Electronic Supplementary Information (ESI)

Coupling 6-chloro-3-methyluracil with copper: Structural features, theoretical analysis, and bio-functional properties

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Electronic Supplementary Information (ESI) contains: supporting Figures S1-S23, Tables S1-S14, and Listings S1-S9 with additional experimental data and details.

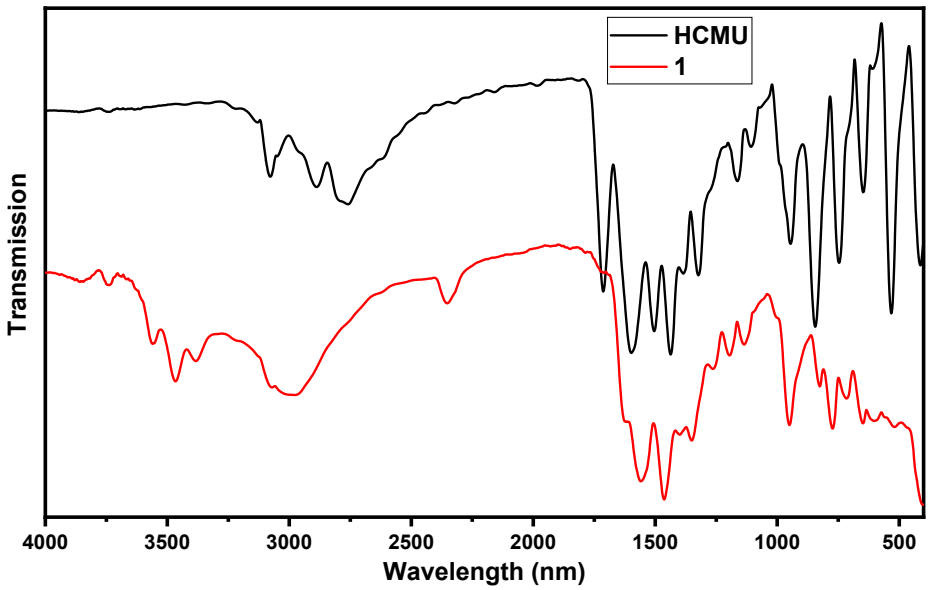


Fig. S1 Solid-state IR spectra of Hcmu (black line) and complex **1** (red line).

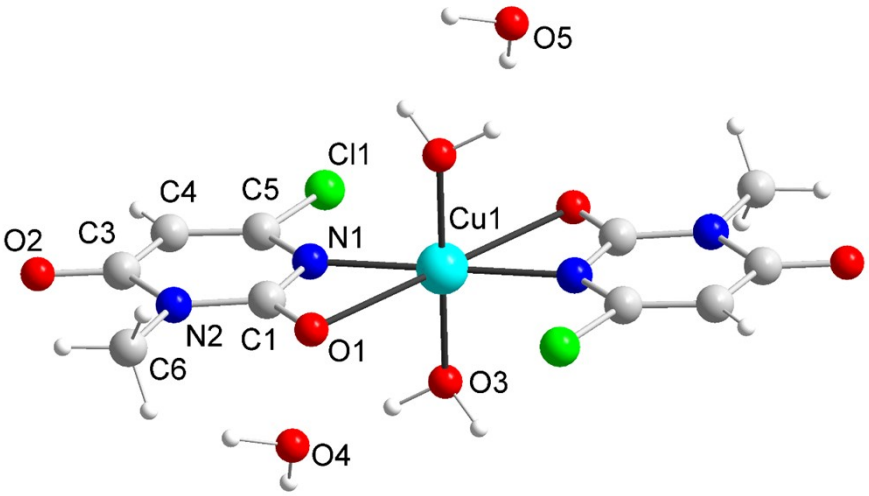


Fig. S2 Ball-and-stick representation of the structure of **1** showing the numbering scheme.

Table S1 Hydrogen bonding parameters for **1**.

D–H…A	d(D–H)	d(H…A)	d(D…A)	<(DHA)
O(3)-H(3W)...O(4)	0.84(3)	1.82(3)	2.663(2)	174(2)
O(3)-H(4W)...O(2)$^{\#1}$	0.70(3)	1.99(3)	2.687(2)	180(4)
O(4)-H(9)…O(1)$^{\#2}$	0.72(4)	2.22(3)	2.918(2)	167(3)
O(4)-H(10)...O(5)$^{\#3}$	0.93(3)	1.86(3)	2.784(3)	173(3)
O(5)-H(11)...O(1)$^{\#4}$	0.86(3)	2.03(3)	2.870(3)	166(3)
O(5)-H(12)...O(2)$^{\#5}$	0.80(3)	2.18(3)	2.974(3)	169(3)

*Symmetry code: (#1) x,-1+y,z; (#2) 1+x,y,z; (#3) x,y,-1+z; (#4) 1-x,1-y,1-z; (#5) 1-x,1-y,-z

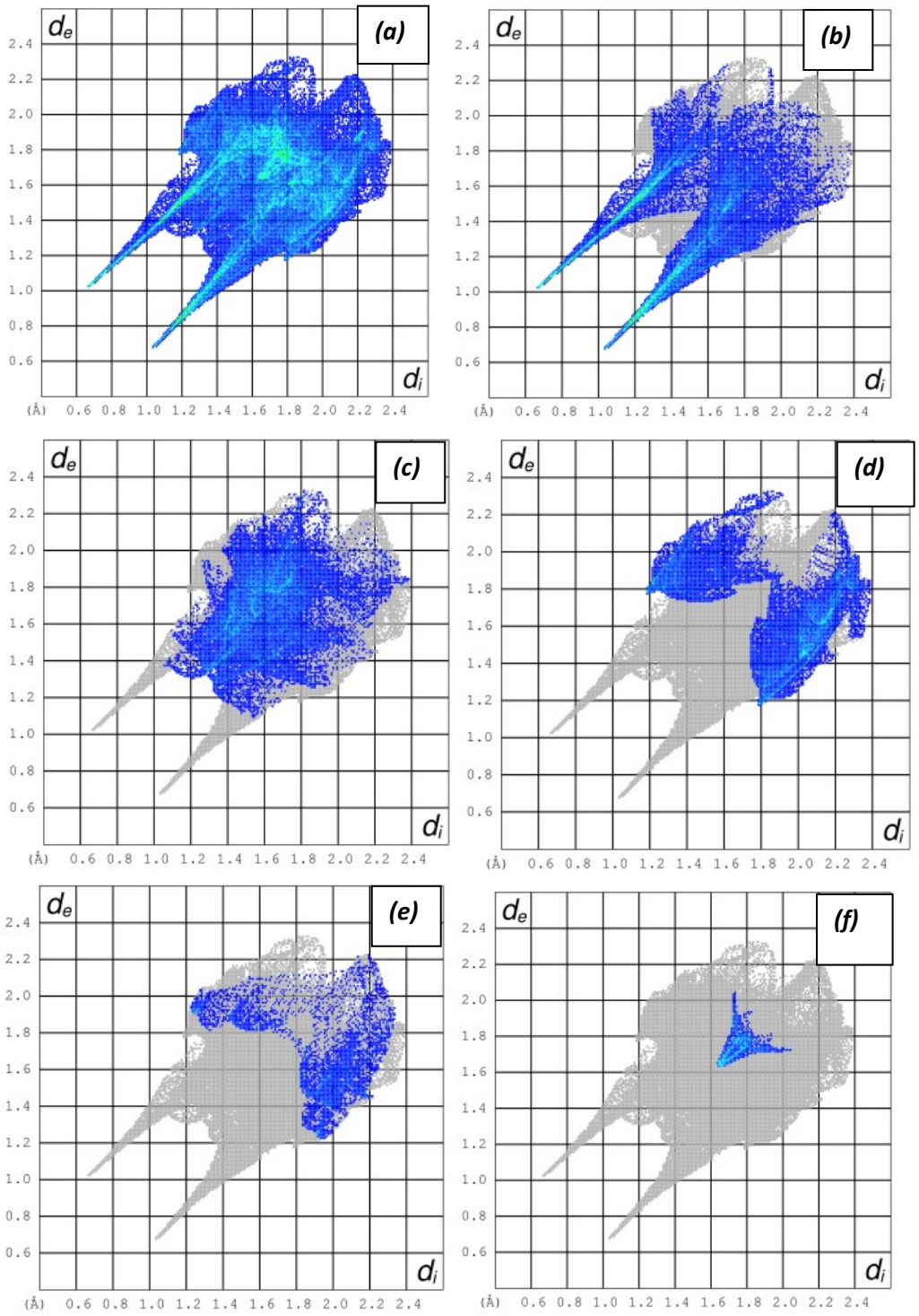


Fig. S3 Fingerprint plots (FP) of the most significant noncovalent interactions in **1**; (*a*) the full two-dimensional fingerprint plot and delineated versions into (*b*) O···H, (*c*) H···H, (*d*) Cl···H, (*e*) C···H, and (*f*) C···C contacts, respectively.

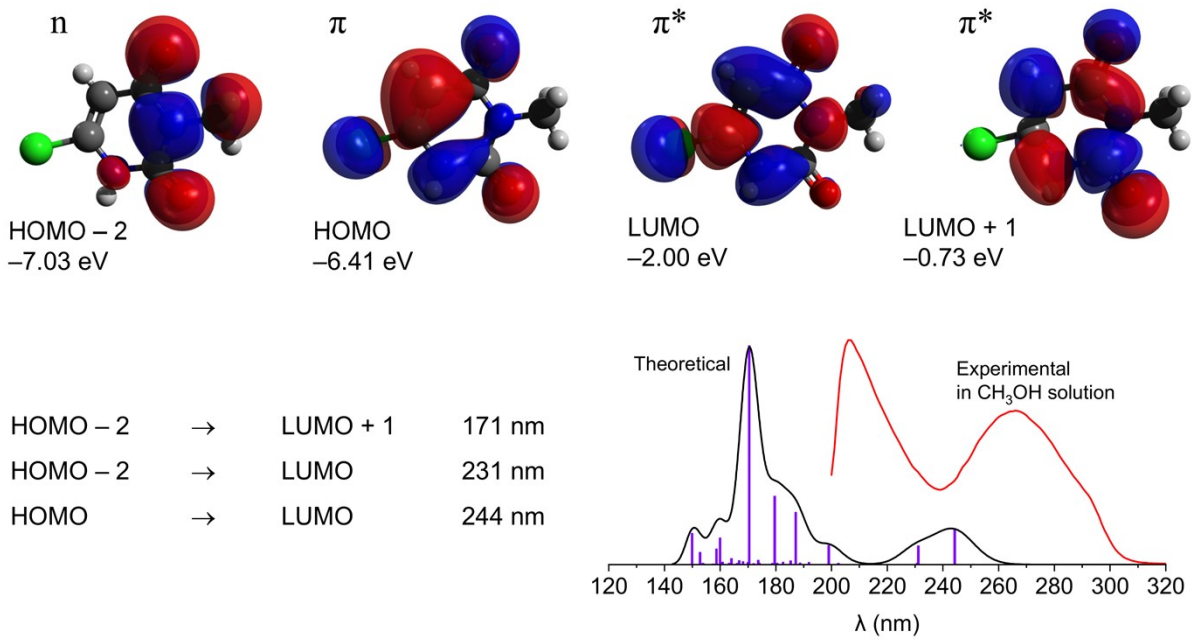


Fig. S4 The 0.02 au isosurfaces of the frontier orbitals of the HCMU ligand. The inset shows the experimental and calculated UV spectra of HCMU in methanol media.

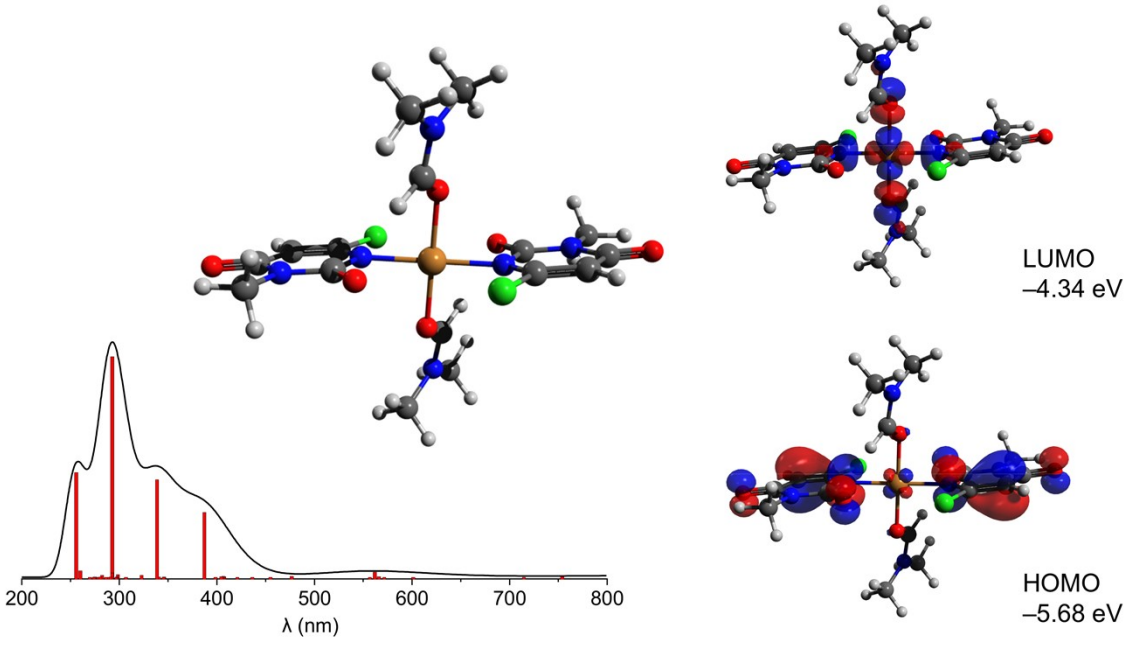


Fig. S5 Optimized geometry of the DMF-substituted **1** (center), the 0.04 au isosurfaces of the spin-down HOMO and LUMO frontier orbitals (right) and calculated UV-Vis spectrum (bottom).

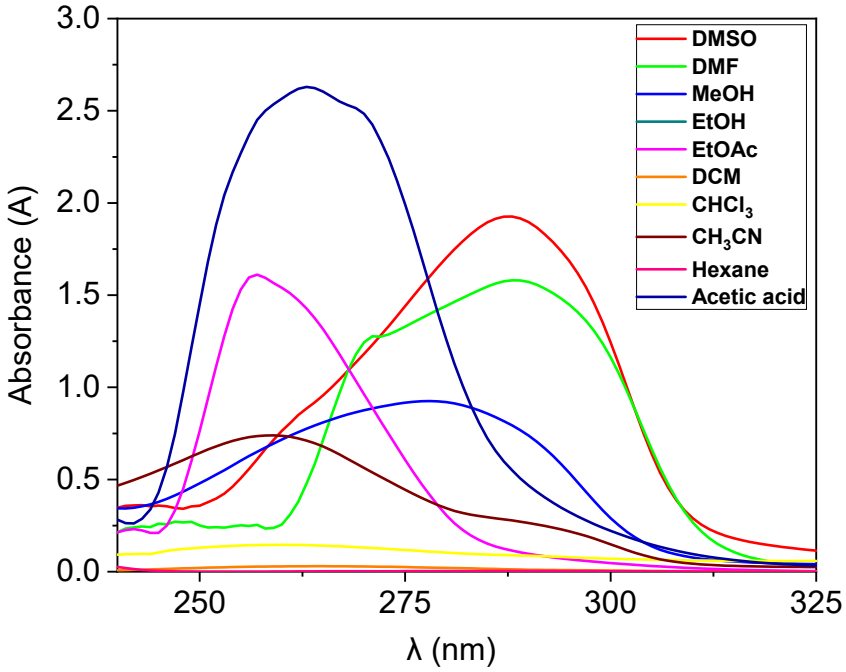


Fig. S6 Experimental UV-spectra of **1** in various solvents.

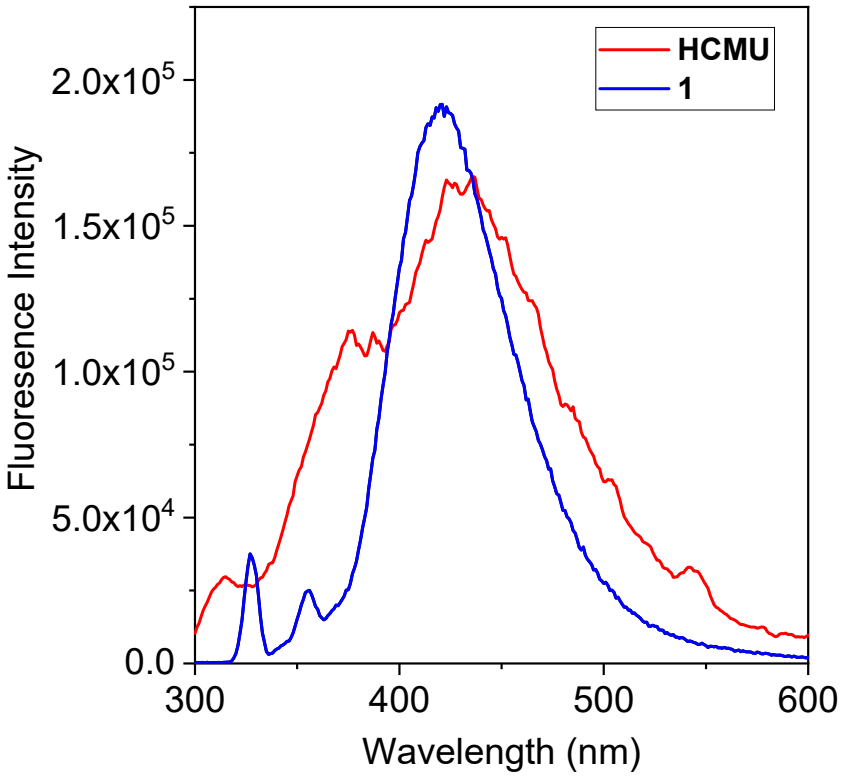


Fig. S7 Experimental fluorescence spectra of **1** and Hcmu in DMF solution upon excitation at 266 and 278 nm, respectively.

Table S2 The solvatochromic shift of **1** in various solvents.

Solvent	Hexane	DCM	$CHCl_3$	EtOAc	CH_3OH	DMF	DMSO	Ac. acid	CH_3CN
λ_{max}	266	265	260	257	278	289	288	263	259

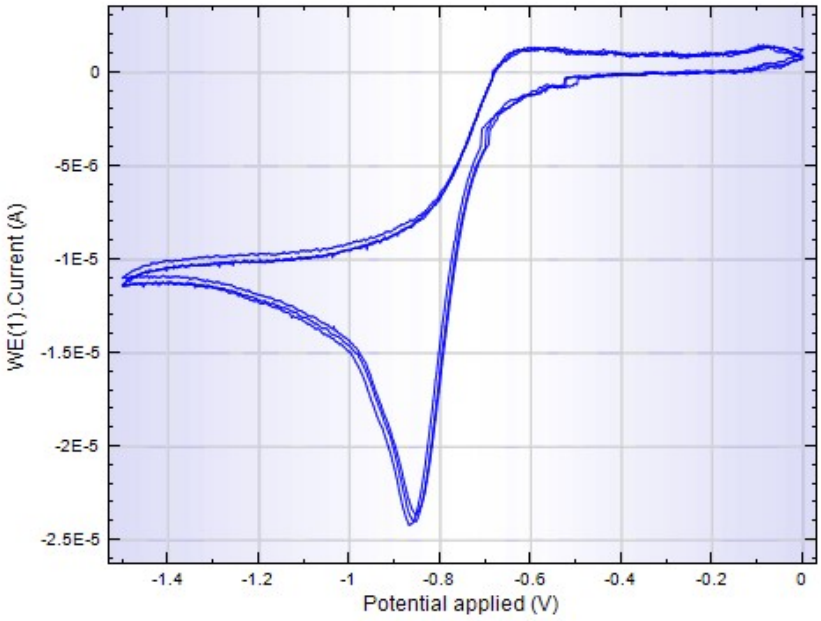


Fig. S8 Cyclic voltammetry of **1** in DMF at a scan rate of 100 mV s^{-1}. The concentration of the metal complex is 0.2 mM along with 0.1 M [n-Bu_4N]PF_6 supporting electrolyte.

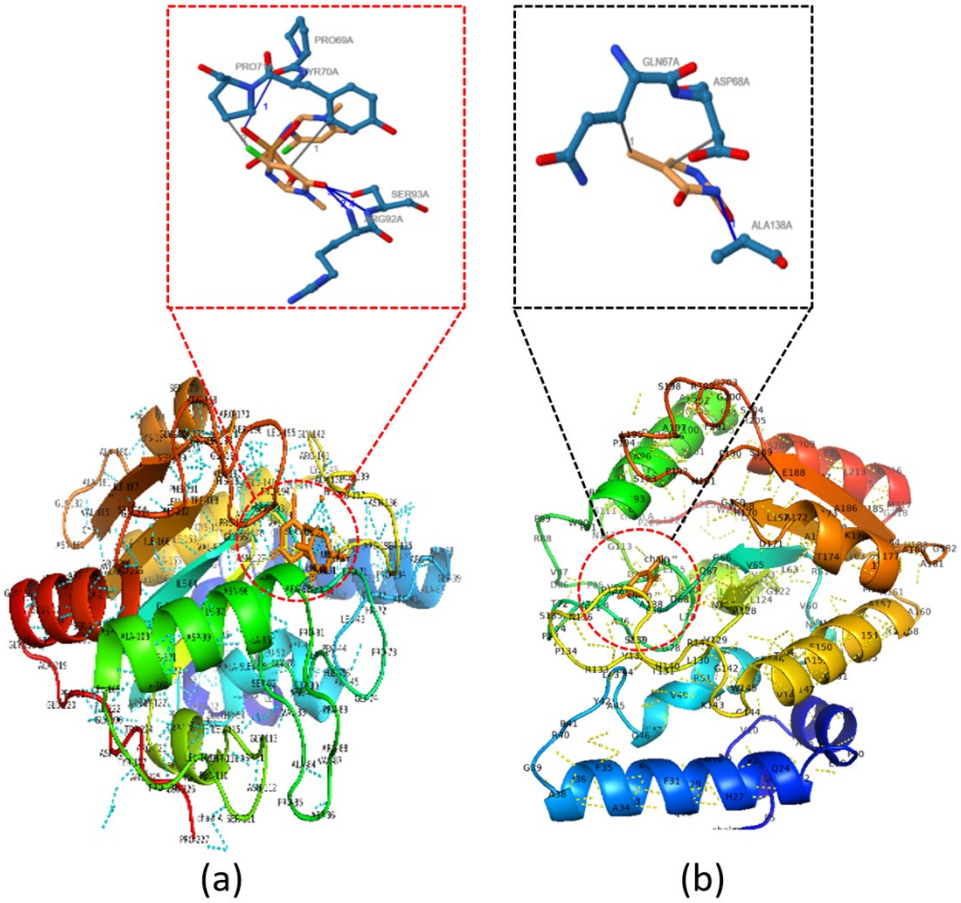


Fig. S9 (a) Docked structure of **1** in the uracil binding site. (b) Docked structure of the pre-existing 5-chlorouracil in the uracil binding motif of UNG enzyme (PDB: 4WS7).

Table S3. Tabulated data showing the interactions between **1**, the reference ligand and the active site of UNG enzyme (PDB: 4WS7).

HYDROPHOBIC INTERACTIONS OF 5-CHLOROURACIL							
RESNR	***RESTYPE***	***RESCHAIN***	***DIST***	***LIGCARBONIDX***	***PROTCARBONIDX***	***LIGCOO***	***PROTCOO***
67	GLN	A	3.80	1713	488	135.942, 2.050, 78.063	136.179, 5.841, 78.151
68	ASP	A	3.41	1709	497	135.187, 1.112, 79.290	134.977, 3.294, 81.907

HYDROGEN BONDING INTERACTIONS OF 5-CHLOROURACIL								
RESNR	***RESTYPE***	***RESCHAIN***	***DIST (H-A)***	***DIST (D-A)***	***DONANGLE***	**PROTISDON**	***PROTCARBONIDX***	**ACCEPTORTYPE**
138	ALA	A	1.52	2.33	135.92	True	1713	N2

HYDROPHOBIC INTERACTIONS OF **1**							
RESNR	***RESTYPE***	***RESCHAIN***	***DIST***	***LIGCARBONIDX***	***PROTCARBONIDX***	***LIGCOO***	***PROTCOO***
70	TYR	A	3.88	1722	514	137.220, -4.765, 76.475	139.871, -3.219, 78.851
71	PRO	A	2.52	1705	525	135.247, -4.970, 78.159	134.062, -4.234, 80.253

HYDROGEN BONDING INTERACTIONS OF **1**								
RESNR	***RESTYPE***	***RESCHAIN***	***D(H-A)***	***D(D-A)***	***DONANGLE***	***PROTISDON***	***PROTCARBONIDX***	***ACCEPTORTYPE***
69	PRO	A	3.62	4.07	110.71	False	1716	O2
92	ARG	A	2.13	2.57	105.39	True	675	O2
93	SER	A	3.34	3.77	108.96	True	691	O2
93	SER	A	2.37	3.27	150.91	True	686	O2

Table S4. The calculated ADME parameters for **1** using SWISS ADME.

Molecule	*H-bond acceptors*	*H-bond donors*	*Heavy atoms*	*MR*	*TPSA*	*BBB permeability*	*iLOGP*	*Silicos-IT LogSw*	*Silicos-IT class*	*GI absorption*	*Lipinski*	*Bioavailability Score*
1	4	1	20	73.31	76.45	No	0	-2.03	Soluble	High	0	0.55

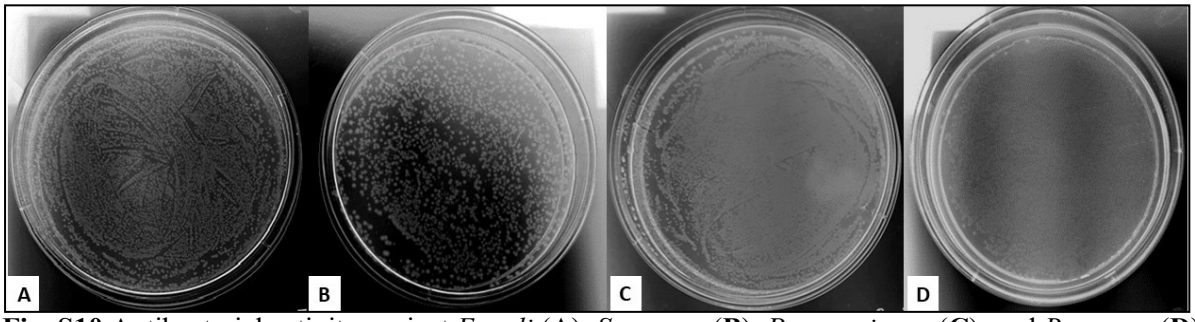
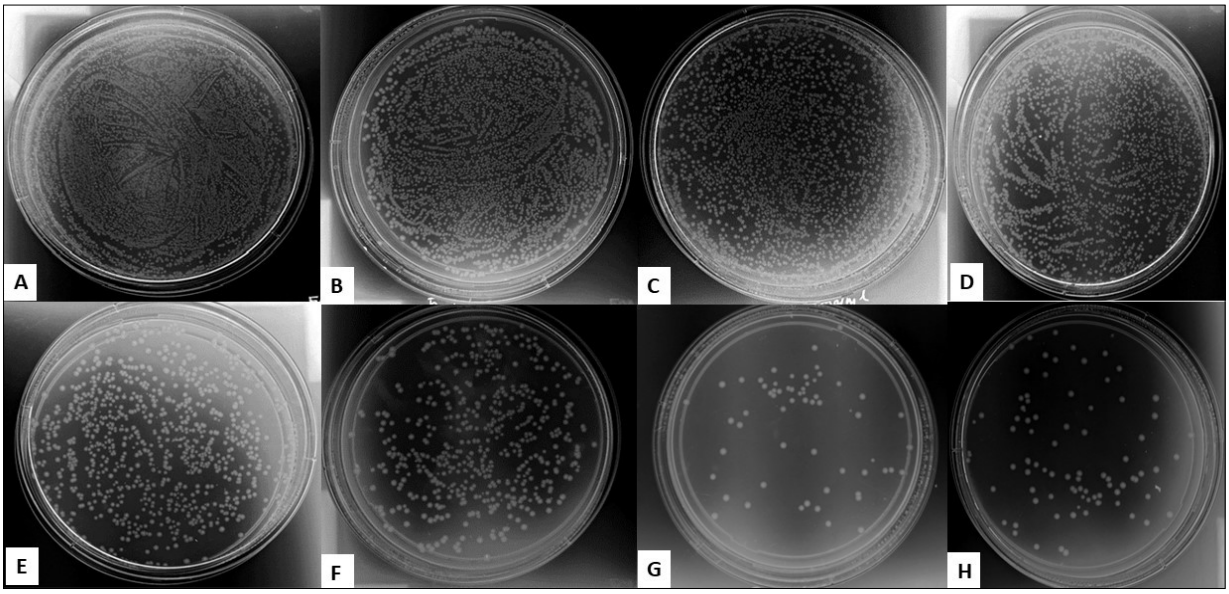


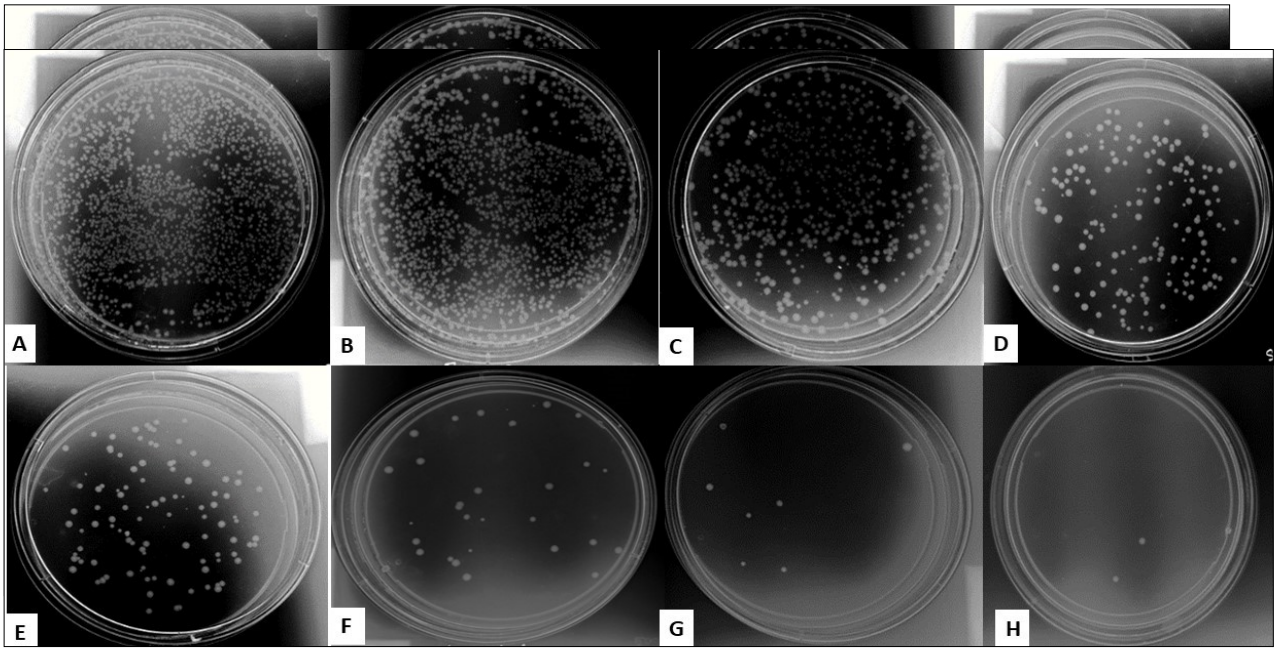
Fig. S10 Antibacterial activity against *E. coli* (**A**)*, S. aureus* (**B**), *P. aeruginosa* (**C**), and *B. cereus* (**D**) in the presence of control test concentrations of DMSO (8%).

Fig. S11 Antibacterial activity against *E. coli* at different concentrations of **1**: (**A**) 0 µg/mL, (**B**) 5 µg/mL,



(**C**) 10 µg/mL, (**D**) 25 µg/mL, (**E**) 50 µg/mL, (**F**) 100 µg/mL, (**G**) 250 µg/mL, (**H**) 500 µg/mL.

Fig. S12 Antibacterial activity against *S. aureus* at different concentrations of **1**: (**A**) 0 µg/mL, (**B**) 5



µg/mL, (**C**) 10 µg/mL, (**D**) 25 µg/mL, (**E**) 50 µg/mL, (**F**) 100 µg/mL, (**G**) 250 µg/mL, (**H**) 500 µg/mL.

Fig. S13 Antibacterial activity against *P. aeruginosa* at different concentrations of **1**: (**A**) 0 μg/mL, (**B**) 5 μg/mL, (**C**) 10 μg/mL, (**D**) 25 μg/mL, (**E**) 50 μg/mL, **(F**) 100 μg/mL, (**G**) 250 μg/mL, (**H**) 500 μg/mL.

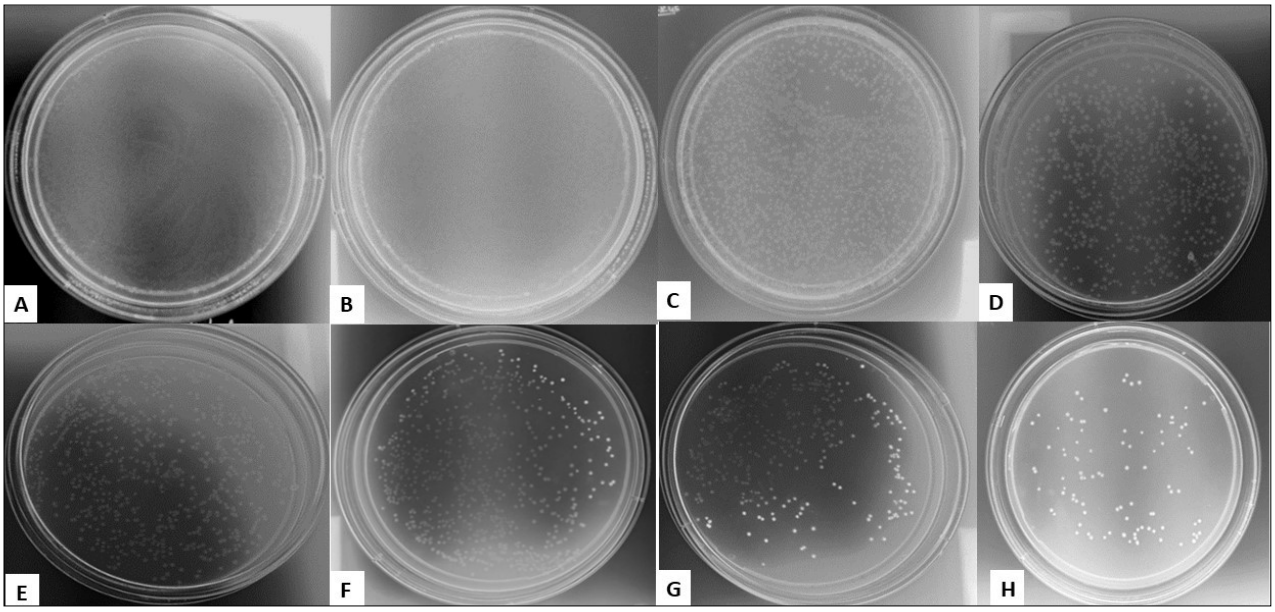


Fig. S14 Antibacterial activity against *B. cereus* at different concentrations of **1**: (**A**) 0 μg/mL, (**B**) 5 μg/mL, (**C**) 10 μg/mL, (**D**) 25 μg/mL, (**E**) 50 μg/mL, **(F**) 100 μg/mL, (**G**) 250 μg/mL, (**H**) 500 μg/mL.

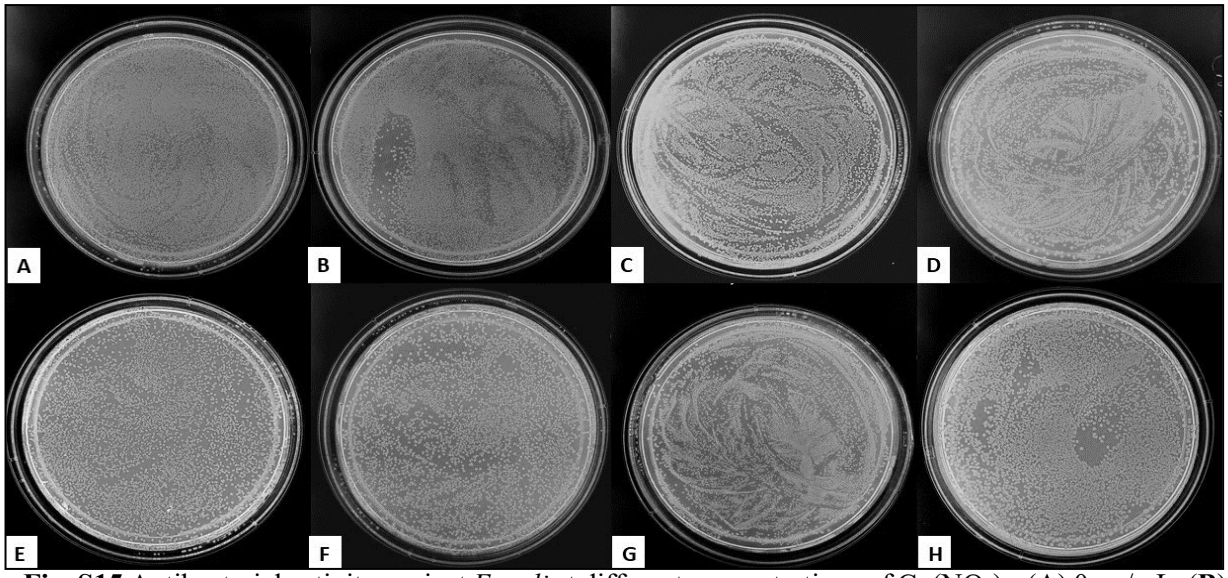


Fig. S15 Antibacterial activity against *E. coli* at different concentrations of $Cu(NO_3)_2$: (**A**) 0 μg/mL, (**B**) 5 μg/mL, (**C**) 10 μg/mL, (**D**) 25 μg/mL, (**E**) 50 μg/mL, **(F**) 100 μg/mL, (**G**) 250 μg/mL, (**H**) 500 μg/mL.

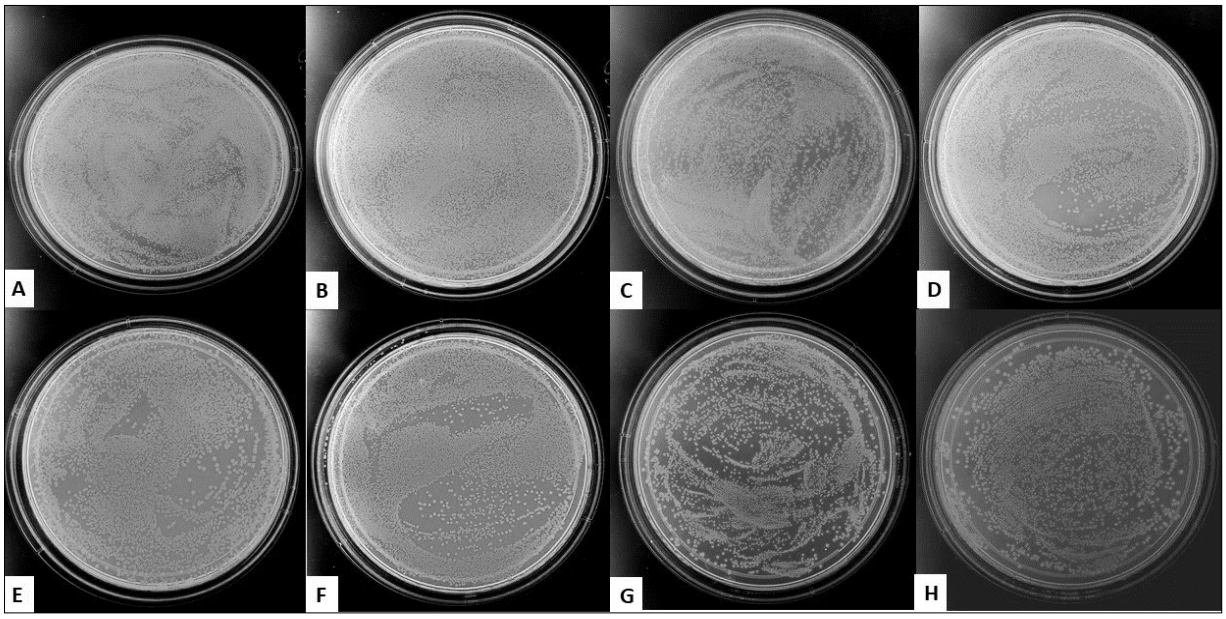


Fig. S16 Antibacterial activity against *E. coli* at different concentrations of Hcmu: (**A**) 0 μg/mL, (**B**) 5 μg/mL, (**C**) 10 μg/mL, (**D**) 25 μg/mL, (**E**) 50 μg/mL, **(F**) 100 μg/mL, (**G**) 250 μg/mL, (**H**) 500 μg/mL.

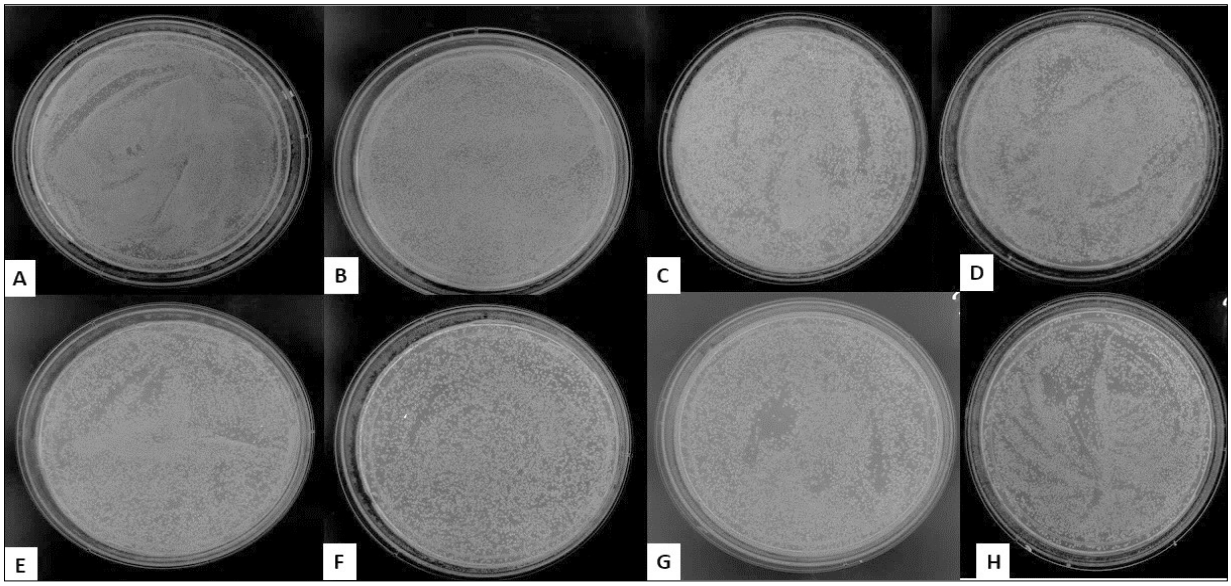


Fig. S17 Antibacterial activity against *S. aureus* at different concentrations of $Cu(NO_3)_2$: (**A**) 0 μg/mL, (**B**) 5 μg/mL, (**C**) 10 μg/mL, (**D**) 25 μg/mL, (**E**) 50 μg/mL, (**F**) 100 μg/mL, (**G**) 250 μg/mL, (**H**) 500 μg/mL.

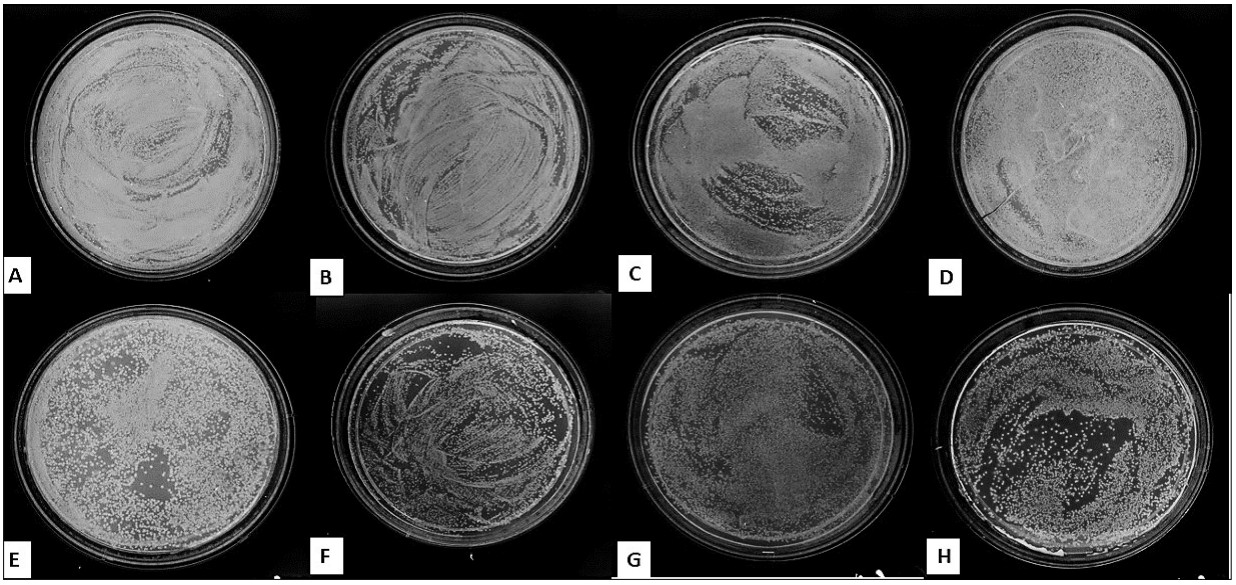


Fig. S18 Antibacterial activity against *S. aureus* at different concentrations of Hcmu: (**A**) 0 μg/mL, (**B**) 5 μg/mL, (**C**) 10 μg/mL, (**D**) 25 μg/mL, (**E**) 50 μg/mL, (**F**) 100 μg/mL, (**G**) 250 μg/mL, (**H**) 500 μg/mL

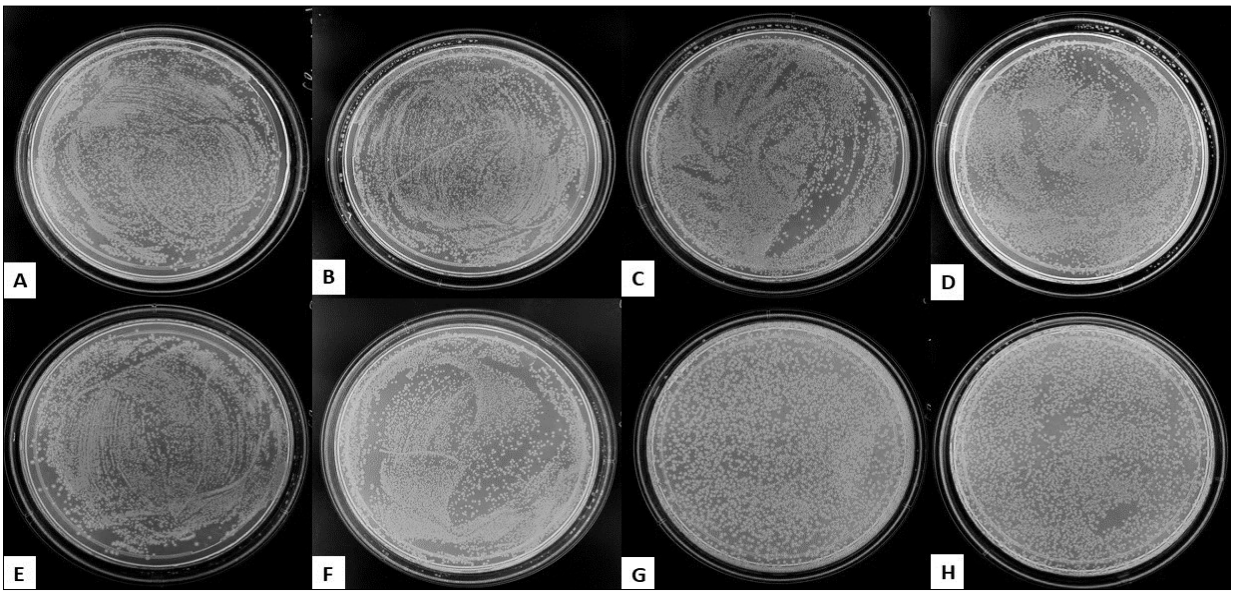


Fig. S19 Antibacterial activity against *P.aeruoginosa* at different concentrations of $Cu(NO_3)_2$: (**A**) 0 μg/mL, (**B**) 5 μg/mL, (**C**) 10 μg/mL, (**D**) 25 μg/mL, (**E**) 50 μg/mL, **(F**) 100 μg/mL, (**G**) 250 μg/mL, (**H**) 500 μg/mL.

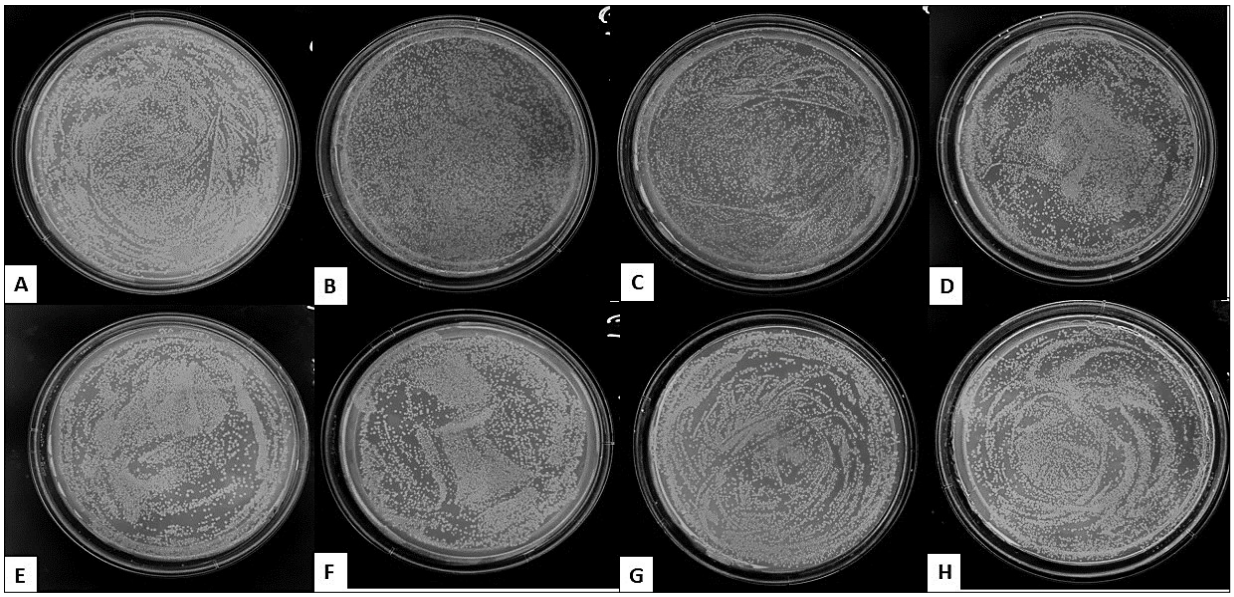


Fig. S20 Antibacterial activity against *P.aeruoginosa* at different concentrations of Hcmu: (**A**) 0 μg/mL, (**B**) 5 μg/mL, (**C**) 10 μg/mL, (**D**) 25 μg/mL, (**E**) 50 μg/mL, **(F**) 100 μg/mL, (**G**) 250 μg/mL, (**H**) 500 μg/mL.

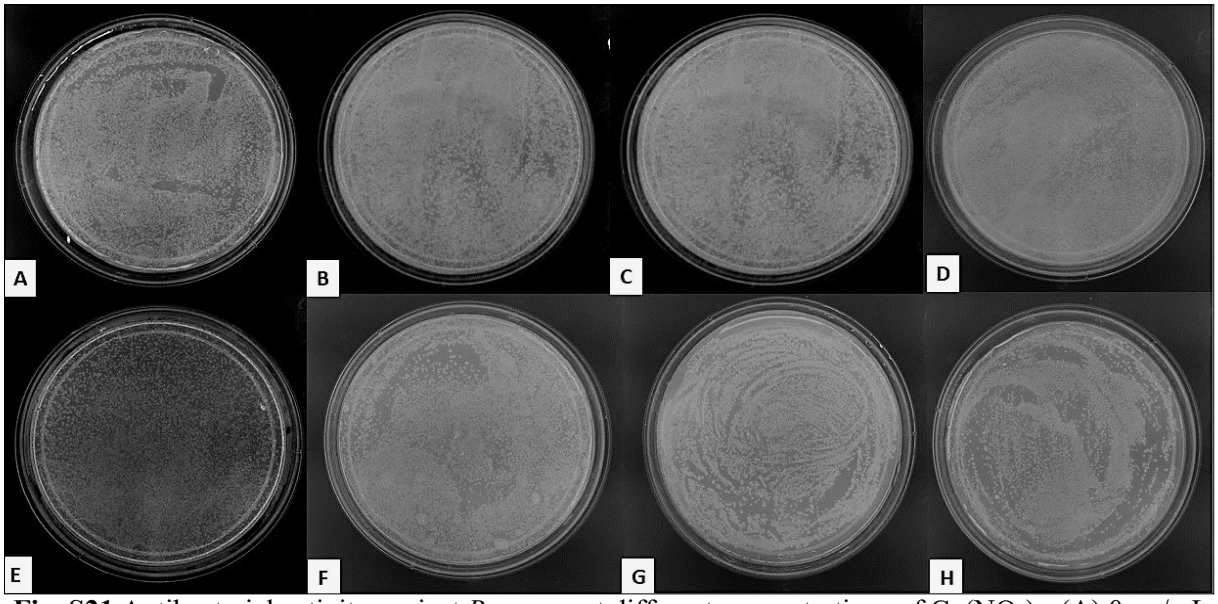


Fig. S21 Antibacterial activity against *B. cereus* at different concentrations of $Cu(NO_3)_2$: (**A**) 0 μg/mL, (**B**) 5 μg/mL, (**C**) 10 μg/mL, (**D**) 25 μg/mL, (**E**) 50 μg/mL, **(F**) 100 μg/mL, (**G**) 250 μg/mL, (**H**) 500 μg/mL.

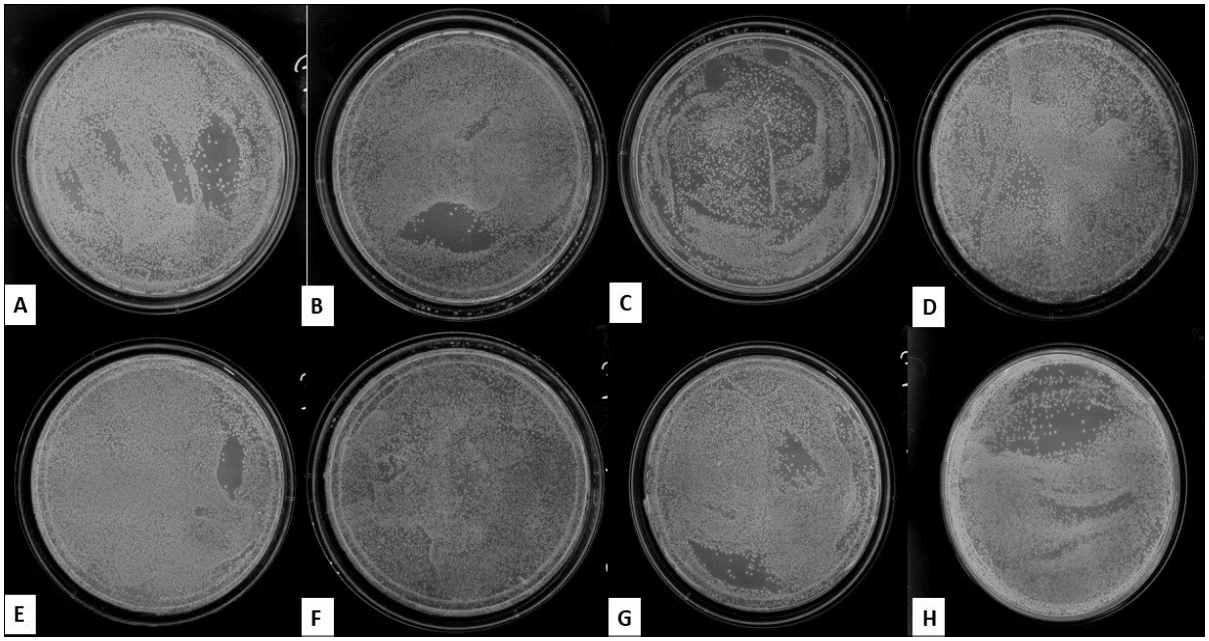


Fig. S22 Antibacterial activity against *B. cereus* at different concentrations of Hcmu: (**A**) 0 μg/mL, (**B**) 5 μg/mL, (**C**) 10 μg/mL, (**D**) 25 μg/mL, (**E**) 50 μg/mL, **(F**) 100 μg/mL, (**G**) 250 μg/mL, (**H**) 500 μg/mL.

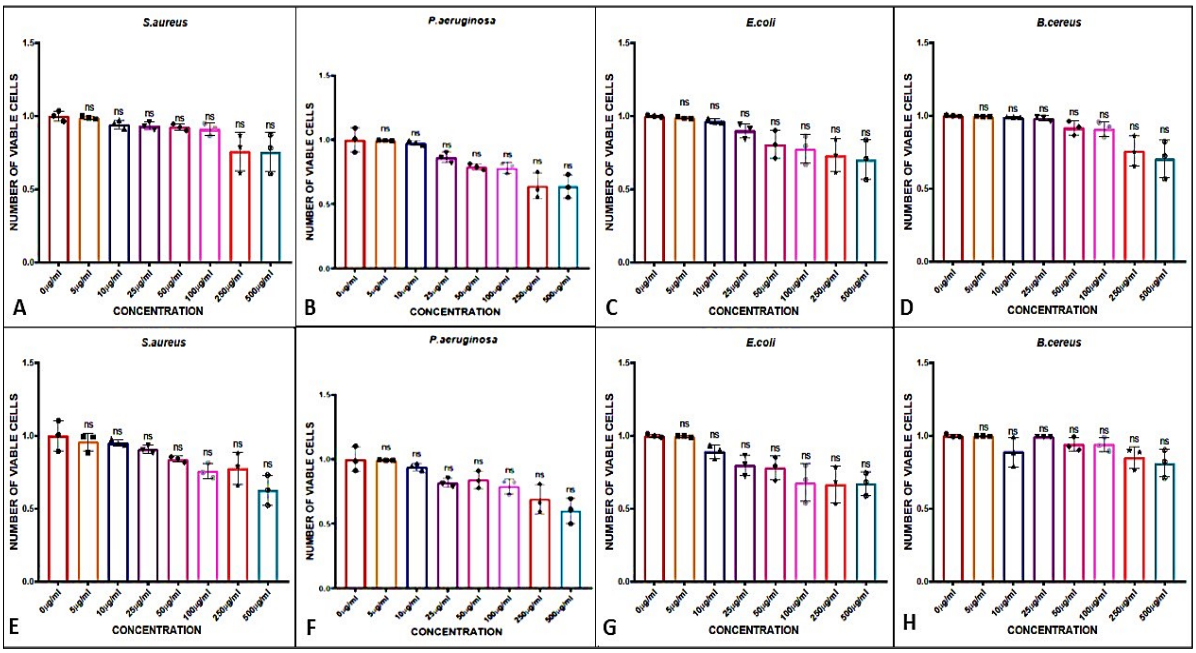


Fig. S23 Graphical representation of antibacterial activity of $Cu(NO_3)_2$ (**A**–**D**) and Hcmu (**E**–**H**) at different concentrations against four bacteria types.

Table S5. Calculated IC_{50} values (µg/mL) for complex **1**.

	SET 1	SET 2	SET 3	N total	Mean	SD	SEM	Median
E. coli	9.568	11.781	12.345	3	11.231	1.467	0.847	11.781
S. aureus	8.966	6.22	6.892	3	7.359	1.431	0.826	6.892
B. cereus	12.406	14.457	8.683	3	11.848	2.927	1.689	12.406
P. aeruginosa	4.965	4.371	4.536	3	4.624	0.370	0.177	4.54
SET 1, SET 2, and SET 3 refer to three independent individual tests (IC_{50} values); N represents the total number of experiments that are carried out for each set; the Mean is calculated by combining the three individual experiments; SD represents the calculated deviation from each set.								

Table S6. Inhibition activity of Hcmu at different concentrations against *E. coli.*

µg/ml	**SET 1**	**SET 2**	**SET 3**	**N total**	**Mean**	**SD**	**SEM**	**Median**	**P-value**
0	0.989	0.998	1.012	3	0.999	0.011	0.006	0.998	
5	0.988	0.998	0.999	3	0.995	0.006	0.003	0.998	0.380
10	0.933	0.901	0.841	3	0.891	0.046	0.026	0.901	0.849
25	0.865	0.805	0.724	3	0.798	0.070	0.040	0.805	0.051
50	0.794	0.852	0.692	3	0.779	0.081	0.046	0.794	0.051
100	0.796	0.54	0.697	3	0.677	0.129	0.074	0.697	0.052
250	0.687	0.784	0.533	3	0.668	0.126	0.073	0.687	0.051
500	0.682	0.745	0.587	3	0.671	0.079	0.045	0.682	0.061
SET 1, SET 2, and SET 3 refer to three independent inhibition evaluations; N represents the total number of experiments that are carried out for each set; the Mean is calculated by combining the three individual experiments; SD represents the calculated deviation from each set.									

μg/ml	SET 1	SET 2	SET 3	N total	Mean	SD	SEM	Median	P-value
0	1.007	0.998	0.994	3	0.999	0.006	0.003	0.998	
5	0.984	0.997	0.986	3	0.989	0.007	0.004	0.986	0.241
10	0.953	0.958	0.984	3	0.965	0.016	0.009	0.958	0.016
25	0.942	0.912	0.845	3	0.899	0.004	0.028	0.912	0.058
50	0.902	0.713	0.803	3	0.806	0.094	0.054	0.803	0.065
100	0.862	0.668	0.796	3	0.775	0.098	0.056	0.796	0.052
250	0.842	0.615	0.735	3	0.730	0.113	0.065	0.735	0.050
500	0.835	0.565	0.070	3	0.703	0.135	0.780	0.709	0.059
SET 1, SET 2, and SET 3 refer to three independent inhibition evaluations; N represents the total number of experiments that are carried out for each set; the Mean is calculated by combining the three individual experiments; SD represents the calculated deviation from each set.									

Table S7. Inhibition activity of $Cu(NO_3)_2$ at different concentrations against *E. coli.*

Table S8. Inhibition activity of Hcmu at different concentrations against *B. cereus*

μg/ml	SET 1	SET 2	SET 3	N total	Mean	SD	SEM	Median	P-value
0	0.999	0.996	1.012	3	1	0.010	0.006	0.995	
5	0.995	0.993	0.998	3	0.997	0.001	0.008	0.998	0.728
10	0.991	0.885	0.789	3	0.888	0.101	0.058	0.885	0.219
25	0.994	0.996	0.992	3	0.994	0.002	0.001	0.994	0.486
50	0.993	0.926	0.902	3	0.940	0.047	0.027	0.926	0.197
100	0.991	0.895	0.934	3	0.940	0.048	0.027	0.934	0.170
250	0.888	0.765	0.900	3	0.851	0.074	0.043	0.888	0.063
500	0.901	0.712	0.822	3	0.811	0.094	0.054	0.822	0.073
SET 1, SET 2, and SET 3 refer to three independent inhibition evaluations; N represents the total number of experiments that are carried out for each set; the Mean is calculated by combining the three individual experiments; SD represents the calculated deviation from each set.									

Table S9. Inhibition activity of $Cu(NO_3)_2$ at different concentrations against *B. cereus.*

μg/ml	SET 1	SET 2	SET 3	N total	Mean	SD	SEM	Median	P-value
0	1.004	0.996	1	3	1.000	0.004	0.002	1	
5	0.995	0.993	0.997	3	0.995	0.002	0.001	0.995	0.129
10	0.986	0.990	0.991	3	0.989	0.002	0.001	0.99	0.092
25	0.99	0.992	0.965	3	0.982	0.015	0.008	0.099	0.192
50	0.962	0.865	0.923	3	0.916	0.048	0.028	0.923	0.084
100	0.954	0.854	0.919	3	0.909	0.050	0.029	0.919	0.078
250	0.862	0.654	0.754	3	0.756	0.010	0.061	0.754	0.051
500	0.822	0.566	0.723	3	0.703	0.129	0.074	0.723	0.054
SET 1, SET 2, and SET 3 refer to three independent inhibition evaluations; N represents the total number of experiments that are carried out for each set; the Mean is calculated by combining the three individual experiments; SD represents the calculated deviation from each set.									

µg/ml	**SET 1**	**SET 2**	**SET 3**	**N total**	**Mean**	**SD**	**SEM**	**Median**	**P-value**
0	1.102	0.912	0.986	**3**	1	0.095	0.055	0.986	
5	0.996	0.993	0.991	3	0.993	0.002	0.001	0.993	0.913
10	0.912	0.945	0.966	3	0.941	0.027	0.015	0.945	0.472
25	0.856	0.812	0.786	3	0.818	0.035	0.020	0.812	0.051
50	0.912	0.834	0.777	3	0.841	0.067	0.039	0.083	0.062
100	0.821	0.823	0.723	3	0.789	0.057	0.033	0.821	0.077
250	0.666	0.595	0.811	3	0.690	0.110	0.063	0.666	0.052
500	0.501	0.612	0.695	3	0.602	0.097	0.056	0.612	0.054

SET 1, SET 2, and SET 3 refer to three independent inhibition evaluations; N represents the total number of experiments that are carried out for each set; the Mean is calculated by combining the three individual experiments; SD represents the calculated deviation from each set.

Table S10. Inhibition activity of Hcmu at different concentrations against *P. aeruginosa.*

Table S11. Inhibition activity of $Cu(NO_3)_2$ at different concentrations against *P. aeruginosa.*

µg/ml	**SET 1**	**SET 2**	**SET 3**	**N total**	**Mean**	**SD**	**SEM**	**Median**	**P-value**
0	1.008	0.902	1.091	3	1.000	0.094	0.05469	1.008	
5	0.998	0.992	0.995	3	0.995	0.003	0.00173	0.995	0.930
10	0.992	0.973	0.957	3	0.974	0.017	0.01012	0.973	0.700
25	0.867	0.901	0.821	3	0.863	0.040	0.02318	0.867	0.219
50	0.765	0.813	0.792	3	0.790	0.024	0.01389	0.792	0.078
100	0.735	0.798	0.812	3	0.781	0.041	0.02368	0.798	.0624
250	0.558	0.754	0.612	3	0.641	0.101	0.05845	0.612	0.077
500	0.552	0.732	0.632	3	0.638	0.090	0.05207	0.632	0.066

SET 1, SET 2, and SET 3 refer to three independent inhibition evaluations; N represents the total number of experiments that are carried out for each set; the Mean is calculated by combining the three individual experiments; SD represents the calculated deviation from each set.

Table S12 Inhibition activity of Hcmu at different concentrations against *S. aureus.*

µg/ml	**SET 1**	**SET 2**	**SET 3**	**N total**	**Mean**	**SD**	**SEM**	**Median**	**P-value**
0	1.006	0.894	1.103	3	1.001	0.104	0.060	1.006	
5	0.995	0.991	*0.886*	3	0.957	0.061	0.035	0.991	0.682
10	0.945	0.975	0.934	3	0.951	0.021	0.012	0.945	0.563
25	0.884	0.903	0.937	3	0.908	0.026	0.015	0.903	0.218
50	0.856	0.843	0.817	3	0.838	0.019	0.011	0.843	0.140
100	0.813	0.748	0.712	3	0.757	0.051	0.029	0.748	0.083
250	0.879	0.66	0.791	3	0.776	0.110	0.063	0.791	0.052
500	0.523	0.729	0.629	3	0.627	0.103	0.059	0.062	0.070

SET 1, SET 2, and SET 3 refer to three independent inhibition evaluations; N represents the total number of experiments that are carried out for each set; the Mean is calculated by combining the three individual experiments; SD represents the calculated deviation from each set.

Table S13. Inhibition activity of $Cu(NO_3)_2$ at different concentrations against *S. aureus.*

µg/ml	SET 1	SET 2	SET 3	N total	Mean	SD	SEM	Median	P-value
0	1.035	0.965	1.000	3	1	0.035	0.020	1.000	
5	0.998	0.989	0.979	3	0.988	0.009	0.005	0.989	0.598
10	0.947	0.969	0.912	3	0.942	0.028	0.016	0.947	0.202
25	0.934	0.959	0.905	3	0.932	0.027	0.015	0.934	0.159
50	0.923	0.945	0.901	3	0.923	0.022	0.012	0.923	0.115
100	0.949	0.917	0.865	3	0.910	0.042	0.024	0.917	0.070
250	0.870	0.61	0.791	3	0.757	0.133	0.076	0.791	0.051
500	0.872	0.782	0.606	3	0.753	0.135	0.078	0.782	0.079
SET 1, SET 2, and SET 3 refer to three independent inhibition evaluations; N represents the total number of experiments that are carried out for each set; the Mean is calculated by combining the three individual experiments; SD represents the calculated deviation from each set.									

Table S14. Antioxidant activity of ascorbic acid and **1**.

DPPH ASSAY								
Antioxidant Activity of Ascorbic acid								
µg/mL	**SET 1**	**SET 2**	**SET 3**	**N**	**Mean**	**SD**	**SEM**	**Median**
10	40.3	40.3	39.8	3	40.19	0.32	0.18	40.37
25	47.9	50.9	49.1	3	49.36	1.52	0.87	49.18
50	58.2	57.1	58.3	3	57.91	0.67	0.39	58.27
75	76.5	77.5	77.8	3	77.30	0.65	0.37	7.76
100	86.7	87.5	87.9	3	87.43	0.61	0.35	87.58
Antioxidant Activity of 1								
10	3.77	4.77	5.39	3	4.643	0.817	0.47	4.77
25	12.3	10.3	12.0	3	11.55	1.082	0.62	12.03
50	39.5	37.9	37.0	3	38.20	1.265	0.73	37.98
75	53.4	53.9	56.2	3	54.53	1.50	0.86	5.39
100	72.5	73.6	71.5	3	72.56	1.050	0.60	72.52
IC_{50} of DPPH Assay								
µg/mL	**SET 1**	**SET 2**	**SET 3**	**N**	**Mean**	**SD**	**SEM**	**Median**
Ascorbic acid	29.3	27.8	28.7	3	28.65	0.80	0.46	28.76
Compound **1**	69.6	69.5	69.6	3	69.63	0.04	0.02	69.65
SET 1, SET 2, and SET3 refer to three independent individual evaluations; N represents the total number of experiments that are carried out for each set; the Mean is calculated by combining the three individual experiments; SD represents the calculated deviation from each set.								

Listing S1. Cartesian coordinates for the DFT optimized **1** with coordinated methanol molecules instead of water ones.

Cu	1.892766	-0.798478	3.939087
Cl	3.290114	1.703850	5.514801
O	0.868960	0.245174	1.531648
O	2.376243	4.618680	1.413844
O	3.677613	-1.262402	3.035566
N	1.991081	1.051616	3.341535
C	1.448564	1.199005	2.076590
N	1.599069	2.435773	1.452925
C	2.284024	3.548393	2.030422
C	2.836222	3.306431	3.349298
H	3.365854	4.119999	3.857278
C	2.660446	2.071094	3.923647
C	1.019484	2.577000	0.117815
H	1.245925	3.598945	-0.229655
H	1.458228	1.829665	-0.571241
H	-0.076017	2.419504	0.155754
Cl	0.511159	-3.297418	2.347452
O	2.908058	-1.851233	6.350404
O	1.394996	-6.222980	6.447011
O	0.114180	-0.326321	4.848535
N	1.796578	-2.651242	4.530698
C	2.330531	-2.802680	5.798869
N	2.174447	-4.040649	6.418677
C	1.492064	-5.151128	5.834186
C	0.948911	-4.905300	4.512161
H	0.422203	-5.717151	3.998407
C	1.129492	-3.668974	3.941840
C	2.746097	-4.186293	7.756671
H	2.517748	-5.209456	8.099317
H	2.302889	-3.441761	8.445953
H	3.841825	-4.028792	7.725792
C	-0.215330	-0.795619	6.174741
H	-1.175370	-0.343022	6.489528
H	0.585119	-0.546761	6.898228
H	-0.331796	-1.891576	6.110042
C	3.991575	-0.817230	1.696708
H	4.953100	-1.267607	1.383457
H	4.098634	0.280769	1.738748
H	3.186900	-1.087787	0.985862
H	0.086612	0.654272	4.834594
H	3.720833	-2.241771	3.070036

Listing S2. Cartesian coordinates for the DFT optimized **1** with coordinated DMF molecules instead of water ones.

Cu	1.912257	-0.803415	3.910225
Cl	3.273451	1.660233	5.488465
O	1.077671	0.258512	1.348283
O	2.000186	4.780995	1.643739
O	3.579843	-1.463420	2.983651
N	2.143389	1.020701	3.216829
C	1.563233	1.215434	1.981878

```
  N       1.547442      2.513583      1.471521
  C       2.059074      3.654810      2.160545
  C       2.623561      3.370443      3.462827
  H       3.031873      4.196284      4.055946
  C       2.623398      2.069530      3.910273
  C       0.949628      2.696629      0.150317
  H       1.052617      3.763590     -0.109802
  H       1.469958      2.065127     -0.595464
  H      -0.120042      2.409354      0.166613
  Cl      0.560027     -3.269796      2.327865
  O       2.721513     -1.860928      6.484232
  O       1.710522     -6.367076      6.229713
  O       0.241941     -0.142201      4.831998
  N       1.673808     -2.625680      4.606501
  C       2.228485     -2.816122      5.853646
  N       2.208929     -4.107635      6.380417
  C       1.684268     -5.246724      5.697643
  C       1.147869     -4.967719      4.382482
  H       0.731897     -5.792649      3.793439
  C       1.181327     -3.672710      3.919223
  C       2.780035     -4.285674      7.714011
  H       2.655227     -5.347983      7.983475
  H       2.256561     -3.638368      8.443950
  H       3.854159     -4.015194      7.714004
  C       0.235783     -0.033129      6.093325
  N      -0.735364      0.586872      6.767133
  H       1.059765     -0.464305      6.704317
  C      -1.865718      1.207551      6.082437
  H      -1.941361      2.272580      6.380595
  H      -2.807999      0.693160      6.361336
  H      -1.712122      1.134525      4.991974
  C      -0.704293      0.659866      8.224396
  H      -0.691960      1.719606      8.550816
  H       0.201383      0.151542      8.602907
  H      -1.601860      0.167255      8.650534
  C       3.582933     -1.554103      1.720782
  N       4.553261     -2.162508      1.035407
  H       2.756440     -1.116214      1.117871
  C       4.517746     -2.215704     -0.422687
  H       4.504525     -3.270953     -0.763266
  H       5.414164     -1.717309     -0.844490
  H       3.611252     -1.702160     -0.791986
  C       5.687042     -2.790792      1.707595
  H       5.762131     -3.851902      1.395654
  H       5.537729     -2.731905      2.799504
  H       6.627564     -2.272229      1.430644
```

Listing S3. Shortened example of the ORCA input TDDFT calculation (atoms coordinates are not shown).

```
! M06L ma-def2-TZVP AutoAux D3Zero RIJCOSX Grid5 FinalGrid6 TightSCF
! LARGEPRINT CPCM(METHANOL) PAL5
%tddft
  maxdim 5
  nroots 50
```

```
end
* xyz 0 2
```

Listing S4. Selected output of the ORCA TDDFT calculations of the complex **1**.

```
----------------
TOTAL SCF ENERGY
----------------

Total Energy       :        -3619.90319587 Eh          -98502.57373 eV

DFT components:
N(Alpha)           :      106.000016468941 electrons
N(Beta)            :      105.000017145421 electrons
N(Total)           :      211.000033614362 electrons

----------------
ORBITAL ENERGIES
----------------
                  SPIN UP ORBITALS
  NO   OCC          E(Eh)            E(eV)
  85   1.0000      -0.358098        -9.7443
  86   1.0000      -0.356204        -9.6928
  87   1.0000      -0.350889        -9.5482
  88   1.0000      -0.335731        -9.1357
  89   1.0000      -0.324023        -8.8171
  90   1.0000      -0.322331        -8.7711
  91   1.0000      -0.317550        -8.6410
  92   1.0000      -0.309068        -8.4102
  93   1.0000      -0.303395        -8.2558
  94   1.0000      -0.297019        -8.0823
  95   1.0000      -0.287145        -7.8136
  96   1.0000      -0.283496        -7.7143
  97   1.0000      -0.258316        -7.0291
  98   1.0000      -0.253431        -6.8962
  99   1.0000      -0.250236        -6.8093
 100   1.0000      -0.249832        -6.7983
 101   1.0000      -0.245770        -6.6877
 102   1.0000      -0.230699        -6.2776
 103   1.0000      -0.228196        -6.2095
 104   1.0000      -0.216978        -5.9043
 105   1.0000      -0.214768        -5.8441
 106   0.0000      -0.061013        -1.6602
 107   0.0000      -0.060326        -1.6415
 108   0.0000      -0.019783        -0.5383
 109   0.0000      -0.017209        -0.4683
 110   0.0000      -0.016293        -0.4434
 111   0.0000      -0.009864        -0.2684
 112   0.0000      -0.004508        -0.1227
 113   0.0000       0.002113         0.0575
 114   0.0000       0.004634         0.1261
 115   0.0000       0.009591         0.2610
 116   0.0000       0.012771         0.3475
 117   0.0000       0.019206         0.5226
 118   0.0000       0.027782         0.7560
```

119	0.0000	0.031004	0.8437
120	0.0000	0.031967	0.8699
121	0.0000	0.035802	0.9742
122	0.0000	0.041751	1.1361
123	0.0000	0.042848	1.1659
124	0.0000	0.044595	1.2135
125	0.0000	0.048345	1.3155

SPIN DOWN ORBITALS

NO	OCC	E(Eh)	E(eV)
84	1.0000	-0.358089	-9.7441
85	1.0000	-0.356708	-9.7065
86	1.0000	-0.352818	-9.6007
87	1.0000	-0.346612	-9.4318
88	1.0000	-0.319634	-8.6977
89	1.0000	-0.318795	-8.6749
90	1.0000	-0.314557	-8.5595
91	1.0000	-0.308847	-8.4042
92	1.0000	-0.297994	-8.1088
93	1.0000	-0.286115	-7.7856
94	1.0000	-0.281945	-7.6721
95	1.0000	-0.281163	-7.6508
96	1.0000	-0.277051	-7.5389
97	1.0000	-0.258036	-7.0215
98	1.0000	-0.250199	-6.8083
99	1.0000	-0.249908	-6.8003
100	1.0000	-0.247750	-6.7416
101	1.0000	-0.230668	-6.2768
102	1.0000	-0.226917	-6.1747
103	1.0000	-0.216013	-5.8780
104	1.0000	-0.213306	-5.8044
105	0.0000	-0.172274	-4.6878
106	0.0000	-0.060749	-1.6531
107	0.0000	-0.060027	-1.6334
108	0.0000	-0.019436	-0.5289
109	0.0000	-0.016059	-0.4370
110	0.0000	-0.014415	-0.3922
111	0.0000	-0.009285	-0.2527
112	0.0000	-0.004309	-0.1173
113	0.0000	0.002671	0.0727
114	0.0000	0.007338	0.1997
115	0.0000	0.010138	0.2759
116	0.0000	0.013497	0.3673
117	0.0000	0.019435	0.5289
118	0.0000	0.028625	0.7789
119	0.0000	0.031718	0.8631
120	0.0000	0.032671	0.8890
121	0.0000	0.036189	0.9848
122	0.0000	0.042226	1.1490
123	0.0000	0.043546	1.1850
124	0.0000	0.046115	1.2548

TD-DFT/TDA EXCITED STATES

STATE 19: E= 0.152151 au 4.140 eV 33393.3 cm**-1

```
    89b -> 105b  :     0.949563 (c=  0.97445515)
   104b -> 106b  :     0.011124 (c= -0.10547245)

STATE 36:  E=   0.182362 au      4.962 eV    40023.7 cm**-1
    99a -> 107a  :     0.010211 (c= -0.10104817)
    99a -> 110a  :     0.011583 (c=  0.10762602)
   100a -> 106a  :     0.014966 (c=  0.12233643)
   100a -> 108a  :     0.015365 (c=  0.12395560)
   101a -> 106a  :     0.288032 (c= -0.53668642)
   104a -> 107a  :     0.157971 (c= -0.39745588)
   105a -> 106a  :     0.127057 (c=  0.35645073)
    89b -> 105b  :     0.012405 (c= -0.11137554)
    98b -> 109b  :     0.012241 (c= -0.11063948)
    99b -> 108b  :     0.012990 (c=  0.11397514)
   103b -> 107b  :     0.148000 (c= -0.38470757)
   104b -> 106b  :     0.114348 (c= -0.33815322)
```

Listing S5. The TDDFT calculated wavenumbers (cm^{-1}) and intensities of the UV/Vis absorptions of the complex **1**.

```
  7353.20   0.000000000000
  8039.70  51.152142865085
  9897.90   0.000000000000
  9031.40   7.585739065389
 14431.00   0.000000000000
 14719.80   0.000000000000
 14615.50  11.256704135966
 17499.40  28.146018182085
 21295.30   0.000000000000
 21591.40   0.000000000000
 22995.50   0.000000000000
 24431.40   0.000000000000
 24071.30  55.350158284226
 29147.10   0.000000000000
 29086.00  25.861753658115
 29711.80   7.000977327418
 29916.50   0.000000000000
 29304.10   0.000000000000
 33393.30 16687.283394691978
 33800.80   0.000813600415
 33801.60  61.223268476928
 34006.00   0.000216960111
 34007.60  30.787724488193
 34631.00   0.246846365783
 34656.90   0.000000000000
 35810.20   4.226382953596
 35937.30   0.000000000000
 35943.40   0.000000000000
 35973.40   0.015675367988
 36170.60   0.000000000000
 36276.20   9.317460427805
 37600.10  30.229757323875
 37596.20   0.028150574344
 38361.60 2347.191688674976
 39632.10   0.000000000000
```

```
 40023.70 9511.857717422135
 40079.20    0.000325440166
 40009.60 2847.411339726897
 40632.90 601.524347312741
 40389.30    0.000433920221
 39656.50  80.966204617139
 40719.90    0.000216960111
 40333.30 1044.702473298583
 40423.40    0.000108480055
 39840.50    0.000000000000
 40731.50  76.309589764314
 40756.60    0.002657761354
 40798.20  20.464436987858
 40873.10    0.000162720083
 41172.80  57.275353825229
```

Listing S6. Selected output of the ORCA TDDFT calculations of the DFT optimized complex **1** with coordinated methanol molecules instead of water ones.

```
----------------
TOTAL SCF ENERGY
----------------

Total Energy       :        -3698.59862609 Eh         -100643.98526 eV

DFT components:
N(Alpha)           :      114.000034425030 electrons
N(Beta)            :      113.000034116126 electrons
N(Total)           :      227.000068541156 electrons

----------------
ORBITAL ENERGIES
----------------
                  SPIN UP ORBITALS
  NO   OCC          E(Eh)            E(eV)
  93   1.0000      -0.349899        -9.5212
  94   1.0000      -0.335943        -9.1415
  95   1.0000      -0.329407        -8.9636
  96   1.0000      -0.325063        -8.8454
  97   1.0000      -0.323769        -8.8102
  98   1.0000      -0.316766        -8.6196
  99   1.0000      -0.311487        -8.4760
 100   1.0000      -0.302434        -8.2296
 101   1.0000      -0.299561        -8.1515
 102   1.0000      -0.289170        -7.8687
 103   1.0000      -0.286387        -7.7930
 104   1.0000      -0.285368        -7.7653
 105   1.0000      -0.265839        -7.2339
 106   1.0000      -0.262314        -7.1379
 107   1.0000      -0.252150        -6.8613
 108   1.0000      -0.251628        -6.8471
 109   1.0000      -0.241718        -6.5775
 110   1.0000      -0.238893        -6.5006
 111   1.0000      -0.235958        -6.4207
```

112	1.0000	-0.219537	-5.9739
113	1.0000	-0.216591	-5.8937
114	0.0000	-0.067016	-1.8236
115	0.0000	-0.066038	-1.7970
116	0.0000	-0.026827	-0.7300
117	0.0000	-0.023870	-0.6495
118	0.0000	-0.022661	-0.6166
119	0.0000	-0.016424	-0.4469
120	0.0000	-0.014814	-0.4031
121	0.0000	-0.002526	-0.0687
122	0.0000	0.001610	0.0438
123	0.0000	0.007443	0.2025
124	0.0000	0.007622	0.2074
125	0.0000	0.016924	0.4605
126	0.0000	0.017622	0.4795
127	0.0000	0.022116	0.6018
128	0.0000	0.026207	0.7131
129	0.0000	0.032440	0.8827
130	0.0000	0.032978	0.8974
131	0.0000	0.035340	0.9616
132	0.0000	0.036335	0.9887
133	0.0000	0.040264	1.0956

SPIN DOWN ORBITALS

NO	OCC	E(Eh)	E(eV)
92	1.0000	-0.349947	-9.5225
93	1.0000	-0.348400	-9.4804
94	1.0000	-0.321197	-8.7402
95	1.0000	-0.320580	-8.7234
96	1.0000	-0.318488	-8.6665
97	1.0000	-0.313806	-8.5391
98	1.0000	-0.311033	-8.4636
99	1.0000	-0.298855	-8.1323
100	1.0000	-0.297409	-8.0929
101	1.0000	-0.284150	-7.7321
102	1.0000	-0.283642	-7.7183
103	1.0000	-0.279865	-7.6155
104	1.0000	-0.273452	-7.4410
105	1.0000	-0.265425	-7.2226
106	1.0000	-0.255742	-6.9591
107	1.0000	-0.252013	-6.8576
108	1.0000	-0.251307	-6.8384
109	1.0000	-0.238801	-6.4981
110	1.0000	-0.235122	-6.3980
111	1.0000	-0.218416	-5.9434
112	1.0000	-0.215429	-5.8621
113	0.0000	-0.177270	-4.8238
114	0.0000	-0.066737	-1.8160
115	0.0000	-0.065697	-1.7877
116	0.0000	-0.026526	-0.7218
117	0.0000	-0.023290	-0.6338
118	0.0000	-0.022168	-0.6032
119	0.0000	-0.016248	-0.4421
120	0.0000	-0.013943	-0.3794
121	0.0000	-0.002178	-0.0593
122	0.0000	0.002453	0.0667
123	0.0000	0.007736	0.2105

```
 124   0.0000       0.008251         0.2245
 125   0.0000       0.017391         0.4732
 126   0.0000       0.018146         0.4938
 127   0.0000       0.022599         0.6149
 128   0.0000       0.026823         0.7299
 129   0.0000       0.032519         0.8849
 130   0.0000       0.033430         0.9097
 131   0.0000       0.036479         0.9927
 132   0.0000       0.036823         1.0020

-------------------------
TD-DFT/TDA EXCITED STATES
-------------------------

STATE 21:  E=   0.147359 au      4.010 eV    32341.5 cm**-1
    94b -> 113b  :     0.845581 (c=  0.91955499)
    95b -> 113b  :     0.106359 (c= -0.32612782)
   111b -> 115b  :     0.011423 (c= -0.10687754)

STATE 42:  E=   0.179318 au      4.879 eV    39355.8 cm**-1
   107a -> 115a  :     0.023619 (c=  0.15368390)
   108a -> 114a  :     0.024107 (c= -0.15526540)
   108a -> 116a  :     0.017763 (c=  0.13327806)
   109a -> 114a  :     0.041296 (c= -0.20321498)
   112a -> 115a  :     0.172510 (c=  0.41534362)
   113a -> 114a  :     0.127043 (c= -0.35643088)
   113a -> 116a  :     0.031052 (c=  0.17621688)
    88b -> 113b  :     0.081321 (c=  0.28516828)
   108b -> 116b  :     0.015307 (c=  0.12372199)
   111b -> 115b  :     0.159780 (c= -0.39972476)
   112b -> 114b  :     0.117977 (c= -0.34347841)
   112b -> 116b  :     0.021496 (c= -0.14661471)
```

Listing S7. The TDDFT calculated wavenumbers (cm^{-1}) and intensities of the UV/Vis absorptions of the DFT optimized complex **1** with coordinated methanol molecules instead of water ones.

```
  7014.70   0.238493401527
  7841.60 351.051710241906
 10788.20   0.138203590423
 10208.80  59.231737382124
 14797.90   0.074742758086
 15156.50   0.249829567303
 14052.10  24.994347136119
 18151.70  39.293862582580
 20347.00   0.100615251270
 20228.90   0.199277861544
 21198.30   0.271579818386
 23329.30   0.019634890005
 23533.90 765.201495516067
 26817.90  14.041549875012
 27270.00 2385.815632676193
 28959.40  15.798818290446
 28996.20   1.255493919749
 27985.20 609.494431213977
```

```
 29420.40   0.112276857212
 31503.80  24.609839580190
 32341.50 12724.455718593543
 24827.30 145.219321037956
 26200.30 162.721276196252
 26167.30  26.905331789881
 25029.30  57.064794037936
 35129.60   0.536542353401
 35173.70   0.000379680193
 36734.20  25.582580235859
 36736.60   3.748365590017
 35884.60  42.306841877874
 36326.90   0.638622085416
 32751.70   1.057192378703
 32742.40  11.236364125602
 37343.20 1404.583158279382
 36752.30   0.652561772519
 36840.70  38.303710878039
 37146.10   8.725647486241
 37403.70 580.318883067285
 37464.60  12.246476160314
 38085.80 1290.452865083150
 36912.90   1.606047218377
 39355.80 13725.603015778152
 39580.60   3.147820004003
 39629.60 2145.340029339446
 39761.40   2.966766791746
 31458.60   1.209661096395
 34598.10  27.108677653498
 31862.60   0.370350908716
 36949.30   9.804590116027
 40073.60   3.524625476008
```

Listing S8. Selected output of the ORCA TDDFT calculations of the DFT optimized complex **1** with coordinated DMF molecules instead of water ones.

```
----------------
TOTAL SCF ENERGY
----------------

Total Energy       :        -3964.26022030 Eh         -107873.00475 eV

DFT components:
N(Alpha)           :      135.999986198351 electrons
N(Beta)            :      134.999986334739 electrons
N(Total)           :      270.999972533090 electrons

----------------
ORBITAL ENERGIES
----------------
                 SPIN UP ORBITALS
  NO   OCC          E(Eh)            E(eV)
 105   1.0000      -0.371513       -10.1094
 106   1.0000      -0.362724        -9.8702
 107   1.0000      -0.362581        -9.8663
```

108	1.0000	-0.359832	-9.7915
109	1.0000	-0.359674	-9.7872
110	1.0000	-0.359317	-9.7775
111	1.0000	-0.352834	-9.6011
112	1.0000	-0.347960	-9.4685
113	1.0000	-0.347882	-9.4663
114	1.0000	-0.331973	-9.0334
115	1.0000	-0.320059	-8.7092
116	1.0000	-0.315937	-8.5971
117	1.0000	-0.313713	-8.5366
118	1.0000	-0.308565	-8.3965
119	1.0000	-0.303948	-8.2708
120	1.0000	-0.295976	-8.0539
121	1.0000	-0.295310	-8.0358
122	1.0000	-0.281750	-7.6668
123	1.0000	-0.278232	-7.5711
124	1.0000	-0.277926	-7.5627
125	1.0000	-0.261139	-7.1059
126	1.0000	-0.258612	-7.0372
127	1.0000	-0.248965	-6.7747
128	1.0000	-0.247699	-6.7402
129	1.0000	-0.247147	-6.7252
130	1.0000	-0.246124	-6.6974
131	1.0000	-0.234787	-6.3889
132	1.0000	-0.232603	-6.3295
133	1.0000	-0.221933	-6.0391
134	1.0000	-0.213291	-5.8039
135	1.0000	-0.210193	-5.7197
136	0.0000	-0.061713	-1.6793
137	0.0000	-0.061274	-1.6674
138	0.0000	-0.043368	-1.1801
139	0.0000	-0.043227	-1.1763
140	0.0000	-0.020518	-0.5583
141	0.0000	-0.020341	-0.5535
142	0.0000	-0.017713	-0.4820
143	0.0000	-0.014305	-0.3893
144	0.0000	-0.012023	-0.3272
145	0.0000	-0.002517	-0.0685
146	0.0000	-0.001147	-0.0312
147	0.0000	0.006503	0.1770
148	0.0000	0.010504	0.2858
149	0.0000	0.012884	0.3506
150	0.0000	0.016883	0.4594
151	0.0000	0.019952	0.5429
152	0.0000	0.023914	0.6507
153	0.0000	0.025878	0.7042
154	0.0000	0.027843	0.7576
155	0.0000	0.031642	0.8610

SPIN DOWN ORBITALS

NO	OCC	E(Eh)	E(eV)
104	1.0000	-0.370399	-10.0791
105	1.0000	-0.367286	-9.9943
106	1.0000	-0.362515	-9.8645
107	1.0000	-0.362235	-9.8569
108	1.0000	-0.359404	-9.7799
109	1.0000	-0.359326	-9.7778

```
 110   1.0000      -0.358842        -9.7646
 111   1.0000      -0.347861        -9.4658
 112   1.0000      -0.347737        -9.4624
 113   1.0000      -0.343994        -9.3606
 114   1.0000      -0.315123        -8.5749
 115   1.0000      -0.315044        -8.5728
 116   1.0000      -0.311767        -8.4836
 117   1.0000      -0.308297        -8.3892
 118   1.0000      -0.299783        -8.1575
 119   1.0000      -0.291346        -7.9279
 120   1.0000      -0.283695        -7.7197
 121   1.0000      -0.277069        -7.5394
 122   1.0000      -0.275453        -7.4955
 123   1.0000      -0.273480        -7.4418
 124   1.0000      -0.263708        -7.1759
 125   1.0000      -0.260849        -7.0981
 126   1.0000      -0.249959        -6.8017
 127   1.0000      -0.248284        -6.7561
 128   1.0000      -0.246683        -6.7126
 129   1.0000      -0.246208        -6.6997
 130   1.0000      -0.242938        -6.6107
 131   1.0000      -0.234735        -6.3875
 132   1.0000      -0.231420        -6.2973
 133   1.0000      -0.212227        -5.7750
 134   1.0000      -0.208657        -5.6778
 135   0.0000      -0.159478        -4.3396
 136   0.0000      -0.061495        -1.6734
 137   0.0000      -0.061018        -1.6604
 138   0.0000      -0.042599        -1.1592
 139   0.0000      -0.042459        -1.1554
 140   0.0000      -0.020096        -0.5468
 141   0.0000      -0.019835        -0.5397
 142   0.0000      -0.017256        -0.4696
 143   0.0000      -0.014096        -0.3836
 144   0.0000      -0.011827        -0.3218
 145   0.0000      -0.002521        -0.0686
 146   0.0000      -0.001137        -0.0309
 147   0.0000       0.006634         0.1805
 148   0.0000       0.010575         0.2877
 149   0.0000       0.012953         0.3525
 150   0.0000       0.017024         0.4633
 151   0.0000       0.020252         0.5511
 152   0.0000       0.024040         0.6542
 153   0.0000       0.025962         0.7065
 154   0.0000       0.027878         0.7586

-------------------------
TD-DFT/TDA EXCITED STATES
-------------------------

STATE 14:  E=   0.114270 au      3.109 eV    25079.5 cm**-1
   120b -> 135b  :     0.392771 (c= -0.62671440)
   121b -> 135b  :     0.558133 (c=  0.74708299)
   122b -> 135b  :     0.035472 (c= -0.18833986)

STATE 19:  E=   0.134496 au      3.660 eV    29518.4 cm**-1
   119b -> 135b  :     0.922155 (c=  0.96028915)
```

```
   123b -> 135b  :     0.055677 (c= -0.23595997)

STATE 26:  E=   0.155595 au      4.234 eV    34149.1 cm**-1
   116b -> 135b  :     0.918642 (c= -0.95845806)
   117b -> 135b  :     0.017616 (c=  0.13272559)

STATE 50:  E=   0.178052 au      4.845 eV    39077.8 cm**-1
   127a -> 138a  :     0.017682 (c= -0.13297196)
   129a -> 138a  :     0.023759 (c= -0.15414002)
   130a -> 138a  :     0.018124 (c=  0.13462649)
   130a -> 139a  :     0.043359 (c=  0.20822716)
   133a -> 138a  :     0.083411 (c= -0.28880878)
   133a -> 139a  :     0.230431 (c= -0.48003250)
   134a -> 137a  :     0.082451 (c= -0.28714289)
   135a -> 136a  :     0.064275 (c=  0.25352460)
   129b -> 139b  :     0.020665 (c= -0.14375168)
   130b -> 136b  :     0.061849 (c=  0.24869543)
   130b -> 138b  :     0.041171 (c= -0.20290736)
   133b -> 137b  :     0.081796 (c=  0.28599960)
   134b -> 136b  :     0.060113 (c= -0.24517986)
```

Listing S9. The TDDFT calculated wavenumbers (cm^{-1}) and intensities of the UV/Vis absorptions of the DFT optimized complex **1** with coordinated DMF molecules instead of water ones.

```
  9321.10   0.695302914299
 10291.30 161.821813817922
 13990.00   0.028638734593
 13261.90  37.983152314695
 16626.30   0.051636506312
 17960.90   0.077183559330
 17791.30 345.932156753187
 17490.70   0.575107013052
 17662.60  53.887738659036
 21970.60   0.031730416169
 20975.70  70.693523062591
 22916.70   0.184090653805
 23748.90   0.066389793830
 25079.50   1.396789191748
 25819.50 4228.331960508796
 28908.70  23.976261817344
 28928.80   0.495048732257
 29344.00  15.030454058918
 29518.40 6345.447106665972
 30952.90 124.100695076749
 24525.40  55.565762394089
 24594.00  66.298616343122
 24664.10  34.723435133673
 24705.60  44.228728777191
 32582.00   1.144627303256
 34149.10 14345.179149409360
 33479.60 188.800478125170
 33604.70  19.512958423023
 35748.90   0.368940667997
 34898.90   0.412658130274
 34544.40   3.301102322110
```

```
35569.70   2.777197895149
35582.40   0.096384529114
34162.20 291.076667521024
34327.30  23.325544205764
36386.80  15.733133616975
36473.00   0.256935010924
35958.60   0.364492985731
35406.20 132.443191007751
35623.50  12.060866785735
36299.00  18.316369173289
36334.10  20.162211553856
36484.70   0.338186572326
33678.50   0.165377844270
33664.70   1.235533589578
37021.40   0.235998360255
37049.20   3.388428766608
38427.10   0.594362222863
38432.60 417.453870797791
39077.80 6822.113296915992
```