Electronic Supplementary Material (ESI) for RSC Advances.

First Principles Study for Electronic and Nonlinear Optical Properties of A-D–π–A and D-A-D–π–A Configured Compounds Containing Novel Quinoline-Carbazole Derivatives

Muhammad Khalid,[a] Akbar Ali,[b] Rifat Jawaria,[a] Muhammad Adnan Asghar,[c] Sumreen Asim,[a] Muhammad Usman Khan,[d] Riaz Hussain,[d] Muhammad Fayyaz ur Rehman[b], Christopher J. Ennis[e], Muhammad Safwan Akram*[e]

corresponding authors: safwan.akram@tees.ac.uk

Table S1: Cartesian coordinates of Q1

	X-axis	Y-axis	Z-axis
C	5.686316	1.802841	0.24438
C	5.086068	0.571849	0.128101
C	3.67643	0.463652	0.066185
C	2.878465	1.653978	0.126864
C	3.535626	2.906343	0.245718
C	4.905147	2.97913	0.303157
H	6.766847	1.873079	0.291329
H	5.684648	-0.32852	0.081395
C	2.945312	-0.74645	-0.06308
H	2.91171	3.790324	0.291682
H	5.393856	3.942455	0.395252
C	0.881406	0.497629	-0.02086
C	1.579912	-0.74354	-0.11179
H	1.040303	-1.6693	-0.24433
C	-0.60339	0.538837	-0.06162
C	-1.24618	1.749891	-0.40265
C	-1.37087	-0.59203	0.240804
C	-2.62633	1.845377	-0.45913
H	-0.62468	2.607973	-0.61787
C	-2.75719	-0.48711	0.186585
H	-0.90714	-1.52432	0.539879
C	-3.40775	0.722541	-0.16537
H	-3.09402	2.785465	-0.72987
Br	3.859141	-2.43033	-0.19332
N	1.522396	1.647606	0.082769
N	-3.72359	-1.4459	0.445792
C	-4.98218	-0.89634	0.266503
C	-6.23947	-1.48333	0.408823
C	-7.35376	-0.68967	0.162243
C	-7.22363	0.656333	-0.21661
C	-5.96958	1.236327	-0.35724
C	-4.82978	0.462027	-0.11635
H	-6.34741	-2.52181	0.701428
H	-8.34343	-1.12008	0.265322
H	-8.11395	1.245974	-0.40093
H	-5.87579	2.275966	-0.65063
H	-3.54006	-2.39729	0.715474

Table S2: Cartesian coordinates of Q1D1

	X-axis	Y-axis	Z-axis
C	-7.44925	-4.56081	0.576698
C	-6.10414	-4.42188	0.330787
C	-5.52435	-3.13589	0.217065
C	-6.35674	-1.97679	0.360929
C	-7.74097	-2.16155	0.614006
C	-8.27409	-3.42203	0.719285
H	-7.88178	-5.55089	0.662351
H	-5.47334	-5.29423	0.220527
C	-4.15456	-2.86732	-0.0423
H	-8.34804	-1.27115	0.720969
H	-9.33308	-3.5488	0.91354
C	-4.60488	-0.50189	0.042771
C	-3.69254	-1.58439	-0.13362
H	-2.65381	-1.39703	-0.36126
C	-4.1408	0.907388	-0.04903
C	-5.08873	1.925576	-0.29058
C	-2.79002	1.241191	0.109261
C	-4.71403	3.255279	-0.38732
H	-6.12513	1.635978	-0.39512
C	-2.42579	2.578351	0.010395
H	-2.04213	0.492285	0.334291
C	-3.3672	3.602431	-0.23937
H	-5.46125	4.017764	-0.57635
Br	-2.90794	-4.3055	-0.29159
N	-5.88918	-0.70627	0.271728
N	-1.15481	3.155598	0.147901
C	-1.27842	4.541718	-0.02777
C	-0.28985	5.521808	0.002809
C	-0.68619	6.839203	-0.204
C	-2.03003	7.170659	-0.43512
C	-3.00906	6.185505	-0.46754
C	-2.63831	4.852474	-0.26489
H	0.747833	5.266853	0.179427
H	0.060705	7.624636	-0.18655
H	-2.30392	8.207466	-0.59104
H	-4.04555	6.446246	-0.64961
C	0.042714	2.467749	0.364689
C	0.765083	2.383583	1.524031
S	0.847533	1.618125	-0.9468
C	1.954697	1.627481	1.385876
H	0.435874	2.843249	2.446199
C	2.148457	1.125081	0.1174
H	2.634776	1.429495	2.203604
C	3.230022	0.294302	-0.36631
C	3.246943	-0.50805	-1.49578
S	4.737575	0.210087	0.504217
C	4.456887	-1.19268	-1.64959
H	2.404135	-0.61117	-2.16617

C	5.400077	-0.93313	-0.65739
H	4.661967	-1.87602	-2.46394
C	6.684208	-1.56078	-0.69844
C	7.843717	-1.48966	0.023312
H	6.739165	-2.25668	-1.52896
C	8.01137	-0.56632	1.163518
C	8.958679	-2.40806	-0.33928
O	9.286827	-0.32408	1.507426
O	8.811132	-2.94747	-1.58539
H	9.548466	-3.56605	-1.68623
O	9.891745	-2.70565	0.362458
O	7.087126	-0.01848	1.732746
H	9.246877	0.29794	2.249004

Table S3: Cartesian coordinates of Q1D2

	X-axis	**Y-axis**	**Z-axis**
C	7.288123	-3.96649	1.165175
C	6.09137	-3.93247	0.490227
C	5.380492	-2.71656	0.351243
C	5.923231	-1.51825	0.923124
C	7.161933	-1.59417	1.611528
C	7.827787	-2.78859	1.729876
H	7.823097	-4.90364	1.265912
H	5.679996	-4.83488	0.05714
C	4.144335	-2.55532	-0.32784
H	7.550228	-0.67657	2.035767
H	8.772688	-2.83295	2.25935
C	4.154226	-0.20827	0.215757
C	3.535839	-1.33387	-0.4045
H	2.610227	-1.2237	-0.94943
C	3.52271	1.136678	0.157212
C	4.315615	2.27722	0.409047
C	2.160866	1.289815	-0.13121
C	3.779854	3.553758	0.371896
H	5.360884	2.124412	0.639036
C	1.63541	2.575108	-0.16843
H	1.514968	0.437062	-0.29321
C	2.421879	3.721089	0.082151
H	4.410349	4.413353	0.569156
Br	3.294993	-4.05158	-1.17827
N	5.310717	-0.31007	0.844497
N	0.312784	2.980533	-0.41891
C	0.254702	4.380131	-0.32239
C	-0.83325	5.230532	-0.50316
C	-0.61145	6.596763	-0.36117
C	0.659824	7.102079	-0.05115
C	1.741327	6.246963	0.119906
C	1.546145	4.869282	-0.01561
H	-1.81492	4.84637	-0.7501

H	-1.43963	7.282925	-0.49579
H	0.797473	8.171877	0.052391
H	2.723192	6.642585	0.353682
C	-0.75903	2.125432	-0.67233
C	-0.94385	1.309322	-1.75746
S	-2.04543	1.914948	0.506374
C	-2.12155	0.529716	-1.67236
H	-0.26014	1.294369	-2.59533
C	-2.84902	0.747042	-0.52199
H	-2.44827	-0.14224	-2.45505
C	-4.11233	0.165483	-0.13234
C	-5.01418	0.619011	0.819273
S	-4.69265	-1.29823	-0.87067
C	-6.1586	-0.18056	0.945791
H	-4.85274	1.521538	1.393461
C	-6.1665	-1.27596	0.09183
H	-6.96241	0.038779	1.633007
C	-7.11373	-2.32166	-0.11298
H	-6.85205	-3.05754	-0.86691
C	-8.31645	-2.53787	0.507307
C	-9.10963	-3.66528	0.137872
N	-9.74767	-4.57995	-0.16613
C	-8.84411	-1.68998	1.522747
N	-9.25875	-0.99121	2.345241

Table S4: Cartesian coordinates of Q1D3

	X-axis	**Y-axis**	**Z-axis**
C	7.23744	-4.40164	1.081842
C	6.063025	-4.25817	0.382502
C	5.441632	-2.99109	0.275376
C	6.051772	-1.85612	0.905317
C	7.264635	-2.0448	1.617743
C	7.843159	-3.28651	1.704001
H	7.703494	-5.37719	1.157364
H	5.600876	-5.11246	-0.0947
C	4.236717	-2.7183	-0.42412
H	7.704832	-1.17322	2.086101
H	8.769323	-3.41663	2.25215
C	4.396203	-0.39932	0.210314
C	3.716813	-1.455	-0.46696
H	2.815823	-1.25925	-1.02882
C	3.861706	0.987954	0.189508
C	4.726738	2.059743	0.500338
C	2.521343	1.247915	-0.12235
C	4.284543	3.37225	0.495746
H	5.752716	1.824841	0.747462
C	2.089169	2.567907	-0.12103
H	1.820982	0.450607	-0.3345
C	2.948967	3.646687	0.183883

H	4.970709	4.177143	0.733983
Br	3.307177	-4.11934	-1.34947
N	5.526695	-0.60589	0.86057
N	0.80773	3.073649	-0.39173
C	0.845009	4.468892	-0.25136
C	-0.18025	5.395498	-0.42119
C	0.129845	6.737945	-0.22769
C	1.425971	7.145012	0.122948
C	2.443564	6.213333	0.28669
C	2.159315	4.856986	0.100356
H	-1.18042	5.083587	-0.69584
H	-0.64739	7.483173	-0.3522
H	1.633073	8.199053	0.265527
H	3.443931	6.533537	0.555177
C	-0.32602	2.307711	-0.67424
C	-0.69119	1.754407	-1.87178
S	-1.48224	1.907387	0.588372
C	-1.89142	1.00684	-1.79719
H	-0.10654	1.885743	-2.7723
C	-2.45429	0.9875	-0.53932
H	-2.32402	0.486815	-2.64171
C	-3.67452	0.34191	-0.10911
C	-4.06936	0.019645	1.179658
S	-4.89274	-0.13691	-1.24955
C	-5.32319	-0.60464	1.254894
H	-3.44939	0.214048	2.044999
C	-5.93326	-0.78653	0.022413
H	-5.77517	-0.93418	2.174023
C	-7.15196	-1.38521	-0.43383
H	-7.20237	-1.43094	-1.51908
C	-8.27164	-1.92	0.150085
C	-9.25139	-2.4504	-0.75129
N	-10.0122	-2.86462	-1.51565
C	-8.67616	-2.04234	1.572153
O	-7.81361	-1.48552	2.457583
H	-8.21422	-1.62021	3.329817
O	-9.69647	-2.57643	1.928009

Table S5: Cartesian coordinates of Q2

	X-axis	**Y-axis**	**Z-axis**
C	-2.24088	5.116576	-0.46469
C	-2.31622	3.755172	-0.28486
C	-1.13929	2.976369	-0.14295
C	0.131565	3.629139	-0.22131
C	0.173026	5.037085	-0.39829
C	-0.98579	5.764236	-0.51348
H	-3.14942	5.69751	-0.57609
C	-1.13025	1.557909	0.049098
H	1.149458	5.503307	-0.44817

H	-0.94155	6.838689	-0.65268
C	1.306209	1.650375	-0.01266
C	0.089206	0.920778	0.102099
H	0.113007	-0.14458	0.288156
C	2.625667	0.965312	0.049343
C	3.783856	1.727214	0.323499
C	2.742636	-0.41219	-0.16975
C	5.037221	1.142956	0.392734
H	3.661447	2.790595	0.475374
C	4.00575	-0.99224	-0.1018
H	1.878705	-1.01907	-0.41173
C	5.168979	-0.23403	0.181446
H	5.907865	1.751855	0.610026
N	1.313966	2.964674	-0.15079
N	4.378339	-2.31523	-0.28561
C	5.748136	-2.43859	-0.12322
C	6.557997	-3.57077	-0.2111
C	7.922664	-3.40655	-0.00184
C	8.471089	-2.14691	0.288054
C	7.660389	-1.02224	0.37515
C	6.283408	-1.15663	0.169604
H	6.141183	-4.5465	-0.43496
H	8.575596	-4.26978	-0.06449
H	9.539347	-2.05476	0.445463
H	8.090239	-0.05244	0.599984
H	3.748913	-3.0729	-0.48817
C	-2.38231	0.766362	0.20209
C	-2.64102	-0.28942	-0.67573
C	-3.28646	1.047299	1.249784
C	-3.80257	-1.03646	-0.49188
H	-1.95779	-0.5014	-1.49045
C	-4.43609	0.292007	1.43435
H	-3.06045	1.856234	1.93375
C	-4.71361	-0.7625	0.559813
H	-5.10826	0.51945	2.254241
C	-5.78857	-1.72584	0.443058
C	-5.48411	-2.54104	-0.67758
C	-6.95934	-1.97066	1.167618
C	-6.32111	-3.58142	-1.07977
C	-7.79646	-3.00612	0.771493
H	-7.21153	-1.36016	2.027566
C	-7.47822	-3.80107	-0.34107
H	-6.08119	-4.19924	-1.93798
H	-8.70659	-3.20484	1.325125
H	-8.14765	-4.60283	-0.63138
N	-4.2851	-2.10901	-1.22234
H	-3.84411	-2.50125	-2.03675
H	-3.28062	3.264206	-0.25932

Table S6: Cartesian coordinates of Q2D1

	X-axis	Y-axis	Z-axis
C	-5.83644	4.900384	1.619365
C	-5.32175	3.748609	1.071886
C	-3.97407	3.690605	0.630507
C	-3.14693	4.84397	0.812193
C	-3.71392	6.021997	1.366112
C	-5.0295	6.052173	1.755823
H	-6.86663	4.923393	1.956444
C	-3.3613	2.537824	0.038392
H	-3.06174	6.879275	1.479716
H	-5.45003	6.955321	2.183892
C	-1.25739	3.774875	0.023083
C	-2.01135	2.596449	-0.24003
H	-1.53104	1.753602	-0.72055
C	0.201142	3.847802	-0.26296
C	0.77104	5.110574	-0.53988
C	1.013615	2.707809	-0.23454
C	2.123001	5.251537	-0.79764
H	0.116812	5.971368	-0.53924
C	2.379302	2.856939	-0.47798
H	0.60189	1.733709	0.002764
C	2.94966	4.123868	-0.7672
H	2.535658	6.230324	-1.01648
N	-1.82533	4.867627	0.503188
N	3.388446	1.905476	-0.49211
C	4.595743	2.523452	-0.76941
C	5.875908	1.974974	-0.88279
C	6.926833	2.836933	-1.17638
C	6.717106	4.213119	-1.35989
C	5.442355	4.754521	-1.25461
C	4.366448	3.912452	-0.95544
H	6.04999	0.912515	-0.76879
H	7.928951	2.43365	-1.2704
H	7.559208	4.855347	-1.59029
H	5.283629	5.817177	-1.402
H	3.306887	0.940852	-0.20272
C	-4.13116	1.303094	-0.27585
C	-3.63943	0.066004	0.151277
C	-5.33282	1.353689	-1.0166
C	-4.36531	-1.0788	-0.15438
H	-2.7234	0.008867	0.724541
C	-6.04931	0.203283	-1.31808
H	-5.68987	2.311312	-1.37414
C	-5.57406	-1.03688	-0.88169
H	-6.96256	0.270771	-1.89846
C	-6.03193	-2.40536	-1.01974
C	-5.0765	-3.22776	-0.37589
C	-7.14706	-2.99596	-1.62023
C	-5.20949	-4.61295	-0.32371

C	-7.28611	-4.37814	-1.57509
H	-7.8933	-2.38511	-2.11562
C	-6.32658	-5.17515	-0.93386
H	-4.47433	-5.22954	0.178476
H	-8.14562	-4.84791	-2.03859
H	-6.45758	-6.25086	-0.90876
N	-4.07053	-2.41523	0.166799
H	-5.94553	2.868522	0.988651
C	-2.82845	-2.8244	0.658622
C	-2.28675	-2.53294	1.880902
S	-1.64587	-3.58681	-0.39638
C	-0.92054	-2.90184	1.98607
H	-2.85348	-2.05317	2.66736
C	-0.42465	-3.49613	0.851807
H	-0.32164	-2.75397	2.874721
C	0.942518	-3.90908	0.576401
C	1.423585	-5.09501	0.057718
S	2.211396	-2.74238	0.800829
C	2.817818	-5.07988	-0.10845
H	0.789716	-5.94141	-0.16958
C	3.427261	-3.88092	0.250447
H	3.39143	-5.92273	-0.47289
C	4.842078	-3.70366	0.156606
C	5.714817	-2.68844	0.419323
C	5.292168	-1.35927	0.90942
C	7.143452	-3.00125	0.116364
O	6.201106	-0.74073	1.676141
H	5.838648	0.130035	1.900833
O	4.207675	-0.85625	0.671987
O	7.922204	-1.9057	-0.00465
H	8.807472	-2.23038	-0.22613
O	7.57262	-4.11675	-0.07136
H	5.342714	-4.60253	-0.19608

Table S7: Cartesian coordinates of Q2D2

	X-axis	**Y-axis**	**Z-axis**
C	3.046281	-4.10986	4.436723
C	2.609002	-3.81827	3.165901
C	3.124055	-2.70031	2.461122
C	4.085742	-1.86175	3.10838
C	4.522248	-2.1969	4.416888
C	4.017175	-3.29707	5.06441
H	2.640057	-4.96518	4.96461
C	2.726823	-2.32872	1.137462
H	5.255382	-1.5467	4.878296
H	4.354765	-3.54094	6.065508
C	4.193706	-0.39013	1.329174
C	3.259012	-1.17882	0.599528
H	2.998495	-0.90836	-0.415

C	4.782314	0.8469	0.748647
C	5.956561	1.382959	1.323988
C	4.194742	1.491912	-0.34608
C	6.551573	2.528813	0.824248
H	6.378905	0.868245	2.175648
C	4.797164	2.644144	-0.84226
H	3.278177	1.124449	-0.79133
C	5.979511	3.180265	-0.27382
H	7.455133	2.91446	1.28331
N	4.598773	-0.74202	2.536813
N	4.411811	3.455766	-1.89857
C	5.313366	4.498344	-2.03635
C	5.331885	5.545849	-2.95716
C	6.368178	6.468179	-2.86523
C	7.36361	6.35359	-1.88158
C	7.341435	5.308079	-0.96733
C	6.311367	4.364447	-1.03578
H	4.566302	5.640853	-3.71924
H	6.406846	7.292736	-3.56806
H	8.156775	7.090725	-1.8385
H	8.113551	5.224897	-0.21058
H	3.610837	3.302202	-2.48681
C	1.780659	-3.15154	0.333463
C	0.597242	-2.57894	-0.1429
C	2.088021	-4.49224	0.019428
C	-0.25136	-3.36655	-0.91388
H	0.342864	-1.5553	0.103273
C	1.237446	-5.26671	-0.75724
H	3.018052	-4.91468	0.379849
C	0.046205	-4.71092	-1.23106
H	1.499253	-6.29212	-0.99247
C	-1.05452	-5.21465	-2.02738
C	-1.98336	-4.15712	-2.16305
C	-1.32827	-6.44503	-2.63157
C	-3.16707	-4.29846	-2.88231
C	-2.50906	-6.59712	-3.34843
H	-0.62965	-7.26933	-2.5428
C	-3.41609	-5.5343	-3.47124
H	-3.86604	-3.47735	-2.98316
H	-2.73363	-7.5464	-3.82025
H	-4.32947	-5.67573	-4.03741
N	-1.4868	-3.0302	-1.48844
H	1.856452	-4.43884	2.696369
C	-2.13919	-1.8031	-1.35108
C	-1.86381	-0.6283	-1.99788
S	-3.45978	-1.60411	-0.2083
C	-2.6994	0.439683	-1.5923
H	-1.08199	-0.54703	-2.74084
C	-3.62506	0.085314	-0.63437
H	-2.61785	1.444201	-1.98614
C	-4.63843	0.909586	-0.01576

C	-5.33725	0.679168	1.159323
S	-5.14113	2.409545	-0.73816
C	-6.25224	1.690634	1.485563
H	-5.17017	-0.19346	1.776577
C	-6.27852	2.730621	0.565694
H	-6.86776	1.66987	2.372799
C	-7.03523	3.938651	0.508957
H	-6.83366	4.585016	-0.33954
C	-7.98916	4.406592	1.373447
C	-8.62594	5.657207	1.113247
C	-8.40102	3.710963	2.546187
N	-8.72428	3.133951	3.494365
N	-9.13795	6.67053	0.896514

Table S8: Cartesian coordinates of Q2D3

	X-axis	**Y-axis**	**Z-axis**
C	-5.49292	5.032447	1.688688
C	-4.99207	3.877524	1.135031
C	-3.64521	3.805686	0.692622
C	-2.80589	4.949264	0.876685
C	-3.35877	6.131541	1.43562
C	-4.67301	6.174624	1.828648
H	-6.52222	5.06532	2.027702
C	-3.04618	2.647588	0.095683
H	-2.69644	6.980811	1.550537
H	-5.08262	7.080524	2.261479
C	-0.9289	3.860133	0.086997
C	-1.69309	2.685837	-0.17091
H	-1.21697	1.839105	-0.6498
C	0.526302	3.92529	-0.21444
C	1.069421	5.159456	-0.63455
C	1.359078	2.811168	-0.05827
C	2.417765	5.294778	-0.91513
H	0.399657	6.003485	-0.72723
C	2.723777	2.959543	-0.3124
H	0.96263	1.86487	0.292478
C	3.266956	4.195635	-0.75456
H	2.811008	6.249372	-1.24739
N	-1.48545	4.960886	0.561493
N	3.754875	2.041807	-0.19951
C	4.948873	2.648532	-0.54792
C	6.241803	2.120228	-0.57083
C	7.273752	2.959913	-0.97201
C	7.034179	4.293743	-1.34364
C	5.747901	4.815825	-1.31614
C	4.688744	3.994806	-0.91381
H	6.431442	1.093774	-0.28188
H	8.28779	2.576077	-0.99811
H	7.864079	4.918931	-1.6525

H	5.567307	5.846593	-1.60119
H	3.695749	1.103971	0.173246
C	-3.84815	1.442316	-0.25342
C	-3.41839	0.177128	0.158874
C	-5.02974	1.559082	-1.01846
C	-4.18862	-0.92927	-0.18258
H	-2.51644	0.071696	0.747549
C	-5.78919	0.448188	-1.35726
H	-5.33728	2.538742	-1.36175
C	-5.37867	-0.81855	-0.93325
H	-6.68627	0.565994	-1.95456
C	-5.90098	-2.15944	-1.10463
C	-5.00307	-3.0388	-0.4553
C	-7.0325	-2.68185	-1.73649
C	-5.2106	-4.41559	-0.42456
C	-7.24458	-4.05533	-1.71522
H	-7.73545	-2.02544	-2.23679
C	-6.34253	-4.91009	-1.06548
H	-4.52217	-5.07789	0.085369
H	-8.11744	-4.47269	-2.20321
H	-6.53068	-5.97751	-1.05733
N	-3.96679	-2.28666	0.119048
H	-5.6263	3.005181	1.048423
C	-2.76562	-2.77528	0.632332
C	-2.20139	-2.48023	1.844425
S	-1.65948	-3.69651	-0.37835
C	-0.87818	-2.97237	1.975915
H	-2.72306	-1.91794	2.606748
C	-0.44015	-3.66739	0.87498
H	-0.27188	-2.84151	2.862332
C	0.880278	-4.22097	0.630207
C	1.257228	-5.45873	0.143381
S	2.256687	-3.19073	0.883363
C	2.64984	-5.59186	0.012724
H	0.546262	-6.24167	-0.08276
C	3.361575	-4.45076	0.363816
H	3.14216	-6.49211	-0.33263
C	4.776278	-4.32091	0.27251
C	5.57564	-3.22241	0.406689
C	5.064443	-1.91668	0.634369
C	7.0426	-3.40815	0.242675
O	7.71507	-2.24537	0.362066
H	8.654402	-2.44775	0.240521
O	7.577935	-4.46786	0.026356
H	5.312748	-5.23606	0.034489
N	4.614849	-0.86261	0.790233

Table S9: Natural bond orbital (NBO) analysis of compound Q1 by using CAM-B3LYP/6-311G (d, p).

Donor (i)	Type	Acceptor(j)	*Type*	E(2)[a][kJ/mol]	E(j)–E(i)[b][a.u.]	F(i,j)c[a.u.]
C_1-C_2	π	C_3-C_4	π^*	23.89	0.36	0.087
C_1-C_2	π	C_5-C_6	π^*	24.78	0.39	0.088
C_1-H_7	σ	C_2-C_3	σ^*	5.17	1.19	0.070
C_2-C_3	σ	C_3-C_9	σ^*	5.63	1.35	0.078
C_2-H_8	σ	C_3-C_4	σ^*	5.16	1.16	0.070
C_3-C_4	σ	C_9-Br_{24}	σ^*	6.93	0.88	0.070
C_3-C_4	π	C_9-C_{13}	π^*	27.43	0.34	0.091
C_5-C_6	π	C_3-C_4	π^*	25.53	0.36	0.090
C_9-C_{13}	π	C_{12}-N_{25}	π^*	28.99	0.39	0.097
C_{12}-N_{25}	π	C_3-C_4	π^*	28.63	0.41	0.103
C_{27}-C_{32}	π	C_{30}-C_{31}	π^*	31.28	0.36	0.097
C_{28}-C_{29}	π	C_{27}-C_{32}	π^*	29.57	0.36	0.097
C_{30}-C_{31}	π	C_{28}-C_{29}	π^*	31.09	0.37	0.096
Br_{24}	LP(3)	C_9-C_{13}	π^*	12.90	0.42	0.069
N_{25}	LP(1)	C_3-C_4	σ^*	11.98	0.98	0.097
N_{25}	LP(1)	C_{12}-C_{13}	σ^*	12.09	0.97	0.098
N_{26}	LP(1)	C_{20}-C_{22}	π^*	46.50	0.36	0.120
N_{26}	LP(1)	C_{27}-C_{32}	π^*	46.95	0.36	0.121
C_{15}-C_{17}	π	C_{16}-C_{18}	π^*	294.44	0.01	0.095
C_{20}-C_{22}	π	C_{16}-C_{18}	π^*	209.96	0.02	0.094
C_{27}-C_{32}	π	C_{28}-C_{29}	π^*	372.21	0.01	0.095
C_{27}-C_{32}	π	C_{30}-C_{31}	π^*	265.38	0.02	0.095

[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.

Table S10: Natural bond orbital (NBO) analysis of compound Q1D1 by using CAM-B3LYP/6-311G (d, p).

Donor(i)	Type	Acceptor(j)	Type	E(2)	E(J)E(i)[b](a.u)	F(I,j)[c](a.u)
N26-C27	∂	C37-C38	∂*	0.55	1.50	0.026
C1-C2	π	C5-C6	π*	24.74	0.39	0.088
C1-H7	∂	C2-C3	∂*	5.18	1.19	0.070
C2-C3	∂	C3-C9	∂*	5.63	1.35	0.078
C2-H8	∂	C3-C4	∂*	5.16	1.16	0.070
C3-C4	∂	C3-C9	∂*	4.89	1.33	0.072
C3-C4	∂	C9-Br24	∂*	6.90	0.88	0.070
C3-C9	∂	C2-C3	∂*	5.69	1.40	0.080
C5-C6	π	C1-C2	π*	24.52	0.39	0.088
C5-H10	∂	C3-C4	∂*	5.02	1.16	0.068
C6-H11	∂	C4-C5	∂*	4.93	1.18	0.068
C9-C13	π	C12-N25	π*	29.16	0.39	0.097
C12-C13	∂	C9-C13	∂*	5.09	1.41	0.076
C12-C13	∂	C9-Br24	∂*	6.70	0.90	0.069
C12-N25	π	C9-C13	π*	15.43	0.42	0.073
C13-H14	∂	C3-C9	∂*	5.43	1.18	0.072
C15-C16	∂	C15-C17	∂*	4.85	1.38	0.073
C15-C16	π	C12-N25	π*	18.78	0.33	0.072
C15-C16	π	C17-C20	π*	28.54	0.35	0.089
C15-C16	π	C18-C22	π*	33.51	0.36	0.098
C15-C17	∂	C20-N26	∂*	6.36	1.25	0.080
C16-C18	∂	C22-C32	∂*	5.23	1.35	0.075
C16-H19	∂	C15-C17	∂*	5.17	1.21	0.070
C17-C20	∂	C20-C22	∂*	6.07	1.39	0.082
C17-C20	π	C15-C16	π*	31.61	0.37	0.098
C17-C20	π	C18-C22	π*	25.31	0.37	0.088
C17-H21	∂	C20-C22	∂*	5.04	1.20	0.069
C18-C22	∂	C20-C22	∂*	5.14	1.37	0.075
C18-C22	∂	C22-C32	∂*	5.90	1.35	0.080
C18-C22	π	C15-C16	π*	31.34	0.35	0.095
C18-C22	π	C17-C20	π*	30.82	0.35	0.093
C18-C22	π	C31-C32	π*	19.77	0.36	0.076
C20-C22	∂	C17-C20	∂*	5.57	1.38	0.079
C20-C22	∂	N26-C37	∂*	5.46	1.22	0.073
C20-C22	∂	C31-C32	∂*	5.30	1.38	0.077
C22-C32	∂	C18-C22	∂*	5.24	1.36	0.076
C22-C32	∂	C31-C32	∂*	5.26	1.36	0.076
N26-C27	∂	C37-C38	π*	1.69	0.90	0.037
C27-C28	∂	C27-C32	∂*	5.87	1.39	0.081
C27-C28	π	C29-C30	π*	34.05	0.37	0.100
C27-C28	π	C31-C32	π*	25.39	0.37	0.088
C28-C29	∂	N26-C27	∂*	6.94	1.25	0.084
C29-C30	π	C27-C28	π*	27.74	0.35	0.089

C29-C30	π	C31-C32	π^*	33.81	0.36	0.100
C31-C32	π	C18-C22	π^*	20.54	0.36	0.077
C31-C32	π	C27-C28	π^*	31.12	0.35	0.094
C31-C32	π	C29-C30	π^*	29.19	0.35	0.091
C40-C42	π	C44-S46	∂^*	0.61	0.61	0.018
C51-C52	π	C54-O56	∂^*	0.69	0.76	0.021
C3	LP(1)	C1-C2	π^*	61.13	0.20	0.125
C3	LP(1)	C9-C13	π^*	72.78	0.18	0.126
N26	LP(1)	C17-C20	π^*	44.30	0.38	0.117
N26	LP(1)	C27-C28	π^*	44.21	0.38	0.118
S39	LP(2)	C37-C38	π^*	30.66	0.35	0.093
S39	LP(2)	C40-C42	π^*	31.44	0.35	0.094
S46	LP(2)	C44-C45	π^*	36.23	0.34	0.099
S46	LP(2)	C47-C49	π^*	30.57	0.33	0.090
O56	LP(2)	C54-O60	π^*	60.13	0.44	0.148
O57	LP(2)	C55-O59	π^*	51.83	0.45	0.139
O59	LP(2)	C55-O57	∂^*	38.99	0.72	0.152
O60	LP(2)	C54-O56	∂^*	35.37	0.76	0.149

[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.

Table S11: Natural bond orbital (NBO) analysis of compound Q1D2 by using CAM-B3LYP/6-311G (d, p).

Donor(i)	Type	Acceptor(j)	Type	E(2)	E(J)E(i)[b](a.u)	F(I,j)[c](a.u)
C1-C2	π	C3-C4	π^*	23.95	0.36	0.087
C1-C2	π	C5-C6	π^*	24.72	0.39	0.088
C1-H7	∂	C2-C3	∂^*	5.18	1.19	0.070
C2-C3	∂	C3-C4	∂^*	4.65	1.34	0.071
C2-C3	∂	C3-C9	∂^*	5.63	1.35	0.078
C2-C8	∂	C3-C4	∂^*	5.15	1.16	0.070
C3-C4	∂	C3-C9	∂^*	4.89	1.33	0.072
C3-C4	∂	C9-Br24	∂^*	6.90	0.88	0.070
C3-C4	π	C1-C2	π^*	22.67	0.37	0.086
C3-C4	π	C5-C6	π^*	19.39	0.37	0.080
C3-C4	π	C9-C13	π^*	27.48	0.34	0.091
C3-C4	π	C12-N25	π^*	20.12	0.34	0.076
C3-C9	∂	C2-C3	∂^*	5.69	1.40	0.080
C5-C6	π	C1-C2	π^*	24.52	0.39	0.088
C5-C6	π	C3-C4	π^*	25.57	0.36	0.090
C5-H10	∂	C3-C4	∂^*	5.02	1.16	0.068
C6-H11	∂	C4-C5	∂^*	4.93	1.18	0.068
C9-C13	π	C3-C4	π^*	18.07	0.39	0.079
C9-C13	∂	C12-N25	∂^*	29.21	0.39	0.098
C12-C13	∂	C9-C13	∂^*	5.09	1.41	0.076
C12-C13	∂	C9-Br24	∂^*	6.68	0.90	0.069
C12-N25	π	C3-C4	π^*	28.44	0.41	0.103

C12-N25	π	C9-C13	π*	15.44	0.42	0.073
C13-H14	∂	C3-C9	∂*	5.43	1.18	0.072
C15-C16	∂	C15-C17	∂*	4.84	1.38	0.073
C15-C17	∂	C15-C16	∂*	4.74	1.38	0.072
C15-C17	∂	C17-C20	∂*	5.03	1.41	0.075
C15-C17	∂	C20-N26	∂*	6.43	1.24	0.080
C15-C17	π	C12-N25	π*	19.64	0.35	0.074
C15-C17	π	C16-C18	π*	24.20	0.38	0.086
C15-C17	π	C20-C22	π*	29.79	0.36	0.096
C16-C18	∂	C22-C32	∂*	5.22	1.35	0.075
C16-C18	π	C15-C17	π*	29.94	0.36	0.095
C16-C18	π	C20-C22	π*	26.11	0.36	0.090
C16-H19	∂	C15-C17	∂*	5.17	1.21	0.070
C17-C20	∂	C15-C17	∂*	4.81	1.42	0.074
C17-C20	∂	C20-C22	∂*	6.13	1.39	0.082
C17-H21	∂	C20-C22	∂*	5.05	1.20	0.069
C18-C22	∂	C20-C22	∂*	5.19	1.37	0.075
C18-C22	∂	C22-C32	∂*	5.90	1.35	0.080
C18-H23	∂	C20-C22	∂*	5.04	1.19	0.069
C20-C22	π	C15-C17	π*	29.41	0.36	0.092
C20-C22	π	C16-C18	π*	28.01	0.37	0.094
C20-C22	π	C27-C32	π*	22.06	0.35	0.080
C20-N26	∂	C37-C38	π*	1.67	0.90	0.037
N26-C27	∂	C37-C38	π*	1.17	0.90	0.031
C27-C32	π	C30-C31	π*	30.02	0.37	0.096
C28-C29	∂	N26-C27	∂*	6.97	1.25	0.084
C30-C31	π	C28-C29	π*	31.40	0.37	0.096
C47-C49	π	C51-C53	π*	34.36	0.38	0.102
C51-C53	∂	C54-N55	π*	1.27	0.98	0.032
C51-C53	∂	C56-N57	π*	1.39	0.98	0.033
C53-C54	∂	C56-N57	π*	3.00	0.96	0.048
C53-C56	∂	C54-N55	π*	2.74	0.97	0.046
N26	LP(1)	C20-C22	π*	39.51	0.37	0.112
N26	LP(1)	C27-C32	π*	40.09	0.37	0.113
S39	LP(2)	C37-C38	π*	31.11	0.35	0.094
S39	LP(2)	C40-C42	π*	31.07	0.35	0.093
S46	LP(2)	C44-C45	π*	35.49	0.34	0.099
S46	LP(2)	C47-C49	π*	28.96	0.34	0.088

[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 orbita

Table S12: Natural bond orbital (NBO) analysis of compound Q1D3 by using CAM-B3LYP/6-311G (d, p).

Donor(i)	Type	Acceptor(j)	Type	E(2)	E(J)E(i)[b](a.u)	F(I,j)[c](a.u)
C1-H7	∂	C1-C6	∂*	0.61	1.20	0.024
C1-C2	π	C5-C6	π*	24.73	0.39	0.088
C1-H7	∂	C2-C3	∂*	5.18	1.19	0.070

C2-C3	∂	C3-C4	∂*	4.65	1.34	0.071
C2-C3	∂	C3-C9	∂*	5.63	1.35	0.078
C2-H8	∂	C3-C4	∂*	5.15	1.16	0.070
C3-C4	∂	C3-C9	∂*	4.89	1.33	0.072
C3-C4	∂	C9-Br24	∂*	6.90	0.88	0.070
C3-C9	∂	C2-C3	∂*	5.69	1.40	0.080
C5-C6	π	C1-C2	π*	24.51	0.39	0.088
C5-H10	∂	C3-C4	∂*	5.02	1.16	0.068
C6-H11	∂	C4-C5	∂*	4.93	1.18	0.068
C9-C13	π	C12-N25	π*	29.18	0.39	0.098
C12-C13	∂	C9-C13	∂*	5.09	1.41	0.076
C12-C13	∂	C9-Br24	∂*	6.69	0.90	0.069
C12-N25	π	C9-C13	π*	15.44	0.42	0.073
C13-H14	∂	C3-C9	∂*	5.43	1.18	0.072
C15-C16	∂	C15-C17	∂*	4.83	1.38	0.073
C15-C17	∂	C15-C16	∂*	4.73	1.38	0.072
C15-C17	∂	C17-C20	∂*	5.01	1.41	0.075
C15-C17	∂	C20-N26	∂*	6.38	1.25	0.080
C15-C17	π	C12-N25	π*	19.67	0.35	0.074
C15-C17	π	C16-C18	π*	24.16	0.38	0.086
C16-C18	∂	C22-C32	∂*	5.23	1.35	0.075
C16-C18	π	C15-C17	π*	29.94	0.36	0.095
C16-H19	∂	C15-C17	∂*	5.16	1.21	0.070
C17-C20	∂	C15-C17	∂*	4.81	1.42	0.074
C17-C20	∂	C20-C22	∂*	6.09	1.39	0.082
C17-H21	∂	C20-C22	∂*	5.06	1.20	0.070
C18-C22	∂	C22-C32	∂*	5.90	1.35	0.080
C20-C22	∂	C17-C20	∂*	5.56	1.38	0.079
C20-C22	∂	N26-C37	∂*	5.36	1.22	0.072
C20-C22	∂	C31-C32	∂*	5.29	1.38	0.077
C22-C32	∂	C18-C22	∂*	5.24	1.36	0.076
C22-C32	∂	C31-C32	∂*	5.25	1.36	0.076
C27-C28	∂	C27-C32	∂*	5.89	1.39	0.081
C27-C32	∂	C18-C22	∂*	5.39	1.38	0.077
C27-C32	∂	N26-C37	∂*	5.46	1.22	0.073
C27-C32	∂	C27-C28	∂*	5.38	1.38	0.077
C27-C32	π	C28-C29	π*	26.54	0.36	0.089
C27-C32	π	C30-C31	π*	30.23	0.37	0.096
C28-C29	∂	N26-C27	∂*	6.94	1.25	0.083
C28-C29	π	C27-C32	π*	30.73	0.36	0.098
C28-C29	π	C30-C31	π*	25.57	0.37	0.088
C30-C31	π	C28-C29	π*	31.34	0.37	0.096
C37-C38	π	C40-C42	π*	20.28	0.40	0.084
C38-C40	∂	N26-C37	∂*	7.16	1.24	0.084
C40-C42	π	C37-C38	π*	22.55	0.39	0.086
C40-C42	π	C44-C45	π*	17.25	0.38	0.075
C47-C49	π	C51-C53	π*	32.17	0.38	0.100
C3	LP(1)	C1-C2	π*	61.09	0.20	0.125

C3	LP(1)	C9-C13	π^*	72.83	0.18	0.126
C22	LP(1)	C16-C18	π^*	78.49	0.19	0.133
C22	LP(1)	C27-C32	π^*	63.01	0.17	0.107
N26	LP(1)	C27-C32	π^*	40.43	0.37	0.113
S39	LP(2)	C37-C38	π^*	30.71	0.35	0.094
S39	LP(2)	C40-C42	π^*	31.79	0.35	0.094
S46	LP(2)	C44-C45	π^*	35.66	0.34	0.099
O57	LP(2)	C56-O59	π^*	54.99	0.45	0.143
O59	LP(2)	C56-O57	∂^*	37.52	0.74	0.151

[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.

Table S13: Natural bond orbital (NBO) analysis of compound Q2 by using CAM-B3LYP/6-311G (d, p).

Donor (i)	Type	Acceptor(j)	*Type*	E(2)[a][kJ/mol]	E(j)–E(i)[b][a.u.]	F(i,j)c[a.u.]
C_1-C_2	π	C_3-C_4	π^*	22.93	0.37	0.086
C_1-C_2	π	C_5-C_6	π^*	25.19	0.39	0.089
C_1-H_7	σ	C_2-C_3	σ^*	5.15	1.19	0.070
C_2-C_3	σ	C_3-C_8	σ^*	5.04	1.35	0.074
C_3-C_4	π	C_1-C_2	π^*	23.49	0.36	0.087
C_3-C_4	π	C_5-C_6	π^*	20.14	0.37	0.081
C_3-C_4	π	C_8-C_{12}	π^*	25.47	0.36	0.091
C_3-C_4	π	C_{11}-N_{23}	π^*	20.03	0.34	0.076
C_8-C_{12}	π	C_{11}-N_{23}	π^*	34.83	0.37	0.103
C_{11}-N_{23}	π	C_3-C_4	π^*	28.09	0.42	0.103
C_{15}-C_{17}	σ	C_{21}-C_{30}	σ^*	5.22	1.36	0.075
C_{25}-C_{30}	π	C_{28}-C_{29}	π^*	31.41	0.36	0.097
C_{26}-C_{27}	σ	N_{24}-C_{25}	σ^*	6.53	1.28	0.082
C_{28}-C_{29}	π	C_{26}-C_{27}	π^*	31.09	0.37	0.096
C_{38}-C_{41}	π	N_{36}-C_{37}	π^*	30.75	0.37	0.097
C_{39}-C_{43}	π	C_{38}-C_{41}	π^*	31.40	0.36	0.097
C_{45}-C_{46}	π	C_{47}-C_{49}	π^*	31.39	0.36	0.097
C_{47}-C_{49}	π	C_{48}-C_{51}	π^*	31.09	0.37	0.096
N_{23}	$LP(1)$	C_3-C_4	σ^*	11.40	0.99	0.096
N_{23}	$LP(1)$	C_{11}-C_{12}	σ^*	11.48	0.99	0.096
N_{24}	$LP(1)$	C_{19}-C_{21}	π^*	46.22	0.36	0.120
N_{24}	$LP(1)$	C_{25}-C_{30}	π^*	46.95	0.36	0.121
N_{55}	$LP(1)$	C_{39}-C_{43}	π^*	47.19	0.36	0.121
N_{55}	$LP(1)$	C_{45}-C_{46}	π^*	46.50	0.37	0.120
C_{14}-C_{16}	π	C_{15}-C_{17}	π^*	326.79	0.01	0.095
C_{25}-C_{30}	π	C_{26}-C_{27}	π^*	386.06	0.01	0.095
C_{45}-C_{46}	π	C_{48}-C_{51}	π^*	391.20	0.01	0.095

[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.

Table S14: Natural bond orbital (NBO) analysis of compound Q2D1 by using CAM-B3LYP/6-311G (d, p).

Donor(i)	Type	Acceptor(j)	Type	E(2)	E(J)E(i)[b](a.u)	F(I,j)[c](a.u)
C73-O75	∂	C73-O77	∂*	0.50	1.66	0.026
C1-C2	π	C3-C4	π*	22.74	0.37	0.085
C1-C2	π	C5-C6	π*	25.07	0.39	0.089
C1-H7	∂	C2-C3	∂*	5.23	1.19	0.070
C2-C3	∂	C3-C8	∂*	4.99	1.35	0.073
C2-H56	∂	C3-C4	∂*	4.91	1.18	0.068
C3-C4	π	C1-C2	π*	23.51	0.36	0.081
C3-C4	π	C5-C6	π*	20.02	0.37	0.091
C3-C4	π	C8-C12	π*	25.50	0.36	0.091
C3-C8	∂	C36-C37	π*	0.65	0.81	0.022
C5-C6	π	C1-C2	π*	24.50	0.39	0.087
C5-C6	π	C3-C4	π*	24.75	0.37	0.089
C5-H9	∂	C3-C4	∂*	5.04	1.17	0.069
C6-H10	∂	C4-C5	∂*	4.87	1.19	0.068
C8-C12	π	C11-N23	π*	34.85	0.37	0.102
C11-N23	π	C3-C4	π*	28.29	0.42	0.103
C12-H13	∂	C3-C8	∂*	5.36	1.18	0.071
C14-C16	∂	C19-N24	∂*	5.97	1.28	0.078
C14-C16	π	C15-C17	π*	23.75	0.38	0.085
C14-C16	π	C19-C21	π*	28.58	0.36	0.094
C15-C17	∂	C21-C30	∂*	5.16	1.36	0.075
C15-C17	π	C14-C16	π*	29.77	0.37	0.095
C15-H18	∂	C14-C16	∂*	5.08	1.21	0.070
C16-C19	∂	C19-C21	∂*	5.46	1.38	0.077
C17-C21	∂	C21-C30	∂*	5.99	1.36	0.081
C19-C21	∂	C16-C19	∂*	5.11	1.37	0.075
C19-C21	∂	C29-C30	∂*	5.47	1.37	0.078
C21-C30	∂	C17-C21	∂*	5.32	1.36	0.076
C21-C30	∂	C29-C30	∂*	5.37	1.36	0.077
C25-C26	∂	C25-C30	∂*	5.34	1.37	0.077
C25-C30	∂	C17-C21	∂*	5.56	1.37	0.078
C25-C30	π	C26-C27	π*	26.02	0.35	0.087
C25-C30	π	C28-C29	π*	31.57	0.36	0.097
C26-C27	∂	N24-C25	∂*	6.47	1.29	0.081
C28-C29	∂	C21-C30	∂*	5.30	1.36	0.076
C29-C30	∂	C21-C30	∂*	6.08	1.35	0.081
C29-C30	∂	C25-C30	∂*	4.97	1.36	0.074
C36-C37	∂	C39-N55	∂*	6.35	1.24	0.079
C37-C39	∂	C39-C43	∂*	6.10	1.39	0.082
C37-H40	∂	C39-C43	∂*	4.98	1.19	0.069
C39-C43	∂	C37-C39	∂*	5.62	1.38	0.079
C46-C48	π	C49-C51	π*	33.48	0.37	0.099
C48-C51	∂	C46-N55	∂*	6.88	1.25	0.083

C58-C60	∂	N55-C57	∂*	6.99	1.23	0.083
C58-H61	∂	C57-S59	∂*	6.40	0.85	0.066
C60-H63	∂	S59-C62	∂*	6.26	0.86	0.066
C65-C67	∂	C62-C64	∂*	6.13	1.32	0.080
N24	∂	C19-C21	π*	46.32	0.36	0.120
N24	LP(1)	C25-C30	π*	47.32	0.36	0.121
N55	LP(1)	C39-C43	π*	38.91	0.38	0.111
N55	LP(1)	C46-C48	π*	43.09	0.38	0.116
S66	LP(2)	C64-C65	π*	35.90	0.34	0.100
S66	LP(2)	C67-C69	π*	30.83	0.33	0.091
O77	LP(2)	C73-O75	∂*	34.12	0.77	0.146
O78	LP(2)	C74-O80	π*	58.35	0.44	0.146
O80	LP(2)	C74-O78	∂*	36.63	0.75	0.150

[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.

Table S15: Natural bond orbital (NBO) analysis of compound Q2D2 by using CAM-B3LYP/6-311G (d, p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**(kcal/mol)	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C1-C2	∂	C2-C3	∂*	4.17	1.39	0.068
C1-C2	π	C3-C4	π*	22.97	0.37	0.086
C1-C2	π	C5-C6	π*	25.13	0.39	0.089
C1-H7	∂	C2-C3	∂*	5.15	1.19	0.070
C2-C3	∂	C3-C4	∂*	4.33	1.35	0.068
C2-C3	∂	C3-C8	∂*	5.05	1.35	0.074
C3-C4	∂	C3-C8	∂*	4.39	1.34	0.069
C3-C4	π	C1-C2	π*	23.43	0.36	0.087
C3-C4	π	C5-C6	π*	20.10	0.37	0.081
C3-C4	π	C8-C12	π*	25.52	0.36	0.091
C3-C8	∂	C36-C37	π*	0.78	0.82	0.024
C5-C6	π	C3-C4	π*	24.76	0.37	0.089
C5-H9	∂	C3-C4	∂*	5.01	1.17	0.069
C8-C12	π	C11-N23	π*	34.49	0.37	0.102
C11-N23	π	C3-C4	π*	28.09	0.42	0.103
C12-H13	∂	C3-C8	∂*	5.44	1.19	0.072
C14-C16	π	C19-C21	π*	29.05	0.36	0.095
C15-C17	∂	C21-C30	∂*	5.22	1.36	0.075
C17-C21	∂	C21-C30	∂*	5.99	1.35	0.080
C25-C30	π	C28-C29	π*	31.38	0.36	0.097
C29-C30	∂	C21-C30	∂*	6.02	1.35	0.081
C36-C37	∂	C8-C12	π*	1.15	0.84	0.029
C36-C38	∂	C8-C12	π*	1.20	0.84	0.030
C39-N55	∂	C57-C58	π*	1.70	0.90	0.038
C46-N55	∂	C57-C58	π*	1.42	0.90	0.034
C47-C49	π	C48-C51	π*	31.35	0.37	0.096
C60-C62	∂	N55-C57	∂*	0.57	1.30	0.024

C67-C69	π	C71-C73	π^*	33.92	0.38	0.101
C71-H72	∂	C67-C69	∂^*	6.22	1.23	0.078
C71-C73	π	C75-N76	π^*	25.75	0.49	0.103
C73-C74	∂	C74-N77	∂^*	9.50	1.78	0.117
C73-C75	∂	C75-N76	∂^*	9.51	1.78	0.117
C74-N77	∂	C73-C74	∂^*	8.57	1.69	0.108
C74-N77	π	C71-C73	∂^*	2.78	1.05	0.048
C74-N77	π	C73-C75	∂^*	3.70	0.97	0.054
N24	LP(1)	C25-C30	π^*	46.86	0.36	0.121
N55	LP(1)	C39-C43	π^*	40.41	0.37	0.113
N55	LP(1)	C45-C46	π^*	39.97	0.37	0.113
S66	LP(2)	C64-C65	π^*	35.36	0.34	0.099
S66	LP(2)	C67-C69	π^*	29.10	0.34	0.089

[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.

Table S16: Natural bond orbital (NBO) analysis of compound Q2D3 by using CAM-B3LYP/6-311G (d, p).

Donor(i)	Type	Acceptor(j)	Type	E(2)	E(J)E(i)[b](a.u)	F(I,j)[c](a.u)
C1-C2	∂	C2-C3	∂^*	4.20	1.39	0.068
C1-C2	π	C3-C4	π^*	22.71	0.37	0.085
C1-C2	π	C5-C6	π^*	25.07	0.39	0.089
C1-H7	∂	C2-C3	∂^*	5.23	1.19	0.070
C3-C4	π	C1-C2	π^*	23.49	0.36	0.087
C3-C4	π	C5-C6	π^*	20.02	0.37	0.081
C3-C4	π	C8-C12	π^*	25.39	0.36	0.091
C5-C6	π	C1-C2	π^*	24.50	0.39	0.087
C5-H9	∂	C3-C4	∂^*	5.05	1.17	0.069
C8-C12	π	C3-C4	π^*	18.33	0.37	0.077
C8-C12	π	C11-N23	π^*	34.83	0.37	0.102
C8-C12	π	C36-C37	π^*	6.90	0.38	0.047
C11-N23	π	C3-C4	π^*	28.22	0.42	0.103
C11-N23	π	C8-C12	π^*	14.28	0.44	0.071
C12-H13	∂	C3-C8	∂^*	5.37	1.18	0.071
C14-C16	∂	C19-N24	∂^*	5.96	1.28	0.078
C14-C16	π	C15-C17	π^*	23.76	0.38	0.085
C14-C16	π	C19-C21	π^*	28.49	0.36	0.094
C15-C17	∂	C21-C30	∂^*	5.14	1.36	0.075
C15-C17	π	C14-C16	π^*	29.94	0.37	0.095
C15-H18	∂	C14-C16	∂^*	5.08	1.21	0.070
C16-C19	∂	C19-C21	∂^*	5.40	1.37	0.077
C17-C21	∂	C21-C30	∂^*	5.99	1.36	0.081
C17-H22	∂	C19-C21	∂^*	5.06	1.18	0.069
C19-C21	∂	C16-C19	∂^*	5.05	1.37	0.075
C19-C21	∂	C29-C30	∂^*	5.48	1.37	0.078

C19-C21	π	C15-C17	π^*	29.79	0.36	0.096
C19-C21	π	C25-C30	π^*	22.44	0.35	0.080
C21-C30	∂	C17-C21	∂^*	5.33	1.36	0.076
C25-C30	π	C19-C21	π^*	23.62	0.34	0.082
C25-C30	π	C26-C27	π^*	25.91	0.36	0.087
C25-C30	π	C28-C29	π^*	31.45	0.36	0.097
C26-C27	∂	N24-C25	∂^*	6.45	1.29	0.081
C26-C27	π	C25-C30	π^*	28.93	0.36	0.096
C26-C27	π	C28-C29	π^*	24.67	0.37	0.087
C28-C29	π	C25-C30	π^*	23.76	0.36	0.086
C28-C29	π	C26-C27	π^*	30.68	0.37	0.096
C29-C30	∂	C21-C30	∂^*	6.08	1.35	0.081
C29-H34	∂	C25-C30	∂^*	5.07	1.18	0.069
C36-C37	π	C3-C8	∂^*	2.22	0.89	0.043
C36-C37	π	C8-C12	∂^*	1.63	0.96	0.038
C36-C37	π	C38-C41	π^*	25.00	0.37	0.086
C36-C37	π	C39-C43	π^*	30.11	0.36	0.096
C37-C39	∂	C39-C43	∂^*	6.08	1.39	0.082
C38-C41	∂	C43-C45	∂^*	5.23	1.35	0.075
C38-C41	π	C36-C37	π^*	30.25	0.37	0.096
C39-C43	π	C36-C37	π^*	28.41	0.36	0.091
C39-C43	π	C38-C41	π^*	29.71	0.37	0.095
C41-C43	∂	C39-C43	∂^*	5.28	1.37	0.076
C45-C47	π	C46-C48	π^*	31.00	0.35	0.094
C45-C47	π	C49-C51	π^*	29.29	0.36	0.091
C46-C48	π	C49-C51	π^*	33.30	0.37	0.099
C46-N55	∂	C57-C58	π^*	0.70	0.90	0.024
C48-C51	∂	C46-N55	∂^*	6.92	1.25	0.083
C49-C51	π	C45-C47	π^*	33.44	0.36	0.099
C60-C62	π	C57-C58	π^*	20.89	0.39	0.084
C60-H63	∂	S59-C62	∂^*	6.24	0.86	0.066
C64-C65	π	C67-C69	π^*	28.85	0.37	0.096
C65-C67	∂	C62-C64	∂^*	6.03	1.32	0.080
C67-C69	∂	C69-C71	∂^*	5.18	1.38	0.076
C67-C69	π	C71-C72	π^*	34.54	0.39	0.105
C71-C72	π	C67-C69	π^*	11.08	0.39	0.061
C71-C72	π	C73-N79	π^*	27.90	0.49	0.107
C71-H78	∂	S66-C69	∂^*	8.92	0.85	0.078
C71-H78	∂	C72-C73	∂^*	7.59	1.16	0.084
C72-C73	∂	C73-N79	∂^*	10.18	1.79	0.121
C73-N79	∂	C72-C73	∂^*	8.41	1.72	0.108
C73-N79	π	C71-C72	π^*	8.00	0.48	0.058
N23	LP(1)	C11-C12	∂^*	11.54	0.99	0.096
N24	LP(1)	C19-C21	π^*	47.48	0.36	0.121
N55	LP(1)	C39-C43	π^*	38.44	0.38	0.111
N55	LP(1)	C46-C48	π^*	42.93	0.38	0.116
S59	LP(2)	C57-C58	π^*	31.00	0.35	0.094
S66	LP(2)	C64-C65	π^*	35.25	0.34	0.100

S66	LP(2)	C67-C69	π^*	30.29	0.34	0.091
O75	LP(2)	C74-O77	π^*	57.92	0.45	0.146
O77	LP(2)	C72-C74	∂^*	22.63	0.80	0.122
O77	LP(2)	C74-O75	∂^*	36.85	0.75	0.150
N79	LP(1)	C72-C73	∂^*	10.77	1.16	0.100

[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.

Table S17: Wave length, excitation energy and oscillator strength of investigated compound **Q1**

λ(*nm*)	E(*eV*)	f_{os}	MO contributions
321.17	3.86040	1.447	H-1→L (83%) H-3→L (5%), H-1→L+1 (4%)
313.46	3.95530	0.086	H→L (63%), H→L+1 (22%)H-1→L+4 (4%), H→L+2 (6%)
283.26	4.37710	0.084	H-2→L (11%), H-1→L+1 (46%)H-3→L+1 (3%),H-2→L+1 (5%), H-2→L+2 (8%)
276.25	4.48820	0.511	H-1→L+1 (13%)H-5→L (2%), H-2→L+1 (5%), H-1→L+2 (4%)
270.80	4.57840	0.004	H-5→L+5 (2%), H-2→L (2%)
254.51	4.87160	0.403	H→L+1 (44%), H→L+2 (11%)H-5→L (2%), H-4→L (4%), H-3→L (2%), H→L+4 (5%)

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

Table S18: Wave length, excitation energy and oscillator strength of investigated compound **Q1D1**

λ (*nm*)	E(*eV*)	*f*	MO contributions
405.005	3.06130	1.353	H-2→L (29%), H→L (66%)
319.687	3.87830	1.438	H-1→L+1 (85%)H-4→L+1 (4%), H-1→L+2 (3%)
308.464	4.01940	0.090	H-2→L+1 (25%), H→L+1 (39%), H→L+2 (11%)H-2→L+2 (8%), H-2→L+4 (2%), H→L+4 (3%)
304.727	4.06870	0.024	H-2→L (53%), H→L (22%), H→L+3 (13%)H-2→L+3 (3%)
283.931	4.36670	0.021	H-6→L (59%), H-5→L (11%) H-8→L (3%), H-7→L (7%), H-2 →L+3 (5%), H→L+3 (5%)
283.043	4.38040	0.046	H-4→L+1 (18%), H-3→L+1 (20%), H-1→L+2 (36%)H-4→L+2 (4%), H-3→L+2 (2%), H-3→L+4 (8%), H-1→L (2%)

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

Table S19: Wave length, excitation energy and oscillator strength of investigated compound **Q1D2**

λ (*nm*)	E(*eV*)	*f*	MO contributions
435.935	2.84410	1.450	H-2→L (31%), H→L (65%)
322.691	3.84220	0.114	H-2→L (48%), H→L (19%), H→L+3 (14%)H-7→L (2%), H-6→L (3%), H-1→L+1 (7%)
319.136	3.88500	1.343	H-1→L+1 (78%)H-4→L+1 (4%), H-2→L (4%), H-1→L+2 (2%), H→L (2%)
309.775	4.00240	0.099	H-2→L+1 (14%), H→L+1 (50%), H→L+2 (15%)H-2→L+2 (5%), H-1→L+6 (2%), H→L+4 (3%)
297.503	4.16750	0.010	H-1→L (92%)H-1→L+3 (4%)
288.550	4.29680	0.056	H-9→L (30%), H-7→L (10%), H-6→L (35%)H-8→L (4%),

			H-5→L (3%), H-2→L (3%), H-2→L+3 (6%), H→L+3 (4%)

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

Table S20: Wave length, excitation energy and oscillator strength of investigated compound **Q2**

λ (*nm*)	E(*eV*)	*f*	MO contributions
319.14	3.88500	1.459	H-1→L (44%), H→L (32%) H-5→L(4%),H-3→L (3%), H-2→L (4%), H-1→L+1 (4%)
310.35	3.99500	0.062	H-1→L (22%), H→L (37%), H→L+1 (19%)
298.26	4.15690	0.383	H-3→L (11%), H-2→L (33%), H-2→L+1 (16%),H-2→L+2 (19%) H-4→L (4%), H-3→L+4 (3%)
294.03	4.21670	0.832	H-3→L (44%) H-4→L (9%), H-3→L+1 (9%), H-3→L+2 (5%), H-2→L(2%), H-2→L+1(4%),H-2→L+2(9%), H-1→L+1 (2%), H→L+1 (2%)
282.19	4.39370	0.236	H-5→L (19%), H-1→L+1 (27%), H→L+1 (13%)H-5→L+2 (2%), H-4→L (6%), H-4→L+3 (5%), H-2→L+1(6%), H-1→L+2 (5%), H→L+2 (2%)
271.77	4.56210	0.038	H-8→L (82%) H-8→L+2 (3%)

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

Table S21: Wave length, excitation energy and oscillator strength of investigated compound **Q2D1**

λ (*nm*)	E(*eV*)	f_{os}	MO contributions
374.65	3.30930	1.078	H-4→L (47%), H-2→L (45%) H-1→L (2%)
316.97	3.91160	1.283	H-1→L+1 (69%)H-6→L+1 (6%), H-3→L+2 (2%),H-2→L+1 (2%), H-1→L+2 (8%), H→L+1 (5%)
309.46	4.00650	0.082	H→L+1 (47%), H→L+2 (32%) H-1→L+1(3%),H-1→L+9 (3%), H→L+4 (2%), H→L+5 (5%)
300.65	4.12390	0.088	H→L (86%)H-3→L+1 (4%), H-1→L (3%)
300.38	4.12760	1.217	H-3→L+1 (63%)H-5→L+1 (6%), H-3→L+2 (6%), H-2→L+1 (3%), H→L (5%)
298.53	4.15320	0.165	H-2→L+1 (35%), H-2→L+2 (17%), H-2→L+4 (13%) H-4→L (4%), H-4→L+1 (5%), H-4→L+2 (3%), H-4→L+4 (2%), H-3→L+6 (2%), H-1→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 Q2D2

λ (*nm*)	E(*eV*)	*f*	MO contributions
425.23	2.91570	1.410	H-4→L (54%), H-2→L (38%)H-3→L (3%)
323.81	3.82890	0.005	H-4→L (33%), H-2→L (47%),H-2→L+2 (12%)
320.03	3.87420	1.454	H-1→L+1 (55%), H→L+1 (25%)H-6→L+1(5%),H-1→L+3 (5%)
310.86	3.98850	0.065	H-1→L+1 (18%), H→L+1 (41%), H→L+3 (20%)H-1→L+3 (4%), H-1→L+8 (3%), H→L+5 (4%)
294.31	4.21270	0.751	H-3→L+1 (36%), H-2→L+1 (15%) H-5→L+1(9%),H-

			3→L (3%), H-3→L+3 (5%), H-3→L+4 (2%),H-2→L+3 (7%), H-2→L+4 (4%), H→L (3%)
294.14	4.21510	0.064	H-3→L (37%), H-1→L (13%), H→L (37%)H-3→L+1(3%), H-3→L+2 (3%)

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

Table S23: Wave length, excitation energy and oscillator strength of investigated compound **Q2D3**

λ (***nm***)	E(***eV***)	***f***	**MO contributions**
393.74	3.14890	1.023	H-4→L (42%), H-2→L (18%), H-1→L (34%)
314.28	3.94500	0.009	H→L (97%)
313.60	3.95360	1.183	H-2→L+1 (46%), H-1→L+1 (27%)H-6→L+1 (6%), H-3→L+2 (2%), H-2→L+2 (6%), H-1→L+2 (3%)
308.20	4.02290	0.134	H→L+1 (47%), H→L+2 (33%),H-2→L+9 (2%), H→L+4 (3%), H→L+5 (6%)
305.95	4.05250	0.168	H-9→L (12%), H-4→L (33%), H-1→L (19%), H-1→L+3 (11%) H-8→L (3%), H-2→L (6%), H-2→L+3 (6%)
300.13	4.13100	1.044	H-3→L+1 (53%)H-5→L+1(4%),H-3→L+2(4%),H-2→L+1 (7%), H-2→L+2 (7%), H-1→L+1 (7%)

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