Exploration of Nonlinear Optical Enhancement in Acceptor-π-Donor Indacenodithiophene Based Derivatives *via* Structural Variations: A DFT Approach

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Table S1: Computed transition energy (*eV*), maximum absorption wavelengths (λ_{max}), oscillator strengths (f_{os}) and transition natures of compound **TNPR** in chloroform at B3LYP functional with 6-311G(d,p) basis set

NO.	λ_{DFT} (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	798.404	1.553	2.624	H→L (96%), H-1→L+1 (2%)
2	740.027	1.675	0.001	H→L+1 (99%),
3	598.293	2.072	0.006	H-1→L (98%),
4	584.418	2.122	1.183	H-1→L+1 (88%), H→L (3%), H→L+2 (5%), H→L+4 (2%)
5	564.026	2.198	0.138	H→L+2 (87%), H-1→L+1 (6%), H-1→L+3 (5%)
6	554.317	2.237	0.000	H→L+3 (93%), H-1→L+2 (5%)

Table S2: Computed transition energy (*eV*), maximum absorption wavelengths (λ_{max}), oscillator strengths (f_{os}) and transition natures of compound **TNPR** in chloroform at CAM-B3LYP functional with 6-311G(d,p) basis set

NO.	λ_{DFT} (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	484.446	2.559	3.611	H-2→L (13%), H-1→L+1 (31%), H→L (25%), H-7→L+1 (2%), H-2→L+1 (3%), H→L+1 (9%), H→L+2 (2%), H→L+4 (4%)
2	472.051	2.627	0.191	H-2→L+1 (15%), H-1→L (38%), H→L+1 (23%), H-7→L (3%), H-2→L (5%), H→L (6%)
3	378.844	3.273	0.212	H-2→L (15%), H→L+4 (35%), H-7→L+1 (6%), H-1→L+1 (7%), H-1→L+3 (2%), H→L (8%), H→L+2 (9%)
4	361.186	3.433	0.019	H-2→L+1 (13%), H-1→L+2 (10%), H→L+1 (17%), H→L+3 (13%), H-7→L (8%), H-2→L (3%), H-2→L+3 (5%), H-1→L (4%), H→L (8%), H→L+5 (3%)
5	353.302	3.509	0.055	H-2→L+3 (13%), H-1→L+3 (16%), H→L+1 (23%), H-7→L+3 (3%), H-2→L+1 (3%), H-2→L+2 (5%), H-1→L+2 (7%), H→L+2 (4%), H→L+3 (8%), H→L+4 (3%)
6	352.508	3.517	0.109	H-2→L+2 (18%), H-1→L+2 (17%), H-1→L+3 (12%), H→L (16%), H→L+2 (10%), H-7→L+2 (3%), H-7→L+3 (2%), H-2→L+3 (4%), H→L+1 (3%), H→L+3 (2%)

Table S3: Computed transition energy (*eV*), maximum absorption wavelengths (λ_{max}), oscillator strengths (f_{os}) and transition natures of compound **TNPR** in chloroform at M06 functional with 6-311G(d,p) basis set

NO.	λ_{DFT} (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	706.785	1.754	2.960	H→L (86%), H-1→L+1 (8%)
2	658.895	1.882	0.016	H→L+1 (89%), H-1→L (7%)
3	538.757	2.301	0.064	H-1→L (83%), H-2→L+1 (5%), H→L+1 (7%)
4	525.513	2.359	0.921	H-1→L+1 (75%), H→L (10%), H-2→L (5%), H→L+2 (3%), H→L+4 (2%)
5	502.530	2.467	0.166	H-1→L+3 (10%), H→L+2 (77%), H-1→L+1 (6%)
6	493.214	2.514	0.002	H-1→L+2 (12%), H→L+3 (82%),

Table S4: Computed transition energy (*eV*), maximum absorption wavelengths (λ_{max}), oscillator strengths (f_{os}) and transition natures of compound **TNPR** in chloroform at MPW1PW91 functional with 6-311G(d,p) basis set

NO.	λ_{DFT} (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	782.926	1.584	3.495	H→L (93%), H-1→L+1 (5%)
2	698.660	1.775	0.001	H→L+1 (96%), H-1→L (3%)
3	573.258	2.163	0.001	H-1→L (93%), H-2→L+1 (3%), H→L+1 (3%)
4	557.583	2.224	0.432	H→L+2 (82%), H-1→L+1 (6%), H-1→L+3 (7%), H→L (3%)
5	546.668	2.268	0.001	H→L+3 (89%), H-1→L+2 (8%)
6	544.053	2.279	0.419	H-1→L+1 (82%), H→L (4%), H→L+2 (7%), H→L+4 (2%)

Table S5: Computed transition energy (*eV*), maximum absorption wavelengths (λ_{max}), oscillator strengths (f_{os}) and transition natures of compound **TNPR** in chloroform at ωB97XD functional with 6-311G(d,p) basis set

NO.	λ_{DFT} (*nm*)	*E*(*eV*)	f_{os}	MO contributions

1	454.638	2.727	3.145	H-2→L (15%), H-1→L+1 (33%), H→L (11%), H→L+1 (10%), H-7→L+1 (5%), H-2→L+1 (8%), H-1→L+3 (2%), H→L+4 (4%)
2	444.420	2.790	0.607	H-2→L (12%), H-2→L+1 (18%), H-1→L (38%), H-7→L (5%), H-1→L+2 (2%), H→L (4%), H→L+1 (9%)
3	362.527	3.420	0.560	H→L+4 (52%), H-7→L+1 (5%), H-2→L (7%), H-2→L+4 (2%), H-1→L+1 (3%), H-1→L+3 (2%), H-1→L+5 (3%), H→L (2%), H→L+2 (6%)
4	342.706	3.618	0.029	H-2→L+3 (20%), H-1→L+2 (23%), H→L+3 (12%), H-24→L+2 (3%), H-23→L+3 (4%), H-20→L+1 (3%), H-7→L (3%), H-7→L+2 (3%), H-2→L+1 (3%), H-1→L+3 (3%)
5	338.477	3.663	0.054	H-2→L+2 (24%), H-1→L+3 (21%), H-24→L+3 (4%), H-23→L+2 (4%), H-23→L+3 (2%), H-20→L (2%), H-7→L+3 (5%), H-1→L+2 (4%), H→L+2 (5%), H→L+4 (7%)
6	335.655	3.694	0.007	H-24→L+2 (24%), H-24→L+3 (12%), H-23→L+2 (11%), H-26→L+2 (2%), H-24→L (5%), H-23→L+3 (5%), H-21→L+2 (7%), H-21→L+3 (4%)

Table S6: Cartesian coordinates of **TNPR**

Atom	X-axis	Y-axis	Z-axis
C	-0.77926	-1.23708	0.545443
C	0.59375	-1.36381	0.50919
C	1.344184	-0.2005	0.352007
C	0.732246	1.062195	0.235569
C	-0.63951	1.191972	0.303464
C	-1.38987	0.028736	0.462267
H	1.076002	-2.33631	0.573084
H	-1.12284	2.162399	0.219167
C	2.764793	0.017902	0.239744
C	3.054492	1.33837	0.017987
C	4.433136	1.607114	-0.14494
C	5.178168	0.446155	-0.02148
S	4.169785	-0.96411	0.289877
C	-5.23504	-0.6436	0.610001
C	-4.49275	-1.81171	0.673955
C	-3.10828	-1.53009	0.616518
C	-2.81269	-0.19579	0.517943
S	-4.21696	0.786814	0.467677
C	-6.66059	-0.43459	0.643906
C	-7.33176	0.681212	1.098364
S	-7.78459	-1.59541	-0.00379
C	-8.71962	0.603712	0.943977
H	-6.82376	1.519592	1.56112
C	-9.15284	-0.57289	0.369073
H	-9.40232	1.377059	1.278014
C	6.602044	0.235529	-0.10091

C	7.259496	-0.90405	-0.51408
S	7.742881	1.427892	0.44934
C	8.650855	-0.81733	-0.4108
H	6.737008	-1.77238	-0.89907
C	9.1035	0.388197	0.08688
H	9.319248	-1.61875	-0.70535
C	-1.82798	-2.35268	0.599817
C	1.774239	2.160017	-0.01055
C	-10.5077	-0.9423	0.072357
C	-11.0567	-2.20527	-0.15765
S	-11.6956	0.323279	-0.01926
C	-12.4283	-2.12051	-0.37209
C	-12.9695	-0.83737	-0.32968
H	-13.055	-2.99081	-0.54596
C	10.46897	0.79071	0.265655
C	10.98644	1.940359	0.86815
S	11.72192	-0.26644	-0.31894
C	12.37684	1.93244	0.849891
C	12.96818	0.821337	0.25422
H	12.97841	2.731421	1.274262
C	-10.3129	-3.50019	-0.14767
H	-9.65163	-3.59911	-1.01559
H	-9.69443	-3.60801	0.749154
H	-11.0144	-4.3372	-0.17461
C	10.19287	3.049333	1.475991
H	9.587099	3.576201	0.730597
H	9.512851	2.686983	2.25449
H	10.8609	3.782205	1.933968
C	-5.06432	-3.18203	0.834866
H	-6.02309	-3.16199	1.359368
H	-5.22352	-3.66952	-0.13459
H	-4.38271	-3.8157	1.409187
C	4.992742	2.952488	-0.47073
H	5.153966	3.554003	0.431938
H	5.946706	2.877555	-0.9983
H	4.300848	3.50774	-1.11049
C	-1.8212	-3.17805	-0.69435
C	-2.34741	-4.46378	-0.73389
C	-1.36515	-2.5941	-1.8788
C	-2.40357	-5.15636	-1.93993
H	-2.70506	-4.93807	0.173967
C	-1.4193	-3.29217	-3.07967
H	-0.96242	-1.58804	-1.85579

C	-1.94297	-4.58485	-3.10936
H	-2.81058	-6.16273	-1.96127
H	-1.9715	-5.1147	-4.05604
C	-1.59222	-3.16767	1.86668
C	-0.64192	-4.19367	1.888331
C	-2.23853	-2.82944	3.044759
C	-0.36915	-4.85722	3.070847
H	-0.1269	-4.47986	0.976571
C	-1.96278	-3.50256	4.236535
H	-2.97437	-2.03006	3.073402
C	-1.02209	-4.52685	4.253551
H	0.367091	-5.65525	3.080443
C	1.462534	2.742233	-1.38956
C	0.523172	3.767335	-1.5384
C	2.008067	2.165137	-2.52577
C	0.161931	4.194641	-2.80352
H	0.079602	4.233447	-0.66418
C	1.636322	2.59383	-3.80113
H	2.731595	1.357063	-2.45506
C	0.708646	3.620082	-3.94591
H	-0.56483	4.994086	-2.91188
H	0.407535	3.975209	-4.92425
C	1.827436	3.189354	1.119535
C	2.334502	4.474896	0.909661
C	1.463998	2.818601	2.405462
C	2.457771	5.352777	1.972343
H	2.624235	4.793436	-0.08599
C	1.591329	3.70424	3.475817
H	1.072393	1.82752	2.616914
C	2.089934	4.985211	3.26143
H	2.847431	6.351459	1.799448
O	-0.98051	-2.79963	-4.26078
O	2.230933	1.945489	-4.82847
C	-0.42811	-1.50052	-4.27949
H	-1.16246	-0.7449	-3.97356
H	0.453954	-1.42486	-3.63022
C	1.889126	2.3308	-6.14234
H	2.468342	1.694287	-6.81044
H	0.820511	2.180566	-6.3401
C	14.372	0.714781	0.186056
C	15.23871	-0.22326	-0.31747
H	14.8296	1.586956	0.644562
C	-14.3532	-0.64188	-0.51567

C	-15.1694	0.461941	-0.53504
H	-14.842	-1.59813	-0.68111
C	16.09885	-2.1673	-1.34476
C	16.23926	-3.38156	-1.98467
C	17.526	-3.84386	-2.22815
C	18.62594	-3.0891	-1.83066
C	18.47835	-1.86541	-1.18625
C	17.19191	-1.39621	-0.93876
H	15.35969	-3.94441	-2.28113
H	17.67916	-4.79411	-2.72864
H	19.62601	-3.46147	-2.02679
H	19.36194	-1.31324	-0.89546
C	-18.2825	2.486128	-0.93698
C	-17.0386	1.8884	-0.75782
C	-15.9198	2.700325	-0.55078
C	-15.9939	4.077418	-0.5123
C	-17.2385	4.667175	-0.69076
C	-18.363	3.874256	-0.90119
H	-19.1826	1.910291	-1.10493
H	-15.0965	4.665376	-0.34731
H	-17.3393	5.747106	-0.66801
H	-19.3293	4.347321	-1.04162
C	16.69107	-0.16498	-0.2914
C	14.84877	-1.47787	-0.98133
C	-14.7217	1.85728	-0.39752
C	-16.6096	0.473666	-0.7335
C	17.49788	0.824232	0.223744
C	-17.4631	-0.59919	-0.85523
O	13.72424	-1.88355	-1.19798
O	-13.5909	2.258128	-0.20549
C	17.01787	2.010891	0.840564
N	16.66979	2.989347	1.348564
C	18.91756	0.770614	0.195485
N	20.0733	0.775766	0.198388
C	-17.0551	-1.95866	-0.78875
N	-16.7655	-3.07671	-0.73749
C	-18.8647	-0.46626	-1.04731
N	-20.0083	-0.41202	-1.20515
H	-0.12806	-1.30944	-5.30944
H	2.146062	3.379813	-6.33385
H	-0.79245	-5.06716	5.164217
O	-2.66272	-3.08471	5.315143
C	-2.42544	-3.72631	6.549192

H	-3.07876	-3.24585	7.276739
H	-2.66774	-4.79505	6.500112
H	-1.38309	-3.60842	6.869939
H	2.193597	5.693962	4.074375
O	1.201086	3.223905	4.678323
C	1.305358	4.075613	5.798111
H	0.685913	4.973313	5.680233
H	0.946183	3.504789	6.653798
H	2.34441	4.37748	5.97901

Table S7: Cartesian coordinates of **TNPD1**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	-0.16107	-0.59366	1.714775
C	1.216395	-0.64691	1.698085
C	1.895584	0.453056	1.178532
C	1.2061	1.581706	0.698193
C	-0.1696	1.661179	0.777658
C	-0.84936	0.559835	1.292949
H	1.752925	-1.53645	2.020286
H	-0.70875	2.531069	0.409846
C	3.294912	0.681803	0.916978
C	3.494204	1.856209	0.240136
C	4.839209	2.087992	-0.12916
C	5.655648	1.060098	0.313219
S	4.751783	-0.18622	1.17035
C	-4.6477	-0.31058	1.60091
C	-3.83417	-1.36904	1.960837
C	-2.46778	-1.01626	1.841576
C	-2.25691	0.267095	1.412061
S	-3.725	1.103576	1.105679
C	-6.08918	-0.21056	1.562006
C	-6.87045	0.884117	1.838191
S	-7.08358	-1.53905	1.021651
C	-8.24622	0.660411	1.648971
H	-6.45512	1.817993	2.201144
C	-8.54867	-0.61006	1.219571
H	-9.00797	1.405212	1.851984
C	7.077994	0.869856	0.179724
C	7.762599	-0.32674	0.139616
S	8.192817	2.206099	0.151367
C	9.150539	-0.17725	0.067414

H	7.261026	-1.28777	0.145108
C	9.574286	1.136113	0.051871
H	9.836098	-1.01584	0.016289
C	-1.13629	-1.73375	2.013005
C	2.166795	2.567222	0.021389
C	-9.84972	-1.15412	0.909653
C	-10.2976	-2.45763	0.882381
S	-11.1344	-0.04383	0.49197
C	-11.6652	-2.54328	0.528497
C	-12.2746	-1.34192	0.286507
H	-12.1818	-3.49413	0.440119
C	10.92442	1.605543	-0.07309
C	11.43337	2.900165	0.047144
S	12.17075	0.439546	-0.41488
C	12.81385	2.915377	-0.13027
C	13.40299	1.681527	-0.38586
H	13.40761	3.823056	-0.07005
C	-9.47638	-3.66898	1.186448
H	-8.8201	-3.93908	0.350779
H	-8.8395	-3.52225	2.064324
H	-10.1248	-4.5272	1.380958
C	10.64164	4.131561	0.340894
H	9.943326	4.372341	-0.46829
H	10.05504	4.030677	1.260448
H	11.30886	4.987531	0.464415
C	-4.32877	-2.68815	2.458365
H	-5.31911	-2.59994	2.912025
H	-4.3963	-3.42637	1.650194
H	-3.64803	-3.09349	3.212817
C	5.293865	3.247928	-0.95197
H	5.491539	4.132648	-0.33492
H	6.20546	3.01715	-1.50847
H	4.522452	3.523959	-1.67677
C	-1.05025	-2.79986	0.908673
C	-1.56229	-4.07756	1.104676
C	-0.53332	-2.46227	-0.34484
C	-1.54928	-5.00044	0.063138
H	-1.96266	-4.36411	2.071646
C	-0.51001	-3.39234	-1.37745
H	-0.14014	-1.46633	-0.51265
C	-1.027	-4.67135	-1.17267
H	-1.94778	-5.9973	0.22596
H	-0.99741	-5.38447	-1.99024

C	-0.87028	-2.25874	3.416962
C	0.112533	-3.22633	3.646996
C	-1.52495	-1.69709	4.501831
C	0.409542	-3.61352	4.941712
H	0.634878	-3.68272	2.811796
C	-1.22487	-2.09138	5.806529
H	-2.28635	-0.93366	4.363301
C	-0.25095	-3.05899	6.032449
H	1.171274	-4.3678	5.114649
C	1.737656	2.589293	-1.44749
C	0.768311	3.487206	-1.90324
C	2.186309	1.596339	-2.3058
C	0.276935	3.377182	-3.19235
H	0.39527	4.268147	-1.24825
C	1.67766	1.479432	-3.59901
H	2.931367	0.871523	-1.98675
C	0.717076	2.377681	-4.05277
H	-0.47416	4.079463	-3.54106
H	0.310106	2.311455	-5.05466
C	2.211089	3.932465	0.704481
C	2.653984	5.071876	0.026184
C	1.90497	4.037668	2.052818
C	2.772128	6.275748	0.697682
H	2.897393	5.020473	-1.02961
C	2.027937	5.251851	2.729109
H	1.563384	3.177055	2.621095
C	2.462709	6.384551	2.048702
H	3.111392	7.156985	0.161564
O	0.00335	-3.14262	-2.60427
O	2.171928	0.450584	-4.32788
C	0.62972	-1.89721	-2.83224
H	-0.08109	-1.06153	-2.76878
H	1.449442	-1.71971	-2.12257
C	1.667008	0.262959	-5.63251
H	2.174918	-0.61278	-6.03646
H	0.584875	0.077747	-5.61993
C	14.79608	1.578353	-0.58711
C	15.64695	0.537795	-0.84868
H	15.25908	2.559559	-0.51151
C	16.52652	-1.60907	-1.25304
C	16.91167	-2.95365	-1.48314
C	18.30839	-3.03364	-1.67955
C	17.56177	-0.7209	-1.27301

C	17.08816	0.638788	-1.03158
C	15.27355	-0.888	-0.99137
C	17.91456	1.736486	-1.00545
O	14.1658	-1.37766	-0.91192
C	17.47662	3.067482	-0.78015
N	17.1497	4.161103	-0.5999
C	19.31253	1.600623	-1.21338
N	20.45069	1.491407	-1.38217
H	1.040347	-1.93921	-3.84036
H	1.876601	1.127109	-6.27429
H	-0.00186	-3.38507	7.035242
O	-1.93479	-1.47558	6.778906
C	-1.67469	-1.83419	8.118308
H	-2.34096	-1.23055	8.733744
H	-1.88356	-2.89596	8.29854
H	-0.63575	-1.62005	8.397852
H	2.561577	7.340751	2.548539
O	1.698209	5.22323	4.040379
C	1.801464	6.422117	4.77665
H	1.139324	7.199382	4.375501
H	1.496267	6.185224	5.795361
H	2.831539	6.799286	4.789333
C	18.94032	-4.24994	-1.92485
C	16.13778	-4.11395	-1.53429
H	20.01267	-4.30489	-2.07473
H	15.06491	-4.06247	-1.38477
S	19.09544	-1.46901	-1.57748
C	18.16658	-5.38837	-1.97309
C	16.77193	-5.32151	-1.77883
C	-13.6589	-1.0871	-0.08978
C	-14.653	-2.03563	0.179151
C	-14.0484	0.092021	-0.73293
C	-15.9677	-1.82423	-0.18567
H	-14.3957	-2.94464	0.71489
C	-15.3614	0.309391	-1.10442
H	-13.3041	0.84608	-0.97546
C	-16.3433	-0.64912	-0.84295
H	-16.7206	-2.56912	0.052229
H	-15.6353	1.22693	-1.61736
N	-17.6779	-0.40745	-1.21382
C	-18.199	0.90808	-1.05066
C	-18.5926	1.658441	-2.19345
C	-18.3083	1.446739	0.206546

C	-19.1426	2.956292	-1.99527
C	-18.8315	2.739348	0.392394
H	-17.9907	0.854044	1.060164
C	-19.2527	3.472416	-0.68328
H	-18.9123	3.142866	1.39654
H	-19.6703	4.466566	-0.54811
C	-18.5399	-1.43914	-1.63674
C	-18.0558	-2.50569	-2.40033
C	-19.9032	-1.3853	-1.34189
C	-18.9146	-3.50125	-2.83466
H	-17.0015	-2.54457	-2.65781
C	-20.7569	-2.38023	-1.79488
H	-20.2915	-0.55816	-0.75528
C	-20.2713	-3.44699	-2.5375
H	-18.5198	-4.32127	-3.42701
H	-21.8143	-2.32099	-1.555
H	-20.9418	-4.22567	-2.88576
C	-18.4317	1.178382	-3.51405
C	-19.544	3.708581	-3.12397
H	-17.9866	0.200088	-3.66893
H	-19.9703	4.69557	-2.96395
C	-19.3918	3.211377	-4.38913
C	-18.8211	1.937463	-4.58462
H	-19.7015	3.799061	-5.24755
H	-18.6874	1.55926	-5.59326
C	16.00474	-6.52362	-1.83582
N	15.38945	-7.49857	-1.88276
H	18.62725	-6.35166	-2.16214

Table S8: Cartesian coordinates of **TNPD2**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	0.579365	0.282831	1.705966
C	-0.79901	0.290462	1.734736
C	-1.4611	-0.74311	1.075562
C	-0.75383	-1.76203	0.411033
C	0.625542	-1.8052	0.440788
C	1.287856	-0.77154	1.098931
H	-1.35165	1.103038	2.200889
H	1.178562	-2.59084	-0.06886
C	-2.86096	-0.98131	0.82485
C	-3.04697	-2.04937	-0.01264
C	-4.39652	-2.27421	-0.3702

C	-5.22859	-1.35285	0.243612
S	-4.33483	-0.21412	1.248406
C	5.067734	0.152517	1.46828
C	4.234973	1.126872	1.986216
C	2.875788	0.758059	1.835709
C	2.689393	-0.45478	1.227406
S	4.171928	-1.19911	0.784853
C	6.51061	0.091769	1.405567
C	7.316584	-1.0111	1.540876
S	7.471743	1.497799	1.02459
C	8.684975	-0.73677	1.369944
H	6.923709	-1.99082	1.790097
C	8.958192	0.582489	1.09412
H	9.462598	-1.48548	1.474459
C	-6.65995	-1.19325	0.180591
C	-7.37794	-0.0254	0.32764
S	-7.73799	-2.54798	0.001232
C	-8.7634	-0.20772	0.277402
H	-6.90261	0.940919	0.452056
C	-9.15059	-1.51905	0.092694
H	-9.47389	0.606675	0.36559
C	1.529817	1.398724	2.144098
C	-1.70607	-2.66662	-0.38097
C	10.24724	1.182365	0.846139
C	10.65761	2.497782	0.902198
S	11.57449	0.134532	0.399707
C	12.02999	2.641907	0.587749
C	12.6802	1.473883	0.294626
H	12.51952	3.61069	0.565151
C	-10.4909	-2.00974	-0.06072
C	-10.965	-3.32211	-0.06405
S	-11.7705	-0.8483	-0.26704
C	-12.3485	-3.3555	-0.21932
C	-12.9717	-2.1183	-0.34042
H	-12.9191	-4.27967	-0.23798
C	9.794165	3.667221	1.249675
H	9.11339	3.931546	0.431935
H	9.17847	3.474095	2.134067
H	10.41109	4.545437	1.45615
C	-10.1375	-4.5549	0.09349
H	-9.46809	-4.71056	-0.75979
H	-9.51612	-4.51773	0.994592
H	-10.7818	-5.43375	0.16925

C	4.70702	2.372075	2.663705
H	5.707031	2.243934	3.085652
H	4.744073	3.220753	1.97022
H	4.030301	2.646587	3.478686
C	-4.84213	-3.31843	-1.33983
H	-4.96582	-4.29526	-0.8571
H	-5.79128	-3.05492	-1.81248
H	-4.09836	-3.44142	-2.13274
C	1.37643	2.612144	1.21271
C	1.857064	3.8645	1.578898
C	0.826446	2.444591	-0.06066
C	1.778249	4.929266	0.686082
H	2.28193	4.02081	2.564999
C	0.736589	3.514638	-0.94289
H	0.459148	1.471313	-0.36366
C	1.221316	4.767287	-0.56771
H	2.152113	5.904763	0.982134
H	1.139902	5.591481	-1.26905
C	1.294842	1.699877	3.617934
C	0.298663	2.594633	4.019965
C	1.995612	0.997865	4.586232
C	0.034018	2.772572	5.366491
H	-0.26029	3.157815	3.279062
C	1.727945	1.18093	5.943479
H	2.768991	0.28485	4.312022
C	0.740368	2.07669	6.3412
H	-0.73858	3.471124	5.673472
C	-1.33169	-2.44141	-1.84795
C	-0.33799	-3.20822	-2.46334
C	-1.85929	-1.35657	-2.53216
C	0.099501	-2.88017	-3.73447
H	0.09561	-4.05796	-1.94566
C	-1.40606	-1.021	-3.80787
H	-2.62626	-0.72856	-2.0855
C	-0.42043	-1.78809	-4.42041
H	0.870299	-3.48111	-4.20743
H	-0.05457	-1.55112	-5.41226
C	-1.6778	-4.12301	0.077064
C	-2.09813	-5.15887	-0.76239
C	-1.32488	-4.4262	1.383299
C	-2.14825	-6.45769	-0.28807
H	-2.37665	-4.95192	-1.79017
C	-1.37823	-5.7362	1.860484

H	-0.99884	-3.65187	2.072038
C	-1.79091	-6.76493	1.019826
H	-2.4704	-7.2571	-0.94855
O	0.185256	3.428534	-2.17562
O	-1.97806	0.076326	-4.35803
C	-0.40941	2.207337	-2.56371
H	0.330258	1.399308	-2.65124
H	-1.19268	1.894922	-1.85927
C	-1.53939	0.478356	-5.63794
H	-2.10663	1.374035	-5.89087
H	-0.46819	0.719065	-5.63661
C	-14.3721	-2.03098	-0.5008
C	-15.2513	-0.99163	-0.64206
H	-14.8108	-3.02618	-0.51039
C	-16.1841	1.161391	-0.84053
C	-16.6022	2.510313	-0.94577
C	-18.0023	2.573869	-1.10395
C	-17.202	0.253962	-0.91379
C	-16.6954	-1.10894	-0.79688
C	-14.9116	0.449791	-0.6685
C	-17.4981	-2.22404	-0.83484
O	-13.8122	0.955319	-0.57153
C	-17.028	-3.55813	-0.72084
N	-16.6753	-4.65493	-0.63071
C	-18.9035	-2.10382	-0.99657
N	-20.0476	-2.00681	-1.12844
H	-0.86293	2.382151	-3.53863
H	-1.73346	-0.29428	-6.39156
H	0.515413	2.239839	7.388461
O	2.481345	0.443544	6.790449
C	2.252968	0.58441	8.175467
H	2.951451	-0.08786	8.672721
H	2.441927	1.611177	8.512362
H	1.228223	0.300663	8.445296
H	-1.83605	-7.79141	1.363703
O	-1.00682	-5.90126	3.15039
C	-1.03583	-7.20556	3.687123
H	-0.35725	-7.87798	3.147816
H	-0.70504	-7.12035	4.721706
H	-2.04872	-7.6265	3.667965
C	-18.6581	3.79039	-1.22948
C	-15.8557	3.69074	-0.91392
H	-19.7334	3.850491	-1.35172

H	-14.7789	3.655201	-0.79273
S	-18.7581	0.988033	-1.11849
C	-17.9047	4.948	-1.1959
C	-16.5055	4.897915	-1.03837
Cl	-18.7255	6.467777	-1.35289
Cl	-15.5668	6.358183	-0.99792
C	14.07955	1.276314	-0.05904
C	15.03884	2.241771	0.2692
C	14.51871	0.133338	-0.73521
C	16.36807	2.079745	-0.06771
H	14.74251	3.123309	0.830068
C	15.84636	-0.03454	-1.07852
H	13.80281	-0.63144	-1.02483
C	16.7936	0.939337	-0.75489
H	17.09326	2.835789	0.216694
H	16.15986	-0.92453	-1.61679
N	18.14455	0.744887	-1.09442
C	18.7005	-0.55688	-0.93724
C	19.16914	-1.26716	-2.07741
C	18.77157	-1.12142	0.311418
C	19.75244	-2.55105	-1.88305
C	19.32791	-2.40082	0.492102
H	18.39749	-0.55953	1.162981
C	19.8205	-3.0945	-0.5793
H	19.37701	-2.8251	1.489723
H	20.26399	-4.07783	-0.4476
C	18.98946	1.813527	-1.45545
C	18.49964	2.887252	-2.20523
C	20.34229	1.79196	-1.11275
C	19.34197	3.920403	-2.5798
H	17.45443	2.901971	-2.49949
C	21.18037	2.824775	-1.50647
H	20.735	0.959956	-0.53602
C	20.68846	3.897851	-2.23567
H	18.94312	4.745474	-3.16234
H	22.22994	2.7902	-1.23023
H	21.34643	4.706081	-2.53737
C	19.05233	-0.76135	-3.39302
C	20.22928	-3.26297	-3.00853
H	18.58247	0.20546	-3.54651
H	20.68044	-4.23923	-2.85094
C	20.1184	-2.74094	-4.26794
C	19.51495	-1.48185	-4.46115

H	20.48613	-3.29774	-5.12405
H	19.41455	-1.08428	-5.4662

Table S9: Cartesian coordinates of **TNPD3**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	1.237842	0.120906	1.669051
C	-0.14127	0.137101	1.662916
C	-0.79433	-0.82623	0.896235
C	-0.07947	-1.78615	0.155774
C	1.299696	-1.82048	0.185273
C	1.952435	-0.85747	0.951448
H	-0.70258	0.889146	2.21234
H	1.861207	-2.55863	-0.38261
C	-2.19327	-1.06649	0.640151
C	-2.37224	-2.09343	-0.24894
C	-3.72449	-2.34801	-0.57266
C	-4.56559	-1.49061	0.117126
S	-3.67722	-0.37512	1.15166
C	5.730764	-0.04504	1.535117
C	4.894696	0.848386	2.179169
C	3.536056	0.524584	1.943938
C	3.352465	-0.5776	1.15294
S	4.837308	-1.2644	0.633022
C	7.173496	-0.11966	1.490047
C	7.954356	-1.24697	1.417552
S	8.172743	1.309933	1.416637
C	9.332033	-0.97785	1.330921
H	7.537066	-2.24717	1.459766
C	9.636424	0.362016	1.333381
H	10.09406	-1.74889	1.299951
C	-6.00363	-1.39292	0.115598
C	-6.77159	-0.27127	0.348099
S	-7.01906	-2.79129	-0.08581
C	-8.14737	-0.52227	0.343312
H	-6.33887	0.710626	0.50259
C	-8.47572	-1.84268	0.112399
H	-8.89378	0.248555	0.500186
C	2.19104	1.119823	2.334285
C	-1.02732	-2.67524	-0.65771
C	10.94159	0.971867	1.229299
C	11.40996	2.181615	1.693782
S	12.20219	0.089481	0.399747

C	12.77656	2.378921	1.380271
C	13.36227	1.352983	0.689554
H	13.31083	3.283536	1.6545
C	-9.79232	-2.39983	-0.01161
C	-10.1936	-3.73731	-0.01957
S	-11.1378	-1.30786	-0.16778
C	-11.5759	-3.84493	-0.13539
C	-12.2695	-2.6416	-0.22358
H	-12.0962	-4.79845	-0.14927
C	10.60905	3.191968	2.450121
H	9.985999	3.800561	1.784155
H	9.941489	2.721827	3.178649
H	11.27084	3.874514	2.989724
C	-9.2959	-4.92443	0.0998
H	-8.6561	-5.04434	-0.78146
H	-8.64019	-4.85479	0.974079
H	-9.88918	-5.83616	0.199826
C	5.356273	1.971442	3.049393
H	6.348985	1.777822	3.463326
H	5.402884	2.917852	2.497281
H	4.666306	2.11769	3.885832
C	-4.16929	-3.3619	-1.57459
H	-4.27038	-4.35792	-1.12694
H	-5.13072	-3.0961	-2.02075
H	-3.43759	-3.44305	-2.38361
C	2.085209	2.503539	1.680249
C	2.487302	3.653906	2.348167
C	1.667815	2.600876	0.350311
C	2.458832	4.883313	1.69589
H	2.814583	3.601773	3.381318
C	1.637352	3.831409	-0.29474
H	1.362619	1.704523	-0.17744
C	2.035819	4.982682	0.385249
H	2.769372	5.778387	2.226346
H	1.999985	5.934648	-0.13463
C	1.918251	1.108674	3.8345
C	0.878892	1.871168	4.377702
C	2.626861	0.256006	4.665677
C	0.58054	1.771766	5.724539
H	0.313188	2.550431	3.747491
C	2.324647	0.159096	6.025262
H	3.434064	-0.36153	4.280572
C	1.294583	0.922754	6.563622

H	-0.22524	2.36886	6.140828
C	-0.68498	-2.43315	-2.12766
C	0.329315	-3.16253	-2.75585
C	-1.28365	-1.3898	-2.81674
C	0.711356	-2.84355	-4.04659
H	0.815471	-3.98179	-2.2355
C	-0.89119	-1.06609	-4.11654
H	-2.06612	-0.78942	-2.35963
C	0.111621	-1.79955	-4.74231
H	1.496973	-3.41634	-4.53006
H	0.430728	-1.57184	-5.75237
C	-0.97795	-4.14151	-0.22433
C	-1.38416	-5.16761	-1.08244
C	-0.62243	-4.46388	1.076752
C	-1.4181	-6.4754	-0.63147
H	-1.66393	-4.94604	-2.10681
C	-0.65957	-5.78272	1.530172
H	-0.30669	-3.69892	1.780591
C	-1.05818	-6.80166	0.670943
H	-1.72929	-7.26675	-1.3068
O	1.229655	4.005204	-1.57328
O	-1.54236	-0.0215	-4.67734
C	0.8073	2.870248	-2.29893
H	1.61711	2.138431	-2.41052
H	-0.05266	2.381408	-1.82278
C	-1.18545	0.354794	-5.98967
H	-1.81564	1.205041	-6.24848
H	-0.13251	0.656932	-6.04916
C	-13.6737	-2.63233	-0.35174
C	-14.616	-1.64454	-0.46871
H	-14.0551	-3.65081	-0.36151
C	-15.6785	0.449448	-0.65024
C	-16.1845	1.768038	-0.75561
C	-17.5819	1.742605	-0.90556
C	-16.6402	-0.51728	-0.71461
C	-16.05	-1.84944	-0.60412
C	-14.3621	-0.18617	-0.49249
C	-16.7873	-3.00849	-0.63232
O	-13.2945	0.383743	-0.4045
C	-16.2384	-4.31297	-0.52594
N	-15.8203	-5.3869	-0.44182
C	-18.1995	-2.97024	-0.77393
N	-19.3491	-2.93992	-0.88929

H	0.511796	3.228065	-3.28491
H	-1.36694	-0.45714	-6.70458
H	1.042692	0.868808	7.616054
O	3.090663	-0.7033	6.731091
C	2.83039	-0.84497	8.110363
H	3.54402	-1.57814	8.484843
H	2.973779	0.101446	8.646288
H	1.812	-1.20993	8.292317
H	-1.09039	-7.83463	0.996404
O	-0.28731	-5.96592	2.817499
C	-0.29988	-7.27975	3.330903
H	0.388257	-7.93356	2.780914
H	0.028303	-7.20865	4.367393
H	-1.30709	-7.71365	3.302602
C	-18.3098	2.918314	-1.03513
C	-15.5236	2.998903	-0.73284
H	-19.3859	2.890931	-1.15324
H	-14.4471	3.018937	-0.61525
S	-18.239	0.117744	-0.90963
C	-17.648	4.130964	-1.01011
C	-16.2372	4.171009	-0.86258
C	14.74036	1.236784	0.230285
C	15.76434	1.94501	0.869774
C	15.09357	0.427666	-0.85415
C	17.07558	1.855394	0.44563
H	15.53249	2.551092	1.740869
C	16.40205	0.336958	-1.28811
H	14.32398	-0.122	-1.38983
C	17.41648	1.052804	-0.64724
H	17.85203	2.398154	0.97538
H	16.64757	-0.28673	-2.14282
N	18.74601	0.930285	-1.08658
C	19.20188	-0.34859	-1.51843
C	19.58146	-0.54024	-2.8758
C	19.26195	-1.38864	-0.6256
C	20.06502	-1.8197	-3.27001
C	19.72013	-2.65644	-1.02813
H	18.95615	-1.21523	0.402618
C	20.12573	-2.86381	-2.31823
H	19.76304	-3.46303	-0.30339
H	20.49297	-3.8364	-2.63481
C	19.66916	1.99298	-1.00681
C	19.263	3.311054	-1.23572

C	21.0166	1.737982	-0.7476
C	20.18201	4.345311	-1.18072
H	18.22193	3.518268	-1.46501
C	21.9315	2.779844	-0.71005
H	21.34444	0.717277	-0.57535
C	21.52291	4.089232	-0.9191
H	19.84767	5.362501	-1.36149
H	22.97554	2.561574	-0.50651
H	22.24086	4.901965	-0.88404
C	19.46933	0.478722	-3.85019
C	20.45152	-2.0195	-4.61597
H	19.07455	1.446992	-3.55739
H	20.827	-2.99693	-4.90767
C	20.34787	-1.00998	-5.53318
C	19.84285	0.24802	-5.14679
H	20.64555	-1.17614	-6.56367
H	19.74721	1.037092	-5.88605
C	-15.4533	5.45641	-0.77435
C	-18.4923	5.364919	-1.21093
F	-14.1445	5.24199	-0.92375
F	-15.8076	6.337565	-1.71096
F	-15.6124	6.04598	0.413766
F	-18.1877	6.338033	-0.35186
F	-18.3525	5.857188	-2.44439
F	-19.791	5.100726	-1.04838

Table S10: Cartesian coordinates of **TNPD4**

Atom	X-axis	Y-axis	Z-axis
C	-0.35046	-0.55719	1.603884
C	1.027157	-0.60497	1.586142
C	1.701218	0.493785	1.05732
C	1.006345	1.615016	0.56736
C	-0.36966	1.689004	0.646437
C	-1.04406	0.589673	1.172836
H	1.567633	-1.48907	1.916651
H	-0.91273	2.553829	0.272538
C	3.10006	0.729977	0.799505
C	3.294139	1.901583	0.116238
C	4.640538	2.145181	-0.24005
C	5.462744	1.129585	0.218928
S	4.563218	-0.12116	1.073707

C	-4.83863	-0.2816	1.524574
C	-4.02015	-1.33631	1.886279
C	-2.6554	-0.98459	1.747589
C	-2.44985	0.294271	1.302435
S	-3.92118	1.126567	1.00196
C	-6.27962	-0.17494	1.510253
C	-7.04475	0.942025	1.741439
S	-7.30037	-1.52252	1.074508
C	-8.42667	0.722154	1.599815
H	-6.61302	1.891124	2.039962
C	-8.75059	-0.56821	1.255583
H	-9.1775	1.483996	1.77875
C	6.890368	0.961483	0.112968
C	7.59592	-0.22282	0.080182
S	7.981689	2.316729	0.127004
C	8.982839	-0.04895	0.04819
H	7.110332	-1.19195	0.064777
C	9.383798	1.271664	0.057648
H	9.684199	-0.87513	0.010998
C	-1.32084	-1.69798	1.914644
C	1.962849	2.601264	-0.11425
C	-10.0646	-1.11709	1.013808
C	-10.5408	-2.4035	1.145992
S	-11.327	-0.03503	0.473761
C	-11.9142	-2.49898	0.815654
C	-12.4979	-1.3211	0.435684
H	-12.4553	-3.43986	0.847114
C	10.72892	1.766356	-0.01449
C	11.21061	3.065817	0.155925
S	12.00608	0.630186	-0.34154
C	12.59636	3.107321	0.033803
C	13.21565	1.889665	-0.22905
H	13.17245	4.021706	0.143937
C	-9.74247	-3.5865	1.590472
H	-9.13374	-3.99786	0.776639
H	-9.06169	-3.33569	2.409625
H	-10.4058	-4.3841	1.935106
C	10.38762	4.275908	0.451878
H	9.711845	4.523948	-0.37397
H	9.773229	4.14248	1.348834
H	11.03484	5.140065	0.617623
C	-4.5071	-2.65086	2.403176
H	-5.47529	-2.5527	2.900885

H	-4.61994	-3.38663	1.59776
H	-3.7987	-3.06537	3.126173
C	5.093165	3.304666	-1.06468
H	5.265066	4.197933	-0.45231
H	6.018938	3.082869	-1.60105
H	4.331749	3.562091	-1.80682
C	-1.2378	-2.76889	0.814452
C	-1.75118	-4.04519	1.016311
C	-0.72121	-2.43774	-0.44088
C	-1.73998	-4.97258	-0.02117
H	-2.15094	-4.32736	1.984793
C	-0.69948	-3.37232	-1.46943
H	-0.32678	-1.44323	-0.61365
C	-1.21804	-4.64968	-1.25883
H	-2.13961	-5.9682	0.146321
H	-1.18989	-5.36651	-2.07319
C	-1.04417	-2.21494	3.31942
C	-0.06248	-3.18397	3.547706
C	-1.68709	-1.64294	4.406032
C	0.245124	-3.56237	4.842647
H	0.450965	-3.64806	2.711245
C	-1.3764	-2.02834	5.71079
H	-2.44728	-0.87811	4.268607
C	-0.40354	-2.9975	5.935098
H	1.005998	-4.3178	5.014317
C	1.538473	2.607793	-1.58462
C	0.562264	3.493295	-2.05006
C	1.997993	1.611914	-2.43368
C	0.075068	3.368555	-3.33935
H	0.180528	4.276102	-1.4024
C	1.493107	1.479724	-3.72697
H	2.748334	0.896148	-2.10673
C	0.525895	2.365842	-4.19043
H	-0.68129	4.061358	-3.69555
H	0.121844	2.287634	-5.19264
C	1.995404	3.972448	0.557557
C	2.427551	5.110362	-0.13003
C	1.689547	4.085404	1.905361
C	2.535513	6.320498	0.531998
H	2.670728	5.052702	-1.18556
C	1.80207	5.305864	2.571973
H	1.356334	3.22618	2.48069
C	2.226128	6.437076	1.882324

H	2.866544	7.200488	-0.01127
O	-0.18603	-3.12831	-2.6974
O	1.99728	0.44869	-4.4459
C	0.441834	-1.88459	-2.93072
H	-0.26807	-1.04782	-2.87123
H	1.261589	-1.70464	-2.22171
C	1.498097	0.247057	-5.75065
H	2.013948	-0.62792	-6.14605
H	0.417363	0.053732	-5.74016
C	14.61839	1.810661	-0.35949
C	15.49711	0.789198	-0.60502
H	15.06295	2.794662	-0.22865
C	16.42619	-1.32613	-1.06179
C	16.8425	-2.65342	-1.33385
C	18.25024	-2.70914	-1.45148
C	17.44881	-0.428	-0.97799
C	16.94508	0.912795	-0.694
C	15.15069	-0.63186	-0.83519
C	17.75576	2.013074	-0.55153
O	14.04729	-1.1367	-0.84192
C	17.29044	3.323088	-0.26604
N	16.94156	4.399878	-0.03336
C	19.1649	1.90139	-0.68495
N	20.312	1.811221	-0.79388
H	0.852778	-1.93153	-3.93853
H	1.703211	1.107786	-6.39845
H	-0.14631	-3.31682	6.938019
O	-2.07526	-1.4028	6.684972
C	-1.80331	-1.75136	8.024671
H	-2.46165	-1.14054	8.641576
H	-2.01383	-2.81092	8.215628
H	-0.76104	-1.53833	8.292393
H	2.31675	7.397997	2.374619
O	1.473655	5.284676	3.883723
C	1.566541	6.490285	4.610326
H	0.897079	7.258287	4.20352
H	1.264231	6.258776	5.631132
H	2.593162	6.876884	4.619202
C	18.9135	-3.90465	-1.71921
C	16.08851	-3.8178	-1.48698
H	19.99333	-3.93896	-1.8083
H	15.00881	-3.80591	-1.40183
S	19.00822	-1.14511	-1.22576

C	18.1614	-5.04921	-1.86929
C	16.76944	-4.98391	-1.7506
C	-13.882	-1.07638	0.051098
C	-14.9036	-1.92001	0.502201
C	-14.2438	-0.00692	-0.77403
C	-16.221	-1.71094	0.144373
H	-14.6641	-2.73636	1.177521
C	-15.5586	0.205503	-1.14145
H	-13.4769	0.658376	-1.16189
C	-16.5709	-0.64558	-0.69062
H	-16.9947	-2.36799	0.528669
H	-15.8112	1.034334	-1.79647
N	-17.9065	-0.40051	-1.0539
C	-18.3532	0.950551	-1.12236
C	-18.7697	1.49266	-2.36981
C	-18.3709	1.722016	0.012098
C	-19.2455	2.833871	-2.40084
C	-18.821	3.054251	-0.03103
H	-18.0381	1.284152	0.949289
C	-19.2617	3.593982	-1.20845
H	-18.8299	3.644003	0.879882
H	-19.6232	4.61807	-1.24852
C	-18.8452	-1.4387	-1.22598
C	-18.467	-2.65581	-1.80068
C	-20.181	-1.24692	-0.87065
C	-19.4017	-3.65982	-1.98971
H	-17.4356	-2.80656	-2.10532
C	-21.1122	-2.25376	-1.07854
H	-20.4871	-0.30293	-0.43002
C	-20.731	-3.46766	-1.63197
H	-19.0892	-4.59829	-2.43777
H	-22.1469	-2.08585	-0.79518
H	-21.4613	-4.25465	-1.78843
C	-18.7022	0.762764	-3.57939
C	-19.6697	3.380529	-3.63462
H	-18.3132	-0.25083	-3.56245
H	-20.0391	4.40269	-3.64878
C	-19.6091	2.644755	-4.78612
C	-19.1113	1.326377	-4.75792
H	-19.9354	3.075995	-5.72722
H	-19.0496	0.757008	-5.68002
N	15.99397	-6.22604	-1.91548
O	16.60794	-7.24649	-2.14944

O	14.78751	-6.15714	-1.80772
H	18.62821	-6.00336	-2.07826

Table S11: Cartesian coordinates of **TNPD5**

Atom	X-axis	Y-axis	Z-axis
C	-0.41998	-0.38734	1.714931
C	0.958285	-0.40228	1.73556
C	1.621448	0.655459	1.116895
C	0.915416	1.704357	0.499361
C	-0.46352	1.752614	0.538961
C	-1.12682	0.695159	1.157117
H	1.509762	-1.23561	2.164869
H	-1.01557	2.56195	0.066774
C	3.020855	0.898745	0.870466
C	3.207826	2.002276	0.080029
C	4.556037	2.236849	-0.27351
C	5.387131	1.284425	0.294074
S	4.492264	0.105802	1.251303
C	-4.90889	-0.22294	1.513806
C	-4.07857	-1.2218	1.987247
C	-2.71813	-0.85468	1.842953
C	-2.52895	0.380882	1.28285
S	-4.00987	1.150213	0.87967
C	-6.35171	-0.1518	1.460821
C	-7.15017	0.949962	1.642068
S	-7.32305	-1.53583	1.028658
C	-8.52089	0.691122	1.465285
H	-6.75015	1.916696	1.927917
C	-8.80314	-0.61457	1.139078
H	-9.29361	1.439822	1.601437
C	6.815667	1.11842	0.213147
C	7.526628	-0.0591	0.325843
S	7.901574	2.467904	0.047156
C	8.911099	0.113032	0.259477
H	7.04563	-1.02428	0.43578
C	9.307168	1.425716	0.096717
H	9.615575	-0.70906	0.319997
C	-1.37347	-1.51572	2.111789
C	1.86761	2.637509	-0.25894
C	-10.0963	-1.19569	0.867974
C	-10.5197	-2.5078	0.88873
S	-11.4092	-0.12409	0.436255

C	-11.8907	-2.63064	0.559345
C	-12.5269	-1.44936	0.289084
H	-12.3894	-3.59367	0.509013
C	10.64826	1.905672	-0.06434
C	11.13386	3.216437	-0.0585
S	11.91547	0.736233	-0.296
C	12.51366	3.240266	-0.22632
C	13.12721	1.997791	-0.36781
H	13.09186	4.159759	-0.24026
C	-9.67005	-3.69333	1.215034
H	-8.99746	-3.955	0.389678
H	-9.04705	-3.52067	2.098421
H	-10.2974	-4.56628	1.41246
C	10.31711	4.453277	0.120228
H	9.634626	4.618084	-0.7208
H	9.71097	4.41453	1.031563
H	10.96835	5.327346	0.190365
C	-4.55428	-2.49025	2.617473
H	-5.55152	-2.37331	3.049082
H	-4.59923	-3.31079	1.891388
H	-3.8753	-2.80038	3.417735
C	5.001232	3.322526	-1.19648
H	5.157795	4.268973	-0.66512
H	5.933384	3.065959	-1.70564
H	4.242244	3.503513	-1.96301
C	-1.23537	-2.68823	1.126869
C	-1.72688	-3.94999	1.44263
C	-0.68777	-2.4726	-0.14035
C	-1.66175	-4.97732	0.506281
H	-2.14902	-4.14318	2.423345
C	-0.61135	-3.50623	-1.06643
H	-0.31174	-1.49076	-0.403
C	-1.10747	-4.76848	-0.74182
H	-2.0439	-5.96072	0.762977
H	-1.03632	-5.56346	-1.47718
C	-1.12599	-1.88623	3.567502
C	-0.12616	-2.79961	3.915205
C	-1.81761	-1.23335	4.575703
C	0.151632	-3.04393	5.24842
H	0.42472	-3.32591	3.141833
C	-1.53717	-1.48396	5.919708
H	-2.5935	-0.50797	4.344398
C	-0.54571	-2.39773	6.263033

H	0.927055	-3.75656	5.512985
C	1.489995	2.468628	-1.733
C	0.496407	3.258332	-2.31876
C	2.015456	1.409125	-2.45752
C	0.05895	2.978756	-3.60153
H	0.062754	4.08789	-1.76941
C	1.561518	1.121531	-3.74456
H	2.781107	0.762881	-2.03539
C	0.577584	1.912705	-4.32833
H	-0.71119	3.597967	-4.05143
H	0.211635	1.713905	-5.32852
C	1.843163	4.074428	0.257136
C	2.250393	5.145436	-0.54351
C	1.506969	4.321827	1.579527
C	2.303543	6.42355	-0.01585
H	2.515582	4.982679	-1.58263
C	1.563445	5.610722	2.110515
H	1.191853	3.518412	2.239472
C	1.962573	6.674871	1.308159
H	2.615146	7.250797	-0.64642
O	-0.06295	-3.3753	-2.29655
O	2.131004	0.043765	-4.33442
C	0.55057	-2.14846	-2.63397
H	-0.17573	-1.3254	-2.68576
H	1.340096	-1.87936	-1.9188
C	1.694277	-0.30797	-5.62976
H	2.259104	-1.19547	-5.91491
H	0.622302	-0.54487	-5.64031
C	14.52131	1.90159	-0.54269
C	15.39224	0.854066	-0.7079
H	14.96991	2.892469	-0.5434
C	16.30224	-1.30287	-0.95432
C	16.70719	-2.65188	-1.08811
C	18.10757	-2.72482	-1.26003
C	17.32797	-0.40632	-1.02076
C	16.83236	0.962528	-0.87443
C	15.03668	-0.58082	-0.75537
C	17.64953	2.066962	-0.90169
O	13.93585	-1.08127	-0.65553
C	17.19625	3.404326	-0.7601
N	16.85515	4.502548	-0.64746
C	19.05122	1.929975	-1.08012
N	20.19201	1.815094	-1.22579

H	0.999515	-2.28899	-3.61655
H	1.893026	0.492025	-6.35298
H	-0.31102	-2.61276	7.298711
O	-2.2828	-0.79046	6.809483
C	-2.043	-1.00204	8.183556
H	-2.73683	-0.35591	8.720346
H	-2.2299	-2.04467	8.468958
H	-1.01582	-0.73286	8.459041
H	2.009733	7.686175	1.694136
O	1.208923	5.720855	3.410923
C	1.242057	7.0018	4.001062
H	0.554944	7.694158	3.499065
H	0.925013	6.872673	5.035391
H	2.25371	7.425886	3.986359
C	18.75581	-3.94262	-1.41443
C	15.94666	-3.82344	-1.0719
H	19.82992	-4.00339	-1.54671
H	14.87155	-3.77438	-0.941
S	18.87475	-1.14947	-1.25239
C	17.99334	-5.09975	-1.39667
C	16.58473	-5.0393	-1.22527
C	-13.9206	-1.22916	-0.07334
C	-14.8933	-2.19133	0.223802
C	-14.3408	-0.06723	-0.7288
C	-16.217	-2.00829	-0.1239
H	-14.6121	-3.08787	0.768457
C	-15.6628	0.121837	-1.08281
H	-13.6141	0.696258	-0.99397
C	-16.6234	-0.84918	-0.7912
H	-16.9529	-2.76277	0.136023
H	-15.961	1.026605	-1.60486
N	-17.9681	-0.63448	-1.14229
C	-18.5108	0.671808	-0.97562
C	-18.9467	1.405951	-2.11363
C	-18.6005	1.21744	0.280174
C	-19.5177	2.693997	-1.91089
C	-19.1446	2.500825	0.46986
H	-18.251	0.637407	1.130018
C	-19.6062	3.217543	-0.6002
H	-19.2091	2.90995	1.472917
H	-20.0401	4.204236	-0.46178
C	-18.8193	-1.68599	-1.53738
C	-18.3303	-2.75148	-2.29937

C	-20.1773	-1.6539	-1.2166
C	-19.1789	-3.76678	-2.7072
H	-17.2807	-2.77383	-2.57693
C	-21.0213	-2.66858	-1.64335
H	-20.5694	-0.82798	-0.63078
C	-20.5305	-3.73389	-2.38467
H	-18.7806	-4.5856	-3.29884
H	-22.0748	-2.62601	-1.38371
H	-21.1932	-4.528	-2.71235
C	-18.8085	0.919525	-3.43447
C	-19.9618	3.429723	-3.03449
H	-18.3478	-0.05079	-3.59362
H	-20.4039	4.409099	-2.87075
C	-19.8308	2.92632	-4.29955
C	-19.2393	1.66274	-4.50032
H	-20.1733	3.501295	-5.15411
H	-19.1227	1.279876	-5.50932
C	15.81992	-6.24295	-1.21195
N	15.20091	-7.21595	-1.20134
C	18.63801	-6.36084	-1.55386
N	19.16204	-7.38053	-1.68134

Table S12: Cartesian coordinates of **TNPD6**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	0.591239	-1.62557	0.606787
C	1.964408	-1.6977	0.499497
C	2.684793	-0.512	0.630255
C	2.041312	0.716573	0.86947
C	0.670257	0.783045	1.011207
C	-0.05027	-0.40181	0.878048
H	2.468057	-2.63792	0.287357
H	0.164658	1.727939	1.196114
C	4.094283	-0.22476	0.52229
C	4.343799	1.117199	0.636596
C	5.704772	1.467538	0.477644
C	6.479893	0.341894	0.257156
S	5.520985	-1.13585	0.244659
C	-3.87598	-1.20642	0.919925
C	-3.10584	-2.32251	0.650532
C	-1.72854	-1.99251	0.642272
C	-1.46664	-0.67393	0.900505

S	-2.899	0.240824	1.144603
C	-5.30947	-1.05823	1.032389
C	-6.00593	-0.22309	1.870623
S	-6.41063	-1.90642	-0.02353
C	-7.4003	-0.27694	1.694092
H	-5.51578	0.389723	2.619292
C	-7.80204	-1.1529	0.714455
H	-8.10382	0.290087	2.293851
C	7.90118	0.211234	0.049817
C	8.557473	-0.7496	-0.68819
S	9.047685	1.252141	0.844877
C	9.952076	-0.64349	-0.63523
H	8.032171	-1.50275	-1.26456
C	10.40538	0.398375	0.146365
H	10.62088	-1.31342	-1.16415
C	-0.43114	-2.74503	0.386029
C	3.046545	1.874552	0.877512
C	-9.14917	-1.42337	0.269438
C	-9.69726	-2.54494	-0.31442
S	-10.3553	-0.17561	0.480634
C	-11.0792	-2.38613	-0.57848
C	-11.5996	-1.17464	-0.2122
H	-11.6732	-3.16273	-1.05073
C	11.77	0.799706	0.349317
C	12.30856	1.676172	1.290255
S	12.98951	0.118513	-0.68865
C	13.69363	1.761671	1.161414
C	14.25308	0.988096	0.151812
H	14.31038	2.380384	1.807224
C	-8.96083	-3.80397	-0.64137
H	-8.37754	-3.70823	-1.56479
H	-8.26463	-4.08852	0.153565
H	-9.66388	-4.62859	-0.785
C	11.5445	2.42689	2.330677
H	10.89869	3.194819	1.890517
H	10.90691	1.765323	2.926632
H	12.2329	2.930345	3.013346
C	-3.64391	-3.70131	0.448124
H	-4.62767	-3.82133	0.908308
H	-3.73962	-3.94464	-0.61695
H	-2.9728	-4.44405	0.890368
C	6.215243	2.870841	0.47846
H	6.412644	3.230789	1.495355

H	7.140215	2.965486	-0.0956
H	5.476248	3.544227	0.03429
C	-0.4405	-3.20273	-1.07847
C	-0.94383	-4.44552	-1.4448
C	-0.02829	-2.31595	-2.0764
C	-1.02094	-4.79634	-2.78961
H	-1.26941	-5.14979	-0.6862
C	-0.10332	-2.67318	-3.41743
H	0.35551	-1.34168	-1.79633
C	-0.60386	-3.92495	-3.77632
H	-1.41027	-5.77112	-3.06747
H	-0.64947	-4.18667	-4.82858
C	-0.14791	-3.85429	1.393118
C	0.818009	-4.83134	1.13091
C	-0.76791	-3.84254	2.632431
C	1.131708	-5.76911	2.098187
H	1.313602	-4.86387	0.165582
C	-0.45026	-4.79087	3.606142
H	-1.51494	-3.09283	2.879714
C	0.505796	-5.76553	3.340195
H	1.879666	-6.52748	1.887272
C	2.653035	2.780991	-0.28913
C	1.700583	3.791374	-0.12516
C	3.129968	2.512233	-1.56289
C	1.257939	4.507727	-1.22298
H	1.307766	4.017263	0.861204
C	2.672868	3.228608	-2.66968
H	3.860129	1.725753	-1.73568
C	1.732502	4.239963	-2.50237
H	0.521091	5.293815	-1.08814
H	1.365645	4.814893	-3.34429
C	3.131683	2.574822	2.23422
C	3.609306	3.883553	2.349688
C	2.82912	1.87264	3.391144
C	3.763473	4.457165	3.599501
H	3.851052	4.458387	1.462202
C	2.987792	2.451693	4.650368
H	2.462033	0.850972	3.350226
C	3.456256	3.757027	4.760453
H	4.129511	5.476368	3.679349
O	0.291905	-1.87489	-4.43615
O	3.199052	2.857887	-3.85968
C	0.833521	-0.60978	-4.12136

H	0.103932	0.0254	-3.60353
H	1.734265	-0.69924	-3.50024
C	2.759464	3.533464	-5.0179
H	3.291488	3.085331	-5.8565
H	1.679932	3.409533	-5.16984
C	15.65035	0.992136	-0.06628
C	16.47847	0.361147	-0.95181
H	16.1366	1.655435	0.645442
C	17.3097	-0.97489	-2.71003
C	17.66702	-1.80818	-3.78269
C	19.01936	-1.78706	-3.97351
C	18.37066	-0.34124	-2.10785
C	17.93059	0.500958	-1.01006
C	16.06891	-0.57612	-2.02565
C	18.78148	1.247283	-0.22807
O	14.9443	-0.94206	-2.2941
C	18.37351	2.071939	0.851377
N	18.07157	2.751726	1.736174
C	20.17973	1.229454	-0.46993
N	21.31778	1.210733	-0.67205
H	1.100847	-0.14454	-5.06981
H	2.995536	4.603793	-4.97413
H	0.767555	-6.51552	4.077061
O	-1.12713	-4.67713	4.771347
C	-0.84729	-5.60745	5.794232
H	-1.48789	-5.34301	6.634926
H	-1.07474	-6.63317	5.478594
H	0.201494	-5.55358	6.111352
H	3.58295	4.232127	5.725976
O	2.656839	1.664037	5.698937
C	2.794253	2.196844	6.997763
H	2.154706	3.076422	7.141995
H	2.482127	1.412864	7.686994
H	3.834674	2.470177	7.213017
S	19.86053	-0.76264	-2.85946
C	-12.9724	-0.70122	-0.33376
C	-14.0342	-1.61077	-0.39951
C	-13.2834	0.660819	-0.39217
C	-15.3417	-1.18374	-0.52387
H	-13.833	-2.67488	-0.31583
C	-14.5883	1.095998	-0.52188
H	-12.4853	1.39804	-0.36459
C	-15.6408	0.180082	-0.59427

H	-16.1465	-1.91157	-0.55016
H	-14.8018	2.159401	-0.58057
N	-16.9646	0.640187	-0.70404
C	-17.3385	1.807111	0.022874
C	-17.7222	2.982764	-0.67994
C	-17.3168	1.792309	1.39464
C	-18.1232	4.121957	0.073674
C	-17.6937	2.929413	2.132322
H	-17.01	0.882948	1.904348
C	-18.101	4.064619	1.486409
H	-17.6727	2.892872	3.216698
H	-18.4057	4.943716	2.047936
C	-17.9566	-0.07325	-1.40725
C	-17.643	-0.76429	-2.5816
C	-19.281	-0.05841	-0.96707
C	-18.6295	-1.44094	-3.27911
H	-16.6209	-0.76091	-2.9482
C	-20.2639	-0.72697	-1.68187
H	-19.5374	0.480555	-0.06005
C	-19.9471	-1.4275	-2.83687
H	-18.3665	-1.97183	-4.18915
H	-21.2885	-0.70413	-1.32311
H	-20.7179	-1.95338	-3.39045
C	-17.6922	3.07212	-2.09112
C	-18.5125	5.294719	-0.61471
H	-17.3607	2.213134	-2.66676
H	-18.8247	6.157747	-0.0323
C	-18.489	5.346783	-1.98137
C	-18.0655	4.226654	-2.72493
H	-18.7878	6.253236	-2.49832
H	-18.033	4.28394	-3.80841
H	16.97512	-2.38877	-4.37915
H	19.59672	-2.32083	-4.7164

Table S13: Natural bond orbitals (NBOs) analysis of **TNPR**

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C38-C39	π	C112-C113	π*	31.17	0.31	0.088
C44-C45	π	C109-C110	π*	31.13	0.31	0.088
C109C110	π	C135-C139	π*	26.97	0.3	0.081
C78-C80	π	C74-C76	π*	25.23	0.31	0.079
C41-C42	π	C44-C45	π*	24.78	0.29	0.078
C66-C70	π	C65-C68	π*	24.04	0.29	0.077

C73-C75	π	C78-C80	π*	23.91	0.3	0.077
C112-C113	π	C137-O142	π*	23.72	0.31	0.078
C117-C118	π	C119-C120	π*	22.29	0.3	0.073
C127-C128	π	C125-C126	π*	21.92	0.3	0.073
C119-C120	π	C117-C118	π*	20.85	0.3	0.072
C26-C27	π	C29-C31	π*	19.61	0.3	0.072
C119-C120	π	C135-C139	π*	18.59	0.29	0.066
C74-C76	π	C78-C80	π*	17.57	0.29	0.065
C136-O141	π	C115-C116	π*	4.09	0.44	0.041
C82-C84	π	C4-C5	π*	1.16	0.31	0.017
C16-C17	π	C63-C64	π*	0.79	0.33	0.015
C109-H111	σ	S43-C45	σ*	10.29	0.73	0.077
C140-C149	σ	C149-N150	σ*	8.17	1.61	0.103
C143-N144	σ	C139-C143	σ*	7.99	1.57	0.101
C109-H111	σ	C110-C136	σ*	6.82	0.99	0.074
C11-C12	σ	C12-C26	σ*	6.27	1.25	0.079
C29-C31	σ	C31-C41	σ*	5.98	1.27	0.078
C44-H46	σ	S43-C45	σ*	5.18	0.74	0.055
C76-C80	σ	C78-O154	σ*	4.98	1.09	0.066
C70-H72	σ	C64-C66	σ*	3.98	1.11	0.059
C115-C120	σ	C136-O141	σ*	2.94	1.29	0.055
C92-C94	σ	C94-H98	σ*	1.99	1.12	0.042
C29-H32	σ	C29-C31	σ*	1.69	1.11	0.039
C125C126	σ	C125-H131	σ*	1.66	1.15	0.039
C95-C99	σ	C99-H159	σ*	1.57	1.13	0.038
C103-H105	σ	C68-O101	σ*	0.52	0.91	0.020
C59-H60	σ	C10-C11	σ*	0.50	1.07	0.021
O154	LP(2)	C78-C80	π*	33.27	0.36	0.104
O102	LP(2)	C87-C89	π*	33.13	0.36	0.104
S37	LP(2)	C35-C36	π*	26.52	0.27	0.076
S18	LP(2)	C14-C15	π*	21.11	0.29	0.07
O141	LP(2)	C115-C136	σ*	20.82	0.76	0.114
N148	LP(1)	C140-C147	σ*	12.64	1.04	0.103
S28	LP(1)	C51-H54	σ*	0.51	1.06	0.021

LP = lone pair, (i) donor; (j) acceptor; $E(2)$ means energy of hyper conjugative interaction (stabilization energy), Unit in *kcal/mol*; $E(j) - E(i)$ is the energy difference between donor and acceptor i and j NBO orbitals; $F(i, j)$ is the Fock matrix element between i and j NBO orbitals

Table S14: Natural bond orbitals analysis for **TNPD1** with its representative values

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i,j*) [*a.u*]**
C44-C45	π	C109-C110	π*	30.87	0.31	0.088
C5-C6	π	C3-C4	π*	25.63	0.3	0.079
C63-C64	π	C66-C70	π*	24.63	0.3	0.077
C150-C152	π	C145-C147	π*	23.95	0.3	0.077

C1-C2	π	C3-C4	π*	22.05	0.3	0.075
C112-C115	π	C116-C118	π*	21.56	0.32	0.075
C5-C6	π	C1-C2	π*	20.68	0.3	0.072
C9-C10	π	C3-C4	π*	14.09	0.32	0.063
C38-C39	π	C145-C147	π*	12.03	0.32	0.058
C14-C15	π	C19-C20	π*	10.74	0.31	0.053
C116-C118	π	C109-C110	π*	7.79	0.34	0.046
C117-O119	π	C112-C115	π*	4.86	0.42	0.044
C117-O119	π	C109-C110	π*	3.62	0.43	0.038
C63-C64	π	C16-C17	π*	1.32	0.29	0.018
C73-C75	π	C1-C2	π*	0.84	0.3	0.014
C122-N123	π	C120-N121	π*	0.64	0.47	0.015
C120-N121	π	C122-N123	π*	0.63	0.47	0.015
C109-H111	σ	S43-C45	σ*	10.01	0.73	0.076
C144-C184	σ	C184-N185	σ*	8.88	1.61	0.107
C3-C4	σ	C9-S13	σ*	7.39	0.91	0.073
C14-C15	σ	C16-C33	σ*	6.69	1.14	0.078
C14-C19	σ	C14-C15	σ*	6.55	1.31	0.083
C29-C31	σ	C31-C41	σ*	5.98	1.27	0.078
C27-H30	σ	C26-S28	σ*	5.68	0.74	0.058
C65-C68	σ	C68-C70	σ*	5.29	1.29	0.074
C139-H141	σ	C113-C114	σ*	4.99	1.06	0.065
C55-H56	σ	C15-C16	σ*	4.46	1.07	0.062
C74-H77	σ	C76-C80	σ*	3.99	1.11	0.059
C44-H46	σ	C41-C42	σ*	3.38	1.1	0.055
C51-H53	σ	C42-C44	σ*	2.44	1.08	0.046
C12-C26	σ	C10-C11	σ*	2.05	1.3	0.046
C115-S142	σ	C110-C116	σ*	1.44	1.2	0.037
C97-O133	σ	C95-C99	σ*	1.03	1.52	0.035
C150-H154	σ	C152-N155	σ*	0.93	0.95	0.027
C12-S13	σ	C10-C34	σ*	0.57	1.07	0.022
C4-C34	σ	C82-C84	σ*	0.52	1.21	0.022
C120-N121	σ	C116-C118	σ*	0.5	1.65	0.026
O127	LP(2)	C78-C80	π*	33.18	0.36	0.104
S43	LP(2)	C41-C42	π*	26.06	0.27	0.076
N155	LP(1)	C156-C158	π*	5.27	0.3	0.036
O119	LP(2)	C112-C117	σ*	21.58	0.75	0.116
O102	LP(1)	C87-C89	σ*	7.36	1.14	0.082
S43	LP(1)	C45-C109	σ*	0.55	1.21	0.023

LP = lone pair, (i) donor; (j) acceptor; $E^{(2)}$ means energy of hyper conjugative interaction (stabilization energy), Unit in *kcal/mol*; E(j) – E(i) is the energy difference between donor and acceptor i and j NBO orbitals; F(i, j) is the Fock matrix element between i and j NBO orbitals

Table S15: Natural bond orbitals analysis for **TNPD2** with its representative values

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2)**	***E*(*j*)-*E*(*i*)**	***F*(*i*,*j*)**

				[*kcal/mol*]	[*a.u*]	[*a.u*]
C44-C45	π	C109-C110	π*	30.53	0.31	0.087
C113-C139	π	C143-C144	π*	26.26	0.25	0.074
C78-C80	π	C74-C76	π*	25.35	0.31	0.079
C63-C64	π	C66-C70	π*	24.64	0.3	0.077
C152-C154	π	C147-C149	π*	23.93	0.3	0.076
C147-C149	π	C148-C150	π*	21.97	0.3	0.073
C112-C115	π	C117-O119	π*	20.84	0.33	0.075
C3-C4	π	C1-C2	π*	19.89	0.3	0.07
C179-C182	π	C178-C183	π*	18.75	0.31	0.069
C63-C64	π	C65-C68	π*	17.98	0.29	0.066
C11-C12	π	C26-C27	π*	13.22	0.3	0.059
C14-C15	π	C19-C20	π*	10.41	0.31	0.053
C117-O119	π	C112-C115	π*	4.84	0.42	0.044
C117-O119	π	C109-C110	π*	3.63	0.43	0.038
C1-C2	π	C73-C75	π*	0.88	0.31	0.015
C167-C169	π	C158-C160	π*	0.66	0.3	0.013
C120-N121	π	C122-N123	π*	0.63	0.47	0.015
C109-H111	σ	S43-C45	σ*	9.97	0.73	0.076
C118-C120	σ	C120-N121	σ*	8.34	1.62	0.104
C109-H111	σ	C110-C117	σ*	7.19	0.97	0.075
C36-C38	σ	C24-C35	σ*	6.07	1.21	0.077
C41-S43	σ	S28-C31	σ*	5.87	0.87	0.064
C47-H50	σ	C35-C36	σ*	5.41	1.1	0.069
C95-C99	σ	C97-O133	σ*	4.98	1.09	0.066
C59-H61	σ	C10-C11	σ*	4.44	1.07	0.062
C70-H72	σ	C64-C66	σ*	3.98	1.11	0.059
C115-S142	σ	C114-C138	σ*	3.66	1.28	0.061
C112-C115	σ	C117-O119	σ*	2.95	1.33	0.056
C182-C183	σ	C178-H180	σ*	2.84	1.12	0.05
C14-C15	σ	C19-C20	σ*	2.15	1.31	0.048
S43-C45	σ	C109-H111	σ*	1.95	1.07	0.041
N157-C167	σ	C168-C170	σ*	1.38	1.38	0.039
C34-C82	σ	C3-C4	σ*	1.07	1.19	0.032
C1-C2	σ	C16-C33	σ*	0.81	1.14	0.027
C1-C33	σ	C73-C75	σ*	0.58	1.21	0.024
C10-C34	σ	C92-C94	σ*	0.52	1.22	0.023
C120-N121	σ	C116-C118	σ*	0.5	1.65	0.026
O127	LP(2)	C78-C80	π*	33.17	0.36	0.078
S28	LP(2)	C29-C31	π*	23.35	0.28	0.104
N157	LP(1)	C158-C160	π*	5.52	0.3	0.082
O119	LP(2)	C112-C117	σ*	21.51	0.76	0.115
O101	LP(2)	C103-H105	σ*	5.76	0.69	0.058
Cl145	LP(2)	C114-C138	σ*	0.53	0.9	0.02

LP = lone pair, (i) donor; (j) acceptor; $E(2)$ means energy of hyper conjugative interaction (stabilization energy), Unit in *kcal/mol*; $E(j) - E(i)$ is the energy difference between donor and acceptor i and j NBO orbitals; $F(i, j)$ is the Fock matrix element between i and j NBO orbitals

Table S16: Natural bond orbitals analysis for **TNPD3** with its representative values

Donor(*i*)	Type	Acceptor(*j*)	Type	*E*(2) [*kcal/mol*]	*E*(*j*)-*E*(*i*) [*a.u*]	*F*(*i,j*) [*a.u*]
C44-C45	π	C109-C110	π*	31.36	0.31	0.088
C109-C110	π	C116-C118	π*	26.83	0.29	0.080
C5-C6	π	C3-C 4	π*	25.61	0.30	0.078
C87-C89	π	C83-C85	π*	25.21	0.31	0.079
C41-C42	π	C44-C45	π*	24.70	0.29	0.078
C66-C70	π	C65-C68	π*	23.98	0.3	0.077
C166-C168	π	C165-C167	π*	22.92	0.29	0.075
C146-C148	π	C150-C152	π*	21.99	0.30	0.074
C170-C172	π	C165-C167	π*	20.63	0.29	0.070
C3-C4	π	C1-C2	π*	19.83	0.30	0.070
C113-C114	π	C139-C144	π*	18.75	0.31	0.070
C156-C158	π	C160-C162	π*	17.97	0.32	0.068
C109-C110	π	C44-C45	π*	11.13	0.30	0.054
C116-C118	π	C112-C115	π*	9.36	0.32	0.050
C117-O119	π	C112-C115	π*	4.83	0.42	0.044
C122-N123	π	C120-N121	π*	0.64	0.47	0.015
C65-C68	π	C65-C68	π*	0.62	0.30	0.012
C109-H111	σ	S43-C45	σ*	10.06	0.73	0.077
C118-C120	σ	C120-N121	σ*	8.35	1.62	0.104
C109-H111	σ	C110-C117	σ*	7.18	0.97	0.075
C24-C35	σ	C35-C36	σ*	6.88	1.32	0.085
C31-C41	σ	C41-C42	σ*	6.00	1.31	0.079
C19-C20	σ	C14-C19	σ*	5.96	1.26	0.077
C29-H32	σ	S28-C31	σ*	5.67	0.74	0.058
C41-S43	σ	C42-C51	σ*	5.31	1.11	0.069
C139-H141	σ	C143-C144	σ*	5.28	1.06	0.067
C39-C145	σ	C38-C39	σ*	4.99	1.30	0.072
C55-H56	σ	C15-C16	σ*	4.47	1.07	0.062
C70-H72	σ	C64-C66	σ*	3.98	1.11	0.059
C114-S142	σ	C113-C139	σ*	3.94	1.25	0.063
C181-H183	σ	C177-C180	σ*	3.61	1.14	0.057
C19-C20	σ	C14-C15	σ*	2.99	1.32	0.056
C73-C75	σ	C75-H79	σ*	2.02	1.12	0.043
C65-C68	σ	C70-H72	σ*	1.98	1.14	0.042
C120-N121	σ	C116-C118	σ*	0.50	1.65	0.026
O127	LP(2)	C78-C80	π*	33.20	0.36	0.104
S142	LP(2)	C112-C115	π*	27.02	0.28	0.078
S13	LP(2)	C9-C10	π*	26.52	0.29	0.078
F187	LP(2)	C139-C144	π*	0.51	0.48	0.015

O119	LP(2)	C112-C117	σ*	21.74	0.75	0.116
O101	LP(1)	C65-C68	σ*	7.46	1.15	0.083
F186	LP(2)	C113-C139	σ*	0.50	1.02	0.020

LP = lone pair, (i) donor; (j) acceptor; $E(2)$ means energy of hyper conjugative interaction (stabilization energy), Unit in *kcal/mol*; $E(j) - E(i)$ is the energy difference between donor and acceptor i and j NBO orbitals; $F(i, j)$ is the Fock matrix element between i and j NBO orbitals

Table S17: Natural bond orbitals analysis for **TNPD4** with its representative values

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C44-C45	π	C109-C110	π*	31.01	0.31	0.088
C143-C144	π	N184-O186	π*	30.58	0.15	0.065
C109-C110	π	C116-C118	π*	26.48	0.30	0.080
C143-C144	π	C113-C139	π*	25.78	0.31	0.079
C83-C85	π	C82-C84	π*	24.75	0.30	0.078
C165-C167	π	C170-C172	π*	23.80	0.30	0.076
C113-C139	π	C114-C138	π*	22.99	0.28	0.072
C145-C147	π	C150-C152	π*	21.83	0.29	0.071
C5-C6	π	C1-C2	π*	20.68	0.30	0.072
C3-C4	π	C1-C2	π*	19.87	0.30	0.070
C66-C70	π	C63-C64	π*	18.34	0.30	0.068
C156-C158	π	C160-C162	π*	17.98	0.32	0.068
C11-C12	π	C9-C10	π*	16.71	0.32	0.068
C35-C36	π	C38-C 39	π*	15.67	0.31	0.065
C22-C24	π	C35-C36	π*	11.78	0.32	0.058
C92-C94	π	C9-C10	π*	1.37	0.29	0.018
C120-N121	π	C122-N123	π*	0.63	0.47	0.015
C109-H111	σ	S43-C45	σ*	10.01	0.73	0.076
C118-C120	σ	C120-N121	σ*	8.34	1.62	0.104
C3-C4	σ	C9-S13	σ*	7.39	0.91	0.073
C1-C6	σ	C17-S18	σ*	7.36	0.91	0.073
C109-H111	σ	C110-C117	σ*	7.18	0.97	0.075
C11-C12	σ	C10-C34	σ*	6.64	1.15	0.078
C158-H161	σ	C156-C157	σ*	5.84	1.08	0.071
C39-C145	σ	C38-C39	σ*	4.99	1.30	0.072
C139-C144	σ	C113-C139	σ*	3.89	1.31	0.064
C94-C97	σ	O133-C134	σ*	3.64	1.01	0.054
C22-C24	σ	C20-C22	σ*	3.63	1.29	0.061
C181-H183	σ	C177-C180	σ*	3.61	1.14	0.057
C170-C172	σ	C167-C170	σ*	3.47	1.30	0.060
C4-C34	σ	C4-C5	σ*	2.99	1.21	0.054
C148-C152	σ	N155-C156	σ*	2.92	1.12	0.051
C165-C166	σ	N155-C165	σ*	2.01	1.14	0.043
C112-C117	σ	C117-O119	σ*	1.99	1.26	0.045

C120-N121	σ	C116-C118	σ*	0.50	1.65	0.026
O127	LP(2)	C78-C80	π*	33.17	0.36	0.104
O102	LP(2)	C87-C89	π*	32.36	0.36	0.103
N155	LP(1)	C156-C158	π*	5.24	0.30	0.036
O119	LP(2)	C112-C117	σ*	21.69	0.75	0.116
O186	LP(2)	N184-O185	σ*	20.60	0.76	0.113
S43	LP(1)	C45-C109	σ*	0.55	1.21	0.023

LP = lone pair, (i) donor; (j) acceptor; *E*(2) means energy of hyper conjugative interaction (stabilization energy), Unit in *kcal/mol*; *E*(j) – *E*(i) is the energy difference between donor and acceptor i and j NBO orbitals; *F*(i, j) is the Fock matrix element between i and j NBO orbitals

Table S18: Natural bond orbitals analysis for **TNPD5** with its representative values

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i,j*) [*a.u*]**
C44-C45	π	C109-C110	π*	32.04	0.31	0.089
C109-C110	π	C116-C118	π*	27.30	0.29	0.081
C5-C6	π	C3-C4	π*	25.70	0.30	0.079
C83-C85	π	C82-C84	π*	24.71	0.30	0.078
C150-C152	π	C145-C147	π*	23.96	0.30	0.077
C113-C114	π	C138-C143	π*	22.77	0.30	0.075
C145-C147	π	C146-C148	π*	21.98	0.30	0.073
C170-C172	π	C165-C167	π*	20.56	0.29	0.070
C3-C4	π	C1-C2	π*	19.88	0.30	0.070
C177-C180	π	C176-C181	π*	18.75	0.31	0.069
C156-C158	π	C160-C162	π*	17.99	0.32	0.068
C44-C45	π	C41-C42	π*	17.05	0.30	0.065
C29-C31	π	C26-C27	π*	16.97	0.31	0.067
C41-C42	π	C29-C31	π*	15.34	0.30	0.061
C35-C36	π	C22-C24	π*	14.45	0.31	0.062
C117-O119	π	C112-C115	π*	4.84	0.41	0.043
C117-O119	π	C109-C110	π*	3.58	0.43	0.038
C122-N123	π	C120-N121	π*	0.63	0.47	0.015
C109-H111	σ	S43-C45	σ*	10.08	0.73	0.077
C143-C186	σ	C186-N187	σ*	8.96	1.62	0.108
C118-C122	σ	C122-N123	σ*	8.13	1.61	0.103
C3-C4	σ	C9-S13	σ*	7.40	0.91	0.073
C118-C120	σ	C116-C118	σ*	6.21	1.34	0.081
C19-C20	σ	C14-C19	σ*	5.99	1.26	0.078
C39-C145	σ	C38-C39	σ*	4.98	1.30	0.072
C10-C11	σ	C9-C10	σ*	4.89	1.27	0.071
C180-H182	σ	C159-C177	σ*	4.64	1.08	0.063
C15-C55	σ	C14-S18	σ*	3.99	0.85	0.052
C143-C144	σ	C184-N185	σ*	3.76	1.60	0.070
C165-C166	σ	N155-C156	σ*	3.16	1.12	0.053
C180-C181	σ	C177-H179	σ*	2.88	1.11	0.051
C82-C84	σ	C83-H86	σ*	2.64	1.13	0.049

C166-C168	σ	C172-H175	σ*	2.40	1.14	0.047
C2-C3	σ	C4-C34	σ*	2.37	1.11	0.046
C78-O127	σ	C78-C80	σ*	1.21	1.51	0.038
C120-N121	σ	C116-C118	σ*	0.50	1.64	0.026
O127	LP(2)	C78-C80	π*	33.18	0.36	0.104
S142	LP(2)	C112-C115	π*	26.91	0.28	0.078
N155	LP(1)	C156-C158	π*	5.38	0.30	0.036
O119	LP(2)	C112-C117	*σ**	21.74	0.75	0.116
O119	LP(2)	C112-C117	σ*	21.85	0.75	0.116
N121	LP(1)	C118-C120	σ*	12.64	1.04	0.103
S43	LP(1)	C45-C109	σ*	0.55	1.21	0.023

LP = lone pair, (i) donor; (j) acceptor*; E*(2) means energy of hyper conjugative interaction (stabilization energy), Unit in *kcal/mol*; *E*(j) – *E*(i) is the energy difference between donor and acceptor i and j NBO orbitals; *F*(i, j) is the Fock matrix element between i and j NBO orbitals

Table S19: Natural bond orbitals analysis for **TNPD6** with its representative values

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i,j*) [*a.u*]**
C44-C45	π	C109–C110	π*	29.78	0.31	0.087
C5-C6	π	C3-C4	π*	25.53	0.30	0.078
C83-C85	π	C82-C84	π*	24.59	0.30	0.078
C66-C70	π	C65-C68	π*	23.99	0.30	0.077
C160-C162	π	C159-C161	π*	22.92	0.29	0.075
C140-C142	π	C144-C146	π*	21.98	0.30	0.074
C5-C6	π	C1-C2	π*	20.81	0.30	0.072
C112-C115	π	C117-O119	π*	19.88	0.32	0.073
C171-C174	π	C170-C 75	π*	18.75	0.31	0.069
C150-C152	π	C154-C156	π*	17.96	0.32	0.068
C29-C31	π	C26-C27	π*	16.96	0.31	0.067
C35-C36	π	C38-C39	π*	15.68	0.31	0.065
C5-C6	π	C16-C17	π*	14.55	0.30	0.059
C117-O119	π	C112-C115	π*	4.65	0.42	0.044
C1-C2	π	C73-C75	π*	1.06	0.31	0.016
C122-N123	π	C120-N121	π*	0.62	0.47	0.015
C109-H111	σ	S43-C45	σ*	9.94	0.73	0.076
C118-C120	σ	C120-N	σ*	8.33	1.62	0.104
C3-C4	σ	C9-S13	σ*	7.4	0.90	0.073
C24-C35	σ	C35-C36	σ*	6.87	1.32	0.085
C19-C20	σ	C14-C9	σ*	5.97	1.26	0.077
C44-H46	σ	S43-C45	σ*	5.23	0.74	0.056
C39-C139	σ	C38-C39	σ*	4.99	1.30	0.072
C166-H169	σ	C161-C164	σ*	3.99	1.11	0.060
C44-H46	σ	C41-C42	σ*	3.33	1.11	0.054
C35-C36	σ	C38-H40	σ*	2.99	1.14	0.052
C1-C33	σ	C16-C33	σ*	1.99	1.03	0.040

C146-N149	σ	C159-C161	σ*	1.90	1.37	0.046
C36-C38	σ	C47-H49	σ*	0.61	1.07	0.023
C120-N121	σ	C116-C118	σ*	0.50	1.64	0.026
O127	LP(2)	C78-C80	π*	33.19	0.36	0.104
S138	LP(2)	C112-C115	π*	27.31	0.28	0.078
N149	LP(1)	C159-C161	π*	25.84	0.30	0.081
N149	LP(1)	C 150-C152	π*	5.07	0.30	0.035
O119	LP(2)	C112-C117	σ*	21.56	0.76	0.116
N123	LP(1)	C118-C122	σ*	12.59	1.04	0.102
S43	LP(1)	C45-C109	σ*	0.55	1.21	0.023

LP = lone pair, (i) donor; (j) acceptor; $E(2)$ means energy of hyper conjugative interaction (stabilization energy), Unit in *kcal/mol*; $E(j) - E(i)$ is the energy difference between donor and acceptor i and j NBO orbitals; $F(i, j)$ is the Fock matrix element between i and j NBO orbitals

Table S20: Calculated energies (E) and energy gap (ΔE) of HOMO-1, LUMO+1, HOMO-2 and LUMO+2 for **TNPR**, **TNPD1-TNPD6**.

Compounds	E_{HOMO-1}	E_{LUMO+1}	ΔE	E_{HOMO-2}	E_{LUMO+2}	ΔE
TNPR	-5.988	-3.26	2.728	-6.483	-2.611	3.872
TNPD1	-5.621	-2.815	2.806	-6.004	-2.047	3.957
TNPD2	-5.621	-2.787	2.834	-6.003	-2.043	3.96
TNPD3	-5.634	-3.501	2.133	-6.02	-2.05	3.97
TNPD4	-5.627	-2.870	2.757	-6.004	-2.591	3.413
TNPD5	-5.639	-2.92	2.719	-6.03	-2.273	3.757
TNPD6	-5.616	-2.645	2.971	-5.997	-2.016	3.981

Table S21: Wavelength, excitation energy and oscillator strength of **TNPR** in gas phase

NO	λ_{DFT}	E (eV)	f_{os}	**MO contributions**
1	671.128	1.847	2.637	H→L (86%), H-1→L+1 (5%), H→L+1 (5%)
2	621.693	1.994	0.029	H→L+1 (91%), H-1→L (2%), H→L (5%)
3	518.090	2.393	0.217	H-1→L (89%), H→L (3%)
4	507.466	2.443	0.949	H-1→L+1 (73%), H→L (5%), H→L+1 (2%), H→L+2 (6%), H→L+4 (4%)
5	485.831	2.552	0.077	H-1→L+1 (10%), H→L+2 (70%), H-1→L+3 (8%), H→L+3 (5%)
6	478.205	2.593	0.002	H-1→L+2 (10%), H→L+3 (79%), H→L+2 (6%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S22: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD1**) in gas phase

NO	**DFT** λ **(*nm*)**	E(eV)	f_{OS}	**MO contributions**
1	807.241	1.536	0.387	H→L (93%), H-1→L (5%)
2	666.045	1.862	0.430	H-1→L (82%), H-2→L (9%), H→L (7%)
3	601.165	2.062	0.658	H-1→L+1 (11%), H→L+1 (83%), H-2→L+1 (2%)

4	561.243	2.209	0.239	H-2→L (74%), H-1→L (12%), H-4→L (7%)
5	518.459	2.391	0.560	H-2→L+1 (12%), H-1→L+1 (66%), H→L+1 (16%), H→L+2 (2%)
6	479.537	2.586	0.446	H-4→L (27%), H-3→L (36%), H-2→L (13%), H→L+2 (13%), H-9→L (5%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S23: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD2**) in gas phase

NO	DFT λ (*nm*)	*E*(*eV*)	f_{OS}	MO contributions
1	783.668	1.582	0.407	H→L (92%), H-1→L (6%)
2	652.034	1.902	0.464	H-1→L (80%), H-2→L (9%), H→L (8%)
3	587.854	2.109	0.699	H-1→L+1 (12%), H→L+1 (82%), H-2→L+1 (2%)
4	550.527	2.252	0.235	H-2→L (71%), H-1→L (13%), H-4→L (7%), H-3→L (4%)
5	509.468	2.434	0.596	H-2→L+1 (12%), H-1→L+1 (63%), H→L+1 (17%), H→L+2 (3%)
6	474.908	2.611	0.842	H-4→L (17%), H-3→L (22%), H-2→L (14%), H→L+2 (33%), H-9→L (4%), H→L+3 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S24: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD3**) in gas phase

NO	DFT λ (*nm*)	*E*(*eV*)	f_{OS}	MO contributions
1	843.602	1.470	0.339	H→L (94%), H-1→L (5%)
2	687.693	1.803	0.384	H-1→L (84%), H-2→L (8%), H→L (6%)
3	608.900	2.036	0.626	H-1→L+1 (10%), H→L+1 (85%), H-2→L+1 (2%)
4	577.772	2.146	0.266	H-2→L (77%), H-1→L (10%), H-4→L (7%)
5	522.831	2.371	0.514	H-2→L+1 (12%), H-1→L+1 (68%), H→L+1 (14%),
6	488.974	2.536	0.281	H-4→L (43%), H-3→L (28%), H-2→L (12%), H-9→L (6%), H→L+2 (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S25: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD4**) in gas phase

NO	λ_{DFT}	*E* (*eV*)	f_{os}	MO contributions
1	816.814	1.518	0.369	H→L (94%), H-1→L (5%)
2	668.523	1.855	0.407	H-1→L (82%), H-2→L (9%), H→L (6%)
3	610.309	2.032	0.594	H→L+1 (85%), H-2→L+1 (2%), H-1→L+1 (9%)
4	566.837	2.187	0.247	H-2→L (74%), H-1→L (13%), H-4→L (7%)
5	523.914	2.367	0.608	H-2→L+1 (12%), H-1→L+1 (63%), H→L+1 (14%), H→L+2 (4%), H→L+3 (3%)
6	501.981	2.470	0.041	H→L+2 (89%), H-1→L+1 (6%), H-1→L+2 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S26: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD5**) in gas phase

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	931.302	1.331	0.264	H→L (96%), H-1→L (3%)
2	742.376	1.670	0.377	H-1→L (88%), H-2→L (6%), H→L (4%)
3	642.372	1.930	0.563	H→L+1 (88%), H-1→L+1 (8%)
4	610.459	2.031	0.246	H-2→L (80%), H-4→L (7%), H-1→L (8%)
5	548.821	2.259	0.564	H-2→L+1 (10%), H-1→L+1 (73%), H→L+1 (11%),
6	517.982	2.394	0.120	H-4→L (18%), H-3→L (67%), H-9→L (2%), H-2→L (8%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S27: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD6**) in gas phase

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	697.442	1.778	0.653	H→L (90%), H-1→L (7%)
2	588.272	2.108	0.600	H-1→L (77%), H→L (10%), H-2→L (9%)
3	542.316	2.286	0.607	H-1→L+1 (12%), H→L+1 (78%), H-2→L+1 (3%), H→L+2 (3%)
4	506.017	2.450	0.410	H-2→L (72%), H-1→L (13%), H-4→L (4%), H-3→L (5%), H→L+2 (2%)
5	474.199	2.615	0.618	H-2→L+1 (11%), H-1→L+1 (51%), H→L+1 (21%), H→L+2 (11%),
6	463.111	2.677	0.910	H-1→L+1 (13%), H→L+2 (67%), H-2→L (6%), H-2→L+1 (2%), H-1→L+3 (3%), H→L+3 (5%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S28: Wavelength, excitation energy and oscillator strength of reference compound (**TNPR**) in chloroform

NO	DFT λ (*nm*)	*E* (*eV*)	f_{os}	MO contributions
1	706.785	1.754	2.960	H→L (86%), H-1→L+1 (8%)
2	658.895	1.882	0.016	H→L+1 (89%), H-1→L (7%)
3	538.757	2.301	0.064	H-1→L (83%), H-2→L+1 (5%), H→L+1 (7%)
4	525.513	2.359	0.921	H-1→L+1 (75%), H→L (10%), H-2→L (5%), H→L+2 (3%), H→L+4 (2%)
5	502.530	2.467	0.166	H-1→L+3 (10%), H→L+2 (77%), H-1→L+1 (6%)
6	493.214	2.514	0.002	H-1→L+2 (12%), H→L+3 (82%),

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S29: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD1**) in chloroform

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	774.127	1.602	0.704	H-1→L (13%), H→L (83%), H-2→L (3%)
2	652.720	1.900	0.382	H-2→L (11%), H-1→L (68%), H→L (17%),

3	583.537	2.125	0.969	H-1→L+1 (19%), H→L+1 (70%), H-2→L+1 (5%), H→L+2 (3%)
4	550.112	2.254	0.165	H-2→L (68%), H-1→L (18%), H-3→L (9%)
5	503.285	2.464	0.242	H-2→L+1 (12%), H-1→L+1 (55%), H→L+1 (27%),
6	478.168	2.593	1.561	H→L+2 (79%), H-1→L+4 (2%), H→L+3 (4%), H→L+4 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S30: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD2**) in chloroform

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	766.754	1.617	0.690	H-1→L (13%), H→L (82%), H-2→L (3%)
2	649.574	1.909	0.395	H-2→L (11%), H-1→L (67%), H→L (18%),
3	576.939	2.149	1.007	H-1→L+1 (20%), H→L+1 (68%), H-2→L+1 (4%), H→L+2 (3%)
4	546.836	2.267	0.170	H-3→L (11%), H-2→L (66%), H-1→L (18%),
5	499.332	2.483	0.243	H-2→L+1 (12%), H-1→L+1 (54%), H→L+1 (28%),
6	479.018	2.588	1.572	H→L+2 (80%), H-1→L+3 (3%), H→L+3 (6%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S31: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD3**) in chloroform

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	799.279	1.551	0.627	H-1→L (11%), H→L (85%), H-2→L (2%)
2	667.910	1.856	0.386	H-2→L (11%), H-1→L (71%), H→L (14%),
3	585.632	2.117	0.953	H-1→L+1 (17%), H→L+1 (72%), H-2→L+1 (5%), H→L+2 (2%)
4	564.463	2.197	0.172	H-2→L (70%), H-1→L (17%), H-3→L (9%)
5	503.755	2.461	0.263	H-2→L+1 (13%), H-1→L+1 (56%), H→L+1 (26%),
6	478.039	2.594	1.035	H-3→L (33%), H-2→L (11%), H→L+2 (39%), H-9→L (4%), H-4→L (3%), H→L+3 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S32: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD4**) in chloroform

NO	DFT λ (*nm*)	*E* (*eV*)	f_{os}	MO contributions
1	780.315	1.589	0.665	H-1→L (11%), H→L (84%), H-2→L (3%)
2	654.236	1.895	0.384	H-2→L (12%), H-1→L (68%), H→L (16%),
3	592.121	2.094	0.868	H-1→L+1 (16%), H→L+1 (72%), H-2→L+1 (4%), H→L+3 (2%)
4	555.186	2.233	0.161	H-2→L (68%), H-1→L (19%), H-3→L (8%)
5	512.925	2.417	0.430	H-2→L+1 (10%), H-1→L+1 (39%), H→L+1 (26%), H→L+2 (15%), H-1→L+2 (4%)
6	498.008	2.490	0.077	H-1→L+1 (20%), H→L+2 (67%), H-2→L+1 (3%), H-1→L+2 (2%), H→L+3 (5%)

Table S33: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD5**) in chloroform

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	852.242	1.455	0.553	H-1→L (10%), H→L (87%),
2	709.413	1.748	0.408	H-1→L (75%), H→L (13%), H-2→L (9%)
3	604.241	2.052	0.966	H-1→L+1 (18%), H→L+1 (73%), H-2→L+1 (4%)
4	586.796	2.113	0.144	H-2→L (73%), H-1→L (14%), H-4→L (2%), H-3→L (8%)
5	521.402	2.378	0.298	H-2→L+1 (11%), H-1→L+1 (58%), H→L+1 (25%),
6	495.145	2.504	0.178	H-3→L (61%), H-2→L (15%), H-9→L (6%), H-4→L (9%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S34: Wavelength, excitation energy and oscillator strength of investigated compound (**TNPD6**) in chloroform

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	694.745	1.785	0.997	H-1→L (14%), H→L (79%), H-2→L (3%)
2	590.204	2.101	0.482	H-2→L (11%), H-1→L (64%), H→L (20%),
3	540.802	2.293	0.786	H-1→L+1 (18%), H→L+1 (67%), H-2→L+1 (5%), H→L+2 (4%)
4	506.948	2.446	0.260	H-3→L (10%), H-2→L (67%), H-1→L (19%),
5	472.645	2.623	1.075	H→L+2 (73%), H-2→L+1 (3%), H-1→L+1 (9%), H-1→L+3 (3%), H→L+3 (5%)
6	470.368	2.636	0.414	H-2→L+1 (11%), H-1→L+1 (45%), H→L+1 (31%), H→L+2 (7%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S35: Percentages of donor, π-spacer and acceptor for HOMOs and LUMOs of **TNPR** and **TNPD1-TNPD6**

Compounds	HOMO			LUMO		
	Acceptor	**Donor**	**π-spacer**	**Acceptor**	**Donor**	**π-spacer**
TNPR	7.6	-----	92.4	62.6	------	37.4
TNPD1	1.1	20.8	78.1	82.0	0.0	18.0
TNPD2	1.0	21.3	77.7	82.5	0.0	17.5
TNPD3	1.0	20.3	78.7	82.9	0.0	17.1
TNPD4	1.1	19.5	79.4	82.7	0.0	17.3
TNPD5	1.0	22.7	76.3	84.0	0.0	16.0
TNPD6	1.0	19.4	79.6	75.4	0.0	24.6

Table S36: Dipole polarizability (*D*) of the studied compounds (**TNPR** and **TNPD1-TNPD6**).

Dipole Moment	**TNPR**	**TNPD1**	**TNPD2**	**TNPD3**	**TNPD4**	**TNPD5**	**TNPD6**
μ_x	0.8570	-7.9798	10.3447	11.3761	-8.2252	-11.7648	-9.4745
μ_y	2.3446	4.0619	-1.9208	-4.9929	4.0918	9.6547	-0.5668

μ_z	0.6720	1.2212	0.7554	0.4143	1.0095	1.5017	-0.4329
μ_{total}	2.5852	9.0370	10.5486	12.4305	9.2421	15.2931	9.5013
Polarizability							
α_{xx}	6.525×10^{-22}	5.628×10^{-22}	$5.638\text{x}10^{-22}$	5.672×10^{-22}	5.653×10^{-22}	5.898×10^{-22}	5.281×10^{-22}
α_{yy}	2.464×10^{-22}	2.897×10^{-22}	$2.967\text{x}10^{-22}$	2.811×10^{-22}	2.873×10^{-22}	2.998×10^{-22}	2.294×10^{-22}
α_{zz}	1.605×10^{-22}	1.948×10^{-22}	$5.859\text{x}10^{-22}$	1.998×10^{-22}	1.930×10^{-22}	1.942×10^{-22}	2.179×10^{-22}
α_{total}	3.532×10^{-22}	3.491×10^{-22}	$3.510\text{x}10^{-22}$	3.494×10^{-22}	3.485×10^{-22}	3.613×10^{-22}	3.251×10^{-22}
2nd Hyper pol.							
γ_X	7.977×10^{-32}	6.057×10^{-32}	5.725×10^{-32}	6.831×10^{-32}	6.216×10^{-32}	9.307×10^{-32}	4.099×10^{-32}
γ_Y	1.620×10^{-34}	4.220×10^{-34}	6.275×10^{-34}	6.512×10^{-34}	4.562×10^{-34}	8.709×10^{-34}	2.990×10^{-34}
γ_Z	2.055×10^{-34}	6.896×10^{-34}	4.780×10^{-34}	4.799×10^{-34}	5.030×10^{-34}	7.766×10^{-34}	2.675×10^{-34}
Average<γ>	8.014×10^{-32}	6.168×10^{-32}	5.835×10^{-32}	6.944×10^{-32}	6.312×10^{-32}	9.472×10^{-32}	4.157×10^{-32}
Magnitude of γ	7.977×10^{-32}	6.058×10^{-32}	5.725×10^{-32}	6.831×10^{-32}	6.216×10^{-32}	9.308×10^{-32}	4.100×10^{-32}

Table S37: Frequency dependent second hyperpolarizability (*esu*) of studied compounds (**TNPR** and **TNPD1-TNPD6**).

Parameters	**Frequency ω**	**TNPR**	**TNPD1**	**TNPD2**	**TNPD3**
$\gamma(-\omega,\omega,0,0)$	0.000	8.014×10^{-32}	6.168×10^{-32}	$5.835\text{x}10^{-32}$	6.944×10^{-32}
	1907.21*nm*	1.084×10^{-31}	9.584×10^{-32}	$8.970\text{x}10^{-32}$	1.148×10^{-31}
$\gamma(-2\omega,\omega,\omega,0)$	0.000	8.014×10^{-32}	6.168×10^{-32}	$5.835\text{x}10^{-32}$	6.944×10^{-32}
	1907.21*nm*	3.716×10^{-31}	-1.689×10^{-28}	$5.788\text{x}10^{-30}$	-1.112×10^{-30}

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TNPD4	**TNPD5**	**TNPD6**
6.312×10^{-32}	9.471×10^{-32}	4.156×10^{-32}
9.937×10^{-32}	1.804×10^{-31}	5.673×10^{-32}
6.312×10^{-32}	9.472×10^{-32}	4.156×10^{-32}
-4.438×10^{-30}	-4.235×10^{-31}	2.270×10^{-31}

Table S38: The computed first hyperpolarizability (β_{tot}) and major contributing tensors (*esu*) of **TNPR** and **TNPD1-TNPD6**.

Polarizability	**TNPR**	**TNPD1**	**TNPD2**	**TNPD3**
$\boldsymbol{\beta_{xxx}}$	-2.968×10^{-30}	-3.421×10^{-27}	$3.243\text{x}10^{-27}$	3.719×10^{-27}
$\boldsymbol{\beta_{xxy}}$	-8.803×10^{-29}	-5.478×10^{-30}	$4.765\text{x}10^{-29}$	1.963×10^{-28}
$\boldsymbol{\beta_{xyy}}$	4.350×10^{-30}	5.916×10^{-29}	$-7.975\text{x}10^{-29}$	-3.971×10^{-29}
$\boldsymbol{\beta_{yyy}}$	3.627×10^{-30}	-5.220×10^{-29}	$1.025\text{x}10^{-28}$	2.843×10^{-29}

β_{xxz}	2.756×10^{-28}	3.248×10^{-28}	$2.434\text{x}10^{-28}$	2.405×10^{-28}
β_{yyz}	-6.078×10^{-30}	-1.173×10^{-29}	$-9.759\text{x}10^{-30}$	-6.791×10^{-31}
β_{xzz}	2.119×10^{-29}	-4.306×10^{-29}	$2.700\text{x}10^{-29}$	2.275×10^{-29}
β_{yzz}	-3.105×10^{-30}	1.686×10^{-30}	$-2.885\text{x}10^{-30}$	2.436×10^{-30}
β_{zzz}	1.552×10^{-30}	3.578×10^{-30}	$4.897\text{x}10^{-31}$	-5.767×10^{-32}
β_{total}	2.858×10^{-28}	3.420×10^{-27}	$3.202\text{x}10^{-27}$	3.717×10^{-27}

Continued…

TNPD4	TNPD5	TNPD6
-3.478×10^{-27}	-4.620×10^{-27}	-2.526×10^{-27}
-5.501×10^{-29}	1.363×10^{-29}	-9.989×10^{-29}
5.923×10^{-29}	2.945×10^{-29}	1.188×10^{-29}
-3.211×10^{-29}	-2.362×10^{-29}	-9.186×10^{-30}
2.544×10^{-28}	3.968×10^{-28}	1.864×10^{-28}
-7.260×10^{-30}	-2.302×10^{-30}	-9.600×10^{-30}
-2.575×10^{-29}	-4.512×10^{-29}	1.134×10^{-30}
5.744×10^{-32}	4.233×10^{-30}	-1.066×10^{-29}
1.650×10^{-30}	2.695×10^{-30}	-1.104×10^{-29}
3.455×10^{-27}	4.653×10^{-27}	2.522×10^{-27}

Table S39: Frequency dependent first hyperpolarizability (*esu*) of studied compounds (**TNPR** and **TNPD1-TNPD6**).

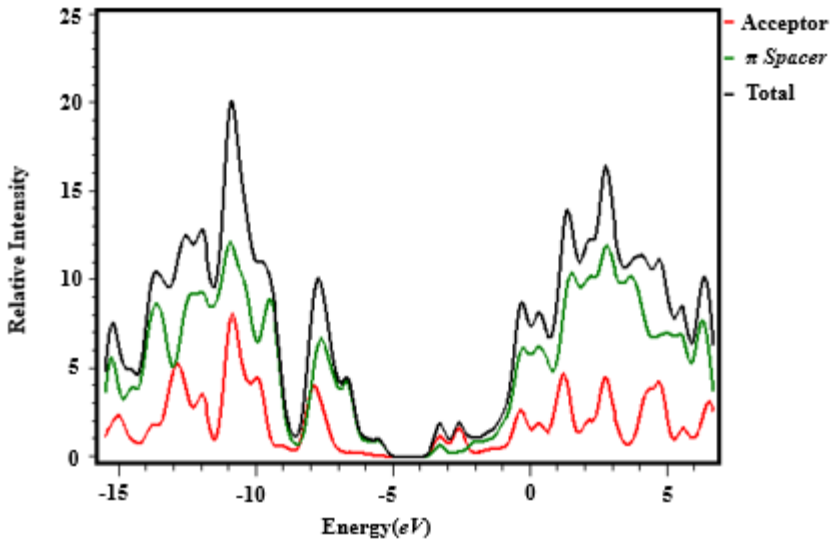
	Parameters	Frequency ω	TNPR	TNPD1	TNPD2	TNPD3
Static	β ($-\omega;\omega,0,$)	0.000	2.858×10^{-28}	3.420×10^{-27}	$3.202\text{x}10^{-27}$	3.717×10^{-27}
	β (-2, $\omega;\omega,\omega$)	0.000	2.858×10^{-28}	3.420×10^{-27}	$3.202\text{x}10^{-27}$	3.717×10^{-27}
Specific	β ($-\omega;\omega,0$)	1907.21*nm*	3.248×10^{-28}	4.315×10^{-27}	$4.039\text{x}10^{-27}$	4.786×10^{-27}
	β ($-2\omega;\omega,\omega$)	1907.21*nm*	6.696×10^{-28}	1.189×10^{-26}	$1.079\ \text{x}10^{-26}$	1.492×10^{-26}

Continued…

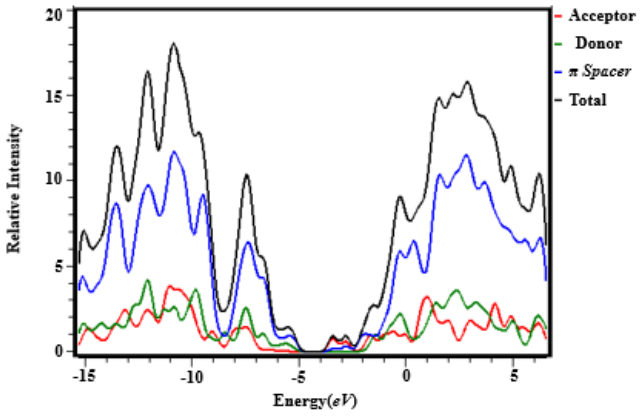
TNPD4	TNPD5	TNPD6
3.455×10^{-27}	4.653×10^{-27}	2.522×10^{-27}
3.455×10^{-27}	4.653×10^{-27}	2.522×10^{-27}
4.382×10^{-27}	6.233×10^{-27}	3.024×10^{-27}
1.238×10^{-26}	2.776×10^{-26}	6.337×10^{-27}

Table S40: IUPAC names of reference and derivative compounds.

TNPR	2,2'-((2*Z*,2'*Z*)-5',5'''-4(4,4,9,9-tetrakis(3-isobutoxyphenyl)-3,8-dimethyl-4,9-dihydro-*s*-indaceno[1,2-*b*:5,6-*b*']dithiophene-2,7-diyl)bis(3-methyl-[2,2'-bithiophene]-5',5-diyl))bis(methanylylidene))bis(3-oxo-2,3-dihydro-1*H*-indene-2,1-diylidene))dimalononitrile
TNPD1	(*Z*)-2-(7-cyano-2-((3-methyl-5'-(4,4,9,9-tetrakis(3-isobutoxyphenyl)-3,8-dimethyl-7-(3'-methyl-5'-(4-naphthalen-1-yl(phenyl)amino)phenyl)-[2,2'-bithiophene]-5-yl)-4,9-dihydro-*s*-indaceno[1,2-*b*:5,6-*b*']dithiophene-2-yl)-[2,2'-bithiophene]-5-yl] methylene)-1-oxo-1*H*-benzo[*b*]cyclopenta[*d*]thiophene-3(2*H*)-ylidene)malonitrile
TNPD2	(*Z*)-2-(6,7-dichloro-2-((3-methyl-5'-(4,4,9,9-tetrakis(3-isobutoxyphenyl)-3,8-dimethyl-7-(3'-methyl-5'-(4-naphthalen-1-yl(phenyl)amino)phenyl)-[2,2'-bithiophene]-5-yl)-4,9-dihydro-*s*-indaceno[1,2-*b*:5,6-*b*']dithiophene-2-yl)-[2,2'-bithiophene]-5-yl] methylene)-1-oxo-1*H*-benzo[*b*]cyclopenta[*d*]thiophen-3(2*H*)-ylidene)malonitrile
TNPD3	(*Z*)-2-(2-((3-methyl-5'-(4,4,9,9-tetrakis(3-isobutoxyphenyl)-3,8-dimethyl-7-(3'-methyl-5'-(4-naphthalen-1-yl(phenyl)amino)phenyl)-[2,2'-bithiophene]-5-yl)-4,9-dihydro-*s*-indaceno[1,2-*b*:5,6-*b*']dithiophene-2-yl) -[2,2'-bithiophene]-5-yl] methylene)-1-oxo-6,7-bis(trifluoromethyl)-1*H*-benzo[*b*]cyclopenta[*d*]thiophen-3(2*H*)-ylidene)malonitrile
TNPD4	(*Z*)-2-(2-((3-methyl-5'-(4,4,9,9-tetrakis(3-isobutoxyphenyl)-3,8-dimethyl-7-(3'-methyl-5'-(4-naphthalen-1-yl(phenyl)amino)phenyl)-[2,2'-bithiophene]-5-yl)-4,9-dihydro-*s*-indaceno[1,2-*b*:5,6-*b*']dithiophene-2-yl)-[2,2'-bithiophen]-5-yl] methylene)-7-nitro-1-oxo-1*H*-benzo[*b*]cyclopenta[*d*]thiophen-3(2*H*)-ylidene)malonitrile
TNPD5	(*Z*)-1-(dicyanomethylene)-2-((3-methyl-5'-(4,4,9,9-tetrakis(3-isobutoxyphenyl)-3,8-dimethyl-7-(3'-methyl-5'-(4-naphthalen-1-yl(phenyl)amino)phenyl)-[2,2'-bithiophene]-5-yl)-4,9-dihydro-*s*-indaceno[1,2-*b*:5,6-*b*']dithiophene-2-yl)-[2,2'-bithiophen]-5-yl] methylene)-3-oxo-2,3-dihydro-1*H*-benzo[*b*]cyclopenta[*d*]thiophene-6,7-dicarbonitrile
TNPD6	(*Z*)-2-(253-methyl-5'-(4,4,9,9-tetrakis(3-isobutoxyphenyl)-3,8-dimethyl-7-(3'-methyl-5'-(4-naphthalen-1-yl(phenyl)amino)phenyl)-[2,2'-bithiophen]-5-yl)-4,9-dihydro-*s*-indaceno[1,2-*b*:5,6-*b*']dithiophen-2-yl)-[2,2'-bithiophen]-5-yl] methylene)-6-oxo-5,6-dihydro-4*H*-cyclopenta[*b*]thiophen-4-ylidene)malonitrile



TNPR



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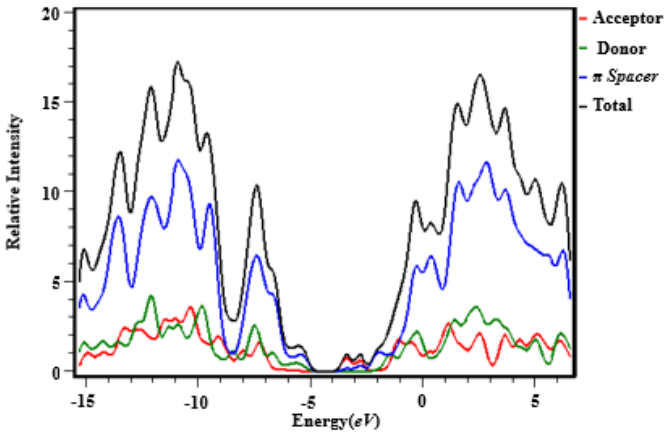

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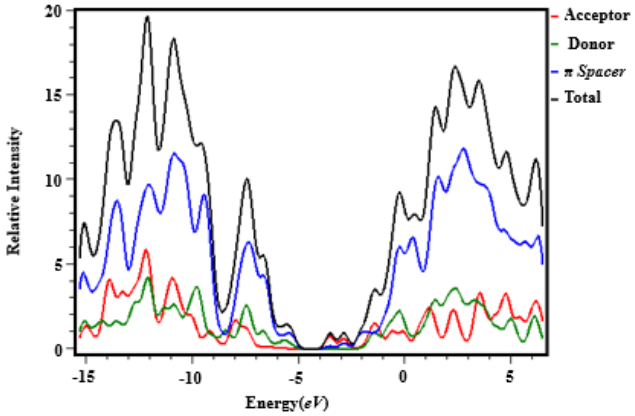

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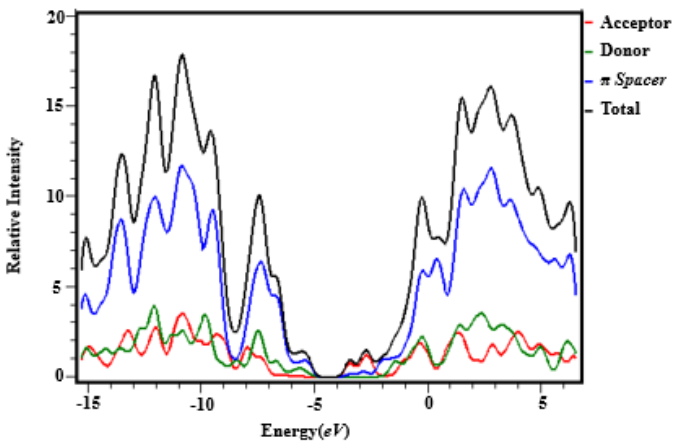
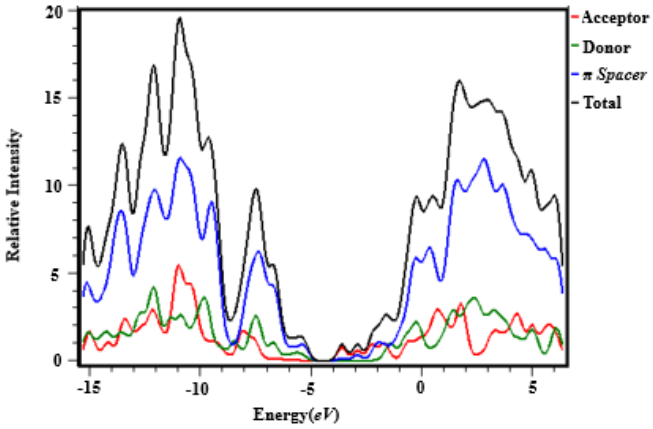
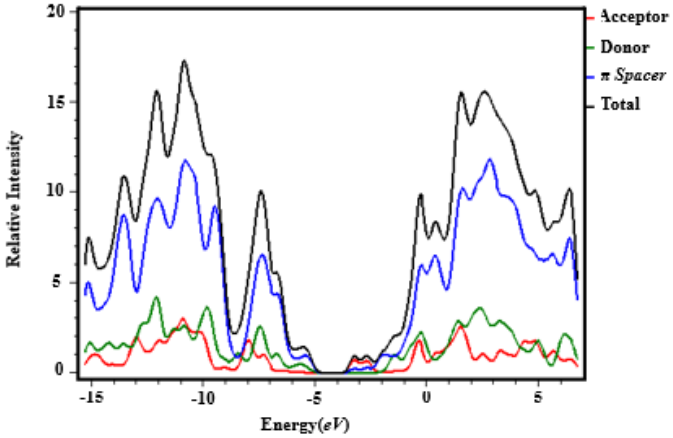


TNPD4

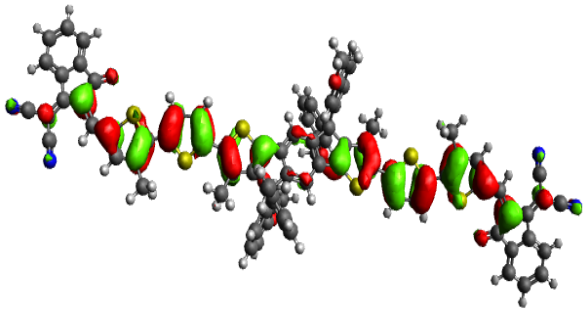


TNPD5

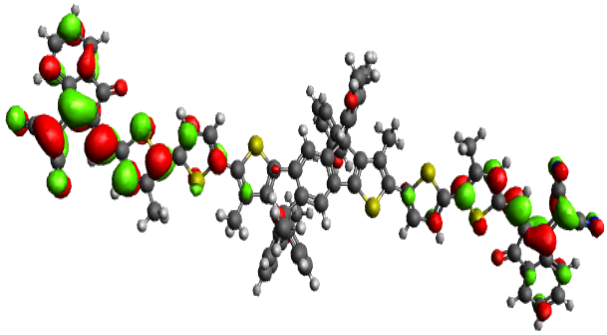


TNPD6

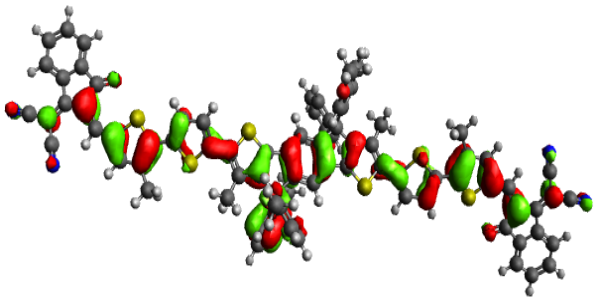
Figure S1: DOS plots of reference (**TNPR**) and designed compounds (**TNPD1** to **TNPD6**)



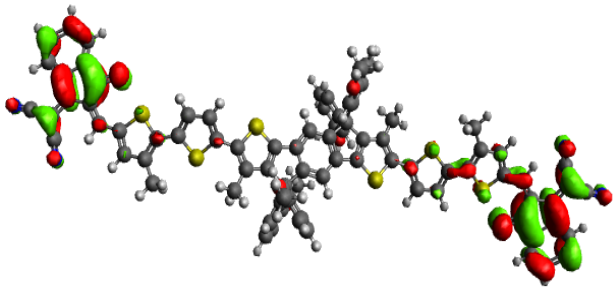
HOMO-1



LUMO+1

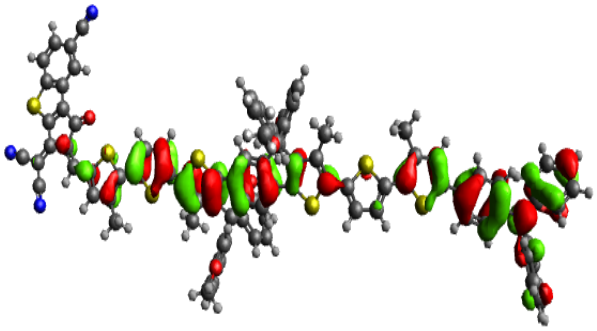


HOMO-2

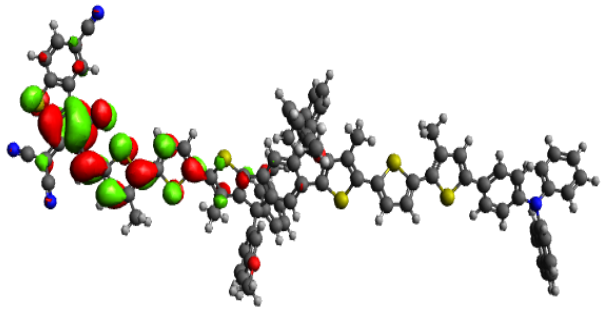


LUMO+2

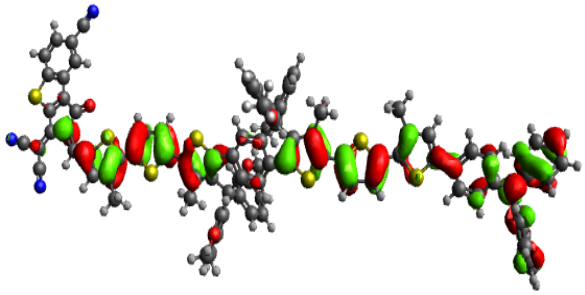
TNPR



HOMO-1



LUMO+1



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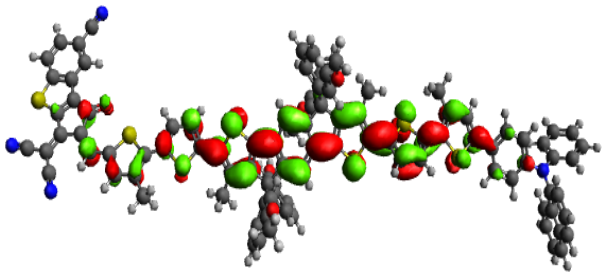
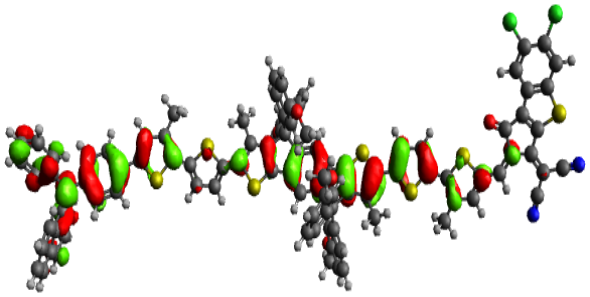
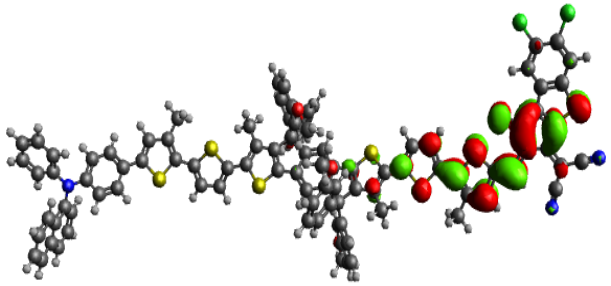


LUMO+2

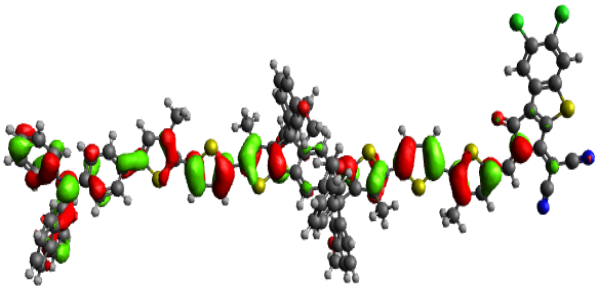
TNPD1



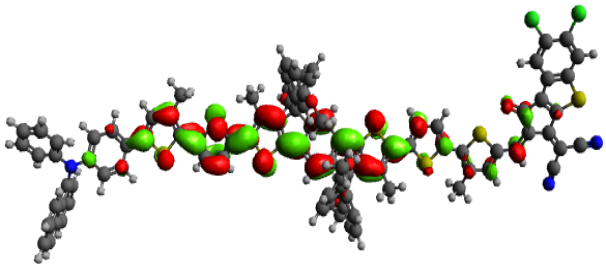
HOMO-1



LUMO+1

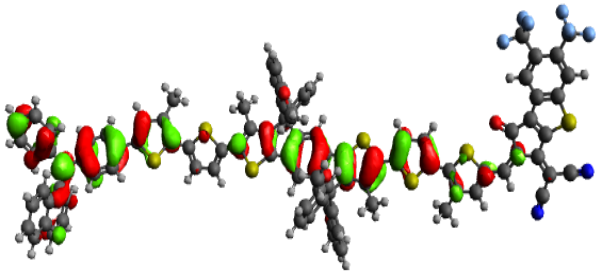


HOMO-2

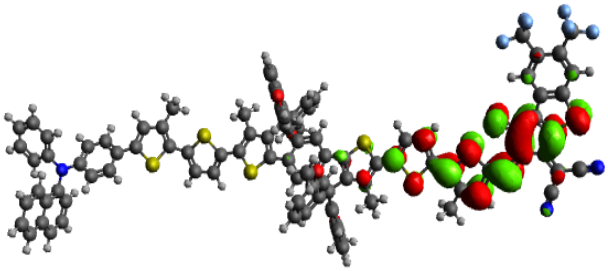


LUMO+2

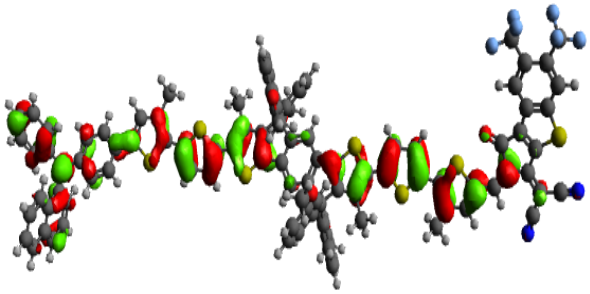
TNPD2



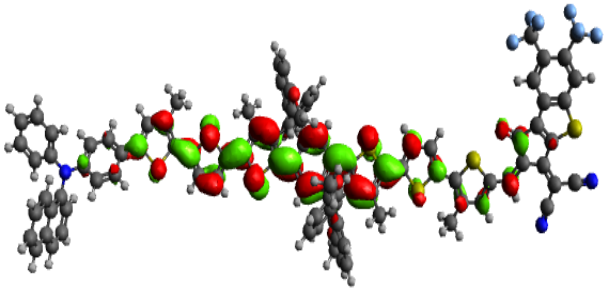
HOMO-1



LUMO+1

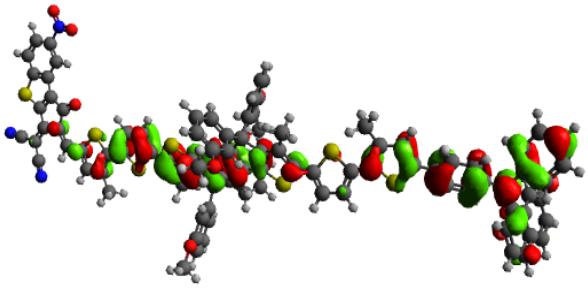


HOMO-2

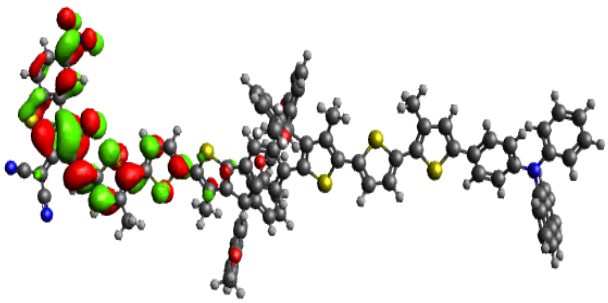


LUMO+2

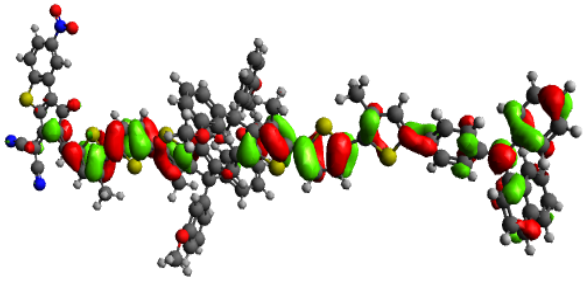
TNPD3



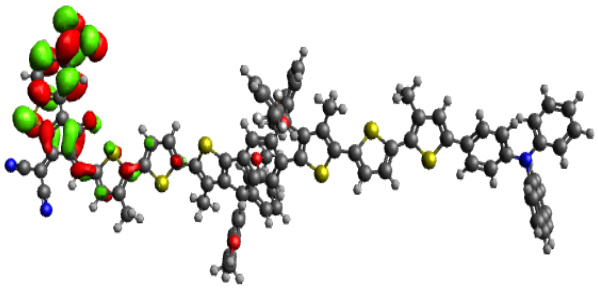
HOMO-1



LUMO+1

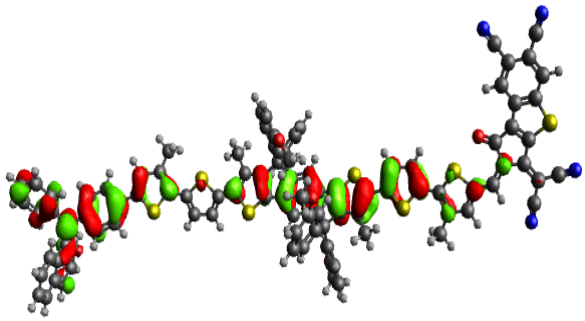


HOMO-2

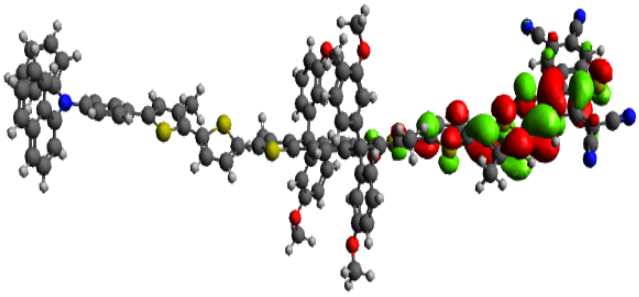


LUMO+2

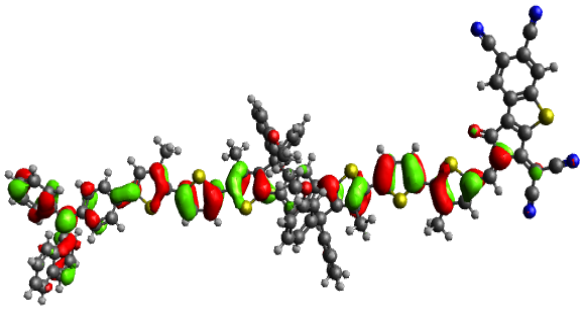
TNPD4



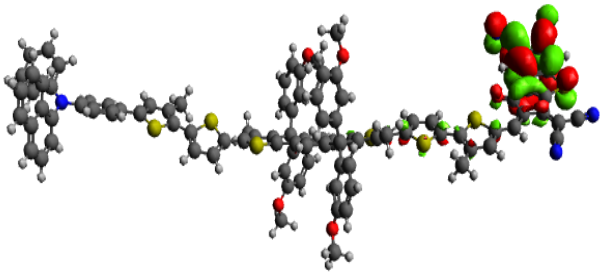
HOMO-1



LUMO+1

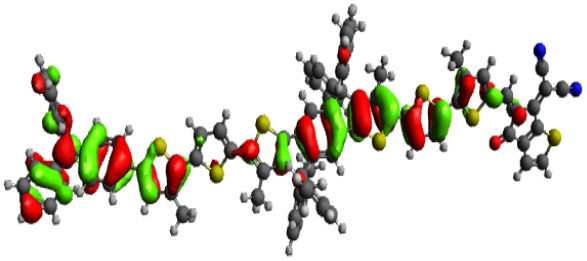


HOMO-2

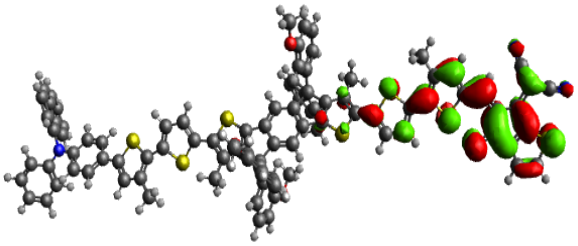


LUMO+2

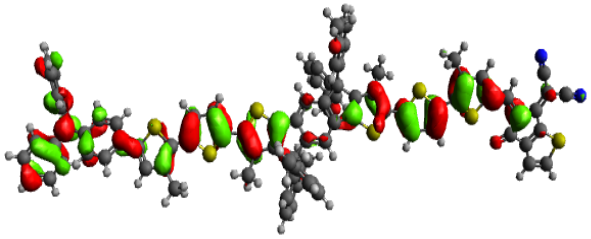
TNPD5

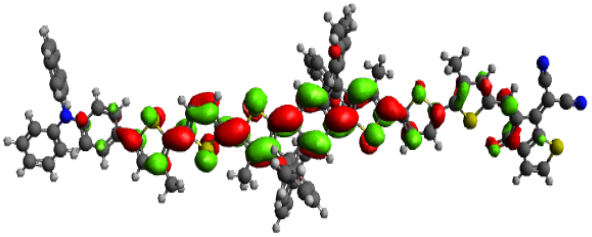


HOMO-1



LUMO+1

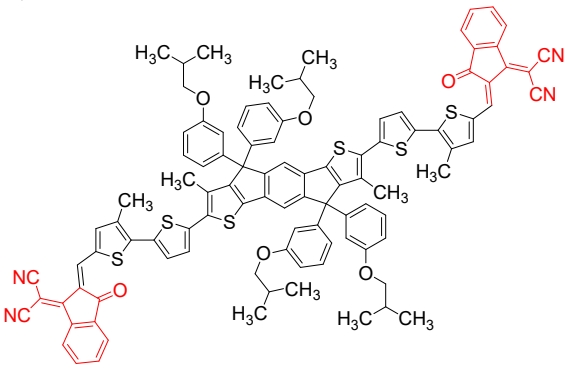




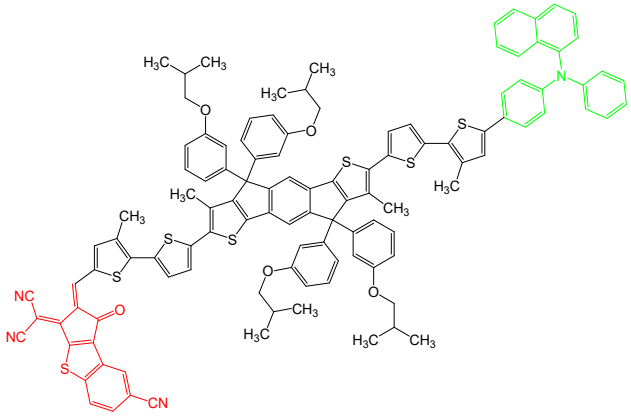
HOMO-2 **LUMO+2**

TNPD6

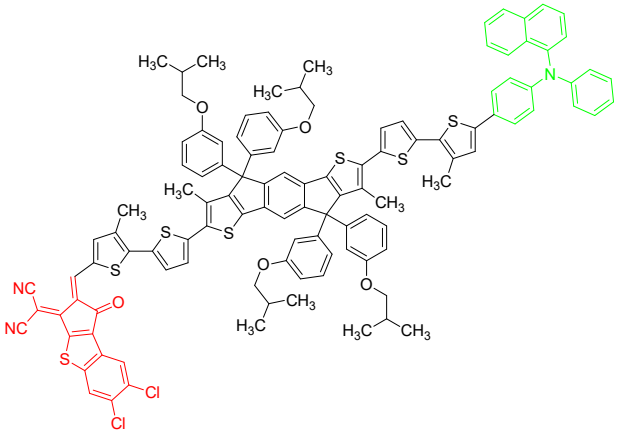
Figure S2: E_{HOMO-1}, E_{LUMO+1}, E_{HOMO-2} and E_{LUMO+2} contoured structures of reference (**TNPR**) and designed compounds (**TNPD1-TNPD6**)



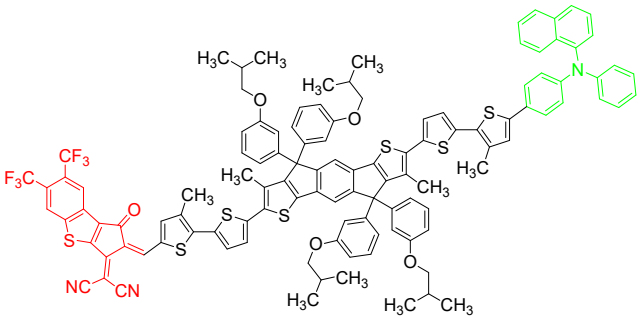
TNPR



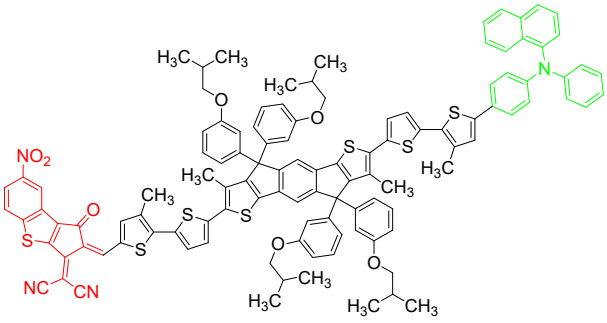
TNPD1



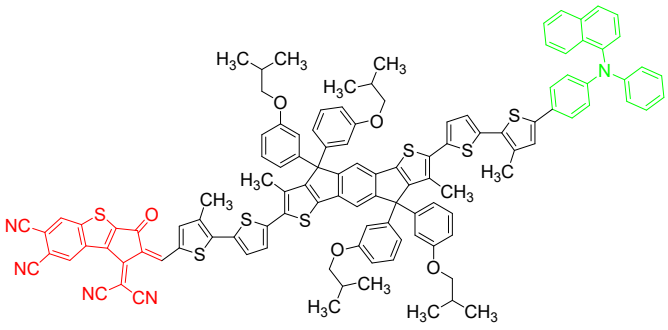
TNPD2



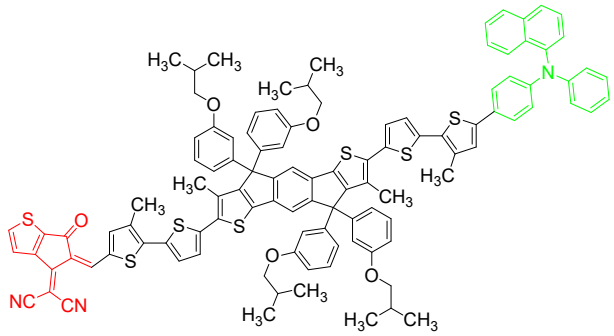
TNPD3



TNPD4



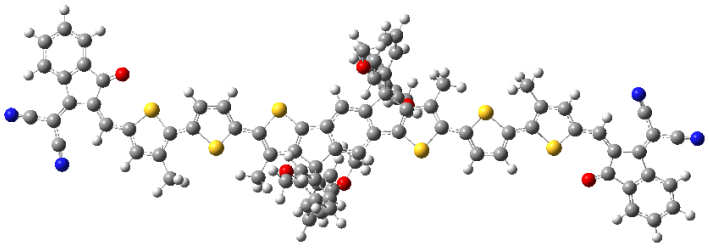
TNPD5



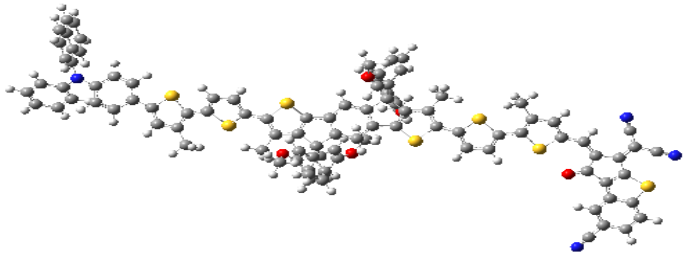
TNPD6

Depicts Donor **Depicts π–linker** **Depicts Acceptor**

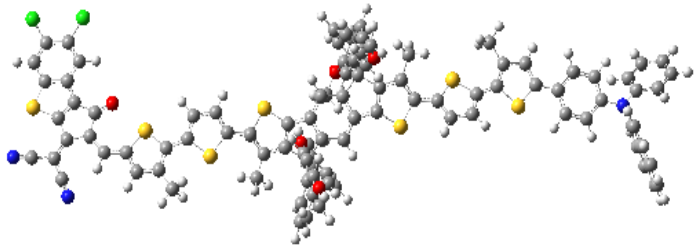
Figure S3: Structures of reference (**TNPR**) and designed compounds (**TNPD1-TNPD6**)



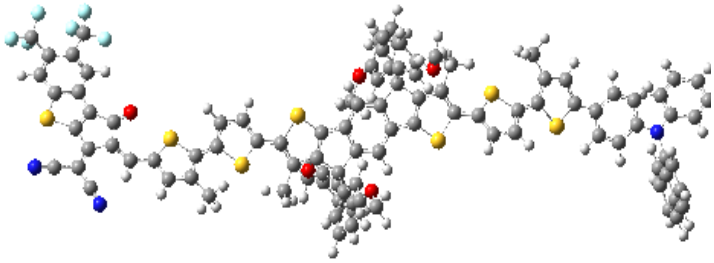
TNPR



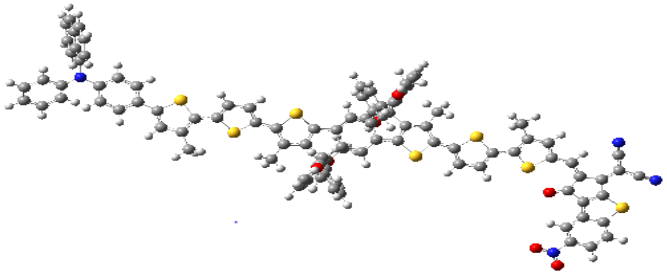
TNPD1



TNPD2



TNPD3



TNPD4

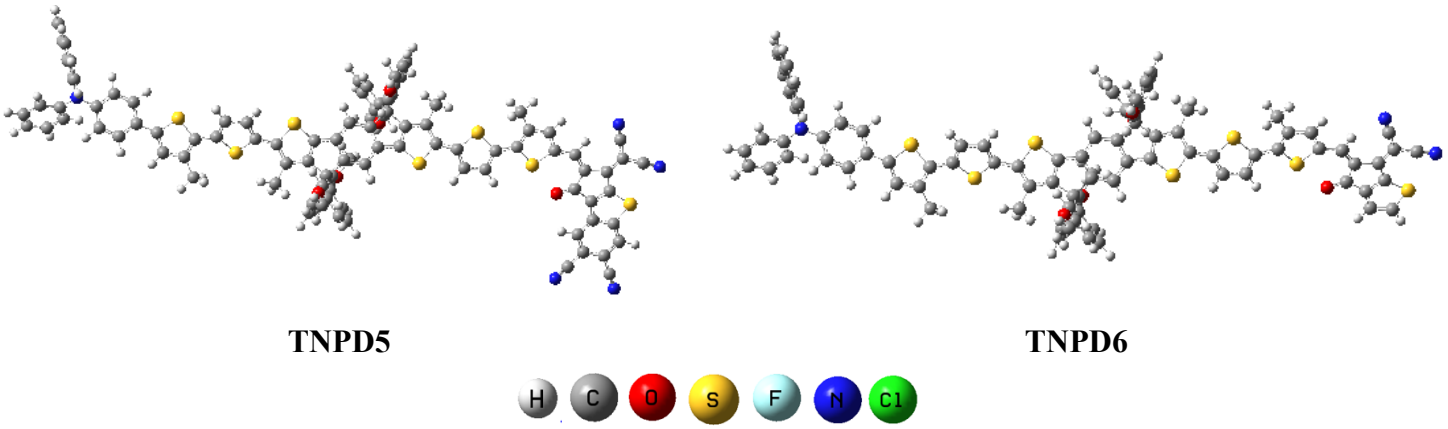


Figure S4: Optimized structures of investigated molecules (**TNPR** and **TNPD1-TNPD6**)