SUPPLEMENTARY INFORMATION

Investigation of photophysical, structural aspects and nonlinear optical properties of Foron blue SR analogs using Density Functional Theory (DFT)

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Table S1. Selected bond lengths, bond angles and torsional angles of **2a** and **2b**, using B3LYP 6-31G(d) in DMF (bond lengths are in Å, dihedral angles are in degree)

Atom number	**2a**			**2b**		
	Gas	DMF		Gas	DMF	
	GS	GS	ES	GS	GS	ES
Bond length						
N_{27}-C_{19}	1.37	1.36	1.36	1.38	1.37	1.36
C_{22}-C_{17}	1.46	1.45	1.50	1.46	1.45	1.50
C_{17}-C_7	1.37	1.38	1.41	1.37	1.38	1.41
bond angle						
C_{22}-C_{17}-C_7	128.79	129.47	122.14	125.77	126.37	121.91
C_{17}-C_7-C_8	124.30	124.57	127.43	125.61	125.85	127.51
C_{17}-C_7-S_{14}	125.90	125.67	121.91	124.26	123.99	121.81
Dihedral angle						
C_{22}-C_{17}-C_7-S_{14}	9.67	11.57	0.10	12.13	15.94	4.91
C_{23}-C_{22}-C_{17}-C_7	25.99	24.30	90.68	43.00	39.50	90.92

Table S2. Selected bond lengths, bond angles and torsional angles of **3a** and **3b**, using B3LYP 6-31G(d) in DMF (bond lengths are in Å, dihedral angles are in degree)

Atom number	**3a**			**3b**		
	Gas	DMF		Gas	DMF	
	GS	GS	ES	GS	GS	ES
Bond length						
N_{26}-C_{18}	1.36895	1.35661	1.35504	1.37151	1.35781	1.35423
C_{21}-C_{16}	1.4341	1.4227	1.48405	1.42759	1.41296	1.4815
C_{16}-C_7	1.37231	1.38166	1.36244	1.37511	1.38765	1.36236
Bond angle						
C_{21}-C_{16}-C_7	132.3531	132.4504	126.1881	131.6421	132.0738	125.769
C_{16}-C_7-C_8	126.9239	126.4101	132.4256	126.55	126.0589	132.4425
C_{16}-C_7-S_{13}	123.0723	123.3975	118.3908	123.3237	123.5224	118.3267
Dihedral angle						
C_{21}-C_7-C_{16}-S_{13}	12.38786	15.7182	1.4734	14.16729	17.67082	2.9818
C_{22}-C_{21}-C_{16}-C_7	17.67245	16.68476	91.50966	20.00739	17.56089	91.33579

Table S3. Selected bond lengths, bond angles and torsional angles of **1a** and **1b**, using B3LYP 6-31G(d) in EA (bond lengths are in Å, dihedral angles are in degree)

Atom number	**1a**		**1b**	
	Gas	EA	Gas	EA

	GS	GS	ES	GS	GS	ES
Bond length						
N_{28}-C_{18}	1.36112	1.36733	1.37404	1.36389	1.3712	1.37371
C_{21}-C_{17}	1.43763	1.43055	1.47923	1.433	1.42372	1.47611
C_{17}-C_7	1.37239	1.36352	1.35709	1.37779	1.36822	1.35849
Bond angle						
C_{21}-C_{17}-C_7	133.6811	134.1668	125.7073	133.0528	133.7498	126.4356
C_{17}-C_7-C_8	120.8806	121.12	126.5021	120.7833	120.9579	125.8129
C_{17}-C_7-S_{14}	128.8208	128.7452	123.1707	128.933	128.8503	123.2158
Dihedral angle						
C_{21}-C_7-C_{17}-S_{14}	4.69675	4.95756	0.43354	5.99833	6.49452	3.58115
C_{22}-C_{21}-C_{16}-C_7	10.65527	9.30751	90.37907	13.30338	11.45619	90.72562

Table S4. Selected bond lengths, bond angles and torsional angles of **2a** and **2b**, using B3LYP 6-31G(d) in EA (bond lengths are in Å, dihedral angles are in degree)

Atom number	**2a**			**2b**		
	Gas	EA		Gas	EA	
	GS	GS	ES	GS	GS	ES
Bond length						
N_{27}-C_{19}	1.37472	1.38056	1.40637	1.36992	1.37646	1.40616
C_{22}-C_{17}	1.46067	1.45224	1.5003	1.4644	1.45498	1.4966
C_{17}-C_7	1.37006	1.36057	1.35851	1.37808	1.36868	1.35896
bond angle						
C_{22}-C_{17}-C_7	128.7936	129.3646	121.7883	125.767	126.3136	121.4828
C_{17}-C_7-C_8	124.2978	124.4839	127.4136	125.6106	125.7831	127.5687
C_{17}-C_7-S_{14}	125.9027	125.77	121.8487	124.2608	124.0955	121.6937
Dihedral angle						
C_{22}-C_{17}-C_7-S_{14}	9.67094	11.02093	1.87261	12.1311	14.73794	5.01798
C_{23}-C_{22}-C_{17}-C_7	25.99396	24.52921	90.53349	43.00418	40.29802	90.79016

Table S5. Selected bond lengths, bond angles and torsional angles of **3a** and **3b**, using B3LYP 6-31G(d) in EA (bond lengths are in Å, dihedral angles are in degree)

Atom number	**3a**			**3b**		
	Gas	EA		Gas	EA	
	GS	GS	ES	GS	GS	ES
Bond length						
N_{26}-C_{18}	1.37231	1.35925	1.36057	1.37511	1.36094	1.3603
C_{21}-C_{16}	1.4341	1.42503	1.4858	1.42759	1.41614	1.48311

C_{16}-C_7	1.36895	1.37956	1.3572	1.37151	1.38468	1.35596
Bond angle						
C_{21}-C_{16}-C_7	132.3531	132.4513	125.9703	131.6421	131.9982	125.5351
C_{16}-C_7-C_8	126.9239	126.5275	132.5587	126.55	126.1485	132.6317
C_{16}-C_7-S_{13}	123.0723	123.3217	118.2164	123.3237	123.5082	118.1283
Dihedral angle						
C_{21}-C_7-C_{16}-S_{13}	12.38786	14.97754	1.80818	14.16729	16.86787	3.09344
C_{22}-C_{21}-C_{16}-C_7	17.67245	16.81219	91.43491	20.00739	18.15935	91.37291

Table S6. Linear polarizability α_0, first order hyperpolarizability β_0 and second order hyperpolarizability γ in DMF solvent

	α_0 (10^{-24} esu)			β_0 (10^{-30} esu)			γ (10^{-36} esu)		
	B3LYP	CAM-B3LYP	BHandHLYP	B3LYP	CAM-B3LYP	BHandHLYP	B3LYP	CAM-B3LYP	BHandHLYP
1a	65.05	58.98	58.98	296.94	222.06	222.06	660.33	475.28	475.28
1b	73.80	67.14	67.14	265.86	199.22	199.22	620.47	415.60	415.60
2a	72.22	65.48	65.48	382.37	337.45	337.45	606.59	680.80	680.80
2b	79.24	68.65	68.65	417.23	314.72	314.72	837.17	764.65	764.65
3a	85.54	77.51	77.51	486.32	416.81	416.81	776.73	851.88	851.88
3b	94.30	85.98	85.98	404.96	352.18	352.18	641.75	609.06	609.06

Table S7. Intrinsic hyperpolarizability of **1a-3b** in DMF solvent

	β_0 (10^{-30} esu)			β limit (10^{-30} esu)	β^{int}		
	B3LYP	CAM-B3LYP	BHandHLYP		B3LYP	CAM-B3LYP	BHandHLYP
1a	296.94	222.06	222.06	2530	0.1174	0.0878	0.0878
1b	265.86	199.22	199.22	2755	0.0965	0.0723	0.0723
2a	382.37	337.45	337.45	4096	0.0934	0.0824	0.0824
2b	417.23	314.72	314.72	4631	0.0901	0.0680	0.0680
3a	486.32	416.81	416.81	4976	0.0977	0.0838	0.0838
3b	404.96	352.18	352.18	5462	0.0741	0.0645	0.0645

Table S8. Intrinsic hyperpolarizability of **1a-3b** in EA solvent

	β_0 (10^{-30} esu)			β limit (10^{-30} esu)	β^{int}		
	B3LYP	CAM	BHandHLYP		B3LYP	CAM-B3LYP	BHandHLYP
1a	232.897	191.179	174.916	2005	0.1162	0.0954	0.0872
1b	211.325	172.061	156.862	2173	0.0973	0.0792	0.0722
2a	290.074	267.341	251.536	3188	0.0910	0.0839	0.0789
2b	319.072	250.598	237.762	3443	0.0927	0.0728	0.0691
3a	373.314	349.919	317.281	3853	0.0969	0.0908	0.0823
3b	322.589	295.244	269.641	4504	0.0716	0.0656	0.0599

Table S9. Amplitude of the sine shaped potential for **1a-3b**

Compound	Solvent	V_0
1a	DMF	0.107608
	EA	0.143918
1b	DMF	0.105557
	EA	0.140998
2a	DMF	-0.32594
	EA	-0.28399
2b	DMF	-0.47953
	EA	-0.44989
3a	DMF	-0.46877
	EA	-0.44106
3b	DMF	-0.45852
	EA	-0.43682

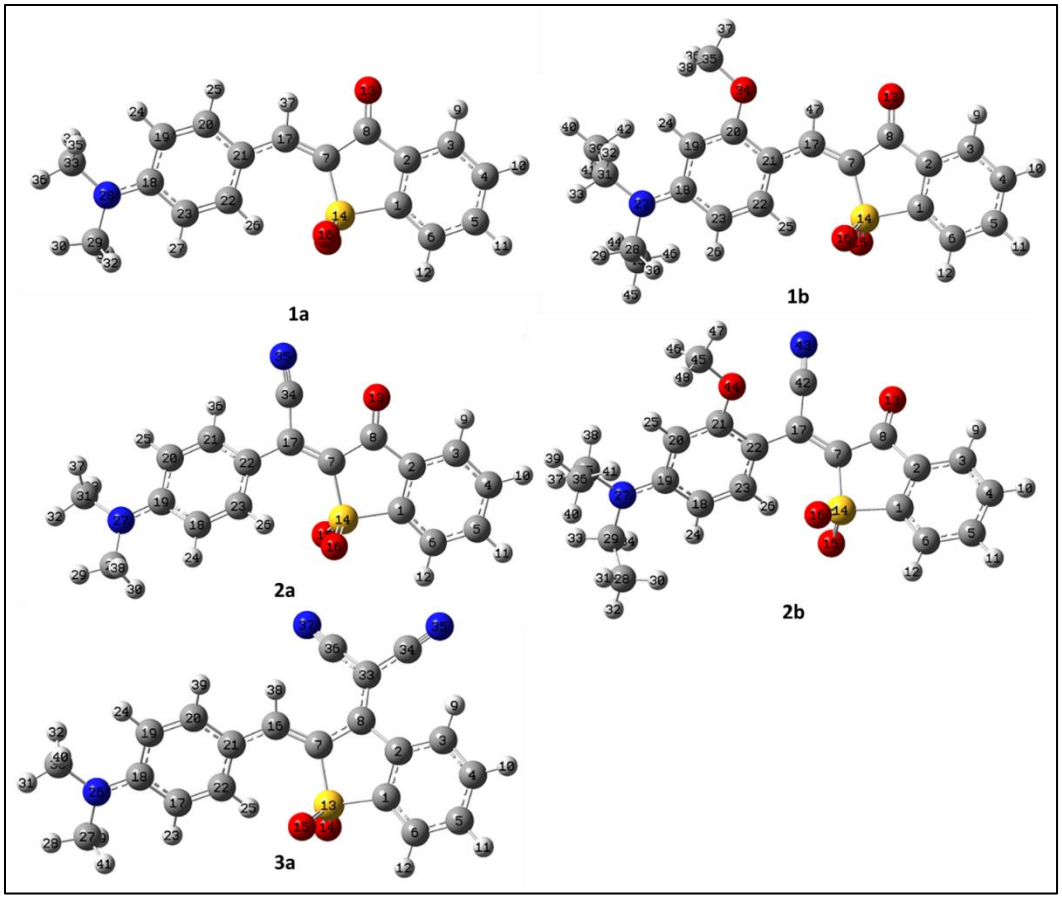

Figure S1. Optimized structures of 1a-3a

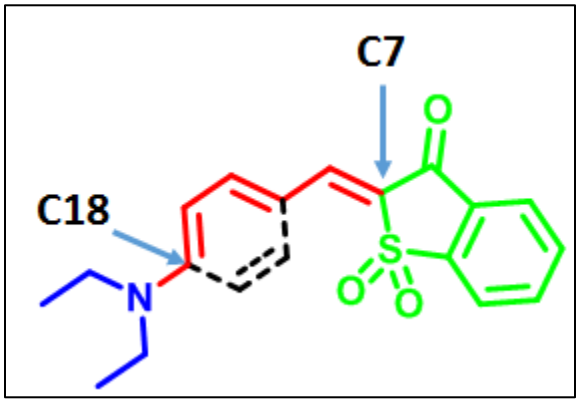

Figure S2. Polyene system considered for calculation of potential (V_0)