Supporting Information

Synthesis of carbon nitride oligomer as a precursor of melon with improved fluorescence quantum yield

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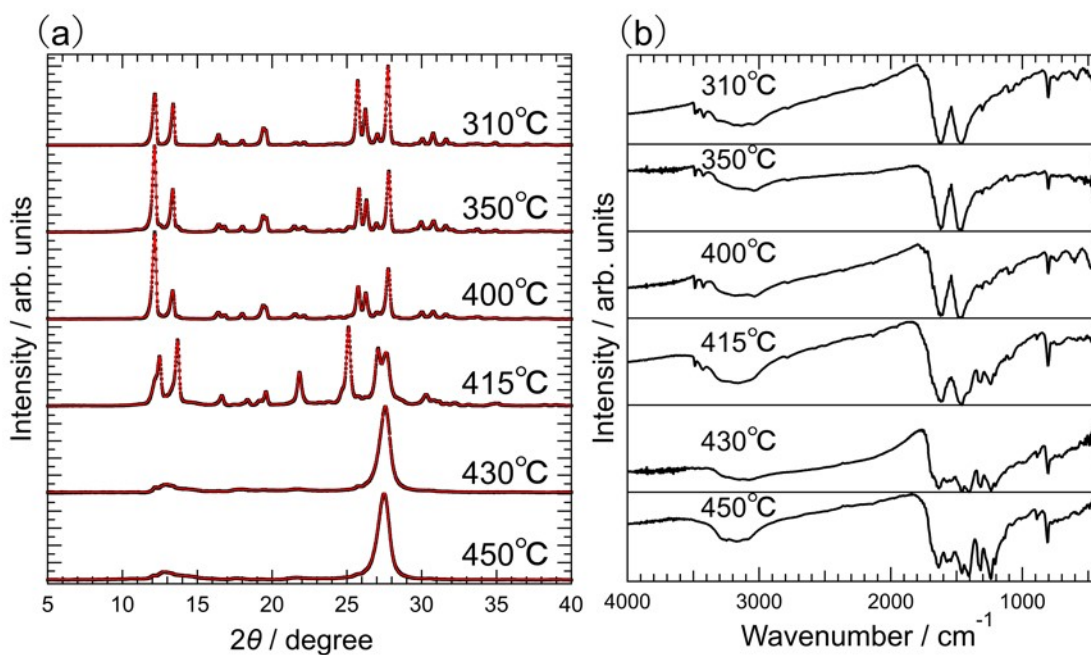
Fig. S1. XRD and FT-IR data of the products obtained by calcination at different temperatures using melamine as the starting material.
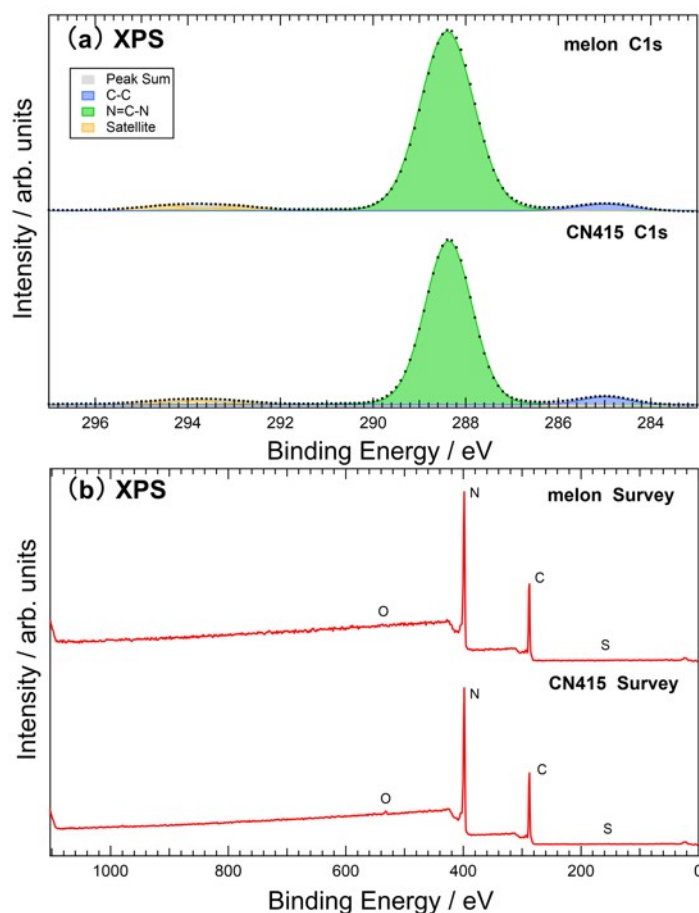
Fig. S2. (a) C 1s XPS data of melon and CN415. (b) XPS data of melon and CN415 obtained in a wide binding energy range (survey measurements). Ratio of C/N is calculated from the ratio of the peak area of N=C-N to the peak areas in N1s XPS data in Figs. 3(a) and 3(b). DMSO treatment was performed during the production of CN415, but no sulfur peaks were observed in the survey spectra. Therefore, DMSO did not remain in the sample and was completely removed by the cleaning process.

Table S1. Binding energies (eV) of nitrogen atoms in different chemical environments reported in prior studies[13].

N_i (C=N-C)	N_{ii} (C-NH$_2$)	N_{iii} ((C)$_2$-NH)	N_{iv} ((C)$_3$-N)
398.8	399.6	400.4	401.3
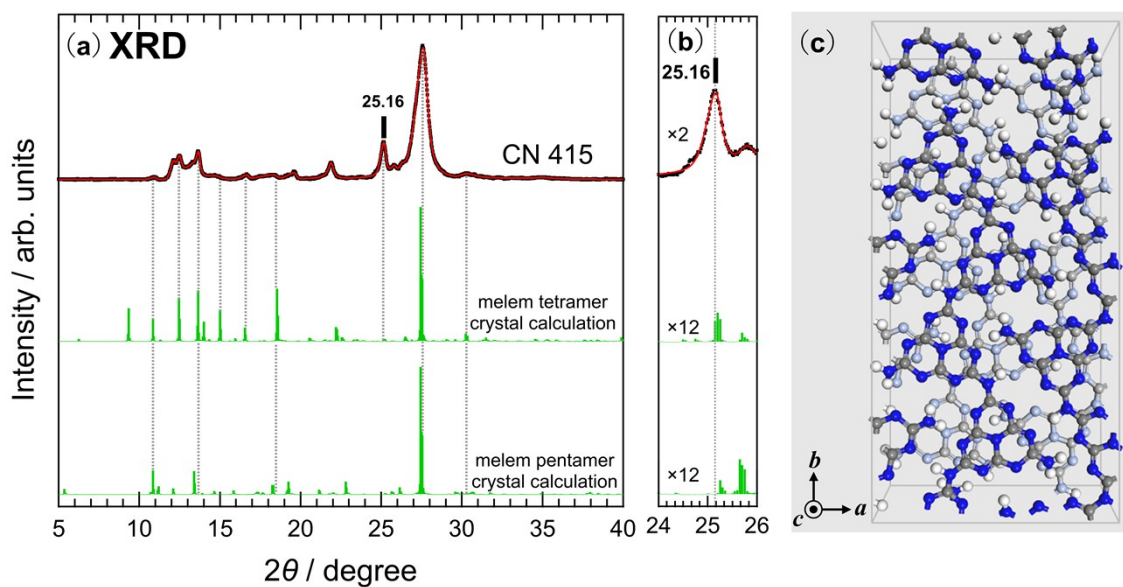
Fig. S3. (a) XRD profiles of melon and CN415 (identical to those in Fig. 2(a)) and calculated XRD patterns for CN415. The results of the XRD simulation for CN415 using the model structures with melem tetramer as a building unit (Fig. 4(c)) and melem pentamer (Fig. S3(c)) are shown. (b) Magnified view of the XRD profiles near $2\theta = 25°$. (c) Unit cell of the model structure of CN415 using melem pentamer viewed from the c-axis direction.
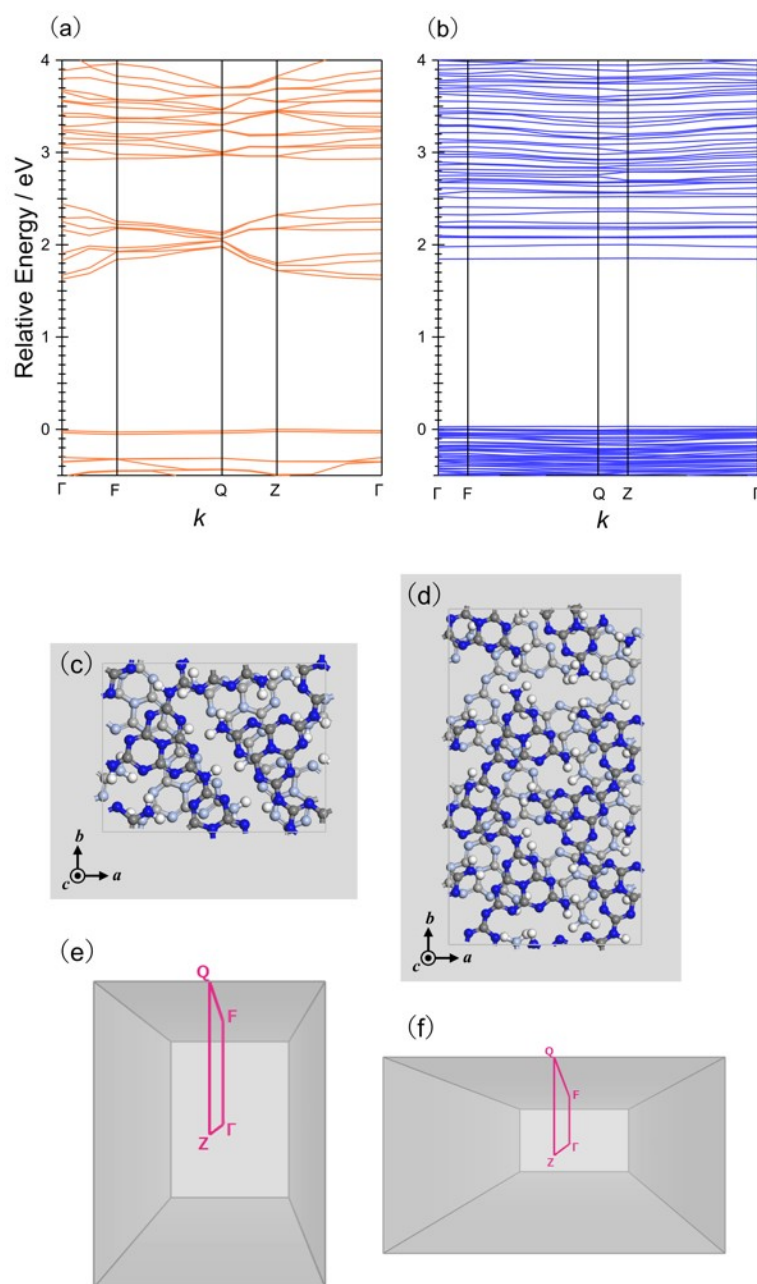
Fig. S4. (a) and (b) show the energy band structures of melon and MT, respectively. (c) and (d) represent the structural models of melon and MT, respectively. (e) and (f) exhibit the Brillouin zones of the melon and MT crystals, respectively. Calculated energy gaps of melon and MT are 1.66 eV and 1.82 eV, respectively.
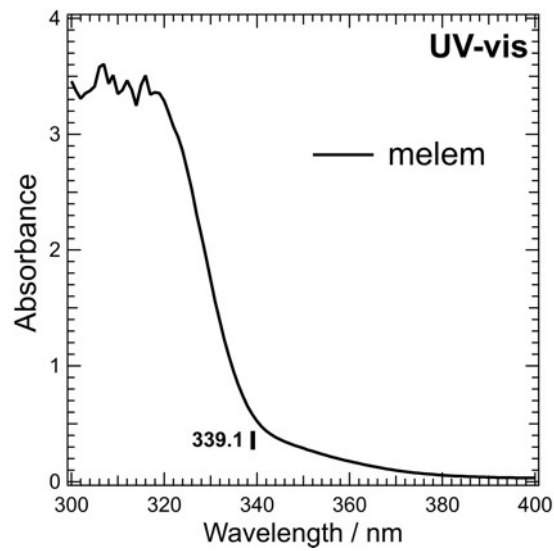
Fig. S5. UV-vis spectrum of the DMSO solution of melem.
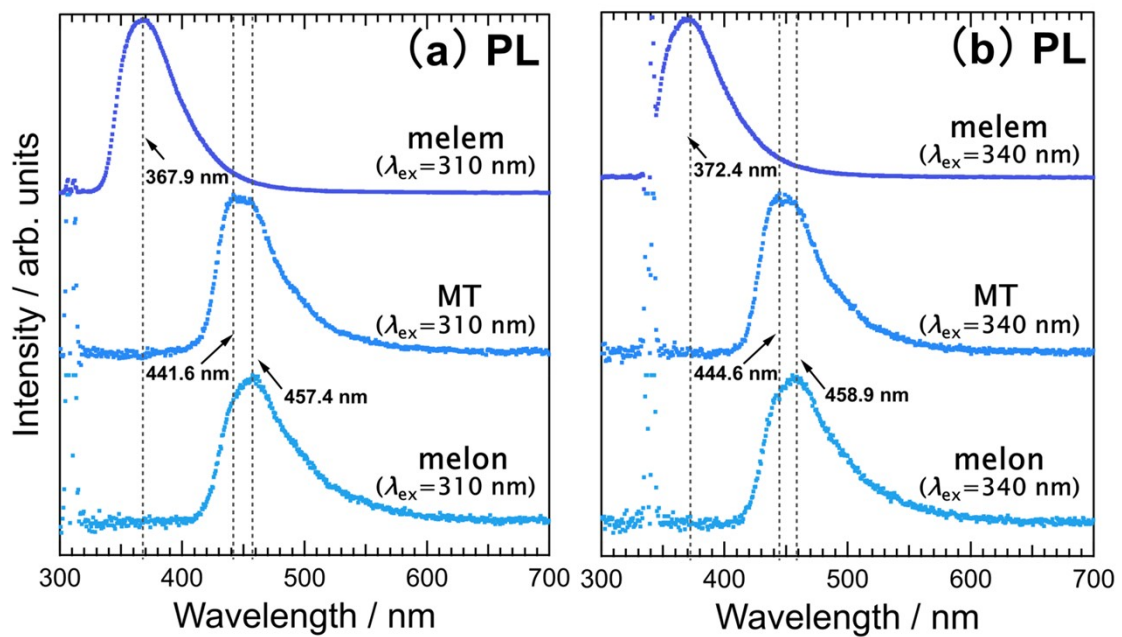
Fig. S6. PL spectra of the powder samples of melem, MT, and melon measured at room temperature. The excitation wavelength λ_{ex} are λ_{ex} = 310 nm (a) and 340 nm (b).
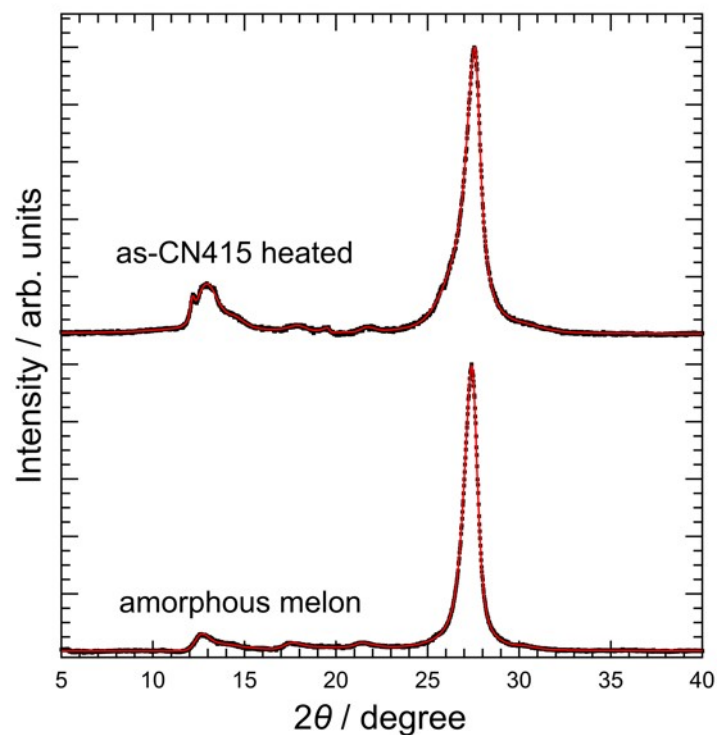
Fig. S7. XRD data of the as-CN415 sample reheated in a tube furnace at 415 °C. The width of the diffraction peak increases and the peak becomes broader in comparison to that for the amorphous melon prepared by reheating melon at 450 °C. This suggests that reheating of MT yields melon with disordered crystal structure, supporting that MT is an intermediate to melon.

Table S2. Atomic coordinates of CN415 (MT). Unit cell parameters: a = 16.3 Å, b = 28.4 Å, c = 6.49 Å, $\alpha = \beta = \gamma = 90$ °.

| Atom	x	y	z
C1	0.68582	0.11696	0.28432
C2	0.23728	0.23485	0.28432
C3	0.80979	0.41124	0.28432
C4	0.28543	0.16149	0.28432
C5	0.15122	0.16935	0.28432
C6	0.00141	0.18463	0.28432
C7	0.0877	0.24445	0.28432
C8	0.95937	0.40163	0.28432
C9	0.86614	0.33527	0.28432
C10	0.18093	0.31082	0.28432
C11	0.74216	0.19293	0.28432
C12	0.79032	0.26628	0.28432
C13	0.25675	0.3798	0.28432
C14	0.65611	0.25842	0.28432
C15	0.39096	0.38766	0.28432
C16	0.50754	0.24314	0.28432
C17	0.53952	0.40294	0.28432
C18	0.59258	0.18332	0.28432
H19	0.91715	0.27755	0.28432
H20	0.3504	0.10163	0.19127
H21	0.64466	0.05063	0.26199
H22	0.39052	0.24923	0.18588
H23	0.61626	0.35187	0.18588
H24	0.43081	0.29422	0.38275
H25	0.65655	0.39686	0.38275
N26	0.15736	0.21913	0.28432
N27	0.8897	0.42696	0.28432
N28	0.10306	0.29466	0.28432
N29	0.94401	0.35142	0.28432
N30	0.2424	0.28113	0.28432
N31	0.80467	0.36496	0.28432
N32	0.29876	0.20646	0.28432

N33	0.21372	0.14315	0.28432
N34	0.07233	0.15189	0.28432
N35	0.01165	0.23048	0.28432
N36	0.34998	0.13442	0.28432
N37	0.69709	0.07504	0.28432
N38	0.66226	0.20865	0.28432
N39	0.60796	0.13311	0.28432
N40	0.74729	0.14665	0.28432
N41	0.80364	0.22131	0.28432
N42	0.7186	0.28462	0.28432
N43	0.32847	0.36146	0.28432
N44	0.57722	0.27589	0.28432
N45	0.46985	0.3702	0.28432
N46	0.5178	0.1973	0.28432
N47	0.85486	0.29335	0.28432
N48	0.19221	0.35273	0.28432
N49	0.44095	0.26279	0.28432
N50	0.60612	0.3833	0.28432
N51	0.24343	0.42477	0.28432
C52	0.35923	0.52913	0.28432
C53	0.68582	0.55358	0.28432
C54	0.23728	0.67146	0.28432
C55	0.80979	0.84786	0.28432
C56	0.28543	0.59811	0.28432
C57	0.76163	0.48459	0.28432
C58	0.15122	0.60597	0.28432
C59	0.89585	0.47673	0.28432
C60	0.00141	0.62125	0.28432
C61	0.0877	0.68107	0.28432
C62	0.95937	0.83825	0.28432
C63	0.86614	0.77189	0.28432
C64	0.18093	0.74744	0.28432
C65	0.74216	0.62955	0.28432
C66	0.3049	0.45315	0.28432
C67	0.79032	0.7029	0.28432
C68	0.25675	0.81642	0.28432

C69	0.65611	0.69504	0.28432
C70	0.39096	0.82428	0.28432
C71	0.50754	0.67976	0.28432
C72	0.53952	0.83956	0.28432
C73	0.59258	0.61994	0.28432
C74	0.45449	0.46276	0.28432
H75	0.91715	0.71417	0.28432
H76	0.4042	0.59469	0.28432
H77	0.60719	0.48719	0.28432
H78	0.39052	0.68585	0.18588
H79	0.61626	0.78849	0.18588
H80	0.43081	0.73084	0.38275
H81	0.65655	0.83348	0.38275
N82	0.15736	0.65575	0.28432
N83	0.8897	0.86358	0.28432
N84	0.10306	0.73128	0.28432
N85	0.94401	0.78804	0.28432
N86	0.2424	0.71775	0.28432
N87	0.80467	0.80158	0.28432
N88	0.29876	0.64308	0.28432
N89	0.74831	0.43962	0.28432
N90	0.21372	0.57977	0.28432
N91	0.83335	0.50293	0.28432
N92	0.07233	0.58851	0.28432
N93	0.97473	0.4942	0.28432
N94	0.01165	0.6671	0.28432
N95	0.34998	0.57104	0.28432
N96	0.69709	0.51166	0.28432
N97	0.66226	0.64527	0.28432
N98	0.38481	0.43744	0.28432
N99	0.60796	0.56973	0.28432
N100	0.43911	0.51297	0.28432
N101	0.74729	0.58327	0.28432
N102	0.29978	0.49944	0.28432
N103	0.80364	0.65793	0.28432
N104	0.7186	0.72124	0.28432

N105	0.32847	0.79808	0.28432
N106	0.57722	0.71251	0.28432
N107	0.46985	0.80682	0.28432
N108	0.5178	0.63392	0.28432
N109	0.52927	0.44879	0.28432
N110	0.85486	0.72997	0.28432
N111	0.19221	0.78935	0.28432
N112	0.44095	0.69941	0.28432
N113	0.60612	0.81992	0.28432
N114	0.24343	0.86139	0.28432
C115	0.35923	0.96575	0.28432
C116	0.76163	0.92121	0.28432
C117	0.89585	0.91335	0.28432
C118	0.3049	0.88977	0.28432
C119	0.45449	0.89938	0.28432
H120	0.64253	0.93855	0.19127
N121	0.74831	0.87624	0.28432
N122	0.83335	0.93955	0.28432
N123	0.97473	0.93082	0.28432
N124	0.69709	0.94828	0.28432
N125	0.38481	0.87406	0.28432
N126	0.43911	0.94959	0.28432
N127	0.29978	0.93606	0.28432
N128	0.52927	0.88541	0.28432
H129	0.40454	0.14416	0.37737
H130	0.7599	0.06083	0.30665
H131	0.69667	0.98108	0.37737
C132	0.68582	-0.14361	0.72269
C133	0.23728	-0.02572	0.72269
C134	0.80979	0.15068	0.72269
C135	0.28543	-0.09907	0.72269
C136	0.15122	-0.09121	0.72269
C137	0.00141	-0.07593	0.72269
C138	0.0877	-0.01611	0.72269
C139	0.95937	0.14107	0.72269
C140	0.86614	0.0747	0.72269

C141	0.18093	0.05025	0.72269
C142	0.74216	-0.06763	0.72269
C143	0.79032	0.00572	0.72269
C144	0.25675	0.11924	0.72269
C145	0.65611	-0.00214	0.72269
C146	0.39096	0.1271	0.72269
C147	0.50754	-0.01742	0.72269
C148	0.53952	0.14238	0.72269
C149	0.59258	-0.07724	0.72269
H150	0.91715	0.01699	0.72269
H151	0.3504	-0.15893	0.62964
H152	0.64466	-0.20994	0.70036
H153	0.39052	-0.01133	0.62425
H154	0.61626	0.0913	0.62425
H155	0.43081	0.03365	0.82112
H156	0.65655	0.13629	0.82112
N157	0.15736	-0.04144	0.72269
N158	0.8897	0.16639	0.72269
N159	0.10306	0.0341	0.72269
N160	0.94401	0.09086	0.72269
N161	0.2424	0.02056	0.72269
N162	0.80467	0.10439	0.72269
N163	0.29876	-0.0541	0.72269
N164	0.21372	-0.11741	0.72269
N165	0.07233	-0.10868	0.72269
N166	0.01165	-0.03008	0.72269
N167	0.34998	-0.12614	0.72269
N168	0.69709	-0.18552	0.72269
N169	0.66226	-0.05192	0.72269
N170	0.60796	-0.12745	0.72269
N171	0.74729	-0.11392	0.72269
N172	0.80364	-0.03925	0.72269
N173	0.7186	0.02406	0.72269
N174	0.32847	0.1009	0.72269
N175	0.57722	0.01532	0.72269
N176	0.46985	0.10963	0.72269

N177	0.5178	-0.06327	0.72269
N178	0.85486	0.03279	0.72269
N179	0.19221	0.09217	0.72269
N180	0.44095	0.00223	0.72269
N181	0.60612	0.12273	0.72269
N182	0.24343	0.16421	0.72269
C183	0.35923	0.26856	0.72269
C184	0.68582	0.29301	0.72269
C185	0.23728	0.4109	0.72269
C186	0.80979	0.5873	0.72269
C187	0.28543	0.33755	0.72269
C188	0.76163	0.22403	0.72269
C189	0.15122	0.34541	0.72269
C190	0.89585	0.21617	0.72269
C191	0.00141	0.36069	0.72269
C192	0.0877	0.42051	0.72269
C193	0.95937	0.57769	0.72269
C194	0.86614	0.51132	0.72269
C195	0.18093	0.48687	0.72269
C196	0.74216	0.36899	0.72269
C197	0.3049	0.19259	0.72269
C198	0.79032	0.44234	0.72269
C199	0.25675	0.55586	0.72269
C200	0.65611	0.43448	0.72269
C201	0.39096	0.56372	0.72269
C202	0.50754	0.4192	0.72269
C203	0.53952	0.579	0.72269
C204	0.59258	0.35938	0.72269
C205	0.45449	0.2022	0.72269
H206	0.91715	0.45361	0.72269
H207	0.4042	0.33412	0.72269
H208	0.644	0.22662	0.72269
H209	0.39052	0.42528	0.62425
H210	0.61626	0.52792	0.62425
H211	0.43081	0.47027	0.82112
H212	0.65655	0.57291	0.82112

N213	0.15736	0.39518	0.72269
N214	0.8897	0.60301	0.72269
N215	0.10306	0.47072	0.72269
N216	0.94401	0.52748	0.72269
N217	0.2424	0.45718	0.72269
N218	0.80467	0.54101	0.72269
N219	0.29876	0.38252	0.72269
N220	0.74831	0.17906	0.72269
N221	0.21372	0.31921	0.72269
N222	0.83335	0.24237	0.72269
N223	0.07233	0.32794	0.72269
N224	0.97473	0.23363	0.72269
N225	0.01165	0.40654	0.72269
N226	0.34998	0.31048	0.72269
N227	0.69709	0.2511	0.72269
N228	0.66226	0.3847	0.72269
N229	0.38481	0.17687	0.72269
N230	0.60796	0.30917	0.72269
N231	0.43911	0.25241	0.72269
N232	0.74729	0.3227	0.72269
N233	0.29978	0.23887	0.72269
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N236	0.32847	0.53752	0.72269
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N241	0.85486	0.46941	0.72269
N242	0.19221	0.52879	0.72269
N243	0.44095	0.43885	0.72269
N244	0.60612	0.55935	0.72269
N245	0.24343	0.60083	0.72269
C246	0.35923	0.70518	0.72269
C247	0.76163	0.66065	0.72269
C248	0.89585	0.65279	0.72269

C249	0.3049	0.62921	0.72269
C250	0.45449	0.63882	0.72269
H251	0.64253	0.67799	0.62964
N252	0.74831	0.61568	0.72269
N253	0.83335	0.67899	0.72269
N254	0.97473	0.67025	0.72269
N255	0.69709	0.68772	0.72269
N256	0.38481	0.61349	0.72269
N257	0.43911	0.68903	0.72269
N258	0.29978	0.67549	0.72269
N259	0.52927	0.62485	0.72269
H260	0.40454	-0.11641	0.81573
H261	0.7599	-0.19973	0.74502
H262	0.69667	0.72051	0.81573
H263	-0.07532	0.13356	0.18588
H264	-0.11561	0.17855	0.38275
N265	-0.06518	0.16499	0.28432
H266	-0.07532	0.57018	0.18588
H267	-0.11561	0.61517	0.38275
N268	-0.06518	0.60161	0.28432
H269	-0.07532	-0.12701	0.62425
H270	-0.11561	-0.08202	0.82112
N271	-0.06518	-0.09558	0.72269
H272	-0.07532	0.30961	0.62425
H273	-0.11561	0.3546	0.82112
N274	-0.06518	0.34104	0.72269
N275	1.03541	0.41561	0.28432
C276	1.04565	0.46145	0.28432
H277	1.16268	0.46754	0.18588
H278	1.12239	0.51253	0.38275
N279	1.03541	0.85223	0.28432
N280	1.11225	0.4811	0.28432
C281	1.04565	0.89807	0.28432
H282	1.16268	0.90416	0.18588
H283	1.12239	0.94915	0.38275
N284	1.11225	0.91772	0.28432

N285	1.03541	0.15504	0.72269
C286	1.04565	0.20089	0.72269
H287	1.16268	0.20698	0.62425
H288	1.12239	0.25196	0.82112
N289	1.03541	0.59166	0.72269
N290	1.11225	0.22054	0.72269
C291	1.04565	0.63751	0.72269
H292	1.16268	0.64359	0.62425
H293	1.12239	0.68858	0.82112
N294	1.11225	0.65715	0.72269
H295	0.28765	1.02283	0.26584
N296	0.34998	1.00766	0.28432
H297	0.40375	1.03127	0.3028
H298	0.28765	0.76226	0.70421
N299	0.34998	0.7471	0.72269
H300	0.40375	0.77071	0.74117