Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

UV-Selective Organic Absorbers for Cosensitization of Greenhouse-Integrated Dye-Sensitized Solar Cells: Synthesis and Computational Study.

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Exchange-Correlation (XC) Functionals Performance.

Here, we justify the choice of the exchange–correlation energy functional $E_{XC}[\rho]$ employed in the time-dependent scheme. In the present work, 12 XC-functionals, grouped into five different categories, were tested. The considered XC-functionals are: **(i)** Three functionals based on hybrid generalized-gradient approximation (H-GGA), B3LYP[1, 2] functional with 20% HFX (Hartree–Fock exact exchange), PBE0[3] with 25% HFX, and APF-D[4] functional with 23% HFX and dispersion effects; **(ii)** Three among hybrid meta-GGA (GGA plus local kinetic energy density): M06-2X[5] (54% HFX), τ-HCTHhyb[6] (15% HFX) and TPSSh[7] (10% HFX); **(iii)** Four range-separated hybrid (RSH) long-range corrected GGA functionals, CAM-B3LYP[8] (short range 19% HFX and long range 65% HFX), LC-ωPBE[9] (short range 0% HFX and long range 100% HFX), ωB97X-D[10] with dispersion effects (short range 22% HFX and long range 100% HFX), and the meta-GGA M11[11] (short range 42.8% HFX and long range 100% HFX); **(iv)** One RSH middle-range corrected functional, HISSb[12, 13] (HFX% = 0-60-0 at short-middle-long interelectronic separations, in that order); **(V)** One among the RSH screened-exchange functionals, MN12-SX[14] (meta-NGA with HFX%= 25-0 at short-long interelectronic separations). The electronic absorption spectra were obtained by calculating a set of 20 excited states for each XC functional. Figure 1 depicts the mean signed deviation (MSD) of calculated λ_{max} to the experimentally measured ones, addition to the mean absolute error (MAE) calculated for each XC functional.

The results show that functionals perform differently depending on the system. In terms of mean absolute error, the best performing functional is MN12-SX with MAE of ca. 6.3 nm (0.11 eV). Typically, the MSD obtained with MN12-SX were +4.1 nm (-0.069 eV), -14 nm (+0.261 eV), +0.2 nm (-0.003 eV) and -4.8 nm (+0.083 eV) for DI-N1, DN-2, DI-CA1 and DI-CA-2, respectively. Therefore, MN12-SX is the best performing functional for DI-CA1 dye and provided comparable accuracy with discrepancy of ca. 2 and 2.5 nm (0.034 and 0.051 eV) to both PBE0 and B3LYP as the best performing functionals for DI-N1 (MSD = +2.1 nm, -0.035 eV) and DI-CA-2 (MSD = +1.9 nm, -0.032 eV) hybrid functionals, respectively. For DI-N2, the hybrid meta-GGA functional τ-HCTHhyb is clearly superior to MN12-SX, PBE0 and B3LYP functionals. Considering that all RSH functionals with long-range correction and the global hybrid meta-GGA functional M06-2X provided poor estimates for all dyes. They tend to severely overestimate the transition energies with following trend of MAE: LC-ωPBE (44.2 nm) > M11 (38.1 nm) > ωB97X-D (31.1 nm) > M06-2X (29.5 nm) > CAM-B3LYP (21.7 nm). Additionally, the hybrids with constant HFX all over the space and the RSH with screened HFX at long range behave very well presenting MAE values of at most 9.1 nm (0.16 eV). A general conclusion could be emerged accordingly: for the present set of dyes, the electronic transitions are local valence excitations (LE) which are energetically below the first ionization potential with unchanging principal quantum number. However, the excited states of DI-N1 and DI-CA1 could not be purely LE, but mixed with charge transfer (CT) excitations between orbitals with appreciable spatial overlap. This could be confirmed by the outperformance of long-range corrected hybrids and M06-2X in reproducing DI-N1 and DI-CA1 excitations than that of DI-N2 and DI-CA2, as can be shown in Figure 1. Especially for CAM-B3LYP, for which HFX increases up to 65% at long range and not all the way up to 100%, and that is known to perform well in CT excitations with intermediate spatial overlap, it delivered MSD of -20.4, -39.4, -19.1 and -38.1 nm for DI-N1, DI-N2, DI-CA1 and DI-CA2, respectively. Although DI-N1 and DI-CA1 dyes are expected to exhibit a partial CT character, global hybrids like PBE0 and the screened-exchange RSH (MN12-SX) accurately reproduced λ_{max} probably for the reason that the distance between the electron donor and the electron acceptor is rather small. Overall, the non-separable functional, MN12-SX that depends on the density, the density gradient, and the kinetic energy density with 25% of HFX at short-range and a screened HFX at long-range, seems to be the most reliable functional for the set of diimide dyes with MAE of ca. 6.3 nm (0.11 eV) attaining the acceptable error (absolute error < 0.15 eV)[15] of TD-DFT scheme.

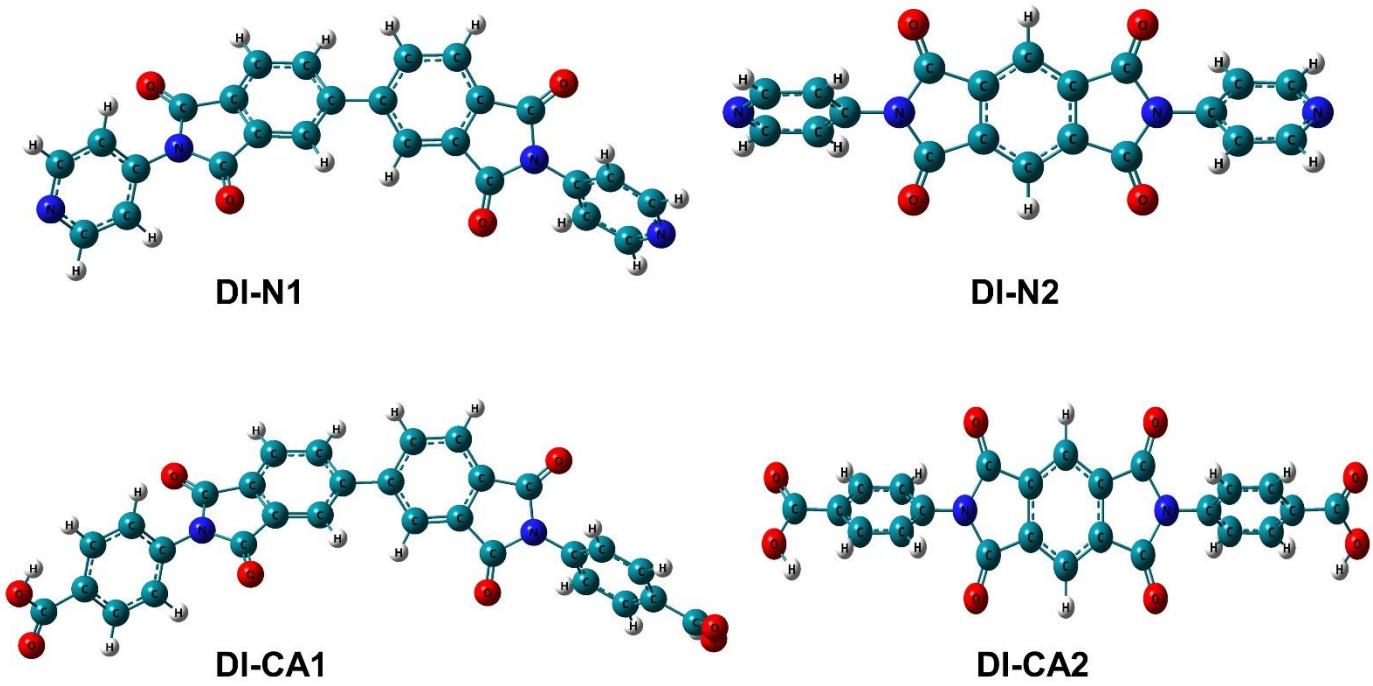


Figure S1. Ground state optimized geometries of studied UV-dyes.

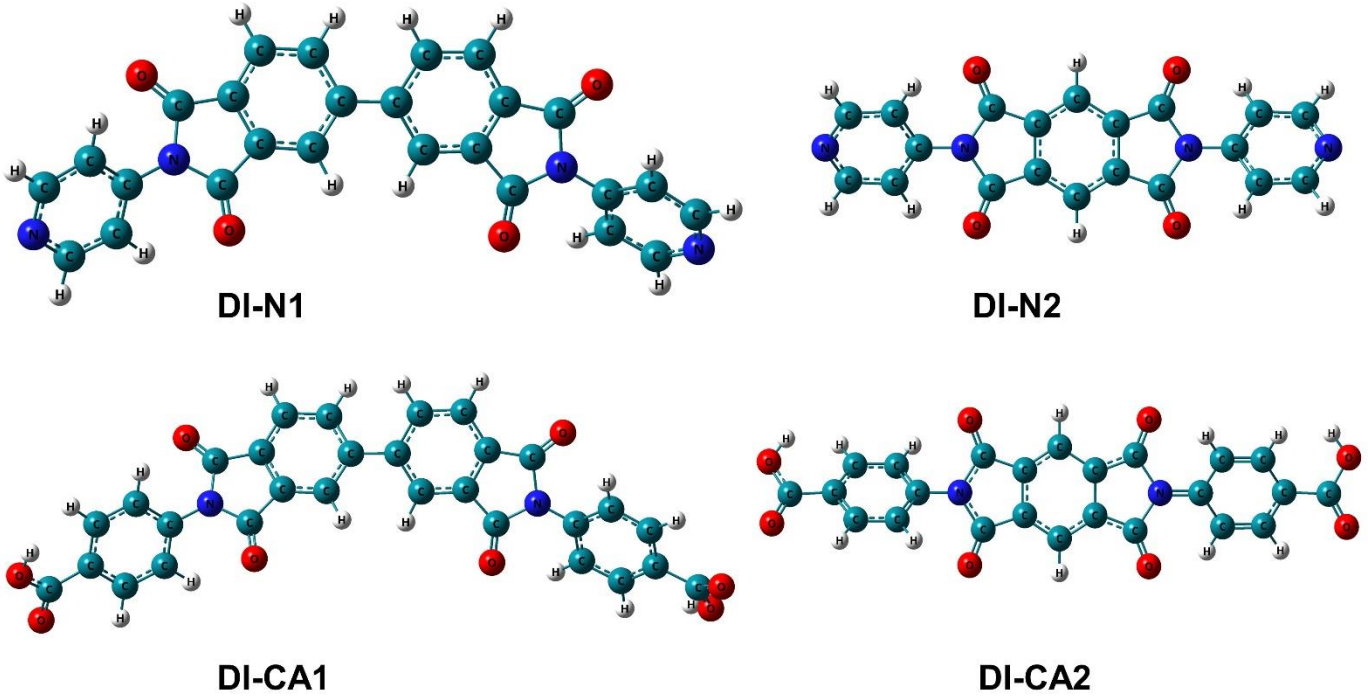


Figure S2. Excited state optimized geometries of studied UV-dyes.

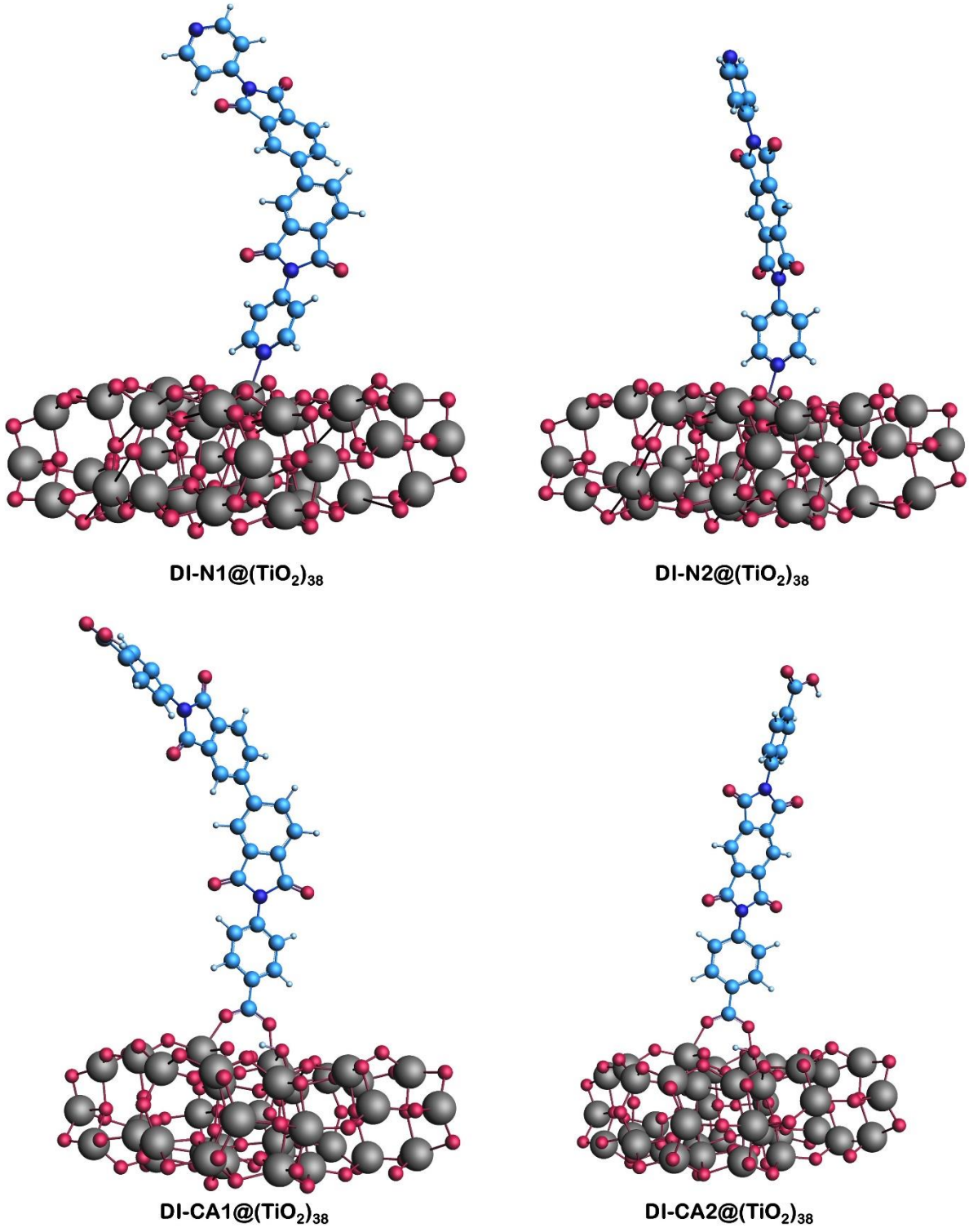


Figure S3. Ground state optimized geometries of dyes adsorbed on a $(TiO_2)_{38}$ cluster (as a model of bulk TiO_2).

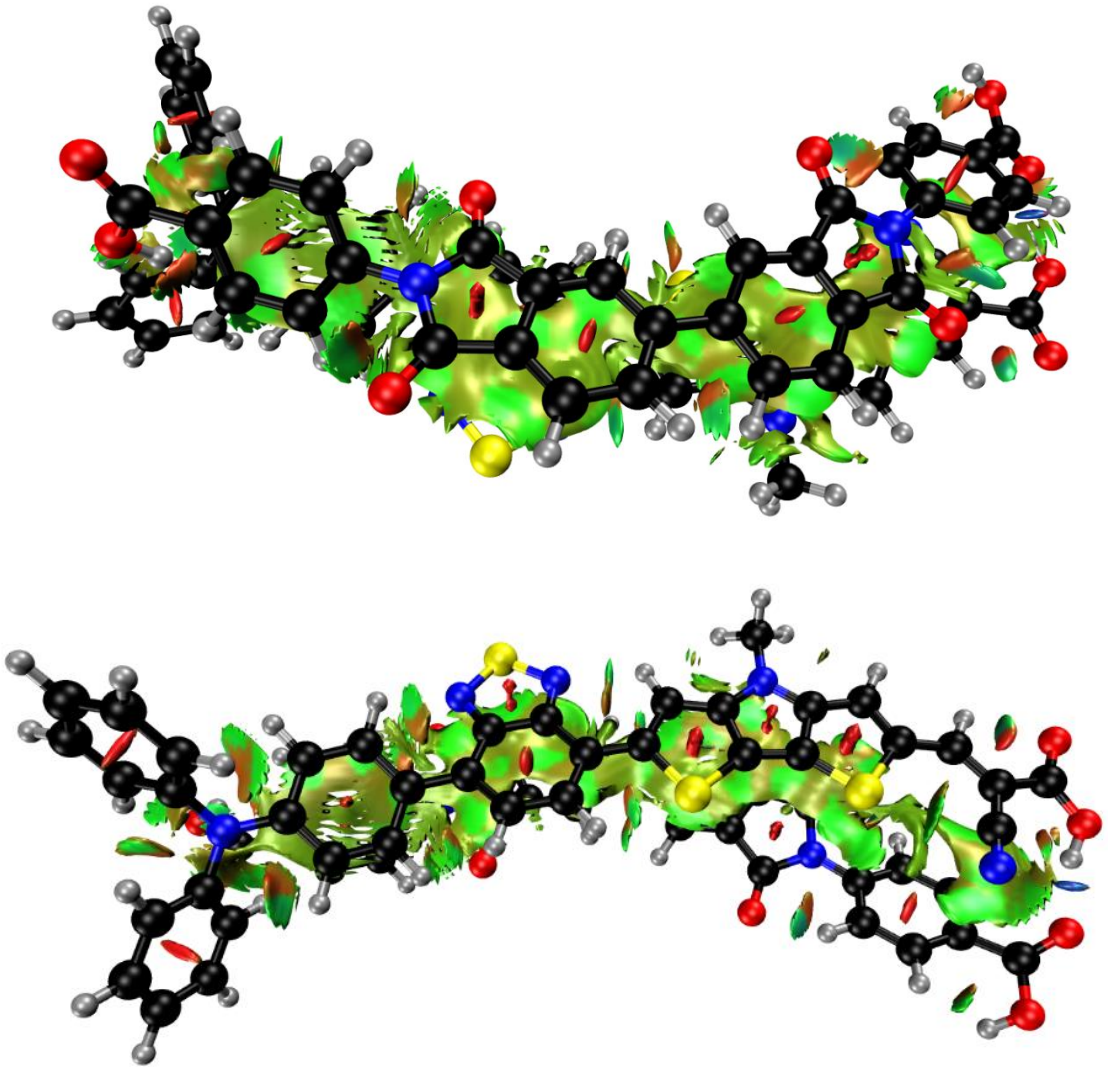


Figure S4. Reduced density gradient isosurface map for the proposed cosensitizers DI-CA1/BTD-DTP1 showing both intra- and inter-molecular interactions.

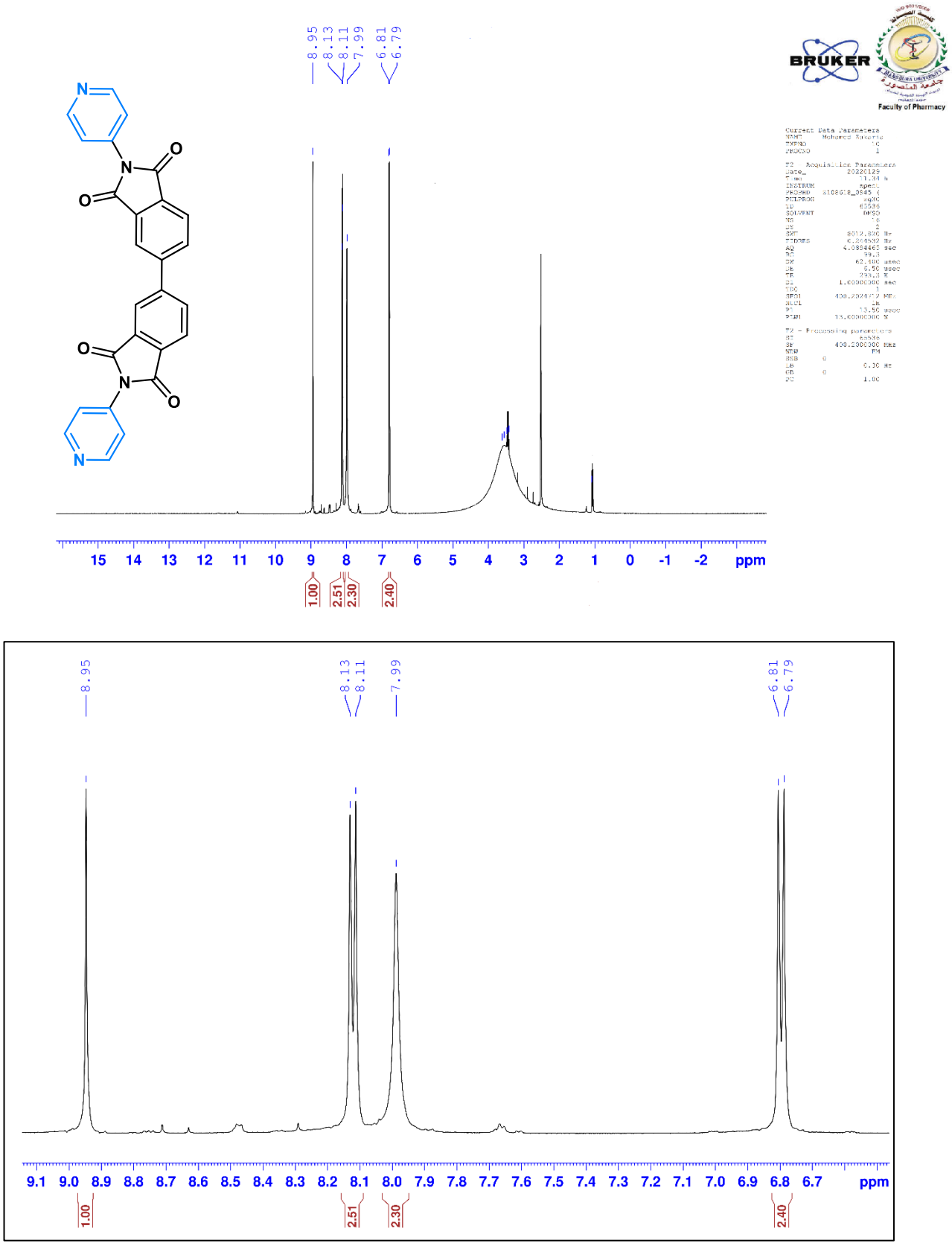


Figure S5. ^{1}**HNMR** (400 MHz, DMSO-*d*$_6$) of 2,2'-di(pyridin-4-yl)-[5,5'-biisoindoline]-1,1',3,3'-tetraone, **DI-N1**

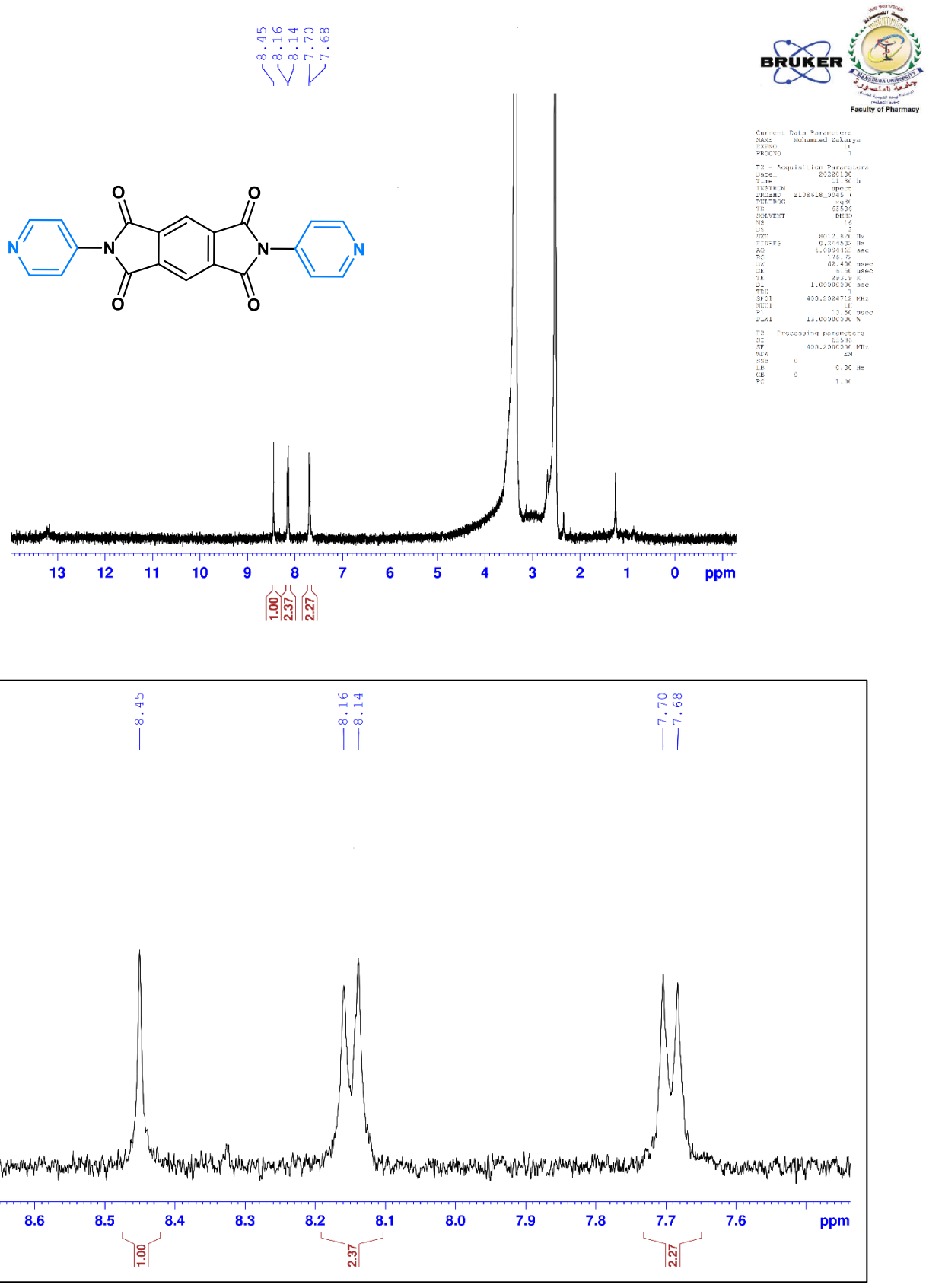


Figure S6. ^{1}**HNMR** (400 MHz, DMSO-d_6) of 2,6-di(pyridin-4-yl)pyrrolo[3,4-f]isoindole-1,3,5,7(2H,6H)-tetraone **DI-N2**

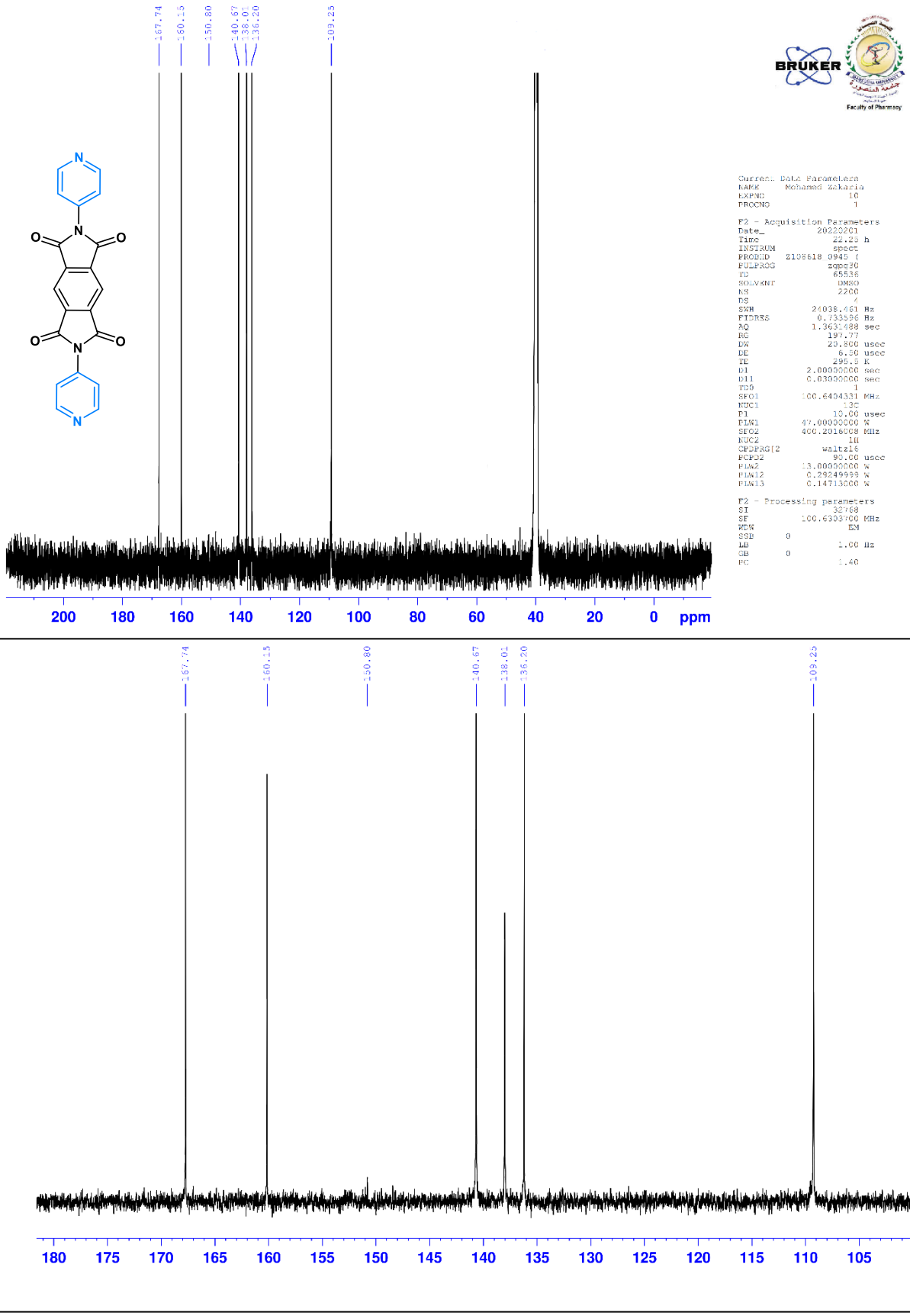


Figure S7. ^{13}**CNMR** (100 MHz, DMSO-*d*$_6$) of 2,6-di(pyridin-4-yl)pyrrolo[3,4-f]isoindole-1,3,5,7(2H,6H)-tetraone **DI-N2.**

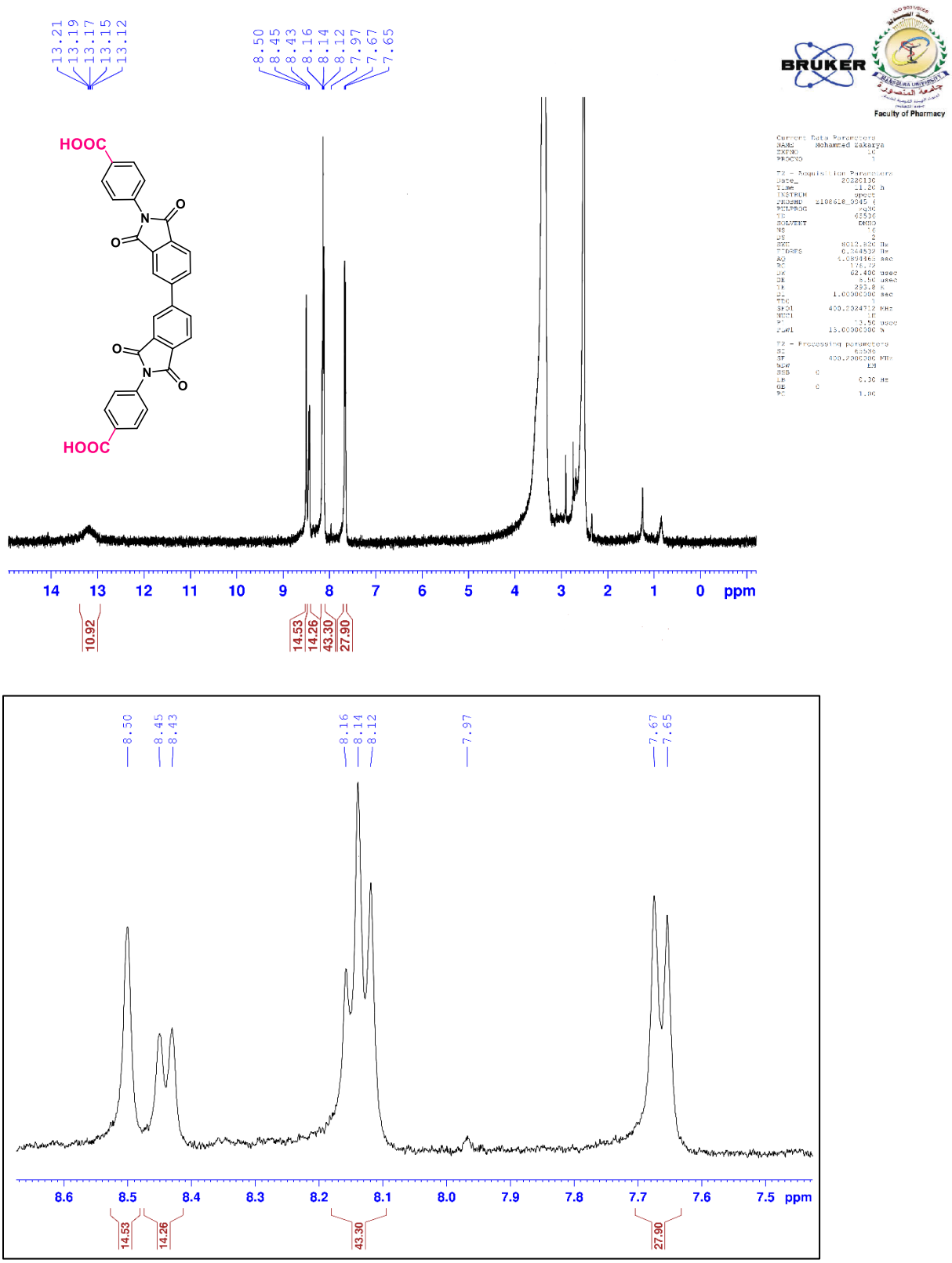
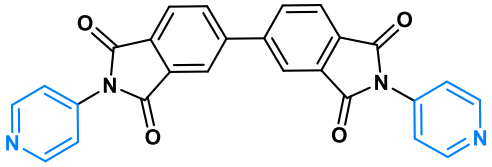


Figure S8. **^{1}HNMR** (400 MHz, DMSO-*d*$_6$) of 4,4'-(1,1',3,3'-tetraoxo-[5,5'-biisoindoline]-2,2'-diyl)dibenzoic acid, **DI-CA1**

Atomic Coordinates of Isolated Dyes:

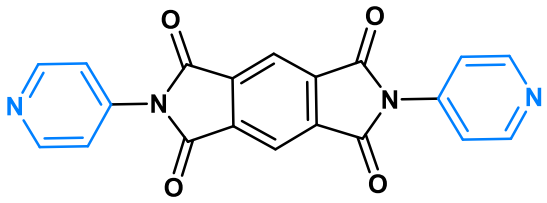
Below, we provide the atomic positions (coordinates) for the optimized geometries of the studied diimide UV-dyes obtained by DFT- B3LYP/6-31+g(d).



DI-N1 (48 atoms)

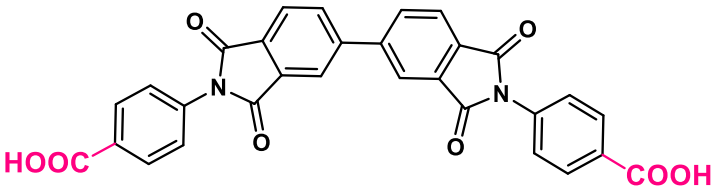
C	-2.79960113	2.57311546	-0.86539615
C	-1.41061947	2.55540589	-0.69244786
C	-0.74113667	1.44084717	-0.14468608
C	-1.48709292	0.30573940	0.24084490
C	-2.86073331	0.33455089	0.06327920
C	-3.51147202	1.44542991	-0.47853492
C	0.73709713	1.45262996	0.01398604
C	1.40962694	2.63392127	0.39200891
C	2.80072921	2.67821517	0.54223397
C	3.51206616	1.50925535	0.30605703
C	2.85814542	0.33279575	-0.06805897
C	1.48220439	0.27607506	-0.21834731
C	-3.88050686	-0.70230093	0.37688122
N	-5.12446932	-0.14835788	-0.00858138
C	-4.96748982	1.15740322	-0.53719705
C	4.97074732	1.23703431	0.37448279
N	5.12528850	-0.12850291	0.02933626
C	3.87785972	-0.73470892	-0.25293934
C	-6.37266608	-0.82160614	0.10725365
C	6.37494635	-0.80671692	-0.02101217
C	-7.43193028	-0.23435224	0.80309891
C	-8.63661367	-0.93433224	0.87943729
N	-8.83054247	-2.14511433	0.33277627
C	-7.79868626	-2.69616969	-0.32598826
C	-6.55643288	-2.07824955	-0.47467378
C	6.76942656	-1.47764833	-1.18089959
C	7.99921332	-2.13675404	-1.17272230
N	8.82958789	-2.15082768	-0.11781365
C	8.43687180	-1.49293812	0.98466212
C	7.22224861	-0.81389245	1.08965963
O	-3.72647725	-1.80195700	0.87465771
O	-5.87132149	1.85626507	-0.95633682
O	3.71864454	-1.90065396	-0.56279399
O	5.88210294	1.99640307	0.64644638
H	-3.29298475	3.43951019	-1.29574740
H	-0.83408244	3.41852839	-1.01087272
H	-1.00083707	-0.56000686	0.67977040
H	0.83441470	3.53255818	0.59320863
H	3.29605401	3.59725311	0.84120359
H	0.99316596	-0.64233422	-0.52810128
H	-7.32632095	0.73377967	1.28038909
H	-9.48106694	-0.50148511	1.41108317
H	-7.97142008	-3.67641688	-0.76480985
H	-5.76374155	-2.56324094	-1.03379887
H	6.14629220	-1.48470776	-2.06854674
H	8.33238273	-2.67210065	-2.05903904
H	9.12032750	-1.51372186	1.83062911
H	6.94796477	-0.31494843	2.01293192

DI-N2 (38 atoms)



C	-1.17325564	0.69979882	0.00091975
C	-1.17325561	-0.69979947	-0.00091559
C	0.00000014	-1.45014802	0.00000188
C	1.17325562	-0.69979928	0.00091950
C	1.17325553	0.69979911	-0.00091624
C	-0.00000009	1.45014769	0.00000150
C	2.58977519	-1.16792001	-0.00196108
N	3.38327822	0.00000005	0.00000045
C	2.58977493	1.16792012	0.00196285
C	4.80910864	0.00000014	-0.00000048
C	5.51372345	-0.62943566	1.02750803
C	6.90821409	-0.60406300	0.97540132
N	7.60497569	0.00000045	-0.00000252
C	6.90821245	0.60406359	-0.97540574
C	5.51372192	0.62943612	-1.02751017
O	3.01061501	2.30781902	0.01796626
O	3.01061527	-2.30781896	-0.01796476
C	-2.58977494	1.16791976	-0.00196086
N	-3.38327825	-0.00000059	0.00000128
C	-2.58977501	-1.16792047	0.00196392
O	-3.01061530	2.30781849	-0.01796503
O	-3.01061489	-2.30781949	0.01796750
C	-4.80910841	-0.00000031	-0.00000031
C	-5.51372372	0.62943773	1.02750685
C	-6.90821414	0.60406562	0.97539982
N	-7.60497579	0.00000066	-0.00000334
C	-6.90821250	-0.60406443	-0.97540497
C	-5.51372176	-0.62943776	-1.02750883
H	0.00000015	-2.53550607	0.00000203
H	-0.00000036	2.53550573	0.00000120
H	4.99990440	-1.11894059	1.84801215
H	7.48827972	-1.08710645	1.75840480
H	7.48827708	1.08710754	-1.75840963
H	4.99990131	1.11894105	-1.84801329
H	-4.99990486	1.11894410	1.84801024
H	-7.48827977	1.08711071	1.75840224
H	-7.48827660	-1.08710965	-1.75840847
H	-4.99990159	-1.11894479	-1.84801103

DI-CA1 (56 atoms)



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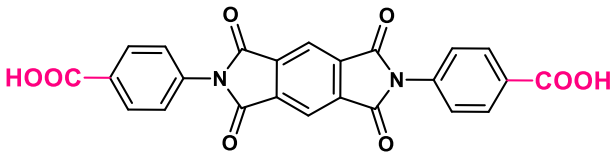
C	-1.48862323	-0.81220671	-0.18711723
C	-2.85934658	-0.84187961	0.01052140
C	-3.50353214	-1.95970466	0.54644503
C	0.73554235	-1.96558664	-0.02060030
C	1.39372755	-3.12997987	-0.46847722
C	2.78006230	-3.16839806	-0.66158812
C	3.50063703	-2.01192180	-0.39411985
C	2.86073784	-0.85394161	0.05512650
C	1.48969059	-0.80217463	0.24554261
C	-3.88359690	0.19936442	-0.27497092
N	-5.11998211	-0.35689677	0.12433231
C	-4.95846437	-1.66746800	0.63343323
C	4.95760988	-1.73426115	-0.49720574
N	5.12414665	-0.39049551	-0.08737327
C	3.88883771	0.20258831	0.25888316
C	-6.36930501	0.32503686	0.03655894
C	6.37554200	0.29268499	-0.05117003
C	-7.39548563	-0.20387076	-0.75183900
C	-8.61369124	0.46846768	-0.84139238
C	-8.81169762	1.67396410	-0.14894804
C	-7.77485106	2.18810872	0.64633665
C	-6.55774053	1.52015755	0.74050878
C	6.85518656	0.79247128	1.16297951
C	8.07051413	1.47473831	1.19622047
C	8.81356662	1.65843060	0.01908544
C	8.31886310	1.15165167	-1.19342265
C	7.10578527	0.47032543	-1.23206169
O	-3.73695738	1.30532966	-0.76206616
O	-5.85860488	-2.36947525	1.05663359
O	3.74307137	1.35255589	0.63047736
O	5.85875130	-2.47588868	-0.84412166
C	10.11061520	2.40267080	-0.01408660
O	10.58844543	2.87063676	-1.03053738
O	10.78126883	2.56504121	1.15120859
C	-10.09520534	2.44082029	-0.19519783
O	-10.40306876	3.27971523	0.63072124
O	-10.95547668	2.18610672	-1.20987912
H	-3.27562475	-3.96745970	1.32709975
H	-0.82086229	-3.94795963	0.99741313
H	-1.00649537	0.05938780	-0.61911039
H	0.80974921	-4.01765194	-0.69256118
H	3.26402069	-4.07314071	-1.01743216
H	1.01072254	0.10195678	0.60874869
H	-7.24421148	-1.13127765	-1.29467907
H	-9.39784138	0.01728386	-1.44420115
H	-7.92820551	3.11380170	1.19095800
H	-5.76109820	1.91855124	1.36070228
H	6.28497151	0.64978414	2.07513425
H	8.40347585	1.87267689	2.15164179
H	8.88754343	1.29890793	-2.10576427
H	6.72199831	0.08820135	-2.17255405
H	10.36020398	2.07898381	1.88564048
H	-10.57882340	1.56417244	-1.86137796

DI-CA2 (46 atoms)



C	-1.17332485	0.71020075	0.00431467
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C	1.17351337	-0.68945838	-0.00346670
C	1.17332264	0.71020508	-0.00432164
C	-0.00000255	1.46035866	-0.00000445
C	2.59113091	-1.15619510	0.00033775
N	3.38321525	0.01096689	-0.00964187
C	2.59035634	1.17767319	-0.01545747
C	4.81148263	0.01242227	-0.00372083
C	5.50794468	-0.54050620	-1.08170091
C	6.90222825	-0.55146116	-1.06703682
C	7.60301810	0.01138305	0.01195535
C	6.88915027	0.58244279	1.07733148
C	5.49728557	0.57124214	1.08015761
O	3.01121160	2.31794428	-0.03794288
O	3.01288320	-2.29622235	0.02118745
C	-2.59036040	1.17766333	0.01545312
N	-3.38321521	0.01095421	0.00963866
C	-2.59112665	-1.15620495	-0.00033841
O	-3.01122034	2.31793260	0.03794056
O	-3.01287277	-2.29623437	-0.02118318
C	-4.81148298	0.01241125	0.00372231
C	-5.50794563	-0.54050630	1.08170747
C	-6.90222920	-0.55145520	1.06704438
C	-7.60301784	0.01138395	-0.01195142
C	-6.88914847	0.58243122	-1.07733324
C	-5.49728408	0.57122599	-1.08016004
C	-9.09736697	0.05467221	-0.07171481
O	-9.71891116	0.86991711	-0.72645873
O	-9.78550812	-0.86777977	0.64178458
C	9.09736697	0.05466688	0.07171526
O	9.71891640	0.86990958	0.72645646
O	9.78550081	-0.86779298	-0.64178081
H	0.00000460	-2.52498900	0.00000029
H	-0.00000514	2.54574880	-0.00000488
H	4.96773287	-0.94911887	-1.92979396
H	7.41827873	-0.96794546	-1.92865943
H	7.42868140	1.01966280	1.91095340
H	4.94707746	0.98727106	1.91829157
H	-4.96773497	-0.94911517	1.92980261
H	-7.41827904	-0.96792907	1.92867227
H	-7.42867939	1.01964626	-1.91095774
H	-4.94707349	0.98724789	-1.91829585
H	-9.19129869	-1.52427322	1.05381134
H	9.19128493	-1.52428398	-1.05380258

Atomic Coordinates of Cosensitizer:

Below, we provide the atomic positions (coordinates) for the optimized geometries of the studied dimer obtained by DFT- B3LYP-D3(BJ)/6-31G(d).

DI-CA1/ BTD-DTP1 (126 atoms)

C	-1.06192300	3.99619600	-1.92699000	H	-9.42257200	0.04891000	-0.42643400	C	5.09339200	0.31470900	1.68836500
C	0.29478900	3.68405200	-1.87869200	C	-3.10777800	-0.05281700	1.17127600	C	3.69168100	0.34746400	1.59238700
C	0.76023400	2.35320300	-1.81938400	C	-2.61059700	1.28938200	1.29756400	C	3.29094800	1.68415400	1.80099500
C	-0.17878100	1.30016300	-1.86729100	C	-2.13289000	-1.03457700	1.13009700	C	1.89610800	1.89614900	1.73525900
C	-1.52371800	1.61875500	-1.94348300	C	-1.17945500	1.56831300	1.39815300	C	1.21521700	0.72056500	1.47091700
C	-1.96013300	2.94277200	-1.94686700	C	-0.75046900	-0.77099200	1.21646700	H	1.38229600	2.83696400	1.87125500
C	2.21357700	2.08026000	-1.71187200	H	-2.44057300	-2.07128200	1.05556200	C	6.90489300	1.78758500	2.03909800
C	3.09409800	3.07180000	-1.22518700	C	-0.21333200	0.49973000	1.36302700	H	7.44144800	2.71640700	2.18970600
C	4.46845500	2.86554500	-1.11567300	H	-0.08375900	-1.62748000	1.19338600	C	7.56747600	0.57264400	1.87143000
C	4.95809400	1.61983300	-1.47250000	N	-3.36197800	2.39751900	1.30312400	S	6.43759700	-0.77953100	1.60737200
C	4.10579600	0.62713000	-1.94258000	N	-0.90553600	2.87397400	1.48786100	S	2.32146600	-0.66851200	1.28037300
C	2.74549000	0.82959200	-2.08385000	S	-2.34086600	3.67708500	1.43743000	N	4.40684300	2.47448600	2.00264100
C	-2.72337000	0.72994800	-2.03730500	C	8.98358200	0.46625700	1.81433200	C	4.40710400	3.88807900	2.31486400
N	-3.83638500	1.60194200	-2.03596600	C	9.80209600	-0.61892500	1.67601700	H	3.57808000	4.37255500	1.79245000
C	-3.44243600	2.96242000	-1.97173600	H	9.51697300	1.41340900	1.85847200	H	5.34251500	4.33453800	1.96862200
C	6.33562800	1.08150600	-1.41349500	C	9.32454100	-1.95500800	1.70572600	H	4.30363600	4.06779400	3.39129600
N	6.24722600	-0.27257800	-1.85783800	C	11.27704100	-0.34144500	1.53130400				
C	4.90461900	-0.59705700	-2.20386800	N	8.95310900	-3.05925000	1.75518600				
C	-5.19960500	1.20640700	-2.08705500	O	12.06585400	-1.32626500	1.09201100				
C	7.31050900	-1.20922500	-1.76911900	H	11.61071200	-2.12663800	0.73714200				
C	-6.08352900	1.73898300	-1.14881900	O	11.73358900	0.75235300	1.79343100				
C	-7.43000900	1.40545200	-1.21510300	C	-4.53316900	-0.39520900	1.08099400				
C	-7.90187000	0.55791200	-2.22335800	C	-4.93312700	-1.52069100	0.34080500				
C	-7.00522500	0.03614000	-3.16460100	C	-5.53770500	0.31750800	1.75923800				
C	-5.65170700	0.34406800	-3.09054200	C	-6.25052000	-1.95082000	0.31498200				
C	7.03053000	-2.56872400	-1.56628100	H	-4.20005700	-2.05794900	-0.25055000				
C	8.07274000	-3.46567800	-1.38193800	C	-6.86408000	-0.08632500	1.71214500				
C	9.40076500	-3.02469800	-1.36758300	H	-5.27656600	1.20250200	2.32676300				
C	9.67372900	-1.67185200	-1.58899400	C	-7.24831300	-1.24349900	1.00575500				
C	8.64216600	-0.76954600	-1.81537200	H	-6.50264800	-2.83796900	-0.24961900				
O	-2.76817100	-0.47909800	-2.11357500	H	-7.61224900	0.49026800	2.24342400				
O	-4.18558500	3.91815500	-1.94004000	N	-8.60663200	-1.64093100	0.97600000				
O	4.50691800	-1.66412300	-2.61971200	C	-9.03443200	-2.75461100	0.17593200				
O	7.34182000	1.65843300	-1.05996300	C	-9.75014900	-3.80628700	0.76045800				
C	10.51291400	-3.93374900	-0.98616500	C	-8.77394800	-2.78765500	-1.19972500				
O	11.48006000	-3.58012600	-0.33878100	C	-10.20948200	-4.86271200	-0.02459000				
O	10.41697700	-5.22123700	-1.37941400	H	-9.95478800	-3.79000700	1.82486000				
C	-9.35486200	0.22532300	-2.34189900	C	-9.22614300	-3.85103100	-1.97538800				
O	-9.91261500	0.01717800	-3.39264100	H	-8.20662200	-1.98938800	-1.65953200				
O	-10.04305400	0.18171000	-1.16766200	C	-9.95203000	-4.89212700	-1.39482200				
H	-1.40855400	5.02388500	-1.95344200	H	-10.76781100	-5.66833100	0.44358100				
H	1.01092200	4.49684300	-1.90298200	H	-9.02287100	-3.85211800	-3.04207800				
H	0.12695000	0.26240100	-1.81011300	H	-10.31451400	-5.71431600	-2.00420100				
H	2.68850800	4.02000300	-0.89250200	C	-9.45124500	-1.32008900	2.09467500				
H	5.13072600	3.63838000	-0.74172600	C	-9.00778800	-1.49231800	3.41071900				
H	2.12168100	0.03598200	-2.47728300	C	-10.75571600	-0.87555500	1.85263700				
H	-5.70913300	2.39433100	-0.37376700	C	-9.85617600	-1.19311700	4.47542400				
H	-8.11745600	1.82813900	-0.48948800	H	-8.00074600	-1.85274000	3.59228900				
H	-7.38665700	-0.60384300	-3.95327200	C	-11.60216100	-0.59108500	2.92275000				
H	-4.94887800	-0.06426300	-3.80732800	H	-11.10497100	-0.76875500	0.83080600				
H	6.00811800	-2.91260000	-1.52599000	C	-11.15546300	-0.74176100	4.23659100				
H	7.83406600	-4.50030900	-1.15242400	H	-9.50304900	-1.32616800	5.49401000				
H	10.70162300	-1.32529000	-1.56448000	H	-12.61236900	-0.24468700	2.72553600				
H	8.86315400	0.27516300	-1.97329500	H	-11.81540200	-0.51308300	5.06803300				
H	9.65968000	-5.32155900	-1.98004100	C	5.51465400	1.64313000	1.94412200				

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