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SUPPLEMENTARY MATERIAL TO

Quantum-chemical study of C–H···O interactions between $HTcO_4$ and aromatic amino acids

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OPTIMIZED GEOMETRIES

This section provides the Cartesian coordinates (XYZ format) of the optimized geometries for phenylalanine (Phe), tyrosine (Tyr), tryptophan (Trp), and pertechnetic acid ($HTcO_4$). Geometry optimizations were carried out using the MP2 method. The def2-TZVP basis set was employed for $HTcO_4$, while the cc-pVTZ basis set was used for the amino acids. The optimized structures serve as the starting point for further computational analyses presented in the main text.

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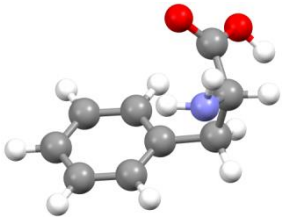
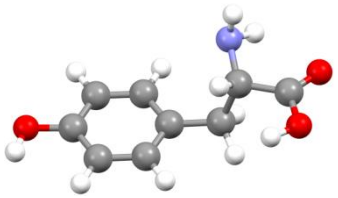
Table S1. Cartesian coordinates (XYZ) of optimized **Phe** at the MP2/cc-pVTZ level.



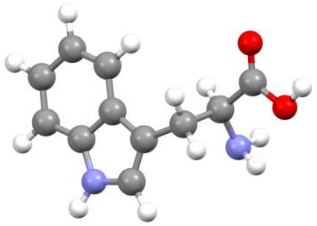
N	1.16448	1.44041	2.24973
C	1.96538	1.36108	1.04665
C	1.68598	2.48823	0.05467
O	0.77677	3.26951	0.15219
C	1.74035	-0.00674	0.37019
C	0.30752	-0.19870	-0.03773
C	-0.59606	-0.82768	0.82429
C	-0.15815	0.29003	-1.26295
C	-1.93690	-0.96484	0.47097
C	-1.49732	0.15407	-1.61815
C	-2.39035	-0.47284	-0.75106
O	2.54592	2.56550	-1.00036
H	3.02018	1.42493	1.33085
H	2.03211	-0.76905	1.09159
H	2.39050	-0.10836	-0.50105
H	-0.24229	-1.20709	1.77453
H	0.53023	0.77873	-1.94161
H	-2.62371	-1.45600	1.14678
H	-1.84220	0.53675	-2.56887
H	-3.43023	-0.57969	-1.02727
H	0.18669	1.44066	1.97527
H	1.31202	2.34361	2.68583
H	3.22153	1.88402	-0.90283

Table S2. Cartesian coordinates (XYZ) of optimized Tyr at the MP2/cc-pVTZ level.



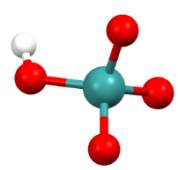
N	1.69351	1.91821	-1.04695
C	2.14635	0.56433	-0.79248
C	3.44810	0.22924	-1.51150
O	3.83835	0.81089	-2.49154
C	1.07272	-0.43929	-1.26216
C	-0.13629	-0.43178	-0.37457
C	-0.27745	-1.39328	0.62794
C	-1.12722	0.54800	-0.49399
C	-1.37047	-1.38262	1.49136
C	-2.22321	0.56729	0.35986
C	-2.34714	-0.39808	1.35782
O	-3.44718	-0.32981	2.16677
O	4.14390	-0.82796	-1.01673
H	2.28386	0.43792	0.28466
H	0.80969	-0.17274	-2.28822
H	1.49593	-1.44554	-1.29190
H	0.46821	-2.17283	0.73284
H	-1.02949	1.30918	-1.25463
H	-1.46617	-2.14157	2.25877
H	-2.99110	1.32230	0.26654
H	-3.40237	-1.05705	2.79612
H	2.27574	2.57315	-0.53848
H	1.86716	2.11559	-2.02851
H	3.70018	-1.14567	-0.22141

Table S3. Cartesian coordinates (XYZ) of optimized **Trp** at the MP2/cc-pVTZ level.



N	-0.50791	3.10300	-1.76549
C	0.61173	2.45668	-1.10309
C	1.97044	3.09398	-1.30539
O	2.87254	3.08085	-0.49936
C	0.71264	0.99188	-1.57380
C	-0.41996	0.17802	-1.05934
C	-1.56780	-0.18913	-1.72448
C	-0.55171	-0.31478	0.27567
N	-2.39295	-0.88836	-0.87520
C	-1.80232	-0.98350	0.35981
C	0.26950	-0.25531	1.41404
C	-2.24345	-1.59347	1.53583
C	-0.16886	-0.85723	2.58291
C	-1.41111	-1.51950	2.64331
O	2.10152	3.64324	-2.54037
H	-1.86208	0.00846	-2.74183
H	-3.28754	-1.27133	-1.12336
H	1.22648	0.25094	1.37995
H	-3.19679	-2.10336	1.58712
H	0.45100	-0.82023	3.46837
H	-1.72229	-1.97924	3.57139
H	0.43436	2.45402	-0.02839
H	0.73544	0.98552	-2.66610
H	1.66003	0.57457	-1.22524
H	-0.66100	4.02361	-1.37259
H	-0.27735	3.24834	-2.74161
H	3.01566	3.96288	-2.58086

Table S4. Cartesian coordinates (XYZ) of optimized **$HTcO_4$** at the MP2/def2-TZVP level.



Tc	-0.03238	0.00466	0.00007
O	-0.63619	-0.84287	-1.39854
O	-0.63702	-0.84664	1.39592
O	-0.71239	1.60410	0.00181
O	1.86083	0.14394	0.00057
H	2.39044	-0.66878	-0.00089