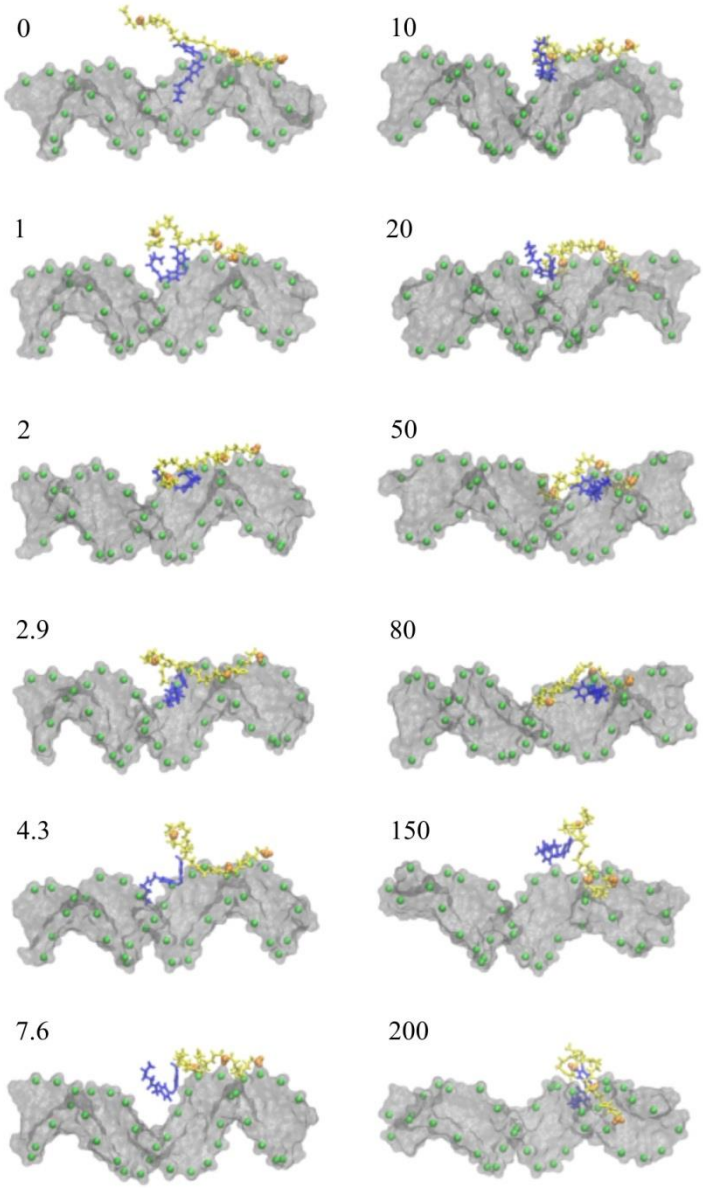


Figure S7. Snapshots from simulation for the protonated *trans* Azo-PM. The time, at which the snapshorts were taken, is shown in the figure in nano-seconds.

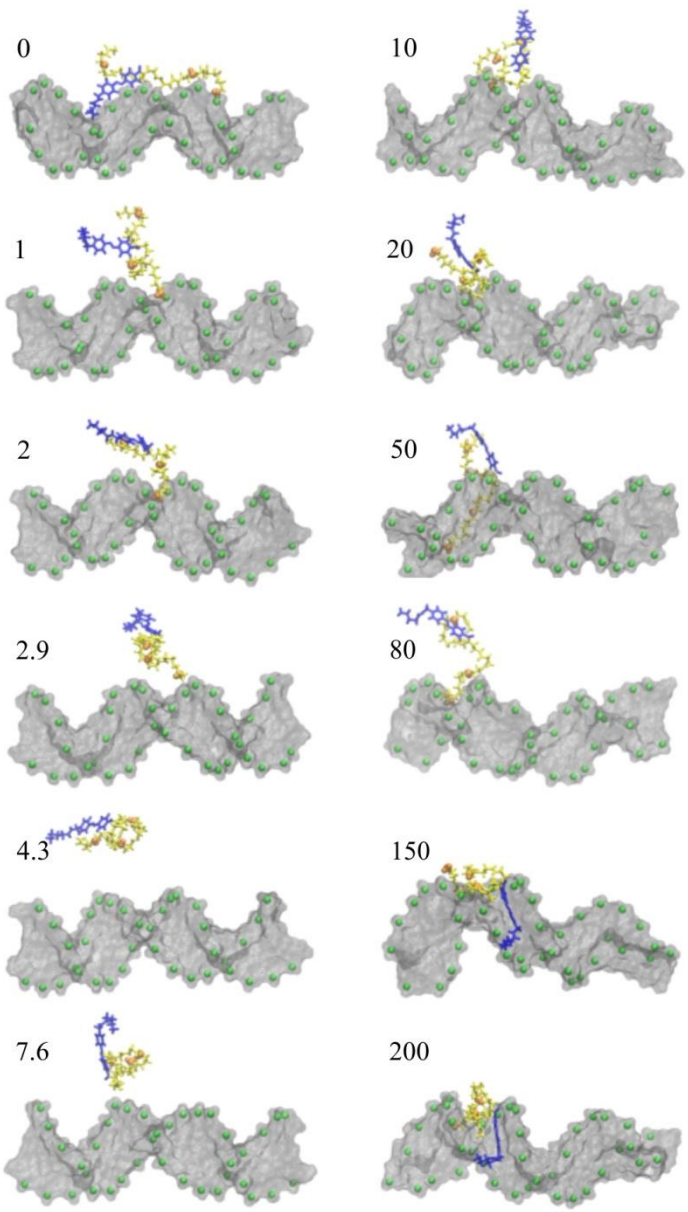


Figure S8. Snapshots from simulation for the protonated *cis* Azo-PM. The time, at which the snapshorts were taken, is shown in the figure in nano-seconds.

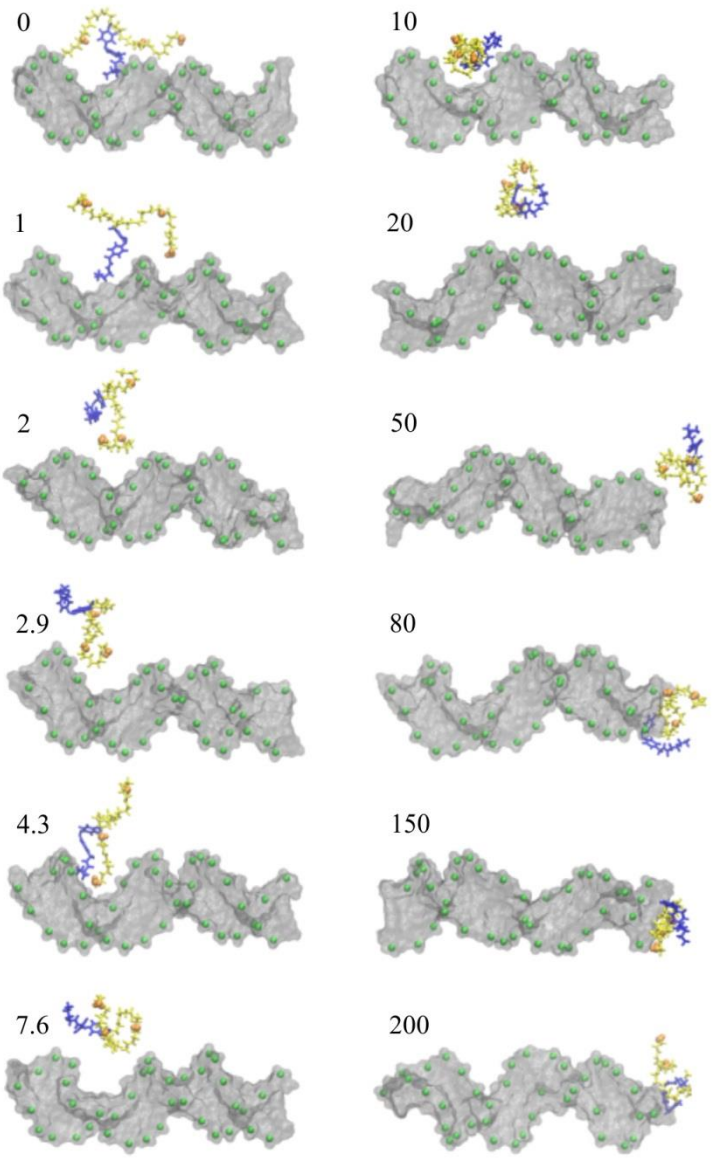


Figure S9. Snapshots from simulation for the unprotonated *trans* Azo-PM. The time, at which the snapshorts were taken, is shown in the figure in nano-seconds.

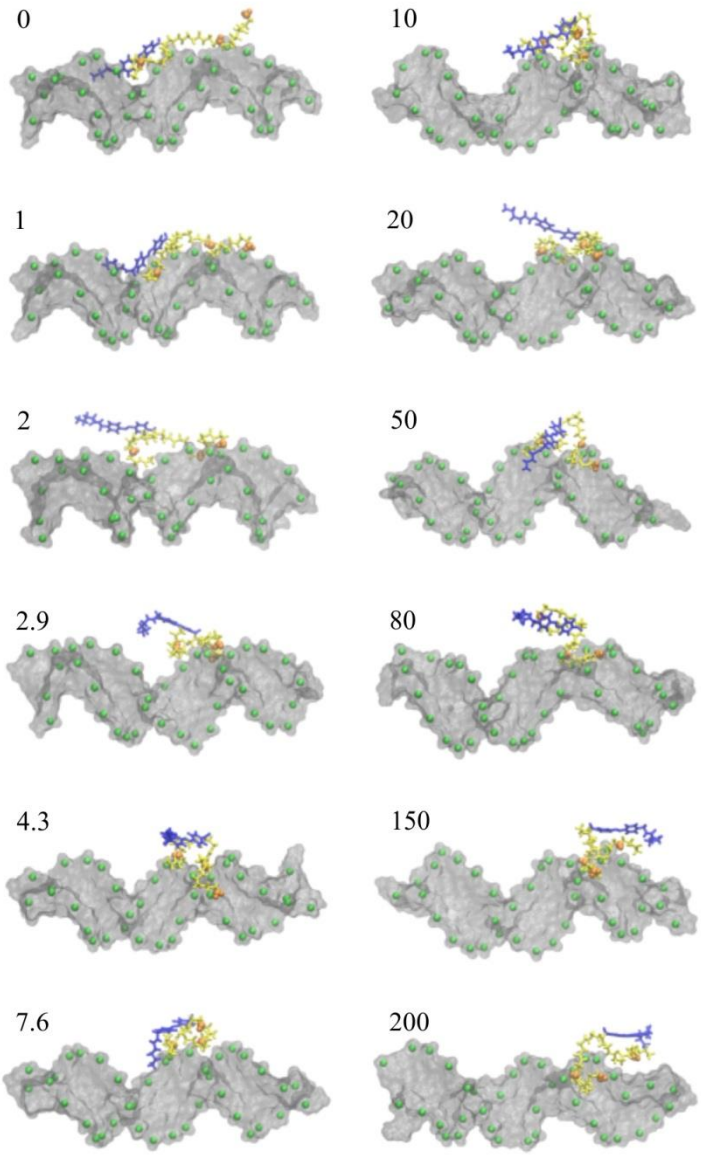


Figure S10. Snapshots from simulation for the unprotonated *cis* Azo-PM. The time, at which the snapshorts were taken, is shown in the figure in nano-seconds.