Supporting Information

for

Synthesis and Rotation Barriers in 2,6-Di-(o-anisyl)anisole

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1d, ^{1}H NMR (500 MHz, CD_2Cl_2) δ 3.143 (s, 3H, OMe), 3.816 (s, 6H, OMe), 7.016 (dd, J = 8.3, 1.2 Hz, 2H, *ortho* to OMe), 7.018 (dt, J = 1.1, 7.6 Hz, 2H, *para* to OMe), 7.147 (A, 1H, *para* to OMe in central ring) and 7.231 (B, 2H, *meta* to OMe in central ring), AB_2 system (J_{AB} = 7.6 Hz), 7.293 (dd, J = 7.7, 1.8 Hz, 2H, *meta* to OMe and *ortho* to central ring), 7.357 (ddd, J = 8.2, 7.5, 1.8 Hz, 2H, *meta* to OMe and *para* to central ring). ^{13}C NMR (125 MHz, CD_2Cl_2) δ 56.00 (OMe), 60.75 (OMe of central ring), 111.34 (CH, *ortho* to OMe in outer ring), 120.79 (CH, *para* to OMe in outer ring), 123.17 (C_q, *ortho* to OMe in outer ring), 128.61 (C_q, *ortho* to OMe in central ring), 129.23 (CH, *meta* to OMe in outer ring), 131.66 / 131.85 (two CH, *meta* to OMe in central ring / *meta* to OMe and *ortho* to central ring in outer ring), 132.54 (CH, *para* to OMe in central ring), 156.72 (C_q-O in central ring), 157.45 (C_q-O in outer ring).

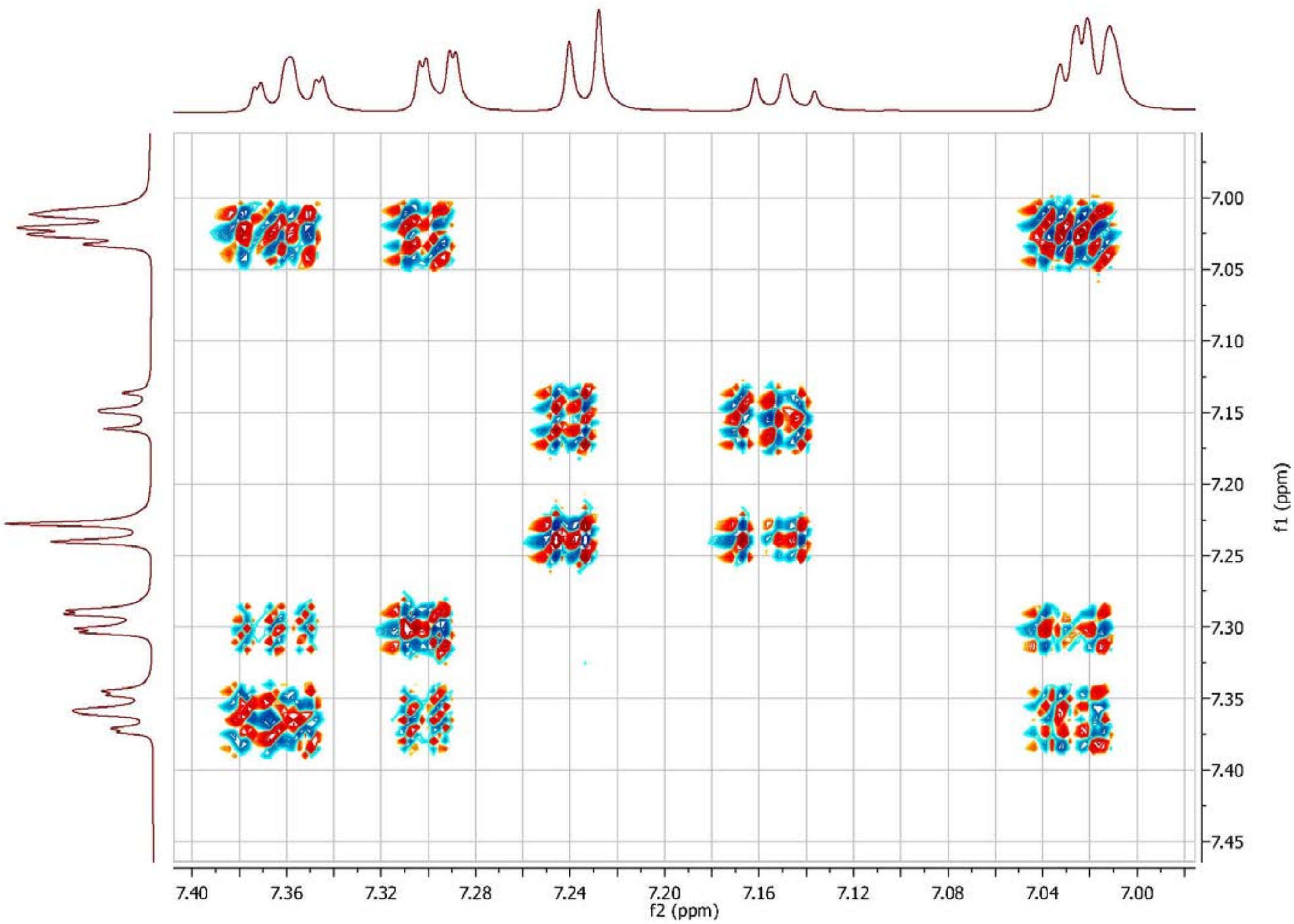


Figure S1. ^{1}H-^{1}H COSY spectrum for **1d**.

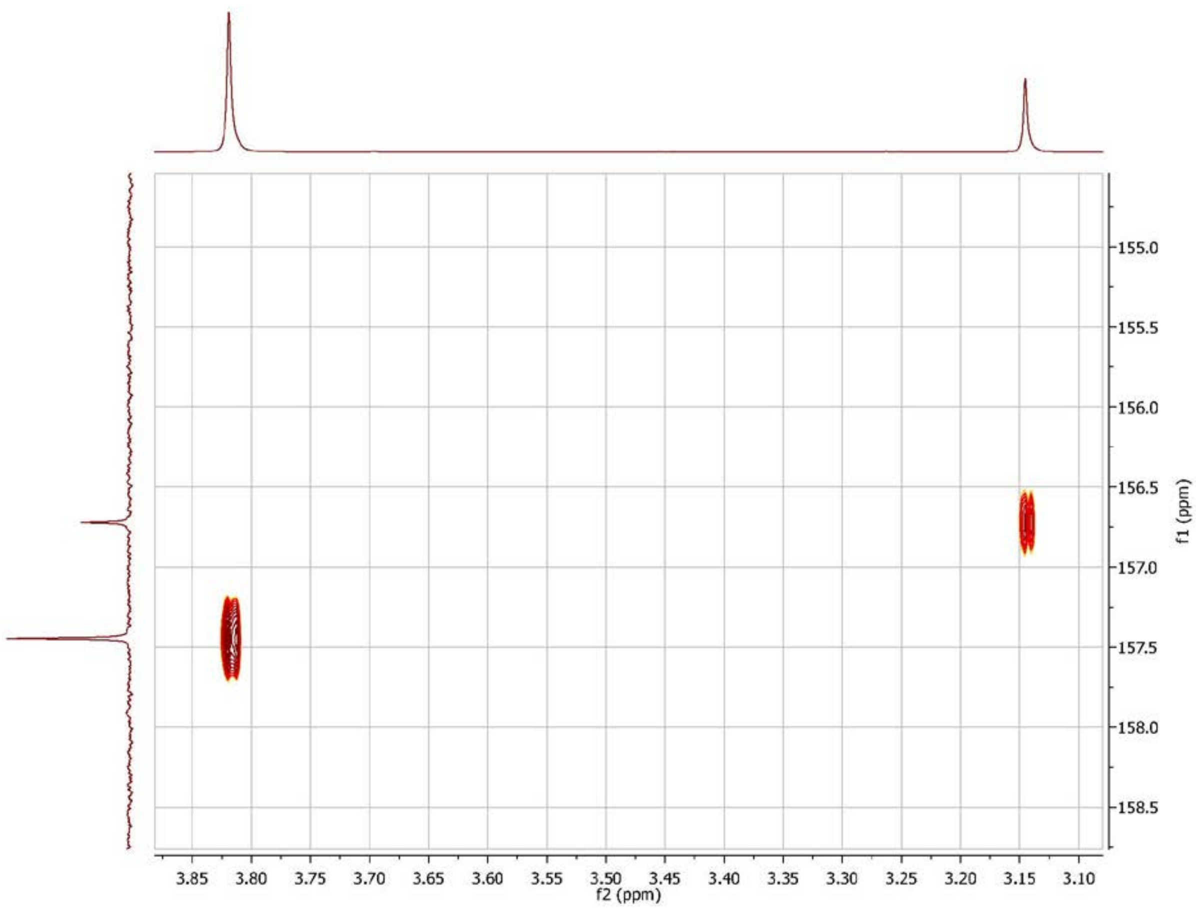


Figure S2. Partial ^{1}H-^{13}C HMBC spectrum for **1d**.
(f_2 dimension: ^{1}H, f_1 dimension: ^{13}C)

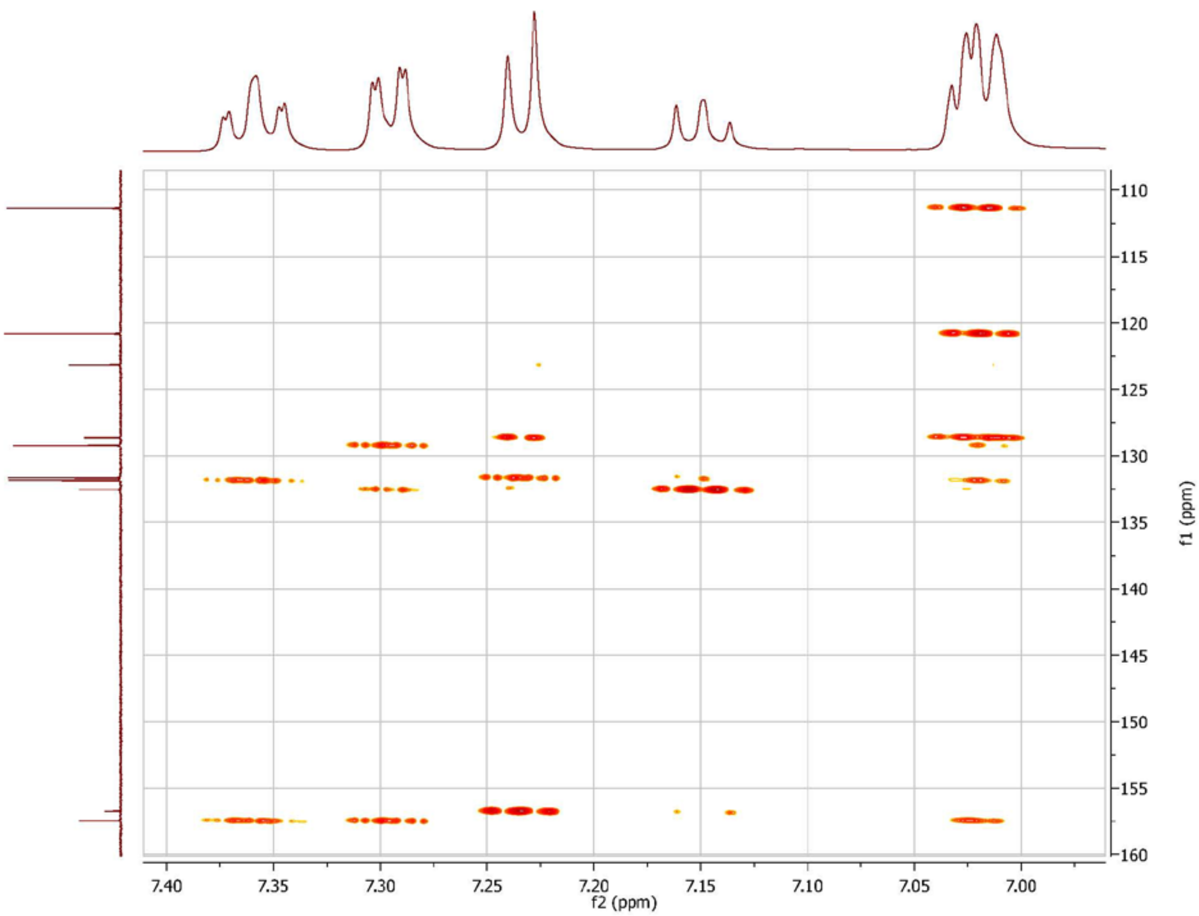


Figure S3. Partial ^{1}H-^{13}C HMBC spectrum for **1d**.
(f_2 dimension: ^{1}H, f_1 dimension: ^{13}C)

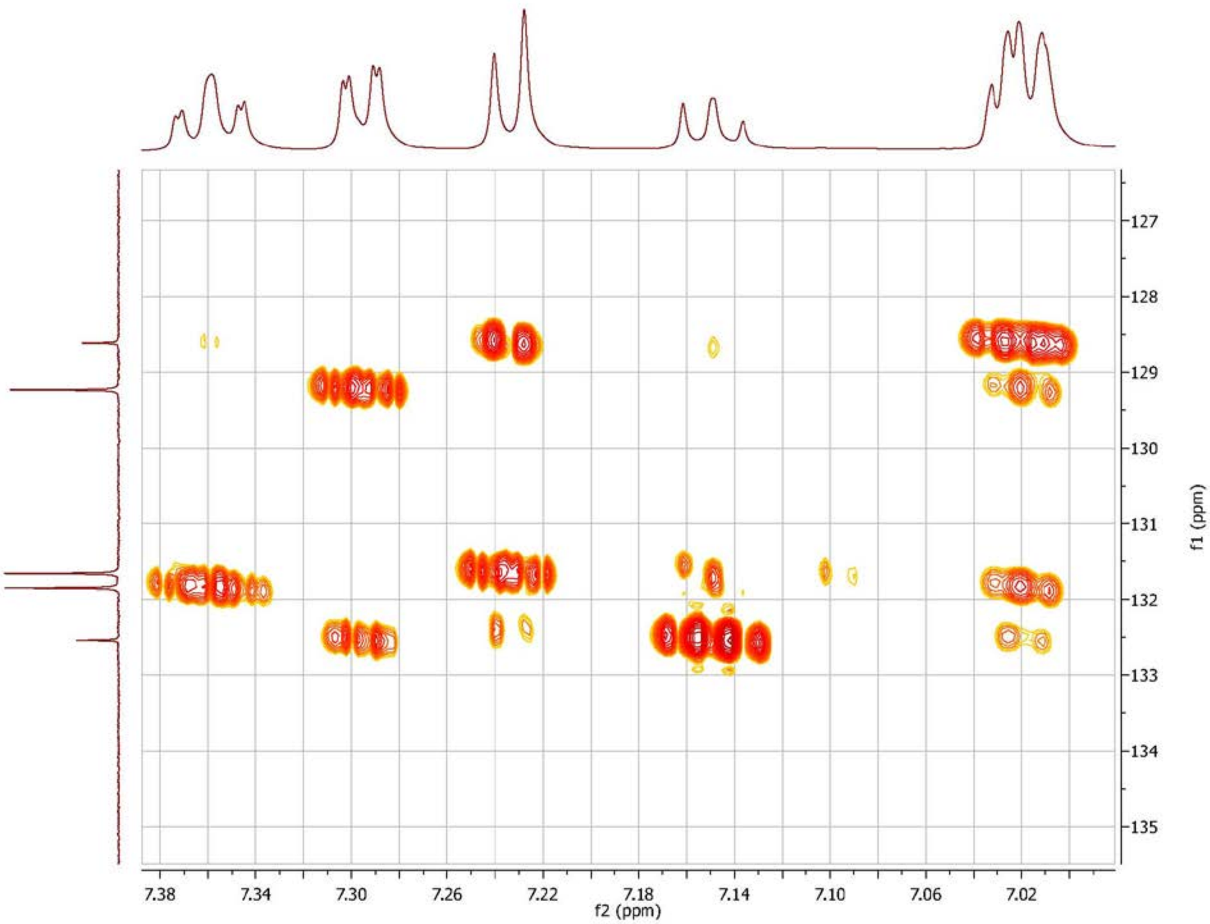


Figure S4. Partial ^{1}H-^{13}C HMBC spectrum for **1d**.
(f_2 dimension: ^{1}H, f_1 dimension: ^{13}C)

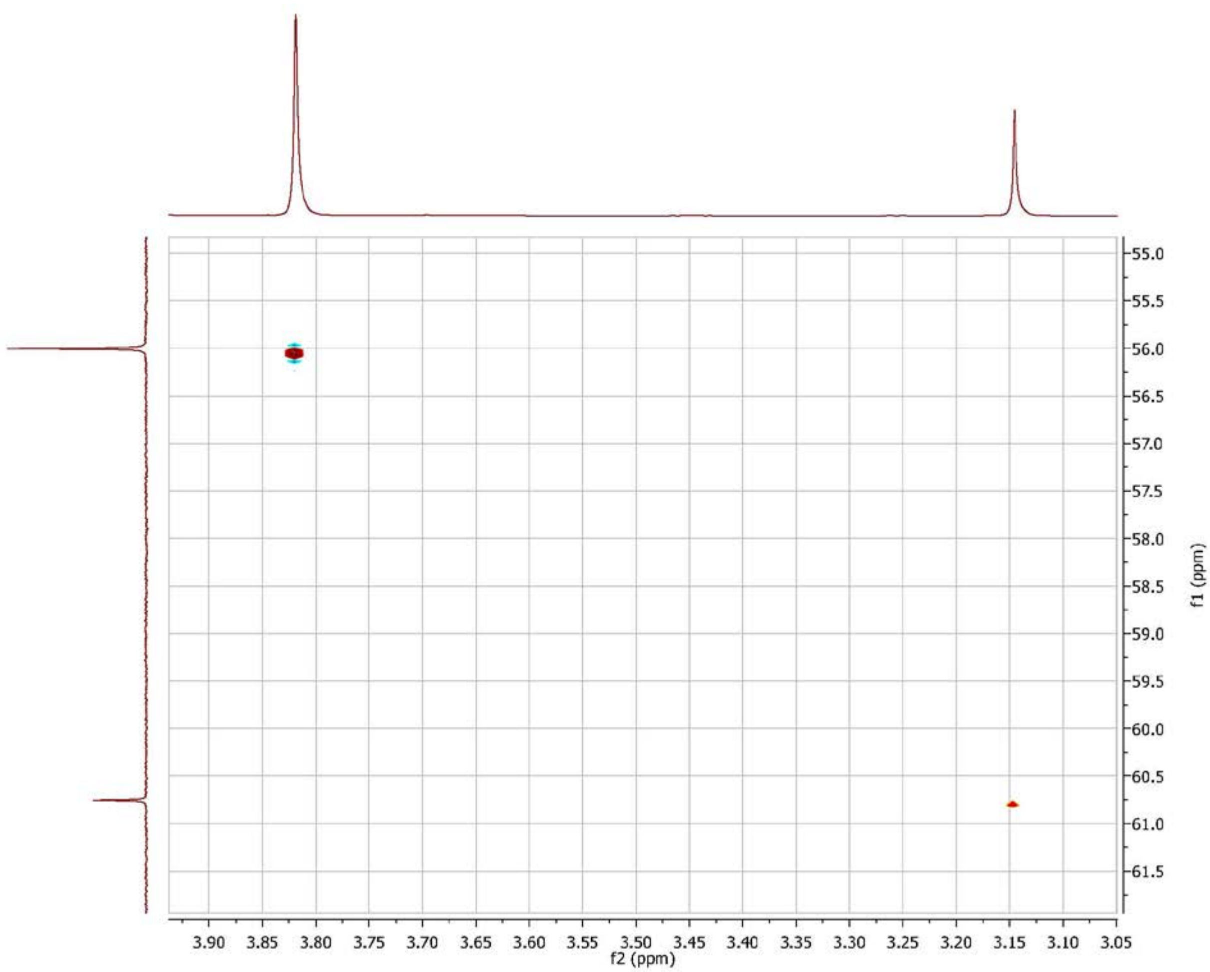


Figure S5. Partial ^{1}H-^{13}C HSQC spectrum for **1d**.
(f_2 dimension: ^{1}H, f_1 dimension: ^{13}C)

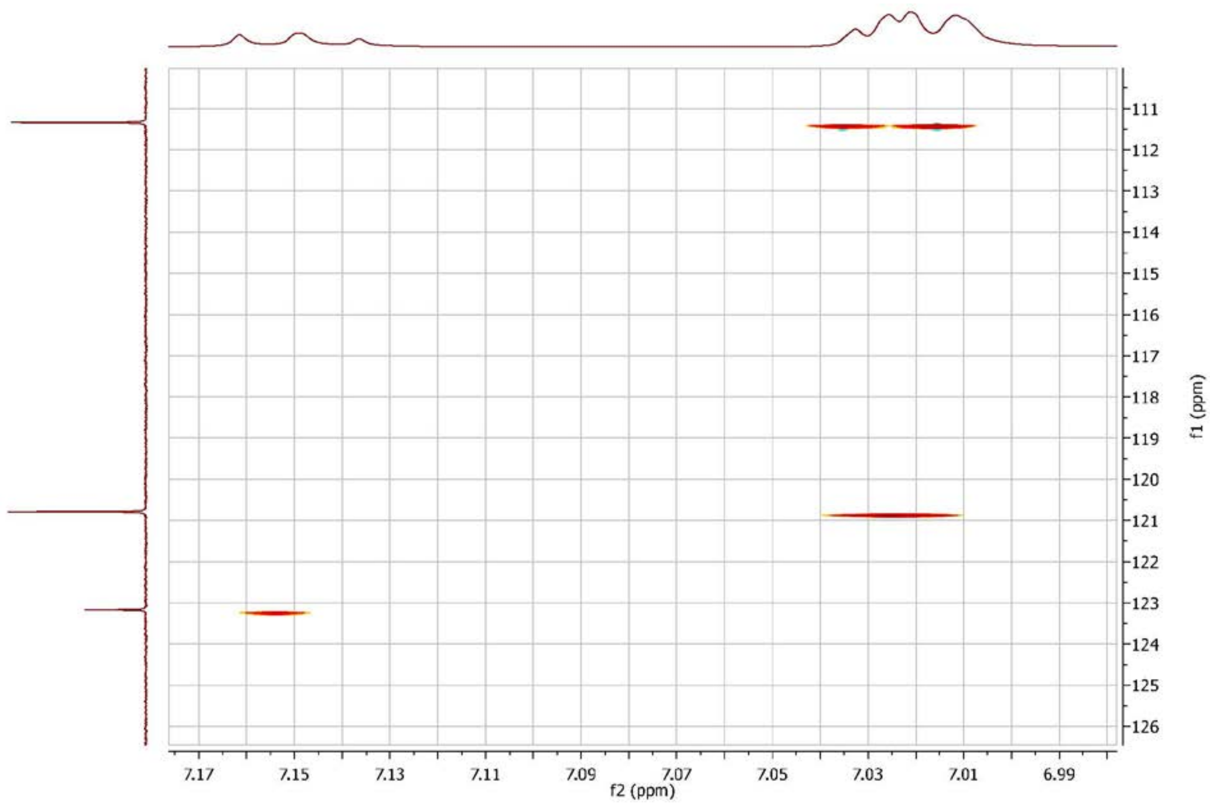


Figure S6. Partial ^{1}H-^{13}C HSQC spectrum for **1d**.
(f_2 dimension: ^{1}H, f_1 dimension: ^{13}C)

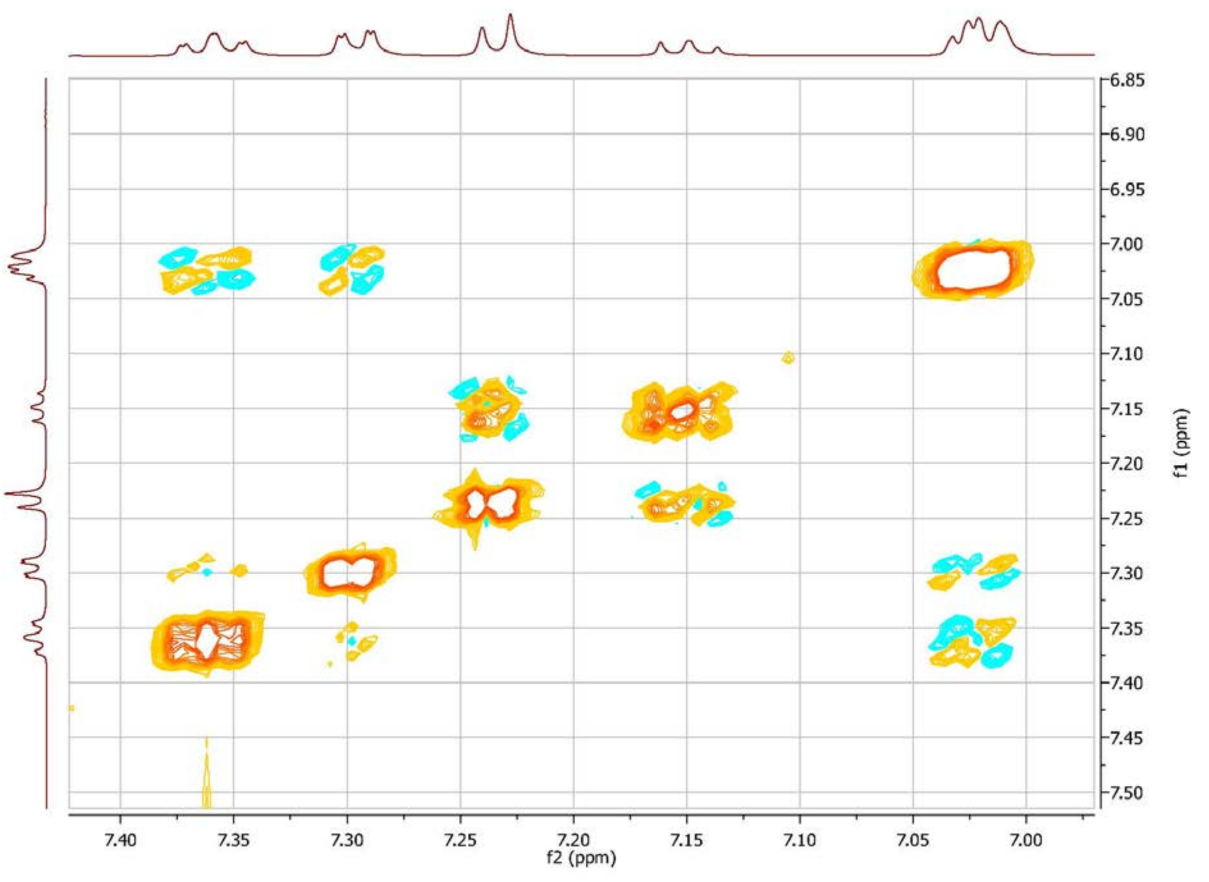
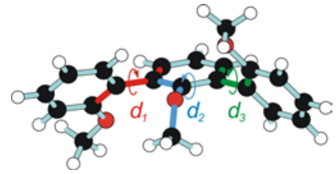
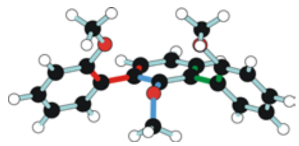
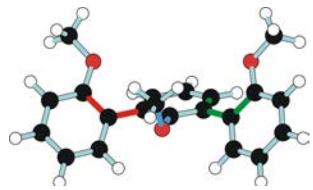
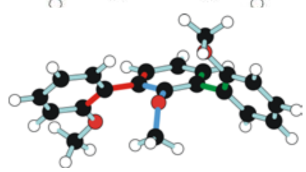
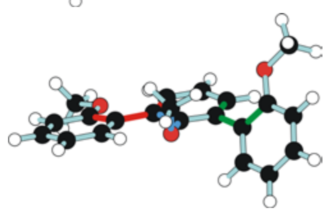
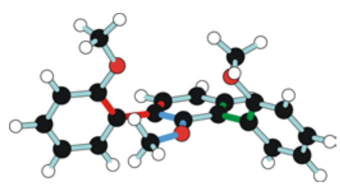
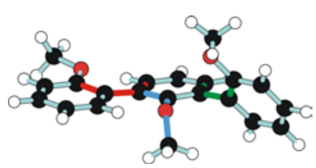
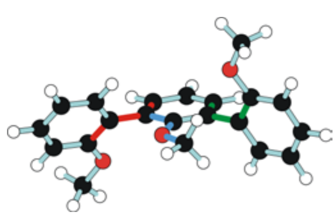


Figure S7. Partial 2-D ^{1}H-^{1}H ROESY spectrum of **1**

Table S1. Geometrical parameters of the species in Figure 3. 

Conformers		Dihedral angles[a]		
		d_1	d_2	d_3
syn-a		*118.81*	*-89.84*	*-118.81*
		123.23	**-89.08**	**-123.23**
syn-s		*-54.36*	*-90.56*	*54.36*
		-51.54	**-89.97**	**51.54**
anti		*53.21*	*84.56*	*118.26*
		50.82	**81.64**	**122.10**
TS(*syn-s* → *anti*)		*6.26*	*-100.31*	*57.57*
		5.64	**-100.47**	**56.07**
TS(*syn-a* → *syn-s*)		*-100.80*	*-1.34*	*116.23*
		-103.75	**-5.20**	**120.06**
TS(*anti* → *syn-a*)		*-7.78*	*95.94*	*118.49*
		-7.38	**95.82**	**121.39**
TS(*anti* → *anti*)[b]		*95.32*	*-179.12*	*114.92*
		96.75	**-177.22**	**118.05**

[a] *italics*B3LYP/6-31G*; **bold** B2PLYPD/cc-pVDZ; [b] lower of the two T

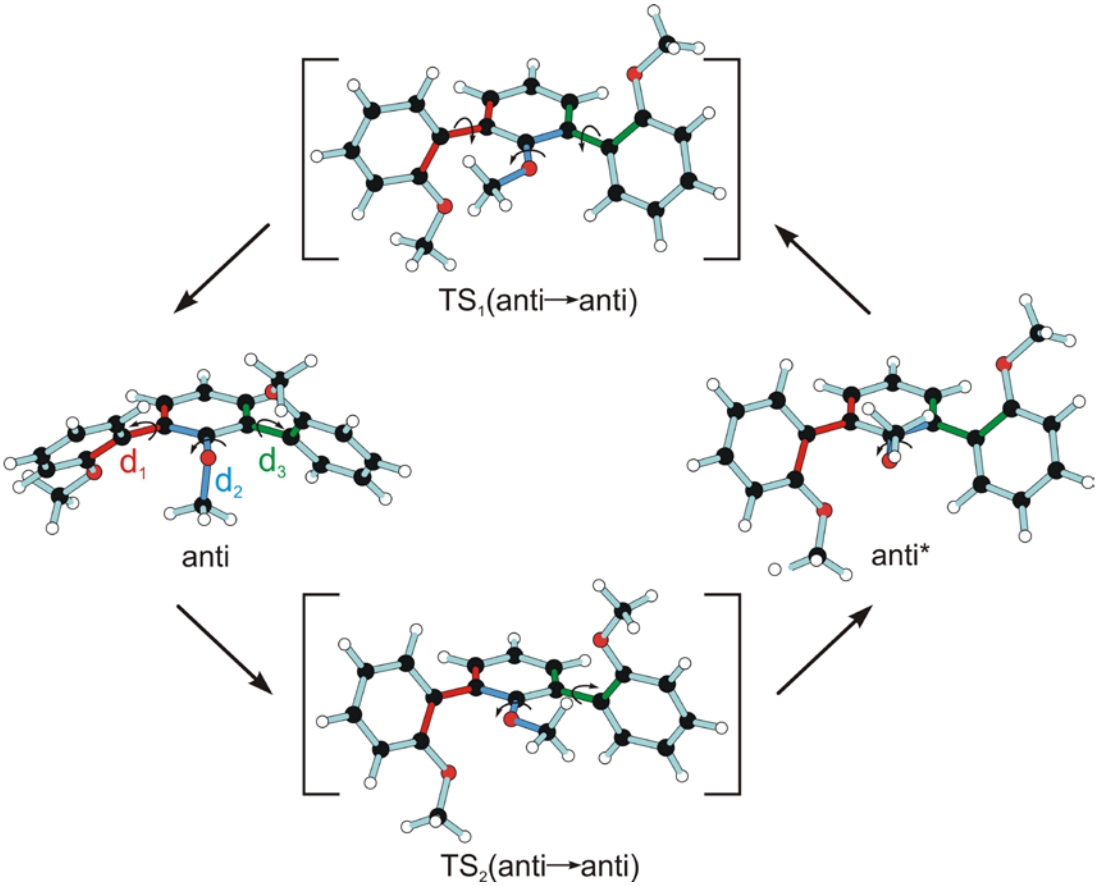


Figure S8. Interconversion of *anti* atropisomer of **1d** (structures from B2PLYPD/cc-pVDZ calculations; note that the two anti structures are identical); the TS_1 lies 2.82 kJ/mol higher than TS_2; (for geometrical parameters see Table S1).

Table S1. Geometrical parameters of the species in Figure S8.

Conformers	Dihedral angles		
	d_1	d_2	d_3
anti	**50.82**	**81.64**	**122.10**
TS(*anti* → *anti*)[a]	**96.75**	**-177.22**	**118.05**
anti*	**122.10**	**81.64**	**50.82**
TS(*anti* → *anti*)[b]	**99.36**	**175.76**	**55.20**