

Electronic Supporting Information

**Quinoline-based compound for explosive 2,4,6-trinitrophenol sensing:
experimental and DFT-D3 studies**

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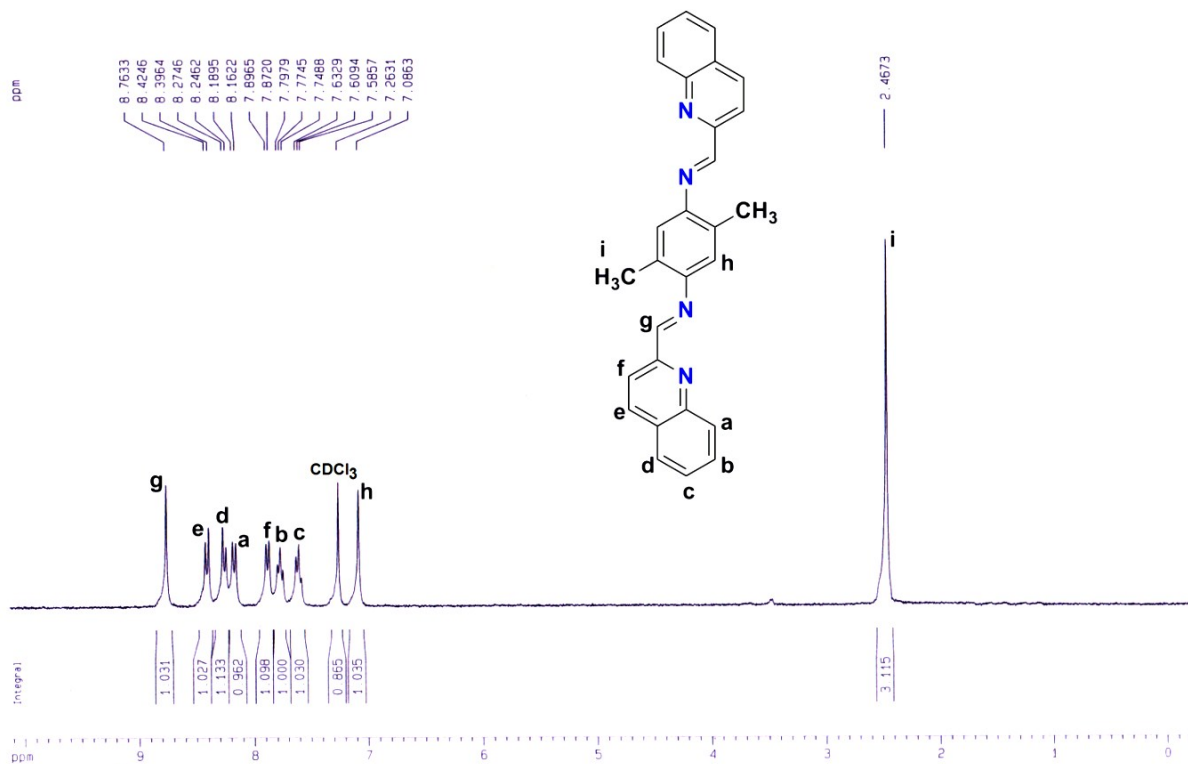


Fig. s1 ¹H NMR spectrum of DQB in CDCl₃.

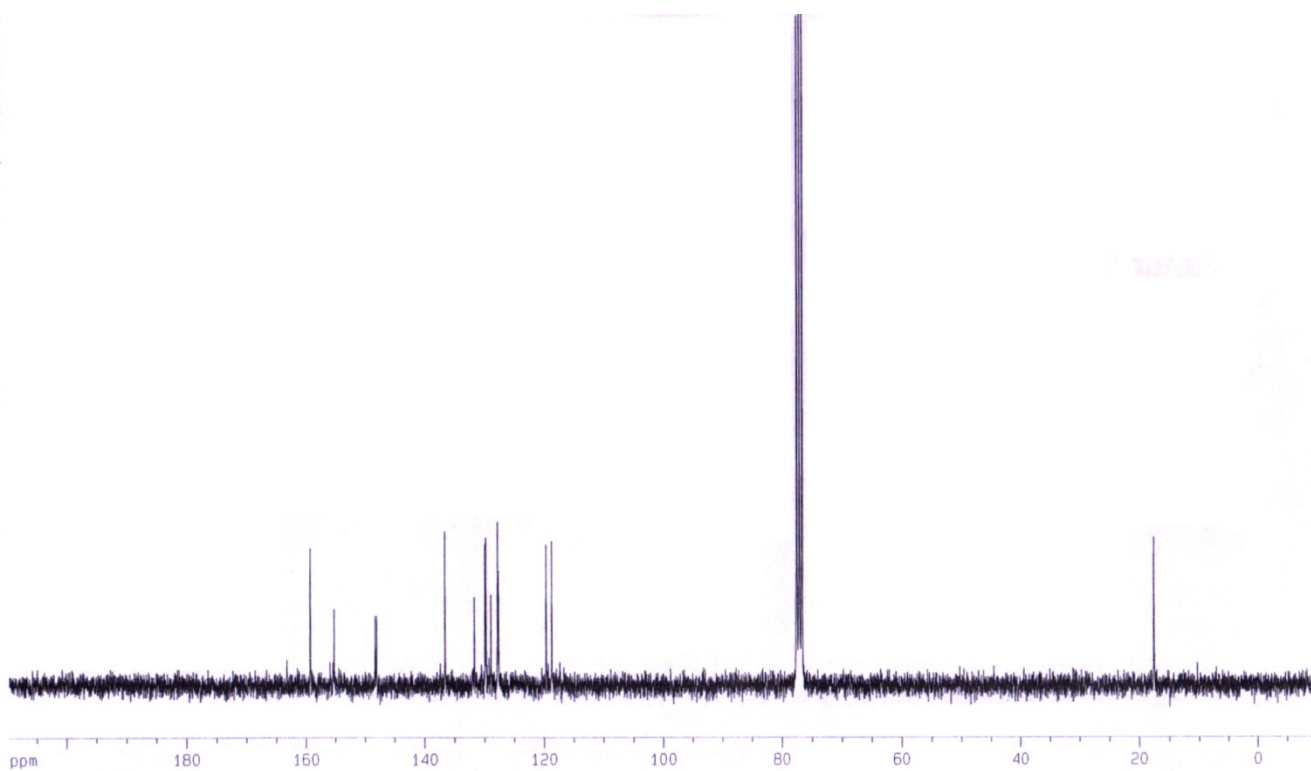


Fig. s2 ¹³C NMR spectrum of DQB in CDCl₃.

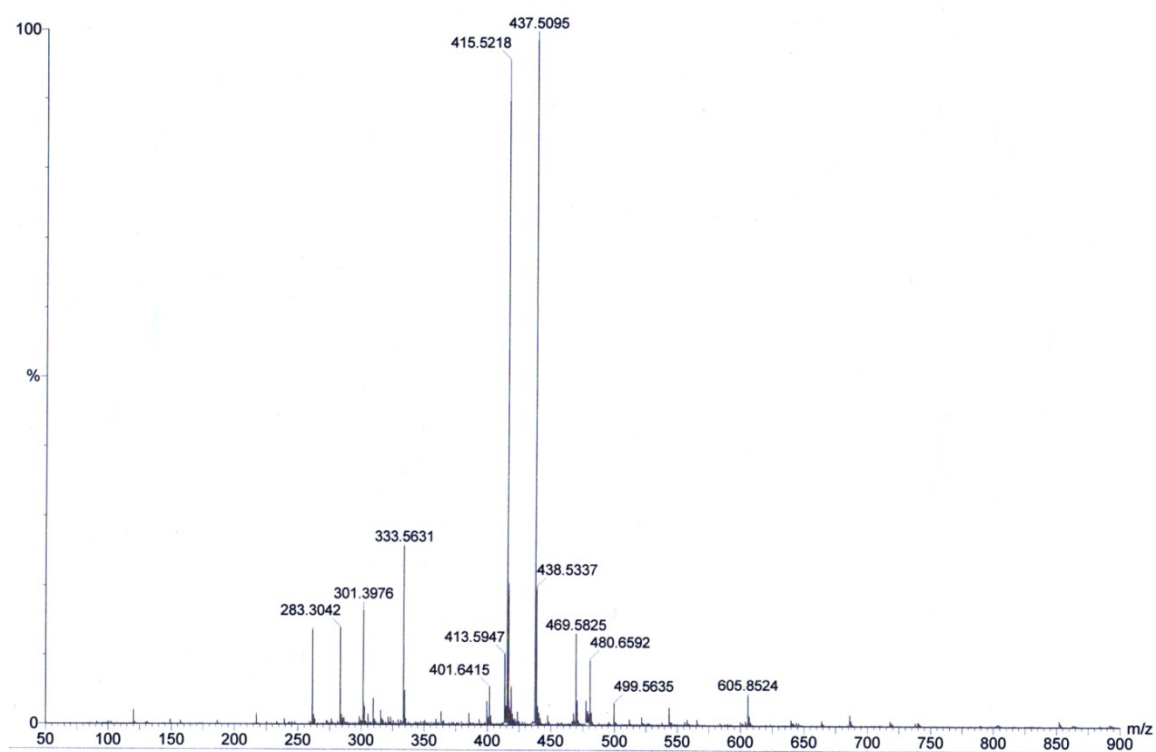


Fig. s3 Mass spectrum of DQB in methanol.

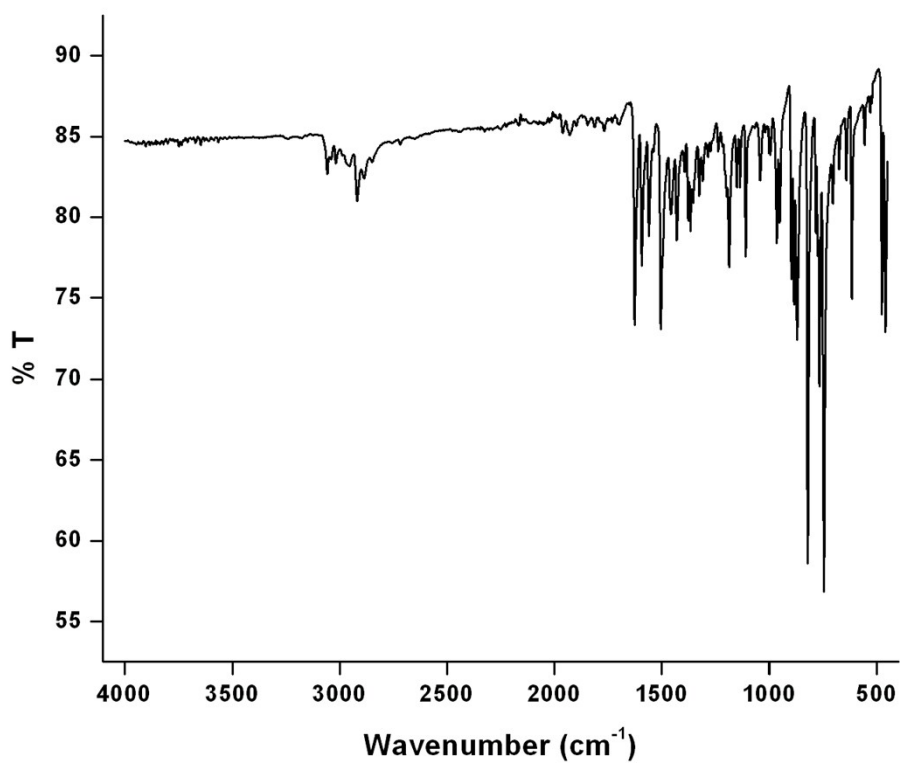


Fig. s4 FT-IR spectrum of DQB.

Detection limit (DL) has been calculated through the following equation^{ref1}

$$DL = CL \times ET$$

CL = Conc. of DQB; ET = Conc. of titrant at which change is observed.

Thus detection limit for TNP: $DL = 1 \times 10^{-4} \times 0.015 \text{ equiv} = 1.5 \times 10^{-6} \text{ M} \approx 1.5 \mu\text{M}$.

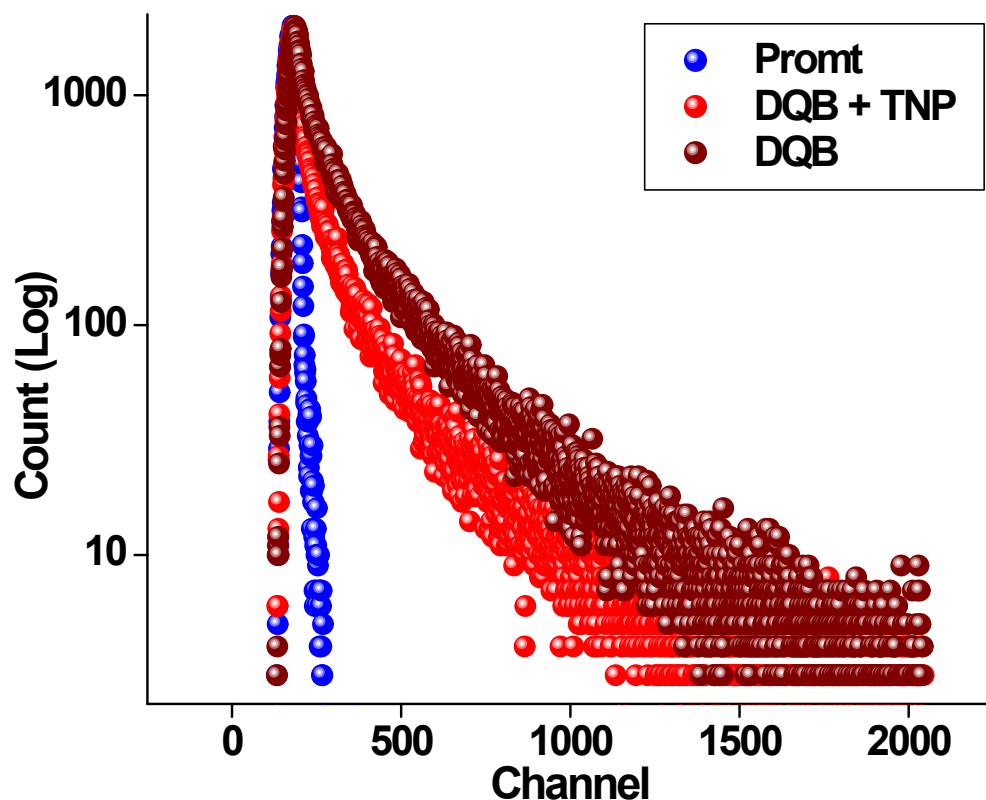


Fig. s5 Fluorescence decay behavior of DQB and DBQ with TNP (5 eqv.).

Table S1 Coordinates of DQB.

C	-0.7080719	2.0007731	-0.3001934
C	0.6815483	2.0611021	-0.3728349
C	1.4194873	0.9645182	0.1401680
C	0.7360878	-0.1172161	0.7234746
C	-0.6605051	-0.1899930	0.7821773
C	-1.3960861	0.8920603	0.2325613
C	-1.3105044	-1.3665176	1.4708655
C	1.3889494	3.2407689	-0.9823670

C	-5.0189298	0.1001011	-0.0053110
C	-5.6601992	1.2850437	0.4617791
C	-7.0389827	-0.9726910	-0.3384937
C	-7.0322952	1.3157198	0.5187734
C	-7.7525985	-2.1341711	-0.7482144
C	-7.7767049	0.1722312	0.1162912
C	-9.1316124	-2.1571142	-0.7078428
C	-9.1954660	0.1177961	0.1453757
C	-9.8592095	-1.0239635	-0.2584438
C	5.0133391	0.0631547	-0.0242134
C	5.6910126	1.2978246	0.2031901
C	7.0034137	-1.1029786	-0.1844550
C	7.0641136	1.3041951	0.2310082
C	7.6833776	-2.3378412	-0.3821773
C	7.7753546	0.0873883	0.0367754
C	9.0621934	-2.3876537	-0.3609184
C	9.1927922	0.0036037	0.0527512
C	9.8234245	-1.2095823	-0.1422153
N	5.6439492	-1.0871078	-0.2112701
N	-5.6801701	-0.9812171	-0.3899931
C	-3.5484068	0.0150175	-0.0822659
C	3.5415673	0.0056809	-0.0625268
N	-2.7939299	0.9863203	0.2640017
N	2.8152031	1.0439283	0.1094183
H	-1.3072424	2.8348585	-0.6736599
H	1.3185697	-0.9189953	1.1839899
H	-2.2227823	-1.0724367	2.0120819

H	-1.5987905	-2.1558471	0.7573858
H	-0.6135853	-1.8185906	2.1918390
H	1.8767465	2.9652198	-1.9326689
H	0.6870891	4.0628070	-1.1842317
H	2.1894827	3.6029010	-0.3184020
H	-5.0448786	2.1345439	0.7598383
H	-7.5618999	2.2057131	0.8692862
H	-7.1743343	-2.9950048	-1.0908516
H	-9.6725655	-3.0527917	-1.0232492
H	-9.7507832	0.9932182	0.4923420
H	-10.9510500	-1.0601497	-0.2337277
H	5.1005135	2.2030087	0.3475175
H	7.6200137	2.2302612	0.4009069
H	7.0796627	-3.2326030	-0.5488963
H	9.5768255	-3.3396788	-0.5132095
H	9.7739564	0.9139820	0.2220266
H	10.9145094	-1.2679176	-0.1289162
H	-3.1712429	-0.9407030	-0.4824392
H	3.1281443	-0.9994757	-0.2622368

Table S2 Coordinates of DQB---DNT.

C	-1.1502976	3.2054523	-3.8155450
C	0.2079005	3.2954700	-4.1135210
C	1.0956526	2.4360689	-3.4197874
C	0.5889954	1.5497017	-2.4534277
C	-0.7766609	1.4428914	-2.1661615
C	-1.6655269	2.2811544	-2.8857172

C	-1.2355732	0.5032050	-1.0775029
C	0.7233497	4.2507375	-5.1551205
C	-5.2185542	1.3044803	-2.4022549
C	-5.8767370	2.5408546	-2.1384904
C	-7.1819029	0.1071658	-2.1931940
C	-7.2241852	2.5294932	-1.8787777
C	-7.8626787	-1.1414785	-2.2360073
C	-7.9288574	1.2942603	-1.8903821
C	-9.2151992	-1.2113285	-1.9717901
C	-9.3196439	1.1908102	-1.6226686
C	-9.9496116	-0.0376724	-1.6586502
C	4.6663633	1.6276341	-3.9750693
C	5.3078025	2.8999749	-4.0341788
C	6.6367367	0.5137323	-4.4429297
C	6.6493671	2.9533385	-4.3219070
C	7.3234115	-0.7129101	-4.6603320
C	7.3651223	1.7456412	-4.5458900
C	8.6675846	-0.7148894	-4.9723394
C	8.7439703	1.7118950	-4.8788319
C	9.3824151	0.5048612	-5.0871699
N	5.3067890	0.4832932	-4.1625416
N	-5.8441176	0.1378916	-2.4337597
C	-3.7658763	1.2619127	-2.6540006
C	3.2186235	1.5217062	-3.7273955
N	-3.0505721	2.3200183	-2.6700544
N	2.4648584	2.5525649	-3.6790768
C	-7.5299071	-0.5062564	1.3988104

C	-6.4568531	-1.3691231	0.7927718
C	-6.6974816	-2.6837059	0.3322765
C	-5.7117792	-3.5139828	-0.2056496
C	-4.3960545	-3.0680692	-0.2775929
C	-4.0971394	-1.7832318	0.1607607
C	-5.1150158	-0.9606850	0.6512603
N	-8.0558711	-3.2530138	0.3442062
N	-4.6805749	0.4043997	1.0010942
O	-8.3276254	-4.0660420	-0.5292698
O	-8.8407282	-2.8965728	1.2080292
O	-5.4030955	1.3455134	0.7136542
O	-3.5788461	0.5211599	1.5202706
C	3.8654555	3.1629012	-7.1890384
C	4.9684886	2.1692429	-7.4405886
C	4.7735270	0.7677286	-7.4383638
C	5.7957387	-0.1550053	-7.6761655
C	7.0955796	0.2865607	-7.8945090
C	7.3557767	1.6516260	-7.8757438
C	6.3039941	2.5504093	-7.6793049
N	3.4439667	0.1808765	-7.1870898
N	6.6993267	3.9702253	-7.7195536
O	3.2437856	-0.9560989	-7.5902960
O	2.6095094	0.8399418	-6.5848719
O	6.0343865	4.7468490	-8.3869472
O	7.7086588	4.2810146	-7.1041034
H	-1.8607328	3.8631450	-4.3224678
H	1.2933581	0.9445731	-1.8772305

H	-2.0442517	0.9403007	-0.4726573
H	-1.6065634	-0.4505727	-1.4865790
H	-0.4016879	0.2627514	-0.4021539
H	1.0230835	3.7101195	-6.0686525
H	-0.0438816	4.9875955	-5.4332966
H	1.6211148	4.7770063	-4.7961025
H	-5.2896003	3.4594619	-2.1364088
H	-7.7645187	3.4543113	-1.6599465
H	-7.2809335	-2.0328319	-2.4747574
H	-9.7241832	-2.1776330	-1.9913815
H	-9.8809918	2.0986457	-1.3868217
H	-11.0188146	-0.1121484	-1.4468511
H	4.7147988	3.7978636	-3.8599740
H	7.1732730	3.9089714	-4.3933496
H	6.7515077	-1.6395785	-4.5796955
H	9.1872117	-1.6609398	-5.1426696
H	9.2860680	2.6554808	-4.9744299
H	10.4436783	0.4849878	-5.3462300
H	-3.3685506	0.2521227	-2.8528855
H	2.8399962	0.4887410	-3.6381131
H	-5.9901356	-4.5063396	-0.5576757
H	-3.0803348	-1.3962316	0.1182023
H	-8.4031814	-0.4527439	0.7335535
H	-3.6131477	-3.7139578	-0.6772030
H	-7.8750924	-0.9547090	2.3398601
H	-7.1749009	0.5084480	1.5826355
H	5.5569918	-1.2168754	-7.6701563

H	8.3639414	2.0360802	-8.0245081
H	3.0167933	2.9700861	-7.8611864
H	7.9016628	-0.4282705	-8.0594758
H	3.4830754	3.0606804	-6.1666966
H	4.2057631	4.1877696	-7.3483041

Table S3. Coordinates of DQB---NBA.

C	-0.4902208	1.5923173	-1.6774508
C	0.8473527	1.9356615	-1.8493036
C	1.8184599	0.9410253	-1.5750324
C	1.4084865	-0.3234021	-1.1192561
C	0.0628724	-0.6778032	-0.9598970
C	-0.9126714	0.3070903	-1.2725028
C	-0.2656401	-2.0513122	-0.4291796
C	1.2675112	3.3016368	-2.3181641
C	-4.3975845	-1.0021101	-1.2557970
C	-5.1482377	0.1233093	-0.8067039
C	-6.2990805	-2.3053623	-1.4438302
C	-6.5110103	0.0055378	-0.6856528
C	-6.8944581	-3.5590234	-1.7584584
C	-7.1402865	-1.2282584	-1.0067016
C	-8.2581740	-3.7339389	-1.6436290
C	-8.5391343	-1.4405164	-0.8951888
C	-9.0872784	-2.6683627	-1.2095771
C	5.4349045	0.8134795	-2.3607405
C	5.9198102	2.0935874	-1.9621638
C	7.5094727	0.1722951	-3.1527733

C	7.2408620	2.3976337	-2.1820229
C	8.3251936	-0.8051307	-3.7874676
C	8.0882178	1.4376317	-2.7995566
C	9.6482669	-0.5350776	-4.0687077
C	9.4522146	1.6850183	-3.1015202
C	10.2159409	0.7192915	-3.7265750
N	6.2004807	-0.1101315	-2.9235604
N	-4.9511991	-2.1681847	-1.5578101
C	-2.9330354	-0.9188776	-1.4130236
C	4.0135144	0.4630116	-2.1992427
N	-2.2978743	0.1577610	-1.1471428
N	3.1647146	1.2876628	-1.7180825
O	-10.0262134	-1.7903811	2.4558621
O	-9.8163835	-3.9384827	1.8432093
C	-5.8258022	-1.3372932	2.2855152
C	-5.0966746	-2.4357651	1.8245448
C	-5.6974157	-3.6538637	1.5061402
C	-7.0788361	-3.7688684	1.6324498
C	-7.8362208	-2.6712990	2.0680935
C	-7.2051511	-1.4646781	2.4065069
N	-3.6467623	-2.2963917	1.6402524
O	-3.0184227	-3.2812233	1.2773935
O	-3.1429889	-1.2011448	1.8445429
C	-9.3261090	-2.7335307	2.1513877
O	9.6070106	-0.0166481	-7.4415585
O	10.3046077	2.0294680	-6.8420223
C	5.7289656	0.8966041	-6.0166571

C	5.5444966	2.1680315	-5.4703038
C	6.5707454	3.1109646	-5.4045881
C	7.8262435	2.7648555	-5.8984141
C	8.0387933	1.4915494	-6.4465869
C	6.9884345	0.5634123	-6.5050113
N	4.2216930	2.5257221	-4.9338660
O	4.0864121	3.6342471	-4.4372277
O	3.3276873	1.6953098	-5.0104930
C	9.3767814	1.0741626	-6.9629036
H	-1.2691043	2.3344769	-1.8683815
H	2.1746826	-1.0536754	-0.8469208
H	-1.1035254	-2.0476943	0.2822330
H	-0.5366375	-2.7497975	-1.2384160
H	0.6112517	-2.4761986	0.0813683
H	1.8251226	3.2414918	-3.2650139
H	0.3962885	3.9587923	-2.4543644
H	1.9554437	3.7673656	-1.5932992
H	-4.6175865	1.0451493	-0.5690799
H	-7.1201472	0.8447861	-0.3399434
H	-6.2380156	-4.3688866	-2.0833475
H	-8.7064776	-4.7016341	-1.8811459
H	-9.1719910	-0.6211261	-0.5454450
H	-10.1635164	-2.8277781	-1.1141489
H	5.2246162	2.8014064	-1.5110583
H	7.6484605	3.3726211	-1.9023871
H	7.8654779	-1.7586885	-4.0545292
H	10.2631467	-1.2836331	-4.5730587

H	9.8812970	2.6563208	-2.8428982
H	11.2614420	0.9214888	-3.9692942
H	-2.4695398	-1.8377249	-1.8039514
H	3.7426392	-0.5422221	-2.5685224
H	-10.7879867	-3.9036300	1.9106871
H	-5.0903371	-4.4816845	1.1443786
H	-5.3165915	-0.4055231	2.5245350
H	-7.5730283	-4.7028706	1.3699251
H	-7.8114851	-0.6231569	2.7432794
H	11.1458675	1.6885433	-7.1967288
H	6.3845501	4.0895326	-4.9659412
H	4.9039564	0.1870935	-6.0411962
H	8.6459038	3.4805078	-5.8486921
H	7.1747229	-0.4240338	-6.9278233

Table S4 Coordinates of DQB---NB.

C	-0.7634616	3.1775452	-2.7581168
C	0.5996002	3.3842708	-2.9578758
C	1.4847165	2.3291179	-2.6214787
C	0.9732376	1.1377998	-2.0802648
C	-0.3973054	0.9210496	-1.8915642
C	-1.2824237	1.9645521	-2.2633244
C	-0.8662424	-0.3663864	-1.2544372
C	1.1345690	4.6732434	-3.5197765
C	-4.7863590	0.7456715	-2.2205575
C	-5.5011478	1.7292511	-1.4778378
C	-6.6390123	-0.6249107	-2.3704955

C	-6.8214077	1.4986994	-1.1774446
C	-7.2211452	-1.8456416	-2.8109856
C	-7.4368733	0.2910767	-1.6060056
C	-8.5280868	-2.1510736	-2.4930846
C	-8.7778623	-0.0525530	-1.2934892
C	-9.3105217	-1.2520138	-1.7232104
C	5.0708963	1.8438153	-3.4086324
C	5.6567590	3.1167369	-3.1462124
C	7.0789821	0.9700628	-4.1470257
C	6.9932705	3.2955742	-3.4057446
C	7.8104413	-0.1279555	-4.6786078
C	7.7565909	2.2164430	-3.9286474
C	9.1480223	0.0071173	-4.9863345
C	9.1332705	2.3245456	-4.2557421
C	9.8145719	1.2422023	-4.7763440
N	5.7560493	0.8127557	-3.8808855
N	-5.3365486	-0.3744452	-2.6631041
C	-3.3475539	0.8988891	-2.4987624
C	3.6296222	1.6219192	-3.2039919
N	-2.6706767	1.8955281	-2.0743671
N	2.8540590	2.5514307	-2.7962626
C	6.2834226	3.4707682	-6.7314293
C	5.1146181	2.7100085	-6.6638814
C	5.0639829	1.3800787	-7.0903896
C	6.2244825	0.8021257	-7.6011683
C	7.4077059	1.5471560	-7.6784831
C	7.4364337	2.8764617	-7.2449416

N	3.8984243	3.3266527	-6.1226688
O	2.8792616	2.6501216	-6.0775730
O	3.9602724	4.4880392	-5.7416070
C	-6.8902297	-1.4674598	1.2294541
C	-6.7678907	-2.6534424	0.5032676
C	-5.5758605	-3.0259610	-0.1230857
C	-4.4739981	-2.1791639	-0.0136695
C	-4.5750180	-0.9855295	0.7102844
C	-5.7784835	-0.6309171	1.3290259
N	-7.9372619	-3.5284819	0.3768831
O	-7.8312042	-4.5408729	-0.3027433
O	-8.9681629	-3.2041883	0.9513200
H	-1.4733601	3.9731093	-2.9980374
H	1.6741787	0.3621336	-1.7615494
H	-1.7448780	-0.2024899	-0.6126443
H	-1.1511947	-1.1225559	-2.0042540
H	-0.0667593	-0.8027597	-0.6381302
H	1.6995235	4.4965151	-4.4474871
H	0.3211668	5.3854743	-3.7212620
H	1.8464235	5.1369782	-2.8167916
H	-4.9781413	2.6297237	-1.1542770
H	-7.4023472	2.2216114	-0.5987018
H	-6.5962648	-2.5303841	-3.3876672
H	-8.9627508	-3.0985624	-2.8192472
H	-9.3768142	0.6425792	-0.6995364
H	-10.3384203	-1.5175081	-1.4666538
H	5.0231748	3.9169792	-2.7643514

H	7.4773268	4.2597235	-3.2288112
H	7.2754357	-1.0653172	-4.8432835
H	9.7014189	-0.8386146	-5.4018912
H	9.6412706	3.2788115	-4.0937675
H	10.8733370	1.3328773	-5.0309447
H	-2.9118447	0.0771934	-3.0919701
H	3.2771274	0.6114636	-3.4782777
H	4.1339311	0.8195915	-7.0115036
H	8.3160021	1.0838851	-8.0690834
H	6.2806073	4.5013767	-6.3807852
H	6.2086886	-0.2382977	-7.9318532
H	8.3623827	3.4517446	-7.2970530
H	-5.5281366	-3.9551694	-0.6885046
H	-3.7118433	-0.3204922	0.7857199
H	-7.8412643	-1.2114256	1.6932040
H	-3.5370629	-2.4472543	-0.5057344
H	-5.8551748	0.3061257	1.8835175

Table S5. Coordinates of DQB---TNP_{Head on}.

C	-1.5726979	-0.3408976	-1.1133988
C	-0.1876987	-0.4949571	-1.1438648
C	0.4059518	-1.1538291	-0.0341502
C	-0.4133677	-1.5678193	1.0356881
C	-1.8039174	-1.4590200	1.0426019
C	-2.4057362	-0.8405331	-0.0901764
C	-2.5611128	-1.9485533	2.2501373
C	0.5795868	0.0505747	-2.3196010

C	-6.1297544	-0.9769512	-0.1174514
C	-6.4589032	0.0145280	-1.0864218
C	-8.3491178	-1.5521346	0.1866675
C	-7.7806313	0.2100809	-1.4073986
C	-9.3198118	-2.3777512	0.8178328
C	-8.7820489	-0.5735958	-0.7704983
C	-10.6590038	-2.2286574	0.5215435
C	-10.1666084	-0.4434165	-1.0525407
C	-11.0868520	-1.2545600	-0.4178354
C	3.9558182	-2.1319806	-0.5527202
C	4.5175047	-2.0915005	0.7567741
C	5.8485080	-3.1265344	-1.4359646
C	5.7902197	-2.5746878	0.9436687
C	6.5147043	-3.7020730	-2.5530749
C	6.5057086	-3.1164402	-0.1595309
C	7.7776775	-4.2379990	-2.4083880
C	7.8096708	-3.6634717	-0.0472744
C	8.4317699	-4.2151282	-1.1496609
N	4.5960840	-2.6236378	-1.6037466
N	-7.0360847	-1.7309375	0.4895911
C	-4.7291772	-1.2591895	0.2362161
C	2.5726222	-1.6984980	-0.8092968
N	-3.7653942	-0.6188743	-0.3131338
N	1.7644482	-1.4326345	0.1469492
H	-2.0663928	0.1808297	-1.9349705
H	0.0889701	-2.0260762	1.8888933
H	-3.3274219	-1.2272882	2.5748499

H	-3.0677205	-2.9054030	2.0496976
H	-1.8680864	-2.1157616	3.0865856
H	0.7736560	-0.7379292	-3.0652924
H	-0.0034284	0.8357368	-2.8217483
H	1.5509597	0.4751276	-2.0240054
H	-5.6529336	0.5778593	-1.5569011
H	-8.0743755	0.9560562	-2.1506864
H	-8.9703926	-3.1240383	1.5335814
H	-11.4005778	-2.8653785	1.0103777
H	-10.4898322	0.3044348	-1.7813984
H	-12.1518973	-1.1514611	-0.6393155
H	3.9212113	-1.6868246	1.5748636
H	6.2569470	-2.5613999	1.9320123
H	5.9881659	-3.7219748	-3.5088079
H	8.2799093	-4.6897364	-3.2671514
H	8.3039390	-3.6554708	0.9274346
H	9.4312397	-4.6460630	-1.0549629
H	-4.6167385	-2.0802865	0.9566275
H	2.2934141	-1.7243400	-1.8711777
O	3.6763145	-5.5753663	-3.1461111
C	3.2712232	-5.3907704	-1.9182404
C	2.0318192	-4.7568550	-1.5941205
C	1.6038315	-4.5663032	-0.2835138
C	2.4449827	-4.9480313	0.7475301
C	3.6862141	-5.5327882	0.4982626
C	4.0772435	-5.7744438	-0.8075657
N	1.2227307	-4.1843360	-2.6509371

N	2.0408962	-4.6892708	2.1292425
N	5.3702128	-6.4469437	-0.9982999
O	0.3322065	-3.4120756	-2.3499675
O	1.4978450	-4.4737200	-3.8228135
O	5.5754698	-7.0191869	-2.0539508
O	6.1571202	-6.4123712	-0.0639896
O	2.8855389	-4.8305937	3.0001562
O	0.8882647	-4.3360198	2.3266312
H	0.6412371	-4.1073873	-0.0774846
H	4.3444429	-5.8101580	1.3187651
H	2.9614166	-5.2425318	-3.7524129
O	-5.0521641	-5.1884162	0.0399860
C	-4.7030885	-4.3753452	-0.9254534
C	-5.6345894	-3.6952317	-1.7624079
C	-5.2299208	-2.7979136	-2.7448338
C	-3.8733873	-2.5933564	-2.9468011
C	-2.9086835	-3.3008838	-2.2268051
C	-3.3315824	-4.1507492	-1.2195620
N	-7.0614807	-3.9133629	-1.5890348
N	-3.4422222	-1.6030301	-3.9339659
N	-2.3012887	-4.8478811	-0.4428329
O	-7.8391346	-3.3133299	-2.3001798
O	-7.4209744	-4.7103233	-0.7109778
O	-2.4472138	-4.9287381	0.7636710
O	-1.3432233	-5.2847814	-1.0623934
O	-2.2427602	-1.4888789	-4.1349486
O	-4.3059751	-0.9361638	-4.4832716

H	-5.9718640	-2.2636297	-3.3340517
H	-1.8487029	-3.1788169	-2.4473574
H	-6.0467683	-5.2448643	0.0314701

Table S6 Coordinates of DQB---TNP_{pi-pi}.

C	-0.6104989	2.0329742	-1.8022771
C	0.7710485	2.0802101	-1.9671081
C	1.5407207	1.0604279	-1.3533111
C	0.9001775	0.0693673	-0.5893685
C	-0.4896834	0.0077280	-0.4361895
C	-1.2621322	1.0088858	-1.0830558
C	-1.0860024	-1.0648655	0.4415894
C	1.4394463	3.1622479	-2.7707314
C	-4.9137821	0.3108694	-1.0219977
C	-5.4755508	1.5972333	-0.7713877
C	-7.0030970	-0.6675095	-1.1900601
C	-6.8422394	1.7291945	-0.7444717
C	-7.7945869	-1.8344322	-1.3909938
C	-7.6619423	0.5877796	-0.9645587
C	-9.1717376	-1.7557008	-1.3735702
C	-9.0805569	0.6345357	-0.9462185
C	-9.8204286	-0.5149918	-1.1447185
C	5.1083944	0.1502857	-1.7456247
C	5.7711897	1.4133109	-1.7653245
C	7.0827718	-0.9910526	-2.1219057
C	7.1285890	1.4474167	-1.9738812
C	7.7552878	-2.2241163	-2.3450885

C	7.8367335	0.2301408	-2.1698282
C	9.1066176	-2.2422988	-2.6238541
C	9.2302832	0.1773431	-2.4373115
C	9.8501998	-1.0339337	-2.6715287
N	5.7402354	-1.0030138	-1.9103971
N	-5.6480485	-0.7765571	-1.2103194
C	-3.4509515	0.1305181	-1.1010432
C	3.6461381	0.0730158	-1.5873764
N	-2.6547280	1.1245047	-1.0058284
N	2.9288322	1.1264747	-1.4947029
H	-1.2373239	2.8082770	-2.2494595
H	1.5139957	-0.6664698	-0.0640112
H	-1.9317659	-0.6927021	1.0359184
H	-1.4562303	-1.9214928	-0.1452531
H	-0.3251805	-1.4527325	1.1349601
H	1.9770721	2.7407387	-3.6338975
H	0.7054175	3.8966824	-3.1325720
H	2.1987754	3.6842550	-2.1659716
H	-4.8041669	2.4393156	-0.6056040
H	-7.3093969	2.6981321	-0.5478011
H	-7.2784087	-2.7828958	-1.5510274
H	-9.7722739	-2.6557873	-1.5220313
H	-9.5768164	1.5910269	-0.7633559
H	-10.9116401	-0.4735305	-1.1231272
H	5.1799548	2.3186062	-1.6281728
H	7.6698191	2.3959419	-2.0100599
H	7.1654844	-3.1422326	-2.3063170

H	9.6108355	-3.1923241	-2.8147694
H	9.7964614	1.1104789	-2.4778152
H	10.9182129	-1.0676064	-2.8973352
H	-3.1307642	-0.9058902	-1.2938518
H	3.2324164	-0.9508352	-1.6064777
O	-6.0292786	1.9480102	2.6175888
C	-6.6761437	0.8405007	2.3726546
C	-8.1028081	0.7772747	2.2971865
C	-8.7949346	-0.4075532	2.0689048
C	-8.0694250	-1.5741552	1.8854557
C	-6.6781535	-1.5768976	1.9280864
C	-5.9946234	-0.3942332	2.1620125
N	-8.8903295	1.9931473	2.4035258
N	-8.7765648	-2.8251771	1.6124450
N	-4.5294517	-0.4717919	2.1564012
O	-10.0927286	1.9318137	2.2540494
O	-8.2900106	3.0580443	2.6189033
O	-3.8891934	0.5649495	2.1147521
O	-4.0311040	-1.5887732	2.1685534
O	-8.1038691	-3.8220572	1.4007584
O	-9.9971680	-2.7949267	1.5989580
H	-9.8810869	-0.4066586	2.0235089
H	-6.1203581	-2.4963135	1.7672208
H	-6.7083524	2.6693817	2.7281114
O	6.8742196	2.2354323	-5.1755140
C	6.7261976	0.9376732	-5.2110744
C	5.4602029	0.2988256	-5.0324101

C	5.3081418	-1.0840832	-5.0587447
C	6.4249845	-1.8710304	-5.2847779
C	7.6822568	-1.3092734	-5.4956764
C	7.8316989	0.0663833	-5.4428471
N	4.2651376	1.0948785	-4.8036908
N	6.2925412	-3.3281107	-5.2570215
N	9.1937937	0.5884319	-5.6151967
O	3.1999130	0.5310146	-4.6666608
O	4.3888570	2.3282344	-4.7525212
O	9.4251613	1.7346863	-5.2735693
O	10.0301935	-0.1773421	-6.0721505
O	7.3058472	-3.9912049	-5.4167817
O	5.1813277	-3.7938683	-5.0578429
H	4.3303401	-1.5309792	-4.8950711
H	8.5483854	-1.9396643	-5.6795706
H	5.9728586	2.6323128	-5.0237626