Supplementary Information

Structural Parameters Modulated Nonlinear Optical Amplitude of Acceptor-π-D-π-Donor Configurated Pyrene Derivatives: A DFT Approach

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Table S1: Cartesian coordinates of **MCPTR**

Atom	X-axis	Y-axis	Z-axis
C	-3.45168	-2.65703	0.260534
C	-4.81187	-2.82556	0.43042
C	-5.68739	-1.74856	0.266557
C	-5.1573	-0.47855	-0.09227
C	-3.75326	-0.30401	-0.27515
C	-2.89681	-1.41532	-0.08143
C	-7.09901	-1.89431	0.450339
C	-6.04691	0.618344	-0.2755
C	-7.44625	0.445994	-0.0878
C	-7.94095	-0.84506	0.282313
C	-8.29955	1.538612	-0.27116
H	-9.36943	1.399943	-0.12418
C	-7.79773	2.781622	-0.63483
C	-6.43402	2.958303	-0.82525
C	-5.54489	1.892014	-0.65224
C	-4.13833	2.030431	-0.86247
C	-3.2877	0.987155	-0.69061
H	-2.22946	1.129849	-0.88753
H	-3.75591	2.999167	-1.17945
H	-7.48048	-2.87491	0.729808
H	-2.78006	-3.49608	0.427724
H	-5.21248	-3.79813	0.71036
H	-9.01382	-0.96466	0.424058
H	-8.47684	3.61926	-0.77273
H	-6.03927	3.930773	-1.11449
C	2.359539	-0.5233	0.174609
H	3.115744	-1.18968	-0.23987
C	2.837706	0.576879	0.816227
C	1.9782	1.548097	1.407477
N	1.249094	2.323463	1.878541
C	4.287437	0.849676	0.946233
O	4.742973	1.819275	1.504935
O	5.036862	-0.10756	0.372793
C	6.454079	0.091934	0.456246
C	7.11632	-1.07094	-0.24274
H	6.748238	0.15287	1.513667
H	6.701608	1.057538	-0.00236
C	8.632847	-1.05536	-0.10274
H	6.709798	-2.00164	0.175297
H	6.835899	-1.05657	-1.30627
H	9.040017	-1.96154	-0.57421
H	8.90519	-1.12483	0.962631

C	9.307256	0.165079	-0.7142
C	10.82469	0.061221	-0.71436
H	9.012256	1.076374	-0.17011
H	8.948684	0.303909	-1.74802
C	11.49627	1.290498	-1.30104
H	11.17512	-0.10236	0.316091
H	11.12368	-0.83584	-1.27769
H	12.58744	1.200117	-1.30267
H	11.17491	1.4581	-2.33663
H	11.23806	2.190856	-0.72989
C	1.021254	-0.95902	-0.04562
C	0.702328	-2.10779	-0.74878
S	-0.43429	-0.15903	0.507128
C	-0.67475	-2.34287	-0.84818
H	1.467686	-2.74572	-1.18261
C	-1.43978	-1.37463	-0.22813
H	-1.11881	-3.18176	-1.37527

Table S2: Cartesian coordinates of **MCPTD1**

Atom	X-axis	Y-axis	Z-axis
C	-6.9636	-3.4116	-0.382
C	-5.66774	-3.77851	-0.68565
C	-4.63824	-2.83229	-0.66851
C	-4.93413	-1.48969	-0.30857
C	-6.27001	-1.11625	0.028371
C	-7.29351	-2.09336	-0.03787
C	-3.29064	-3.1841	-0.98065
C	-3.88388	-0.52422	-0.28113
C	-2.5554	-0.88846	-0.65151
C	-2.29756	-2.26019	-0.97191
C	-1.54039	0.100184	-0.65276
C	-1.85344	1.397526	-0.2243
C	-3.13307	1.744778	0.16177
C	-4.16872	0.806095	0.126269
C	-5.50142	1.141463	0.507799
C	-6.50371	0.228386	0.463492
H	-7.49993	0.516478	0.784266
H	-5.7	2.156528	0.847234
H	-3.0725	-4.22477	-1.21494
H	-7.76231	-4.14744	-0.44381
H	-5.43832	-4.80646	-0.96023
H	-1.27612	-2.5596	-1.18674
H	-1.07019	2.152893	-0.2321
H	-3.35287	2.762907	0.477855

C	-12.3369	-0.36047	0.082756
H	-13.1552	-0.86664	0.594759
C	-12.6763	0.779647	-0.5777
C	-11.7217	1.560228	-1.29283
N	-10.9183	2.176556	-1.86686
C	-14.0624	1.299973	-0.59982
O	-14.3915	2.313888	-1.16866
O	-14.9115	0.514259	0.084911
C	-16.2744	0.959393	0.102405
C	-17.0664	-0.03098	0.921356
H	-16.6467	1.022683	-0.93005
H	-16.3093	1.974002	0.518387
C	-18.5621	0.257088	0.901896
H	-16.8734	-1.03809	0.528226
H	-16.6932	-0.02077	1.955883
H	-19.0811	-0.53396	1.462343
H	-18.9367	0.185582	-0.13192
C	-18.9501	1.610018	1.482612
C	-20.4557	1.787688	1.606756
H	-18.5465	2.423564	0.859227
H	-18.4831	1.73293	2.474437
C	-20.8417	3.149087	2.157954
H	-20.9187	1.637081	0.61958
H	-20.8604	0.99256	2.25111
H	-21.9269	3.261501	2.250639
H	-20.4046	3.309544	3.151542
H	-20.4783	3.954731	1.508104
C	-11.0763	-1.01079	0.216773
C	-10.8874	-2.16715	0.95381
S	-9.56457	-0.48766	-0.49286
C	-9.56262	-2.6234	0.957313
H	-11.705	-2.65089	1.481704
C	-8.70776	-1.82043	0.228512
H	-9.21739	-3.502	1.493811
C	-0.1759	-0.18422	-1.09744
C	0.263406	-0.84944	-2.21567
S	1.186711	0.426375	-0.19022
C	1.670315	-0.86304	-2.35363
H	-0.42012	-1.27228	-2.94668
C	2.331545	-0.20897	-1.34286
H	2.186718	-1.31017	-3.19833
C	3.767829	-0.03893	-1.15769
C	4.30034	1.012271	-0.39993
C	4.671165	-0.93699	-1.74353

C	5.665877	1.158899	-0.22647
H	3.630496	1.735933	0.062184
C	6.038044	-0.78314	-1.597
H	4.291519	-1.77832	-2.31949
C	6.559994	0.266056	-0.82927
H	6.052724	1.976877	0.376164
H	6.718762	-1.48868	-2.0675
N	7.950819	0.410009	-0.66443
C	8.771829	-0.74017	-0.54391
C	9.976048	-0.81451	-1.25479
C	8.383248	-1.79624	0.285464
C	10.80046	-1.93022	-1.14095
H	10.25583	0.018887	-1.89521
H	7.448308	-1.7309	0.839694
C	10.41129	-2.98434	-0.33066
H	11.73474	-1.9725	-1.70051
C	8.541916	1.695218	-0.58706
C	9.546348	1.945314	0.352793
C	8.132952	2.712208	-1.46029
H	9.858623	1.152953	1.030941
C	8.704783	3.97946	-1.39224
H	7.358516	2.496717	-2.19249
C	9.706319	4.227114	-0.4678
H	8.371989	4.760329	-2.07582
C	10.12748	3.20509	0.395426
C	11.18278	3.736628	1.256382
C	10.47411	5.508248	-0.21094
C	9.201251	-2.91412	0.375581
C	9.046263	-4.14779	1.144777
C	11.12139	-4.2968	-0.06605
C	10.15999	-4.96422	0.898427
C	10.26803	-6.20393	1.506958
C	8.033259	-4.56726	2.00036
C	9.253603	-6.62551	2.366367
H	11.13132	-6.84187	1.318253
C	8.146856	-5.81335	2.609546
H	7.16807	-3.93468	2.19151
H	9.325706	-7.59616	2.851598
H	7.365083	-6.15807	3.282389
C	11.3987	5.079516	0.912358
C	12.35696	5.826805	1.577374
C	11.92382	3.134361	2.267171
C	13.10102	5.22406	2.591339
H	12.52933	6.870344	1.314183

C	12.8852	3.889453	2.932204
H	11.75681	2.092022	2.533505
H	13.85714	5.798751	3.12123
H	13.4743	3.434916	3.72532
C	11.26975	-5.11396	-1.35196
H	10.29534	-5.27879	-1.82551
H	11.917	-4.593	-2.06889
H	11.71898	-6.09266	-1.14084
C	12.4913	-4.07256	0.577085
H	12.96971	-5.03106	0.815208
H	13.15432	-3.52564	-0.10519
H	12.40013	-3.49483	1.503701
C	9.538409	6.632113	0.241345
H	8.828792	6.888404	-0.55554
H	8.966346	6.333138	1.126882
H	10.10853	7.536271	0.489798
C	11.26365	5.944762	-1.44675
H	10.58492	6.185384	-2.27478
H	11.8612	6.839405	-1.23025
H	11.94214	5.151086	-1.77908

Table S3: Cartesian coordinates of **MCPTD2**

Atom	X-axis	Y-axis	Z-axis
C	7.168105	-1.50244	3.507513
C	5.857444	-1.49365	3.938431
C	4.805422	-1.49386	3.016703
C	5.099273	-1.53202	1.627047
C	6.455481	-1.54134	1.180972
C	7.495934	-1.50643	2.14344
C	3.442841	-1.42975	3.435384
C	4.026529	-1.55892	0.686208
C	2.671182	-1.54813	1.131418
C	2.424999	-1.44678	2.538427
C	1.626449	-1.60425	0.17528
C	1.952598	-1.60989	-1.18812
C	3.263623	-1.60323	-1.62077
C	4.318152	-1.59546	-0.70279
C	5.679955	-1.64538	-1.12215
C	6.699794	-1.62932	-0.22742
H	7.722419	-1.69781	-0.5846
H	5.88795	-1.71043	-2.18877
H	3.236694	-1.34875	4.501317
H	7.974286	-1.45912	4.23631
H	5.629735	-1.46395	5.002301

H	1.39829	-1.36281	2.881994
H	1.147715	-1.66168	-1.91842
H	3.489504	-1.62868	-2.68529
C	12.47243	-0.49292	0.47965
H	13.28435	-1.02135	0.975694
C	11.2284	-0.8971	1.027576
C	11.19373	-1.85093	2.044124
S	9.596699	-0.38609	0.63239
C	9.911651	-2.16333	2.490462
H	12.1067	-2.30055	2.427112
C	8.922098	-1.4629	1.818843
H	9.690799	-2.89516	3.261404
C	0.2156	-1.67313	0.556744
C	-0.40478	-2.44303	1.510106
S	-0.97272	-0.74515	-0.32671
C	-1.81044	-2.29295	1.537712
H	0.142402	-3.12841	2.151236
H	-2.4547	-2.81675	2.238024
N	-7.69883	-0.01609	-0.51109
C	-8.12743	1.335279	-0.50082
C	-8.92564	1.820656	-1.54451
C	-7.76155	2.181402	0.550487
C	-9.37078	3.139273	-1.5444
H	-9.19376	1.14808	-2.35587
H	-7.14816	1.797324	1.363923
C	-9.00094	3.982898	-0.51
H	-9.99347	3.500304	-2.36267
C	-8.61928	-1.033	-0.86924
C	-9.91659	-1.01588	-0.348
C	-8.23495	-2.04801	-1.75516
H	-10.2115	-0.22467	0.339283
C	-9.12496	-3.05751	-2.10948
C	-10.4119	-3.04063	-1.59773
H	-8.80789	-3.84183	-2.7965
C	-10.804	-2.01447	-0.72524
C	-12.1972	-2.24349	-0.34486
C	-11.5469	-4.0148	-1.8399
C	-8.19161	3.501164	0.530063
C	-7.96141	4.592183	1.476253
C	-9.34951	5.441992	-0.29734
C	-8.63068	5.732009	1.005577
C	-8.57486	6.920059	1.715222
C	-7.2318	4.635572	2.659371
C	-7.84402	6.964827	2.902107

H	-9.0926	7.808167	1.353382
C	-7.17861	5.831778	3.368502
H	-6.70992	3.752368	3.023928
H	-7.7918	7.890973	3.469819
H	-6.61227	5.884256	4.295428
C	-12.6446	-3.40733	-0.9879
C	-13.941	-3.85754	-0.80029
C	-13.0457	-1.5228	0.488757
C	-14.7926	-3.13635	0.036321
H	-14.2925	-4.76142	-1.29761
C	-14.3472	-1.97951	0.67414
H	-12.7003	-0.61834	0.986831
H	-15.8129	-3.47849	0.193347
H	-15.0244	-1.42846	1.322583
C	-8.81244	6.314773	-1.43416
H	-7.72983	6.188824	-1.54725
H	-9.29099	6.049066	-2.38535
H	-9.01645	7.37525	-1.23911
C	-10.8607	5.637012	-0.1521
H	-11.0977	6.686108	0.06624
H	-11.3779	5.360484	-1.07958
H	-11.2592	5.019075	0.660389
C	-11.183	-5.42096	-1.35775
H	-10.3399	-5.82134	-1.93496
H	-10.9003	-5.41099	-0.29911
H	-12.0311	-6.10627	-1.48065
C	-11.9461	-4.05006	-3.31684
H	-11.1205	-4.42928	-3.93246
H	-12.8104	-4.70874	-3.46953
H	-12.2099	-3.0488	-3.67551
C	12.75074	2.04257	-2.18992
C	14.1021	1.731073	-1.98812
C	15.07032	2.390689	-2.74472
C	14.65045	3.337617	-3.67636
C	13.30015	3.634498	-3.8657
C	12.32938	2.980938	-3.11398
C	11.9162	1.232717	-1.28385
C	12.84066	0.394163	-0.49774
C	14.20108	0.693843	-0.93858
H	16.12962	2.19006	-2.6287
H	15.39911	3.856844	-4.26927
H	13.01141	4.379435	-4.6027
H	11.26762	3.184373	-3.23013
O	10.69907	1.268072	-1.21148

C	15.38174	0.139257	-0.498
C	16.65858	0.515859	-1.01006
N	17.71608	0.800093	-1.40569
C	15.46124	-0.86896	0.507683
N	15.54641	-1.69267	1.326771
H	-7.22498	-2.03564	-2.15848
C	-3.67265	-1.02629	0.332689
C	-3.99946	0.165614	-0.32683
C	-4.72992	-1.86386	0.715686
C	-5.31291	0.500001	-0.60889
H	-3.20809	0.849624	-0.62968
C	-6.04664	-1.52625	0.459717
H	-4.51396	-2.8065	1.214221
C	-6.36119	-0.34202	-0.21952
H	-5.53748	1.423918	-1.13615
H	-6.84958	-2.19049	0.770465
C	-2.29091	-1.40653	0.604602

Table S4: Cartesian coordinates of **MCPTD3**

Atom	X-axis	Y-axis	Z-axis
C	6.652865	-4.20884	-0.06605
C	5.348465	-4.54589	0.229635
C	4.328968	-3.59265	0.138735
C	4.646636	-2.27462	-0.28789
C	5.993729	-1.93155	-0.61545
C	7.007455	-2.91316	-0.47273
C	2.972814	-3.91603	0.441675
C	3.605674	-1.30448	-0.39053
C	2.265998	-1.63703	-0.0297
C	1.988301	-2.98594	0.361199
C	1.258953	-0.64338	-0.10781
C	1.592488	0.625364	-0.60204
C	2.883279	0.941105	-0.97705
C	3.909906	-0.00148	-0.86577
C	5.252127	0.300514	-1.23904
C	6.245871	-0.61615	-1.12279
H	7.249156	-0.35389	-1.44299
H	5.465435	1.291735	-1.63549
H	2.740762	-4.94058	0.727514
H	7.439147	-4.95006	0.057125
H	5.103221	-5.55496	0.555419
H	0.959833	-3.26459	0.570822
H	0.815324	1.384945	-0.65722
H	3.117947	1.937694	-1.34672

C	12.10335	-1.31981	-0.64083
H	12.82826	-1.99186	-1.09664
C	10.80753	-1.88802	-0.7061
C	10.62069	-3.13407	-1.30606
S	9.270202	-1.2679	-0.12842
C	9.300777	-3.57565	-1.30446
H	11.45343	-3.68316	-1.73873
C	8.43033	-2.6738	-0.70992
H	8.96486	-4.51038	-1.74262
C	-0.11824	-0.89099	0.318405
C	-0.59357	-1.47622	1.46616
S	-1.44994	-0.32285	-0.65907
C	-2.00332	-1.45943	1.572119
H	0.066241	-1.86037	2.239141
H	-2.543	-1.84249	2.433443
N	-8.20985	-0.1156	-0.35756
C	-8.71281	1.161406	-0.72268
C	-9.59496	1.271502	-1.80373
C	-8.34115	2.299259	-0.00126
C	-10.1117	2.509399	-2.17492
H	-9.8687	0.370396	-2.34812
H	-7.66223	2.203824	0.844745
C	-9.73463	3.641302	-1.47111
H	-10.7969	2.580461	-3.01927
C	-9.12874	-1.18651	-0.21709
C	-10.3271	-0.97986	0.472043
C	-8.85477	-2.4368	-0.78627
H	-10.531	-0.00417	0.910579
C	-9.76034	-3.48657	-0.65987
C	-10.9519	-3.28256	0.01702
H	-9.53368	-4.45432	-1.10693
C	-11.2322	-2.0268	0.575636
C	-12.5382	-2.09509	1.228718
C	-12.0832	-4.25764	0.274389
C	-8.84894	3.532407	-0.38839
C	-8.64434	4.867027	0.173447
C	-10.1517	5.081485	-1.69122
C	-9.39966	5.781407	-0.57621
C	-9.3902	7.128434	-0.25392
C	-7.87677	5.295524	1.250953
C	-8.62235	7.559204	0.827587
H	-9.97489	7.842423	-0.83372
C	-7.8731	6.649425	1.572555
H	-7.29019	4.587194	1.833516

H	-8.60734	8.613555	1.093647
H	-7.28012	7.002025	2.413201
C	-13.0472	-3.39161	1.062559
C	-14.2817	-3.73242	1.59029
C	-13.2611	-1.13182	1.923821
C	-15.0076	-2.76777	2.288769
H	-14.6818	-4.73819	1.462957
C	-14.5004	-1.47941	2.452794
H	-12.8659	-0.12562	2.053022
H	-15.978	-3.02119	2.709421
H	-15.0798	-0.73947	3.000044
C	-9.69995	5.5851	-3.06418
H	-8.6175	5.467522	-3.18764
H	-10.2001	5.026845	-3.86572
H	-9.94618	6.647182	-3.18827
C	-11.6643	5.253011	-1.53759
H	-11.9476	6.308674	-1.63497
H	-12.1981	4.688479	-2.31261
H	-12.0025	4.895902	-0.55841
C	-11.6087	-5.45469	1.101585
H	-10.8607	-6.03626	0.547794
H	-11.1581	-5.12549	2.04471
H	-12.4478	-6.12162	1.336753
C	-12.7125	-4.73849	-1.03528
H	-11.986	-5.31033	-1.6266
H	-13.5729	-5.39	-0.8366
H	-13.0562	-3.89129	-1.63935
C	12.76814	1.954474	0.929866
C	14.06103	1.592856	0.53419
C	15.12611	2.450059	0.815879
C	14.84363	3.630416	1.481366
C	13.5438	3.974945	1.869013
C	12.48251	3.133613	1.595303
C	11.81561	0.900883	0.535207
C	12.60564	-0.1488	-0.1321
C	14.00161	0.280178	-0.143
H	16.1579	2.248446	0.54811
H	11.46859	3.387913	1.891332
O	10.61322	0.921945	0.737059
C	15.09342	-0.37029	-0.67133
C	16.4139	0.165344	-0.61798
N	17.5004	0.582579	-0.58691
C	15.02648	-1.63602	-1.32464
N	14.99184	-2.66942	-1.86064

H	-7.9232	-2.5754	-1.33013
F	15.8232	4.475652	1.768996
F	13.35803	5.123794	2.502147
C	-4.05809	-0.67206	0.273581
C	-4.53782	0.282952	-0.63239
C	-5.00787	-1.44219	0.959182
C	-5.89225	0.458673	-0.85137
H	-3.8336	0.907983	-1.17964
C	-6.36526	-1.25667	0.767189
H	-4.67461	-2.2071	1.657559
C	-6.83415	-0.30445	-0.14895
H	-6.23307	1.200106	-1.56952
H	-7.07754	-1.85927	1.32519
C	-2.63182	-0.86334	0.505597

Table S5: Cartesian coordinates of **MCPTD4**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	6.472233	-4.34735	-0.07316
C	5.16507	-4.67695	0.217671
C	4.150444	-3.71907	0.118904
C	4.476057	-2.40476	-0.31304
C	5.825943	-2.06984	-0.63821
C	6.835277	-3.05505	-0.48411
C	2.792039	-4.03405	0.420097
C	3.440392	-1.42958	-0.42152
C	2.098547	-1.75277	-0.05991
C	1.812737	-3.09869	0.335004
C	1.097658	-0.75295	-0.14056
C	1.439031	0.511786	-0.63997
C	2.731398	0.817869	-1.017
C	3.752288	-0.13045	-0.90186
C	5.096008	0.16214	-1.27611
C	6.084861	-0.75907	-1.15368
H	7.089148	-0.50312	-1.47534
H	5.315165	1.149935	-1.67776
H	2.553929	-5.05627	0.709209
H	7.25408	-5.09168	0.059078
H	4.913773	-5.68323	0.547422
H	0.782393	-3.37085	0.544125
H	0.667075	1.276468	-0.69695
H	2.972225	1.811599	-1.39031
C	11.92916	-1.45795	-0.63365
H	12.65865	-2.13893	-1.06814
C	10.63687	-2.03169	-0.69311

C	10.45822	-3.29161	-1.26875
S	9.091802	-1.40304	-0.14562
C	9.139762	-3.73465	-1.2736
H	11.29661	-3.8484	-1.68025
C	8.260494	-2.82099	-0.70826
H	8.810601	-4.67841	-1.69717
C	-0.28002	-0.98854	0.290231
C	-0.75667	-1.5686	1.440188
S	-1.60991	-0.40468	-0.68056
C	-2.16552	-1.53511	1.553155
H	-0.09774	-1.9598	2.210366
H	-2.70493	-1.91175	2.41746
N	-8.36399	-0.10852	-0.34633
C	-8.84999	1.172013	-0.72204
C	-9.73185	1.285321	-1.803
C	-8.46028	2.310865	-0.01176
C	-10.23	2.527434	-2.18545
H	-10.0198	0.383583	-2.33893
H	-7.78155	2.213043	0.83413
C	-9.83456	3.660131	-1.4931
H	-10.9149	2.600939	-3.02984
C	-9.29581	-1.16741	-0.20023
C	-10.4911	-0.94325	0.488857
C	-9.03715	-2.42342	-0.76391
H	-10.6831	0.036724	0.923166
C	-9.95466	-3.46202	-0.63168
C	-11.1429	-3.24076	0.04541
H	-9.73992	-4.43445	-1.07442
C	-11.4083	-1.97901	0.597927
C	-12.7152	-2.02832	1.251017
C	-12.2853	-4.20133	0.30859
C	-8.94946	3.547891	-0.41019
C	-8.72303	4.884537	0.138222
C	-10.2282	5.104599	-1.72758
C	-9.46453	5.80338	-0.61973
C	-9.43341	7.153193	-0.31084
C	-7.94734	5.311503	1.210505
C	-8.65749	7.582451	0.765514
H	-10.0075	7.870513	-0.89709
C	-7.92172	6.668323	1.518539
H	-7.37128	4.599815	1.799431
H	-8.62567	8.638987	1.021206
H	-7.3221	7.0198	2.354937
C	-13.2392	-3.31966	1.091698

C	-14.4783	-3.64301	1.619765
C	-13.4279	-1.05258	1.939241
C	-15.194	-2.66582	2.311148
H	-14.8898	-4.64479	1.497485
C	-14.6721	-1.38246	2.468207
H	-13.0214	-0.05019	2.06287
H	-16.168	-2.90523	2.731624
H	-15.2437	-0.63236	3.009785
C	-9.7682	5.587031	-3.10545
H	-8.68767	5.451392	-3.22722
H	-10.2766	5.02857	-3.90158
H	-9.9977	6.651544	-3.2405
C	-11.7378	5.302619	-1.57598
H	-12.0035	6.361835	-1.68364
H	-12.2807	4.739523	-2.34567
H	-12.082	4.960648	-0.59351
C	-11.8244	-5.39876	1.142808
H	-11.0837	-5.99239	0.592038
H	-11.3693	-5.06913	2.083629
H	-12.6711	-6.05434	1.382572
C	-12.9206	-4.68256	-0.99802
H	-12.2009	-5.26577	-1.58653
H	-13.7882	-5.32334	-0.7952
H	-13.2553	-3.83497	-1.60662
C	12.57053	1.867994	0.826562
C	13.87097	1.505933	0.442933
C	14.93761	2.369346	0.678682
C	14.66132	3.580413	1.29593
C	13.37307	3.949297	1.679469
C	12.3146	3.078794	1.441495
C	11.62471	0.791636	0.476863
C	12.4278	-0.27047	-0.15626
C	13.81785	0.164751	-0.18215
H	15.96659	2.155031	0.41229
O	10.42417	0.794575	0.678956
C	14.91572	-0.49943	-0.68166
C	16.23454	0.041435	-0.65246
N	17.32091	0.460169	-0.64208
C	14.85595	-1.79183	-1.28121
N	14.82799	-2.84669	-1.77407
H	-8.1077	-2.57531	-1.30785
F	15.64156	4.435788	1.540501
F	13.16225	5.115788	2.262666
C	-4.21707	-0.72099	0.265202

C	-4.68809	0.234901	-0.64443
C	-5.17408	-1.47223	0.961628
C	-6.04105	0.428935	-0.85711
H	-3.97809	0.845948	-1.19995
C	-6.52966	-1.26811	0.775968
H	-4.84825	-2.23697	1.66367
C	-6.98989	-0.31552	-0.14425
H	-6.37505	1.170509	-1.57834
H	-7.24759	-1.85629	1.342076
C	-2.79233	-0.93117	0.489964
F	11.09898	3.433281	1.808415

Table S6: Cartesian coordinates of **MCPTD5**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	-6.12326	-4.55365	0.020523
C	-4.80896	-4.84749	-0.27616
C	-3.8175	-3.86696	-0.16561
C	-4.17443	-2.56677	0.283087
C	-5.53164	-2.26895	0.61501
C	-6.51718	-3.27667	0.450624
C	-2.45234	-4.14581	-0.47159
C	-3.16197	-1.56833	0.401976
C	-1.81313	-1.85477	0.034921
C	-1.49539	-3.1886	-0.37638
C	-0.8363	-0.83222	0.126507
C	-1.20676	0.417327	0.642652
C	-2.50569	0.687539	1.024674
C	-3.50394	-0.2833	0.89866
C	-4.85356	-0.02796	1.278704
C	-5.82037	-0.97115	1.147391
H	-6.82919	-0.74314	1.47558
H	-5.09551	0.949084	1.693422
H	-2.19061	-5.15864	-0.77305
H	-6.88694	-5.31504	-0.12048
H	-4.53393	-5.84287	-0.61977
H	-0.45901	-3.43353	-0.58965
H	-0.45267	1.198929	0.70886
H	-2.76976	1.670292	1.411143
C	-11.6475	-1.80797	0.673229
H	-12.3593	-2.51491	1.095754
C	-10.3422	-2.35375	0.707784
C	-10.1273	-3.61948	1.256514
S	-8.81874	-1.67564	0.15943
C	-8.79784	-4.02863	1.24227

H	-10.9477	-4.20522	1.66372
C	-7.94648	-3.08278	0.687035
H	-8.44196	-4.97116	1.646474
C	0.544949	-1.03115	-0.31101
C	1.028828	-1.58258	-1.47196
S	1.866383	-0.43926	0.666411
C	2.43645	-1.52215	-1.58739
H	0.374585	-1.97335	-2.24637
H	2.980563	-1.8745	-2.45895
N	8.617616	-0.05332	0.331456
C	9.093646	1.224401	0.727915
C	9.981481	1.326592	1.805182
C	8.687893	2.372611	0.041863
C	10.46906	2.56644	2.208101
H	10.28219	0.418263	2.322598
H	8.005164	2.283989	-0.8018
C	10.05677	3.708049	1.540773
H	11.15832	2.631073	3.049641
C	9.55612	-1.10472	0.172068
C	10.74574	-0.86814	-0.52235
C	9.30729	-2.3665	0.726966
H	10.92975	0.116327	-0.94992
C	10.22922	-3.39927	0.580777
C	11.41198	-3.16596	-0.10186
H	10.02246	-4.37647	1.016769
C	11.66758	-1.89833	-0.64567
C	12.97087	-1.93554	-1.30684
C	12.55783	-4.11827	-0.3793
C	9.166176	3.606929	0.461275
C	8.921125	4.951351	-0.05919
C	10.43496	5.151998	1.801727
C	9.656376	5.863663	0.712583
C	9.607641	7.218845	0.430981
C	8.134111	5.390411	-1.11828
C	8.820226	7.660334	-0.63202
H	10.17718	7.93074	1.028158
C	8.090736	6.752695	-1.39892
H	7.562807	4.683917	-1.71801
H	8.774512	8.721304	-0.86635
H	7.481973	7.113746	-2.22456
C	13.50235	-3.22538	-1.16085
C	14.74044	-3.53788	-1.69768
C	13.67508	-0.95057	-1.9907
C	15.4477	-2.55138	-2.38443

H	15.15778	-4.53842	-1.58531
C	14.91843	-1.26955	-2.52854
H	13.26286	0.050721	-2.10405
H	16.42089	-2.78217	-2.81149
H	15.48333	-0.51199	-3.0667
C	9.97807	5.60146	3.19177
H	8.899756	5.451837	3.316945
H	10.49701	5.032545	3.973596
H	10.19704	6.665448	3.347166
C	11.94113	5.371336	1.644937
H	12.19474	6.431291	1.772857
H	12.49577	4.799175	2.399418
H	12.28322	5.053961	0.653496
C	12.09874	-5.31192	-1.21981
H	11.36491	-5.914	-0.66909
H	11.63613	-4.97782	-2.15537
H	12.94781	-5.96073	-1.46953
C	13.20364	-4.60562	0.919943
H	12.49084	-5.19734	1.508355
H	14.07367	-5.2398	0.707214
H	13.53704	-3.76066	1.532866
C	-12.3668	1.556303	-0.66565
C	-13.651	1.155624	-0.28087
C	-14.7169	2.029523	-0.47522
C	-14.4644	3.277042	-1.04578
C	-13.1679	3.659977	-1.42409
C	-12.1038	2.785735	-1.23194
C	-11.4	0.48259	-0.36971
C	-12.1718	-0.61749	0.233062
C	-13.5724	-0.2087	0.287188
H	-15.7392	1.787416	-0.2039
O	-10.2019	0.528288	-0.59205
C	-14.6536	-0.91427	0.763995
C	-15.9802	-0.39166	0.76495
N	-17.0721	0.012107	0.778299
C	-14.568	-2.23081	1.305406
N	-14.5179	-3.30557	1.751244
H	8.381386	-2.52727	1.27445
C	4.477186	-0.70014	-0.28853
C	4.937723	0.247427	0.635043
C	5.442237	-1.42954	-0.99692
C	6.288682	0.453475	0.850213
H	4.221188	0.841918	1.200111
C	6.795438	-1.21294	-0.80868

H	5.124722	-2.18755	-1.70995
C	7.245399	-0.26963	0.126058
H	6.6148	1.187807	1.582437
H	7.519761	-1.78465	-1.38344
C	3.055127	-0.92622	-0.51495
H	-11.0913	3.058889	-1.51704
C	- 12.863200	5.208994	-2.13008
C	-15.797993	4.354726	-1.27775

Table S7: Cartesian coordinates of **MCPTD6**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	-5.7301	-4.603	-0.12352
C	-4.41442	-4.8671	-0.44041
C	-3.44136	-3.86801	-0.3314
C	-3.81987	-2.57747	0.126933
C	-5.17973	-2.30779	0.472341
C	-6.14457	-3.33758	0.321531
C	-2.07308	-4.12056	-0.64575
C	-2.82467	-1.56161	0.247044
C	-1.47145	-1.82362	-0.12169
C	-1.13206	-3.14834	-0.54462
C	-0.51035	-0.7875	-0.01842
C	-0.90076	0.452973	0.504147
C	-2.20516	0.701059	0.883087
C	-3.18744	-0.28532	0.751025
C	-4.54059	-0.05493	1.134457
C	-5.49012	-1.01607	1.007074
H	-6.50134	-0.80632	1.339772
H	-4.79955	0.917242	1.550323
H	-1.79531	-5.12629	-0.95643
H	-6.4795	-5.37998	-0.25583
H	-4.12296	-5.85419	-0.79421
H	-0.09219	-3.37392	-0.76222
H	-0.15753	1.244173	0.579035
H	-2.48585	1.677206	1.274533
C	-11.3036	-2.0268	0.787124
H	-11.961	-2.75811	1.252717
C	-9.98328	-2.53101	0.740338
C	-9.70326	-3.78929	1.278211
S	-8.50984	-1.80859	0.116922
C	-8.36482	-4.15742	1.200464
H	-10.4846	-4.39711	1.728138
C	-7.5701	-3.18555	0.606193
H	-7.96107	-5.08642	1.590528

C	0.877088	-0.96752	-0.44525
C	1.377176	-1.49506	-1.61025
S	2.183574	-0.39463	0.562596
C	2.786422	-1.43231	-1.70409
H	0.733936	-1.87201	-2.40069
H	3.344406	-1.76713	-2.57384
N	8.942215	-0.05035	0.351589
C	9.425792	1.221199	0.758973
C	10.29235	1.311688	1.854365
C	9.049547	2.374518	0.064717
C	10.78881	2.544915	2.266675
H	10.57017	0.39961	2.37794
H	8.383333	2.294863	-0.79289
C	10.40665	3.691565	1.59014
H	11.46136	2.600212	3.122251
C	9.871683	-1.11162	0.2061
C	11.07974	-0.88409	-0.459
C	9.596566	-2.37449	0.746299
H	11.2845	0.101035	-0.87543
C	10.51031	-3.41633	0.613966
C	11.7113	-3.19187	-0.03932
H	10.28234	-4.39394	1.038298
C	11.99318	-1.92334	-0.5677
C	13.31126	-1.96999	-1.19786
C	12.85326	-4.15458	-0.2966
C	9.536564	3.602388	0.49304
C	9.322241	4.949719	-0.03342
C	10.80164	5.129942	1.85705
C	10.05622	5.851759	0.751542
C	10.03434	7.207052	0.467084
C	8.563159	5.399211	-1.10843
C	9.275247	7.658909	-0.61202
H	10.60302	7.91105	1.074338
C	8.546781	6.761499	-1.39189
H	7.992532	4.700718	-1.71811
H	9.250775	8.720035	-0.84883
H	7.960104	7.13061	-2.22985
C	13.82642	-3.26597	-1.0476
C	15.07338	-3.58765	-1.55791
C	14.04023	-0.9881	-1.85974
C	15.80558	-2.60418	-2.22267
H	15.47807	-4.59302	-1.44254
C	15.29212	-1.31642	-2.3712
H	13.6402	0.017673	-1.97676

H	16.78584	-2.84222	-2.62909
H	15.87634	-0.5617	-2.89247
C	10.32377	5.588228	3.237123
H	9.24114	5.454602	3.341192
H	10.81886	5.012851	4.029623
H	10.55539	6.649063	3.395627
C	12.31393	5.32555	1.730926
H	12.5815	6.381611	1.862432
H	12.84399	4.746292	2.497579
H	12.67144	5.001015	0.747269
C	12.40179	-5.33539	-1.15914
H	11.64636	-5.93267	-0.63297
H	11.96781	-4.98746	-2.10335
H	13.24906	-5.99256	-1.3925
C	13.4606	-4.66071	1.013878
H	12.72618	-5.24872	1.578963
H	14.32801	-5.30357	0.817364
H	13.78857	-3.82516	1.642408
C	-12.2429	1.304647	-0.51723
C	-13.4752	0.853349	-0.02018
C	-14.6006	1.661106	-0.11224
C	-14.4741	2.913042	-0.70786
C	-13.2503	3.372494	-1.21515
C	-12.1163	2.549776	-1.11413
C	-11.2146	0.260792	-0.27847
C	-11.9034	-0.8567	0.389015
C	-13.3037	-0.50153	0.550035
H	-15.5748	1.363401	0.258986
O	-10.0356	0.316181	-0.5749
C	-14.3165	-1.24179	1.118732
C	-15.6628	-0.78453	1.223097
N	-16.7709	-0.44168	1.324619
C	-14.1327	-2.5461	1.665675
N	-14.0045	-3.61177	2.117774
H	8.657053	-2.52933	1.27182
C	4.808565	-0.64571	-0.35651
C	5.260587	0.293251	0.579862
C	5.779246	-1.38272	-1.04899
C	6.6093	0.483187	0.82295
H	4.539221	0.893491	1.132585
C	7.130732	-1.1823	-0.83253
H	5.467056	-2.13468	-1.77072
C	7.572091	-0.24863	0.115822
H	6.929067	1.210857	1.56462

H	7.860202	-1.76016	-1.39448
C	3.389124	-0.85929	-0.61039
C	-13.139994	4.92386	-1.95014
C	-15.885648	3.9068	-0.80712
C	-10.597326	3.088861	-1.72373

Table S8: Cartesian coordinates of **MCPTD7**

Atom	X-axis	Y-axis	Z-axis
C	6.358431	-4.43185	-0.00862
C	5.047294	-4.73741	0.285814
C	4.0485	-3.76267	0.183334
C	4.395786	-2.45556	-0.25344
C	5.751039	-2.14368	-0.58083
C	6.744196	-3.14674	-0.42533
C	2.685896	-4.05574	0.484616
C	3.375315	-1.46489	-0.36564
C	2.028194	-1.76607	-0.00449
C	1.721027	-3.10562	0.394399
C	1.041956	-0.75183	-0.09084
C	1.40273	0.505253	-0.59624
C	2.700183	0.790147	-0.97186
C	3.706901	-0.17294	-0.85092
C	5.05439	0.096819	-1.2264
C	6.02927	-0.83958	-1.10168
H	7.035602	-0.59969	-1.42886
H	5.288916	1.079041	-1.63301
H	2.431984	-5.07317	0.776804
H	7.126321	-5.18969	0.127584
H	4.779465	-5.73753	0.620887
H	0.686246	-3.36144	0.6022
H	0.641948	1.280554	-0.65882
H	2.956398	1.778361	-1.34949
C	11.8632	-1.65473	-0.625
H	12.58169	-2.36346	-1.03278
C	10.56413	-2.20179	-0.66615
C	10.35855	-3.47806	-1.20122
S	9.031307	-1.52418	-0.13846
C	9.03414	-3.89278	-1.19107
H	11.18512	-4.06485	-1.59435
C	8.171322	-2.94316	-0.65274
H	8.686062	-4.84123	-1.58755
C	-0.33888	-0.96759	0.338333
C	-0.82328	-1.53692	1.490636
S	-1.66096	-0.37716	-0.6392

C	-2.23178	-1.49164	1.599255
H	-0.16958	-1.92915	2.264788
H	-2.77746	-1.85902	2.463562
N	-8.41616	-0.07413	-0.34538
C	-8.90517	1.203012	-0.72973
C	-9.77923	1.307549	-1.81769
C	-8.52769	2.346146	-0.01973
C	-10.2817	2.545574	-2.20776
H	-10.058	0.402465	-2.35286
H	-7.85565	2.255008	0.832212
C	-9.89841	3.682598	-1.51576
H	-10.9605	2.612383	-3.05755
C	-9.34641	-1.13527	-0.20042
C	-10.541	-0.91421	0.49054
C	-9.08636	-2.38915	-0.7678
H	-10.7337	0.064713	0.926952
C	-10.0021	-3.42953	-0.63693
C	-11.1897	-3.21162	0.042473
H	-9.78667	-4.4006	-1.0823
C	-11.4565	-1.95169	0.598556
C	-12.7622	-2.00502	1.253667
C	-12.3299	-4.17487	0.305091
C	-9.02105	3.579107	-0.42568
C	-8.80731	4.918716	0.12049
C	-10.2995	5.123821	-1.75737
C	-9.54875	5.830606	-0.64584
C	-9.52866	7.181456	-0.34058
C	-8.04278	5.353593	1.197624
C	-8.76398	7.618634	0.740588
H	-10.1028	7.893417	-0.93326
C	-8.0283	6.711367	1.502025
H	-7.46679	4.647285	1.793076
H	-8.74086	8.676044	0.993548
H	-7.43756	7.06908	2.342064
C	-13.284	-3.29697	1.092137
C	-14.5214	-3.62401	1.62178
C	-13.4753	-1.0323	1.945676
C	-15.2376	-2.64989	2.317011
H	-14.9313	-4.62624	1.497873
C	-14.7179	-1.36591	2.476245
H	-13.0705	-0.02945	2.071006
H	-16.2102	-2.89223	2.738816
H	-15.2898	-0.6183	3.020808
C	-9.83268	5.60513	-3.1333

H	-8.75048	5.47601	-3.24706
H	-10.332	5.04119	-3.93133
H	-10.068	6.667734	-3.27312
C	-11.8115	5.312315	-1.61749
H	-12.0833	6.369444	-1.73014
H	-12.3451	4.743604	-2.38957
H	-12.1609	4.970911	-0.63662
C	-11.8653	-5.37367	1.135322
H	-11.1247	-5.96471	0.581618
H	-11.409	-5.04577	2.076175
H	-12.7104	-6.03125	1.374981
C	-12.9665	-4.65384	-1.00172
H	-12.2469	-5.23454	-1.59282
H	-13.8327	-5.29644	-0.79901
H	-13.3035	-3.80532	-1.60771
C	12.56774	1.72445	0.697672
C	13.85701	1.320466	0.333574
C	14.92281	2.192509	0.537864
C	14.66409	3.447882	1.098942
C	13.35409	3.837513	1.457207
C	12.2914	2.956321	1.252215
C	11.60364	0.644073	0.393144
C	12.38312	-0.45576	-0.1887
C	13.78185	-0.05023	-0.22869
H	15.94731	1.943191	0.281519
O	10.40369	0.699368	0.600657
C	14.8714	-0.75495	-0.68699
C	16.19761	-0.23165	-0.67368
N	17.28864	0.174401	-0.6743
C	14.79247	-2.07421	-1.22308
N	14.74502	-3.15102	-1.66381
H	-8.15729	-2.538	-1.3133
C	-4.27349	-0.67729	0.297088
C	-4.73934	0.282674	-0.61089
C	-5.23406	-1.43407	0.982517
C	-6.091	0.474982	-0.83293
H	-4.02641	0.898456	-1.15742
C	-6.58845	-1.23261	0.786975
H	-4.91176	-2.20215	1.682524
C	-7.04392	-0.2764	-0.13227
H	-6.42098	1.219693	-1.55271
H	-7.30921	-1.82588	1.344004
C	-2.8506	-0.88957	0.53008
H	11.27227	3.225011	1.518126

C	13.10917	5.126245	2.025874
N	12.88515	6.168502	2.488197
C	15.75531	4.349164	1.310069
N	16.64677	5.075044	1.478135

Table S9: Cartesian coordinates of **MCPTD8**

Atom	X-axis	Y-axis	Z-axis
C	-6.20941	-4.35579	-0.25549
C	-4.89625	-4.62648	-0.57923
C	-3.91673	-3.6346	-0.46834
C	-4.28574	-2.34427	-0.00187
C	-5.64264	-2.06856	0.350198
C	-6.61399	-3.09132	0.199536
C	-2.55085	-3.89366	-0.78908
C	-3.28392	-1.33527	0.120796
C	-1.93307	-1.60424	-0.25198
C	-1.6033	-2.92845	-0.68508
C	-0.96492	-0.57582	-0.14225
C	-1.34579	0.664475	0.386858
C	-2.64843	0.919939	0.767875
C	-3.63737	-0.05911	0.632352
C	-4.98881	0.178073	1.019562
C	-5.94424	-0.77669	0.890607
H	-6.95438	-0.56305	1.22456
H	-5.24054	1.150227	1.439999
H	-2.28066	-4.89918	-1.10728
H	-6.96449	-5.12739	-0.3872
H	-4.6124	-5.61367	-0.93909
H	-0.56569	-3.15891	-0.90823
H	-0.596	1.449129	0.466589
H	-2.92185	1.895818	1.165178
C	-11.77	-1.7677	0.700573
H	-12.4264	-2.49499	1.173966
C	-10.4475	-2.27488	0.650768
C	-10.165	-3.52747	1.195403
S	-8.98028	-1.55814	0.008174
C	-8.82596	-3.89842	1.108104
H	-10.9434	-4.13085	1.655992
C	-8.03731	-2.93365	0.498765
H	-8.41996	-4.8256	1.500545
C	0.422506	-0.76544	-0.56681
C	0.921022	-1.28096	-1.73757
S	1.731048	-0.23107	0.458702
C	2.331884	-1.23966	-1.82157

H	0.276527	-1.63569	-2.53725
H	2.89072	-1.56929	-2.69281
N	8.498433	-0.0331	0.311337
C	9.011883	1.234245	0.692222
C	9.870308	1.332642	1.793651
C	8.668463	2.378571	-0.03332
C	10.39304	2.563915	2.178346
H	10.12218	0.428355	2.343084
H	8.007547	2.292896	-0.89441
C	10.04421	3.701827	1.469627
H	11.05992	2.624807	3.038021
C	9.387262	-1.13325	0.224082
C	10.64364	-0.96478	-0.36525
C	9.020599	-2.38225	0.742853
H	10.92348	0.00823	-0.76575
C	9.888196	-3.46772	0.661967
C	11.13594	-3.30205	0.083334
H	9.585646	-4.43287	1.067902
C	11.51045	-2.04746	-0.42015
C	12.8639	-2.15558	-0.96249
C	12.24328	-4.31835	-0.10761
C	9.180257	3.605192	0.368501
C	9.000057	4.943608	-0.19249
C	10.47331	5.13668	1.701532
C	9.749667	5.84792	0.574871
C	9.75942	7.196111	0.257478
C	8.257035	5.38346	-1.28259
C	9.016255	7.638266	-0.83661
H	10.33988	7.902245	0.850973
C	8.272333	6.73852	-1.59895
H	7.674326	4.68305	-1.87846
H	9.01614	8.693707	-1.0988
H	7.69838	7.099988	-2.44899
C	13.30626	-3.47521	-0.78579
C	14.56977	-3.85245	-1.20969
C	13.68275	-1.20611	-1.56375
C	15.39262	-2.90106	-1.8122
H	14.91909	-4.87602	-1.07503
C	14.95149	-1.5899	-1.98682
H	13.33984	-0.18186	-1.69971
H	16.38755	-3.18303	-2.1489
H	15.60691	-0.86099	-2.45779
C	10.00366	5.641865	3.067765
H	8.918018	5.536342	3.172496

H	10.48369	5.075652	3.875977
H	10.26003	6.700653	3.199325
C	11.99033	5.291359	1.574894
H	12.28385	6.343498	1.679946
H	12.50416	4.718854	2.357516
H	12.34149	4.932913	0.600754
C	11.7907	-5.47053	-1.00758
H	10.97533	-6.03232	-0.53434
H	11.43376	-5.09605	-1.97363
H	12.61766	-6.16754	-1.19335
C	12.73907	-4.86114	1.234678
H	11.94158	-5.41366	1.747583
H	13.5836	-5.54641	1.088937
H	13.06782	-4.04627	1.889416
C	-12.6828	1.563375	-0.59974
C	-13.9377	1.11806	-0.1019
C	-15.0327	1.944894	-0.20418
C	-14.8903	3.221392	-0.80478
C	-13.6207	3.652201	-1.3034
C	-12.509	2.783672	-1.18517
C	-11.6697	0.52063	-0.37145
C	-12.3619	-0.59848	0.296919
C	-13.7682	-0.23625	0.458754
H	-16.0156	1.660294	0.159092
O	-10.4903	0.584117	-0.68019
C	-14.7809	-0.98324	1.02291
C	-16.1234	-0.51504	1.12576
N	-17.2273	-0.15727	1.223137
C	-14.6044	-2.29176	1.559735
N	-14.4804	-3.36178	2.003626
H	8.043271	-2.49142	1.207433
C	4.35826	-0.51437	-0.44761
C	4.82354	0.407514	0.499153
C	5.317016	-1.26974	-1.13713
C	6.174401	0.561158	0.75713
H	4.111607	1.021677	1.048696
C	6.67074	-1.10438	-0.90565
H	4.992803	-2.00838	-1.86728
C	7.12479	-0.19111	0.055789
H	6.505923	1.275295	1.50693
H	7.391799	-1.69604	-1.4641
C	2.936453	-0.69558	-0.71449
H	-11.5271	3.079576	-1.55188
C	-13.5145	4.930636	-1.89703

H	-12.5451	5.251428	-2.27415
C	-15.9999	4.092367	-0.92104
H	-16.963	3.758746	-0.53947
C	-15.8642	5.327986	-1.50171
H	-16.7242	5.987565	-1.58402
C	-14.6107	5.750866	-1.99396
H	-14.5166	6.732519	-2.45151

Table S10: Calculated energies (E) and energy gap (ΔE) for **MCPTR**, **MCPTD1**, **MCPTD2**, **MCPTD3**, **MCPTD4**, **MCPTD5**, **MCPTD6**, **MCPTD7** and **MCPTD8**.

System	$E_{(HOMO-1)}$	$E_{(LUMO-1)}$	ΔE	$E_{(HOMO-2)}$	$E_{(LUMO-2)}$	ΔE
MCPTR	-6.667	-1.648	5.019	-6.955	-0.819	6.136
MCPTD1	-5.698	-1.847	3.851	-6.212	-1.057	5.155
MCPTD2	-5.687	-2.418	3.269	-6.214	-1.909	4.305
MCPTD3	-5.719	-2.520	3.199	-6.229	-1.930	4.299
MCPTD4	-5.722	-2.569	3.153	-6.229	-1.936	4.293
MCPTD5	-5.726	-2.627	3.099	-6.230	-1.960	4.270
MCPTD6	-5.734	-2.703	3.780	-6.229	-1.974	4.255
MCPTD7	-5.762	-3.089	2.673	-6.236	-2.072	4.164
MCPTD8	-5.704	-2.304	3.400	-6.221	-1.947	4.274

E= energy, $\Delta E(eV) = E_{LUMO} - E_{HOMO}$; HOMO= highest occupied molecular orbital; LUMO= lowest unoccupied molecular orbital, MO, molecular orbital

Table S11: Dipole moments, dipole polarizability and major contributing tensor (a.u) of **(MCPTR – MCPTD8).**

System	α_{xx}	α_{yy}	α_{zz}	μ_x	μ_y	μ_z
MCPTR	868.3	564.5	244.6	-0.669	-2.910	-1.848
MCPTD1	1967.8	1239.7	715.8	1.052	-2.880	1.556
MCPTD2	2339.5	1007.5	1081.0	-4.031	-0.383	0.422
MCPTD3	2430.9	1379.5	696.0	-4.715	0.561	-0.268
MCPTD4	2473.9	1386.2	686.5	-4.341	0.778	-0.052
MCPTD5	2518.8	1472.2	699.3	-4.950	-0.701	0.154
MCPTD6	2560.5	1471.1	718.2	-4.605	-0.746	0.189
MCPTD7	2668.8	1493.9	700.2	-6.337	-3.325	-0.792
MCPTD8	2509.3	1563.6	716.7	-3.860	1.232	0.95

Table S12: The computed first-order hyperpolarizabilities (β_{tot}) and major contributing tensors (a.u) of the studied compounds **(MCPTR – MCPTD8).**

Compound	β_{xxx}	β_{xxy}	β_{xyy}	β_{yyy}	β_{xxz}	β_{yyz}	β_{xzz}	β_{yzz}	β_{zzz}
MCPTR	-23469.6	-1493.0	-49.1	343.8	-2612.2	95.6	-268.1	60.7	12.0
MCPTD1	74202.8	-2823.4	-948.3	-674.2	-829.9	-384.6	145.7	130.2	-55.9
MCPTD2	-145431	16235.8	-2046.2	884.9	16526.6	157.6	-3473.1	-552.8	538.2
MCPTD3	-190677	15355.4	-1103.0	-1658.1	-578.5	-1741.3	494.6	531.0	-257.0
MCPTD4	-213956	15659.2	-1185.1	-1614.1	-1702.9	-1611.3	432.4	-382.3	-164.2
MCPTD5	-221413	-14432.4	-578.0	3673.8	2347.7	2292.9	490.4	567.8	238.0
MCPTD6	-234466	-10854	440.3	3055.4	7854.0	2005.1	227.8	325.9	136.5

MCPTD7	-323771	-24682.8	-3571.6	-1480.9	2616.69	282.1	238.8	-204.1	-68.5
MCPTD8	-193705	-15936.1	1081.4	6106.6	4871.31	3172.3	625.7	696.4	200.6

Table S13: Second order hyper polarizability **<γ>** and major contributing tensor γ ($a.u.$) of the studied compounds **(MCPTR – MCPTD8).**

Systems	γ_x	γ_y	γ_z	**<γ>**
MCPTR	2.0926×10^{6}	3.4699×10^{4}	1.7853×10^{4}	2.1452×10^{6}
MCPTD1	1.2703×10^{7}	4.1332×10^{5}	9.2633×10^{4}	1.3209×10^{7}
MCPTD2	2.8913×10^{7}	8.2481×10^{5}	5.0194×10^{5}	3.02404×10^{7}
MCPTD3	4.0204×10^{7}	7.9625×10^{5}	9.7075×10^{4}	4.1097×10^{7}
MCPTD4	4.6731×10^{7}	8.0632×10^{5}	9.4683×10^{4}	4.7632×10^{7}
MCPTD5	4.8823×10^{7}	1.0162×10^{6}	1.2087×10^{5}	4.9960×10^{7}
MCPTD6	5.2915×10^{7}	9.4374×10^{5}	1.7328×10^{5}	5.4032×10^{7}
MCPTD7	8.4527×10^{7}	1.3547×10^{6}	1.4219×10^{5}	8.6024×10^{7}
MCPTD8	4.043×10^{7}	1.215×10^{6}	1.640×10^{5}	4.180×10^{7}

Table S14: Wave length, excitation energy and oscillator strength of investigated compound **(MCPTR)**

NO.	**DFT λ (*nm*)**	**E (eV)**	***f***	**MO contributions**
1	481.212(424)[a]	2.577	0.619	H→L (99%)
2	368.332	3.3661	0.3682	H-1→L (68%), H→L+1 (25%), H→L+2 (3%)
3	349.517	3.5473	0.21	H-2→L (14%), H-1→L (16%), H→L+1 (57%), H→L+2 (7%)
4	336.858	3.6806	0.3255	H-2→L (58%), H→L+1 (12%), H→L+2 (12%), H-1→L (8%), H-1→L+1 (3%), H-1→L+2 (2%)
5	315.795	3.9261	0.0039	H-2→L (24%), H-1→L+1 (23%), H→L+2 (38%), H-2→L+1 (6%)
6	297.788	4.1635	0.0196	H-2→L (24%), H-1→L+1 (23%), H→L+2 (38%), H-2→L+1 (6%),

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S15: Wave length, excitation energy and oscillator strength of investigated compound **(MCPTD1)**

NO.	**DFT λ (*nm*)**	**E (eV)**	***f***	**MO contributions**
1	547.050	2.2664	0.07388	H-1 → L (15%), H→ L (82%) H→ L+1 (2%)
2	470.168	2.6370	0.3224	H-1→ L (81%), H → L (16%)
3	435.978	2.8438	0.8646	H→ L+1 (85%), H → L+1 (5%), H→ L+2 (4%)
4	375.889	3.2984	0.1911	H-5→ L (13%), H-1→ L+1 (62%) H → L1 (5%), H-3→ L (8%),

				H→ L+1 (4%)
5	369.846	3.3523	0.0635	H-4→ L (11%), H-3→ L (46%), H-2 → L (12%), H-5→ L (4%), H-1→ L+1 (9%), H-1→ L+4 (3%), H→ L+2 (5%)
6	364.036	3.4058	0,1113	H-5 → L (39%), H-1→1→ L+1 (15%), H→ L+2 (20%), H-5 → L+1 (2%), H-3→ L (3%), H-2→ L (2%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S16: Wave length, excitation energy and oscillator strength of investigated compound (MCPTD2)

NO.	DFT λ (*nm*)	E (eV)	*f*	MO contributions
1	664.505	1.8658	0.4558	H-1→ L (11%), H→ L (87%)
2	569.070	2.1787	0.5143	H-1→ L (82%), H→ L (12%)
3	494.450	2.5075	0.2124	H-1→ L+1 (10%), H → L+1 (83%), H→ L+2 (3%)
4	445.855	2.7808	1.0276	H-4→ L (14%), H→ L+2 (51%), H-5 → L (9%), H-3 → L(8%), H-1 → L+2 (6%), H→ L+1 (2%), H → L+3 (2%)
5	440.626	2.8138	0.106	H-1→ L+1 (78%), H → L+1 (11%), H-4→ L+1 (2%), H-3 → L+1 (2%)
6	435.755	2.8518	0.1345	H-4→ L (19%), H-3→ L (28%), H→ L+2 (30%),H-5→ L (4%), H-2 → L(8%), H→ L+1 (2%

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength.

Table S17: Wave length, excitation energy and oscillator strength of investigated compound **(MCPTD3)**

NO.	DFT λ (*nm*)	E (eV)	*f*	MO contributions
1	697.123	1.7785	0.4535	H→L (90%), H-1→L (8%)
2	578.658	2.1426	0.5421	H-1→L (84%), H→L (9%)
3	517.827	2.3943	0.1583	H→L+1 (86%), H-1→L+1 (8%)
4	453.122	2.7362	0.9009	H-4→L (13%), H→L+2 (46%), H-5→L (9%), H-3→L (8 %)
5	451.736	2.7446	0.3275	H-1→L+1 (72%), H→L+1 (11%), H-4→L+1 (2%),
6	441.882	2.8058	0.1248	H-4→L (15%), H-3→L (31%), H-2→L(10 %), H→L+2 (33%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength.

Table S18: Wave length, excitation energy and oscillator strength of investigated compound **(MCPTD4)**

NO.	DFT λ (*nm*)	E (eV)	*f*	MO contributions
1	720.205	1.7215	0.4299	H → L (91%), H-1 →L (8%)
2	593.108	2.0904	0.5408	H-1→ L (86%), H→ L (9%)
3	529.052	2.3435	0.1662	H→L+1 (87%), H-1→ L+1 (8%)
4	459.266	2.6996	0.2444	H-1→ L+1 (77%), H→ L+1 (10%), H-4→ L+1 (2%), H-3→ L+1 (2%)
5	457.132	2.7122	0.8075	H-5→ L (13%), H-4 (20%), H-3→ L (20%), H→ L+2 (27%), H-2→ L (5%), H-1→ L (3%), H-1→ L+1 (6%), H-1→ L+2 (3%)
6	446.529	2.7766	0.3056	H-3 → L (23%), H-2→ L (11%), H→ L+2 (53%), H-4→ L (5%), H → L+3 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength.

Table S19: Wave length, excitation energy and oscillator strength of investigated compound **(MCPTD5)**

NO.	DFT λ (*nm*)	E (eV)	*f*	MO contributions
1	724.286	1.7118	0.4375	H→ L (91%), H-1 → L (8%)
2	596.246	2.0794	0.5567	H-1 → L (85%), H→ L (9%)
3	539.011	2.3002	0.1093	H → L+1 (88%), H-1→ L (2%), H-1 → L+1 (8%)
4	467.368	2.6528	0.1173	H-1 → L+1 (82%), H→L+1 (10%), H-4 → L+1 (2%), H-3→ L+1 (2%)
5	459.283	2.6995	1.0156	H-5 →L (12%), H-4→ L (18%), H-3→ L (18%), H→ L+2 (34%), H-1 → L (3%), H-1→ L+2 (4%)
6	448.840	2.7623	0.2484	H-3 → L (25%), H-2→ L (13%), H-4 → L (7%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength.

Table 20: Wave length, excitation energy and oscillator strength of investigated compound **(MCPTD6)**

NO.	DFT λ(*nm*)	E (eV)	*f*	MO contributions
1	743.667	1.6672	0.3876	H-1→L (92%),
2	609.738	2.0334	0.5522	H-1→L (86%), H→L (8%)
3	554.739	2.2350	0.0937	H→L+1 (88%), H-1→L (2%), H-1→L+1 (8%)

4	479.592	2.5852	0.1313	H-1→L+1 (83%), H-4→L+1 (2%), H-3→L+1 (2%), H→L+1 (9%)
5	464.482	2.6693	0.7603	H-5→L (14%), H-4→L (21%), H-3→L (30%), H→L+2 (14%) , H-1→L (3%), H-1→L+2 (3%)
6	452.348	2.7409	0.4850	H-3→L (15%), H-2→L (16%), H→L+2 (59%), H-1→L+2 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table 21: Wave length, excitation energy and oscillator strength of investigated Compound **(MCPTD7)**

NO.	DFT λ (*nm*)	E (eV)	*F*	MO contributions
1	832.33	1.4896	0.2774	H → L (94%), H-1→L (4%)
2	669.85	1.8509	0.4875	H-1 → L (22%), H → L+1 (66%), H-1→ L+1 (7%), H→ L (3%)
3	653.85	1.8962	0.1131	H-1 → L (69%), H → L+1 (26%), H→ L (2%)
4	552.51	2.2440	0.2039	H-1 → L+1 (87%), H→ L+1 (7%)
5	491.33	2.5234	0.286	H-4 → L (14%), H-3 → L (44%), H-2 → L (26%), H-5 →L (8%), H-1→L (3%)
6	477.96	2.5940	0.1161	H-3 → L (15%), H-2 → L (73%), H-5 → L (4%), H-4→ L (4%), H → L+2 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength.

Table S22: Wave length, excitation energy and oscillator strength of investigated Compound **(MCPTD8)**

NO.	DFT λ (*nm*)	E (eV)	*f*	MO contributions
1	691.60	1.7927	0.4879	H-1 → L (10%), H →L (89%)
2	581.04	2.1338	0.5772	H-1→ L (84%), H → L (11%)
3	475.58	2.6070	0.4446	H → L+1 (74%), H → L+2 (12%), H-1→ L+1 (7%)
4	452.44	2.7403	0.5511	H-4→ L (40%), H-3→ L (25%), H→ L+1 (10%), H-5 → L (5%), H-2→ L (3%), H→L (2%), H-1→ L+2 (3%), H→ L+2 (9%)
5	444.13	2.7916	0.3673	H-6→ L (11%), H → L+2 (54%), H-5→ L (7%), H-4→ L (8%), H-3 → L (4%), H-1→ L+1 (3%), H-1→ L+2 (3%), H → L+1 (4%)
6	434.91	2.8508	0.1283	H-6 → L (27%), H-5→ L (26%), H-3 → L (20%), H-4 → L (3%), H-2→ L(9%), H → L+1 (2%), H→ L+2 (8%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S23: Natural bond orbital (NBO) analysis of investigated compound **(MCPTR**)

Donor(i)	Type	Acceptor(j)	Type	E (2)[a] [kcal/mol]	E(J)E(i)[b] (a.u)	F(I→j) [c] (a.u)
C26-C28	π	C31-O32	π^*	24.36	0.31	0.079
C3-C4	π	C8-C15	π^*	22.41	0.29	0.072
C5-C6	π	C1-C2	π^*	20.91	0.3	0.072
C5-C6	π	C3-C4	π^*	18.37	0.29	0.067
C9-C11	π	C7-C10	π^*	17.66	0.3	0.069
C53-C54	π	C56-C58	π^*	15.98	0.3	0.063
C3-C4	π	C7-C10	π^*	13.88	0.3	0.062
C26-C28	π	C53-C54	π^*	9.95	0.31	0.052
C31-O32	π	C31-O32	π^*	0.75	0.42	0.017
O32	LP(2)	C31-O33	σ*	35.28	0.66	0.138
S55	LP(2)	C56-C58	π^*	25.1	0.28	0.075
S55	LP(2)	C53-C54	π^*	22.52	0.27	0.07
O32	LP(2)	C28-C31	σ*	20.86	0.73	0.112
N30	LP(1)	C28-C29	σ*	12.75	1.07	0.105
O33	LP(1)	C31-O32	σ*	8.19	1.19	0.088
O33	LP(2)	C34-H36	σ*	4.75	0.76	0.056
O33	LP(2)	C34-H37	σ*	4.55	0.76	0.055
O32	LP(1)	C28-C31	σ*	2.60	1.16	0.05
S55	LP(1)	C56-C58	σ*	2.30	1.25	0.048
S55	LP(1)	C53-C54	σ*	2.09	1.24	0.046
S55	LP(2)	C17-H18	σ*	1.48	0.71	0.032
O32	LP(1)	C31-O33	σ*	1.41	1.1	0.036
O33	LP(1)	C34-C35	σ*	1.01	1.01	0.03
O33	LP(1)	C34-H37	σ*	1.02	1.01	0.029
O33	LP(1)	C34-H36	σ*	1.00	1.01	0.028
O33	LP(1)	C26-H27	σ*	0.96	1.01	0.028
O32	LP(2)	C29-N30	π^*	0.87	0.39	0.017
O32	LP(2)	C34-C35	σ*	0.8	0.7	0.022
O33	LP(1)	C28-C31	σ*	0.68	1.03	0.024
O33	LP(1)	C35-C38	σ*	0.61	1.01	0.022
C26-H27	σ	C28-C29	σ*	6.92	1.07	0.077
C29-N30	σ	C28-C29	σ*	5.99	1.58	0.088
C28-C29	σ	C29-N30	σ*	5.47	1.6	0.084
C17-H18	σ	C4-C5	σ*	4.00	1.09	0.059
C38-H42	σ	C43-H46	σ*	3.00	0.92	0.047
C8-C15	σ	C14-H25	σ*	2.04	1.13	0.043
C56-H59	σ	C56-C58	σ*	1.96	1.11	0.042
C1-C6	σ	C1-H21	σ*	1.00	1.15	0.03
C34-C35	σ	C35-H40	σ*	0.51	1.06	0.021
C34-H36	σ	C34-C35	σ*	0.51	0.94	0.019
C35-H39	σ	C35-C38	σ*	0.51	0.91	0.019

Table S24: Natural bond orbital (NBO) analysis of **(MCPTD1**)

Donor(i)	Type	Acceptor(j)	Type	E(2)	E(J)E(i)b(a.u)	F(I→j)e(a.u)
C2-C3	π	C1-C6	π^*	25.17	0.28	0.076
C25-C27	π	C30-O31	π^*	24.34	0.31	0.079
C11-C12	π	C13-C14	π^*	22.04	0.3	0.073
C8-C9	π	C4-C5	π^*	21.99	0.28	0.07
C77-C79	π	C78-C80	π^*	20.00	0.3	0.069
C69-C73	π	C68-C71	π^*	19.25	0.3	0.069
C15-C16	π	C13-C14	π^*	16.44	0.31	0.067
C7-C10	π	C8-C9	π^*	14.41	0.31	0.063
C94-C110	π	C91-C93	π^*	13.72	0.3	0.058
C25-C27	π	C52-C53	π^*	9.99	0.31	0.052
C28-N29	π	C25-C27	π^*	7.14	0.38	0.049
C55-C57	π	C1-C6	π^*	6.48	0.32	0.042
C30-O31	π	C25-C27	π^*	3.98	0.43	0.039
C25-C27	π	C25-C27	π^*	2.21	0.32	0.024
C55-C57	π	C55-C57	π^*	0.66	0.3	0.013
O31	LP(2)	C30-O32	σ*	35.26	0.66	0.138
N76	LP(1)	C69-C73	π^*	24.99	0.29	0.079
S54	LP(2)	C55-C57	π^*	24.97	0.28	0.075
S61	LP(2)	C62-C64	π^*	23.61	0.29	0.074
S54	LP(2)	C52-C53	π^*	22.58	0.27	0.07
S61	LP(2)	C59-C60	π^*	22.50	0.29	0.072
O31	LP(2)	C27-C30	σ*	20.85	0.73	0.112
N76	LP(1)	C85-C86	π^*	19.69	0.29	0.07
N76	LP(1)	C77-C79	π^*	17.41	0.29	0.066
N29	LP(1)	C27-C28	σ*	12.76	1.07	0.105
O32	LP(1)	C30-O31	σ*	8.18	1.19	0.088
O32	LP(2)	C33-H35	σ*	4.78	0.76	0.056
O32	LP(2)	C33-H36	σ*	4.52	0.76	0.055
N76	LP(1)	C77-C78	σ*	3.53	0.84	0.052
N76	LP(1)	C77-C79	σ*	3.51	0.84	0.052
N76	LP(1)	C85-C87	σ*	3.17	0.84	0.049
N76	LP(1)	C85-C86	σ*	3.01	0.84	0.049
O31	LP(1)	C27-C30	σ*	2.60	1.16	0.05
N76	LP(1)	C71-C73	σ*	2.60	0.84	0.044
N76	LP(1)	C69-C73	σ*	2.57	0.84	0.044
S54	LP(1)	C55-C57	σ*	2.31	1.25	0.048
S61	LP(1)	C59-C60	σ*	2.12	1.25	0.046
S61	LP(1)	C62-C64	σ*	2.12	1.26	0.046
S54	LP(1)	C52-C53	σ*	2.09	1.24	0.046
O31	LP(1)	C30-O32	σ*	1.40	1.1	0.036
S54	LP(2)	C16-H17	σ*	1.37	0.71	0.031

O32	LP(1)	C33-C34	σ*	1.10	1.01	0.03
O32	LP(1)	C33-H36	σ*	1.05	1.01	0.029
O32	LP(1)	C33-H35	σ*	0.98	1.01	0.028
O32	LP(1)	C25-H26	σ*	0.94	1.01	0.028
O31	LP(2)	C28-N29	σ*	0.89	0.39	0.017
O31	LP(2)	C33-C34	σ*	0.81	0.7	0.022
O32	LP(1)	C27-C30	σ*	0.68	1.03	0.024
C25-H26	σ	C27-C28	σ*	6.92	1.07	0.077
C86-C93	σ	C91-C93	σ*	5.00	1.3	0.072
C77-C79	σ	C77-C78	σ*	4.00	1.29	0.064
C66-C68	σ	C68-C71	σ*	3.00	1.31	0.056
C55-C57	σ	C5-C6	σ*	2.01	1.31	0.046
C1-C6	σ	C1-H20	σ*	1.00	1.15	0.03
S54-C57	σ	C6-C57	σ*	0.51	1.17	0.022
C121-H124	σ	C98-C121	σ*	0.50	0.89	0.019

Table S25: Natural bond orbital (NBO) analysis of **(MCPTD2)**

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)b(a.u)**	**F(I→j)e(a.u)**
C104-C110	π	C111-N112	π^*	23.02	0.4	0.088
C47-C59	π	C41-C43	π^*	22.98	0.28	0.071
C96-C101	π	C102-O109	π^*	20.01	0.29	0.071
C49-C50	π	C51-C53	π^*	19.97	0.3	0.069
C37-C126	π	C34-C35	π^*	17.70	0.31	0.069
C34-C35	π	C37-C126	π^*	16.33	0.31	0.066
C116-C117	π	C37-C126	π^*	15.58	0.28	0.06
C25-C103	π	C27-C28	π^*	10.75	0.29	0.052
C11-C12	π	C34-C35	π^*	9.89	0.29	0.048
C102-O109	π	C96-C101	π^*	4.04	0.43	0.041
C102-O109	π	C25-C103	π^*	3.70	0.43	0.038
C113-N114	π	C111-N112	π^*	0.70	0.46	0.016
N40	LP(1)	C119-C123	π^*	25.12	0.29	0.079
S36	LP(2)	C37-C126	π^*	23.71	0.29	0.074
S36	LP(2)	C34-C35	π^*	22.56	0.29	0.072
S29	LP(2)	C27-C28	π^*	22.5	0.27	0.069
O109	LP(2)	C96-C102	σ*	21.82	0.76	0.117
O109	LP(2)	C102-C103	σ*	19.45	0.76	0.11
N40	LP(1)	C49-C50	π^*	18.42	0.29	0.068
N40	LP(1)	C41-C43	π^*	17.99	0.29	0.067
N112	LP(1)	C110-C111	σ*	13.41	1.06	0.107
N114	LP(1)	C110-C113	σ*	13.41	1.06	0.107
O109	LP(1)	C102-C103	σ*	3.60	1.18	0.059
N40	LP(1)	C41-C42	σ*	3.55	0.84	0.052
N40	LP(1)	C49-C51	σ*	3.49	0.84	0.051
N40	LP(1)	C41-C43	σ*	3.28	0.84	0.05

O109	LP(2)	S29-C32	σ*	3.22	0.51	0.037
N40	LP(1)	C49-C50	σ*	3.19	0.84	0.049
S29	LP(1)	C30-C32	σ*	2.60	1.24	0.051
N40	LP(1)	C119-C123	σ*	2.58	0.84	0.044
N40	LP(1)	C121-C123	σ*	2.55	0.84	0.044
S36	LP(1)	C37-C126	σ*	2.12	1.26	0.046
S36	LP(1)	C34-C35	σ*	2.11	1.25	0.046
S29	LP(1)	C27-C28	σ*	1.85	1.23	0.043
O109	LP(1)	S29-C32	σ*	1.79	0.93	0.037
S29	LP(2)	C16-H17	σ*	1.52	0.71	0.032
O109	LP(1)	C96-C102	σ*	1.30	1.19	0.035
C25-H26	σ	C102-C103	σ*	6.78	1	0.074
C96-C101	σ	C96-C97	σ*	5.00	1.3	0.072
C1-H20	σ	C2-C3	σ*	4.00	1.11	0.06
C116-C126	σ	C116-C118	σ*	3.00	1.27	0.055
N40-C49	σ	C119-C123	σ*	2.00	1.35	0.046
C98-C99	σ	C99-H106	σ*	1.00	1.17	0.031

Table S26: Natural bond orbital (NBO) analysis of **(MCPTD3)**

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)b(a.u)**	**F(I→j)e(a.u)**
C25-C103	π	C104-C108	π^*	25.98	0.3	0.079
C54-C56	π	C49-C50	π^*	23.03	0.28	0.072
C65-C67	π	C60-C64	π^*	21.00	0.3	0.072
C49-C50	π	C51-C53	π^*	20.02	0.3	0.069
C8-C9	π	C13-C14	π^*	19.80	0.29	0.068
C2-C3	π	C7-C10	π^*	17.02	0.31	0.068
C27-C28	π	C30-C32	π^*	16.52	0.3	0.063
C8-C9	π	C7-C10	π^*	15.10	0.3	0.064
C1-C6	π	C30-C32	π^*	12.31	0.27	0.052
C37-C126	π	C116-C117	π^*	11.73	0.32	0.058
C25-C103	π	C27-C28	π^*	10.73	0.29	0.052
C11-C12	π	C34-C35	π^*	9.34	0.29	0.047
C30-C32	π	C1-C6	π^*	7.44	0.32	0.044
C111-N112	π	C104-C108	π^*	6.76	0.38	0.049
C49-C50	π	C41-C43	π^*	0.71	0.29	0.013
C109-N110	π	C111-N112	π^*	0.70	0.46	0.016
S29	LP(2)	C30-C32	π^*	26.63	0.27	0.077
S36	LP(2)	C37-C126	π^*	23.63	0.29	0.073
S36	LP(2)	C34-C35	π^*	22.43	0.29	0.072
S29	LP(2)	C27-C28	π^*	22.35	0.27	0.069
O107	LP(2)	C96-C102	σ*	22.19	0.76	0.118
F115	LP(3)	C99-C100	π^*	21.62	0.44	0.095
F114	LP(3)	C99-C100	π^*	21.40	0.44	0.095
O107	LP(2)	C102-C103	σ*	19.40	0.76	0.11

N40	LP(1)	C49-C50	π^*	17.38	0.29	0.066
N40	LP(1)	C41-C43	π^*	14.92	0.29	0.061
N110	LP(1)	C108-C109	σ^*	13.43	1.06	0.107
N112	LP(1)	C108-C111	σ^*	13.43	1.06	0.107
F115	LP(2)	C99-C100	σ^*	8.30	0.97	0.08
F114	LP(2)	C99-C100	σ^*	8.22	0.97	0.08
F115	LP(2)	C100-C101	σ^*	6.87	1.01	0.075
F114	LP(2)	C98-C99	σ^*	6.72	1.01	0.074
N40	LP(1)	C41-C42	σ^*	3.98	0.84	0.055
N40	LP(1)	C41-C43	σ^*	3.86	0.84	0.054
N40	LP(1)	C49-C51	σ^*	3.62	0.84	0.052
O107	LP(1)	C102-C103	σ^*	3.62	1.18	0.059
N40	LP(1)	C49-C50	σ^*	3.41	0.84	0.051
O107	LP(2)	S29-C32	σ^*	3.18	0.51	0.037
S29	LP(1)	C30-C32	σ^*	2.6	1.24	0.051
S36	LP(1)	C34-C35	σ^*	2.12	1.25	0.046
S36	LP(1)	C37-C126	σ^*	2.11	1.26	0.046
N40	LP(1)	C121-C123	σ^*	2.03	0.83	0.039
N40	LP(1)	C119-C123	σ^*	1.92	0.84	0.038
S29	LP(1)	C27-C28	σ^*	1.86	1.23	0.043
O107	LP(1)	S29-C32	σ^*	1.78	0.94	0.037
F114	LP(1)	C98-C99	σ^*	1.63	1.63	0.046
F115	LP(1)	C100-C101	σ^*	1.63	1.63	0.046
S29	LP(2)	C16-H17	σ^*	1.55	0.71	0.033
O107	LP(1)	C96-C102	σ^*	1.31	1.18	0.036
F115	LP(1)	C99-C100	σ^*	1.05	1.59	0.037
F114	LP(1)	C99-C100	σ^*	0.98	1.59	0.036
C25-H26	σ	C102-C103	σ^*	6.77	1.00	0.074
C101-H106	σ	C96-C97	σ^*	5.06	1.11	0.067
C98-H105	σ	C96-C97	σ^*	4.00	1.11	0.06
C116-C118	σ	C118-C121	σ^*	3.01	1.31	0.056
C37-C126	σ	C116-C117	σ^*	2.01	1.31	0.046
C1-C6	σ	C1-H20	σ^*	1.00	1.15	0.03
C30-C32	σ	C27-S29	σ^*	0.51	0.93	0.02

TableS27: Natural bond orbital (NBO) analysis of **(MCPTD4)**

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)b(a.u)**	**F(I→j)e(a.u)**
C25-C103	π	C104-C107	π^*	26.74	0.3	0.08
C13-C14	π	C11-C12	π^*	23.09	0.29	0.073
C65-C67	π	C60-C64	π^*	21.00	0.3	0.072
C4-C5	π	C1-C6	π^*	20.01	0.28	0.068
C97-C98	π	C96-C101	π^*	19.80	0.29	0.069
C7-C10	π	C2-C3	π^*	17.53	0.31	0.069
C2-C3	π	C7-C10	π^*	16.99	0.31	0.068

C8-C9	π	C7-C10	π^*	15.14	0.3	0.065
C7-C10	π	C8-C9	π^*	14.44	0.31	0.063
C25-C103	π	C27-C28	π^*	10.71	0.29	0.052
C11-C12	π	C34-C35	π^*	9.44	0.29	0.047
C108-N109	π	C104-C107	π^*	6.79	0.38	0.049
C102-O106	π	C96-C101	π^*	4.22	0.41	0.041
S29	LP(2)	C30-C32	π^*	26.83	0.27	0.077
S36	LP(2)	C37-C125	π^*	23.64	0.29	0.073
O106	LP(2)	C96-C102	σ^*	23.56	0.75	0.121
F126	LP(3)	C96-C101	π^*	23	0.46	0.1
F113	LP(3)	C99-C100	π^*	22.47	0.44	0.097
S36	LP(2)	C34-C35	π^*	22.41	0.29	0.072
S29	LP(2)	C27-C28	π^*	22.27	0.26	0.069
F114	LP(3)	C99-C100	π^*	21.10	0.44	0.094
O106	LP(2)	C102-C103	σ^*	19.08	0.75	0.109
N40	LP(1)	C49-C50	π^*	17.39	0.29	0.066
N40	LP(1)	C41-C43	π^*	14.92	0.29	0.061
N109	LP(1)	C107-C108	σ^*	13.46	1.06	0.107
N111	LP(1)	C107-C110	σ^*	13.45	1.06	0.107
F126	LP(2)	C100-C101	σ^*	8.35	0.98	0.081
F113	LP(2)	C99-C100	σ^*	8.34	0.98	0.081
F114	LP(2)	C99-C100	σ^*	8.04	0.98	0.079
F114	LP(2)	C100-C101	σ^*	8.03	0.98	0.079
F126	LP(2)	C96-C101	σ^*	7.66	1.02	0.079
F113	LP(2)	C98-C99	σ^*	6.7	1.01	0.074
N40	LP(1)	C41-C42	σ^*	4.00	0.84	0.055
N40	LP(1)	C41-C43	σ^*	3.84	0.84	0.054
O106	LP(1)	C102-C103	σ^*	3.81	1.18	0.06
N40	LP(1)	C49-C51	σ^*	3.63	0.84	0.053
N40	LP(1)	C49-C50	σ^*	3.39	0.84	0.051
O106	LP(2)	S29-C32	σ^*	3.35	0.51	0.038
S29	LP(1)	C30-C32	σ^*	2.61	1.24	0.051
S36	LP(1)	C34-C35	σ^*	2.12	1.25	0.046
S36	LP(1)	C37-C125	σ^*	2.10	1.26	0.046
N40	LP(1)	C120-C122	σ^*	2.02	0.83	0.039
N40	LP(1)	C118-C122	σ^*	1.94	0.84	0.038
S29	LP(1)	C27-C28	σ^*	1.85	1.23	0.043
O106	LP(1)	S29-C32	σ^*	1.82	0.94	0.037
F126	LP(1)	C96-C101	σ^*	1.73	1.64	0.048
F113	LP(1)	C98-C99	σ^*	1.65	1.63	0.046
S29	LP(2)	C16-H17	σ^*	1.59	0.71	0.033
F114	LP(1)	C99-C100	σ^*	1.37	1.6	0.042
F114	LP(1)	C100-C101	σ^*	1.37	1.61	0.042

F126	LP(1)	C100-C101	σ^*	1.18	1.6	0.039
O106	LP(1)	C96-C102	σ^*	1.17	1.18	0.033
F113	LP(1)	C99-C100	σ^*	0.94	1.6	0.035
S29	LP(1)	C16-H17	σ^*	0.67	1.13	0.024
C25-H26	σ	C102-C103	σ^*	6.77	1	0.074
C37-H39	σ	S36-C125	σ^*	5.20	0.74	0.056
C12-H23	σ	C13-C14	σ^*	4.00	1.11	0.06
C115-C117	σ	C117-C120	σ^*	3.01	1.31	0.056
C28-H31	σ	C28-C30	σ^*	1.00	1.13	0.03
C28-H31	σ	C25-H26	σ^*	0.51	0.97	0.02

TableS28: Natural bond orbital (NBO) analysis of **(MCPTD5)**

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)b(a.u)**	**F(I→j)e(a.u)**
C25-C103	π	C104-C107	π^*	26.37	0.3	0.079
C2-C3	π	C1-C6	π^*	25.7	0.28	0.077
C62-C63	π	C65-C67	π^*	22.92	0.29	0.073
C99-C100	π	C97-C98	π^*	19.23	0.33	0.071
C96-C101	π	C102-O106	π^*	18.94	0.3	0.07
C34-C35	π	C37-C123	π^*	16.28	0.31	0.066
C15-C16	π	C4-C5	π^*	15.32	0.3	0.065
C4-C5	π	C15-C16	π^*	14.42	0.3	0.063
C57-C73	π	C54-C56	π^*	13.74	0.3	0.058
C60-C64	π	C47-C59	π^*	13.70	0.3	0.058
C1-C6	π	C30-C32	π^*	12.75	0.27	0.053
C104-C107	π	C97-C98	π^*	9.05	0.32	0.05
C104-C107	π	C25-C103	π^*	7.77	0.33	0.046
C102-O106	π	C96-C101	π^*	4.16	0.43	0.041
C102-O106	π	C25-C103	π^*	3.66	0.43	0.038
S29	LP(2)	C30-C32	π^*	26.8	0.27	0.077
S36	LP(2)	C37-C123	π^*	23.64	0.29	0.073
S36	LP(2)	C34-C35	π^*	22.43	0.29	0.072
O106	LP(2)	C96-C102	σ^*	22.29	0.76	0.118
S29	LP(2)	C27-C28	π^*	22.28	0.27	0.069
O106	LP(2)	C102-C103	σ^*	19.38	0.76	0.11
N40	LP(1)	C49-C50	π^*	17.03	0.29	0.065
Cl125	LP(3)	C99-C100	π^*	16.02	0.31	0.07
Cl126	LP(3)	C99-C100	π^*	15.77	0.31	0.069
N40	LP(1)	C41-C43	π^*	15.26	0.29	0.061
N109	LP(1)	C107-C108	σ^*	13.45	1.06	0.107
N111	LP(1)	C107-C110	σ^*	13.44	1.06	0.107
Cl125	LP(2)	C99-C100	σ^*	5.38	0.86	0.061
Cl126	LP(2)	C99-C100	σ^*	5.25	0.86	0.06
Cl125	LP(2)	C100-C101	σ^*	3.97	0.89	0.053
N40	LP(1)	C41-C42	σ^*	3.95	0.84	0.055

Cl126	LP(2)	C98-C99	σ*	3.90	0.89	0.053
N40	LP(1)	C41-C43	σ*	3.77	0.84	0.054
N40	LP(1)	C49-C51	σ*	3.69	0.84	0.053
O106	LP(1)	C102-C103	σ*	3.63	1.18	0.059
N40	LP(1)	C49-C50	σ*	3.44	0.84	0.051
O106	LP(2)	S29-C32	σ*	3.19	0.51	0.037
S29	LP(1)	C30-C32	σ*	2.59	1.24	0.051
S36	LP(1)	C34-C35	σ*	2.12	1.25	0.046
S36	LP(1)	C37-C123	σ*	2.10	1.26	0.046
N40	LP(1)	C118-C120	σ*	2.02	0.83	0.039
N40	LP(1)	C116-C120	σ*	1.96	0.84	0.039
S29	LP(1)	C27-C28	σ*	1.86	1.23	0.043
O106	LP(1)	S29-C32	σ*	1.79	0.94	0.037
S29	LP(2)	C16-H17	σ*	1.63	0.71	0.034
Cl125	LP(1)	C100-C101	σ*	1.45	1.51	0.042
Cl126	LP(1)	C98-C99	σ*	1.45	1.50	0.042
Cl125	LP(1)	C99-C100	σ*	1.37	1.47	0.041
O106	LP(1)	C96-C102	σ*	1.31	1.18	0.036
Cl126	LP(1)	C99-C100	σ*	1.29	1.47	0.039
O106	LP(1)	C96-C102	σ*	1.17	1.18	0.033
F113	LP(1)	C99-C100	σ*	0.94	1.60	0.035
S29	LP(1)	C16-H17	σ*	0.69	1.13	0.025
S29	LP(1)	C16-H17	σ*	0.67	1.13	0.024
Cl126	LP(2)	C97-C98	σ*	0.54	0.91	0.02
Cl125	LP(2)	C96-C101	σ*	0.52	0.93	0.02
C25-H26	σ	C102-C103	σ*	6.74	1.00	0.074
C57-C73	σ	C57-C71	σ*	4.91	1.3	0.071
C65-H69	σ	C62-C63	σ*	3.78	1.13	0.058
C34-C35	σ	C37-H39	σ*	2.77	1.18	0.051
C102-O106	σ	C102-C103	σ*	1.69	1.57	0.047
C30-C32	σ	C27-S29	σ*	0.52	0.93	0.02

Table S29: Natural bond orbital (NBO) analysis of **(MCPTD6)**

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)b(a.u)**	**F(I→j)e(a.u)**
C25-C103	π	C104-C107	π^*	27.31	0.29	0.08
C97-C98	π	C96-C101	π^*	23.00	0.28	0.073
C65-C67	π	C60-C64	π^*	21.00	0.3	0.072
C4-C5	π	C1-C6	π^*	20.00	0.28	0.068
C99-C100	π	C96-C101	π^*	18.31	0.32	0.069
C99-C100	π	C97-C98	π^*	18.25	0.33	0.07
C37-C123	π	C34-C35	π^*	17.83	0.31	0.069
C8-C9	π	C7-C10	π^*	15.13	0.3	0.065
C7-C10	π	C8-C9	π^*	14.46	0.31	0.063
C11-C12	π	C34-C35	π^*	9.02	0.29	0.046

C104-C107	π	C25-C103	π*	7.97	0.33	0.047
C110-N111	π	C108-N109	π*	0.72	0.46	0.016
S29	LP(2)	C30-C32	π*	26.90	0.27	0.077
O106	LP(2)	C96-C102	∂*	23.96	0.74	0.121
S36	LP(2)	C37-C123	π*	23.65	0.29	0.074
S36	LP(2)	C34-C35	π*	22.48	0.29	0.072
S29	LP(2)	C27-C28	π*	22.22	0.26	0.069
O106	LP(2)	C102-C103	∂*	18.85	0.76	0.109
N40	LP(1)	C49-C50	π*	17.21	0.29	0.065
Cl124	LP(3)	C99-C100	π*	16.58	0.31	0.071
Cl125	LP(3)	C99-C100	π*	16.33	0.31	0.07
Cl126	LP(3)	C96-C101	π*	15.86	0.34	0.071
N40	LP(1)	C41-C43	π*	15.19	0.29	0.061
N109	LP(1)	C107-C108	σ*	13.50	1.06	0.107
N111	LP(1)	C107-C110	σ*	13.47	1.06	0.107
Cl125	LP(2)	C99-C100	σ*	5.47	0.86	0.061
Cl126	LP(2)	C100-C101	σ*	5.18	0.85	0.059
Cl124	LP(2)	C100-C101	σ*	5.11	0.85	0.059
Cl124	LP(2)	C99-C100	σ*	5.02	0.86	0.059
Cl126	LP(2)	C96-C101	σ*	4.75	0.9	0.059
N40	LP(1)	C41-C42	σ*	3.95	0.84	0.055
N40	LP(1)	C41-C43	σ*	3.80	0.84	0.054
Cl125	LP(2)	C98-C99	σ*	3.73	0.89	0.052
N40	LP(1)	C49-C51	σ*	3.66	0.84	0.053
O106	LP(1)	C102-C103	σ*	3.63	1.18	0.059
N40	LP(1)	C49-C50	σ*	3.42	0.84	0.051
O106	LP(2)	S29-C32	σ*	3.23	0.51	0.037
S29	LP(1)	C30-C32	σ*	2.60	1.24	0.051
S36	LP(1)	C34-C35	σ*	2.13	1.25	0.046
S36	LP(1)	C37-C123	σ*	2.11	1.26	0.046
N40	LP(1)	C118-C120	σ*	2.04	0.83	0.039
N40	LP(1)	C116-C120	σ*	1.96	0.84	0.039
S29	LP(1)	C27-C28	σ*	1.85	1.23	0.043
O106	LP(1)	S29-C32	σ*	1.82	0.94	0.037
S29	LP(2)	C16-H17	σ*	1.70	0.71	0.034
Cl126	LP(1)	C96-C101	σ*	1.56	1.52	0.044
Cl124	LP(1)	C99-C100	σ*	1.48	1.48	0.042
Cl125	LP(1)	C98-C99	σ*	1.47	1.51	0.042
Cl124	LP(1)	C100-C101	σ*	1.46	1.47	0.042
Cl126	LP(1)	C100-C101	σ*	1.41	1.47	0.041
Cl125	LP(1)	C99-C100	σ*	1.27	1.47	0.039
O106	LP(1)	C96-C102	σ*	1.24	1.16	0.034
S29	LP(1)	C16-H17	σ*	0.75	1.13	0.026

C25-H26	σ	C102-C103	σ^*	6.84	1	0.074
C108-N109	σ	C107-C108	σ^*	6.28	1.57	0.089
C35-C37	σ	C113-C123	σ^*	4.70	1.2	0.067
C3-C4	σ	C3-C7	σ^*	3.01	1.24	0.055
C35-H38	σ	C34-C35	σ^*	2.01	1.12	0.042
C25-H26	σ	C25-C27	σ^*	1.00	1.08	0.03

TableS30: Natural bond orbital (NBO) analysis of **(MCPTD7)**

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)b(a.u)**	**F(I→j)e(a.u)**
C25-C103	π	C104-C107	π^*	27.52	0.29	0.08
C54-C56	π	C49-C50	π^*	23.06	0.28	0.072
C62-C63	π	C65-C67	π^*	22.93	0.29	0.073
C65-C67	π	C60-C64	π^*	21.00	0.3	0.072
C49-C50	π	C51-C53	π^*	20.04	0.3	0.069
C8-C9	π	C13-C14	π^*	19.75	0.29	0.068
C96-C101	π	C102-O106	π^*	17.64	0.3	0.068
C27-C28	π	C30-C32	π^*	16.7	0.29	0.063
C7-C10	π	C3-C4	π^*	15.97	0.31	0.067
C5-C6	π	C15-C16	π^*	15.34	0.31	0.065
C102-O106	π	C96-C101	π^*	4.25	0.42	0.041
C102-O106	π	C25-C103	π^*	3.66	0.43	0.038
C30-C32	π	C30-C32	π^*	1.12	0.29	0.016
C49-C50	π	C41-C43	π^*	0.72	0.29	0.013
C108-N109	π	C110-N111	π^*	0.70	0.46	0.016
S36	LP(2)	C37-C123	π^*	27.26	0.29	0.074
O106	LP(2)	C96-C102	σ^*	23.68	0.75	0.118
S36	LP(2)	C34-C35	π^*	22.80	0.29	0.072
S29	LP(2)	C27-C28	π^*	22.41	0.26	0.068
O106	LP(2)	C102-C103	σ^*	21.90	0.76	0.11
O106	LP(2)	S29-C32	σ^*	19.20	0.51	0.036
S29	LP(2)	C16-H17	σ^*	16.94	0.71	0.034
N40	LP(1)	C116-C120	π^*	14.83	0.29	0.085
N40	LP(1)	C49-C50	π^*	13.51	0.29	0.065
N40	LP(1)	C41-C43	π^*	13.48	0.29	0.06
N109	LP(1)	C107-C108	σ^*	13.2	1.06	0.107
N111	LP(1)	C107-C110	σ^*	13.18	1.06	0.107
N128	LP(1)	C99-C127	σ^*	4.00	1.06	0.106
N126	LP(1)	C100-C125	σ^*	3.85	1.07	0.106
N40	LP(1)	C41-C42	σ^*	3.69	0.84	0.055
N40	LP(1)	C41-C43	σ^*	3.67	0.84	0.054
N40	LP(1)	C49-C51	σ^*	3.45	0.84	0.053
O106	LP(1)	C102-C103	σ^*	3.11	1.19	0.06
N40	LP(1)	C49-C50	σ^*	2.59	0.84	0.051
S29	LP(1)	C30-C32	σ^*	2.12	1.23	0.051

S36	LP(1)	C34-C35	σ*	2.11	1.25	0.046
S36	LP(1)	C37-C123	σ*	1.96	1.26	0.046
N40	LP(1)	C118-C120	σ*	1.88	0.83	0.039
N40	LP(1)	C116-C120	σ*	1.86	0.84	0.038
S29	LP(1)	C27-C28	σ*	1.74	1.22	0.043
O106	LP(1)	S29-C32	σ*	1.65	0.94	0.036
O106	LP(1)	C96-C102	σ*	1.30	1.17	0.035
C25-H26	σ	C102-C103	σ*	6.66	1.01	0.074
C73-C76	σ	C56-C57	σ*	4.88	1.23	0.069
C12-H23	σ	C13-C14	σ*	4.00	1.11	0.06
C13-C14	σ	C8-C14	σ*	3.98	1.28	0.064
C35-H38	σ	C34-C35	σ*	2.00	1.12	0.042
C114-H117	σ	C113-C114	σ*	1.00	1.11	0.03

Table S31: Natural bond orbital (NBO) analysis of **(MCPTD8)**

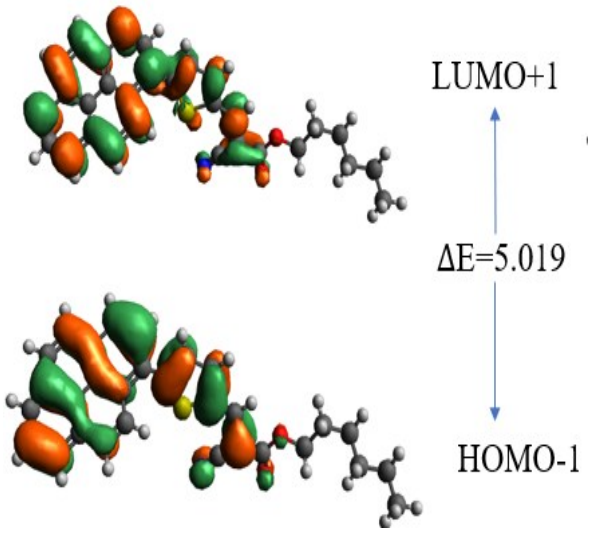
Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)b(a.u)**	**F(I→j)e(a.u)**
C25-C103	π	C104-C107	π^*	25.87	0.3	0.079
C116-C120	π	C113-C114	π^*	24.29	0.30	0.077
C71-C72	π	C74-C76	π^*	22.92	0.29	0.073
C49-C50	π	C54-C56	π^*	22.50	0.31	0.076
C115-C118	π	C116-C120	π^*	21.37	0.29	0.073
C62-C63	π	C60-C64	π^*	21.01	0.3	0.072
C51-C53	π	C54-C56	π^*	20.99	0.31	0.073
C97-C98	π	C104-C107	π^*	20.16	0.29	0.068
C2-C3	π	C4-C5	π^*	19.60	0.29	0.068
C96-C101	π	C97-C98	π^*	17.98	0.31	0.067
C8-C9	π	C7-C10	π^*	15.05	0.3	0.064
C7-C10	π	C8-C9	π^*	14.47	0.31	0.064
C60-C64	π	C47-C59	π^*	13.69	0.3	0.058
C127-C129	π	C90-C100	π^*	18.35	0.29	0.069
C113-C114	π	C37-C123	π^*	15.88	0.28	0.060
C99-C100	π	C96-C101	π^*	17.47	0.29	0.068
C99-C100	π	C97-C98	π^*	18.22	0.29	0.068
C99-C100	π	C125-C131	π^*	16.27	0.29	0.066
C97-C98	π	C96-C101	π^*	17.72	0.32	0.068
C97-C98	π	C99-C100	π^*	16.43	0.30	0.066
S29	LP(2)	C27-C28	π^*	22.47	0.27	0.069
S36	LP(2)	C34-C35	π^*	22.55	0.29	0.72
S36	LP(2)	C37-C123	π^*	23.61	0.29	0.73
N40	LP(1)	C41-C43	π^*	15.85	0.29	0.063
N40	LP(1)	C49-C50	π^*	3.08	0.84	0.049
N40	LP(1)	C49-C50	π^*	19.20	0.29	0.069
O106	LP(2)	C96-C102	σ*	21.67	0.77	0.117
O106	LP(2)	C102-C103	σ*	19.44	0.75	0.110

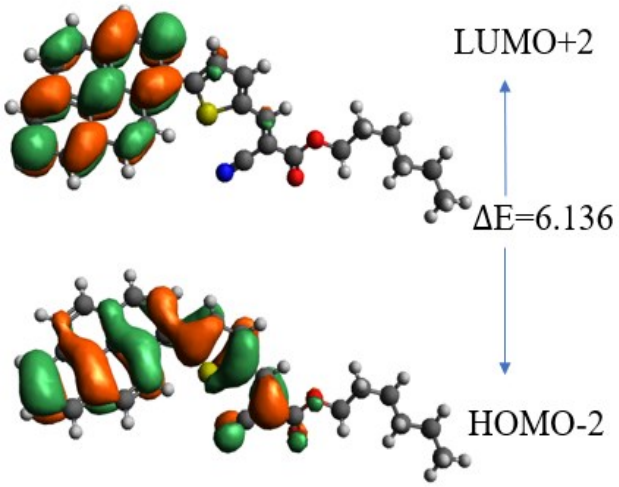
N109	LP(1)	C107-C108	σ^*	13.38	1.07	0.107
N111	LP(1)	C107-C110	σ^*	13.40	1.07	0.107
O106	LP(1)	C102-C103	σ^*	3.61	1.18	0.059
N40	LP(1)	C41-C42	σ^*	3.87	0.84	0.054
C50-C56	σ	C54-C56	σ^*	4.99	1.3	0.072
C2-H21	σ	C1-C6	σ^*	4.20	1.09	0.060
C2-H21	σ	C3-C4	σ^*	4.71	1.09	0.064
C25-C103	σ	C25-C27	σ^*	4.37	1.30	0.067
C27-C28	σ	C25-C27	σ^*	4.18	1.27	0.065
C57-C71	σ	C50-C56	σ^*	4.10	1.29	0.065
C57-C71	σ	C57-C73	σ^*	4.36	1.28	0.067
C7-H19	σ	C9-C10	σ^*	4.76	1.07	0.064
C8-C14	σ	C8-C9	σ^*	3.63	1.25	0.060
C10-H22	σ	C3-C7	σ^*	4.67	1.08	0.063
C15-C18	σ	C8-C14	σ^*	4.33	1.10	0.062
C15-C18	σ	C5-C16	σ^*	4.89	1.07	0.064
C57-C73	σ	C54-C56	σ^*	4.08	1.24	0.063
C56-C57	σ	C50-C56	σ^*	3.69	1.26	0.061
C57-C71	σ	C50-C56	σ^*	4.10	1.29	0.065
C42-C44	σ	N40-C41	σ^*	4.09	1.13	0.061
C127-H128	σ	C129-C131	σ^*	4.00	1.09	0.059
C99-C100	σ	C100-C101	σ^*	3.00	1.25	0.055
N40-C49	σ	C116-C120	σ^*	2.01	1.35	0.047
N40-C41	σ	N40-C49	σ^*	1.98	1.2	0.044
C1-C6	σ	C1-H20	σ^*	1.00	1.15	0.03

[a] E (2) means energy of hyper conjugative interaction (stabilization energy).

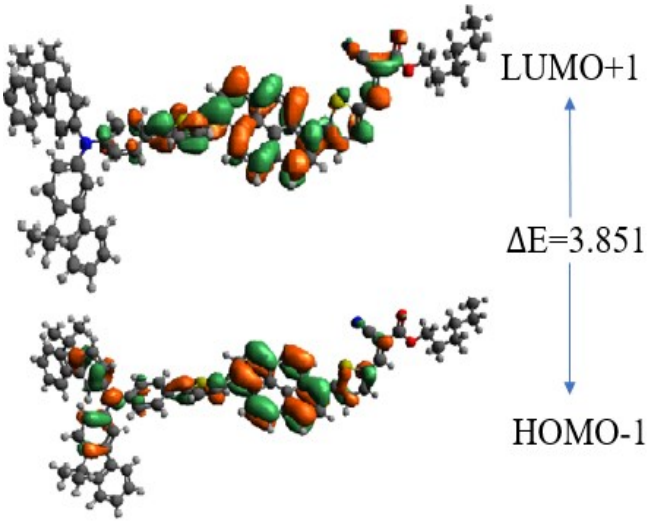
[b] Energy difference between donor and acceptor i and j NBO orbitals.

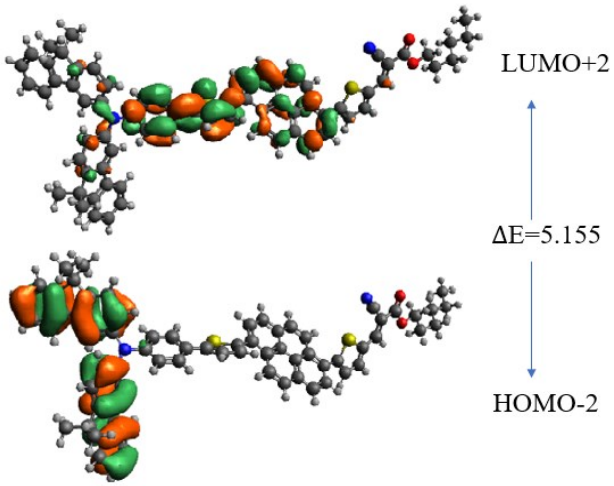
[c] F(i→j) is the Fock matrix element between i and j NBO orbitals.



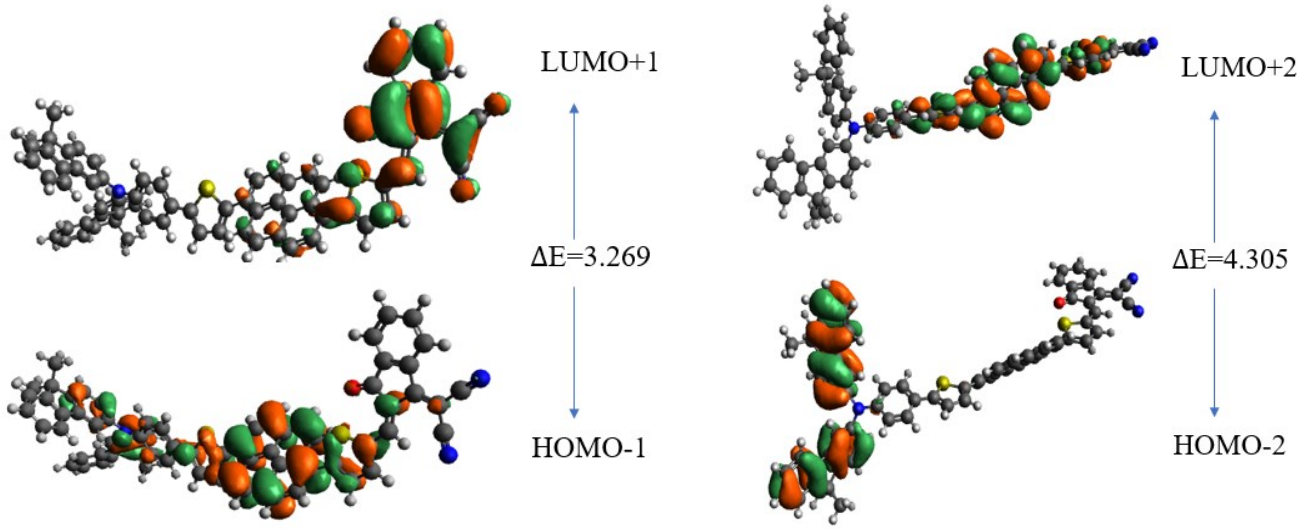


MCPTR

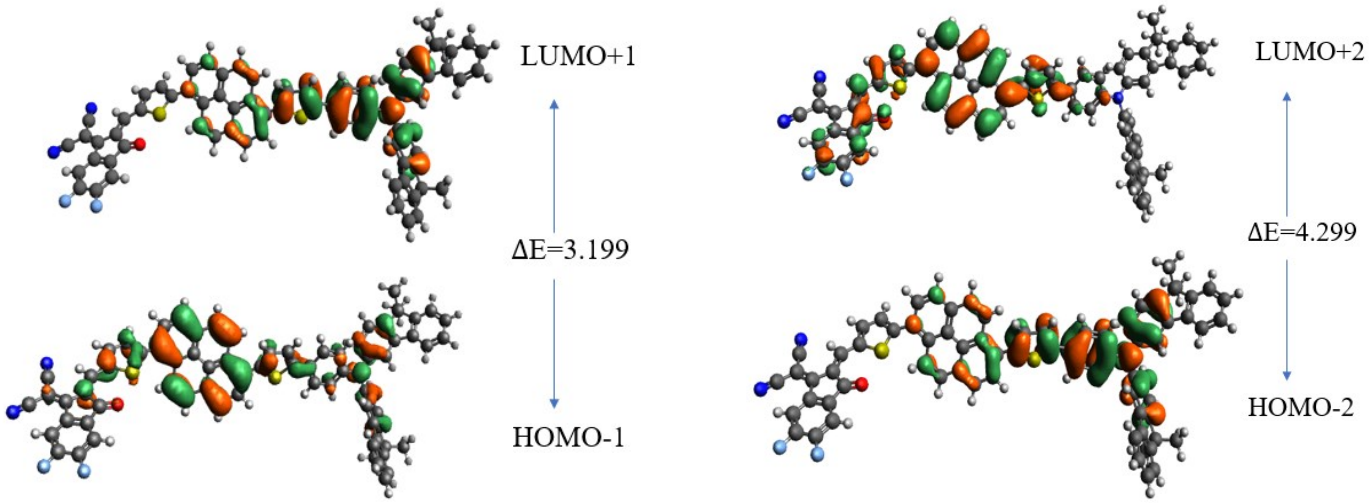




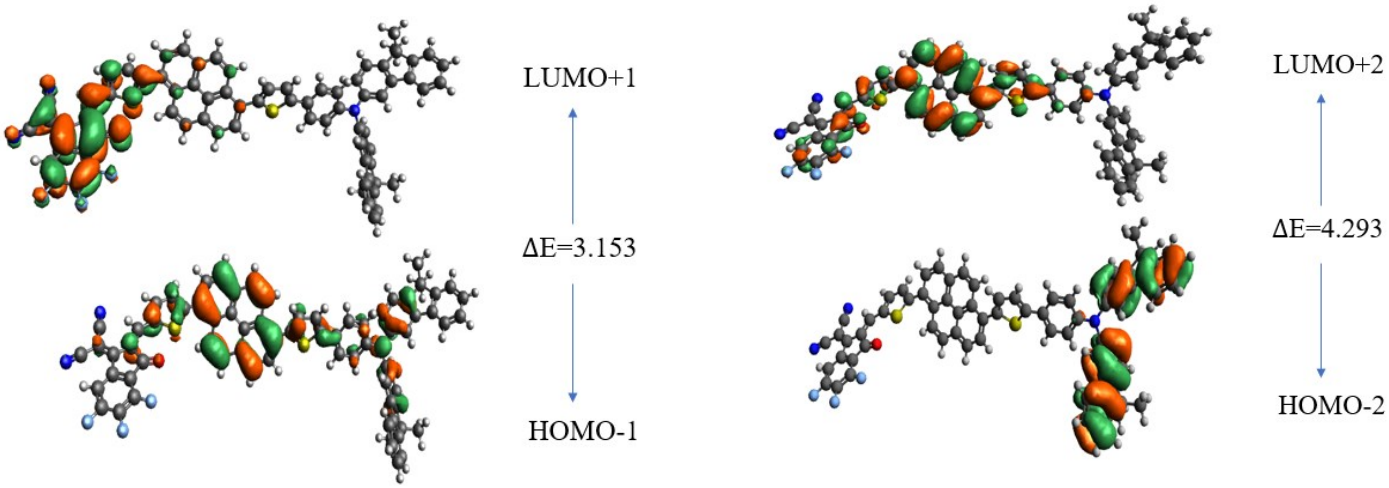
MCPTD1



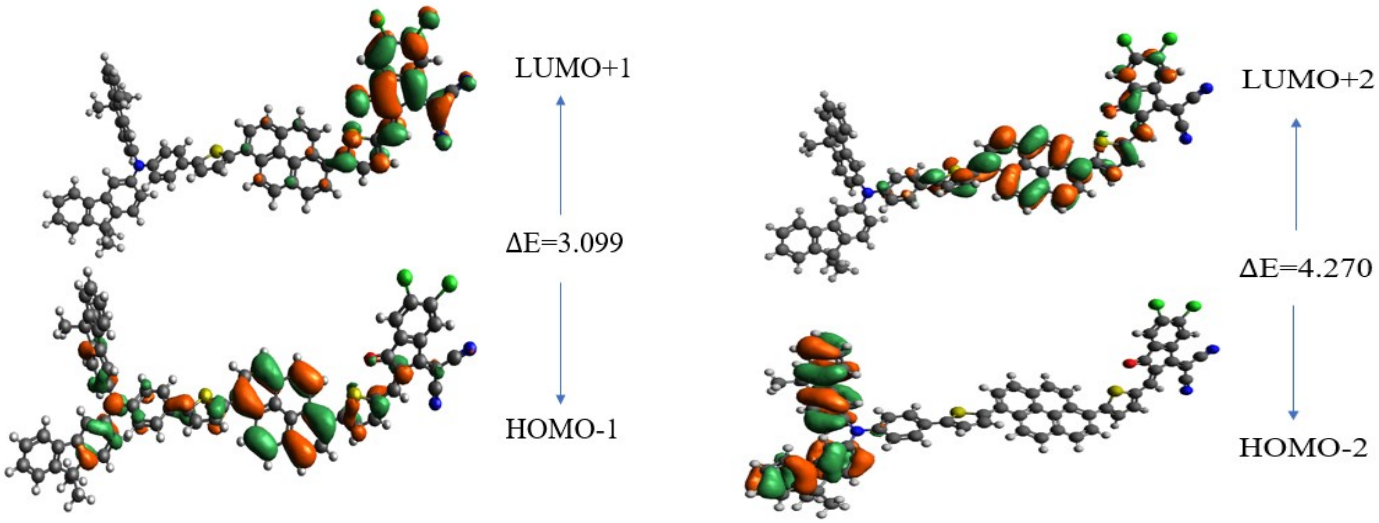
MCPTD2



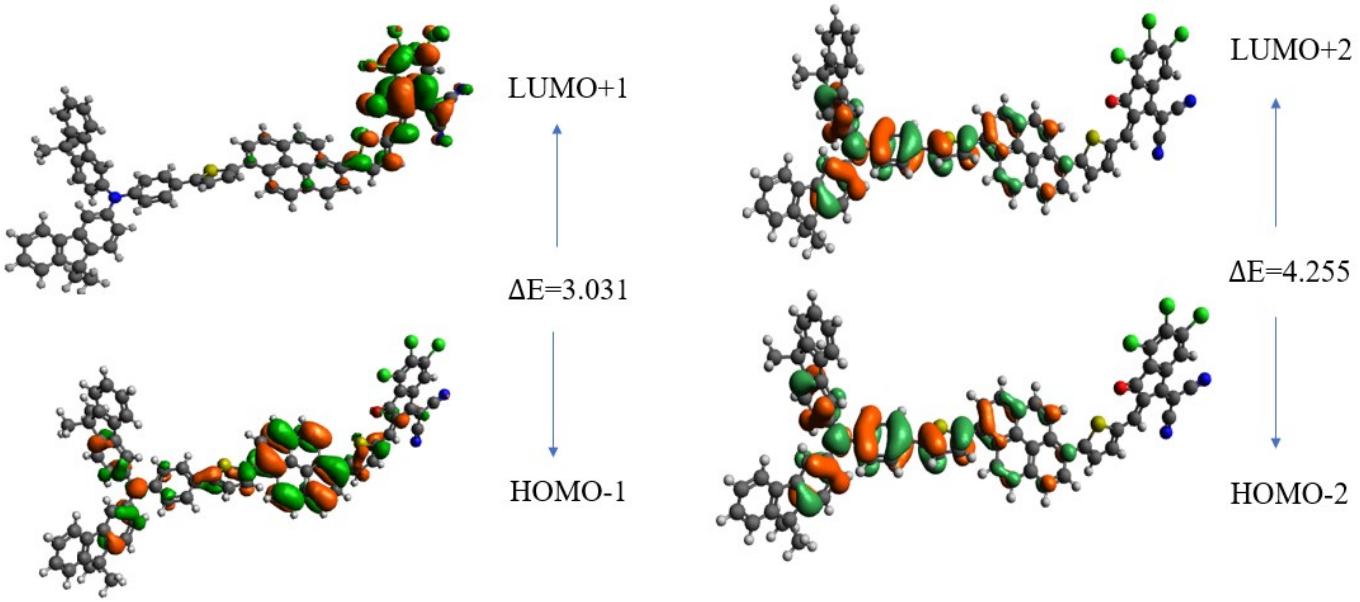
MCPTD3



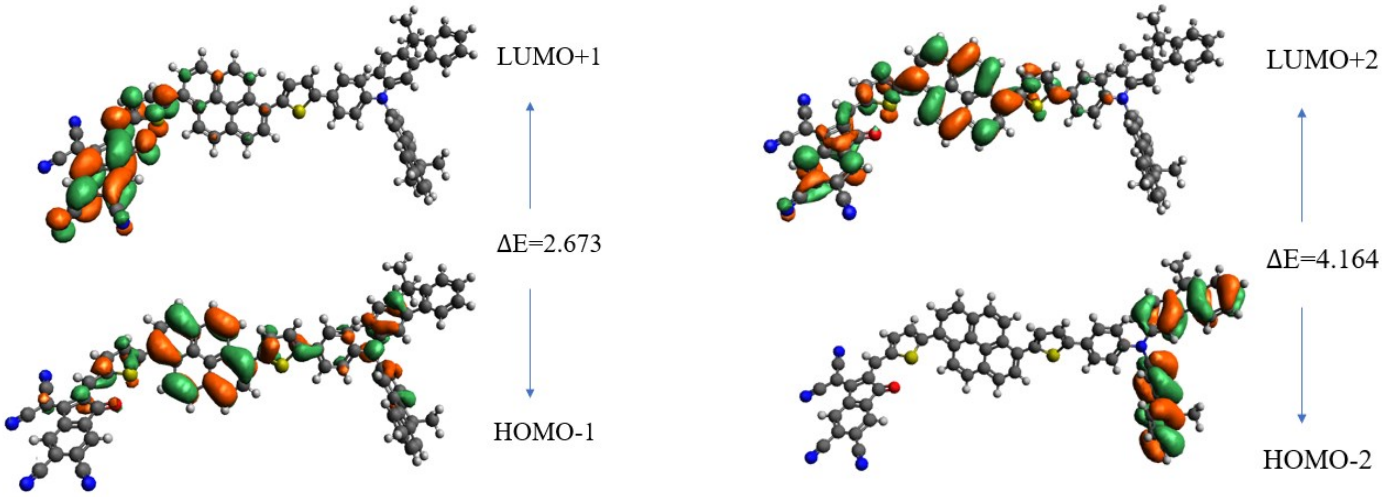
MCPTD4



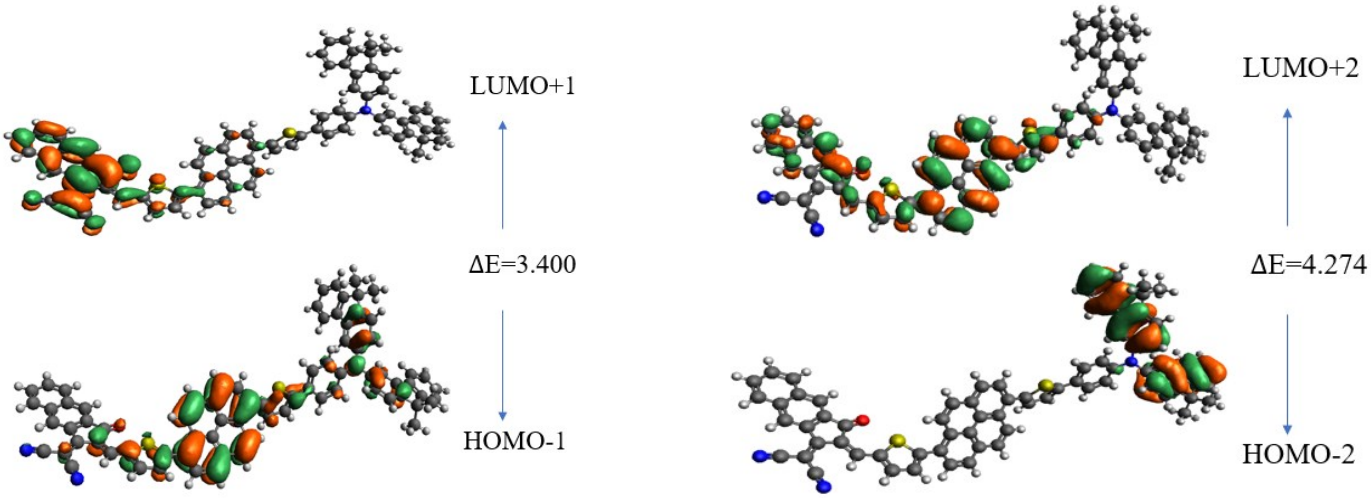
MCPTD5



MCPTD6



MCPTD7



MCPTD8

Figure S1:Pictographic display of HOMO and LUMO of MCPTR-MCPTD8

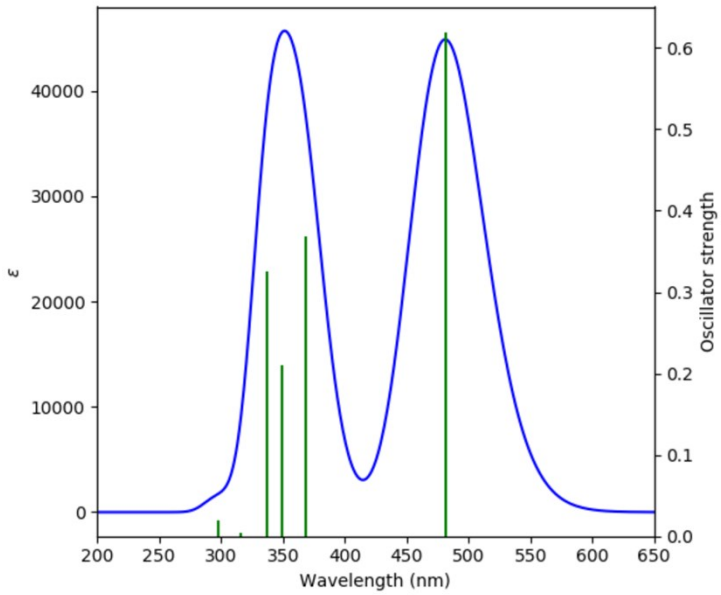


Figure S2: Graph of investigated compound **MCPTR**

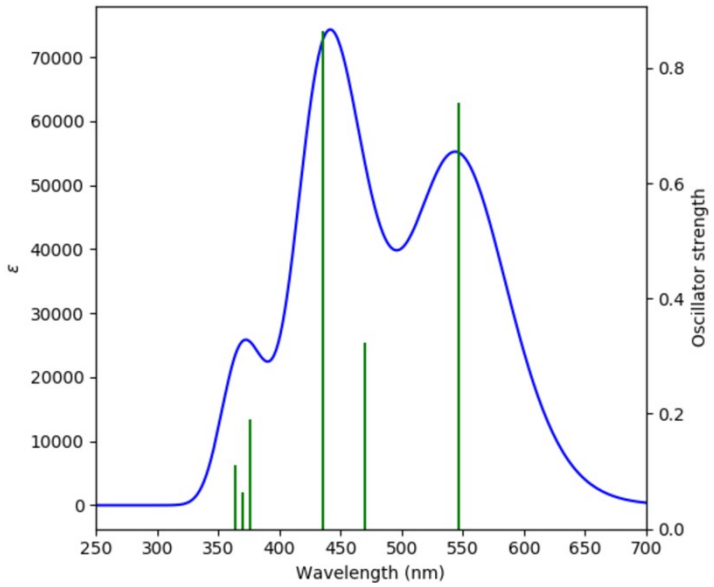


Figure S3: Graph of investigated compound **MCPTD1**

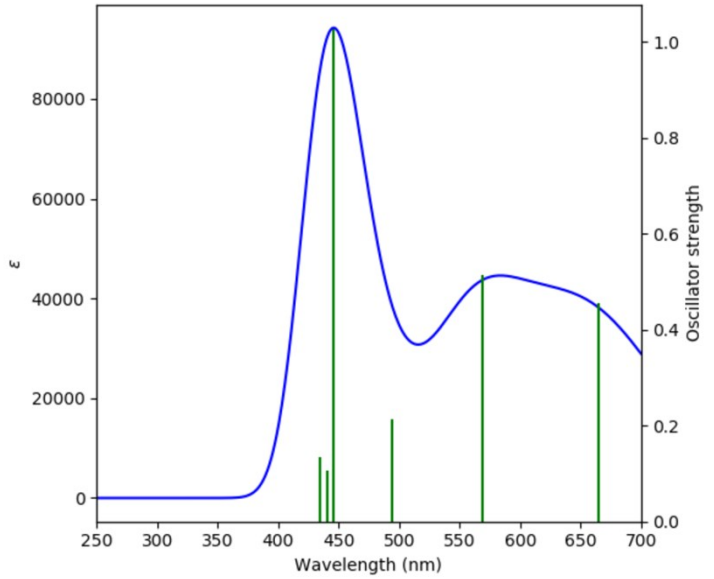


Figure S4: Graph of investigated compound **MCPTD2**

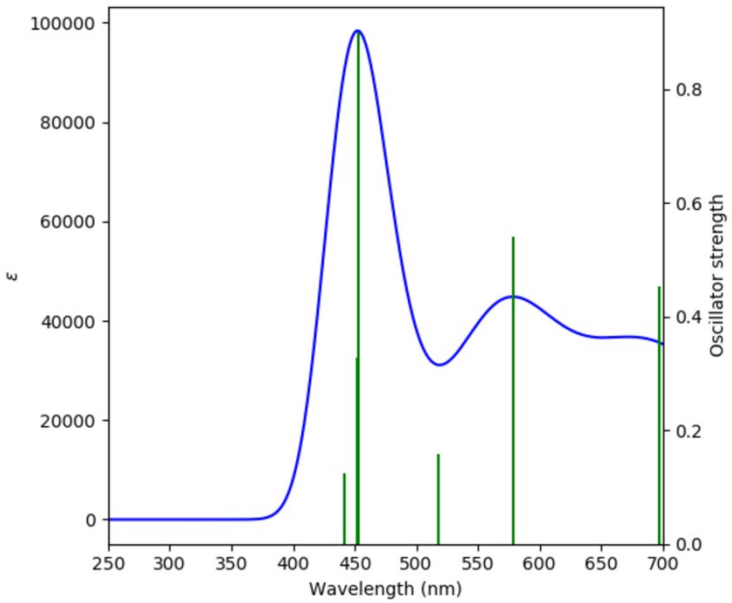


Figure S5: Graph of investigated compound **MCPTD3**

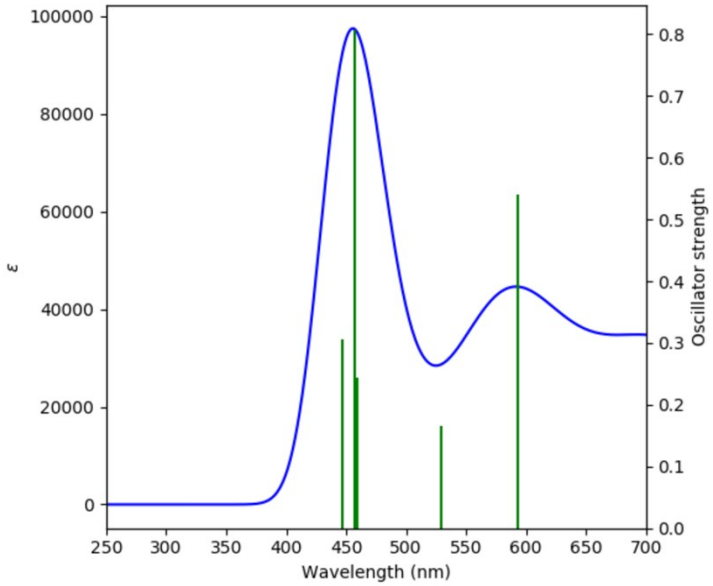


Figure S6: Graph of investigated compound **MCPTD4**

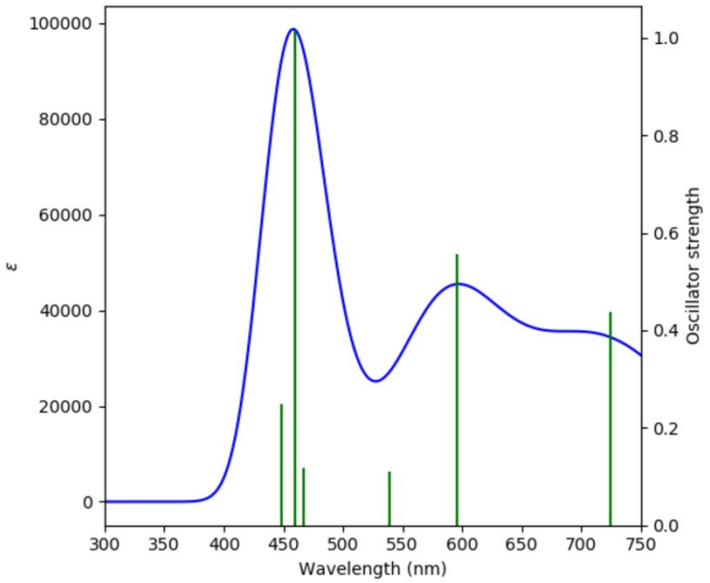


Figure S7: Graph of investigated compound **MCPTD5**

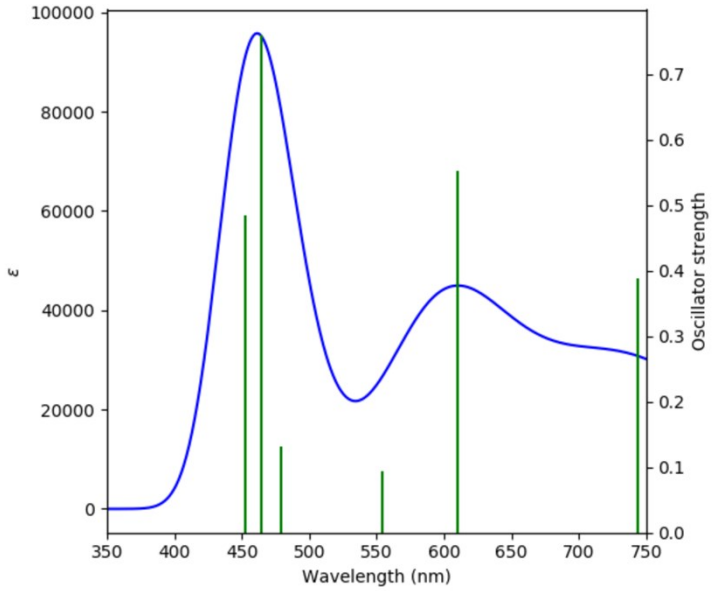


Figure S8: Graph of investigated compound **MCPTD6**

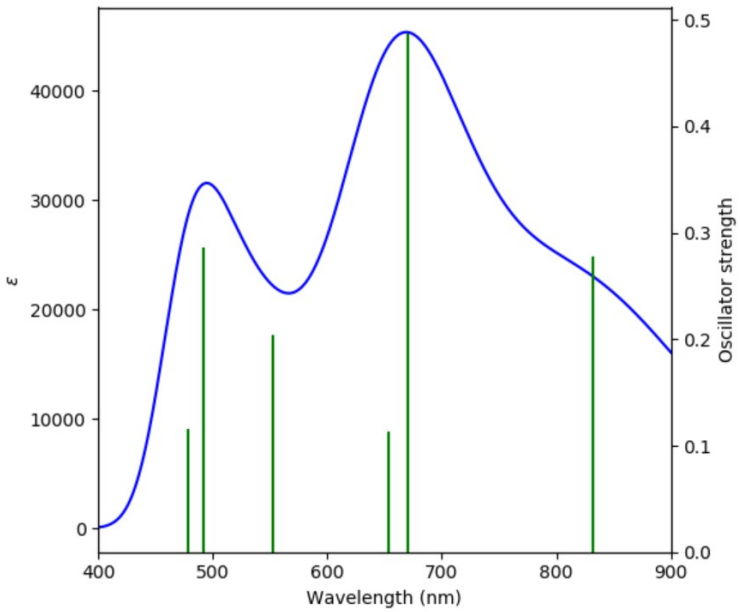


Figure S9: Graph of investigated compound **MCPTD7**

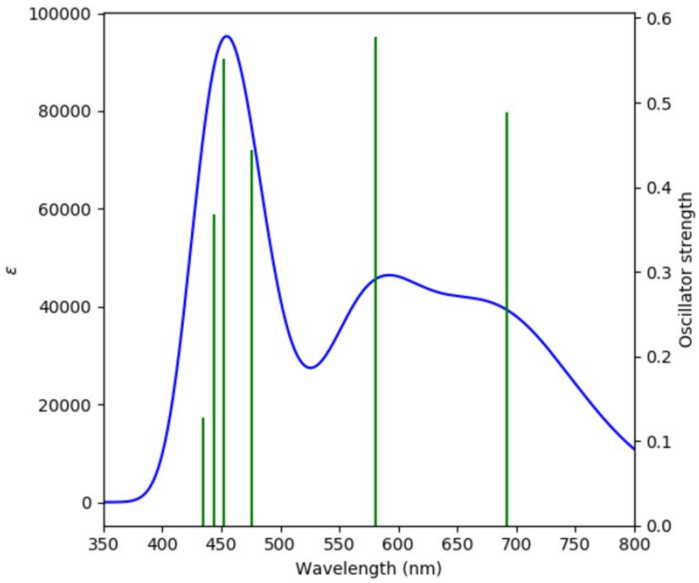


Figure S10: Graph of investigated compound **MCPTD8**