Supplementary information for manuscript:

Bis(4-nitroanilines) in interaction through a π-conjugated bridge: conformational effects and potential molecular switches

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(B3PW91/6-31G*) DFT computed conformations

1. Isomer *OFF* (E = 0) - No constraint

C	5.464228	2.025491	-8.534751
H	4.892097	2.949645	-8.548472
C	6.826610	2.067404	-8.178475
C	7.573689	0.850086	-8.165608
C	6.940721	-0.347713	-8.508736
H	7.492787	-1.279815	-8.502645
C	5.596881	-0.348448	-8.856067
C	4.852222	0.833786	-8.870788
H	3.804404	0.796442	-9.145362
C	10.118975	0.919490	-7.478125
C	8.943865	0.871722	-7.799768
C	13.520160	2.111358	-6.519497
H	14.044151	3.045506	-6.342032
C	14.218176	0.895132	-6.382881
C	13.525795	-0.308665	-6.617817
H	14.049680	-1.254134	-6.512850
C	12.188349	-0.298580	-6.975180
H	11.664355	-1.232729	-7.152635
C	11.490336	0.917646	-7.111810
C	12.182712	2.121442	-6.876853
H	11.658821	3.066912	-6.981785
C	15.589541	0.893271	-6.016580
C	16.764664	0.941024	-5.694982
C	20.111933	2.160832	-4.639125
C	20.856721	0.978711	-4.625708
H	21.904624	1.015875	-4.351396
C	20.244759	-0.212843	-4.962474
H	20.817073	-1.136901	-4.949962
C	18.882283	-0.254640	-5.318318
C	18.135023	0.962617	-5.329837
C	18.767944	2.160215	-4.985967
H	18.215765	3.092257	-4.990940
N	7.440237	3.244774	-7.879011
H	6.879772	4.057201	-7.674911
N	18.268594	-1.431808	-5.618406
H	18.829037	-2.244101	-5.823115
N	4.953782	-1.602498	-9.208030
O	3.763149	-1.568994	-9.507867
O	5.636033	-2.623332	-9.185717
N	20.754976	3.414695	-4.286348
O	20.072294	4.435282	-4.306621
O	21.945572	3.380986	-3.986397
H	8.359552	3.211083	-7.462189
H	17.349203	-1.397821	-6.035030

2. Isomer *ON* state (E = 0)* - No constraint

C	7.608951	0.291079	1.162022
H	8.192269	0.050544	2.047207
C	6.208135	0.148601	1.203726
C	5.447680	0.463034	0.036337
C	6.107516	0.898097	-1.116433
H	5.545563	1.141639	-2.010098
C	7.489735	1.024483	-1.119164
C	8.246859	0.723585	0.015802
H	9.324288	0.835133	-0.021510
C	2.822980	0.217978	0.119714
C	4.035434	0.334624	0.064494
C	-0.721873	0.322590	-1.013885
H	-1.290831	0.594550	-1.897618
C	-1.404150	-0.151816	0.124186
C	-0.652607	-0.501265	1.262601
H	-1.164344	-0.874698	2.144715
C	0.726764	-0.380833	1.264144
H	1.292966	-0.658473	2.148336
C	1.408999	0.093499	0.127228
C	0.657188	0.442987	-1.012337
H	1.172393	0.809431	-1.894897
C	-2.818357	-0.275190	0.114428
C	-4.032509	-0.372457	0.060236
C	-7.541284	-0.479191	-1.159519
C	-8.245930	-0.740196	0.018317
H	-9.325480	-0.828780	-0.019164
C	-7.554758	-0.878258	1.206227
H	-8.096333	-1.084533	2.125978
C	-6.151622	-0.761447	1.247584
C	-5.445444	-0.495097	0.035037
C	-6.158615	-0.356817	-1.158969
H	-5.638461	-0.152892	-2.087261
N	8.160317	1.481029	-2.324547
O	9.383740	1.585188	-2.291965
O	7.466801	1.736563	-3.305034
N	-8.268649	-0.331001	-2.408610
O	-7.620796	-0.100587	-3.425959
O	-9.491122	-0.445114	-2.373618
N	-5.464876	-0.928014	2.411680
H	-5.963010	-0.891729	3.287281
H	-4.492591	-0.655353	2.432397
N	5.579849	-0.309536	2.321061
H	6.075830	-0.321109	3.198288
H	4.574117	-0.230891	2.368162

* after steps 1 and 2 in Figure 4 (manuscript).