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SECOND ORDER HYPERPOLARIZABILITY OF TRIPHENYLAMINE BASED ORGANIC SENSITIZERS: A FIRST PRINCIPLE THEORETICAL STUDY

M. Prakasam[a,b] and P. M. Anbarasan[a,b] *

[a]*Department of Physics, Periyar University, Salem - 636 011, Tamil Nadu, India.*
[b]*Centre for Nanoscience and Nanotechnology, Periyar University, Salem - 636 011, Tamil Nadu, India*

Supporting Information

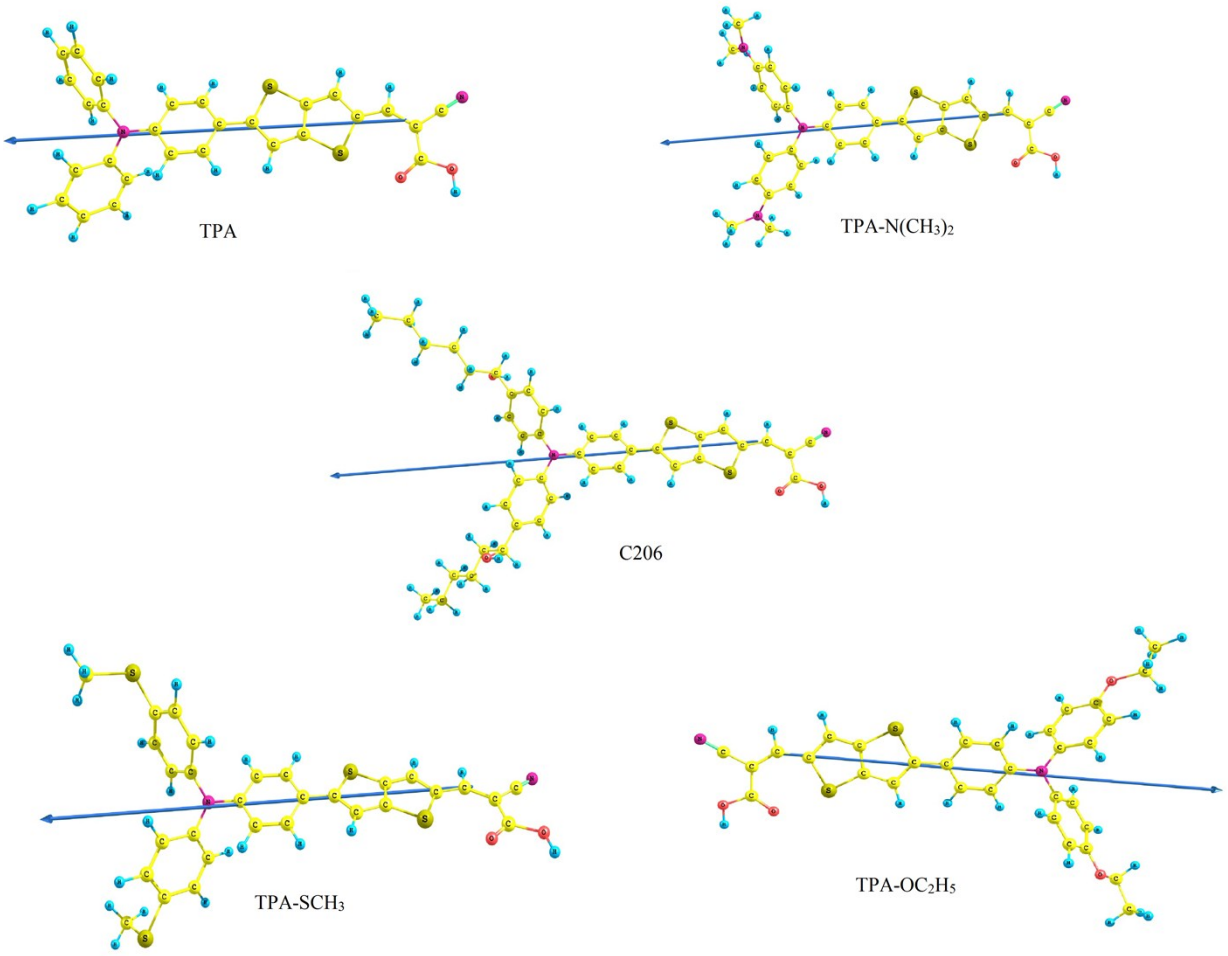

Fig. S1 Dipole moment of the designed molecules

Table S1: Computed excitation energies, electronic transition configurations and oscillator Strengths (f) for the optical transitions of the absorption bands in visible and near–UV region for the dyes in chloroform

Dye	Energy (cm^{-1})	Wavelength (nm)	Oscillator strength (f)	Major Transition
C206	19679.26	508	0.6834	HOMO->LUMO (99%)
	25813.95	387	0.6391	H-1->LUMO (95%)
	28331.23	352	0.1873	H-3->LUMO (55%), H-2->LUMO (38%)
TPA	21342.38	468	1.3948	HOMO->LUMO (98%)
	22461.89	445	0.0008	H-2->LUMO (96%)
	27450.46	364	0.0734	H-3->LUMO (69%), H-1->LUMO (-29%)
TPA-$N(CH_3)_2$	17340.23	576	0.8052	HOMO->LUMO (100%)
	23126.49	432	0.0003	H-3->LUMO (96%)
	23816.91	419	0.0151	H-1->LUMO (100%)
TPA-SCH_3	21265.76	470	0.8095	HOMO->LUMO (98%)
	21656.14	461	0.0009	H-1->LUMO (100%)
	21831.16	458	0.3915	H-2->LUMO (98%)
TPA-OC_2H_5	19186.45	521	0.9716	HOMO->LUMO (99%)
	23133.75	432	0.0003	H-3->LUMO (96%)
	26784.24	373	0.979	H-1->LUMO (93%)