Supporting Information to the article

UV-Vis spectra of the anticancer campothecin family drugs in aqueous solution: specific spectroscopic signatures unraveled by a combined computational and experimental study

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Additional calculated data report

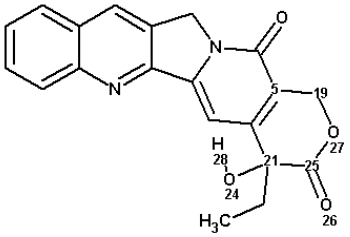
1. Structural parameters.

CPT calculations were performed at the HF/3-21G and B3LYP/6-31G* either in vacuo and with CPCM modeling of the solvent effects. Both lactone (l-) and carboxylated forms of the CPT and its derivatives were taken into account. The energetics of the two tautomers of the lactone form have been evaluated with the *keto* form of the ring D CO significantly more stable than its *enol* counterpart. In Table 1 we report the leading structural parameters of l-CPT forms (see Figure 1 for details) optimized at the PCM(B3LYP/6-31G*) level in various solvents. For the sake of readability, we have tabulated only the most flexible structural features of l-CPT, that is, the atoms of ring E. The table reports the ring E optimized geometries in water and other less polar solvent for comparison purposes. The full set of structural parameters and energetics data of CPT and its derivatives discussed in the main text, could be obtained by the interested reader contacting one of the corresponding authors.

Table 1 *CPT Ring-E structural parameters (Å, degrees) optimized in various solvents at the PCM(B3LYP/6-31G*) level of calculation; D stands for "dihedral angle, A for "angle" and R for "distance".*

CPT-Lactone form	Benzene	Chloroform	Acetone	Methanol	Water
$D(H_{28}O_{24}C_{21}C_{25})$	-24.896	-42.575	-54.151	-54.235	-52.960
$D(O_{24}C_{21}C_{25}O_{26})$	22.666	26.034	25.925	26.427	26.062
$D(C_5C_{19}O_{20}H_{33})$	---------	---------	---------	---------	---------
$A(O_{26}C_{25}O_{27})$	120.413	119.910	119.538	119.536	119.59
$R(C_{25}O_{26})$	1.215	1.215	1.214	1.214	1.215
$R(C_{25}O_{27})$	1.338	1.340	1.342	1.342	1.342
$R(C_{21}O_{24})$	1.413	1.413	1.412	1.412	1.412
$R(O_{24}H_{28})$	0.979	0.981	0.984	0.985	0.986
$R(O_{20}H_{33})$	---------	---------	---------	---------	---------

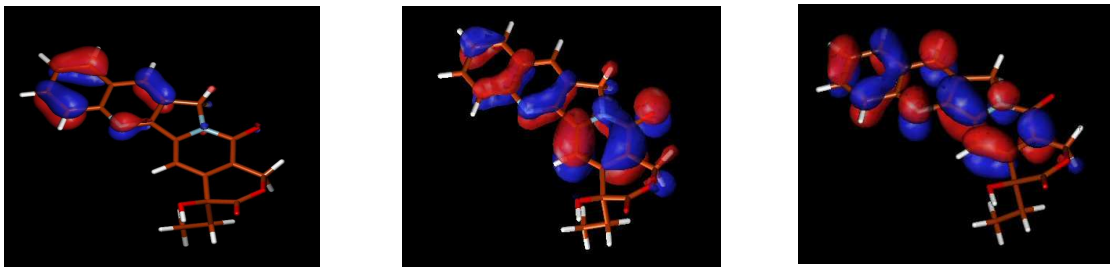
Figure 1 Atom numbering used for the data in Table 1.



2. TD-DFT Kohn-Sham (KS) orbitals.

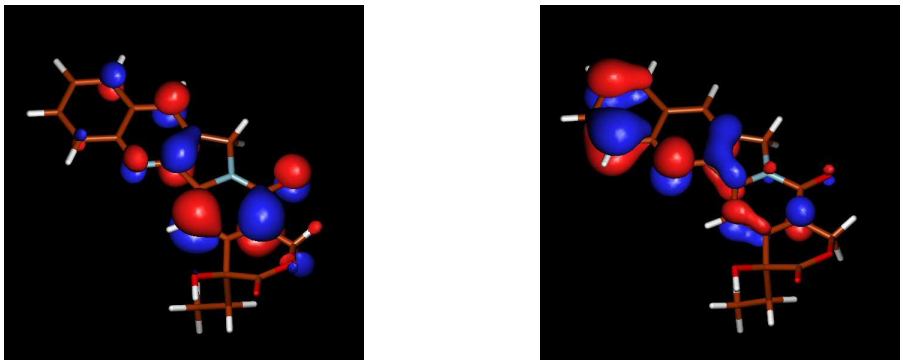
In Figure 2 we report the B3LYP/6-31G* HOMO-1 (left), HOMO (center) and LUMO (right) KS orbitals involved in the UV-Vis transitions λ_1 and λ_3 of l-CPT.

Figure 2 B3LYP/6-31G* HOMO-1 (left), HOMO (center) and LUMO (right) KS orbitals.



Moreover, in Figure 3 we report the sums of the B3LYP/6-31G* KS orbitals involved in the UV-Vis transitions λ_1, $\mathbf{\Psi_{HOMO} - (-\Psi_{LUMO})}$ and λ_3, $\mathbf{\Psi_{HOMO-1} - (-\Psi_{LUMO})}$ where the reader can qualitatively identify the relative contributions of the various parts of the l-CPT molecule to the λ_1, λ_3 **($\pi \rightarrow \pi^*$)** absorption bands. On the left side of the Figure, the leading contributions to the λ_1 arise from the ring D (and only partially from the A and B rings) of CPT, compared to the λ_3 (right side of Figure 3) where the leading contributions arise from the rings A and C (and only partially from the rings B and D) of the CPT system.

Figure 3 B3LYP/6-31G* KS orbitals. Left: $\Psi_{HOMO} - (-\Psi_{LUMO})$. Right: $\Psi_{HOMO-1} - (-\Psi_{LUMO})$. -



3. UV-Vis data.

In Table 2 we report additional, calculated, absorption bands for the l-CPT and its C20 derivatives in aqueous solution also adding, when applicable, two explicit water molecules hydrogen bonded to the CO group of the D ring. In all cases TD-DFT computations have been performed employing geometries optimized at the PCM(B3LYP/6-31G*) level of theory. The table also includes the data for the C20 substituted derivatives not discussed in the main text and for all systems also the λ_4 band position and oscillator strength are given.

Table 2 TD//PCM(B3LYP/6-31G*) UV-Vis band positions in nm and oscillator strength (in parenthesis) of the l–CPT and some of its derivatives. In italics the data already discussed into the main text. H=HOMO. L=LUMO

Substituent		**λ_1 / λ_2 (H→L)**	**λ_3 (H-1→L)**	**λ_4 (H→L+1)**
OH (CPT)	PCM	*367 (0.474)*	*329 (0.035)*	297 (0.086)
	PCM+2w/D	*353 (0.593)*	*336 (0.032)*	292 (0.045)
OCH_2SCH_3	PCM	*366 (0.480)*	*330 (0.030)*	297 (0.079)
	PCM+2w/D	*353 (0.576)*	*335 (0.030)*	292 (0.053)
OCH_3	PCM	367 (0.477)	329 (0.035)	298 (0.088)
	PCM+2w/D	355 (0.577)	335 (0.034)	293 (0.053)
OCH_2CH_3	PCM	368 (0.473)	329 (0.035)	298 (0.091)
H	PCM	368 (0.463)	328 (0.036)	297 (0.091)
NH_2	PCM	369 (0.467)	328 (0.036)	298 (0.093)
Cl	PCM	364 (0.502)	333 (0.034)	299 (0.055)
Br	PCM	362 (0.507)	331 (0.035)	302 (0.032)

4. QM minimum energy molecular geometries of the CPT-nH_2O models investigated.

In the following we report the molecular geometries (xyz format) optimized at PCM(B3LYP/6-31G*) level of theory for the whole set of CPT-nH_2O models investigated.

Legend:
Nw/R(A), **N:** *no. of explicit water molecules;* **R:** *CPT ring (B,D,E);* **A:** *atom involved in the interaction.*

1w D(O)				1w B(N)			
NAT	X	Y	Z	NAT	X	Y	Z
1	-2.75302	-2.96419	3.40155	1	-3.33984	-2.19371	3.31497
6	-2.30819	-2.73188	2.42810	1	-2.01946	-1.27630	2.57378
1	-1.52109	-1.98753	2.58786	1	1.02700	3.25739	1.05148
1	-1.84404	-3.64245	2.03791	6	-2.85253	-1.95517	2.36357
1	-4.20021	-2.95532	1.39738	1	6.24660	1.72389	0.03724
1	-3.83632	-1.29892	1.86863	1	7.60925	-0.34402	-0.10599
6	-3.38825	-2.21907	1.47306	1	3.99779	2.82728	0.12036
1	-4.11879	0.82815	0.93263	6	5.76827	0.74647	-0.01874
6	-2.87753	-1.97535	0.01710	6	6.52220	-0.40414	-0.09860
1	-3.05989	-3.81862	-0.61397	1	-2.44288	-2.88013	1.94702
8	-2.33442	-3.15559	-0.53453	1	-4.25413	-0.39189	1.82491
1	-0.08631	-2.24855	-0.07794	6	3.53357	1.84188	0.06674
6	-1.80997	-0.89688	-0.03815	6	4.34989	0.68016	-0.00897
6	-0.43247	-1.22199	-0.06566	6	5.89136	-1.67237	-0.17313
1	4.51402	-3.08610	-0.12896	6	2.17313	1.67438	0.06731
6	-3.69087	0.74187	-0.07518	6	1.04283	2.66426	0.12910
6	-4.09832	-1.53854	-0.81983	1	6.50196	-2.57162	-0.23786
6	-2.22887	0.41635	-0.04975	6	3.71434	-0.60783	-0.08155
6	0.46159	-0.18376	-0.08432	6	-3.86463	-1.32711	1.40360
7	2.70642	-1.22638	-0.11595	6	4.51773	-1.77539	-0.16508
6	4.94207	-2.08557	-0.14819	1	-4.33007	1.78921	0.98971
1	1.09606	2.76867	0.73325	6	1.64282	0.35748	-0.00407
8	-4.75222	-2.33846	-1.45780	8	-1.64098	3.51050	0.15996
8	-4.46808	-0.24832	-0.79941	7	-0.13941	1.78443	0.08101
1	6.97982	-2.73909	-0.17890	7	2.35364	-0.74951	-0.07570
6	1.92593	-0.16624	-0.11285	1	4.01819	-2.73964	-0.22401
6	4.05099	-0.97903	-0.14387	6	-1.43572	2.28801	0.09759
6	-1.29318	1.51446	-0.05739	1	-4.72677	-1.99656	1.27808
6	6.30455	-1.88482	-0.17581	6	0.18038	0.44695	0.00884
7	0.03615	1.12517	-0.08073	1	1.63925	-2.51857	-0.20490
1	-3.86728	1.68501	-0.59616	1	1.02101	3.36157	-0.71711
8	-1.61057	2.72412	-0.05197	8	1.29745	-3.43535	-0.31609
6	2.35285	1.19062	-0.13646	6	-2.45485	1.26077	0.03337
6	4.59363	0.35439	-0.16856	6	-0.79266	-0.51680	-0.04091
6	1.15231	2.09470	-0.12870	1	-0.53325	-1.56601	-0.10386
6	6.84024	-0.57153	-0.20008	6	-2.14241	-0.07888	-0.01313
6	3.69667	1.45797	-0.16493	6	-3.88319	1.70755	-0.01014
1	7.91987	-0.43222	-0.22173	6	-3.29673	-1.06645	-0.02801
6	6.00342	0.52317	-0.19643	1	-3.96423	2.68384	-0.49266
1	4.08868	2.47541	-0.18509	1	1.14260	-3.49831	-1.27174
1	6.40909	1.53439	-0.21530	8	-2.84114	-2.26436	-0.61835
1	1.06156	2.70649	-1.03527	8	-4.72215	0.81931	-0.79521
1	-0.77688	3.98021	1.01360	6	-4.45615	-0.49411	-0.87041
8	-0.27067	4.58960	1.59372	1	-3.61926	-2.85612	-0.74410
1	0.08742	5.24261	0.97214	8	-5.15567	-1.20795	-1.56043

2w D(O)				2w E(O)			
NAT	X	Y	Z	NAT	X	Y	Z
1	-2.75380	-2.99512	3.38761	1	-5.08917	-3.94607	-1.66350
6	-2.30739	-2.74804	2.41856	8	-4.21859	-3.54736	-1.81673
1	-1.52512	-2.00129	2.59101	1	-4.29125	-2.67675	-1.38298
1	-1.83706	-3.65111	2.01866	1	-7.63185	0.18008	-1.55289
1	-4.19691	-2.96933	1.38379	8	-6.89366	0.12682	-2.17894
1	-3.84151	-1.31670	1.87140	1	-6.15266	-0.18652	-1.62421
6	-3.38826	-2.23026	1.46723	8	-4.68272	-0.92287	-0.60892
1	-4.11939	0.76875	0.96711	1	-3.12736	-2.62891	0.62861
6	-2.87703	-1.97367	0.01374	8	-2.39143	-2.03966	0.34017
1	-3.04729	-3.81386	-0.62650	6	-3.86298	-0.17514	-0.09209
8	-2.32598	-3.14625	-0.54396	1	4.38331	-3.13794	0.14957
1	-0.09341	-2.24342	-0.07981	6	-2.67756	-0.71734	0.73528
6	-1.81329	-0.89047	-0.03550	1	0.00757	-1.49616	0.47317
6	-0.43833	-1.21652	-0.06353	8	-4.02495	1.13922	-0.21054
1	4.50739	-3.08582	-0.12391	1	6.85171	-3.24259	-0.16462
6	-3.70399	0.73156	-0.04885	6	4.96475	-2.23935	-0.04821
6	-4.09631	-1.53871	-0.82542	6	-0.15794	-0.43136	0.36213
6	-2.23541	0.42496	-0.04480	6	-1.45273	0.13836	0.44719
6	0.45758	-0.17988	-0.07645	6	6.33023	-2.28844	-0.22340
7	2.70043	-1.22478	-0.10859	1	-4.01402	-1.24849	2.33368
6	4.93558	-2.08539	-0.14332	7	2.91707	-1.00049	0.05510
1	1.09602	2.77380	0.73839	6	4.27307	-1.00062	-0.12297
8	-4.74127	-2.33840	-1.47224	1	-1.73856	-2.19799	2.94592
8	-4.46836	-0.24973	-0.80039	6	0.88898	0.41979	0.12357
1	6.97306	-2.73933	-0.17653	6	-3.09724	-0.64981	2.23722
6	1.92149	-0.16360	-0.10482	6	2.32591	0.17309	-0.02476
6	4.04503	-0.97841	-0.13792	6	-1.64798	1.49095	0.27709
6	-1.29458	1.51459	-0.05438	1	-3.09773	2.94815	-0.32839
6	6.29802	-1.88488	-0.17245	6	-3.02871	2.06625	0.31134
7	0.03128	1.12808	-0.07007	6	7.06809	-1.10456	-0.48077
1	-0.73844	4.01129	0.99539	1	8.14678	-1.16284	-0.61673
8	-0.22805	4.64210	1.54559	6	5.02127	0.20158	-0.38330
1	-3.91720	1.68717	-0.52937	7	0.68946	1.77195	-0.03140
8	-1.58932	2.73772	-0.05434	6	6.42767	0.11304	-0.55867
6	2.34874	1.19241	-0.12922	6	-2.02824	-1.17374	3.19938
1	-3.11424	3.65350	-0.52600	1	1.86327	3.04218	-1.24729
6	4.58853	0.35493	-0.16332	6	-0.54954	2.40205	0.02955
6	1.14919	2.09754	-0.12142	1	-3.36922	0.37916	2.50097
6	6.83439	-0.57179	-0.19735	6	2.96562	1.41938	-0.27482
1	0.13605	5.26261	0.89506	1	-3.34875	2.35330	1.32125
1	-4.43157	4.24269	-0.01087	6	4.32366	1.43867	-0.45662
8	-3.94303	4.07797	-0.83217	6	1.93716	2.51658	-0.28754
6	3.69269	1.45926	-0.15877	1	6.98877	1.02612	-0.75591
1	7.91409	-0.43325	-0.22016	1	-1.12880	-0.54972	3.18422
6	5.99828	0.52340	-0.19270	8	-0.64644	3.62968	-0.12375
1	4.08547	2.47642	-0.17884	1	-2.42084	-1.17381	4.22162
1	6.40386	1.53458	-0.21166	1	4.87293	2.36012	-0.65300
1	1.05646	2.70579	-1.02990	1	2.08602	3.26991	0.49549

	1w B(N) + 2w D(O)				1w B(N) + 2w E(O)		
NAT	X	Y	Z	NAT	X	Y	Z
1	-2.75429	-2.84711	3.44542	1	2.49582	1.11905	4.20671
6	-2.31465	-2.60168	2.47280	6	2.09690	1.09370	3.18723
1	-1.55406	-1.83039	2.63440	1	1.21421	0.44603	3.18723
1	-1.81788	-3.49605	2.08567	1	1.77836	2.10576	2.91999
1	-4.19745	-2.89199	1.44325	1	4.07790	1.20004	2.31275
1	-3.88715	-1.22208	1.90335	1	3.46537	-0.43811	2.49629
6	-3.40955	-2.12954	1.51387	6	3.17243	0.58313	2.22510
1	-4.24910	0.85010	0.96083	1	3.49194	-2.41251	1.34175
6	-2.90619	-1.88172	0.05582	6	2.74697	0.62938	0.72471
1	-3.02465	-3.72600	-0.57773	1	3.15511	2.54777	0.60872
8	-2.31775	-3.04514	-0.48221	8	2.43211	1.94235	0.31998
1	-0.11281	-2.05830	-0.03866	1	0.04262	1.34387	0.45803
6	-1.87928	-0.76392	-0.00913	6	1.54230	-0.25658	0.44431
6	-0.49248	-1.04385	-0.03584	6	0.23394	0.28318	0.35353
1	4.52882	-2.71234	-0.14107	1	-4.37290	2.86804	0.08077
6	-3.82582	0.79624	-0.05127	6	3.16661	-2.14584	0.32776
6	-4.13946	-1.50062	-0.78882	6	3.94318	0.11095	-0.10218
6	-2.34862	0.53509	-0.03144	6	1.77180	-1.60483	0.28748
6	0.36426	0.02708	-0.05911	6	-0.78977	-0.59856	0.12264
7	2.65568	-0.91705	-0.10216	7	-2.86246	0.75969	0.02851
6	4.91912	-1.69795	-0.15928	6	-4.93355	1.95511	-0.10309
1	0.88513	2.99691	0.76263	1	-1.91656	-3.47440	0.52399
8	-4.75675	-2.33073	-1.42487	8	4.73549	0.87699	-0.63196
8	-4.55724	-0.22650	-0.78001	8	4.13962	-1.20123	-0.20591
1	6.98000	-2.26957	-0.21224	1	-6.84368	2.90859	-0.24351
6	1.82596	0.10567	-0.09329	6	-2.23201	-0.39497	-0.03286
6	3.99035	-0.62413	-0.14244	6	-4.21691	0.73052	-0.15556
6	-1.44847	1.65881	-0.03988	6	0.69703	-2.54661	0.04870
6	6.27192	-1.44245	-0.19919	6	-6.29886	1.96669	-0.28452
7	-0.10974	1.31895	-0.05953	7	-0.55717	-1.94787	-0.01863
1	-4.06265	1.72993	-0.56457	1	3.25728	-3.03388	-0.30064
8	-1.78549	2.86999	-0.02985	8	0.82437	-3.77252	-0.09133
6	2.20165	1.47530	-0.12069	6	-2.84089	-1.65682	-0.27030
6	4.47641	0.72933	-0.16988	6	-4.93003	-0.49398	-0.40151
6	0.96822	2.33247	-0.10539	6	-1.78439	-2.72729	-0.26800
6	6.75584	-0.10899	-0.22417	6	-7.00655	0.76101	-0.52581
6	3.53478	1.79444	-0.15794	6	-4.19825	-1.71205	-0.45572
1	7.82905	0.07151	-0.25537	1	-8.08571	0.79143	-0.66663
6	5.87818	0.95306	-0.21002	6	-6.33743	-0.44220	-0.58339
1	3.88507	2.82701	-0.17998	1	-4.72186	-2.65037	-0.64234
1	6.24382	1.97930	-0.23003	1	-6.87555	-1.37119	-0.76951
1	0.85026	2.94418	-1.00854	1	-1.69559	-3.26216	-1.22127
8	1.89137	-3.72568	-0.10038	8	-1.62616	3.36085	0.45714
1	2.13510	-2.77433	-0.07022	1	-2.02726	2.46988	0.35259
1	1.75240	-3.88487	-1.05437	1	-1.36547	3.59021	-0.45617
8	-4.09357	3.97477	-1.27726	8	4.08176	3.40208	-2.02801
8	-0.46749	4.54825	1.88490	8	7.03371	-0.09121	-2.17037
1	-3.27772	3.67051	-0.82928	1	7.71363	-0.20238	-1.47894
1	-4.65494	4.27500	-0.53544	1	6.24388	0.17081	-1.66031
1	-1.00254	4.04518	1.23739	1	5.01082	3.70184	-2.00076
1	-0.15365	5.31472	1.36542	1	4.11262	2.55693	-1.54537

1w B(N) + 2w D(O) + 2w E(O)				1w B(N) + 1w D(O)			
NAT	X	Y	Z	NAT	X	Y	Z
1	-2.35455	-1.60507	4.26565	1	-2.20012	-1.68371	4.26364
6	-1.94953	-1.58451	3.24852	6	-1.84530	-1.63599	3.22858
1	-1.09601	-0.89853	3.24050	1	-0.98645	-0.95730	3.19937
1	-1.58477	-2.58673	3.00502	1	-1.50284	-2.63329	2.93724
1	-3.91344	-1.80330	2.35775	1	-3.85245	-1.81002	2.43217
1	-3.38453	-0.13441	2.51980	1	-3.29363	-0.14989	2.60195
6	-3.03872	-1.14380	2.26838	6	-2.97512	-1.15943	2.31360
1	-3.49513	1.76102	1.35399	1	-3.46635	1.81250	1.39630
6	-2.59408	-1.19937	0.77259	6	-2.61054	-1.18673	0.79477
1	-2.90995	-3.13401	0.66226	1	-3.04172	-3.06402	0.46626
8	-2.20075	-2.49928	0.40281	8	-2.24683	-2.48677	0.38455
1	0.13461	-1.78630	0.51843	1	0.10638	-1.78837	0.47468
6	-1.43426	-0.25899	0.47879	6	-1.45767	-0.25252	0.46861
6	-0.10624	-0.73769	0.39342	6	-0.13056	-0.73803	0.35873
1	4.60534	-3.12394	0.08021	1	4.58711	-3.12317	0.06624
6	-3.15720	1.53620	0.33410	6	-3.17064	1.55710	0.36965
6	-3.80592	-0.76319	-0.07833	6	-3.87191	-0.74574	0.02427
6	-1.73021	1.07774	0.29149	6	-1.74925	1.08417	0.29300
6	0.87564	0.18346	0.12970	6	0.85323	0.18064	0.10088
7	3.00346	-1.08382	0.02204	7	2.98282	-1.08571	-0.00081
6	5.12013	-2.19169	-0.13809	6	5.10445	-2.18855	-0.13491
1	1.87203	3.13231	0.41046	1	1.85499	3.10909	0.45170
8	-4.55489	-1.58032	-0.59431	8	-4.66646	-1.55416	-0.41200
8	-4.06576	0.53443	-0.21312	8	-4.11178	0.56550	-0.12362
1	7.06512	-3.06540	-0.31179	1	7.05448	-3.05688	-0.27850
6	2.32182	0.04071	-0.05070	6	2.30082	0.03872	-0.07035
6	4.34982	-1.00029	-0.19713	6	4.33303	-0.99824	-0.19738
6	-0.69657	2.04638	0.03091	6	-0.71472	2.05656	0.02355
6	6.47909	-2.14877	-0.35693	6	6.46749	-2.14105	-0.32739
7	0.57772	1.51606	-0.03666	7	0.55889	1.51621	-0.05363
1	-3.32037	2.42429	-0.27819	1	-3.33249	2.43679	-0.25586
8	-0.86820	3.27909	-0.13687	8	-0.87326	3.28544	-0.13149
6	2.86749	1.32094	-0.33403	6	2.85056	1.32328	-0.32889
6	5.00228	0.24816	-0.48874	6	4.98837	0.25367	-0.46489
6	1.76672	2.34286	-0.34234	6	1.74841	2.34619	-0.32858
6	7.12711	-0.91929	-0.64281	6	7.11825	-0.90812	-0.58998
6	4.21678	1.43120	-0.55345	6	4.20225	1.43693	-0.52787
1	8.20239	-0.90686	-0.81305	1	8.19657	-0.89193	-0.73930
6	6.40552	0.25268	-0.70717	6	6.39519	0.26294	-0.65762
1	4.69314	2.38647	-0.77689	1	4.68182	2.39526	-0.73052
1	6.89756	1.19945	-0.92799	1	6.88943	1.21269	-0.86004
1	1.62768	2.82697	-1.31700	1	1.62428	2.86239	-1.28807
8	1.86382	-3.71190	0.54406	8	1.86306	-3.72902	0.48473
1	2.24704	-2.82174	0.38346	1	2.22700	-2.82568	0.35453
1	1.58927	-3.99676	-0.34932	1	1.61099	-3.99476	-0.42115
8	-3.18956	4.63898	-1.07214	8	-3.13404	4.58228	-1.23960
8	0.87041	5.18733	1.12419	1	-2.32793	4.19296	-0.83983
1	-2.36935	4.24005	-0.71686	1	-3.55360	5.04408	-0.48730
1	-3.60736	5.03278	-0.28096				
1	0.22364	4.59391	0.69163				
1	1.23022	5.70512	0.37728				
8	-3.79277	-4.09870	-1.93679				
8	-6.94608	-0.75612	-2.10663				
1	-7.65284	-0.73872	-1.43352				
1	-6.15293	-0.98435	-1.58656				
1	-4.61913	-4.61925	-1.91679				
1	-4.04388	-3.26754	-1.49374				

“Bare” CPT

NAT	X	Y	Z
6	4.79129	-0.94389	0.20931
6	3.60536	-0.17458	0.07205
6	3.71134	1.25911	-0.12162
6	5.00784	1.85208	-0.17152
6	6.13633	1.09569	-0.03419
6	6.07611	-0.33346	0.16144
6	2.28617	-0.72451	0.09594
6	1.21747	0.12166	-0.05246
6	1.44913	1.50927	-0.22949
7	2.63970	2.08057	-0.26748
6	-0.26353	-0.14104	-0.06725
7	-0.81482	1.21423	-0.27051
6	0.16047	2.18147	-0.36433
6	-2.18279	1.45650	-0.34342
6	-2.51418	2.85093	-0.53805
6	-1.54227	3.82280	-0.65051
6	-0.16851	3.50197	-0.55008
6	-3.96388	3.22256	-0.58253
8	-4.21967	4.53766	-0.00639
6	-3.29919	5.49996	-0.08400
6	-2.01274	5.24711	-0.89025
6	-2.34755	5.51416	-2.39191
6	-1.13745	5.38487	-3.31937
8	-1.02976	6.16234	-0.44025
8	-3.49401	6.57839	0.44881
8	-2.99908	0.52400	-0.24382
1	-1.52889	6.92522	-0.08896
1	7.12643	1.54788	-0.06851
1	5.06218	2.92952	-0.32017
1	2.12302	-1.79225	0.22598
1	-0.65025	-0.56452	0.87976
1	0.60341	4.26014	-0.60974
1	-3.14823	4.84081	-2.72238
1	-2.74890	6.53486	-2.44261
1	-1.41720	5.67326	-4.33833
1	-0.32518	6.03948	-2.98972
1	-0.75949	4.35764	-3.35291
1	-4.55885	2.52844	0.01423
1	-4.37391	3.23070	-1.60085
1	-0.58612	-0.79496	-0.88453
1	4.90437	-2.01638	0.36060
1	7.08639	-0.73129	0.24501

5. Non averaged radial distribution functions