Supplementary Material (ESI) for *PCCP*

Electronic supplementary information for

Enantioselective interaction of carbamoylated quinine and (*S*)-3,5-dinitrobenzoyl alanine: theoretical and experimental circular dichroism study

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S1: BHandH/6-31+G** structure of (*S*)-DNB-Ala.

N	-2.13736	-0.17421	0.02540
H	-2.02803	0.77608	-0.29742
C	-3.47612	-0.67293	0.03884
C	-3.94056	-1.06533	1.42328
C	-4.33644	0.39944	-0.54369
O	-5.60146	0.05236	-0.61342
O	-3.92289	1.46653	-0.89949
C	-1.11207	-1.01998	0.15308
O	-1.26736	-2.21008	0.32017
C	0.25697	-0.44488	0.08525
C	0.52602	0.90666	0.16954
C	1.29604	-1.34789	-0.04573
C	1.83543	1.32834	0.10495
H	-0.24280	1.65641	0.30450
C	2.58418	-0.87501	-0.11030
H	1.08282	-2.40829	-0.08996
C	2.89137	0.46302	-0.03730
H	3.91227	0.81532	-0.08521
N	3.67025	-1.82090	-0.25585
O	4.78329	-1.37300	-0.30562
O	3.38089	-2.98348	-0.31720
N	2.11104	2.74489	0.20057
O	3.25888	3.08766	0.13591
O	1.16943	3.47853	0.33770
H	-6.09925	0.78671	-0.99024
H	-3.28167	-1.84433	1.80325
H	-3.90512	-0.20764	2.09656
H	-3.54112	-1.55227	-0.61207
H	-4.95982	-1.44719	1.38783

S2: BHandH/6-31+G** structure of *anti*-closed conformer of *t*BuCQN.

C	-0.25283	-0.23924	0.25572
C	0.78330	-0.87102	1.12847
C	2.08998	-1.15583	0.66633
C	0.48153	-1.17741	2.42011
C	2.52665	-0.90784	-0.63979
C	2.98801	-1.73994	1.58902
C	1.45477	-1.74982	3.25181
C	3.79781	-1.22194	-1.02331
C	4.28880	-2.04733	1.16559
N	2.66021	-2.02327	2.86345
C	4.69470	-1.79899	-0.10929
O	4.13065	-0.94522	-2.29300
C	5.41236	-1.25765	-2.72595
O	-1.52109	-0.68584	0.68837
C	-2.35495	-1.14560	-0.24739
O	-2.09813	-1.15606	-1.42670
N	-3.49249	-1.57040	0.30524
C	-4.60416	-2.12442	-0.44682
C	-5.13354	-1.09359	-1.41901
C	-4.16280	-3.36925	-1.18436
C	-5.66613	-2.47237	0.56686
H	-0.13524	-0.54840	-0.78334
H	-0.51311	-0.99294	2.80347
H	1.88103	-0.44425	-1.37002
H	1.20658	-1.98861	4.28110
H	4.95462	-2.49194	1.89349
H	5.70277	-2.04733	-0.40933
H	5.46506	-0.96147	-3.77039
H	6.17311	-0.70966	-2.16193
H	5.61294	-2.33054	-2.65025
H	-3.55151	-1.52260	1.30733
H	-5.46852	-0.20228	-0.88479
H	-4.35680	-0.80906	-2.12827
H	-5.98042	-1.50265	-1.97282
H	-3.79829	-4.12056	-0.48120
H	-5.00258	-3.79341	-1.73778
H	-3.36531	-3.12940	-1.88700
H	-6.53603	-2.89469	0.06382
H	-5.29852	-3.21338	1.28105
H	-5.99205	-1.58459	1.11445
C	-0.24612	1.27561	0.36040
C	-1.50271	1.93563	-0.21255
H	-0.17493	1.50484	1.42969
C	0.78146	1.90496	-1.69344
C	1.12374	3.16888	0.26337
C	-1.07833	3.25482	-0.83891
H	-1.95251	1.30511	-0.98621
H	-2.25584	2.07698	0.56469

H	1.75492	2.13539	-2.13151
H	0.49956	0.91781	-2.06515
C	-0.28268	2.93383	-2.08811
C	-0.15327	4.02698	0.10123
H	1.96287	3.62395	-0.26745
H	1.41075	3.10152	1.31575
H	-1.95167	3.86520	-1.07582
H	0.17344	3.84609	-2.48308
H	-0.93557	2.53500	-2.86761
H	0.10244	4.97410	-0.38529
N	0.93654	1.83500	-0.25423
C	-0.79062	4.34925	1.40149
C	-1.04461	5.57334	1.83087
H	-1.05393	3.50703	2.03907
H	-1.50896	5.75582	2.79132
H	-0.79171	6.44008	1.22945

S3: BHandH/6-31+G** structure of *anti*-open conformer of *t*BuCQN.

N	-0.00928	1.91936	-1.06873
C	0.27826	1.21463	0.16442
C	-0.36690	1.92046	1.36765
C	-1.22399	3.05864	0.84131
C	-2.21929	2.49085	-0.15344
C	-1.42935	1.94512	-1.35100
C	0.46417	3.27486	-0.93627
C	-0.35397	4.07223	0.10005
C	-0.09000	-0.25757	0.04728
O	-1.42691	-0.45101	0.44807
C	-2.21741	-1.16193	-0.36227
N	-3.43525	-1.28557	0.17135
C	-4.53908	-1.97070	-0.47689
C	-5.71173	-1.86716	0.46671
C	0.51800	4.86806	0.99413
C	0.47680	6.18386	1.11562
C	0.80508	-1.11078	0.88078
C	2.14804	-1.31918	0.48196
C	2.95416	-2.11685	1.32097
N	2.50469	-2.67571	2.46218
C	1.26939	-2.46960	2.79078
C	0.37696	-1.69445	2.03013
C	4.28611	-2.34708	0.95272
C	4.80423	-1.81926	-0.19072
C	3.99545	-1.02935	-1.02421
C	2.69218	-0.78311	-0.69195
O	4.44095	-0.48512	-2.16282
C	5.75431	-0.72421	-2.54715
O	-1.86645	-1.59946	-1.42821
C	-4.86774	-1.29212	-1.78855
C	-4.18417	-3.42303	-0.70632
H	-0.00856	-0.55391	-1.00117
H	-0.64660	-1.56677	2.35517
H	2.10311	-0.16930	-1.36366
H	0.92549	-2.93074	3.71112
H	4.88515	-2.96225	1.61131
H	5.83462	-2.01435	-0.45147
H	5.89707	-0.20412	-3.49059
H	6.46581	-0.33328	-1.81380
H	5.94138	-1.79152	-2.69695
H	-3.58031	-0.86029	1.07041
H	-5.13887	-0.24784	-1.61986
H	-4.01037	-1.32946	-2.46017
H	-5.70986	-1.79349	-2.26893
H	-3.96580	-3.91701	0.24243
H	-5.01976	-3.94101	-1.18041
H	-3.31054	-3.50290	-1.35254
H	-6.58022	-2.36578	0.03635

H	-5.48882	-2.34646	1.42313
H	-5.97902	-0.82305	0.64781
H	1.36484	1.24328	0.27062
H	-0.98899	1.22861	1.93817
H	0.39715	2.29618	2.05096
H	-1.56439	2.57745	-2.23136
H	-1.75967	0.94741	-1.64333
H	0.42714	3.76116	-1.91337
H	1.51712	3.23822	-0.64089
H	-1.74147	3.55456	1.66534
H	-2.92292	3.26583	-0.46796
H	-2.79920	1.69614	0.32244
H	-1.02513	4.76739	-0.41683
H	1.25028	4.31010	1.57583
H	1.14457	6.71547	1.78106
H	-0.23193	6.77606	0.54666

S4: BHandH/6-31+G** structure of *syn*-closed conformer of *t*BuCQN.

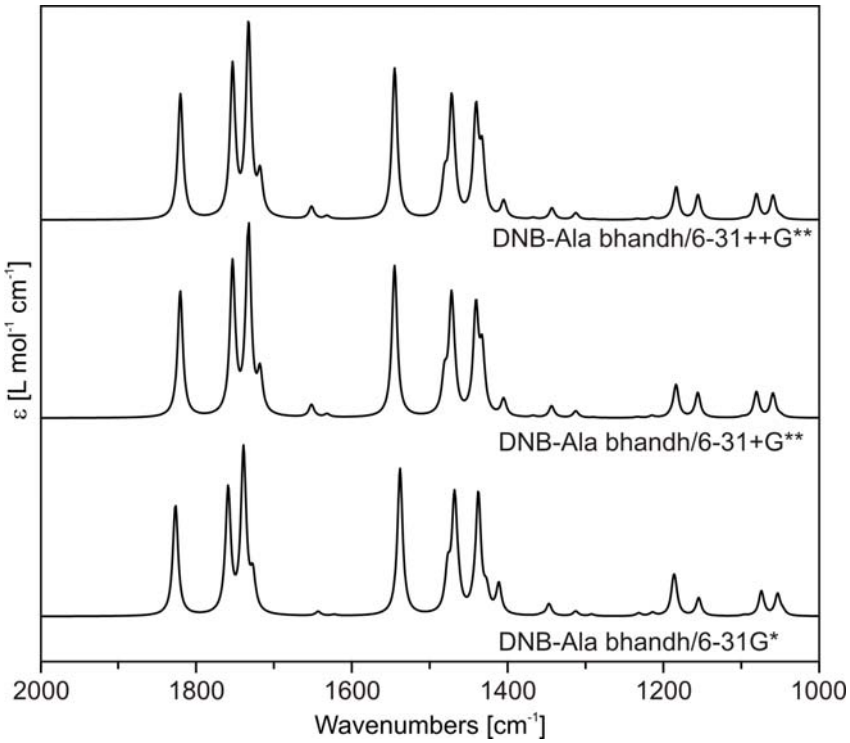
C	-0.27748	0.23185	-0.98271
C	0.85780	-0.53526	-1.57106
C	1.76317	-1.28969	-0.78335
C	1.07869	-0.46984	-2.90998
C	1.65122	-1.44652	0.60489
C	2.84159	-1.90664	-1.45599
C	2.18189	-1.12807	-3.47621
C	2.57331	-2.17408	1.30180
C	3.76835	-2.64968	-0.71182
N	3.03347	-1.81770	-2.78641
C	3.64879	-2.78496	0.63745
O	2.38711	-2.27083	2.62676
C	3.30748	-2.99316	3.37555
O	-1.01751	-0.59932	-0.11159
C	-2.32712	-0.71764	-0.34601
O	-2.91165	-0.10772	-1.20811
N	-2.87705	-1.58219	0.50772
C	-4.28417	-1.93880	0.50970
C	-5.12720	-0.71029	0.77079
C	-4.66288	-2.56888	-0.81260
C	-4.46458	-2.93505	1.62834
H	-0.95117	0.54136	-1.78252
H	0.41183	0.09970	-3.54545
H	0.82174	-1.01659	1.14729
H	2.35133	-1.06864	-4.54639
H	4.58340	-3.11024	-1.25456
H	4.37901	-3.36286	1.18570
H	2.97588	-2.93588	4.40901
H	3.34015	-4.04319	3.07012
H	4.31168	-2.56587	3.29992
H	-2.24957	-2.04835	1.14006
H	-4.86446	-0.26573	1.73268
H	-4.97261	0.03007	-0.01358
H	-6.18426	-0.98128	0.79313
H	-4.06973	-3.46795	-0.99091
H	-5.71812	-2.84794	-0.80594
H	-4.49178	-1.86758	-1.62895
H	-5.50796	-3.24542	1.68495
H	-3.85715	-3.82782	1.46005
H	-4.18963	-2.49703	2.59083
C	0.17412	1.45396	-0.20821
C	-0.95926	2.09647	0.59480
H	0.96785	1.13329	0.47407
C	-0.22541	3.16472	-1.82644
C	1.54586	3.34499	-0.28953
C	-0.76555	3.60234	0.53095
H	-1.93169	1.84479	0.15863
H	-0.96494	1.73070	1.62326

H	0.28284	3.76038	-2.58733
H	-0.86215	2.45834	-2.36147
C	-1.06135	4.04418	-0.88869
C	0.68677	3.96980	0.83518
H	1.94214	4.12197	-0.94702
H	2.40374	2.81494	0.13209
H	-1.42535	4.10413	1.24114
H	-0.81013	5.10194	-1.00849
H	-2.12690	3.93887	-1.10480
H	0.77040	5.06100	0.79782
N	0.78054	2.42387	-1.09429
C	1.11900	3.53047	2.18451
C	1.46283	4.34558	3.16659
H	1.15912	2.45624	2.35786
H	1.77482	3.97295	4.13365
H	1.44409	5.42190	3.03182

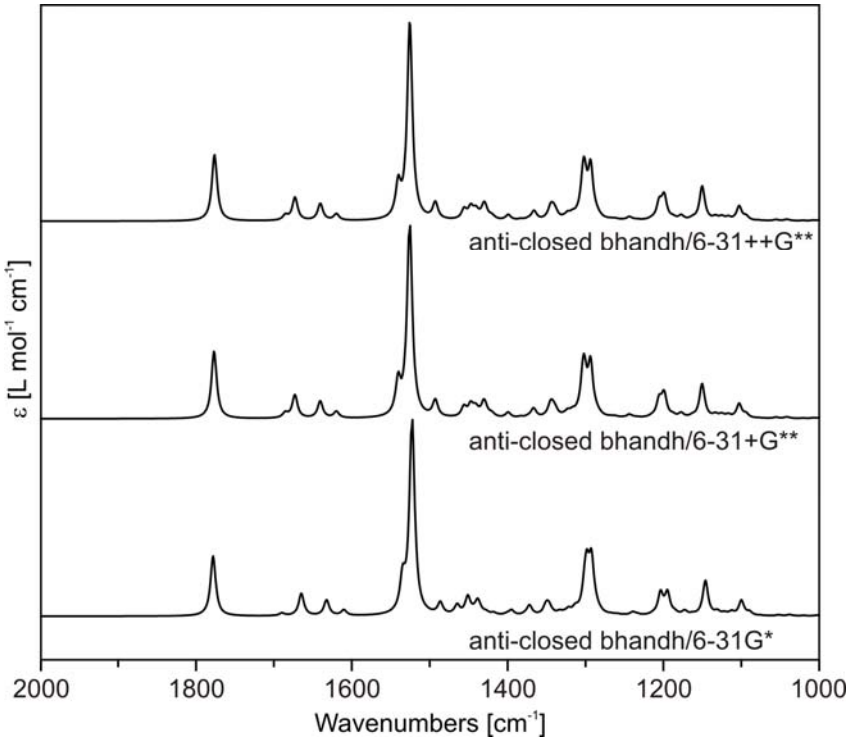
S5: BHandH/6-31+G** structure of complex of (*S*)-DNB-Ala and *t*BuCQN.

C	-0.94383	-0.26806	-0.68568
C	0.28816	-0.43595	-1.51666
C	1.31678	-1.31473	-1.10536
C	0.44034	0.24373	-2.68874
C	1.29466	-2.02561	0.11346
C	2.42502	-1.44504	-1.96878
C	1.59844	0.05594	-3.45316
C	2.33478	-2.85535	0.43387
C	3.47676	-2.31040	-1.60280
N	2.55179	-0.75956	-3.11650
C	3.43408	-2.99828	-0.43831
O	2.41343	-3.56783	1.55036
C	1.39290	-3.43414	2.49664
O	-1.64136	0.87870	-1.12214
C	-1.69953	1.93947	-0.32298
O	-1.25632	1.95012	0.80959
N	-2.33777	2.94475	-0.90174
C	-2.57206	4.24351	-0.28469
C	-3.43604	4.07063	0.94427
C	-1.26084	4.90910	0.06846
C	-3.30188	5.06407	-1.31973
H	-0.67238	-0.12793	0.36249
H	-0.31520	0.94474	-3.01541
H	0.48640	-1.87928	0.81919
H	1.73109	0.61289	-4.37467
H	4.32021	-2.38216	-2.27811
H	4.23972	-3.65250	-0.13108
H	1.63362	-4.12586	3.29904
H	1.35508	-2.41552	2.88961
H	0.42233	-3.69908	2.06729
H	-2.57148	2.82174	-1.87232
H	-4.39499	3.62103	0.67912
H	-2.94227	3.43334	1.67789
H	-3.62655	5.04235	1.40259
H	-0.62245	4.99814	-0.81128
H	-1.45368	5.90535	0.46995
H	-0.72643	4.33179	0.82228
H	-3.52963	6.05065	-0.91692
H	-2.68934	5.20113	-2.21427
H	-4.24500	4.59038	-1.60287
C	-1.83953	-1.49324	-0.80453
C	-2.63349	-1.54839	-2.11526
H	-1.16149	-2.34827	-0.74833
C	-3.72708	-0.57451	0.42102
C	-3.43145	-2.91017	0.20770
C	-4.11158	-1.62253	-1.77892
H	-2.44039	-0.65907	-2.71784
H	-2.32619	-2.40630	-2.71532

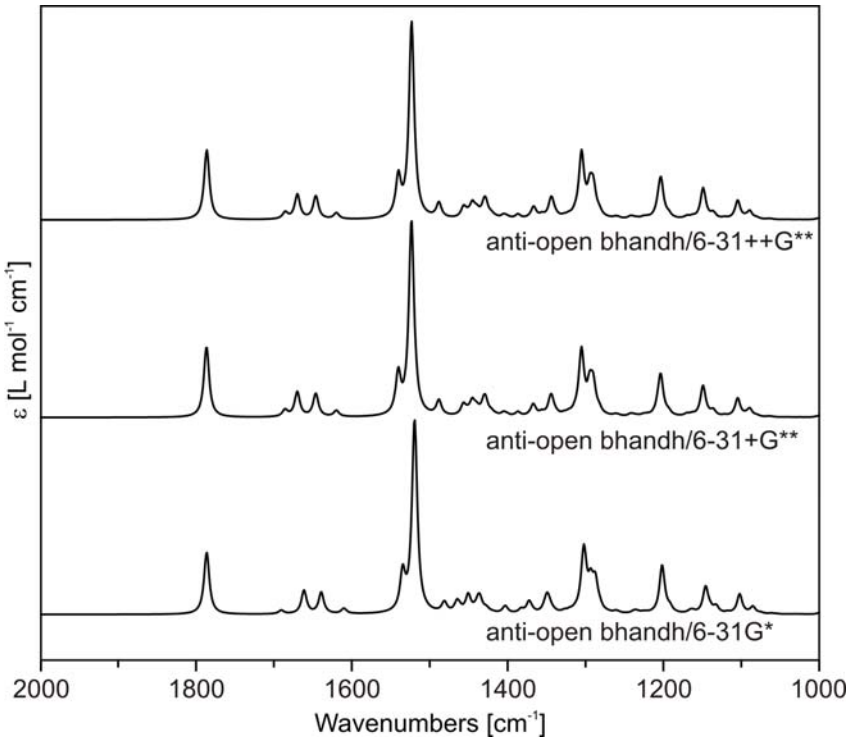
H	-4.39791	-0.83856	1.23920
H	-3.23952	0.34512	0.74226
C	-4.46299	-0.42979	-0.91028
C	-4.40834	-2.89025	-0.97934
H	-3.95195	-3.11908	1.14375
H	-2.68032	-3.69386	0.07411
H	-4.70575	-1.62245	-2.69455
H	-5.54214	-0.38057	-0.74948
H	-4.16557	0.49085	-1.41767
H	-5.43518	-2.81264	-0.60644
N	-2.73574	-1.64295	0.34178
C	-4.31164	-4.13093	-1.78519
C	-5.31423	-4.96260	-2.00772
H	-3.33389	-4.35880	-2.20682
H	-5.18992	-5.85712	-2.60394
H	-6.30008	-4.77494	-1.59582
C	-1.09580	1.50162	4.66878
C	-0.50537	0.40045	3.83509
H	-1.64000	2.20594	4.03706
H	-1.80312	1.09576	5.38990
N	0.38631	0.90900	2.83258
C	-1.58475	-0.40702	3.15055
H	0.08657	-0.28586	4.44740
H	-0.05629	1.42983	2.08489
C	1.60648	0.39734	2.66199
O	-1.10957	-1.25711	2.27786
O	-2.75747	-0.25871	3.36536
O	2.11394	-0.40025	3.42504
C	2.34420	0.81772	1.43798
H	-1.84895	-1.54082	1.61218
C	1.83959	1.69812	0.50453
C	3.55438	0.18932	1.20171
C	2.54821	1.92050	-0.65730
H	0.88653	2.19818	0.62226
C	4.22535	0.44916	0.03173
H	3.94105	-0.51623	1.92635
C	3.74399	1.30634	-0.93225
N	1.96142	2.77485	-1.65865
N	5.46196	-0.25086	-0.22993
H	4.26651	1.45805	-1.86657
O	2.61396	3.03029	-2.63199
O	0.83527	3.16437	-1.46385
O	5.97467	-0.07871	-1.30302
O	5.88674	-0.96615	0.63556
H	-0.30539	2.03501	5.19521



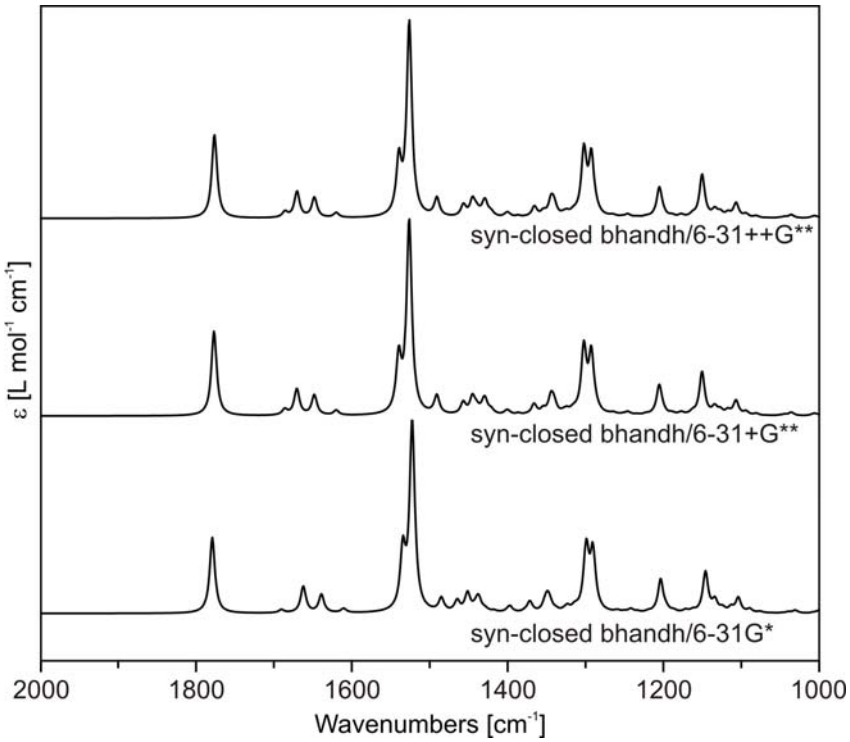
S6: BHandH IR absorption spectra of (*S*)-DNB-Ala using various basis sets.



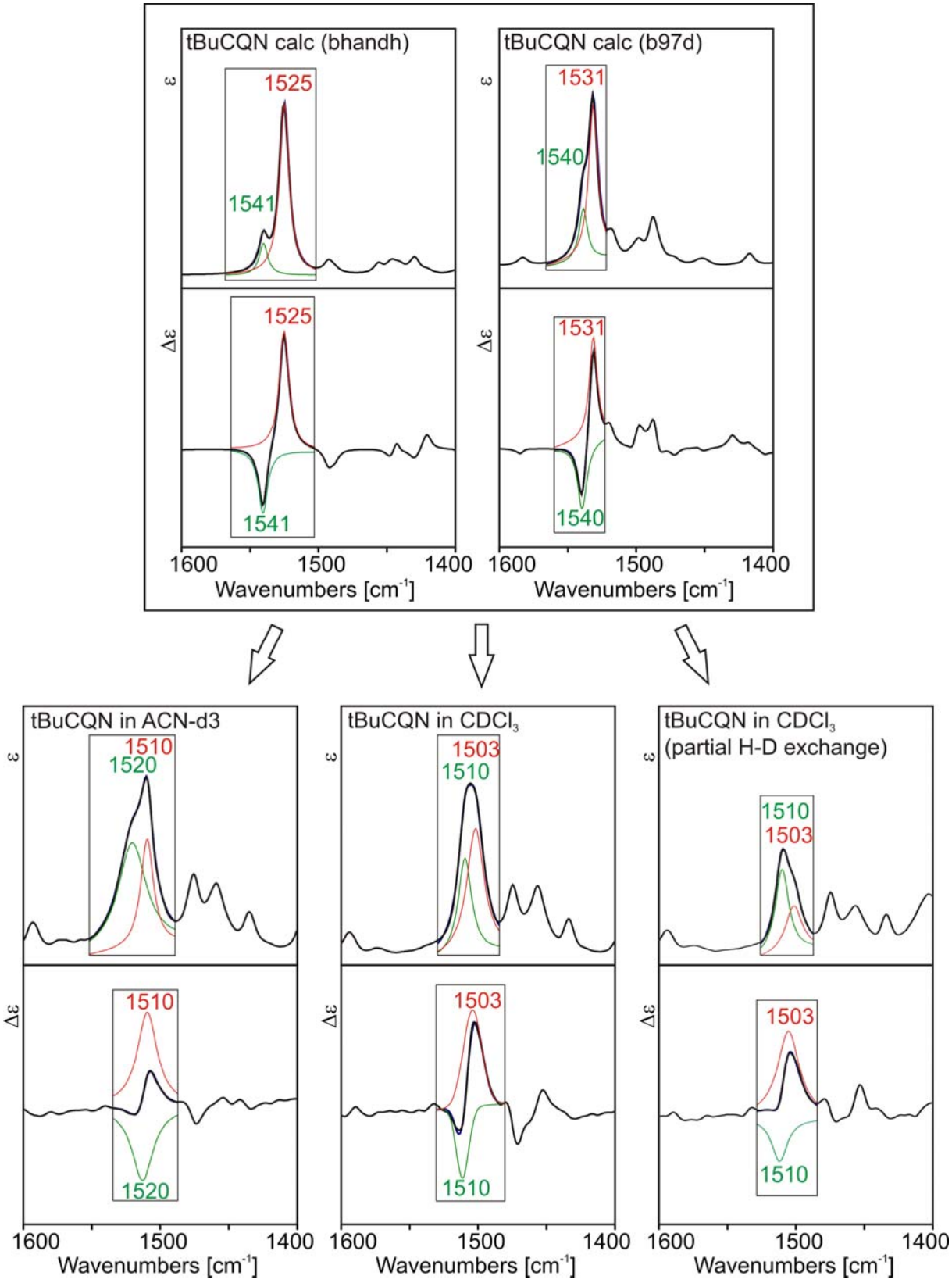
S7: BHandH IR absorption spectra of *anti*-closed conformer of tBuCQN using various basis sets.



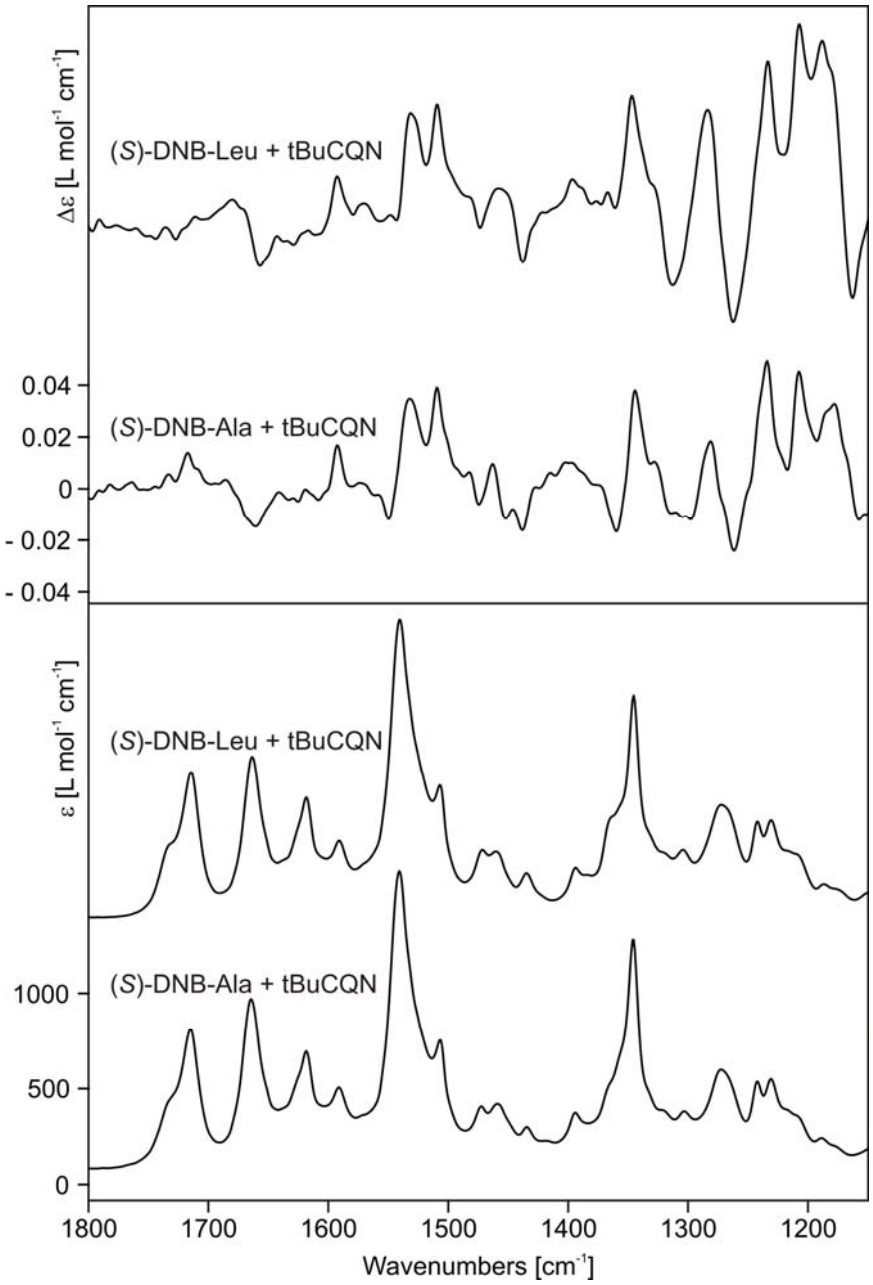
S8: BHandH IR absorption spectra of *anti*-open conformer of tBuCQN using various basis sets.



S9: BHandH IR absorption spectra of *syn*-closed conformer of tBuCQN using various basis sets.



S10: Assignment of Carbamate II vibration (green) and quinoline deformation vibration (red) modes in the IR absorption and VCD spectrum of tBuCQN.



S11: Experimental VCD and IR absorption spectra of complexes of tBuCQN with (S)-DNB-Ala and (S)-DNB-Leu in deuterated acetonitrile.

S12: Details about the conformational analysis

a) *t*BuCQN

Relative energies and populations of *t*BuCQN conformers.

Name	Relative free energy (kJ/mol)	Population (T=298K)
anti-closed-E	0	65%
anti-open-E	2.27	26%
syn-closed-E	4.94	9%

The analysis of conformational degrees of freedom was performed for those not present in previous works. (N. M. Maier, S. Schefzick, G. M. Lombardo, M. Feliz, K. Rissanen, W. Lindner and K. B. Lipkowitz, *Journal of the American Chemical Society*, 2002, **124**, 8611) :
(i) The ethylene group on quinuclidine can be oriented syn (over) or anti (away) from the bicyclic system. The anti orientation is preferred by 5 kJ/mol, the barrier for rotation is approximately 15 kJ/mol.
(ii) The orientation of methoxy group on the quinoline group was modelled by 4-methyl-6-methoxyquinoline. The anti orientation of methoxy group (toward the C5) is preferred by 5 kJ/mol with relatively low lying barrier (15 kJ/mol above the anti orientation).
(iii) Carbamate moiety can be seen as posessing C=N double bond. The E orientation is preferred by 9 kJ/mol above the Z, with high barrier for rotation (estimated ~60 kJ/mol).

The geometries of whole *t*BuCQN were optimized at the B3LYP/6-311++G(2df,2pd) level of theory and the Gibbs free energy was considered for Boltzmann population analysis.

b) DNB-Ala

Relative energies and populations of DNB-Ala conformers.

Conformer no.	Relative free energy (kJ/mol)	Population (T=298K)
1	0	91.8%
2	7.15	4.9%
3	9.47	1.9%
4	11.10	1.0%
5	12.69	0.5%

The conformational analysis of DNB-Ala was carried out at B3LYP/6-31G* level of theory. In the process, two dihedral angles were changed. The first one changed the *E*/*Z* conformation of the amide (i.e. dihedral angle 0 and 180°), the second one defined as N(amide)-Cα-C(carboxyle)-O(carboxyle) changed the angle between the amide and the carboxyle group (dihedral angle 0-330° with a step of 30°). With regard to the results of the Boltzmann population analysis we considered the conformer no.1 as the only significantly populated conformer.