SUPPLEMENTARY INFORMATION

Investigation of the linear and nonlinear optical properties in the crystalline phase of a Pyrimidine Derivative - a potential nonlinear optical material: Analysis of structure, reactivity, and docking studies

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Figures

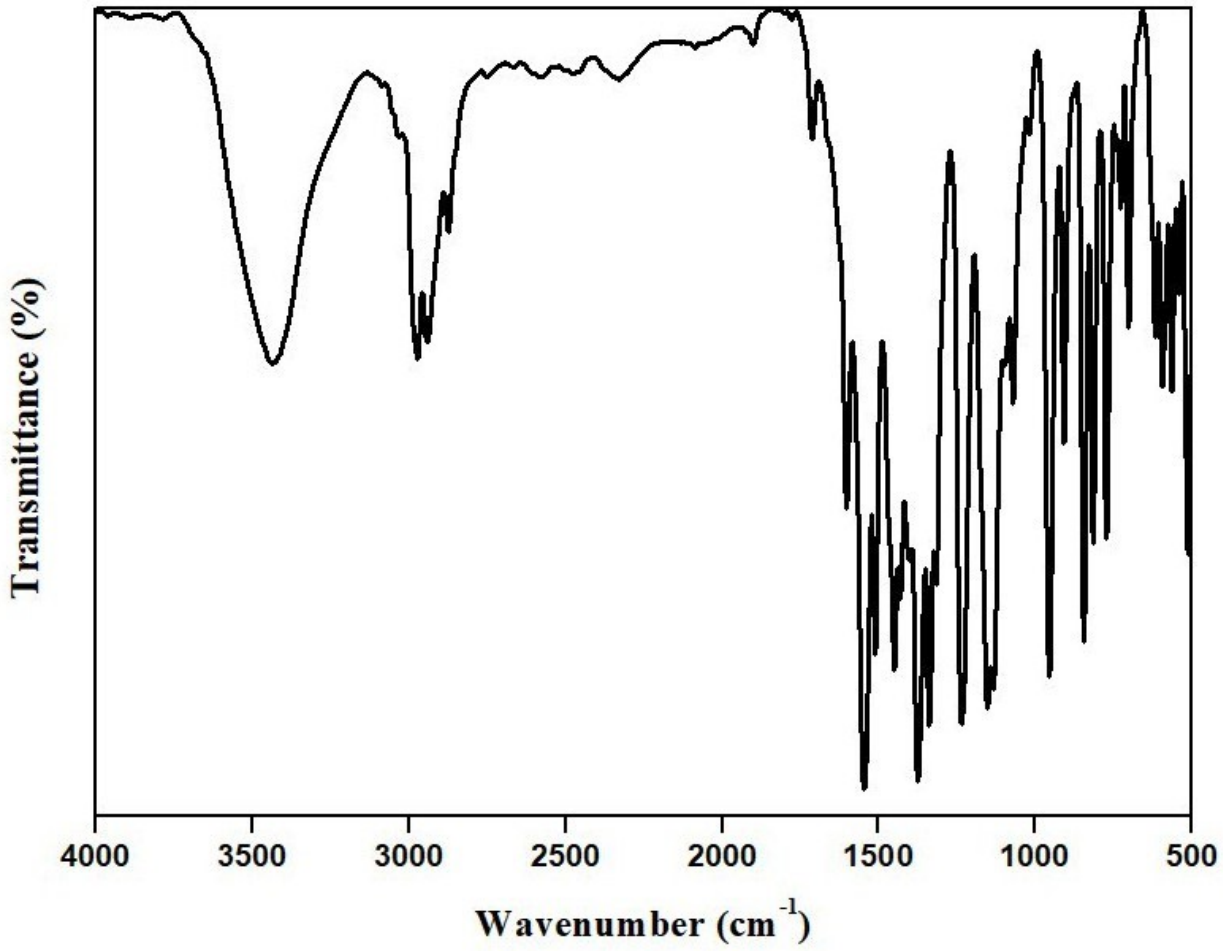

Figure S1. FT-IR spectrum of PMMS compound.

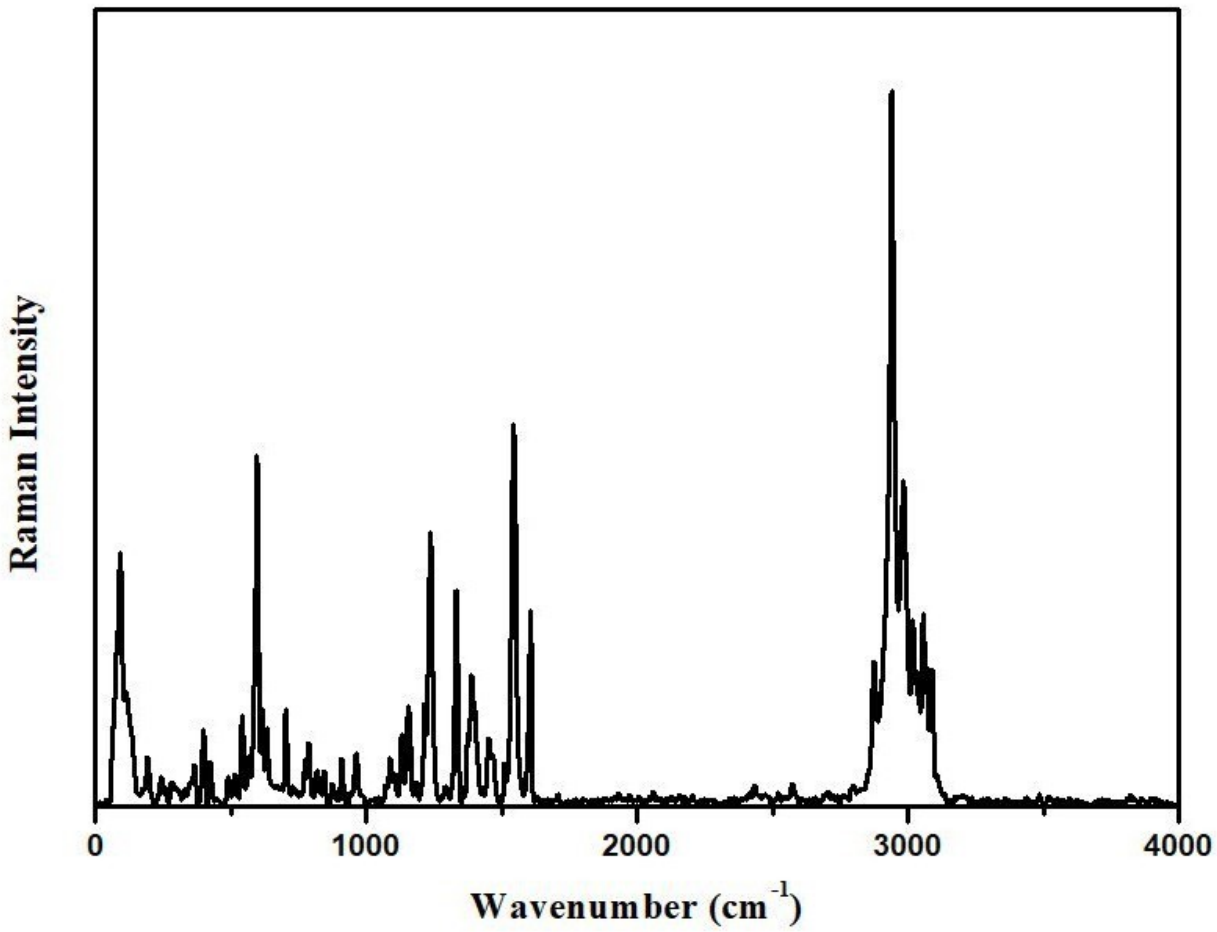

Figure S2. FT-Raman spectrum of PMMS compound.

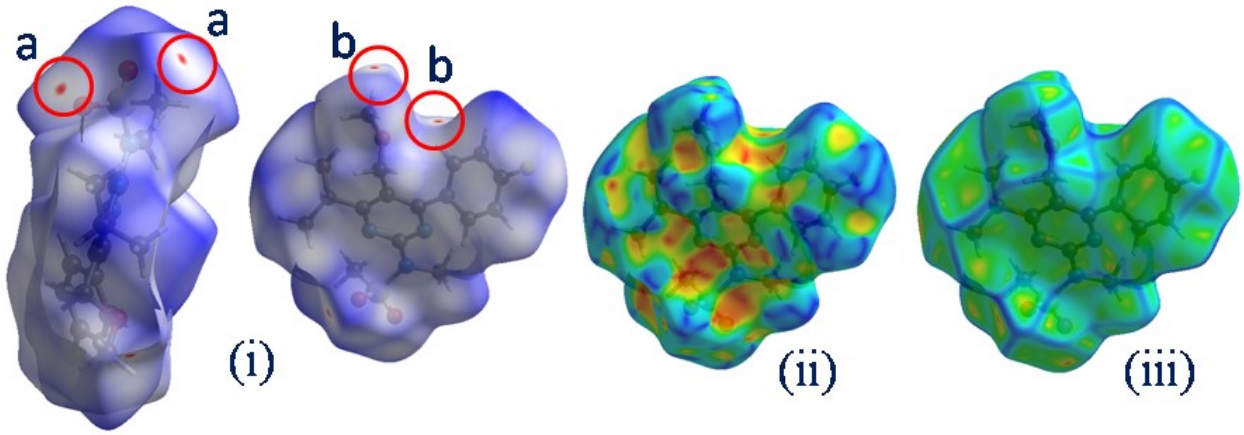

Figure S3. Hirshfeld surface of PMMS compound: d_{norm} (i), shape index (ii), and curvedness (iii).

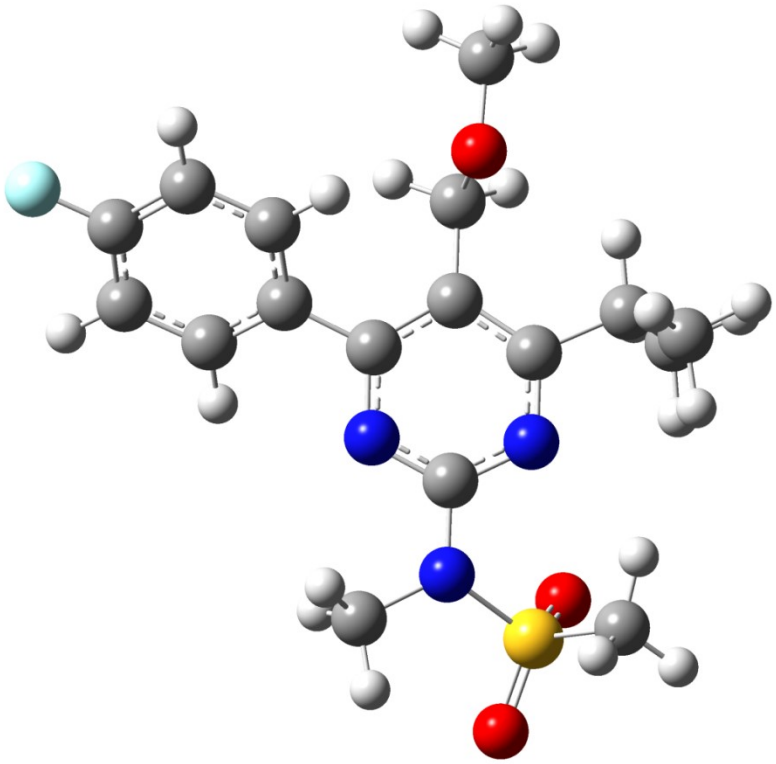

Figure S4. Optimized geometry of the PMMS molecule.

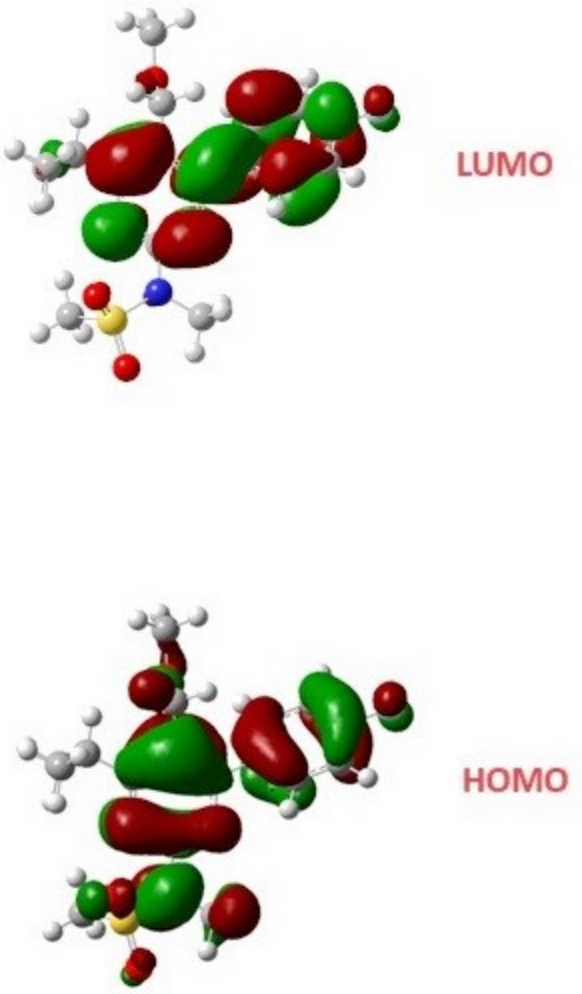

Figure S5. HOMO-LUMO plots of PMMS molecule.

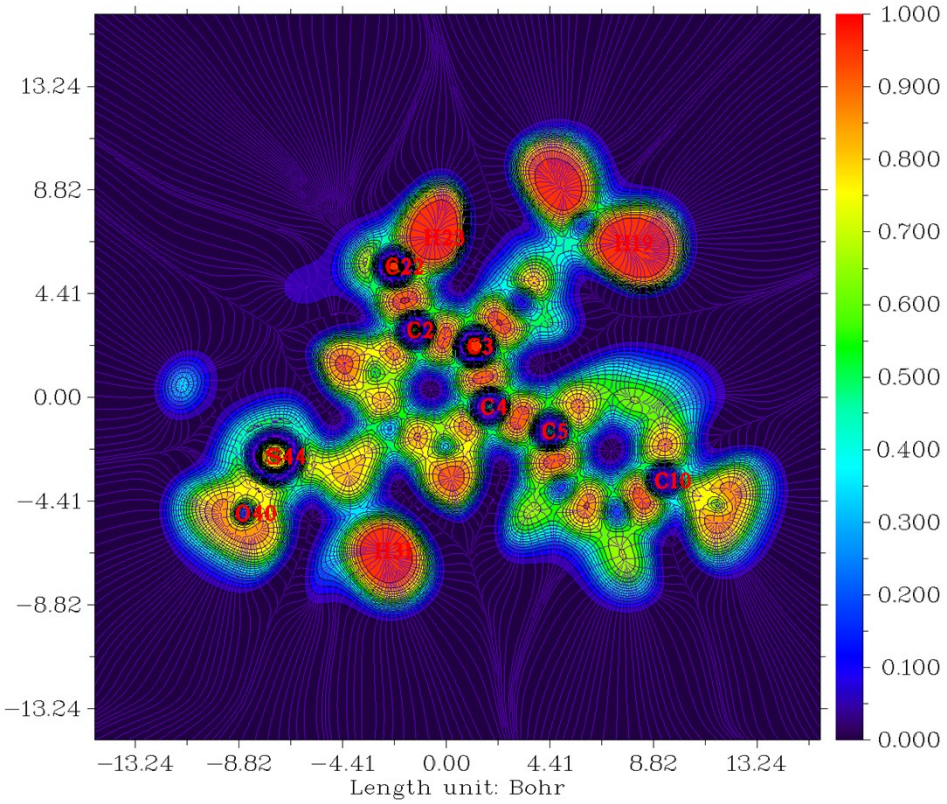

Figure S6. ELF plot for PMMS.

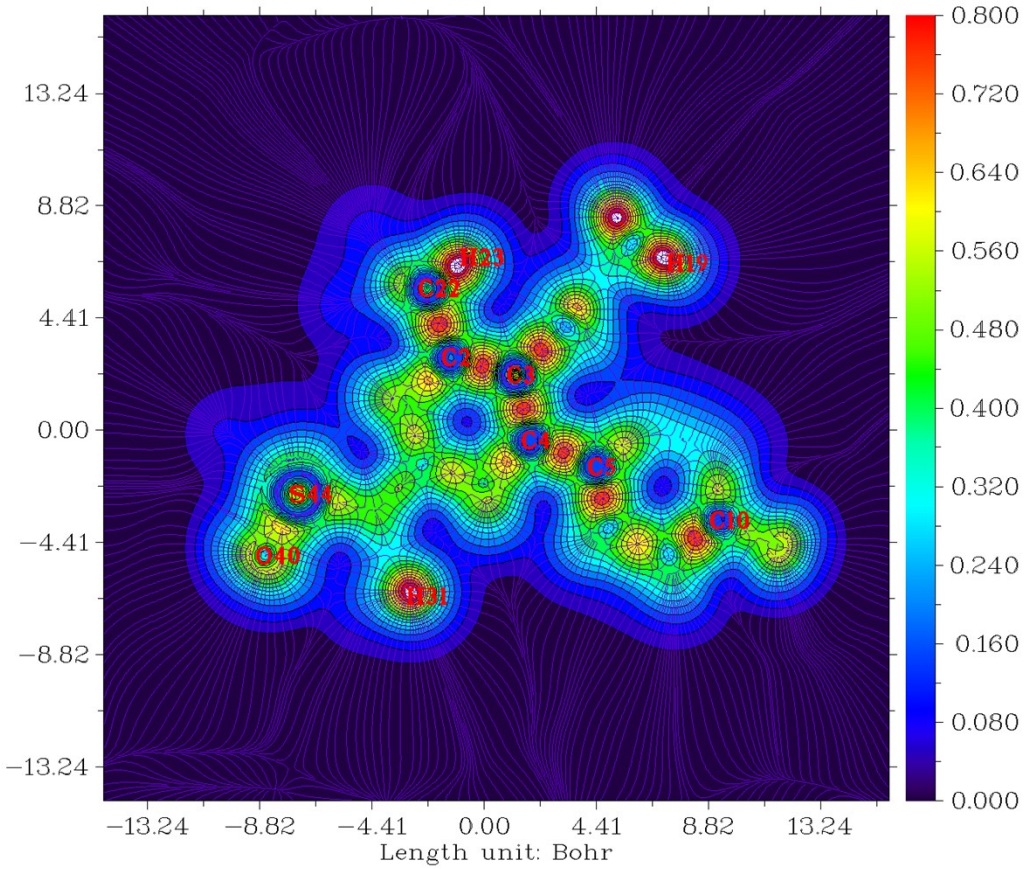

Figure S7. LOL plot for PMMS.

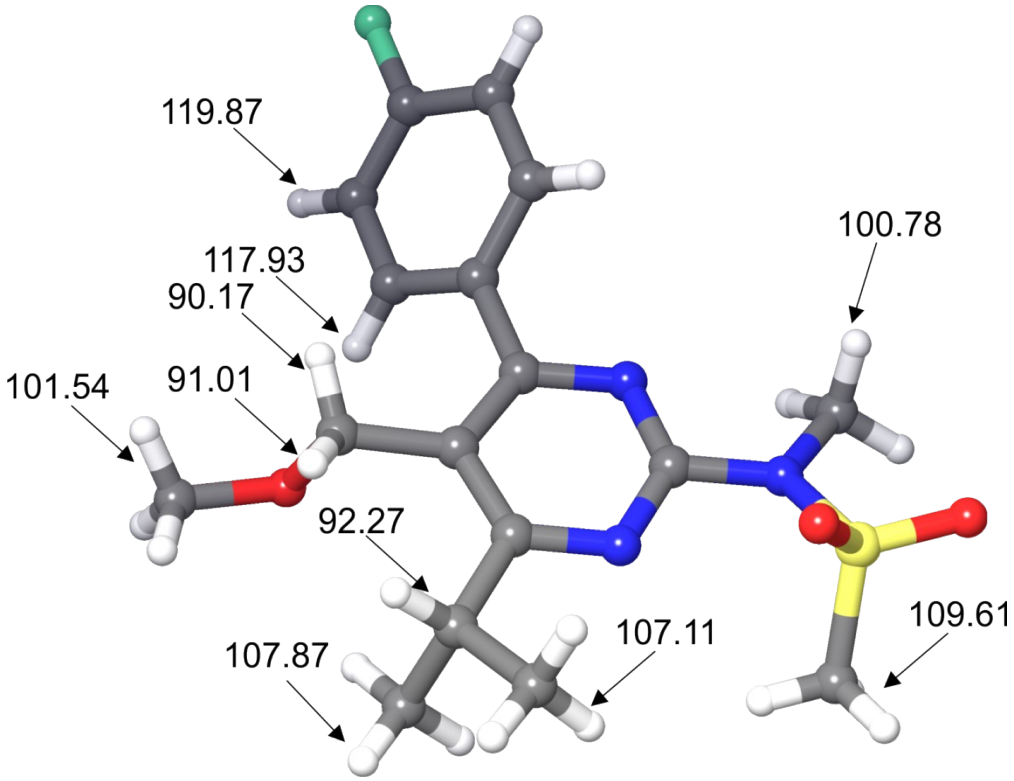

Figure S8. H-BDE values of the PMMS molecule.

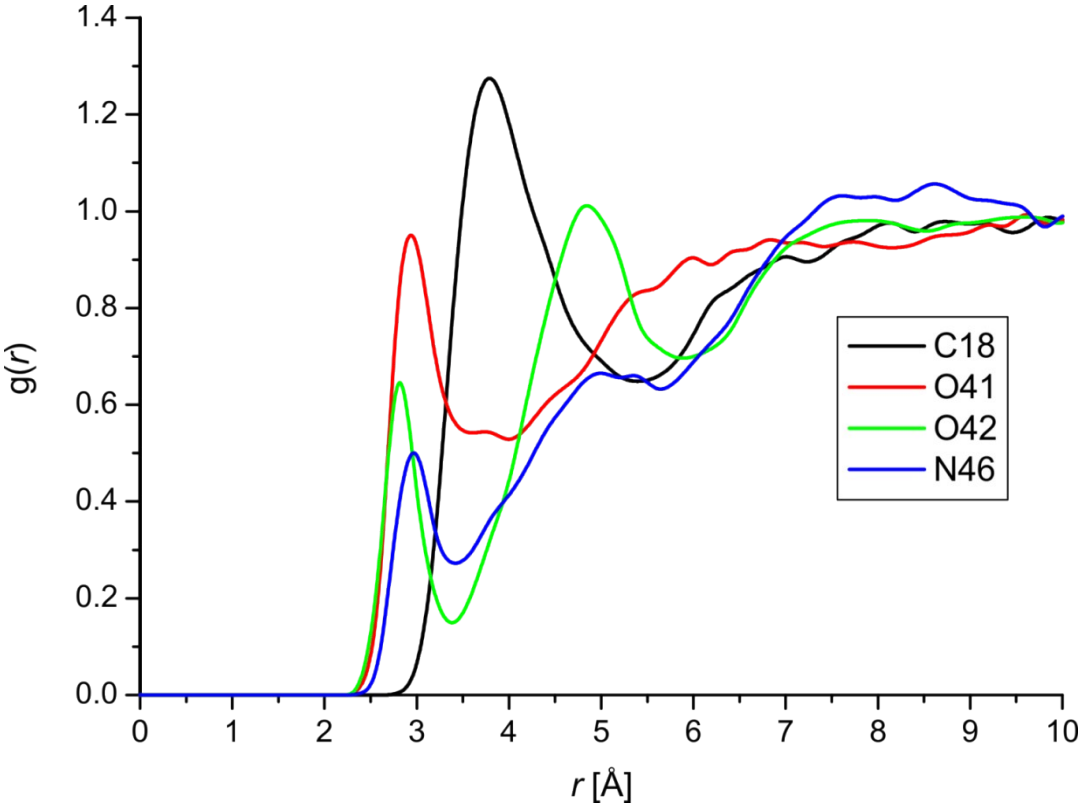

Figure S9. RDFs of the PMMS molecule.

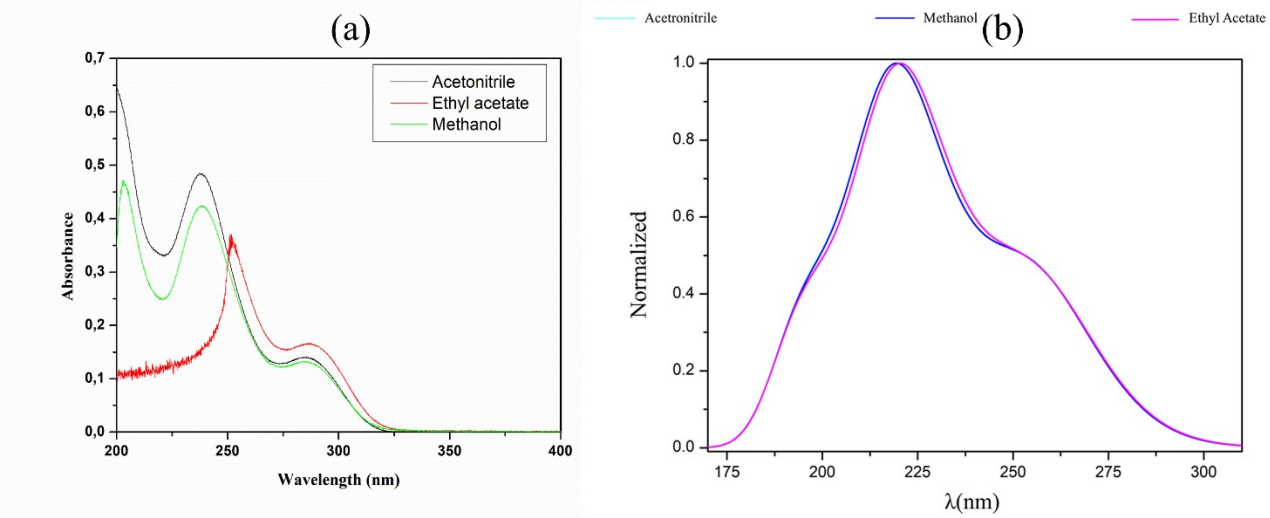

Figure S10. UV-Visible Spectra of the PMMS Compound: (a) Experimental Results; (b) Theoretical Results

Table

Table S1.

Geometrical parameters of the PMMS molecule.

Bond lengths (Å) (XRD/DFT)			
C1—N1	1.32/1.33	C9—C10	1.37/1.39
C1—N2	1.32/1.33	C3—C11	1.49/1.50
C1—N3	1.41/1.42	C11—O3	1.42/1.42
C2—N1	1.33/1.33	C12—O3	1.40/1.41
C2—C3	1.40/1.40	C2—C13	1.51/1.52
C3—C4	1.40/1.40	C13—C14	1.53/1.54
C4—C5	1.48/1.48	C13—C15	1.51/1.53
C4—N2	1.34/1.34	C16—N3	1.46/1.47
C5—C6	1.38/1.40	C17—S1	1.74/1.79
C6—C7	1.38/1.39	O1—S1	1.42/1.46
C7—C8	1.37/1.38	O2—S1	1.42/1.45
C8—C9	1.36/1.38	S1—N3	1.66/1.73
C8—F1	1.35/1.35		
Bond angles (°) (XRD/DFT)			
N1—C1—N2	127.7/125.99	C7—C8—F1	118.4/118.86
N1—C1—N3	116.6/117.55	C9—C8—F1	119.3/118.82
N2—C1—N3	115.6/116.39	C14—C13—C15	111.5/111.51
C3—C2—N1	121.1/121.59	C11—O3—C12	112.1/112.47
C2—C3—C4	116.6/116.01	C17—S1—O1	109.0/107.80
C3—C4—N2	121.9/121.43	C17—S1—O2	109.1/109.27
C5—C4—N2	113.5/114.65	C17—S1—N3	105.3/103.60
C4—C5—C6	122.3/121.70	O1—S1—O2	118.9/119.99
C4—C5—C10	119.4/119.39	O1—S1—N3	104.9/104.82
C6—C5—C10	118.2/118.82	O2—S1—N3	108.7/110.07
C7—C8—C9	122.4/122.31	C1—N1—C2	116.8/125.99
C1—N3—S1	120.9/119.88	C1—N2—C4	115.8/117.15
C16—N3—S1	118.8/117.40	C1—N3—C16	119.6/118.78
Dihedralangles (°) (XRD/DFT)			
N2—C1—N1—C2	-2.4/-6.75	C6—C7—C8—F1	-178.2/-179.65
N3—C1—N1—C2	178.5/175.99	F1—C8—C9—C10	178.8/-179.55
N1—C1—N2—C4	-0.1/3.29	C17—S1—N3—C1	77.0/76.77
N3—C1—N2—C4	179.0/-179.42	C17—S1—N3—C16	-112.5/-125.74
N1—C1—N3—C16	162.9/-27.61	O1—S1—N3—C1	-168.0/-170.30
N1—C1—N3—S1	-26.6/-27.61	O2—S1—N3—C1	-39.8/-39.96
N2—C1—N3—C16	-16.3/-2.30	O1—S1—N3—C16	2.5/-12.82
N2—C1—N3—S1	154.2/154.86	O2—S1—N3—C16	130.7/117.51
C13—C2—C3—C4	179.7/-176.25	N2—C4—C5—C6	135.3/137.09
C13—C2—C3—C11	2.5/5.81	N2—C4—C5—C10	-42.4/-39.76