Effect of Ring Size on Photoisomerization Properties of Stiff Stilbene macrocycles

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

Supplementary

Table of Contents

1. NMR spectra

^{1}H and ^{13}C NMR spectra of synthesized compounds and ^{1}H spectra of photoisomerization studies.

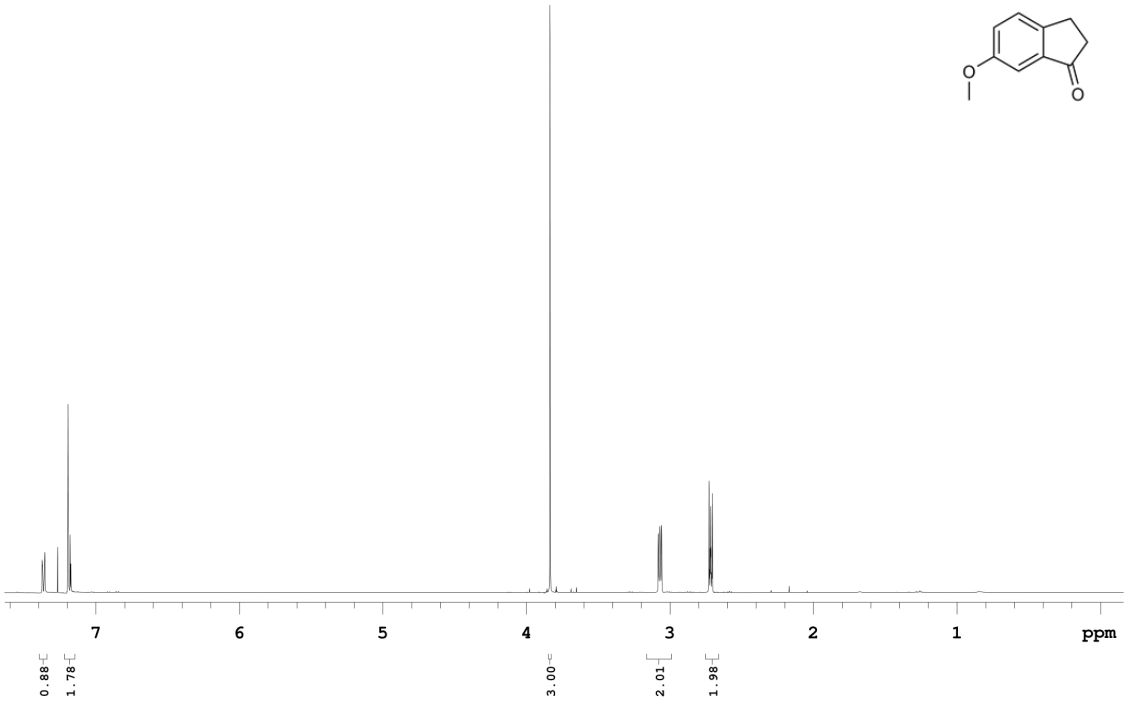


*Figure 1. ^{1}H NMR spectrum of compound **3**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

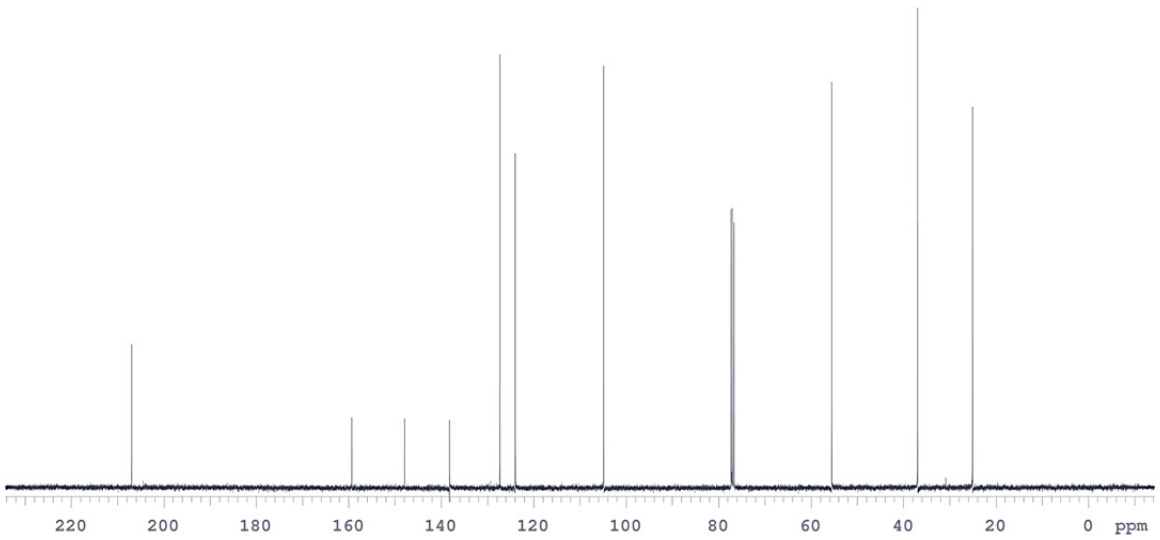


*Figure 2. ^{13}C NMR spectrum of compound **3**.*

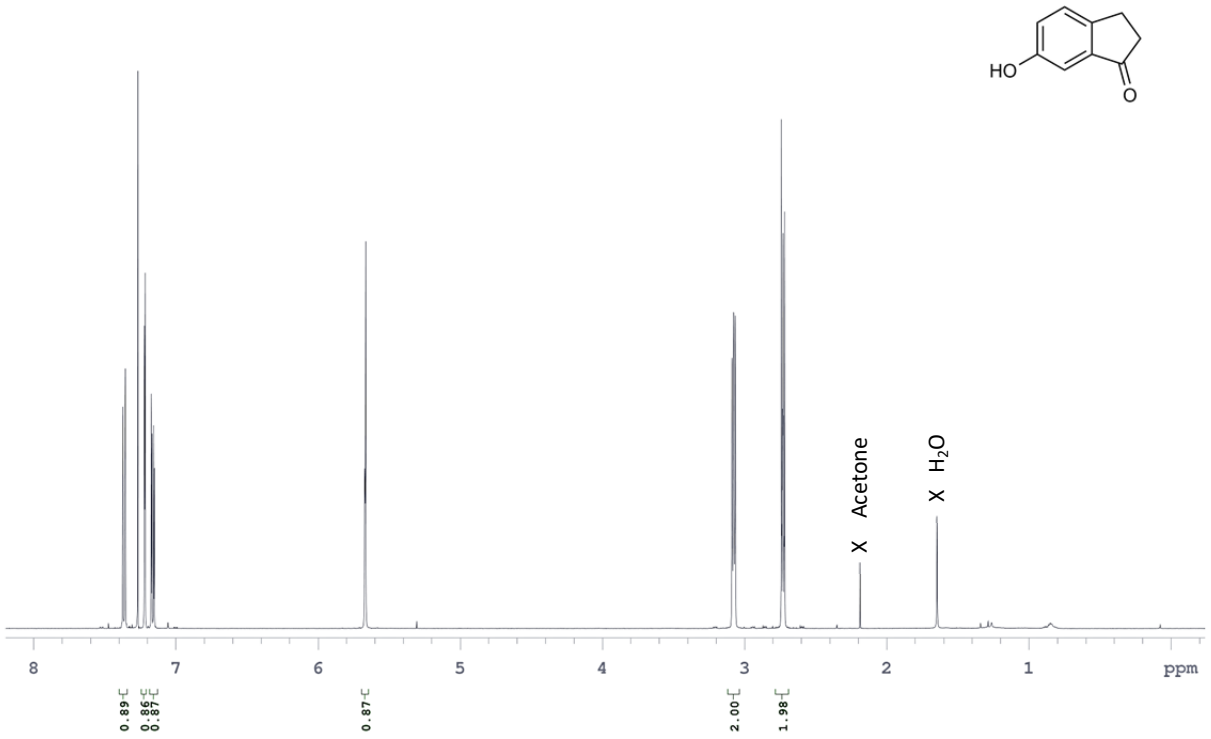


*Figure 3. ^{1}H NMR spectrum of compound **4**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

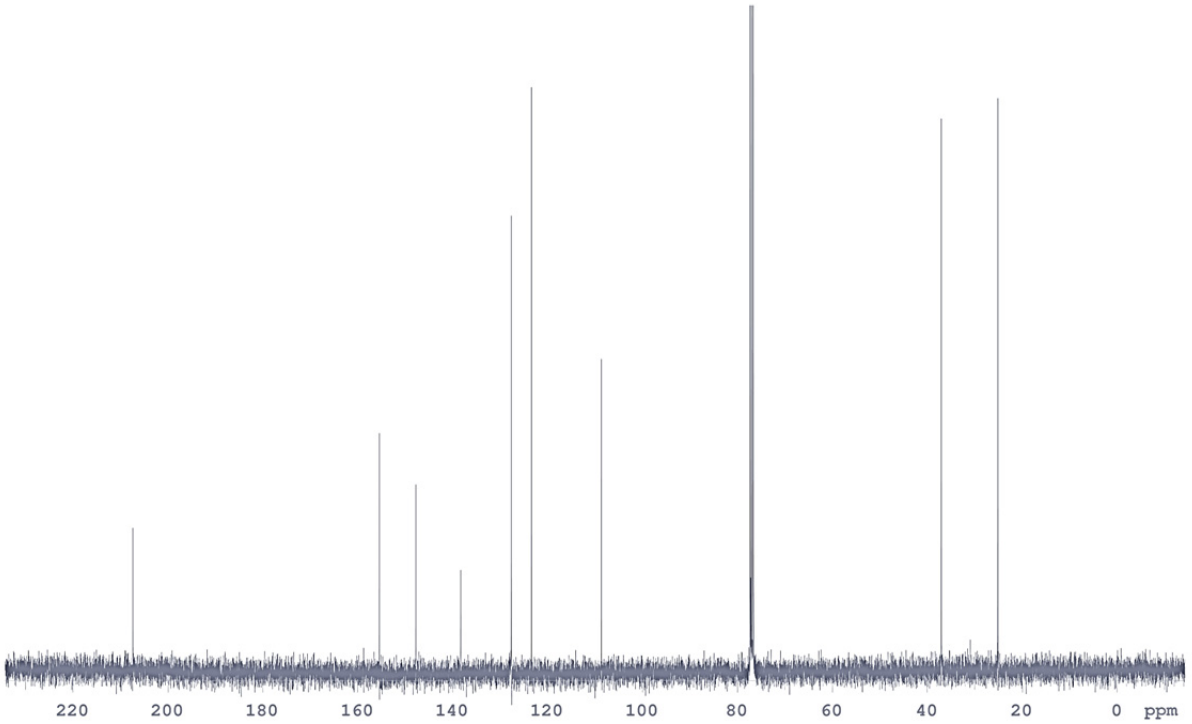


*Figure 4. ^{13}C NMR spectrum of compound **4**.*

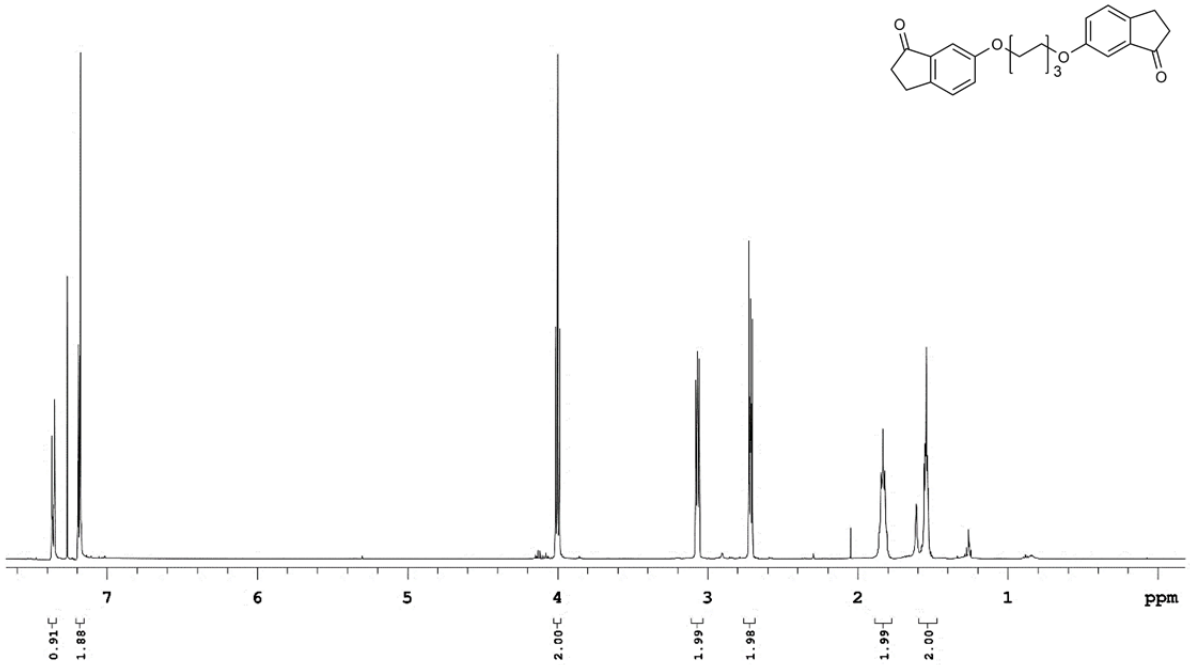


*Figure 5. ^{1}H NMR spectrum of compound **6a**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

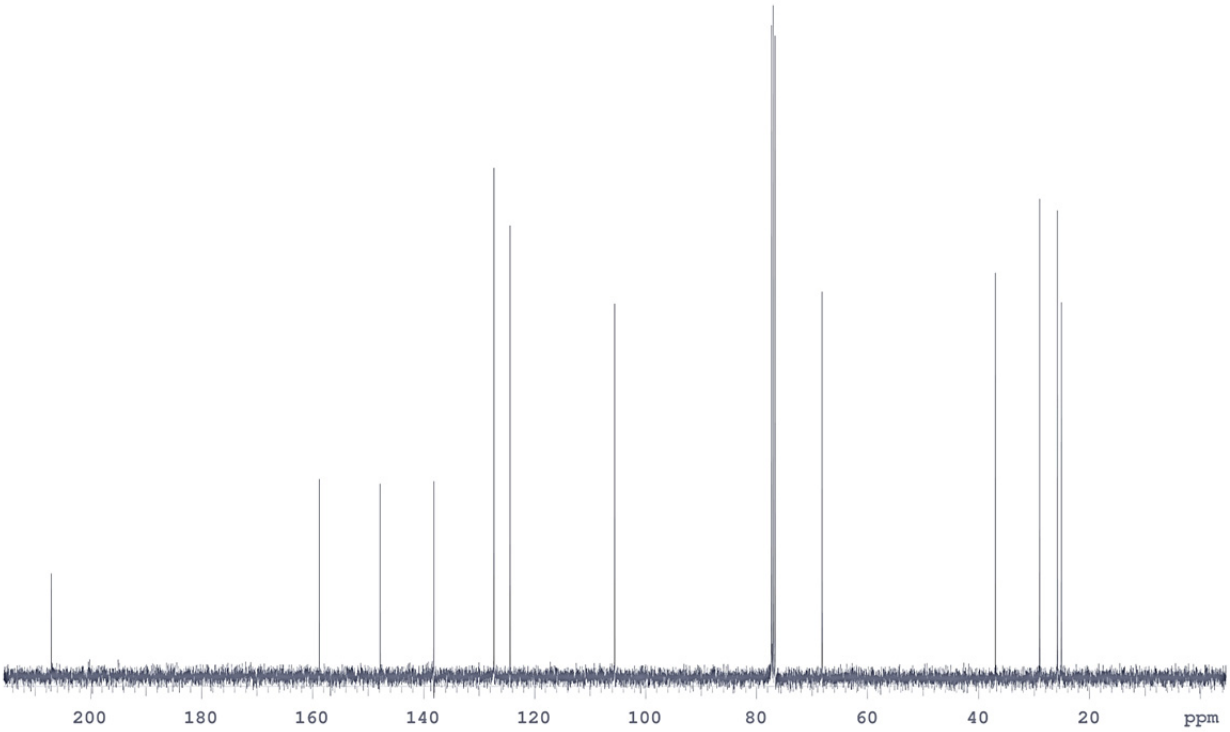


*Figure 6. ^{13}C NMR spectrum of compound **6a**.*

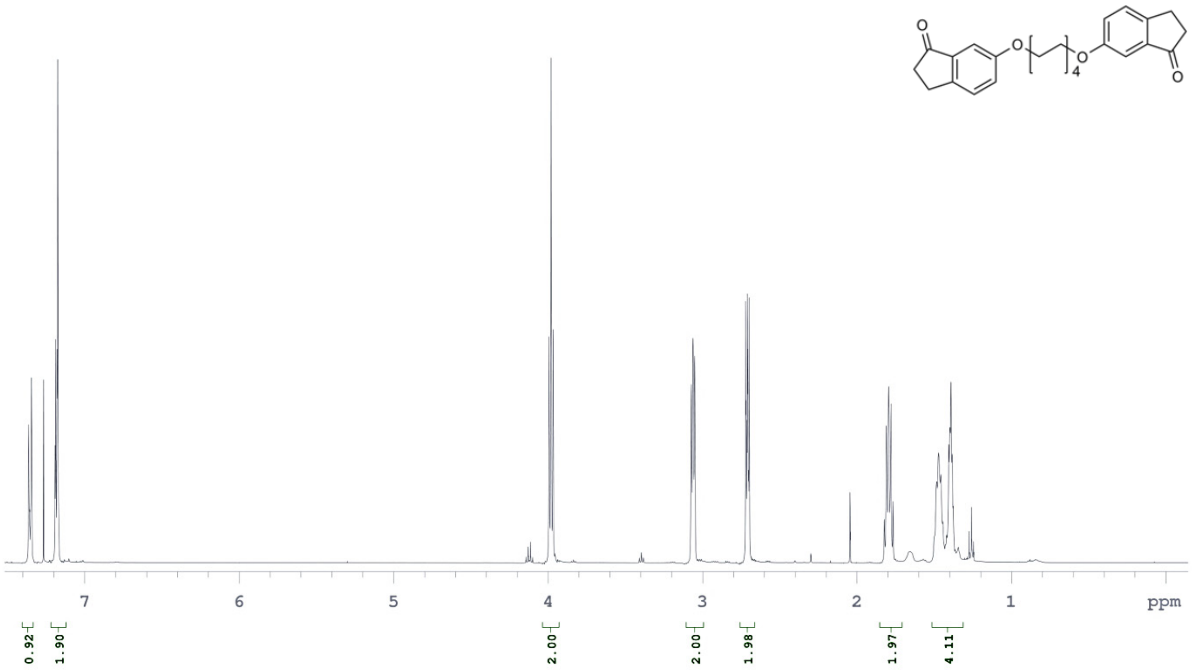


*Figure 7. ^{1}H NMR spectrum of compound **6b**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

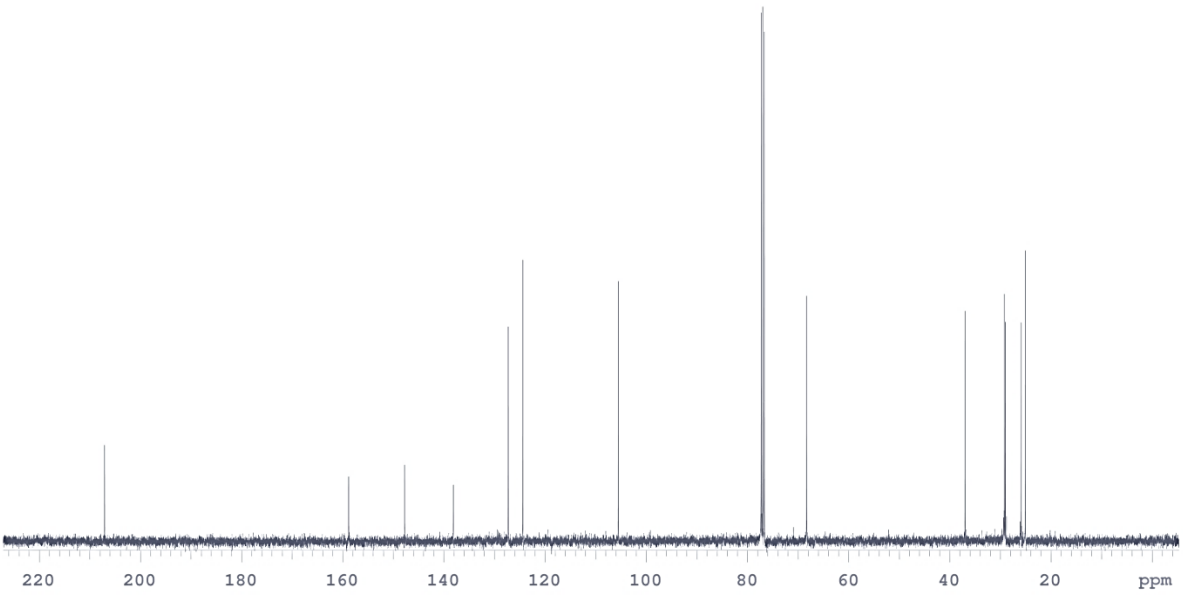


*Figure 8. ^{13}C NMR spectrum of compound **6b**.*

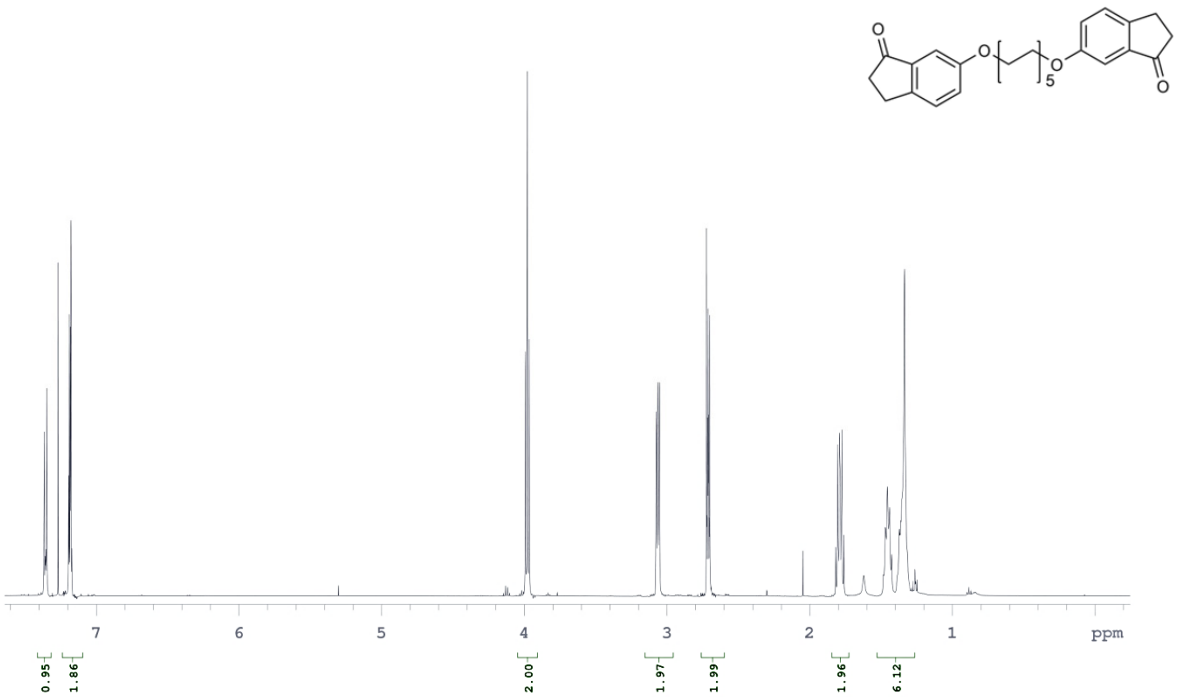


*Figure 9. ^{1}H NMR spectrum of compound **6c**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

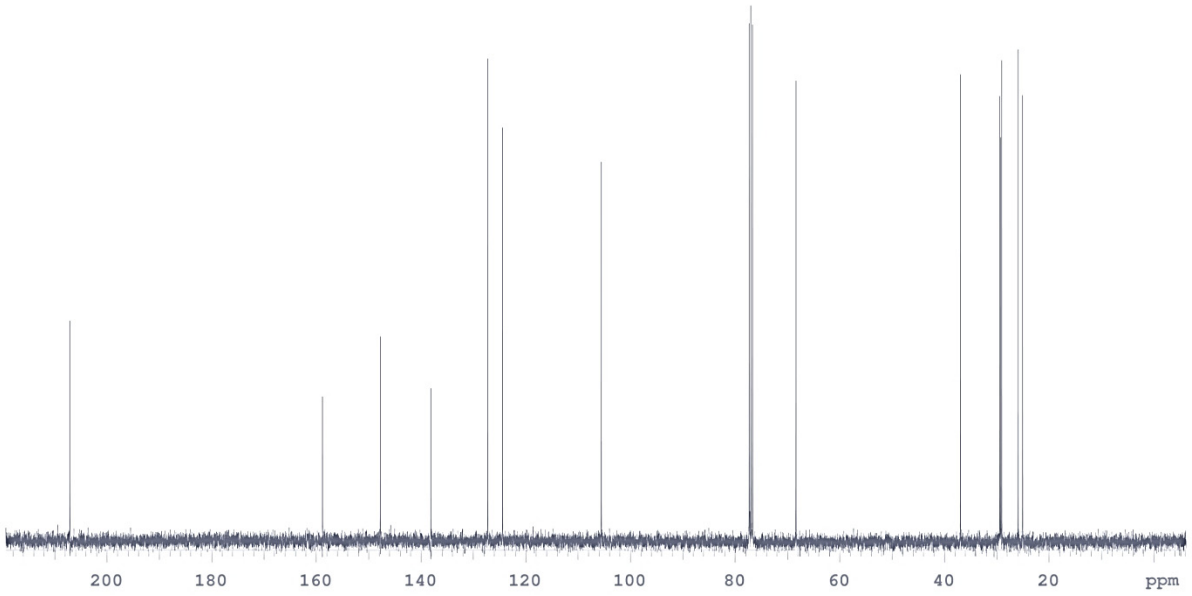


*Figure 10. ^{13}C NMR spectrum of compound **6c**.*

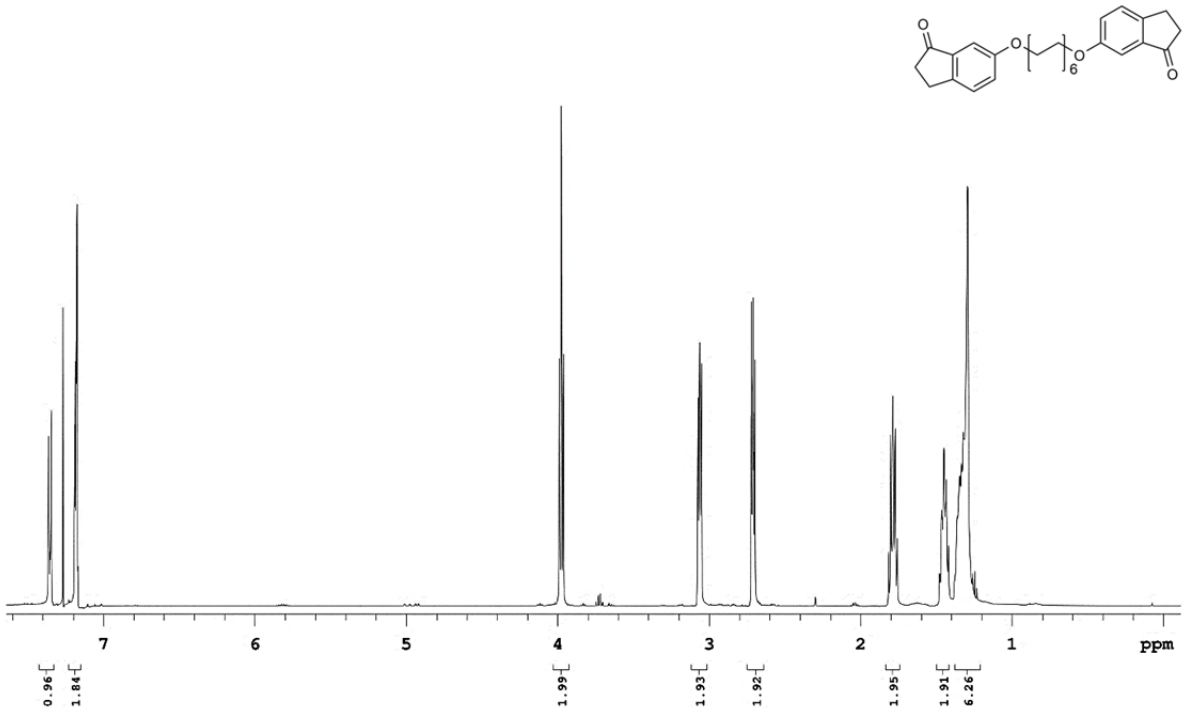


*Figure 11. ^{1}H NMR spectrum of compound **6d**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

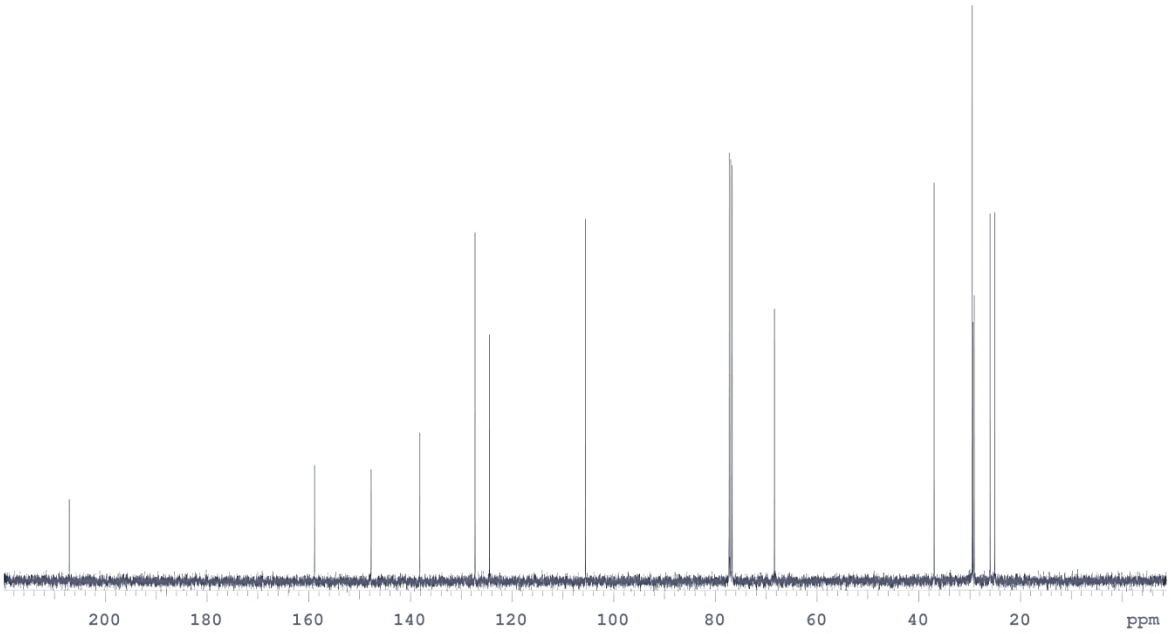


*Figure 12. ^{13}C NMR spectrum of compound **6d**.*

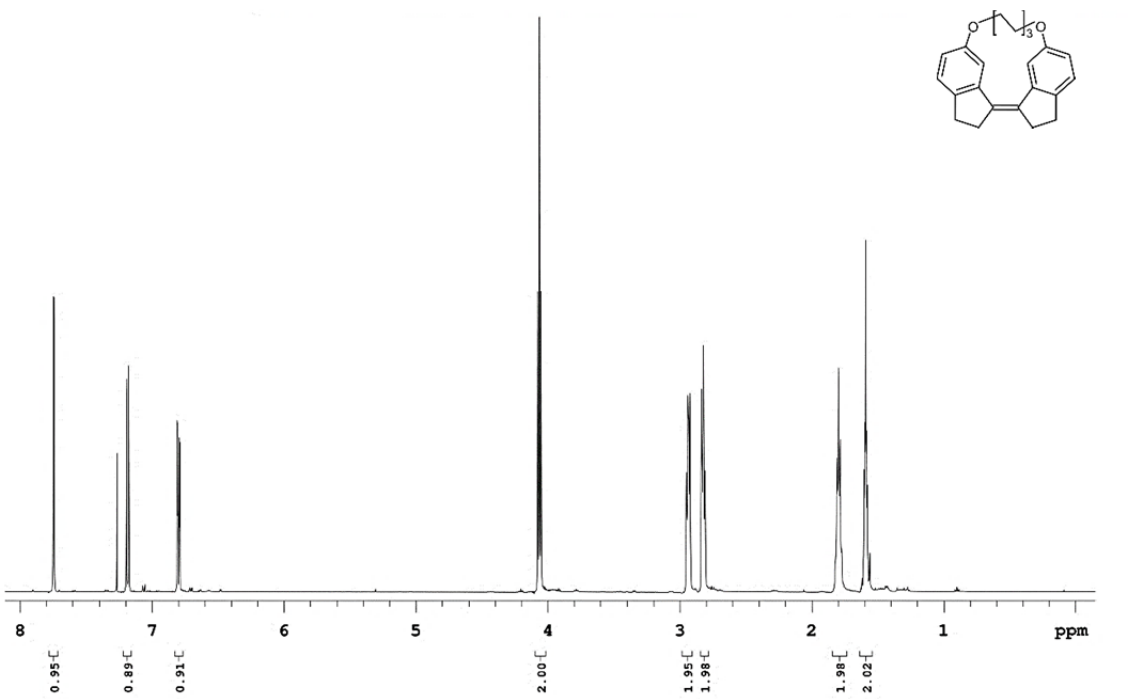


*Figure 13. ^{1}H NMR spectrum of compound **Z-1a**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

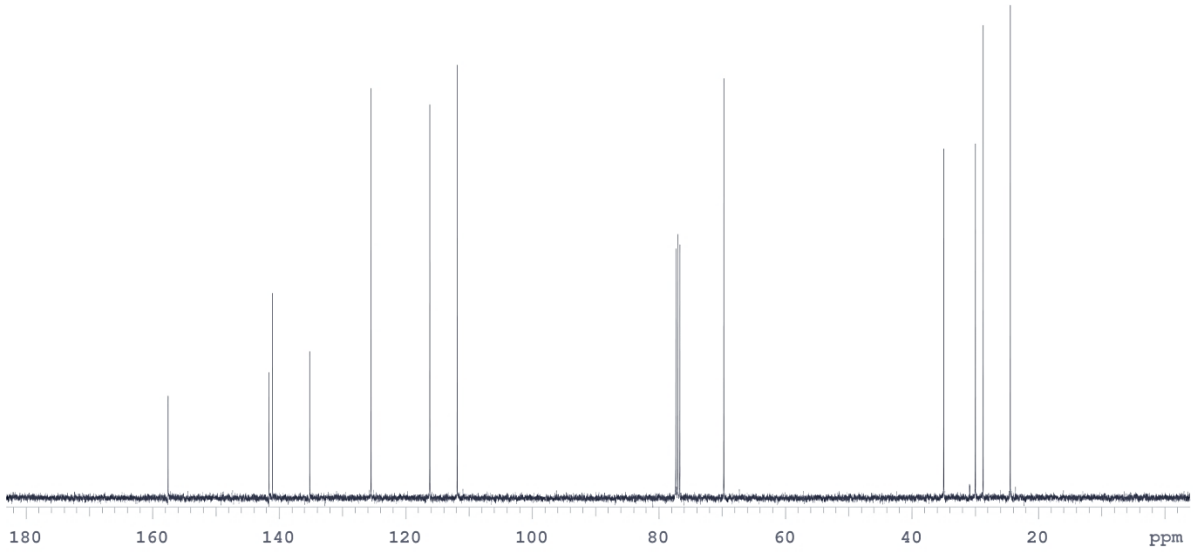


*Figure 14. ^{13}C NMR spectrum of compound **Z-1a**.*

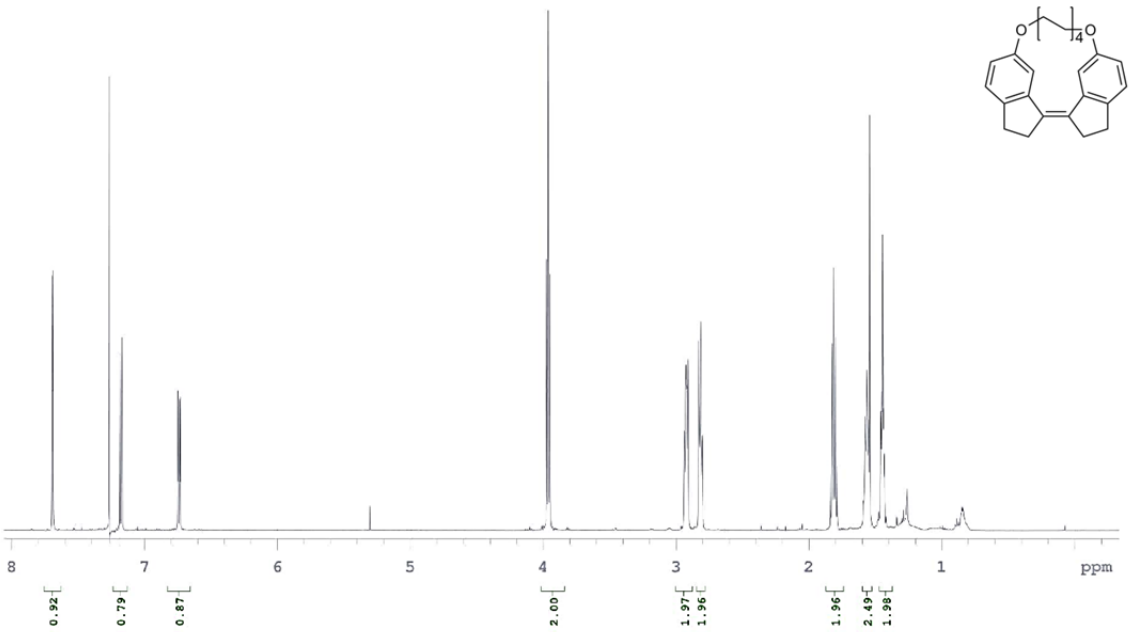


*Figure 15. ^{1}H NMR spectrum of compound **Z-1b**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

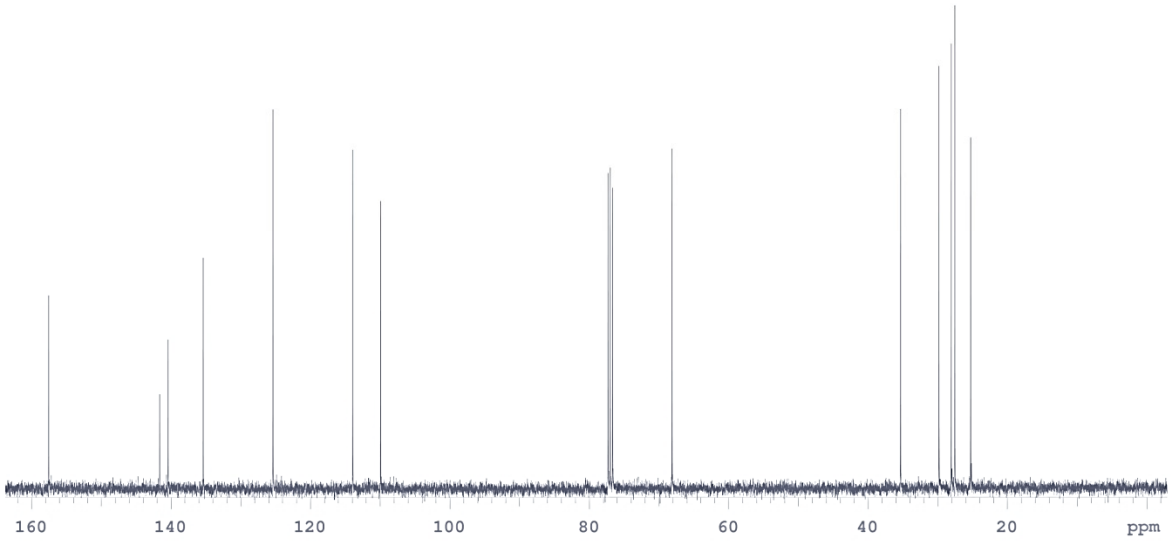


*Figure 16. ^{13}C NMR spectrum of compound **Z-1b**.*

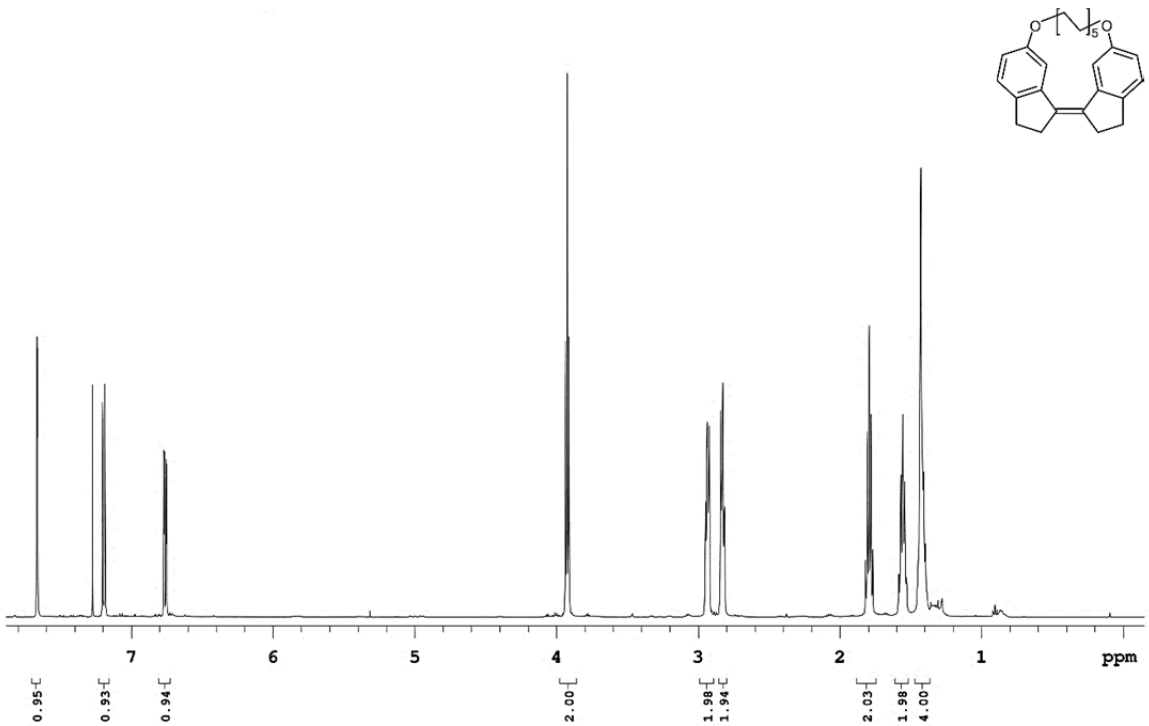


*Figure 17. ^{1}H NMR spectrum of compound **Z-1c**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

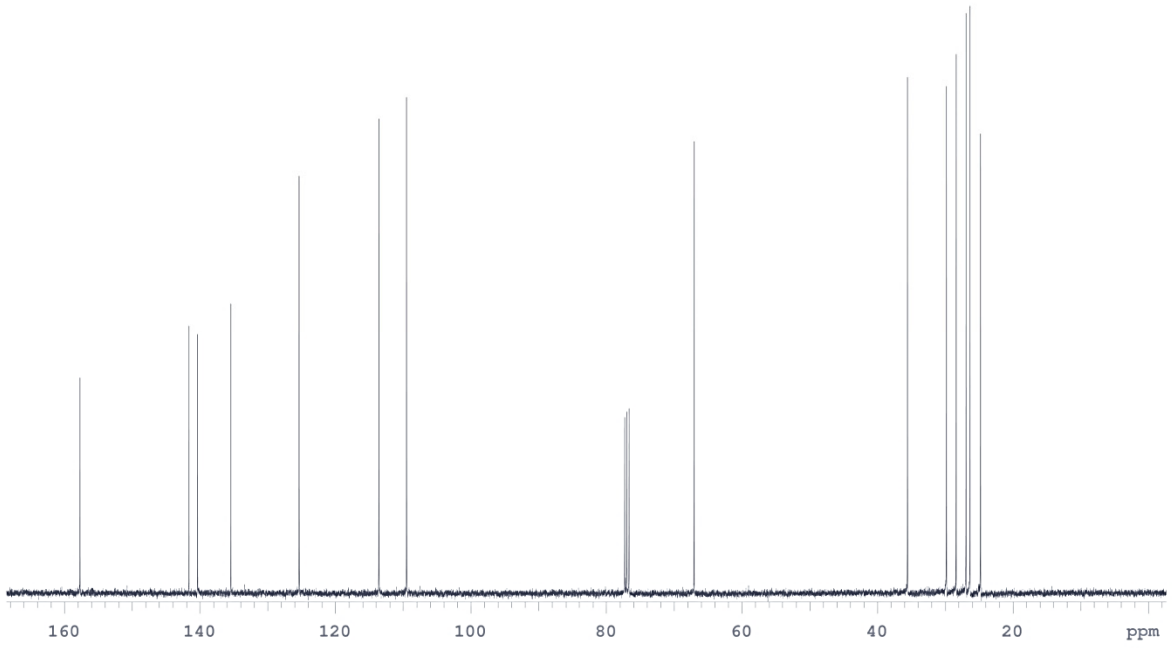


*Figure 18. ^{13}C NMR spectrum of compound **Z-1c**.*

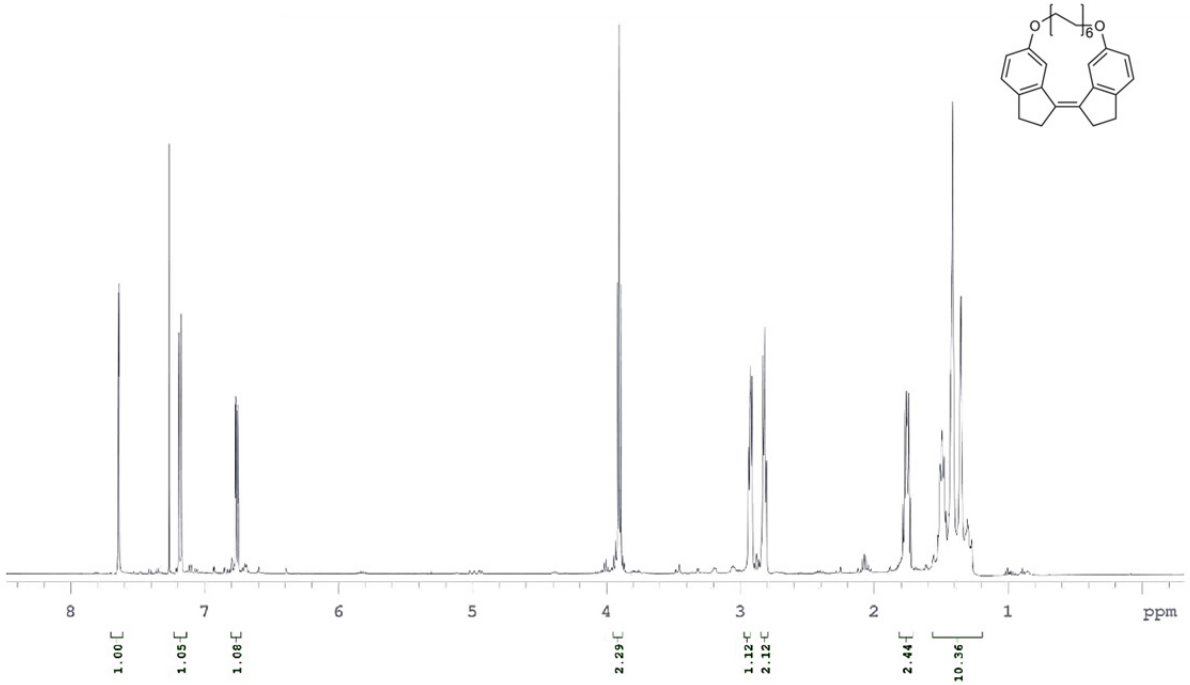


*Figure 19. ^{1}H NMR spectrum of compound **Z-1d**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

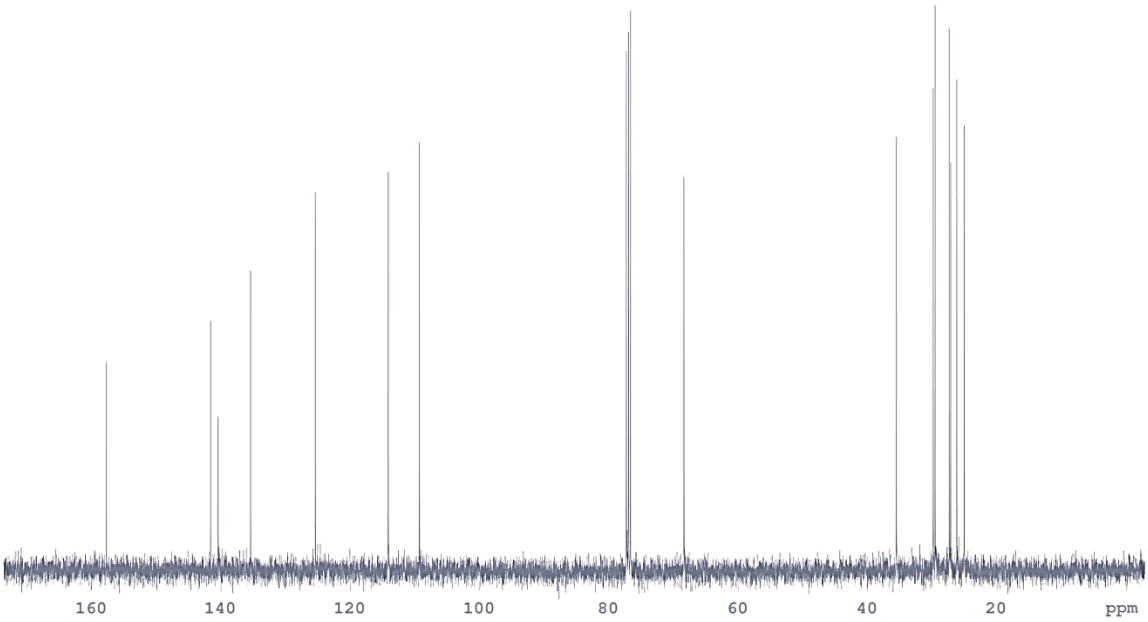


*Figure 20. ^{13}C NMR spectrum of compound **Z-1d**.*

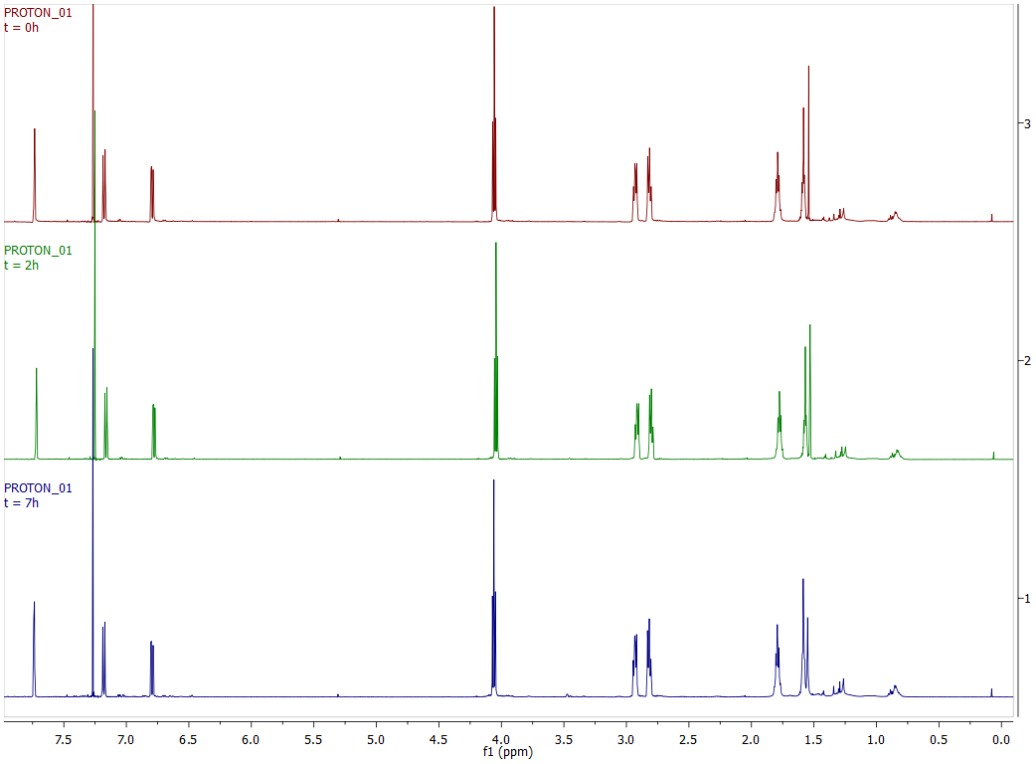


*Figure 21. Photo-isomerization process of compound **Z-1a** monitored by ^{1}H NMR spectroscopy. Initial sample (top), after 2h (middle) and after 7h (bottom).*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a] Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden
[b] Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.

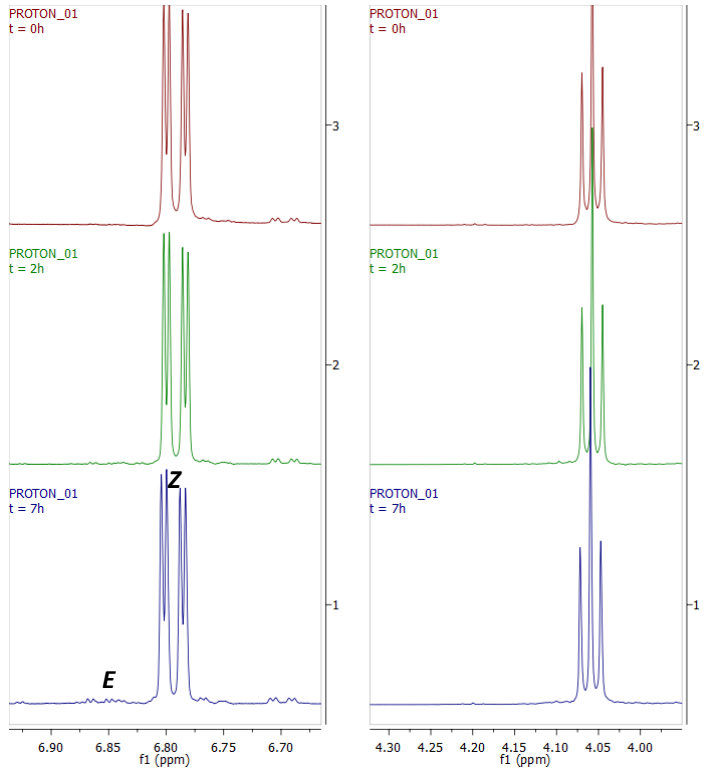


Figure 22. Expansions of ^{1}H NMR spectra of Figure 21 showing an aromatic proton shift (left) and the signals corresponding to the hydrogens bonded to the first carbon of the linker between the two aromatic rings of stiff-stilbene (right).

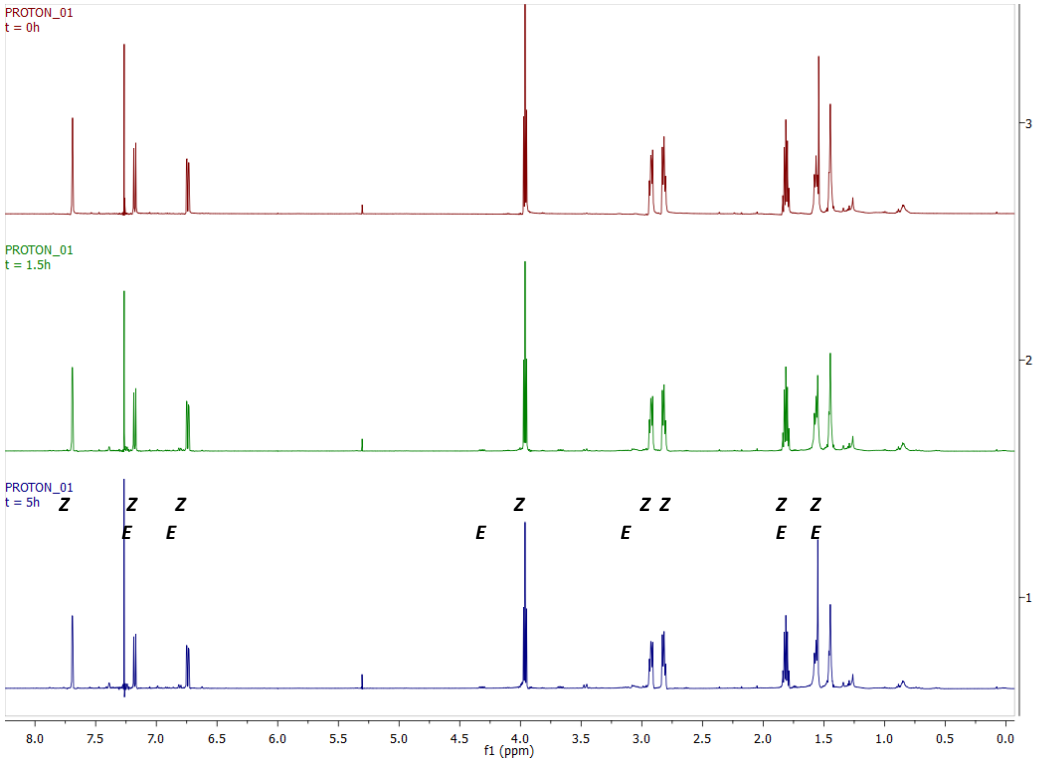


*Figure 23. Photo-isomerization process of compound **Z-1b** followed by ^{1}H NMR spectroscopy. Initial sample (top), after 1.5h (middle) and after 5h (bottom).*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

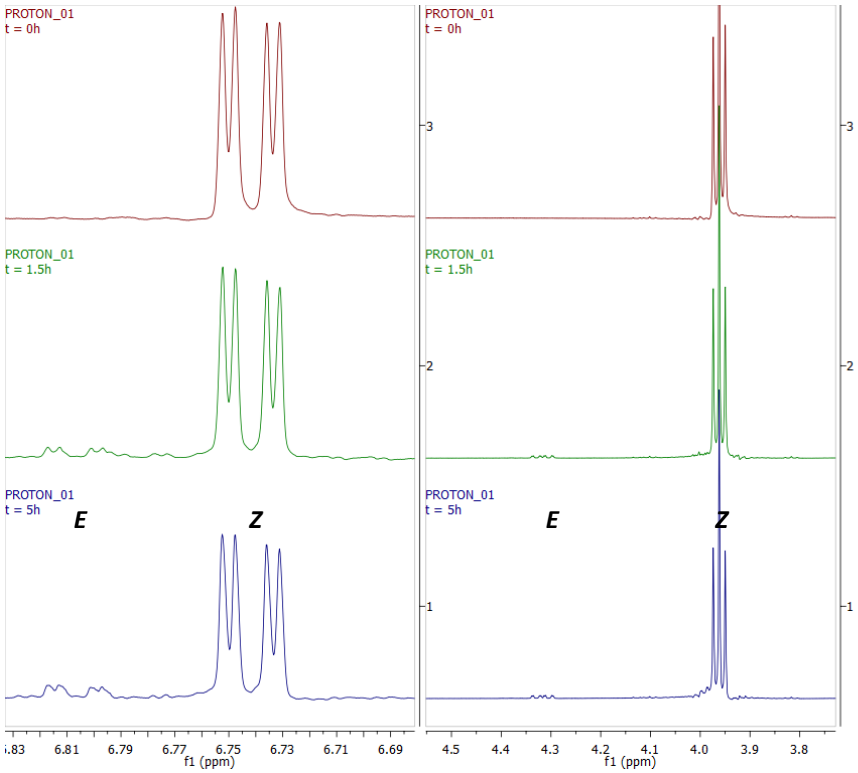


Figure 24. Expansions of ^{1}H NMR spectra of Figure 23 showing an aromatic proton chemical shift (left) and the signals corresponding to the hydrogens bonded to the first carbon of the linker between the two aromatic rings of stiff-stilbene (right).

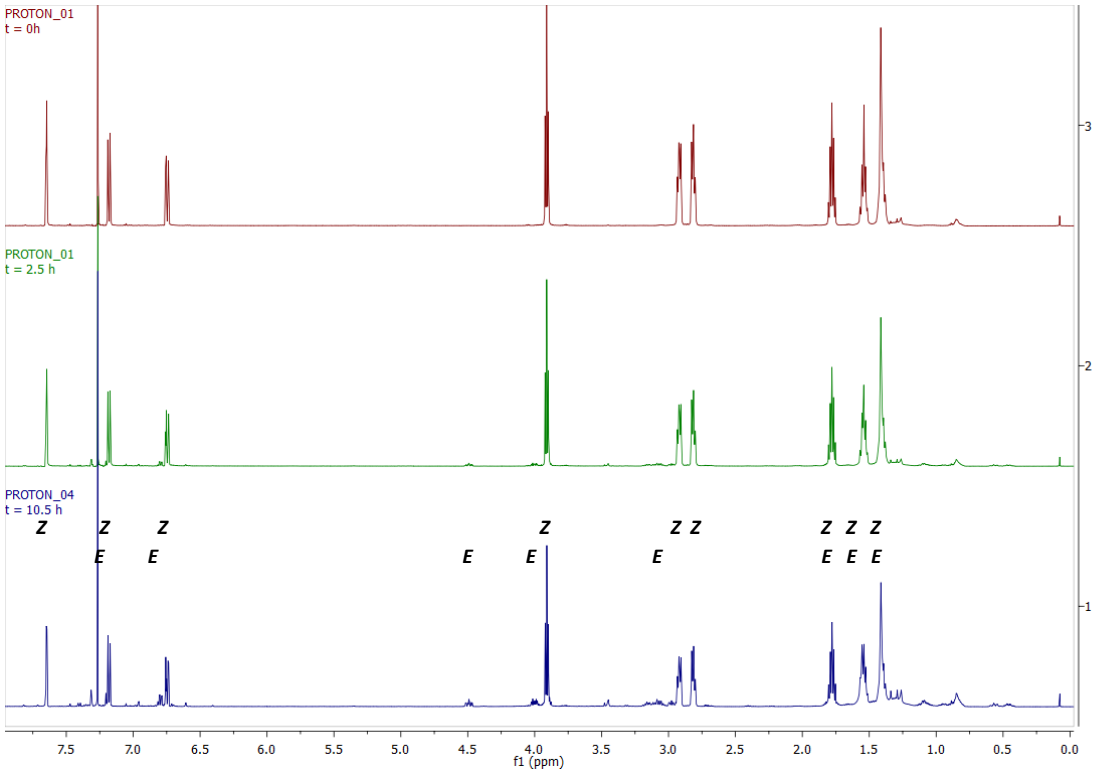


*Figure 25. Photo-isomerization process of compound **Z-1c** followed by ^{1}H NMR spectroscopy. Initial sample (top), mixture composition after 2.5h (middle) and after 10.5h (bottom).*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a] Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden
[b] Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.

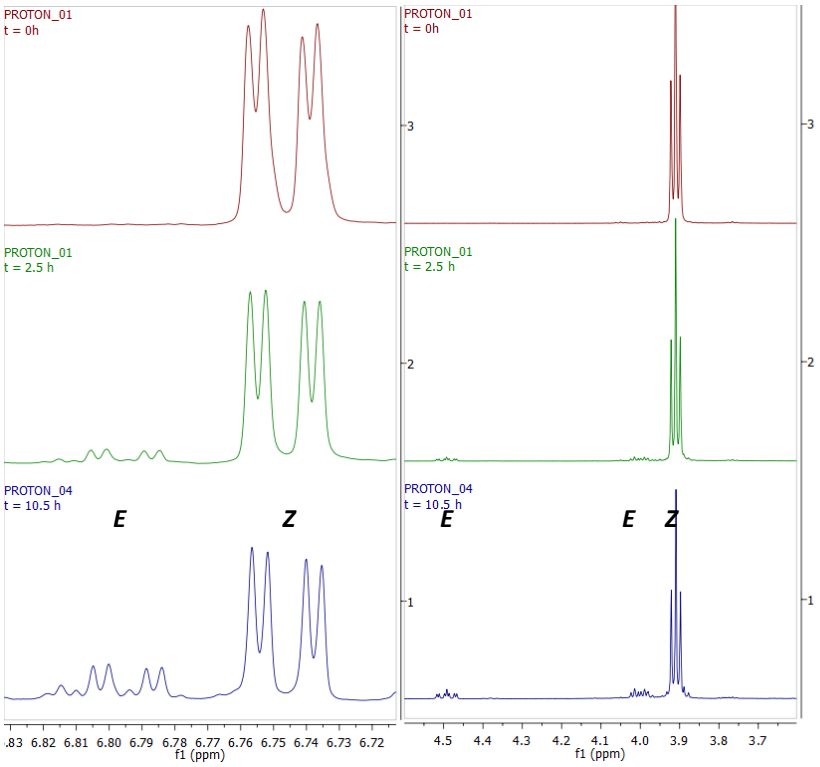


Figure 26. Expansions of ^{1}H NMR spectra of Figure 25 showing an aromatic proton shift (left) and the signals corresponding to the hydrogens bonded to the first carbon of the linker between the two aromatic rings of stiff-stilbene (right).

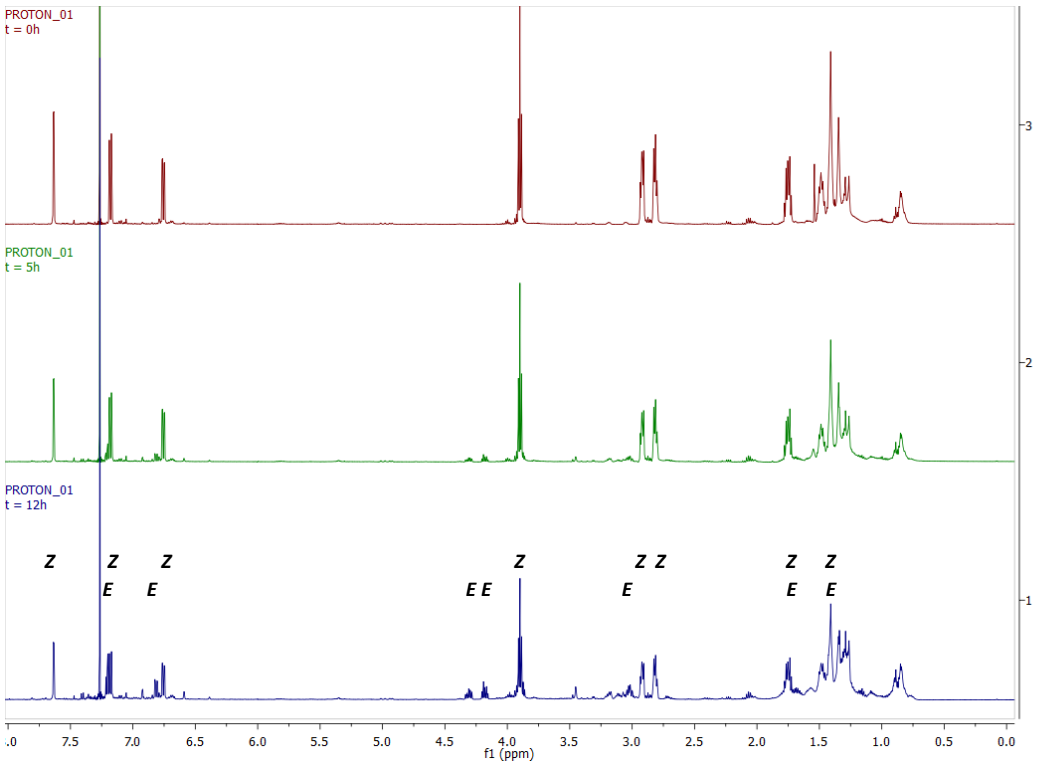


*Figure 27. Photo-isomerization process of compound **Z-1d** followed by ^{1}H NMR. Initial sample (top), mixture composition after 5h (middle) and after 12h (bottom).*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

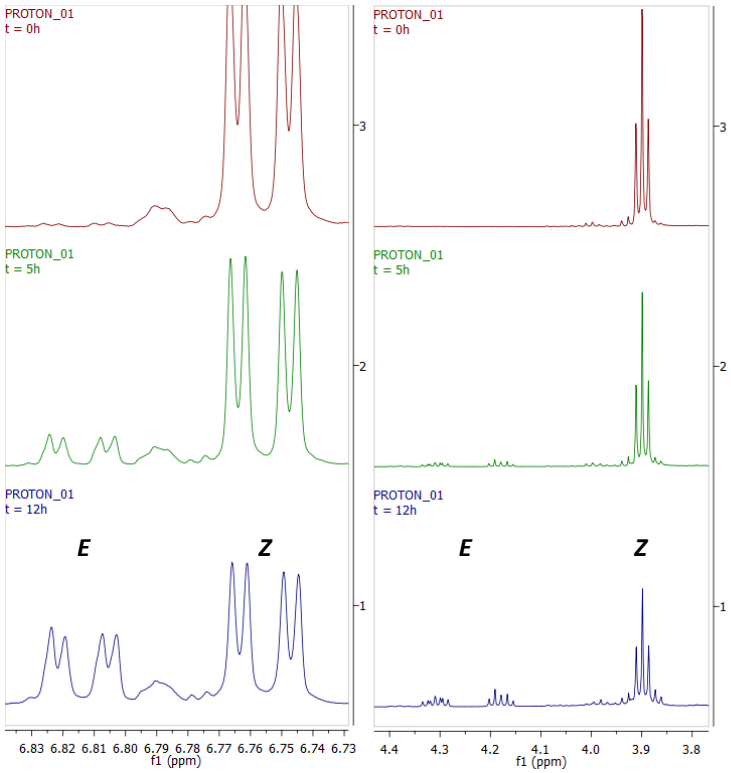


Figure 28. Expansions of ^{1}H NMR spectra of Figure 27 showing an aromatic proton shift (left) and the signals corresponding to the hydrogens bonded to the first carbon of the linker between the two aromatic rings of stiff-stilbnene.(right).

2. UV/Vis spectra

UV/Vis spectra of synthesized compounds.

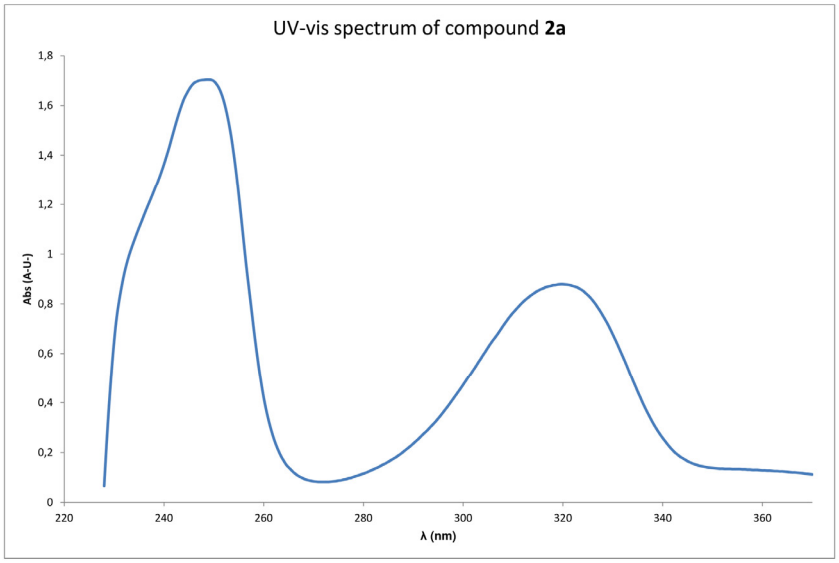


*Figure 29. UV/Vis spectrum of compound **2a**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

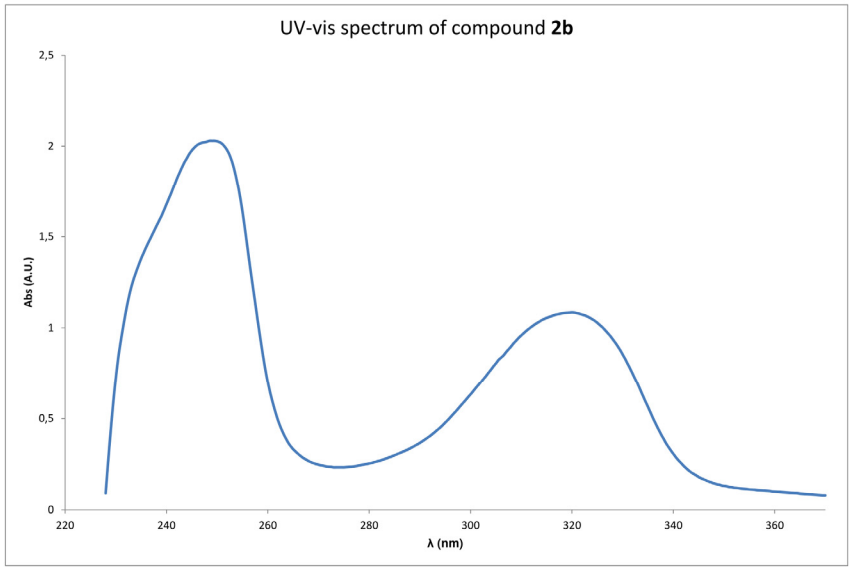


*Figure 30. UV/Vis spectrum of compound **2b**.*

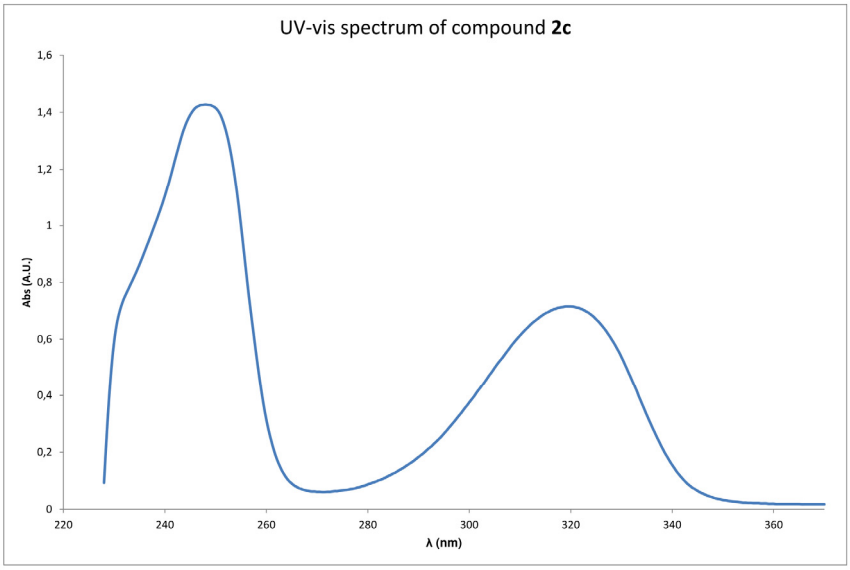


*Figure 31. UV/Vis spectrum of compound **2c**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

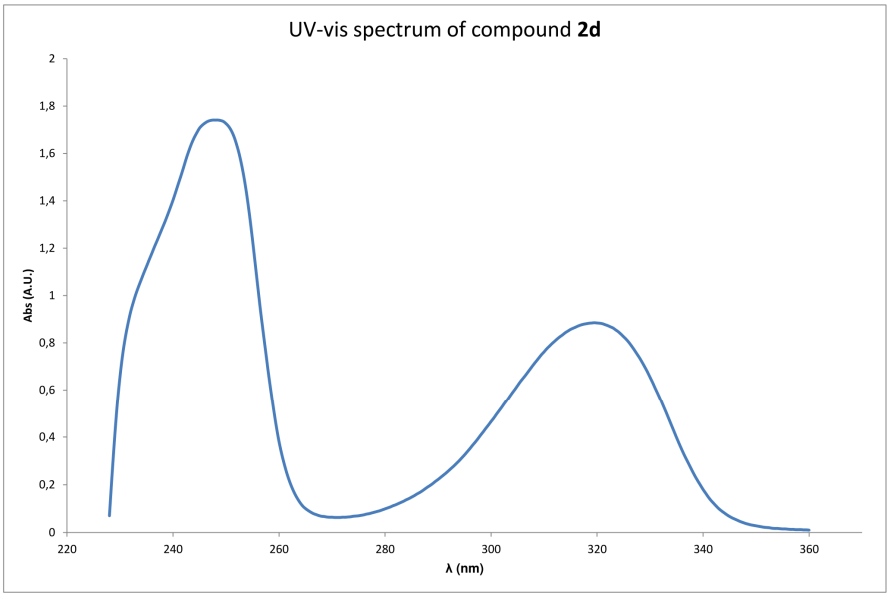


*Figure 32. UV/Vis spectrum of compound **2d**.*

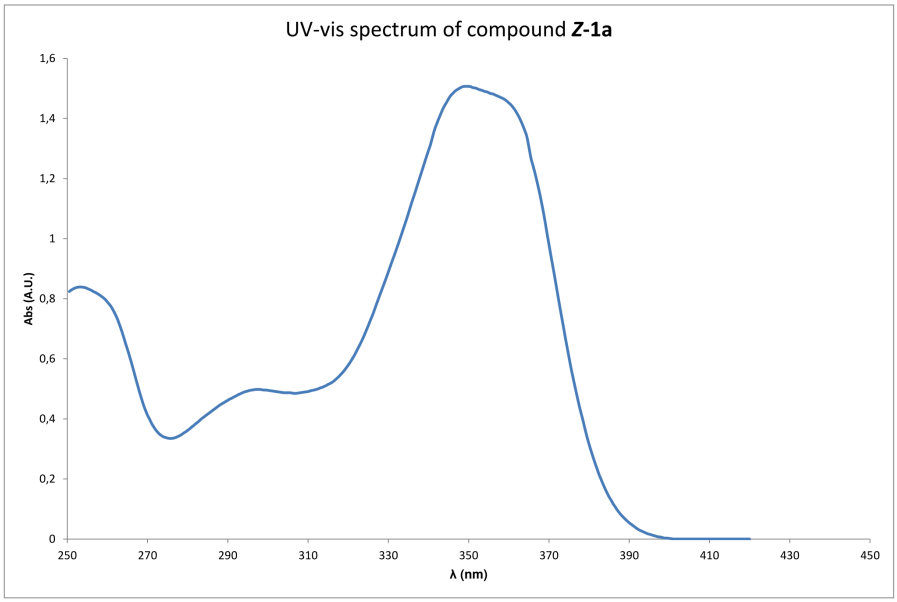


*Figure 33. UV/Vis spectrum of compound **Z-1a**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

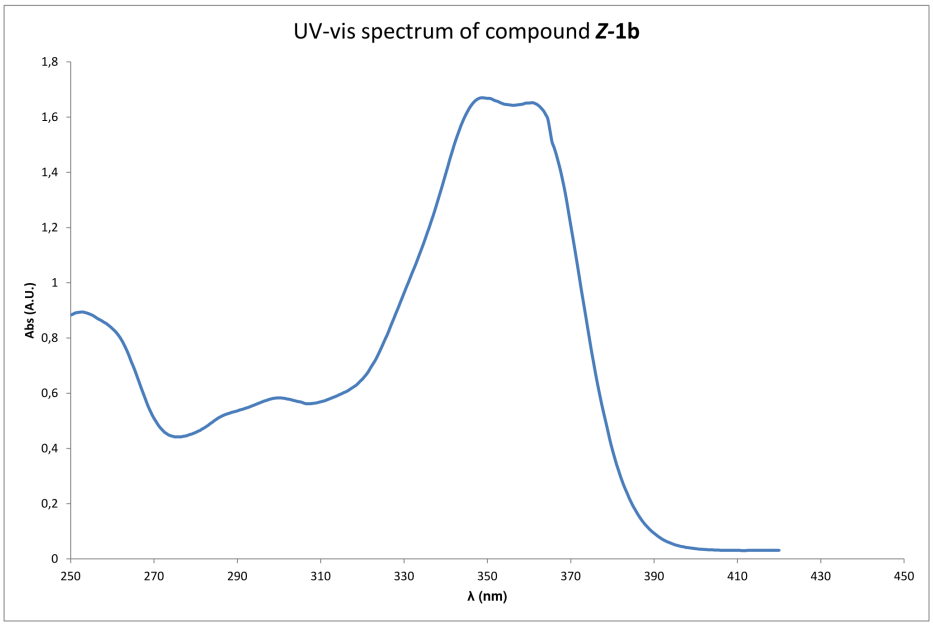


*Figure 34. UV/Vis spectrum of compound **Z-1b**.*

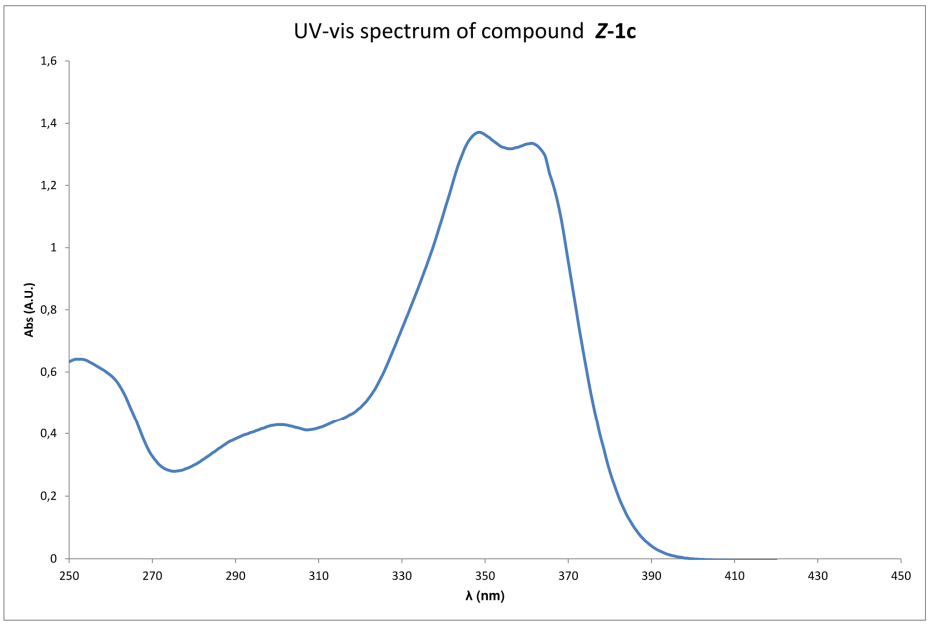


*Figure 35. UV/Vis spectrum of compound **Z-1c**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

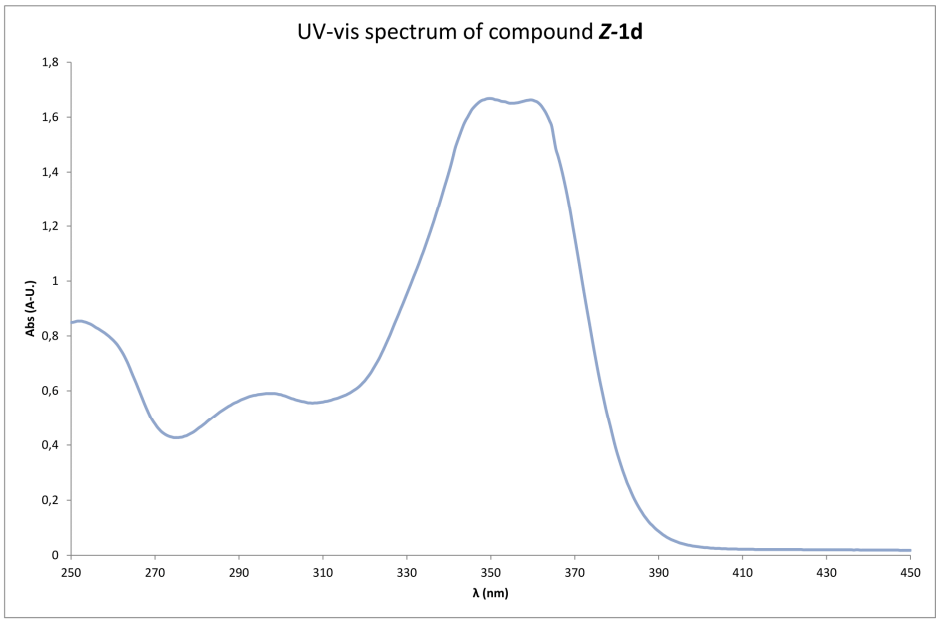


*Figure 36. UV/Vis spectrum of compound **Z-1d**.*

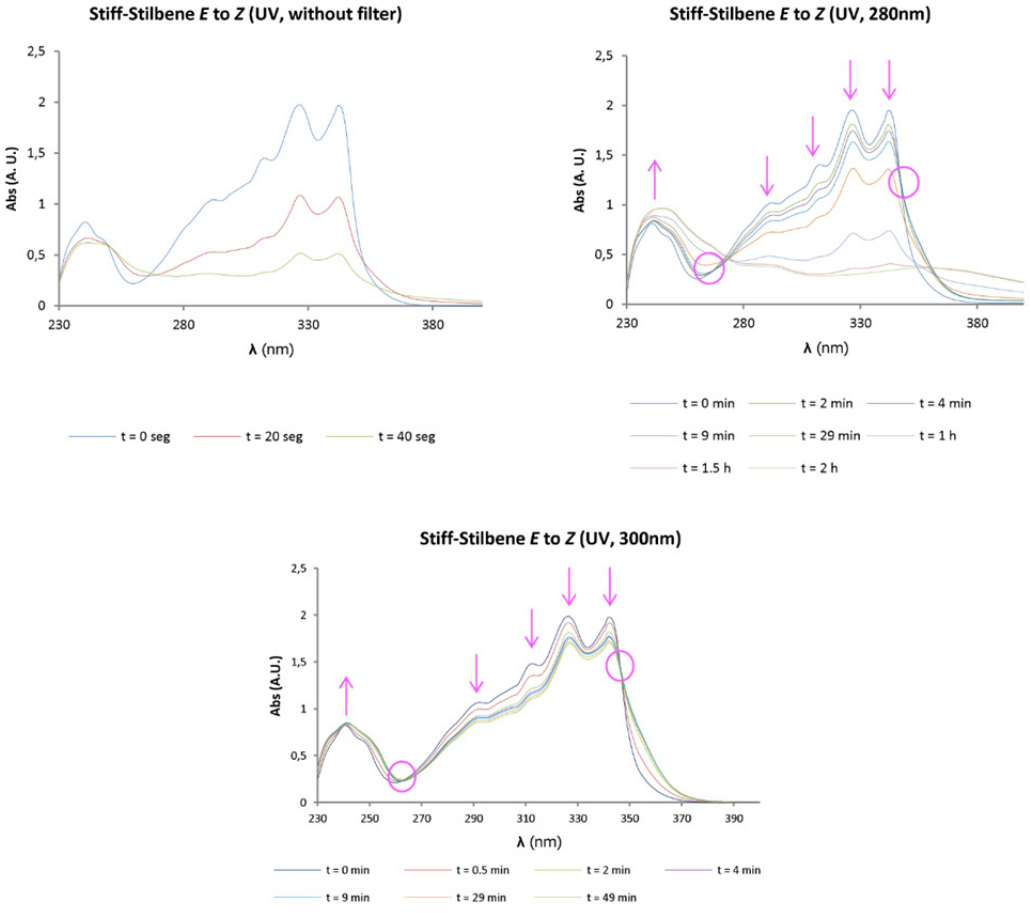


Figure 37. Photo-isomerizations from *E*-stiff-stilbene to *Z*-stiff-stilbene followed by UV-vis spectroscopy. The samples were irradiated with UV light without filter (top, left), UV light of 280 nm (top, right) and UV light of 300 nm (bottom).

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

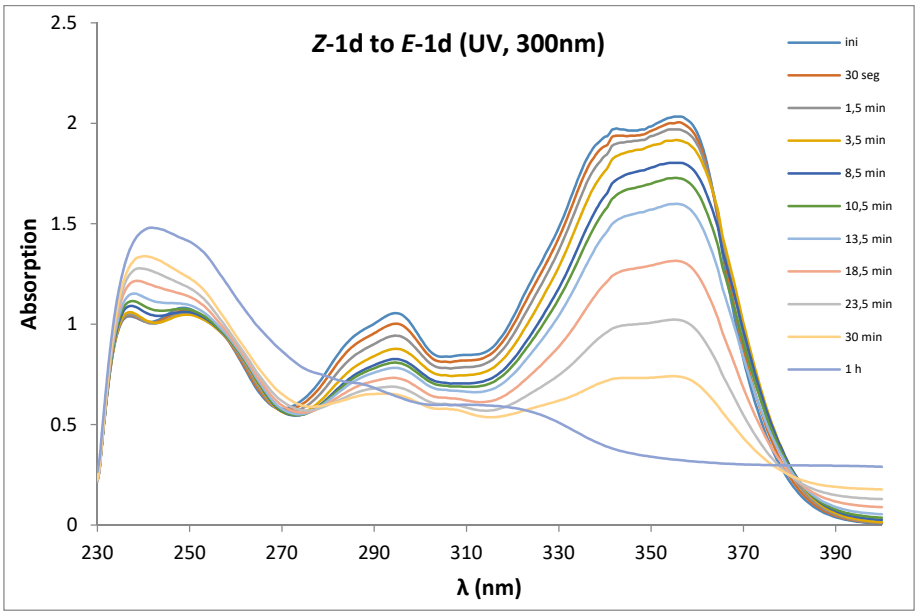


Figure 38. Photo-isomerization from ***E*-1d** to ***Z*-1d** followed by UV-vis spectroscopy. The sample was irradiated with UV light of 300 nm.

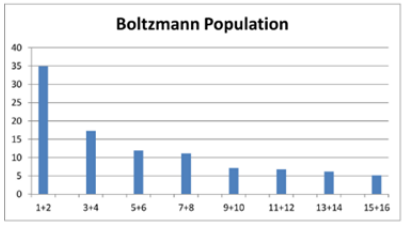
Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

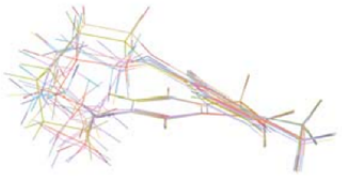
3. Conformational analysis

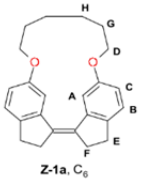
Data from MM (OPLS3) conformational analysis.

***Z*-1a** conformational analysis

Entry ID	Potential Energy-OPLS3e	RMS Derivative-OPLS3e	Relative Potential Energy-OPLS3e	Boltzmann Population	enatiomers	Entry ID	Boltzmann Population	Boltzmann Population w/o enantiomers
1	16.416	0.039	0	17.510664		1+2	17.510664	34.945729
2	16.427	0.037	0.011	17.435065	*		17.435065	
3	18.161	0.046	1.744	8.663045		3+4	8.663045	17.304307
4	18.167	0.036	1.751	8.641262	*		8.641262	
5	19.086	0.034	2.67	5.963962		5+6	5.963962	11.900138
6	19.098	0.032	2.681	5.936176	*		5.936176	
7	19.258	0.038	2.841	5.565757		7+8	5.565757	11.116891
8	19.264	0.045	2.848	5.551134	*		5.551134	
9	20.343	0.042	3.927	3.591659		9+10	3.591659	7.171812
10	20.351	0.041	3.935	3.580153	*		3.580153	
11	20.472	0.036	4.055	3.41045	*	11+12	3.41045	6.804958
12	20.483	0.049	4.067	3.394508			3.394508	
13	20.962	0.04	4.546	2.798056		13+14	2.798056	6.192564
14	20.987	0.045	4.571	2.769804	*		2.769804	
15	21.149	0.034	4.733	2.594582	*	15+16	2.594582	5.188306
16	21.15	0.033	4.734	2.593724			2.593724	
								100.000001







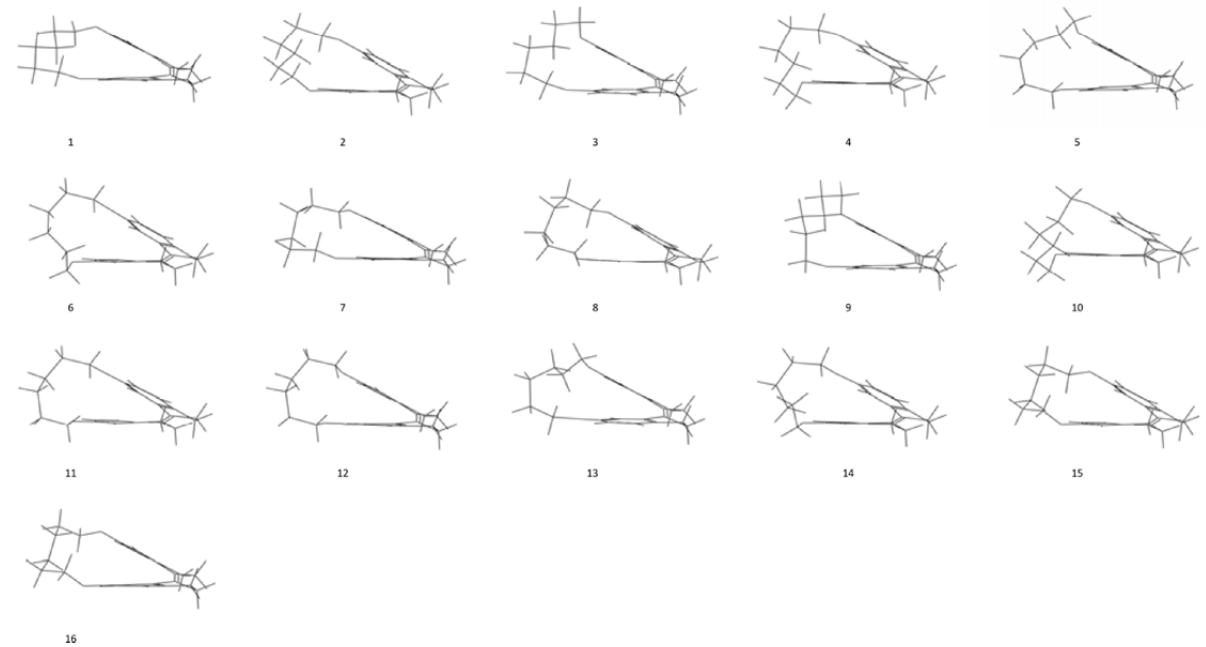


*Figure 39. Conformational analysis of **Z-1a**.*

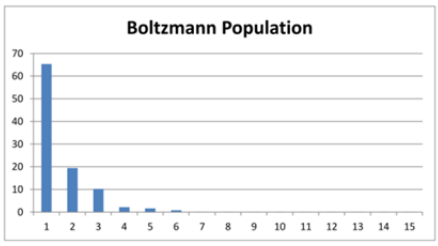
Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

[a] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

***E*-1a** conformational analysis

Entry ID	Potential Energy-OPLS3e	RMS Derivative-OPLS3e	Relative Potential Energy-OPLS3e	Boltzmann Population
1	169.749	0.047	0	65.368285
2	172.751	0.042	3.002	19.470553
3	174.337	0.033	4.589	10.266941
4	178.188	0.027	8.44	2.171404
5	178.905	0.031	9.157	1.625883
6	180.584	0.047	10.836	0.825936
7	186.724	0.047	16.975	0.069386
8	187.738	0.029	17.989	0.046089
9	188.912	0.033	19.164	0.028699
10	188.921	0.039	19.173	0.028593
11	189.682	0.031	19.934	0.021035
12	189.718	0.028	19.97	0.020733
13	189.8	0.035	20.052	0.020055
14	189.902	0.04	20.154	0.019248
15	190.187	0.03	20.438	0.01716
				100



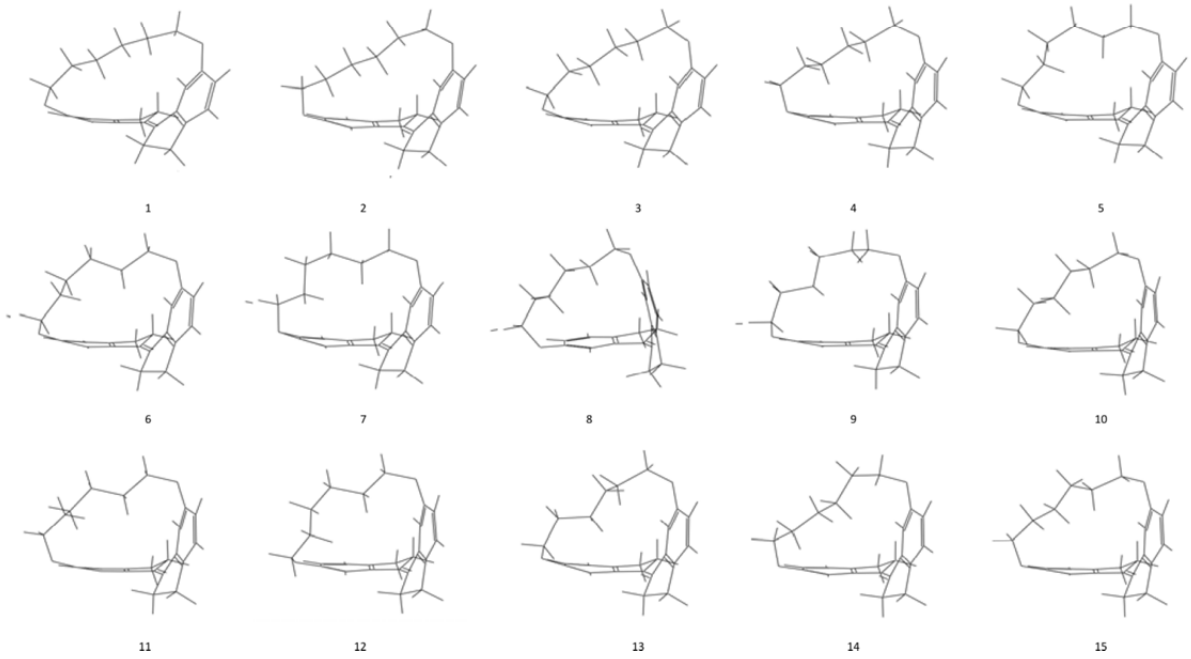


*Figure 40. Conformational analysis of **E-1a**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

[a] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

***Z*-1b** conformational analysis

Entry ID	Potential Energy-OPLS3e	RMS Derivative-OPLS3e	Relative Potential Energy-OPLS3e	Boltzmann Population	enatiomer	Entries	Boltzmann Population w/o enantiomers
1	0.8	0.043	0	28.280308		1	28.280308
2	3.265	0.034	2.465	10.463016		2+3	20.922542
3	3.266	0.041	2.466	10.459526	*	8+9+10+11	16.531972
4	3.899	0.042	3.099	8.1002	*	4+5	16.177061
5	3.906	0.043	3.106	8.076861		6	6.550279
6	4.426	0.045	3.626	6.550279		7	6.247828
7	4.543	0.048	3.743	6.247828		12+13	5.290011
8	5.475	0.037	4.675	4.290365			
9	5.479	0.042	4.679	4.282768	*		
10	5.653	0.039	4.853	3.992008	*		
11	5.669	0.045	4.869	3.966831	*		
12	6.65	0.038	5.85	2.670545	*		
13	6.698	0.046	5.898	2.619466			
							100.000001

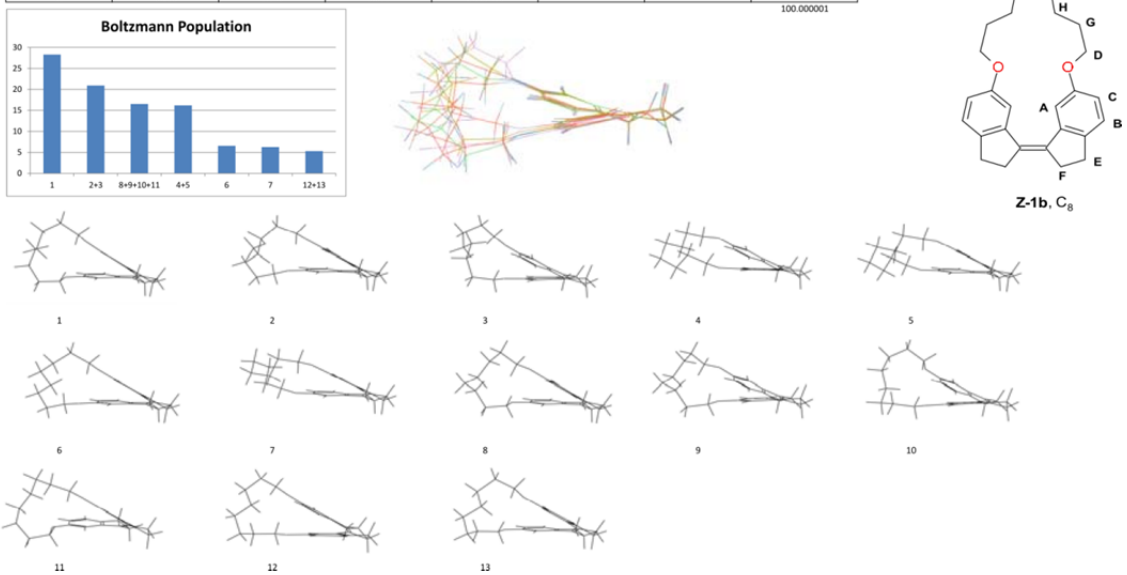


*Figure 41. Conformational analysis of **Z-1b**.*

***E*-1b** conformational analysis

Entry ID	Potential Energy-OPLS3e	RMS Derivative-OPLS3e	Relative Potential Energy-OPLS3e	Boltzmann Population
1	71.765	0.035	0	91.534935
2	77.709	0.042	5.944	8.320544
3	87.756	0.034	15.991	0.144521

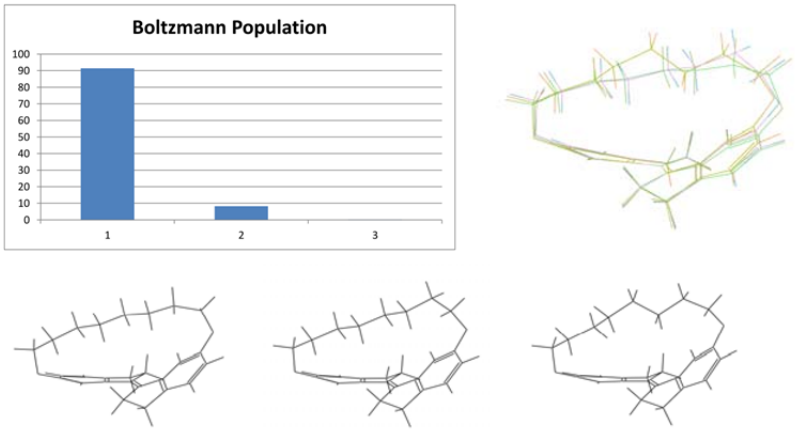


*Figure 42. Conformational analysis of **E-1b**.*

Effect of Ring Size on Photoisomerization Properties of Stiff Stilbene macrocycles

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

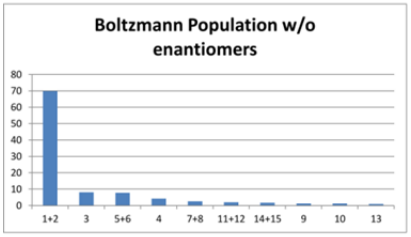
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

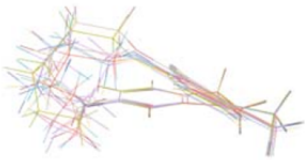
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

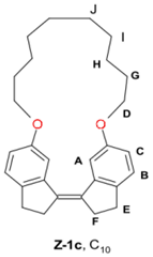
***Z*-1c** conformational analysis

Entry ID	Potential Energy-OPLS3e	RMS Derivative-OPLS3e	Relative Potential Energy-OPLS3e	Boltzmann Population	enatiomers	Entry ID	Boltzmann Population w/o enantiomers
1	0.765	0.041	0	36.706599		1+2	69.900258
2	1.015	0.035	0.249	33.193659	*	3	8.113675
3	4.507	0.049	3.742	8.113675	*	5+6	7.824915
4	6.103	0.045	5.338	4.260882	*	4	4.260882
5	6.314	0.027	5.548	3.914211	*	7+8	2.674599
6	6.316	0.035	5.551	3.910704		11+12	2.01951
7	8.965	0.044	8.2	1.343151	*	14+15	1.718937
8	8.987	0.044	8.221	1.331448		9	1.273828
9	9.096	0.05	8.331	1.273828		10	1.243654
10	9.156	0.042	8.391	1.243654		13	0.969741
11	9.658	0.046	8.893	1.015556			
12	9.686	0.042	8.921	1.003954	*		
13	9.772	0.03	9.007	0.969741	*		
14	9.991	0.045	9.226	0.887901	*		
15	10.155	0.042	9.39	0.831036			

99.999999







Z-1c, C_{10}

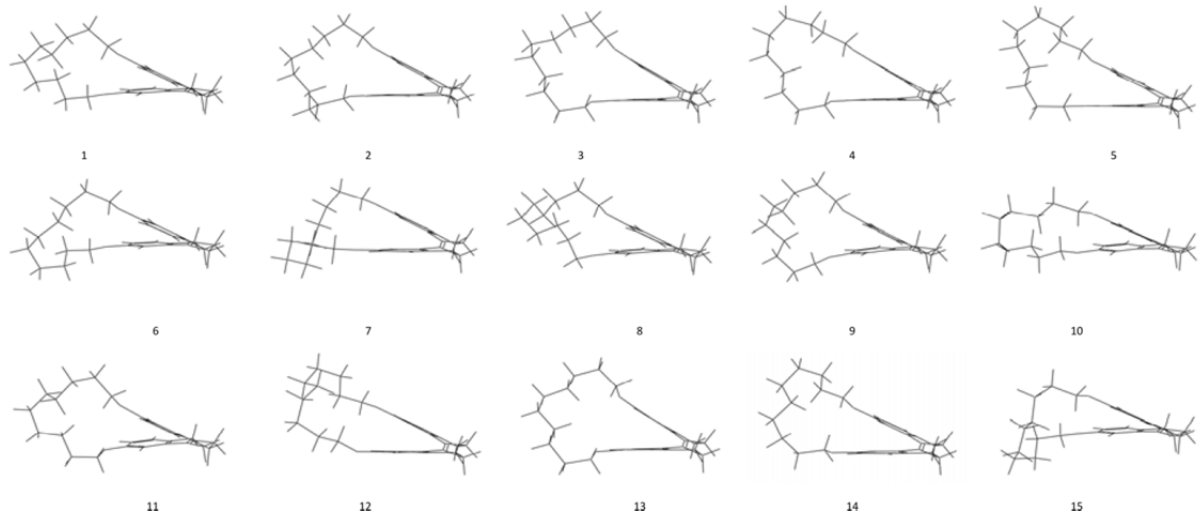
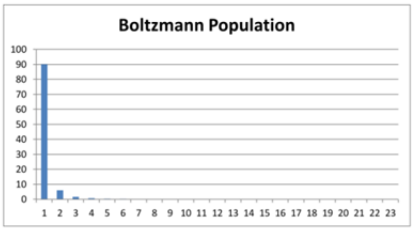


*Figure 43. Conformational analysis of **Z-1c**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

***E*-1c** conformational analysis

Entry ID	Potential Energy-OPLS3e	RMS Derivative-OPLS3e	Relative Potential Energy-OPLS3e	Boltzmann Population
1	17.733	0.04	0	90.043783
2	24.439	0.044	6.706	6.020084
3	27.67	0.024	9.937	1.634638
4	29.576	0.036	11.843	0.757804
5	31.661	0.038	13.928	0.32676
6	32.8	0.043	15.068	0.206338
7	33.436	0.041	15.703	0.15965
8	33.445	0.03	15.712	0.159099
9	34.897	0.047	17.164	0.088555
10	35.014	0.037	17.281	0.084489
11	35.322	0.035	17.59	0.074595
12	35.41	0.028	17.677	0.071999
13	35.929	0.048	18.196	0.058405
14	36.304	0.035	18.571	0.050205
15	36.496	0.034	18.763	0.046469
16	36.867	0.033	19.134	0.040009
17	37.444	0.045	19.711	0.031699
18	37.518	0.046	19.785	0.030765
19	37.91	0.044	20.177	0.026261
20	37.92	0.031	20.187	0.026163
21	38.349	0.041	20.616	0.022005
22	38.427	0.045	20.694	0.021318
23	38.725	0.038	20.992	0.018905



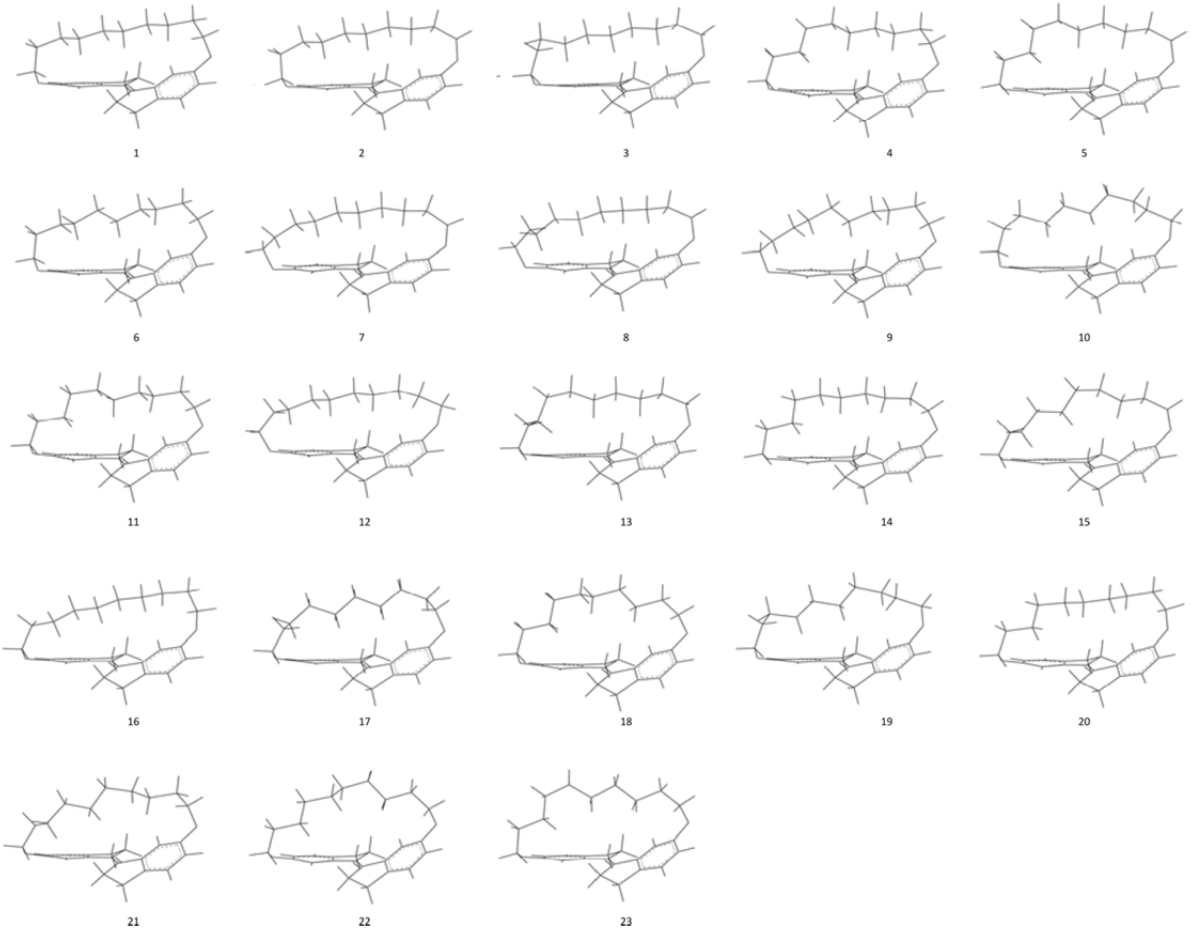


*Figure 44. Conformational analysis of **E-1c**.*

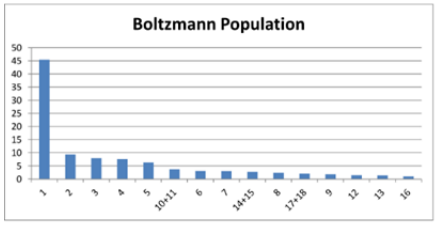
Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

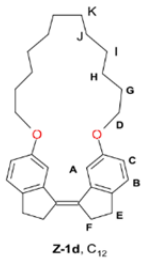
[a] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

***Z*-1d** conformational analysis

Entry ID	Potential Energy-OPLS3e	RMS Derivative-OPLS3e	Relative Potential Energy-OPLS3e	Boltzmann Population	enatiomers	Entry ID	Boltzmann Population w/o enantiomers
1	7.765	0.041	0	45.496109		1	45.4961
2	11.678	0.042	3.914	9.382472		2	9.3825
3	12.079	0.049	4.314	7.982229		3	7.9822
4	12.18	0.046	4.415	7.663767		4	7.6638
5	12.644	0.026	4.879	6.356358		5	6.3564
6	14.392	0.047	6.627	3.139533		10+11	3.7215
7	14.466	0.032	6.701	3.047318		6	3.1395
8	14.993	0.048	7.229	2.463321		7	3.0473
9	15.641	0.042	7.876	1.897164		14+15	2.7615
10	15.675	0.034	7.91	1.870885		8	2.4633
11	15.702	0.04	7.937	1.850606	*	17+18	2.0846
12	16.235	0.041	8.471	1.492442		9	1.8972
13	16.38	0.036	8.616	1.4077		12	1.4924
14	16.397	0.041	8.632	1.398119		13	1.4077
15	16.46	0.035	8.695	1.363372	*	16	1.1040
16	16.983	0.039	9.218	1.103958			
17	17.12	0.029	9.355	1.044591			
18	17.131	0.038	9.366	1.040056	*		





Z-1d, C_{12}

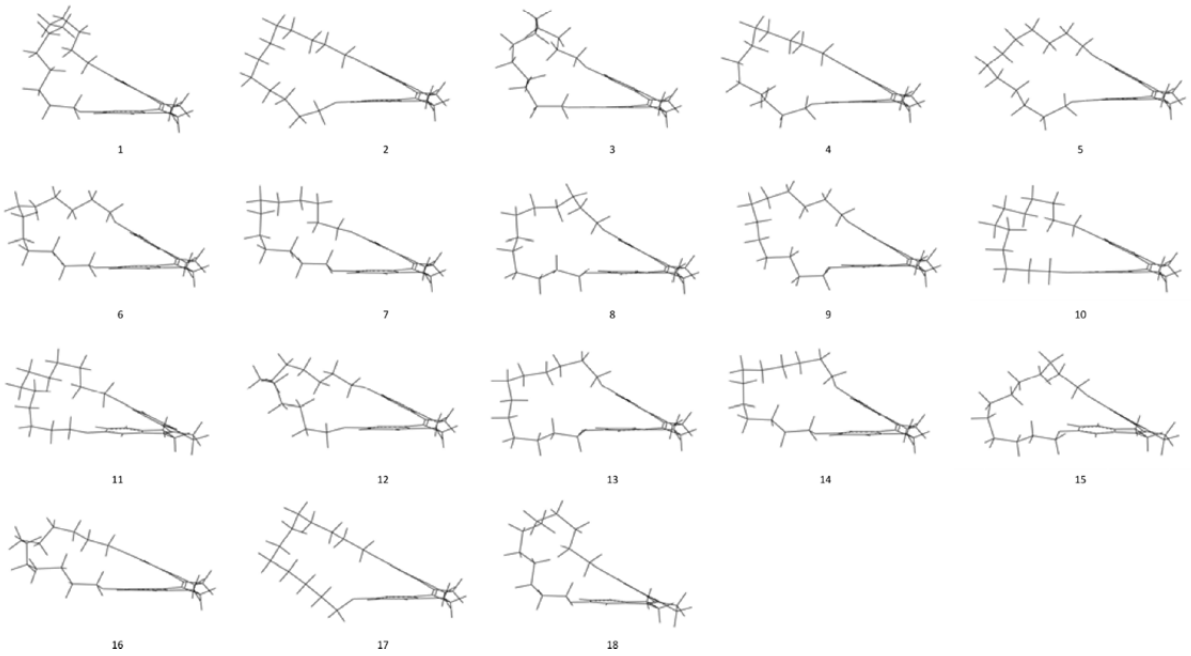


*Figure 45. Conformational analysis of **Z-1d**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

***E*-1d** conformational analysis

Entry ID	Potential Energy-OPLS3e	RMS Derivative-OPLS3e	Relative Potential Energy-OPLS3e	Boltzmann Population	enantiomer	Entry ID	Boltzmann Population
1	7.85	0.032	0	16.70512		1	16.70512
2	8.544	0.039	0.694	12.624384		2	12.624384
3	9.024	0.043	1.174	10.404704		3	10.404704
4	9.353	0.048	1.503	9.109486		4	9.109486
5	9.913	0.041	2.063	7.267577	*	5	7.267577
6	10.227	0.046	2.376	6.40449		6	6.40449
7	11.041	0.045	3.191	4.610556		7	4.610556
8	11.471	0.024	3.621	3.876944		8	3.876944
9	11.486	0.031	3.636	3.85389		9	3.85389
10	11.814	0.027	3.964	3.375726	*	10	3.375726
11	11.839	0.046	3.989	3.341298	*	11	3.341298
12	12.254	0.043	4.404	2.82645		12	2.82645
13	12.551	0.04	4.701	2.507599		13	2.507599
14	12.636	0.049	4.786	2.423038		14	2.423038
15	13.194	0.024	5.344	1.934374		15	1.934374
16	13.199	0.048	5.349	1.930384		16	1.930384
17	13.391	0.043	5.541	1.786966		17	1.786966
18	13.394	0.024	5.544	1.784469		18	1.784469
19	13.482	0.034	5.632	1.722437		19	1.722437
20	13.808	0.041	5.958	1.510107		20	1.510107

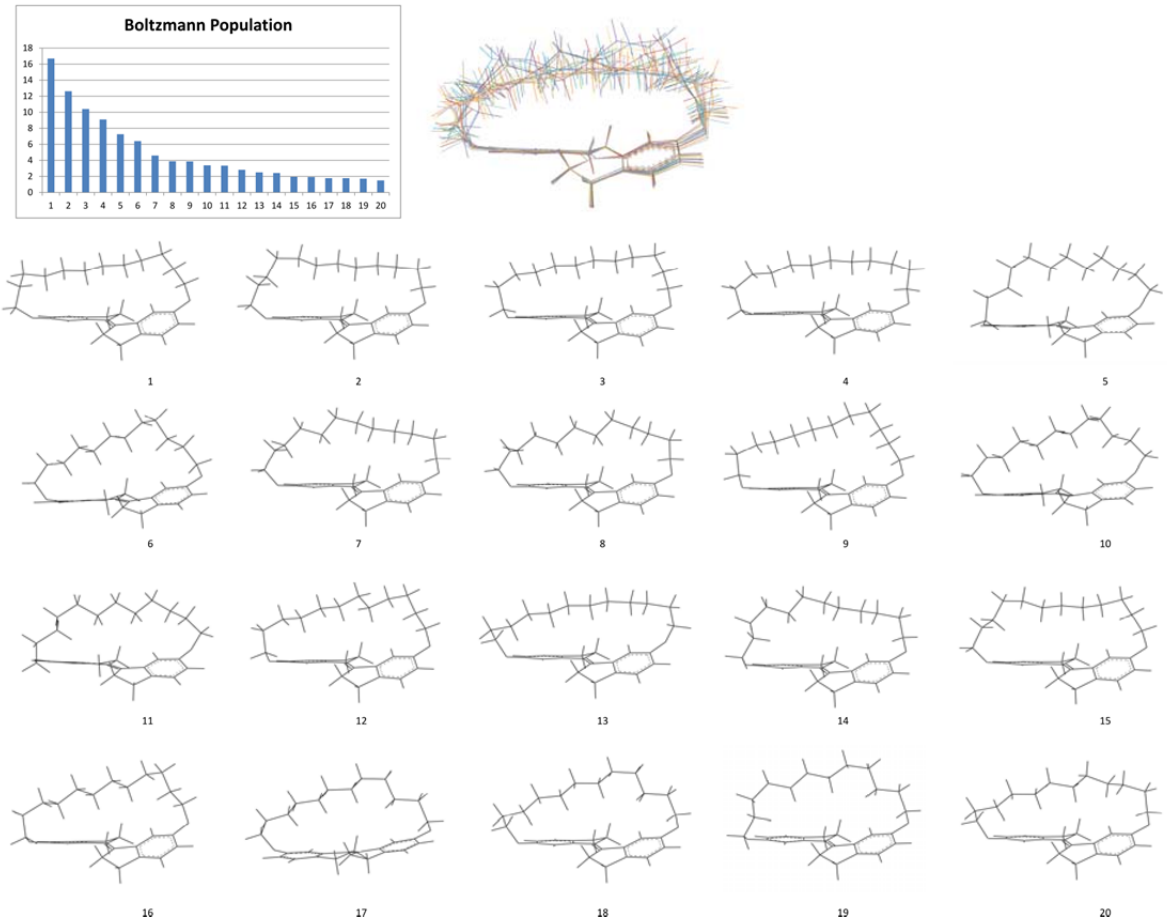


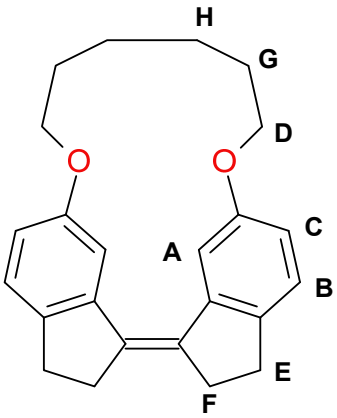
*Figure 46. Conformational analysis of **E-1d**.*

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

4. NOE buildup

*Table 1. NOE buildup for **Z-1a** SS-hexanedioldiether, 14 mg.*

No	δ f2	δ f1	f1	f2	σ	R^2	DISTANCE, r_{AB}
2	7.73	4.05	**A**	**D**	4.26E-05	0.9997	**2.31**
3	7.73	1.58	**A**	**H**	1.02E-05	0.9988	**2.94**
4	7.73	2.92	**A**	**E**	1.03E-06	0.7310	**4.30**
5	7.73	1.78	**A**	**G**	8.58E-06	0.9961	**3.02**
6	7.73	2.8	**A**	**F**	1.82E-06	0.8385	**3.91**
8	7.17	2.81	**B**	**F**	1.68E-06	0.8989	**3.96**
9	7.17	2.93	**B**	**E**	1.77E-05	0.9985	**2.68**
10	7.17	6.79	**B**	**C**	2.61E-05	0.7868	**2.51 ref**
12	6.78	4.05	**C**	**D**	2.63E-05	0.9998	**2.51**
16	4.05	1.79	**D**	**G**	5.25E-05	0.9999	**2.23**
17	4.05	1.58	**D**	**H**	3.78E-05	0.9993	**2.36**



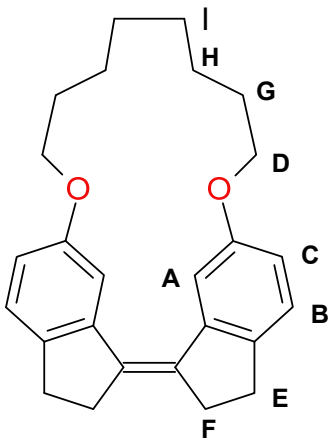
Z-1a, C_6

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

*Table 2. NOE buildup for **Z-1b** SS-octanedioldiether, 4 mg.*

No	δ f2	δ f1	ass. f1	ass. f2	σ	R^2	DISTANCE, r_{AB}
2	7.69	1.56	**A**	**H**	2.03E-06	0.8521	**4.10**
3	7.69	1.8	**A**	**G**	3.63E-06	0.9869	**3.72**
4	7.69	2.92	**A**	**E**	1.16E-06	0.9131	**4.50**
5	7.69	1.44	**A**	**I**	2.51E-06	0.9564	**3.96**
6	7.68	2.8	**A**	**F**	2.23E-06	0.9946	**4.04**
7	7.68	3.95	**A**	**D**	4.96E-05	0.9998	**2.41**
9	7.18	6.74	**B**	**C**	3.86E-05	0.9846	**2.51 (ref)**
10	7.17	3.96	**B**	**D**	1.5E-06	0.9730	**4.31**
11	7.17	2.81	**B**	**F**	3.28E-06	0.3621	**3.79**
12	7.17	2.92	**B**	**E**	2.03E-05	0.8102	**2.79**
14	6.74	1.82	**C**	**G**	1.4E-06	0.8510	**4.36**
15	6.74	1.56	**C**	**H**	7.52E-07	0.7091	**4.84**
17	6.73	3.95	**C**	**D**	3.87E-05	0.9993	**2.51**
20	3.96	1.81	**D**	**G**	5.36E-05	1.0000	**2.38**
22	3.95	1.44	**D**	**I**	2.73E-05	0.9999	**2.66**
25	3.95	1.56	**D**	**H**	1.99E-05	0.9996	**2.80**
32	1.82	1.54	**G**	**H**	2.95E-05	0.9961	**2.62**
34	1.81	1.43	**G**	**I**	3.61E-05	0.9994	**2.54**

Data with greyed R^2 values not taken into account.



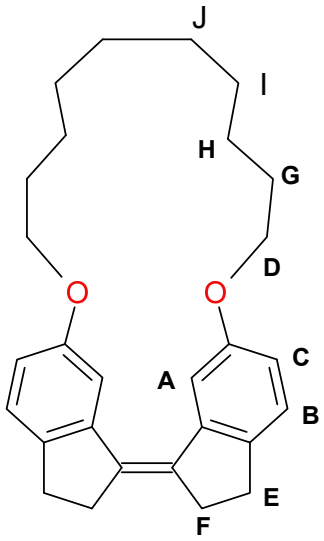
Z-1b, C_8

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

*Table 3. NOE buildup for **Z-1c** SS-decanedioldiether, 12 mg.*

No	δ f2	δ f1	ass. f1	ass. f2	σ	R^2	DISTANCE, r_{AB}
1	7.65	2.91	**A**	**F**	1.07E-06	0.8234	**4.71**
2	7.65	1.77	**A**	**H**	1.45E-06	0.9413	**4.48**
3	7.64	3.91	**A**	**E**	5.8E-05	0.7263	**2.42**
4	7.64	2.8	**A**	**G**	1.22E-06	0.0217	**4.61**
7	7.64	1.54	**A**	**I**	1.22E-06	0.8885	**4.61**
9	7.18	2.93	**C**	**F**	2.59E-05	0.9921	**2.77**
10	7.18	2.81	**C**	**G**	3.43E-06	0.9740	**3.88**
12	7.18	6.75	**C**	**D**	4.67E-05	0.9827	**2.51 (ref)**
13	7.17	3.95	**C**	**E**	9.02E-07	0.0703	**4.85**
14	6.76	3.89	**D**	**E**	5.22E-05	0.9995	**2.46**
17	6.75	1.54	**D**	**I**	4.35E-07	0.2727	**5.47**
19	6.74	1.77	**D**	**H**	2.17E-06	0.9475	**4.19**
22	3.91	1.53	**E**	**I**	2.41E-05	0.9994	**2.80**
25	3.91	1.76	**E**	**H**	6.65E-05	1.0000	**2.37**
26	3.9	2.81	**E**	**G**	1.49E-07	0.0879	**6.55**

Data with greyed R^2 values not taken into account.

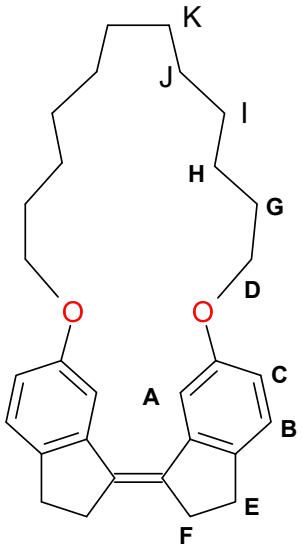


Z-1c, C_{10}

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

*Table 4. NOE buildup for **Z-1d** SS-dodecanedioldiether, 10 mg.*

No	δ f2	δ f1	ass. f1	ass. f2	σ	R^2	DISTANCE, r_{AB}
1	7.63	3.89	**A**	**D**	6.3653E-05	0.9999	2.40
2	7.63	1.75	**A**	**G**	1.3619E-06	0.5091	4.55
3	7.63	2.81	**A**	**F**	2.7143E-06	0.9530	4.05
4	7.63	2.92	**A**	**E**	2.1838E-06	0.9817	4.20
6	7.18	6.75	**B**	**C**	4.8100E-05	0.9604	2.51 (ref)
7	7.17	2.81	**B**	**F**	3.9361E-06	0.8914	3.81
9	7.17	2.92	**B**	**E**	2.6125E-05	0.9971	2.78
10	6.75	7.18	**C**	**B**	4.8100E-05	0.9604	2.51
12	6.75	3.89	**C**	**D**	4.5482E-05	0.9978	2.53
13	3.9	7.63	**D**	**A**	6.3653E-05	0.9999	2.40
14	3.89	1.4	**D**	**I**	1.1242E-05	0.9786	3.20
15	3.89	1.74	**D**	**G**	6.3306E-05	0.9987	2.40
17	3.89	1.49	**D**	**H**	3.0916E-05	0.9935	2.70
26	1.75	1.34	**G**	**J**	1.2303E-05	0.6422	3.15
27	1.74	1.39	**G**	**I**	2.6610E-05	0.9793	2.77



Z-1d, C_{12}

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

5. DFT, optimized geometries

Coordinates compound ***Z*-1a**:

C	2.76129845	0.40718128	-0.17315222
C	2.22047485	-0.96879609	-0.09738357
C	3.24951808	-1.89549972	-0.37237364
C	4.53308478	-1.18912002	-0.73668620
C	4.28226719	0.26509188	-0.27109918
C	2.16386893	1.62429220	-0.09837610
C	0.74190928	2.01766752	-0.09403134
C	0.61031056	3.31097189	0.45778253
C	1.96607769	3.87342650	0.82074837
C	2.95119054	2.92061219	0.09344949
C	-0.38775907	1.35495617	-0.58173297
C	-1.65199764	1.93576620	-0.43043873
C	-0.64905554	3.88451727	0.60284499
C	0.95967365	-1.43754719	0.30939069
C	0.73021880	-2.81452894	0.40008249
C	3.01681942	-3.26543143	-0.26708926
H	5.41319904	-1.64097055	-0.26772343
H	4.69869467	-1.22364495	-1.82218113
H	4.73721144	0.42317831	0.71691177
H	4.72516250	1.00373896	-0.94519093
H	2.08540573	4.91959944	0.52064398
H	2.12783333	3.83220387	1.90660009
H	3.22540093	3.34727627	-0.88199348
H	3.87929448	2.77207146	0.65158027
H	-0.32100776	0.39891637	-1.08481146
H	-0.75735152	4.87391010	1.04086446
H	0.17361041	-0.75400817	0.59766623
H	3.81279171	-3.97613596	-0.47585783
C	1.75494004	-3.72828177	0.10970525
C	-1.79040189	3.19273237	0.17757814
H	-2.77096411	3.64169988	0.29359792
H	1.54682691	-4.79060702	0.19295200
C	-3.94300611	1.23496013	-0.20759567
H	-4.43362980	2.21181518	-0.30910213
H	-3.73976646	1.07012870	0.85898781
C	-4.84335295	0.14842689	-0.78183846
H	-5.09038197	0.41742868	-1.81673668
H	-5.78535421	0.17656804	-0.21813118
C	-4.26543814	-1.27783441	-0.76375645
H	-4.98098526	-1.92109225	-1.28907728
H	-3.35311956	-1.28982868	-1.36898625
C	-3.98858591	-1.87258530	0.64201527
H	-4.40124029	-2.88880439	0.68706020
H	-4.53941371	-1.29779509	1.39756490
C	-2.51023541	-1.95103656	1.07215382
H	-2.05562680	-0.95359736	1.07807753
H	-2.46280755	-2.32887278	2.10114826
C	-1.68804944	-2.89995542	0.19576555
H	-2.26155818	-3.81850680	0.01810098
H	-1.45336209	-2.45915887	-0.77895620
O	-0.46573816	-3.33667728	0.82918807
O	-2.70444723	1.21599901	-0.93403621

Effect of Ring Size on Photoisomerization Properties of Stiff Stilbene macrocycles

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

Coordinates compound ***E*-1a**:

C	0.54716192	-1.85357162	-0.39615919
C	0.62239489	-2.00131722	-1.90288656
C	2.09796864	-2.38495553	-2.15538794
C	2.78872096	-1.62606063	-1.05524279
C	1.89393107	-1.45738222	0.01380473
C	-0.55780330	-1.89217328	0.38050085
C	-0.62445237	-2.01463194	1.89018599
C	-2.09942996	-2.38811274	2.15680106
C	2.17793885	-0.55477726	1.03755849
C	3.29524432	0.25789940	0.91524395
C	4.24886875	0.01882795	-0.07900828
C	3.99729121	-0.94008211	-1.06374513
H	-2.95778399	3.36555934	-1.72136716
H	-0.10389654	-2.71792649	-2.30314219
H	2.44880055	-2.10913644	-3.15559184
H	2.23158489	-3.47111706	-2.04560151
H	-0.43515602	-1.03592198	2.36156638
H	0.10140854	-2.72672942	2.29997867
H	-2.44111568	-2.10441853	3.15799399
H	-2.24143451	-3.47390881	2.05379266
H	1.45484482	-0.31811100	1.81424119
H	5.13291550	0.65132206	-0.13473964
H	4.70178013	-1.06916770	-1.88442121
O	3.33234151	1.38175679	1.70084857
C	3.11320141	2.59127281	0.95432595
H	2.96084871	3.36530249	1.71753551
H	4.03419098	2.84763437	0.40688943
C	1.94973787	2.57827893	-0.03196671
H	2.09799292	1.77504096	-0.77121423
H	2.03598529	3.51704087	-0.60092478
C	0.53940661	2.48784821	0.54251363
H	0.42836204	1.57414634	1.14898730
H	0.37125632	3.33208694	1.23119675
C	-0.53690674	2.49016413	-0.54569720
H	-0.43007115	1.57685374	-1.15361269
H	-0.36666637	3.33466623	-1.23353413
C	-1.94631993	2.58404670	0.03026581
H	-2.09449024	1.78261565	0.77148524
H	-2.03110072	3.52427775	0.59696608
C	-3.11006780	2.59423177	-0.95540442
H	0.43921087	-1.03092346	-2.39399701
H	-4.03110821	2.85270961	-0.40908700
C	-2.18478270	-0.56266401	-1.03823066
H	-1.46462272	-0.33162362	-1.81944779
C	-4.24304317	0.03119422	0.09208390
H	-5.12067003	0.67193110	0.15400853
C	-3.99214911	-0.92849554	1.07598078
H	-4.69055663	-1.04926833	1.90314737
C	-2.79144326	-1.62798584	1.05801588
C	-1.90249480	-1.46899303	-0.01746242
C	-3.29416037	0.26010991	-0.90901274
O	-3.32776485	1.38212309	-1.69754479

Effect of Ring Size on Photoisomerization Properties of Stiff Stilbene macrocycles

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

Coordinates compound ***Z*-1b**:

C	-3.18229949	-0.20513389	0.15612866
C	-2.32086586	-1.39135906	-0.03551873
C	-2.94406428	-2.52396590	0.53194095
C	-4.27885873	-2.15198891	1.13571633
C	-4.55837282	-0.74747246	0.54250853
C	-2.92173859	1.12441161	0.06674908
C	-1.65198680	1.86500605	-0.07595852
C	-1.91847013	3.22455293	-0.35752518
C	-3.40685514	3.46752214	-0.45846100
C	-4.02165363	2.18417454	0.15720975
C	-0.33374536	1.44768131	0.11252956
C	0.72075756	2.35609026	-0.05008408
C	-0.86974206	4.12773861	-0.48964156
C	-1.10754705	-1.54629259	-0.72201810
C	-0.49167198	-2.79964897	-0.76365418
C	-2.32905534	-3.77333362	0.48003461
H	-5.06519115	-2.87779925	0.90469614
H	-4.20620453	-2.09757506	2.23053082
H	-5.19221869	-0.84276332	-0.35069729
H	-5.08631044	-0.09384027	1.24200948
H	-3.72479992	4.37929763	0.05779460
H	-3.71304640	3.57374039	-1.50812032
H	-4.28287570	2.36537251	1.20948472
H	-4.94056307	1.87574113	-0.34929236
H	-0.08747374	0.43382152	0.39561810
H	-1.06979909	5.17559386	-0.70075965
H	-0.63642787	-0.72580590	-1.24731214
H	-2.80984768	-4.64239099	0.92262740
C	-1.09154973	-3.91220401	-0.15640732
C	0.45939866	3.70204148	-0.34675599
H	1.26679199	4.41690125	-0.45511078
H	-0.59837356	-4.87813370	-0.21250696
C	3.12964073	2.63022939	-0.06219160
H	3.18461967	3.36081991	0.75812080
H	3.06269172	3.18572906	-1.00691156
C	4.32879424	-1.60850131	0.97400441
H	5.38108046	-1.74532979	1.26109352
H	3.78088292	-2.41860005	1.47419069
C	4.22551276	-1.80918691	-0.55086444
H	4.68764618	-2.77572715	-0.79697451
H	4.83340481	-1.05405497	-1.06285631
C	2.80815850	-1.77959978	-1.15074213
H	2.31754603	-0.82443643	-0.93138158
H	2.88640370	-1.84782032	-2.24317644
C	1.91166289	-2.92452404	-0.68278739
H	2.41347885	-3.88928134	-0.83656784
H	1.66644526	-2.83994064	0.38096544
O	0.69019007	-2.93684080	-1.46084040
O	1.96534692	1.81263704	0.10054899
C	4.67994508	0.98190749	1.22591623
H	5.73981628	0.69245196	1.20955008
H	4.58451570	1.70051308	2.05173449
C	3.83719602	-0.27060311	1.56422464
H	3.85166306	-0.38973745	2.65574563
H	2.79173446	-0.09368153	1.29703948
C	4.36560306	1.73655346	-0.08231621
H	5.20927646	2.40069942	-0.31188815
H	4.28168316	1.04529829	-0.92753211

Effect of Ring Size on Photoisomerization Properties of Stiff Stilbene macrocycles

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

Coordinates compound ***E*-1b**:

C	0.22362244	-1.34905435	-0.61237470
C	0.00642479	-1.19135223	-2.11827428
C	1.25817820	-1.86500049	-2.75746232
C	2.30912950	-1.68544773	-1.68212231
C	1.67349998	-1.50608839	-0.44015921
C	-0.73138884	-1.49742678	0.33390201
C	-0.56539733	-2.07968763	1.73700493
C	-1.93390779	-2.77289443	2.02462257
C	-2.89427876	-1.97246818	1.16801180
C	-2.17777335	-1.32655625	0.15026171
C	2.40334407	-1.08275852	0.67627622
C	3.74829958	-0.75296695	0.52221229
C	4.41351275	-1.03564686	-0.68141032
C	3.68985550	-1.51762448	-1.78320647
C	-4.83387825	-0.64102221	0.60021212
C	-4.24873392	-1.67686622	1.33919703
H	-0.93523587	-1.63116691	-2.45823424
H	1.54098730	-1.41297380	-3.71269767
H	1.05737660	-2.92850766	-2.94618883
H	-0.41219944	-1.27864862	2.47338565
H	0.28464663	-2.76318540	1.81583497
H	-2.19658739	-2.76167502	3.08674211
H	-1.89533565	-3.82498865	1.71029218
H	1.91267565	-0.83506413	1.61050070
H	5.47017306	-0.80440519	-0.77969133
H	4.19933412	-1.66997794	-2.73172187
H	-5.85274027	-0.32430699	0.80289862
H	-4.83446026	-2.17644761	2.10719972
O	4.33814902	-0.05866141	1.55914274
C	4.69081936	1.32241706	1.27442287
H	4.86439367	1.75821641	2.26368264
H	5.64501487	1.34215024	0.73048767
C	3.66242209	2.14274973	0.48115802
H	4.14103800	3.11194698	0.28485934
H	3.53253399	1.67418352	-0.50142252
C	2.27444402	2.37032059	1.11488982
H	1.91529951	1.43407097	1.55456222
H	2.35428459	3.08783146	1.94291883
C	1.23761079	2.85389231	0.07797466
H	1.29475770	2.17977100	-0.78782867
H	1.52181076	3.84712718	-0.29741080
C	-0.22365629	2.87641676	0.57157306
H	-0.41414824	1.95645293	1.14098702
H	-0.37635629	3.70738653	1.27399557
H	-0.00632453	-0.13006194	-2.40244681
C	-2.71851250	2.74522592	-0.12336340
H	-2.73161592	1.99317082	0.67150172
H	-3.10920096	3.66586367	0.32500288
C	-3.67592492	2.27354419	-1.24968568
H	-4.32682538	3.08362790	-1.58668486
H	-3.11334564	1.92779567	-2.12598871
C	-1.25423021	2.94844020	-0.57548114
H	-1.00086601	2.16317431	-1.30037446
H	-1.15279467	3.89918140	-1.11612852
C	-2.77238115	-0.32956306	-0.63348659
H	-2.16761947	0.22791344	-1.33510085
C	-4.07019519	0.08453050	-0.33324005
O	-4.60741126	1.24252022	-0.83434866

Effect of Ring Size on Photoisomerization Properties of Stiff Stilbene macrocycles

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

Coordinates compound ***Z*-1c**:

C	-3.55438936	-0.35831139	0.08417511
C	-2.61811654	-1.49582298	-0.03158565
C	-3.26331508	-2.68474349	0.37330852
C	-4.67963070	-2.39853559	0.81572917
C	-4.94258328	-0.97660185	0.25913072
C	-3.35688959	0.98375795	0.04384524
C	-2.12435913	1.80012122	0.05541014
C	-2.43305634	3.12528767	-0.32770471
C	-3.90470901	3.26159323	-0.64303991
C	-4.51568099	1.97981789	-0.02172921
C	-0.82734406	1.48610604	0.47061888
C	0.17228656	2.47041175	0.45294816
C	-1.43582119	4.09304836	-0.35568224
C	-1.31972392	-1.56367179	-0.55657744
C	-0.66858545	-2.79734829	-0.63025109
C	-2.60194583	-3.90955401	0.30999787
H	-5.39620424	-3.14035155	0.44883810
H	-4.75085407	-2.40014089	1.91203211
H	-5.44812278	-1.04862774	-0.71439421
H	-5.58777265	-0.38279652	0.91217340
H	-4.34292843	4.18057795	-0.24038561
H	-4.07287411	3.27631722	-1.72871703
H	-4.88192603	2.19910893	0.99140761
H	-5.36551863	1.59931529	-0.59474786
H	-0.56334417	0.50289549	0.83931761
H	-1.66517274	5.11148143	-0.66026159
H	-0.80895043	-0.69125420	-0.94423364
H	-3.10276056	-4.82188035	0.62487328
C	-1.29562467	-3.96949019	-0.18581104
C	-0.12474071	3.77252567	0.02159013
H	0.64079433	4.53890521	-0.00642917
H	-0.77273289	-4.91818649	-0.26200130
C	4.26927034	-2.00630389	1.19635356
H	5.25908876	-2.20430011	1.63098518
H	3.55566501	-2.54443626	1.83480601
C	4.23964385	-2.63094557	-0.21194780
H	4.45421464	-3.70365871	-0.10813866
H	5.05876160	-2.22140187	-0.81529836
C	2.93303960	-2.45995137	-1.00387208
H	2.75728035	-1.40218445	-1.22784454
H	3.03160491	-2.97035884	-1.97024571
C	1.69321375	-3.00316116	-0.30507262
H	1.81292964	-4.06696859	-0.05174614
H	1.48794668	-2.45750755	0.62381190
O	0.58252731	-2.83357879	-1.20940865
O	1.39129116	2.05395077	0.91402944
C	5.01033763	0.46942617	0.71473380
H	6.01294070	0.03285501	0.82820608
H	5.02902907	1.38667921	1.31572351
C	3.97384186	-0.49864810	1.32971380
H	3.92015901	-0.28947427	2.40619815
H	2.97291125	-0.27218461	0.94436693
C	4.82621152	0.86442396	-0.76482320
H	5.65235085	1.53740620	-1.03592742
H	4.95040336	-0.02454327	-1.39558044
C	3.50126309	1.53894963	-1.17441449
H	2.65678409	0.86774563	-0.98170516
H	3.53455856	1.66159578	-2.26434308

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

C	3.18098890	2.91906270	-0.56452220
H	2.50252614	3.44738126	-1.24478602
H	4.09056158	3.53279462	-0.50368524
C	2.54450238	2.90570302	0.82925528
H	3.22838267	2.49529928	1.57434553
H	2.29121896	3.92404829	1.14775931

Effect of Ring Size on Photoisomerization Properties of Stiff Stilbene macrocycles

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

Coordinates compound ***E*-1c**:

C	0.45291401	-1.54709303	-0.50368637
C	0.15916832	-1.71087545	-1.99403534
C	1.44704109	-2.35760545	-2.57834363
C	2.51575427	-1.93258520	-1.59564477
C	1.91885637	-1.54154832	-0.38056276
C	-0.45296965	-1.54704503	0.50382287
C	-0.15915164	-1.71012296	1.99423835
C	-1.44698337	-2.35664535	2.57889439
C	-2.51575562	-1.93212751	1.59602769
C	-1.91890948	-1.54159514	0.38075553
C	2.69583995	-0.96884525	0.63308028
C	4.05637819	-0.74710596	0.41032183
C	4.66800353	-1.20574346	-0.76607106
C	3.89228727	-1.80609198	-1.76792096
C	-4.66803471	-1.20555478	0.76622744
C	-3.89227624	-1.80546758	1.76831372
H	-0.73749460	-2.30662997	-2.18453534
H	1.65603141	-2.03459527	-3.60278836
H	1.34549382	-3.45138299	-2.59941310
H	-0.00357113	-0.72951923	2.46484623
H	0.73754334	-2.30578528	2.18492970
H	-1.65598139	-2.03310987	3.60316949
H	-1.34535156	-3.45040315	2.60055710
H	2.25271748	-0.58349162	1.54337811
H	5.73134379	-1.04679337	-0.91850781
H	4.36500456	-2.11867122	-2.69593771
H	-5.73136638	-1.04651634	0.91864116
H	-4.36499368	-2.11774559	2.69643182
O	4.73450291	-0.02784486	1.37213057
C	5.33624709	1.21822217	0.94273260
H	5.65503759	1.69065829	1.87733393
H	6.23733566	1.00973067	0.35059381
C	4.40255447	2.13652120	0.14690466
H	4.98453107	3.02780740	-0.12190497
H	4.16043505	1.64071972	-0.80055562
C	3.09323569	2.53683906	0.85646247
H	2.75347744	1.69868163	1.47441832
H	3.27950503	3.36914764	1.54854390
C	1.96813615	2.89782830	-0.13170267
H	1.91848044	2.10312257	-0.88891273
H	2.22422682	3.81796124	-0.67591358
C	0.57643409	3.03088373	0.51053603
H	0.42836611	2.17993447	1.19060334
H	0.52934014	3.93287837	1.13685288
H	0.00362189	-0.73048102	-2.46511025
C	-1.96816988	2.89775896	0.13143102
H	-1.91840125	2.10286159	0.88844256
H	-2.22447428	3.81769973	0.67588462
C	-0.57644916	3.03109294	-0.51065399
H	-0.42840942	2.18037597	-1.19102963
H	-0.52929711	3.93329559	-1.13666980
C	-2.69587838	-0.96902856	-0.63297982
H	-2.25274857	-0.58398880	-1.54340188
C	-4.05644179	-0.74737748	-0.41036384
O	-4.73458974	-0.02833178	-1.37229533
C	-4.40251916	2.13645197	-0.14736605
H	-4.16041476	1.64068153	0.80011339
H	-4.98451067	3.02774474	0.12139829

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

C	-3.09314683	2.53675524	-0.85684930
H	-3.27930739	3.36897592	-1.54906708
H	-2.75331650	1.69850203	-1.47463737
C	-5.33616813	1.21802554	-0.94315950
H	-6.23734693	1.00980419	-0.35104961
H	-5.65478983	1.69042001	-1.87783865

Effect of Ring Size on Photoisomerization Properties of Stiff Stilbene macrocycles

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

Coordinates compound ***Z*-1d**:

C	3.86985342	0.50896757	0.34620417
C	2.85707089	1.58443456	0.38362202
C	3.36722620	2.68842984	1.10478329
C	4.74707188	2.38124741	1.63903819
C	5.18159129	1.16415143	0.78410148
C	3.80184395	-0.78247862	-0.06060100
C	2.65922278	-1.68146337	-0.34786508
C	3.12537005	-2.78952487	-1.09341322
C	4.60900254	-2.67099989	-1.35427912
C	5.05243851	-1.62963458	-0.29621941
C	1.34217077	-1.66712845	0.12760716
C	0.48924834	-2.74931176	-0.15647944
C	2.25533990	-3.81512961	-1.43611332
C	1.63426838	1.69644083	-0.28404375
C	0.92053815	2.90323333	-0.22264948
C	2.63071438	3.86322451	1.20017337
H	5.43469136	3.22893437	1.55581844
H	4.70543159	2.10457855	2.70166261
H	5.73960117	1.51385408	-0.09605884
H	5.83508412	0.47783192	1.32945758
H	5.13484229	-3.62664475	-1.26284235
H	4.80513995	-2.28931299	-2.36592706
H	5.34104635	-2.14856495	0.62907791
H	5.91180487	-1.03709663	-0.62042770
H	0.97218408	-0.86954307	0.76289825
H	2.59965705	-4.65574742	-2.03389603
H	1.23274057	0.88968825	-0.88668914
H	3.01589837	4.71164787	1.76085046
C	1.39966627	3.97824418	0.54142453
C	0.93045180	-3.79635560	-0.98262990
H	0.26942895	-4.61121197	-1.25048287
H	0.84403990	4.90779140	0.59392187
C	-5.25996407	1.48817016	0.74305558
H	-6.25255120	1.53831938	1.21182826
H	-4.66037763	2.26098716	1.24187120
C	-5.40488984	1.85822874	-0.75112060
H	-5.63249723	2.93087428	-0.81331543
H	-6.27993290	1.34779985	-1.17417346
C	-4.19514606	1.52103368	-1.64506036
H	-4.13839860	0.43005273	-1.74577987
H	-4.38903818	1.89893777	-2.65866728
O	-0.21431083	2.95391184	-0.97975738
O	-0.74035653	-2.71801458	0.44455381
C	-5.34859713	-1.13041867	0.57709163
H	-5.85550501	-0.93481939	-0.37633097
H	-6.14023449	-1.38628473	1.29521768
C	-4.60495848	0.13068504	1.05297213
H	-4.45128163	0.06834662	2.13745799
H	-3.59997867	0.11992636	0.61771389
C	-4.40502315	-2.33486015	0.38304042
H	-4.99682815	-3.22468166	0.12618617
H	-3.76341674	-2.13151105	-0.48522185
C	-2.82026792	2.01754829	-1.16787481
H	-2.70073791	1.80859038	-0.09886868
H	-2.04607869	1.42695390	-1.66734367
C	-2.50298847	3.50008831	-1.40537725
H	-2.39461556	3.69285394	-2.48050543
H	-3.31465854	4.14664183	-1.04791550

Effect of Ring Size on Photoisomerization Properties of Stiff Stilbene macrocycles

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]

[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*

[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

C	-1.22966473	3.91971328	-0.67248128
H	-1.39985254	3.93126495	0.41288319
H	-0.90724113	4.92420890	-0.97818112
C	-3.51927233	-2.64184484	1.59910704
H	-2.88598032	-1.77644276	1.82058815
H	-4.15627914	-2.79013280	2.48214157
C	-2.61842542	-3.87717888	1.45354481
H	-2.07336810	-4.03151632	2.39324318
H	-3.23515118	-4.77370606	1.30118093
C	-1.60219846	-3.86119668	0.31500371
H	-1.01023869	-4.78166484	0.37130250
H	-2.09016992	-3.83627236	-0.66841493

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

Coordinates compound ***E*-1d**:

C	-0.42072052	-1.52605438	0.59895116
C	0.10917158	-1.43722478	2.02908485
C	-1.07691726	-1.87770781	2.92944794
C	-2.28569161	-1.65471476	2.04961680
C	-1.89049067	-1.51072721	0.70294796
C	0.31881870	-1.68340576	-0.52823927
C	-0.23458696	-2.00588371	-1.91590676
C	0.93914710	-2.67382977	-2.67704699
C	2.15547919	-2.20708865	-1.91419573
C	1.78827553	-1.69113780	-0.65668744
C	-2.84846677	-1.21324430	-0.27487204
C	-4.18575130	-1.04105613	0.09581377
C	-4.58549059	-1.23274864	1.42637959
C	-3.62813249	-1.54311599	2.40165321
C	4.45447910	-1.62456296	-1.48068624
C	3.49148223	-2.19490978	-2.31147036
H	1.00069166	-2.05089291	2.18390824
H	-1.12498925	-1.31738806	3.86860486
H	-0.98066201	-2.93913640	3.19585129
H	-0.52786112	-1.08266510	-2.43398427
H	-1.12130707	-2.64369083	-1.87337225
H	0.96867884	-2.39623106	-3.73565431
H	0.84844896	-3.76814470	-2.63742584
H	-2.58014609	-1.03267148	-1.30776174
H	-5.62814168	-1.11118469	1.70320690
H	-3.93880932	-1.66372648	3.43673848
H	5.49552806	-1.56892321	-1.78383964
H	3.78554607	-2.59850409	-3.27734023
O	-5.05617932	-0.67635007	-0.90751689
C	-5.89087580	0.48361527	-0.68905387
H	-6.38029184	0.63621995	-1.65612974
H	-6.67295395	0.25378683	0.04662651
C	-5.11640926	1.73158673	-0.25621108
H	-5.84002388	2.55259211	-0.17154863
H	-4.73303020	1.56216157	0.75690861
C	-3.94336878	2.11815422	-1.17981240
H	-3.51479773	1.20175055	-1.59933497
H	-4.30934652	2.70216812	-2.03463250
C	-2.82672853	2.87598056	-0.43932051
H	-2.66627552	2.37611396	0.52598160
H	-3.15159110	3.89824984	-0.19934663
C	-1.47729496	2.90284560	-1.17666979
H	-1.26280788	1.88529294	-1.53250298
H	-1.53739757	3.53404350	-2.07420111
H	0.38506105	-0.40120299	2.26957105
C	1.08382539	3.02553373	-0.82905460
H	1.08489271	1.98140660	-1.17235366
H	1.30124092	3.63899242	-1.71477585
C	-0.31352568	3.35342844	-0.27704660
H	-0.41978120	2.84488124	0.69205404
H	-0.39325612	4.42868379	-0.06343477
C	2.75907733	-1.13370949	0.19584056
H	2.47272429	-0.68998320	1.13798850
C	4.08805473	-1.06999398	-0.24013374
O	5.10287859	-0.45308042	0.43406459
C	3.56503059	2.63702420	-0.20806031
H	3.42524425	1.66648222	-0.69973962
H	4.00507011	3.30159680	-0.96350985

Sandra Olsson [a], Oscar Benito Perez[b], Magnus Blom[a], Adolf Gogoll[a]
[a.] *Department of Chemistry-BMC, Uppsala University, S-751 23 Uppsala, Sweden*
[b.] *Faculty of Chemistry, Universitat de Barcelona, C/ Martí i Franquès 1, 08028 Barcelona, Spain.*

C	2.19420364	3.18892077	0.22154400
H	2.29727858	4.24723787	0.50107748
H	1.86683826	2.67071025	1.13286404
C	4.55749131	2.47243637	0.96228698
H	5.56233960	2.28735756	0.56318766
H	4.61641621	3.42483636	1.50475376
C	4.18195246	1.34675557	1.95498609
H	4.40422988	1.66074273	2.98292139
H	3.10104318	1.17974382	1.92911066
C	4.93217896	0.01713615	1.78026548
H	5.96151345	0.13735675	2.13182876
H	4.46178976	-0.76642879	2.38921910