Supporting Information

The important role of the hydroxyl group on the conformational adaptability in bis(L-threoninato)copper(II) compared to bis(L-*allo*-threoninato)copper(II): Quantum Chemical study

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Assignment of chair / boat / twisted boat / envelope / other twist conformations in the Oo coordination mode

The procedure for the assignment of the chelate-ring conformations in the Oo coordination mode has been as follows:

1. Definition of the torsion angles (atom numbering is defined in Figure 5):

tau1 = Cu–O9–C7–C5 = Cu–O_h–C^{β}–C^{α}
tau2 = O9–C7–C5–C15 = O_h–C^{β}–C^{α}–C′
tau3 = O9–Cu–O17–C5 = O_h–Cu–O–C^{α}
tau4 = O9–Cu–O17–C15 = O_h–Cu–O–C′
tau5 = Cu–O17–C15–C5 = Cu–O–C′–C^{α}
tau6 = O17–C15–C7–O9 = O–C′–C^{β}–O_h
tau7 = C7–C5–C15–O17 = C^{β}–C^{α}–C′–O
tau8 = O17–Cu–O9–C7 = O–Cu–O_h–C^{β}
tau9 = Cu–O9–C5–C15 = Cu–O_h–C^{α}–C′
tau0 = H10–O9–Cu–O17= H_h–O_h–Cu–O

2. The applicable criterions used for the assignment chair / boat / twisted boat / envelope / other twist forms:

chair 1 (ch 1):

$|tau1+tau2+tau5+tau7| < 15°$ and
$\min(tau1, tau2, tau5, tau7) \geq 45°$ and
$\max(tau1, tau2, tau5, tau7) \leq 90°$ and $tau1 > 0$

chair 2 (ch2):

$|tau1+tau2+tau5+tau7| < 15°$ and
$\min(tau1, tau2, tau5, tau7) \geq 45°$ and
$\max(tau1, tau2, tau5, tau7) \leq 90°$ and $tau1 \leq 0$

boat 1 (bt1):

$|tau1| \leq 20°$ and
$|tau5| \leq 20°$ and
$|tau6| \leq 10°$ and $tau2 < 0$

boat 2 (bt2):

$|tau1| \leq 20°$ and
$|tau5| \leq 20°$ and
$|tau6| \leq 10°$ and $tau2 \geq 0$

boat 3 (bt3):

$|tau8| \leq 22$ ° and
$|tau7| \leq 22$ ° and
$|tau9| \leq 20$ ° and $tau1 < 0$

boat 4 (bt4):

$|tau8| \leq 22$ ° and
$|tau7| \leq 22$ ° and
$|tau9| \leq 20$ ° and $tau1 \geq 0$

twisted boat 1 (tb1):

$|tau1| \leq 29$ ° and
$|tau5| \leq 29$ ° and
$|tau6| \leq 40$ ° and $tau2 < 0$

twisted boat 2 (tb2):

$|tau1| \leq 29$ ° and
$|tau5| \leq 29$ ° and
$|tau6| \leq 40$ ° and $tau2 \geq 0$

envelope 4 down (e4d): $|tau4| \leq 40$ ° and $|tau8| \leq 40$ ° and $|tau6| \leq 20$ ° and $tau2 > 0$

envelope 4 up (e4u): $|tau4| \leq 40$ ° and $|tau8| \leq 40$ ° and $|tau6| \leq 20$ ° and $tau2 \leq 0$

envelope 3 up (e3u): $|tau5| \leq 33$ ° and $|tau4| \leq 33$ ° and $|tau9| \leq 20$ ° and $tau1 > 0$

envelope 3 down (e3d): $|tau5| \leq 33$ ° and $|tau4| \leq 33$ ° and $|tau9| \leq 20$ ° and $tau1 \leq 0$

twist 1 (tw1): $|tau8-tau4| \leq 22$ ° and $tau8*tau4 > 0$ ° and $|tau3| \leq 15$ °

twist2 (tw2): $|tau8-tau5| \leq 22$ ° and $tau8*tau5 > 0$ ° and $|tau4| \leq 15$ °

3. For all of the above, the sign minus (m) was used to define the value $tau0 > 0$, whereas the sign plus (p) defined the values with $tau0 \leq 0$.

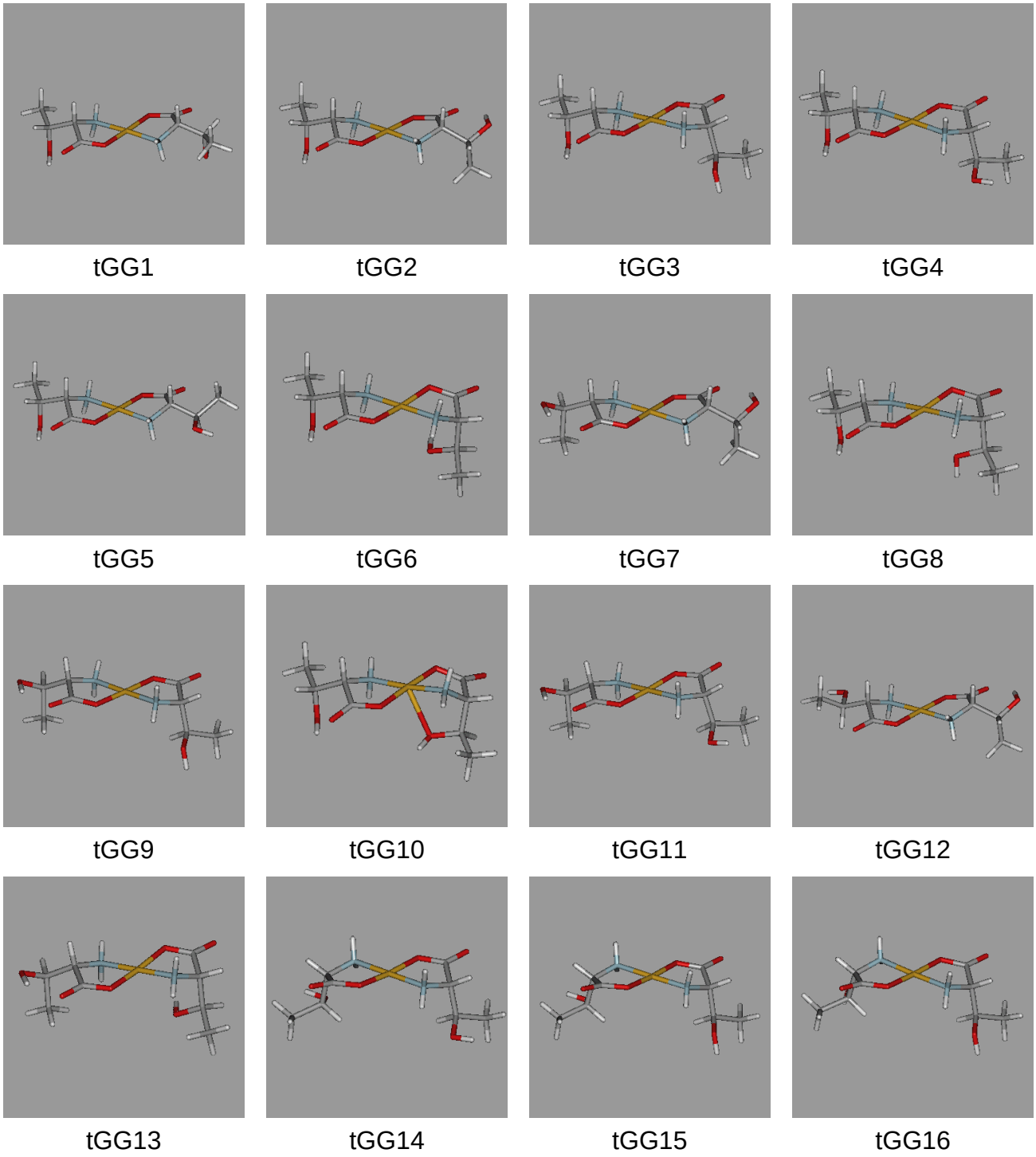
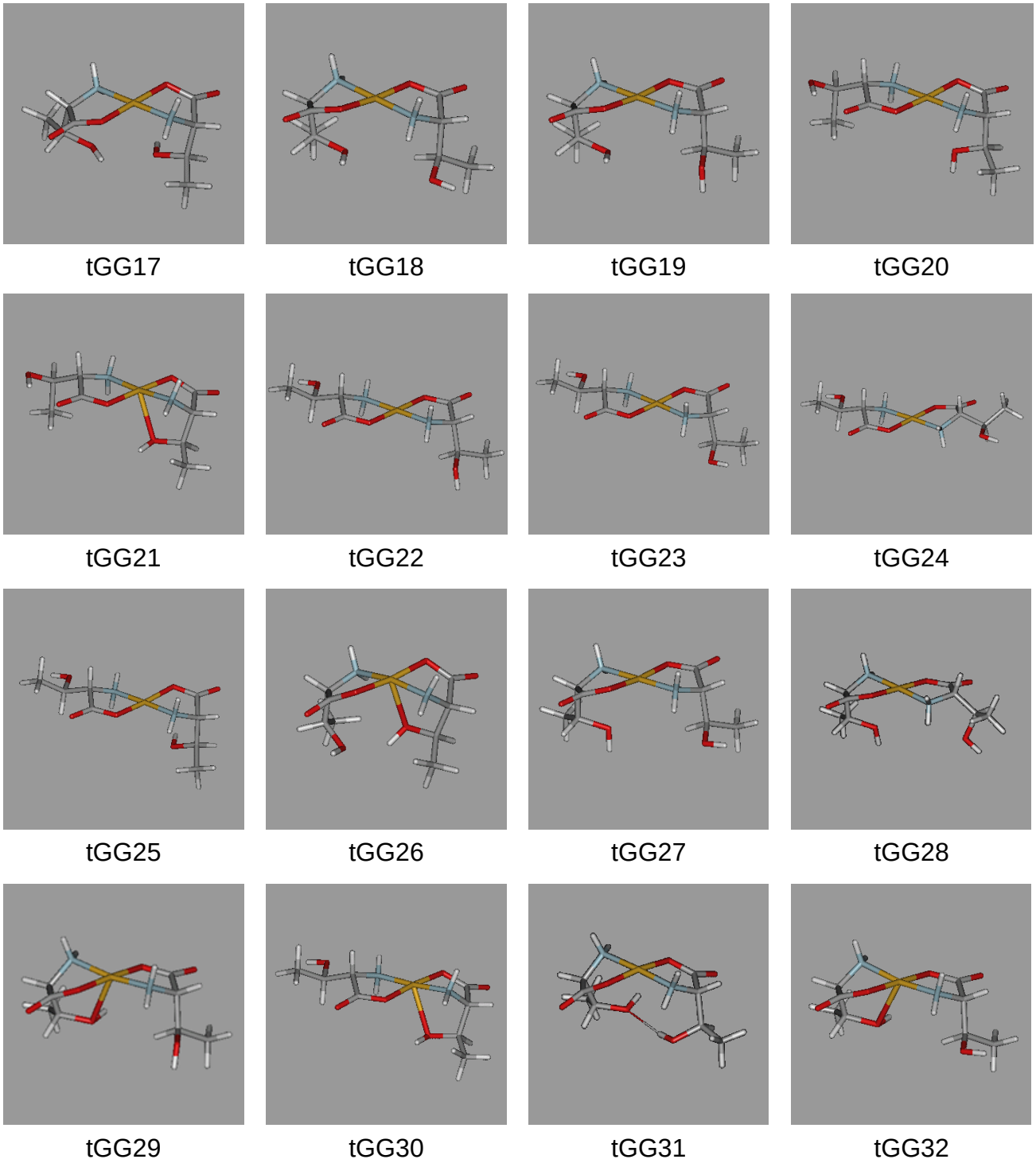


Figure S1. Illustrations and names of 196 Cu(L-Thr)$_2$ and 267 Cu(L-*a*Thr)$_2$ conformers computed using B3LYP/BS0 in the gas phase.



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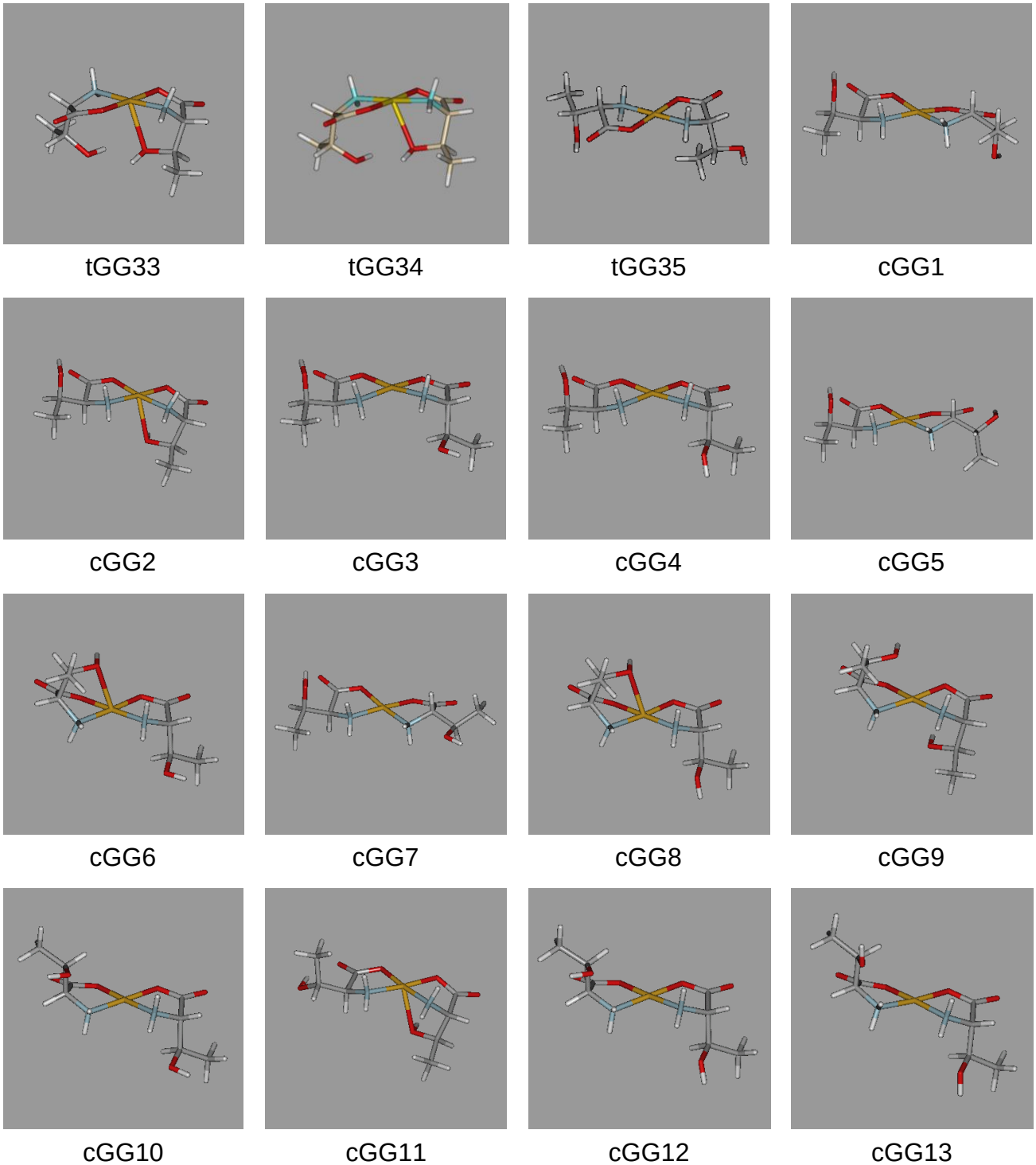

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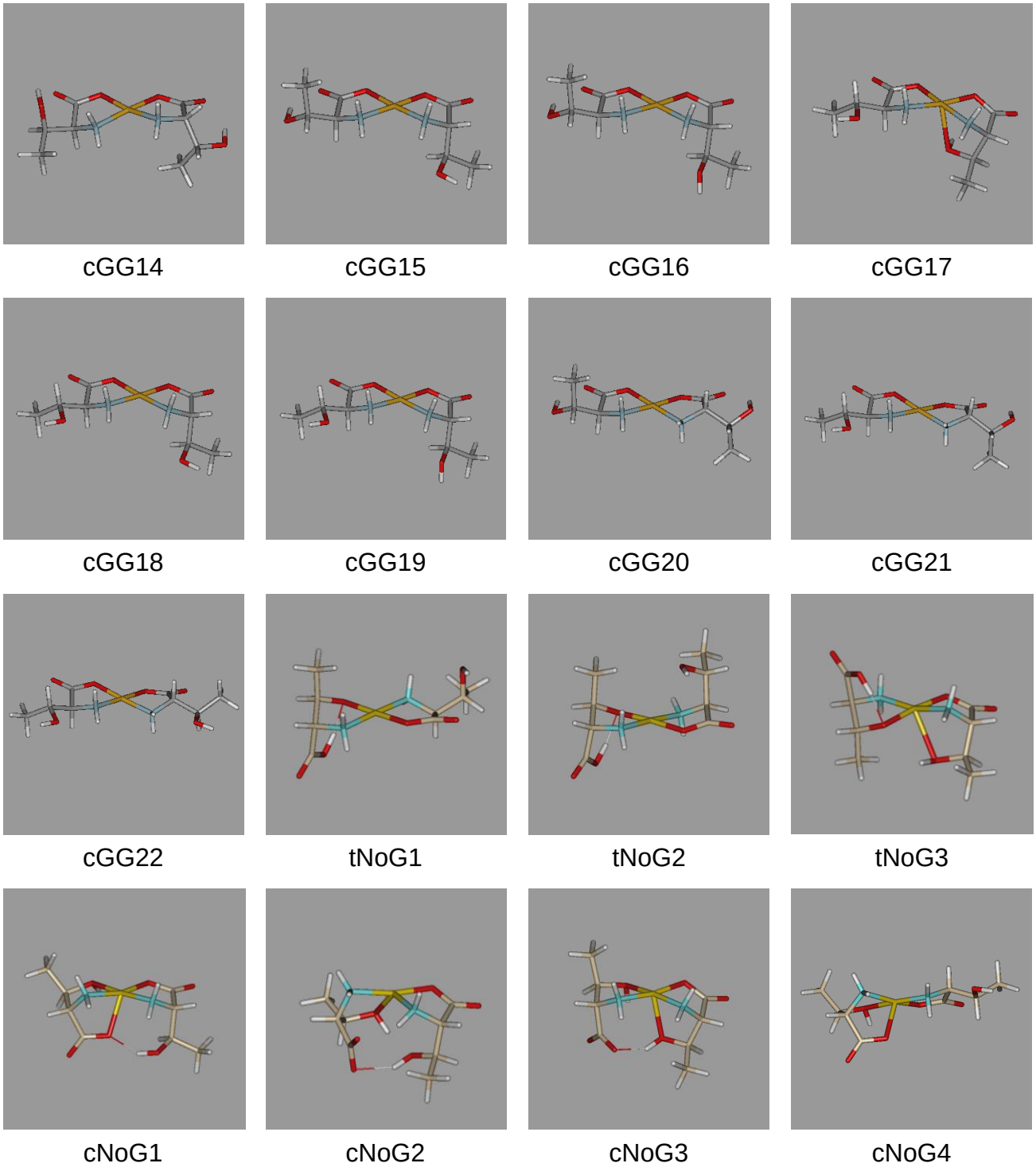

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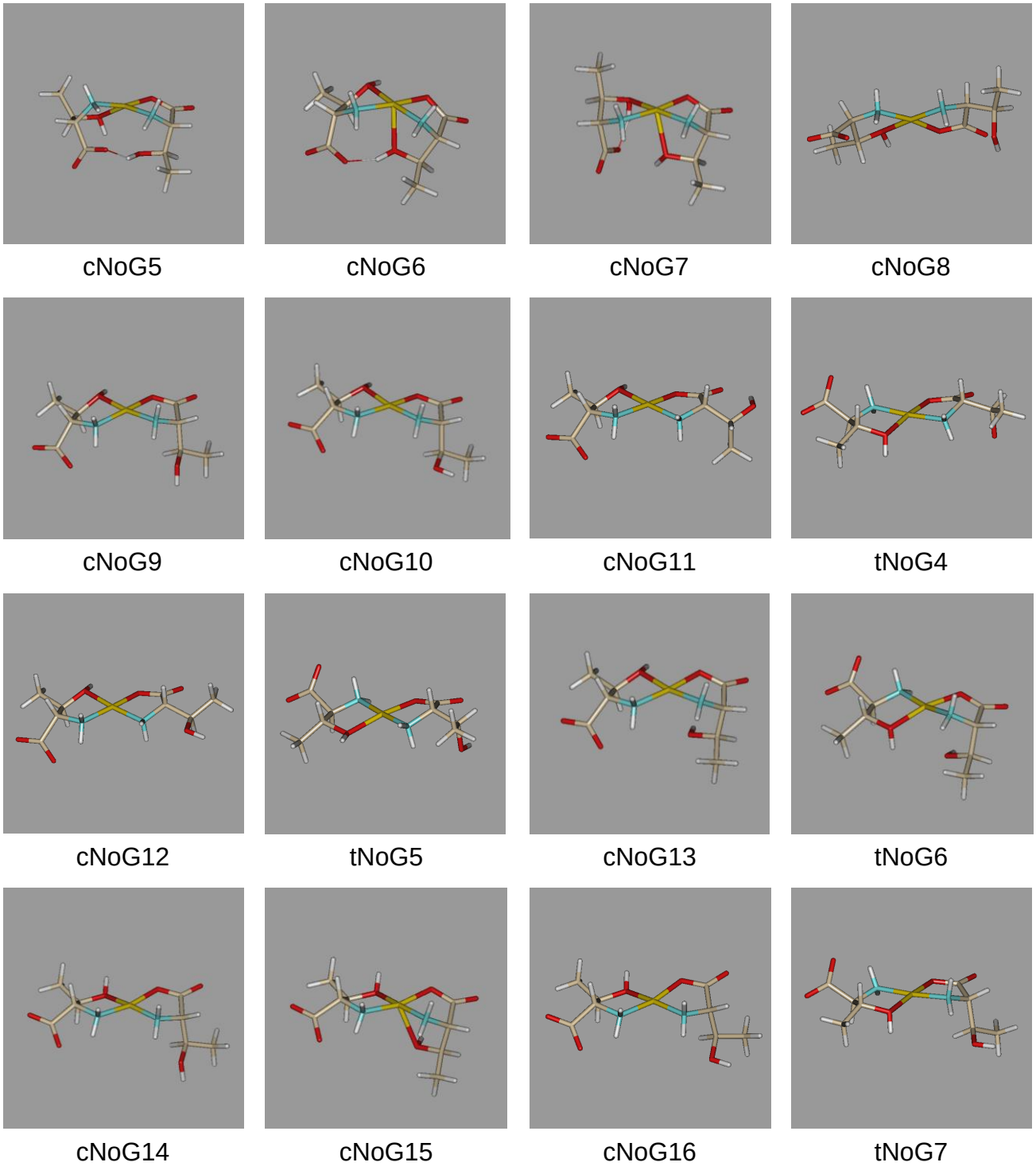

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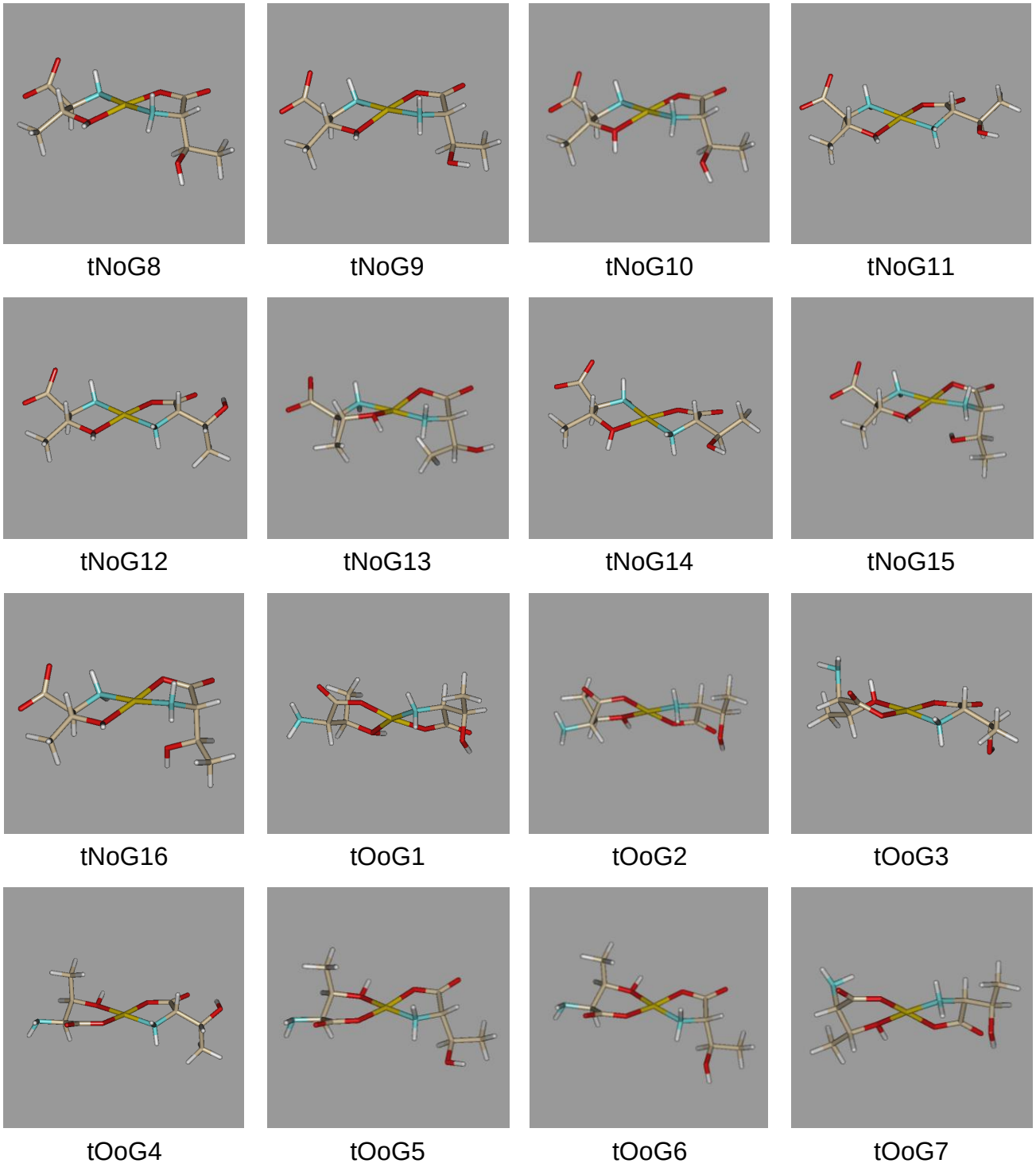

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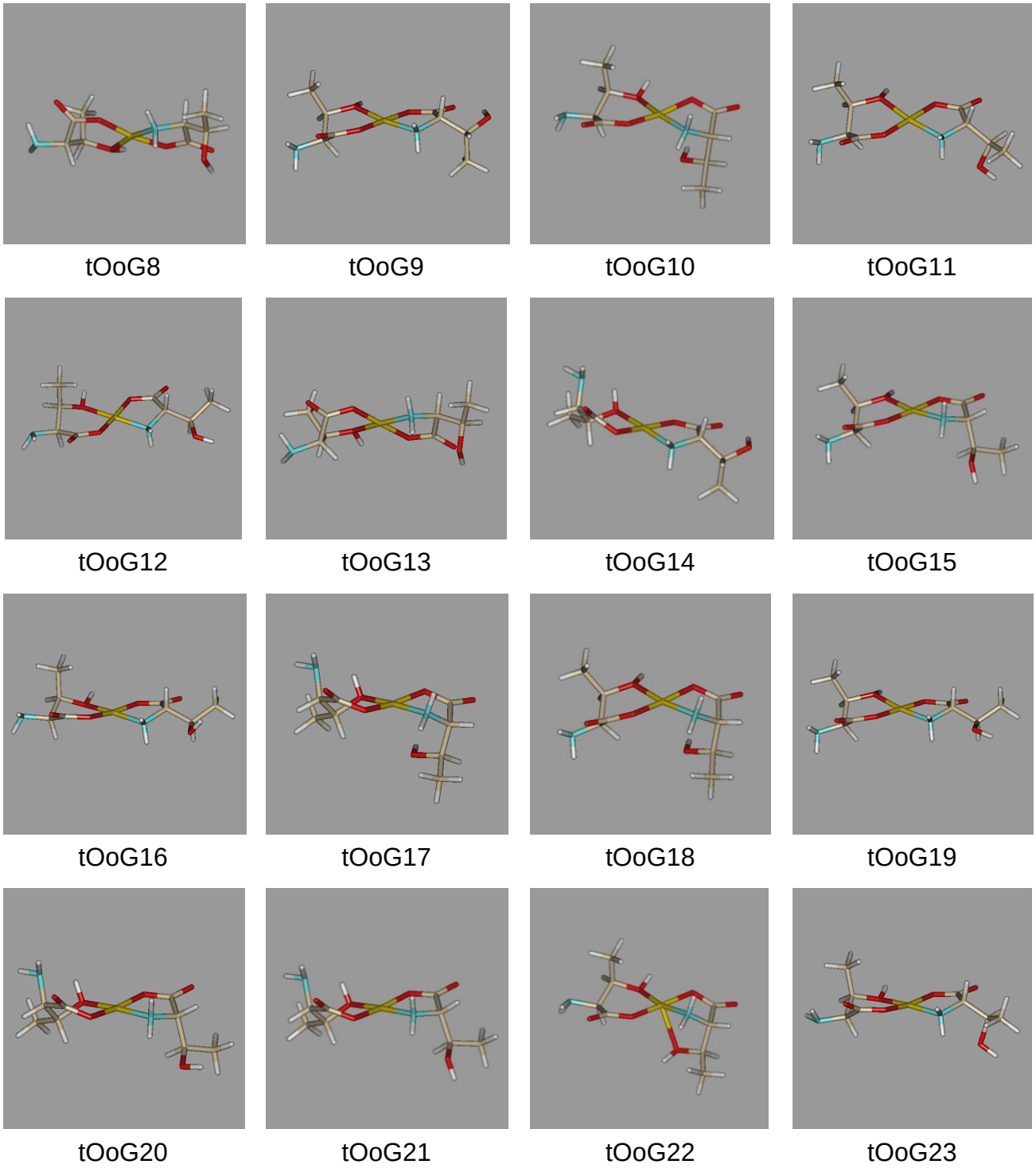

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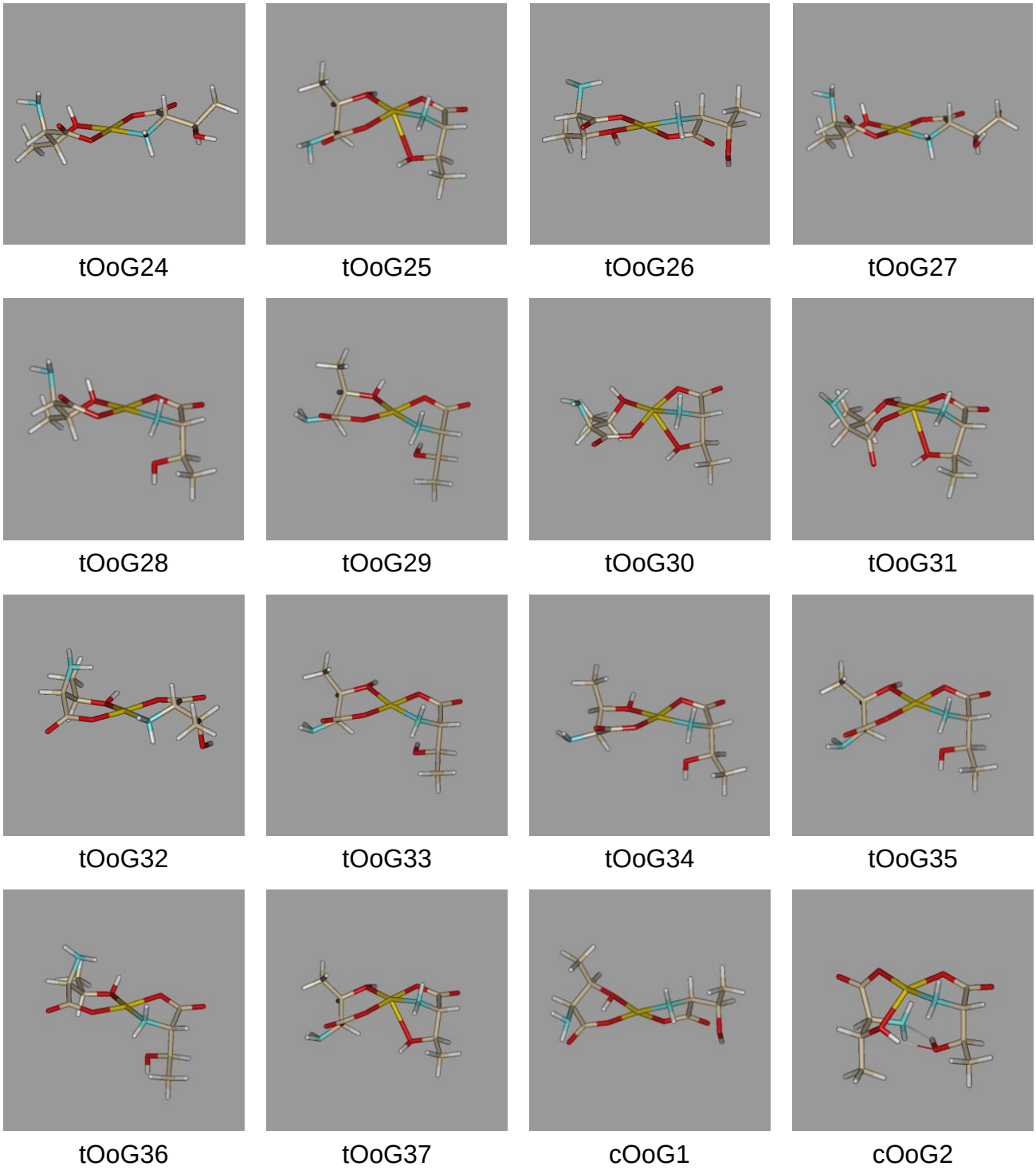

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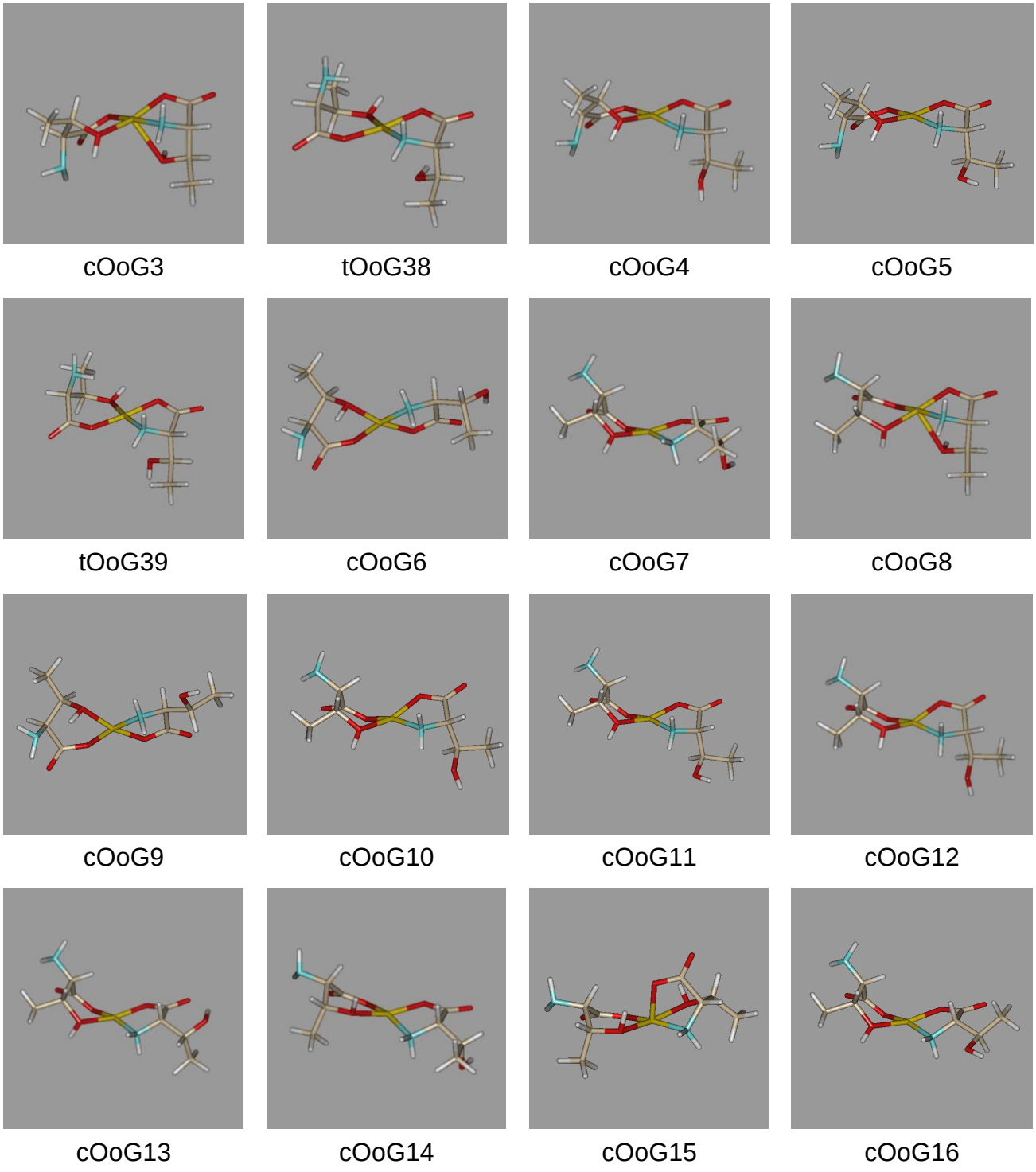

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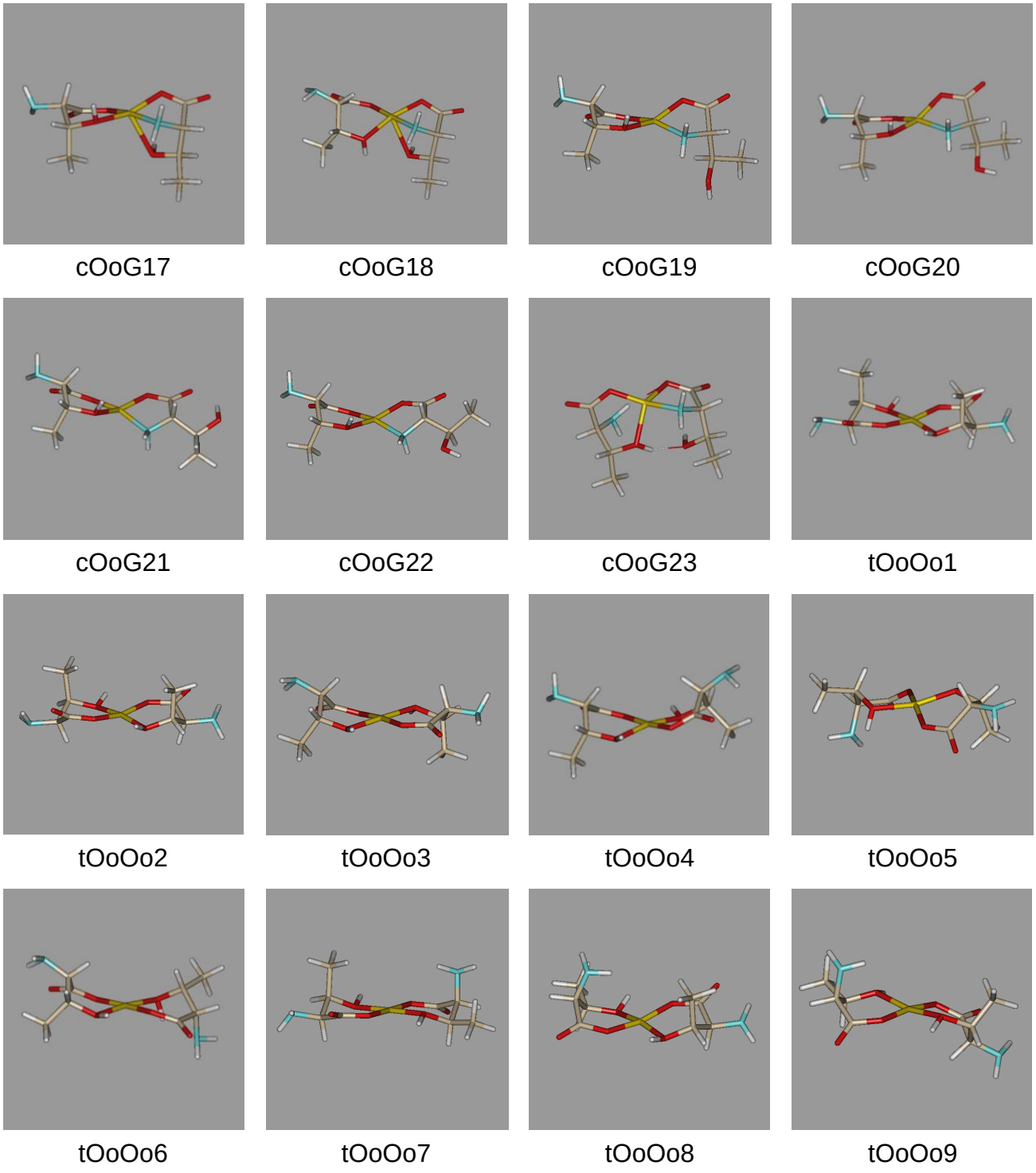

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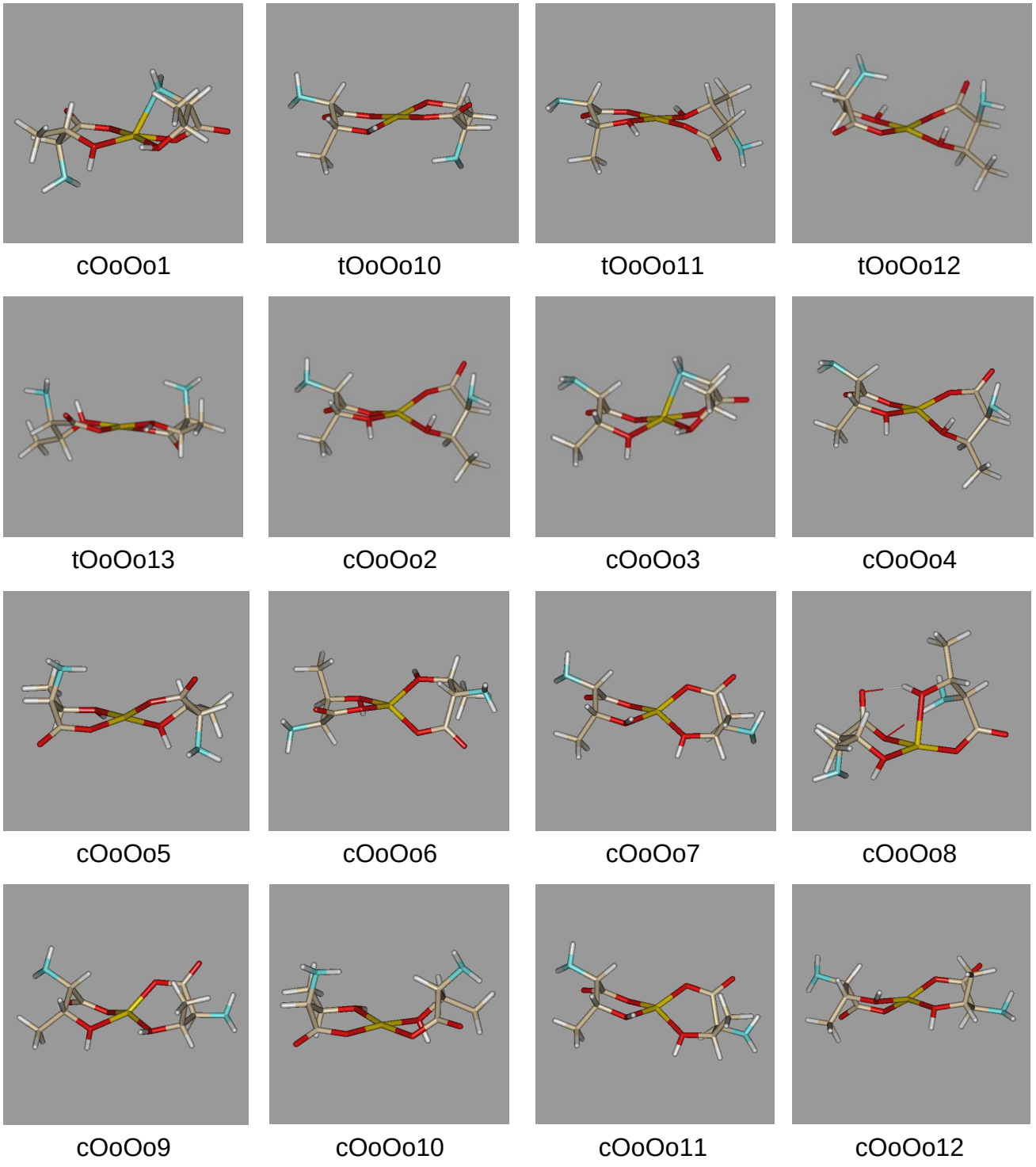

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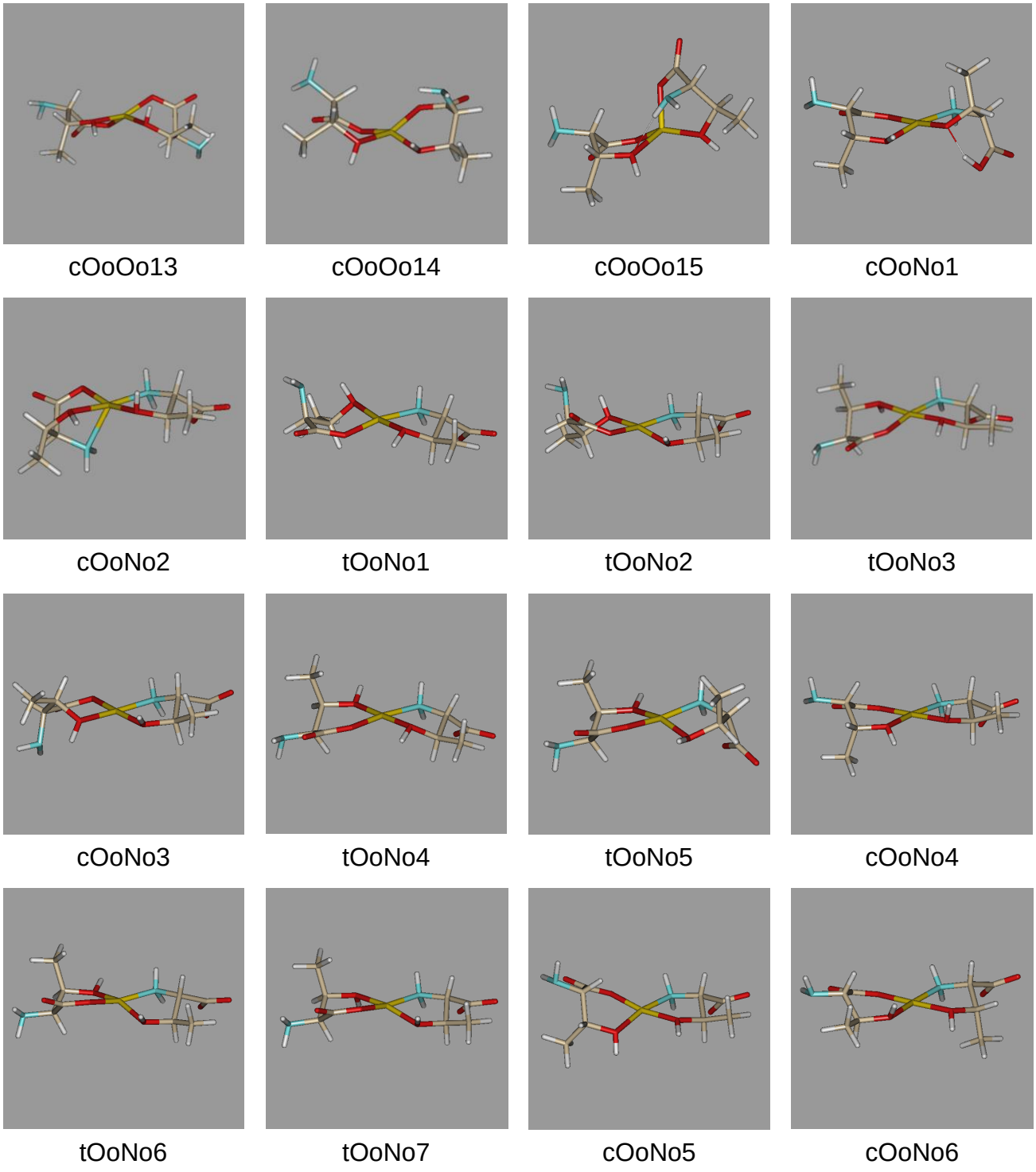

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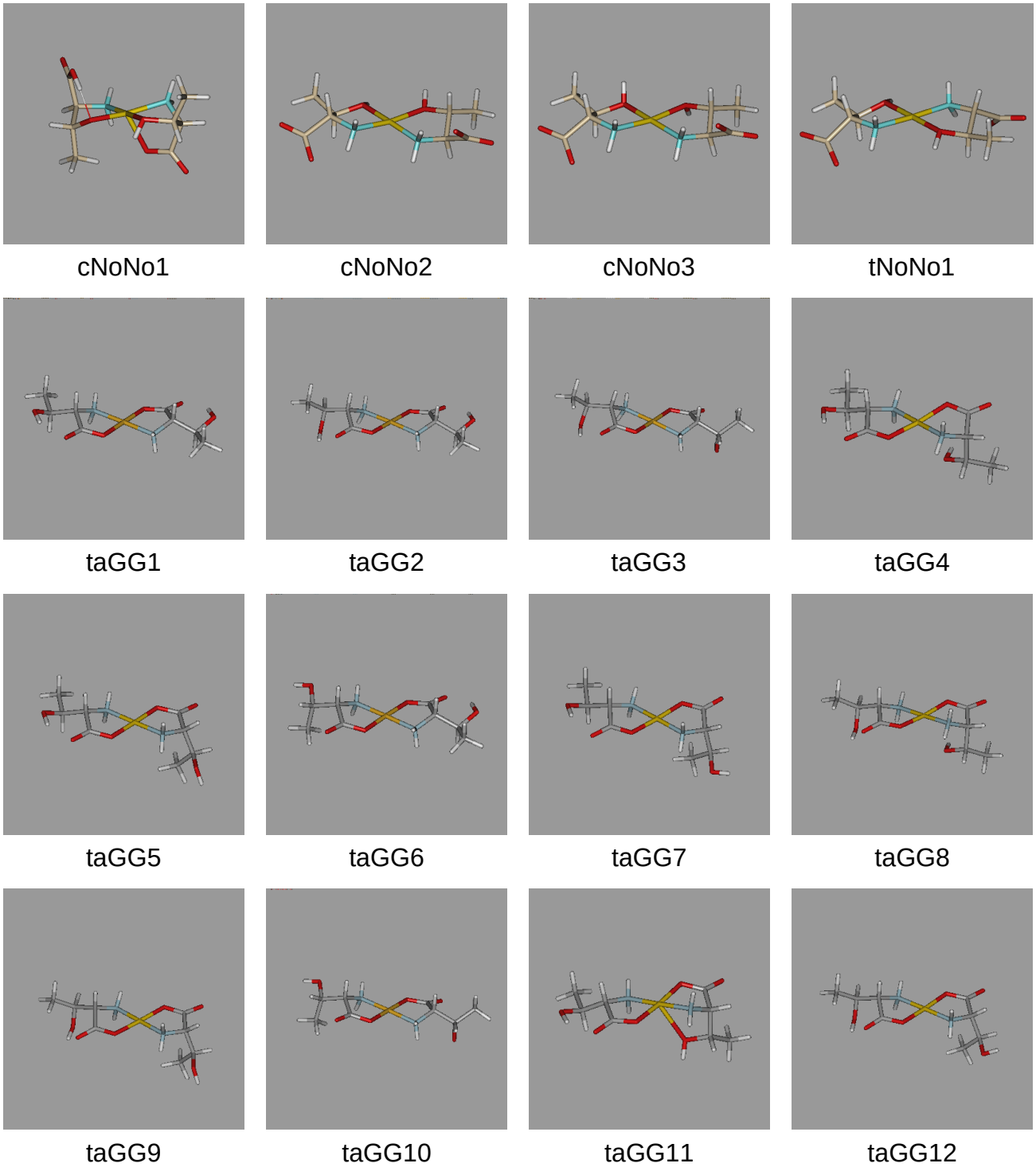

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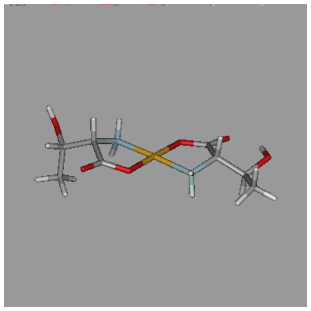
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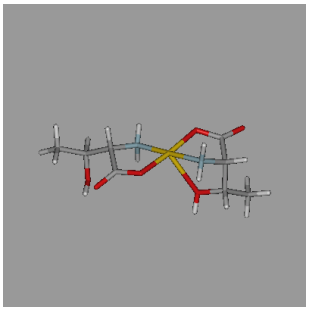
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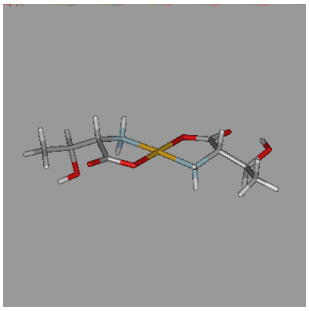
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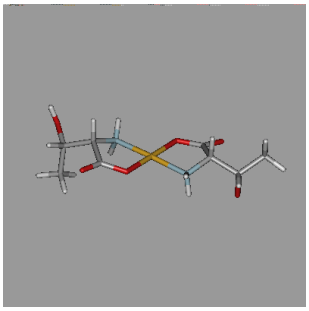
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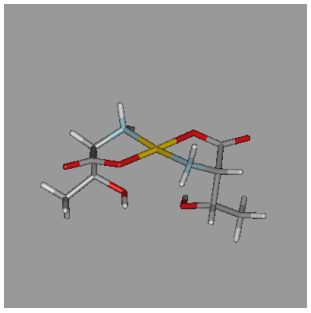
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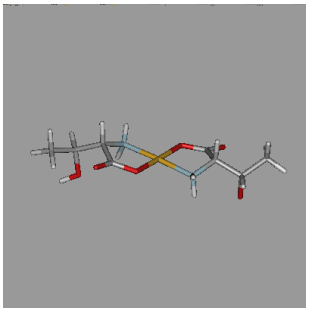
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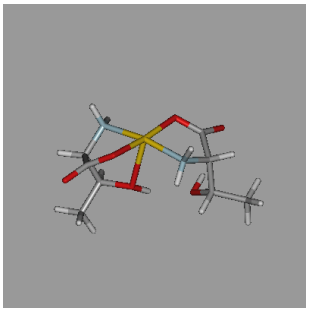
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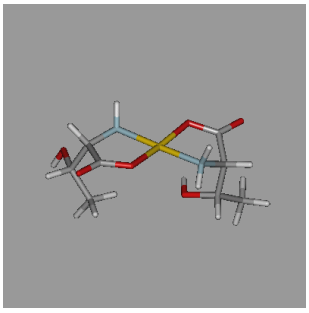
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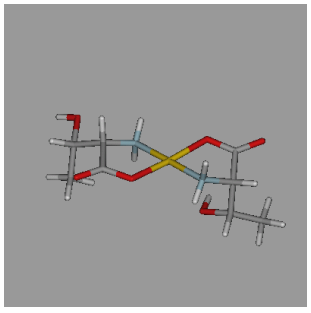
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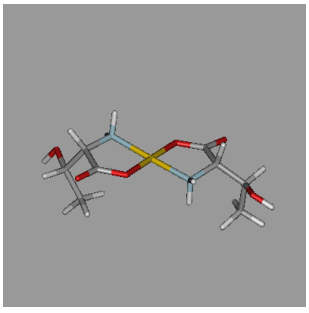
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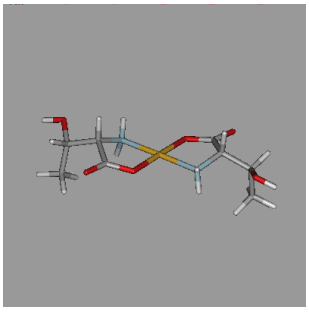
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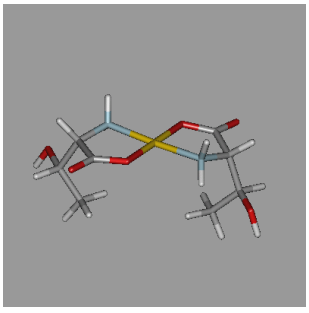
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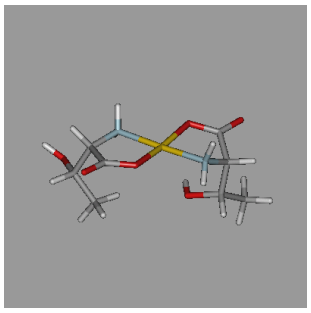
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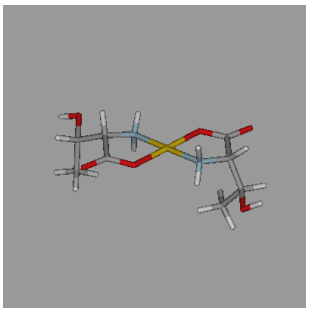
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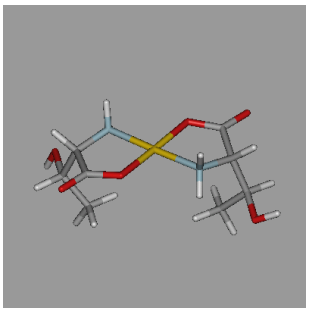
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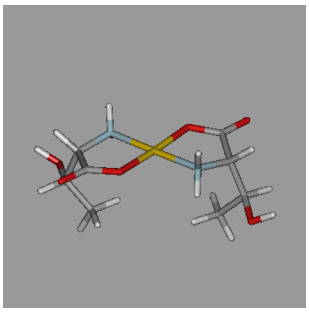
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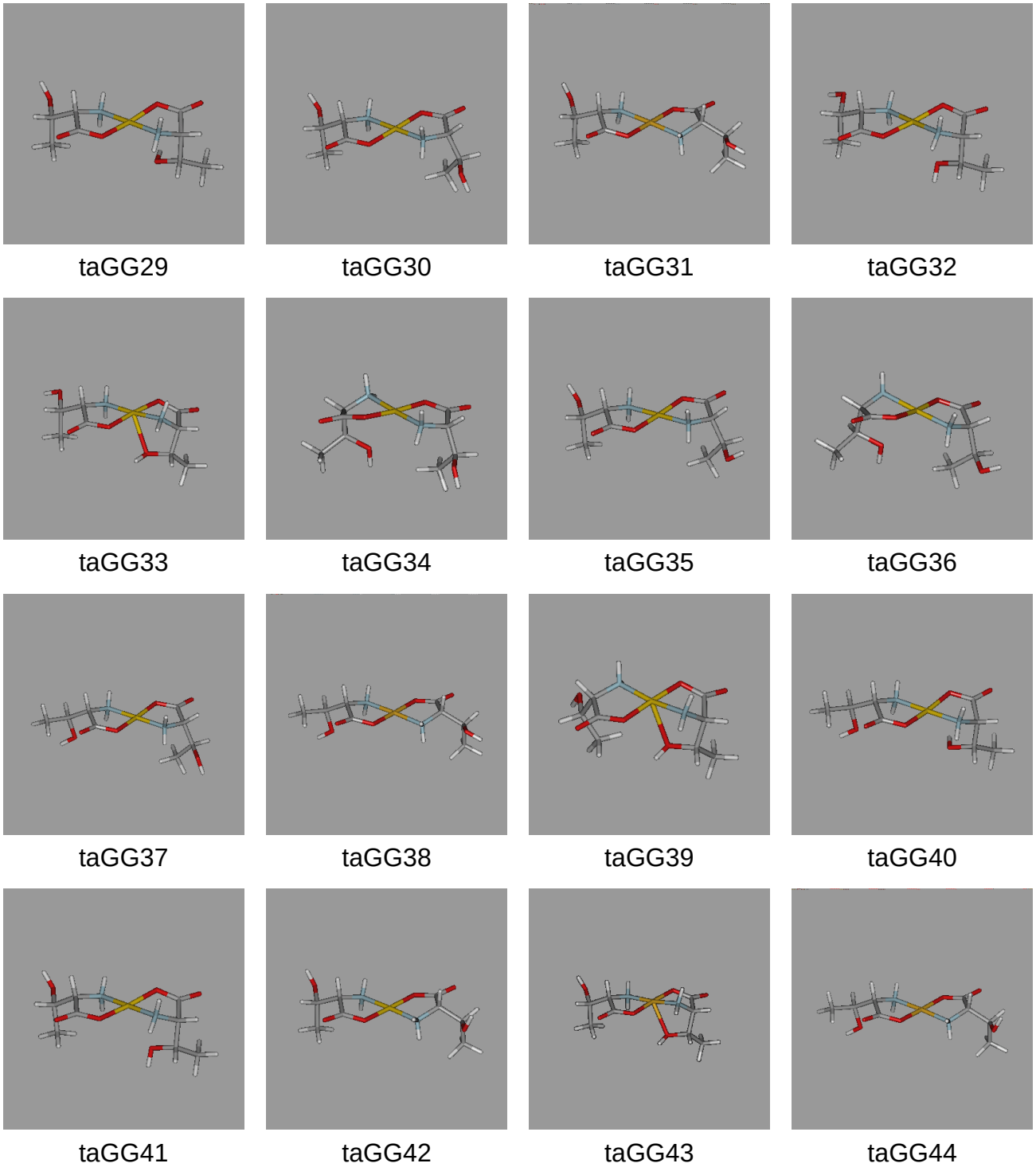

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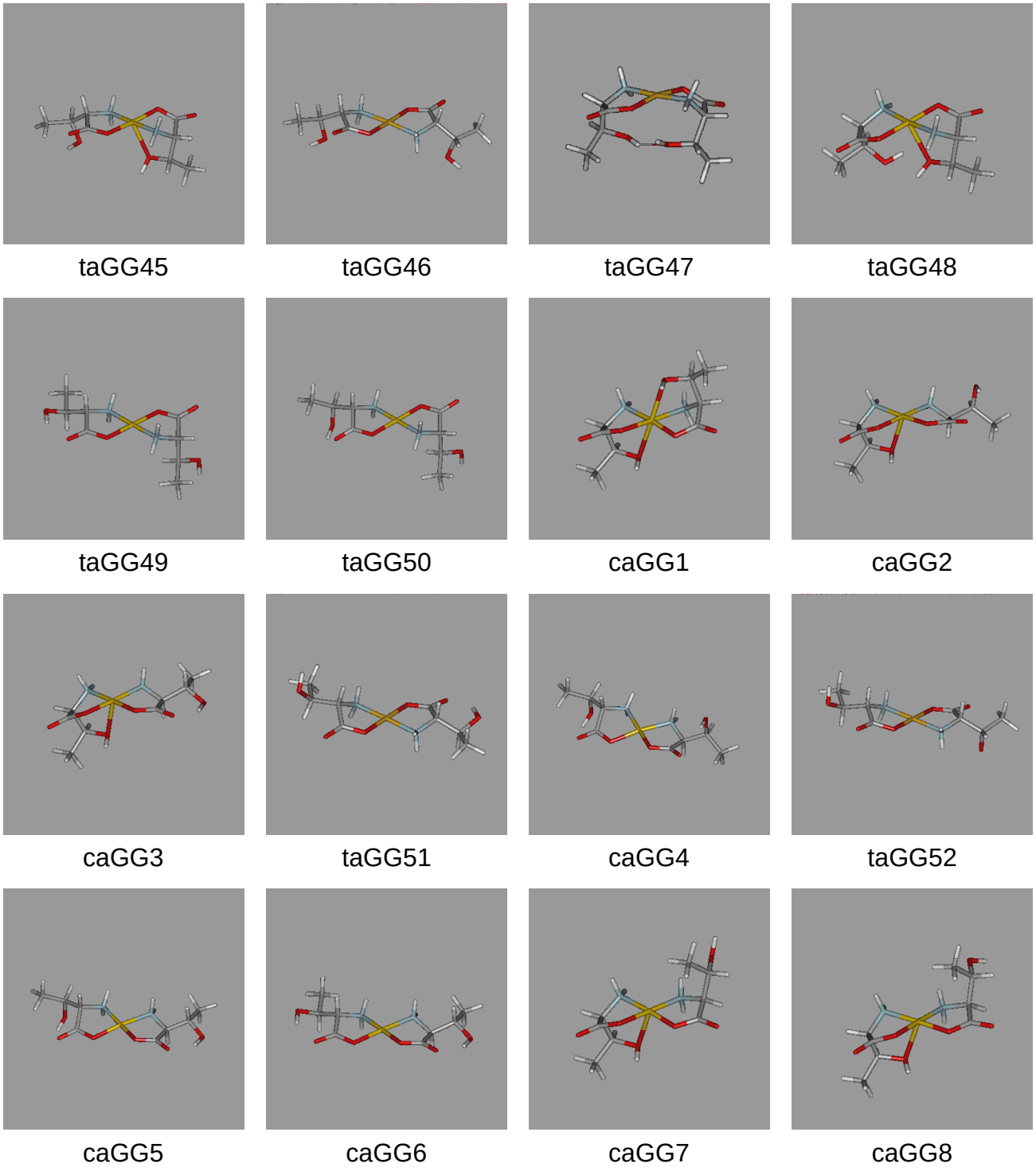

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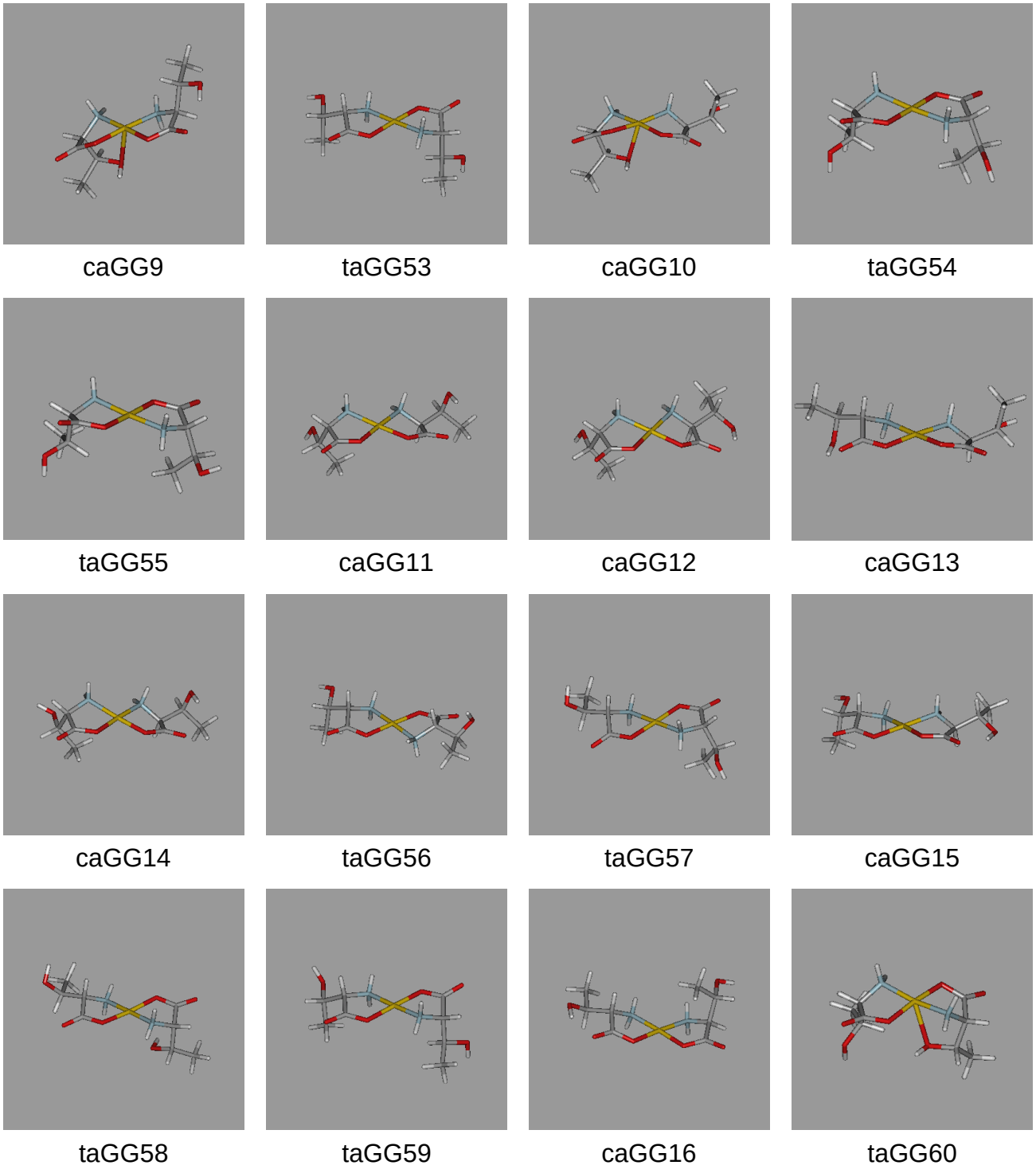

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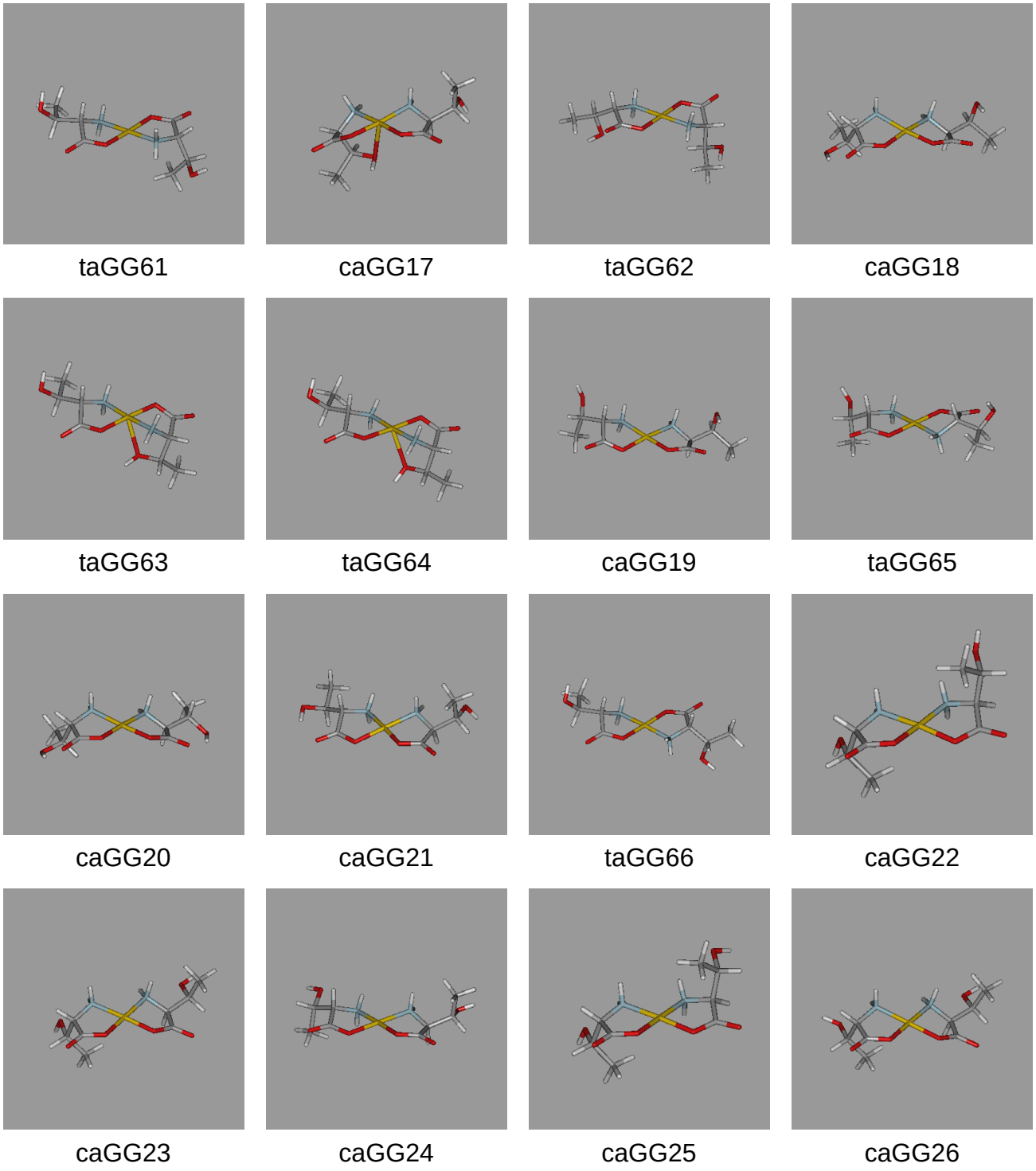

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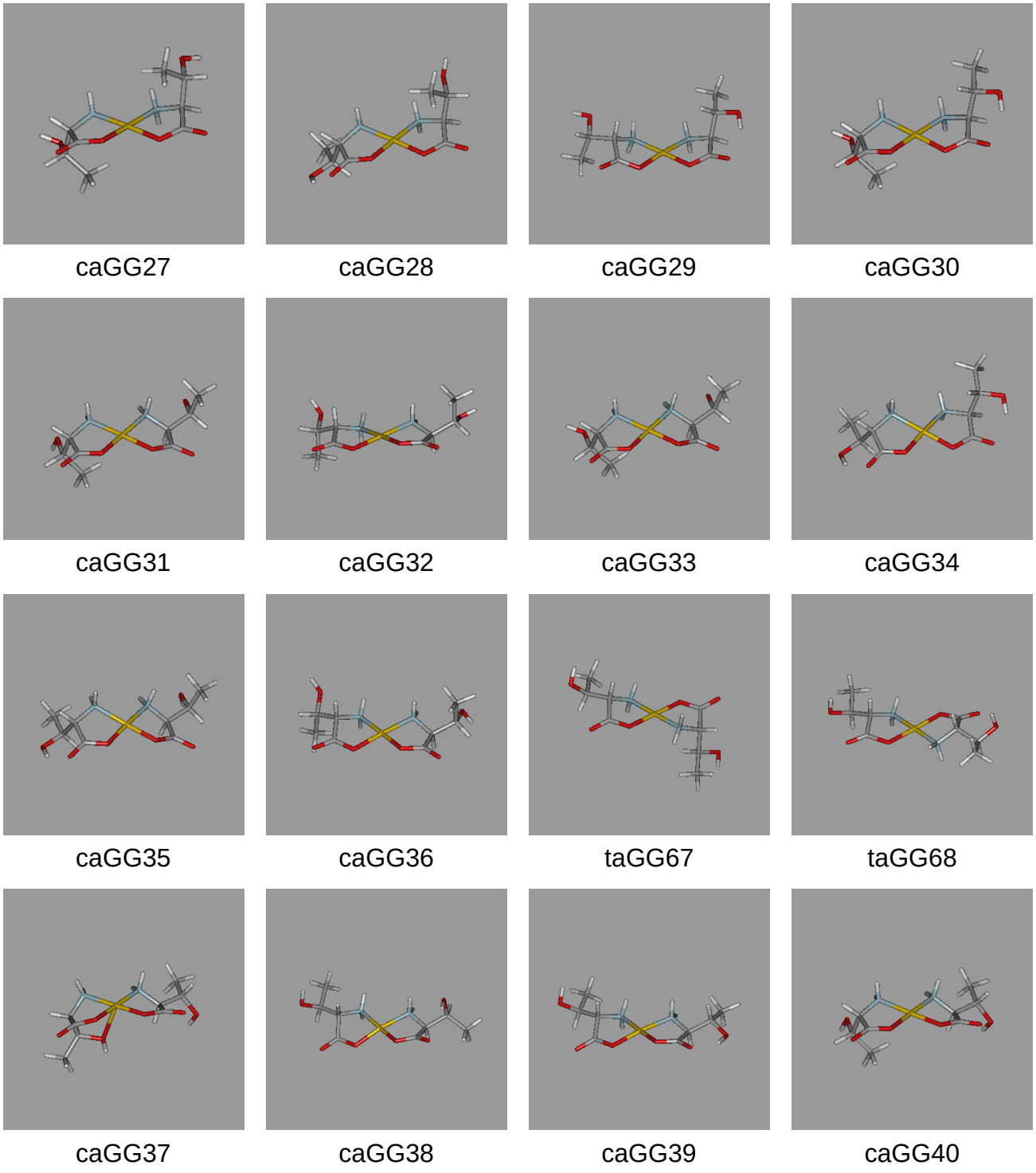

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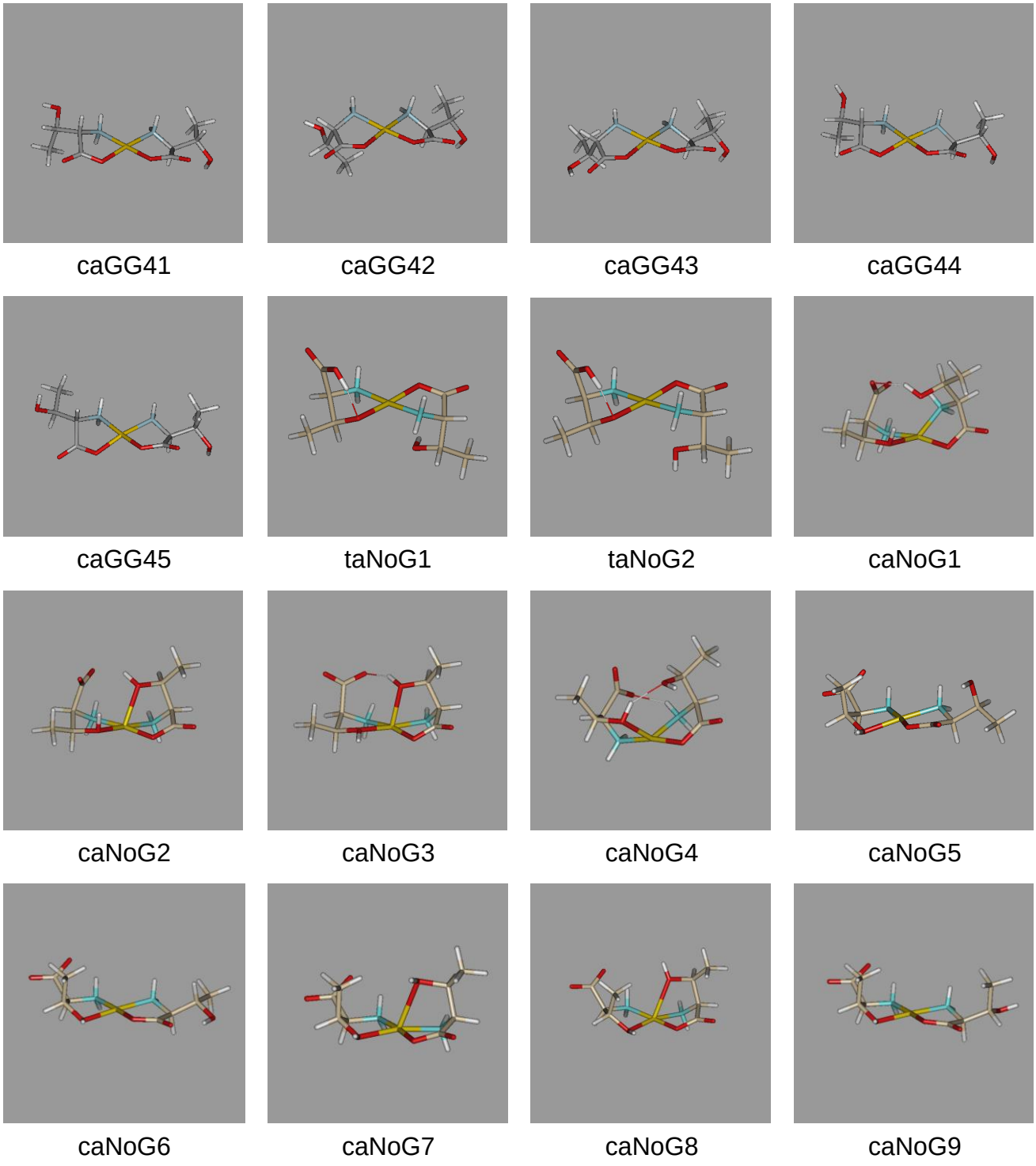

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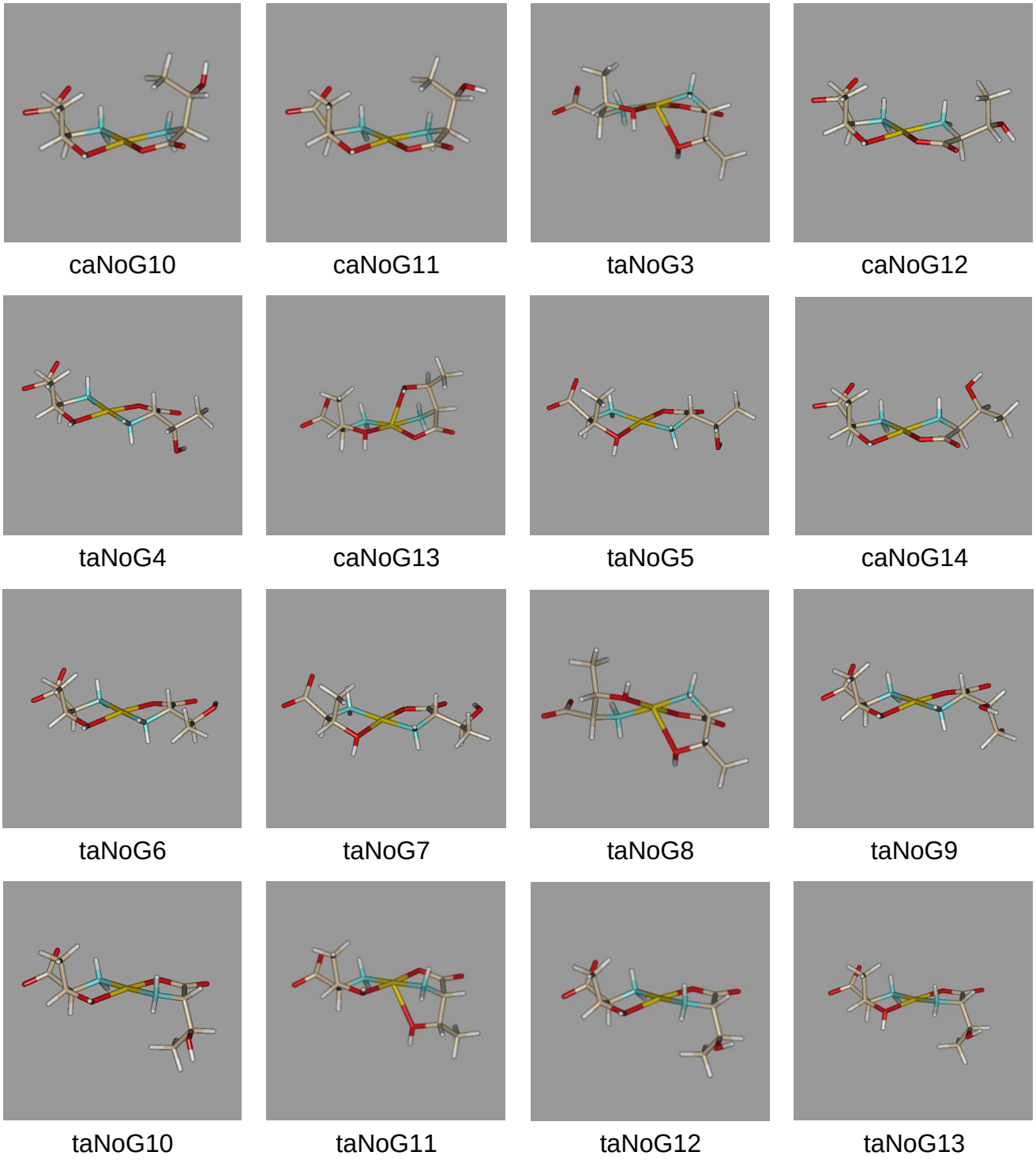

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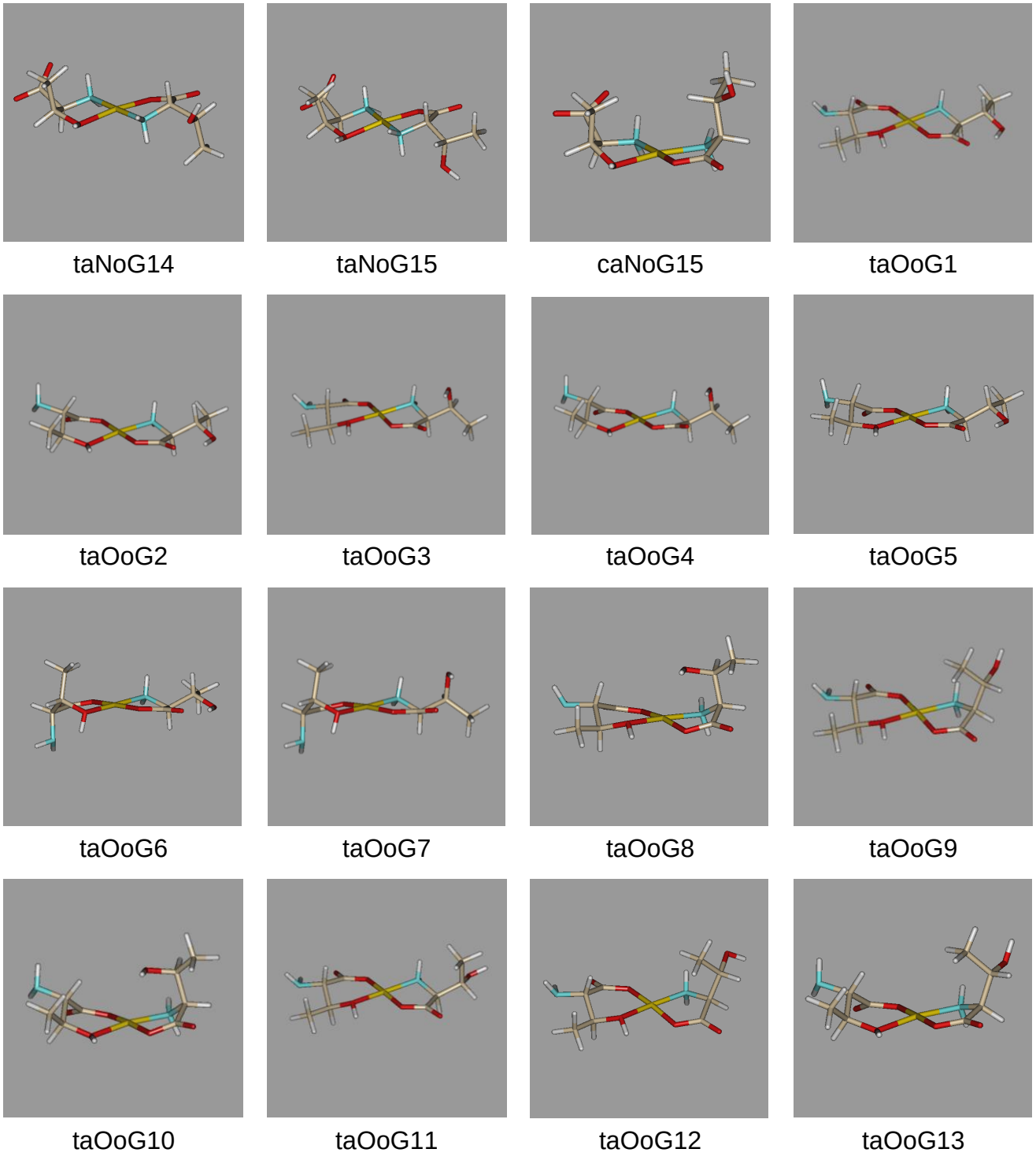

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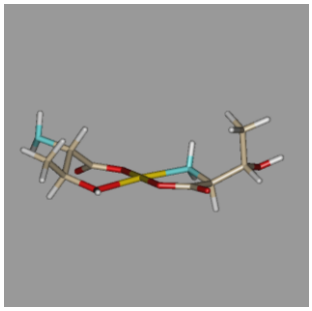

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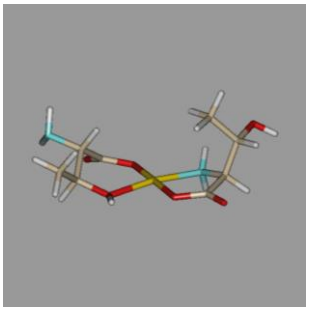

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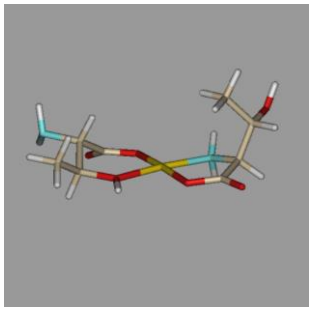

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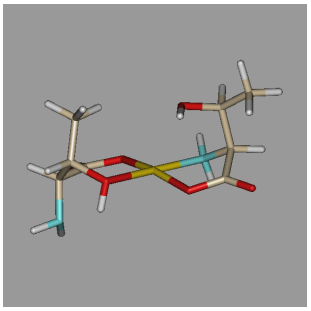

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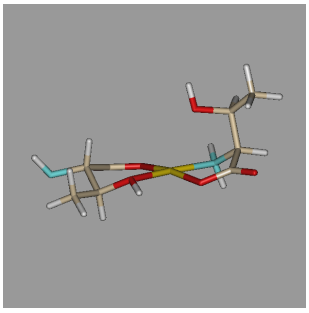

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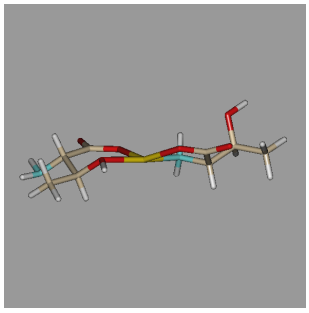

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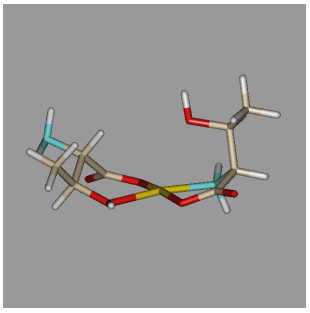

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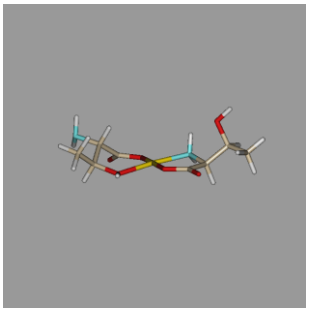

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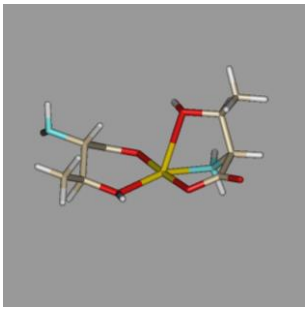

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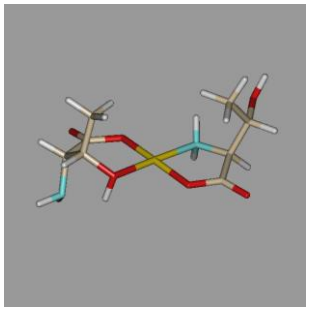

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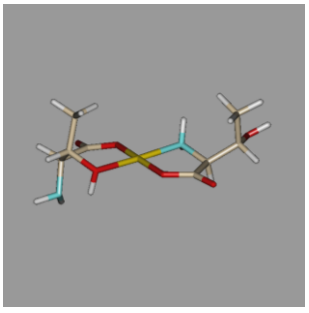

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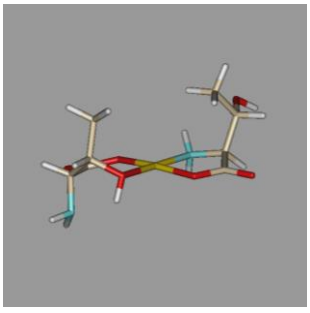
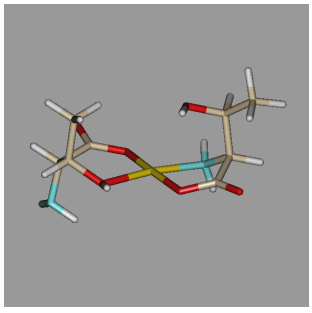


taOoG25



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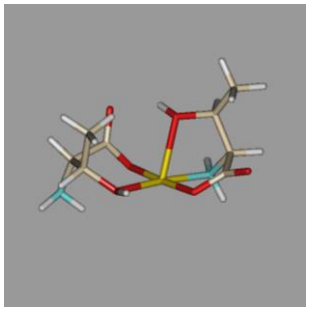
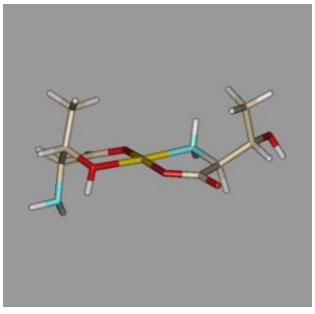


taOoG27

taOoG28



taOoG29

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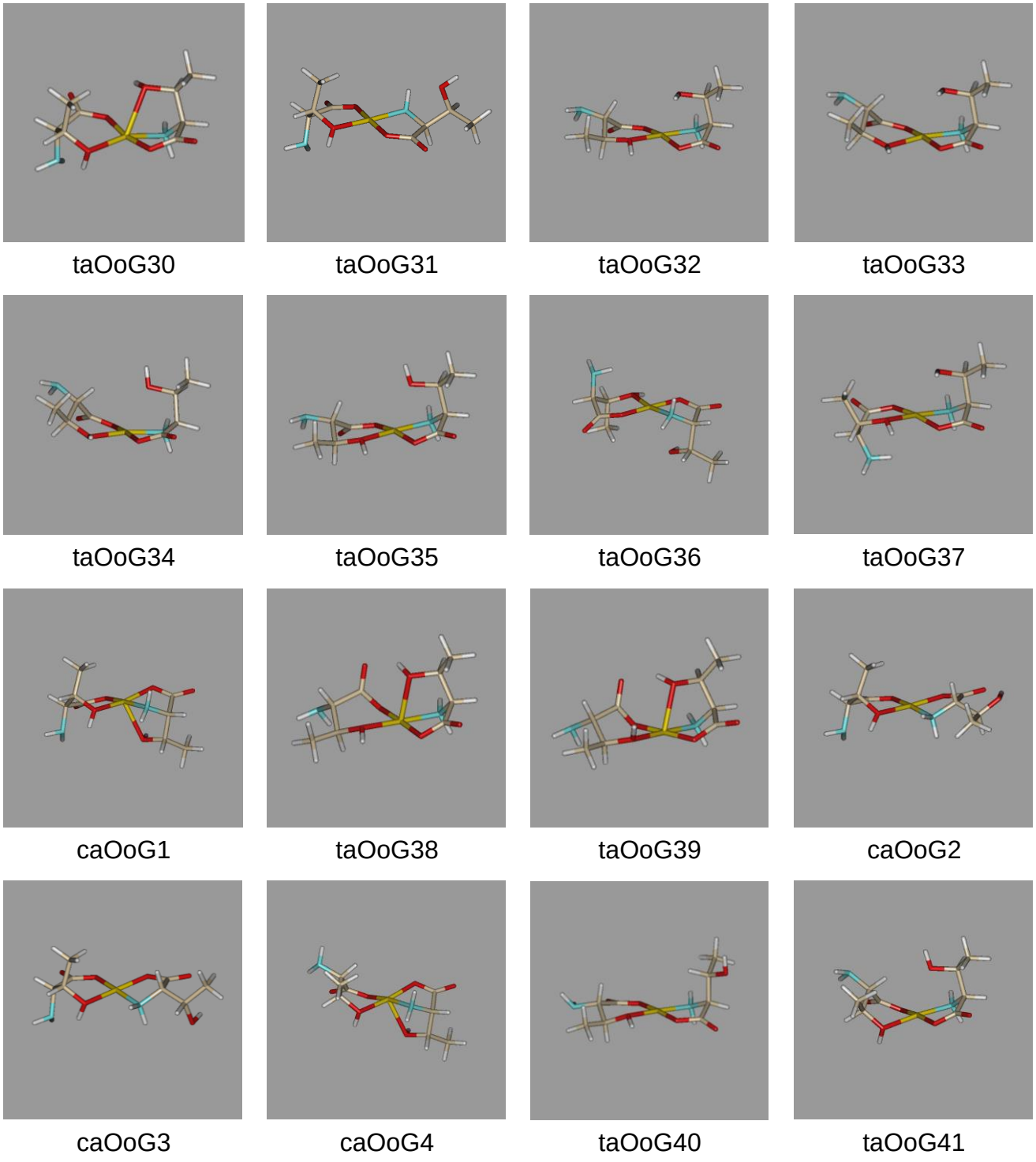


Figure S1. continued

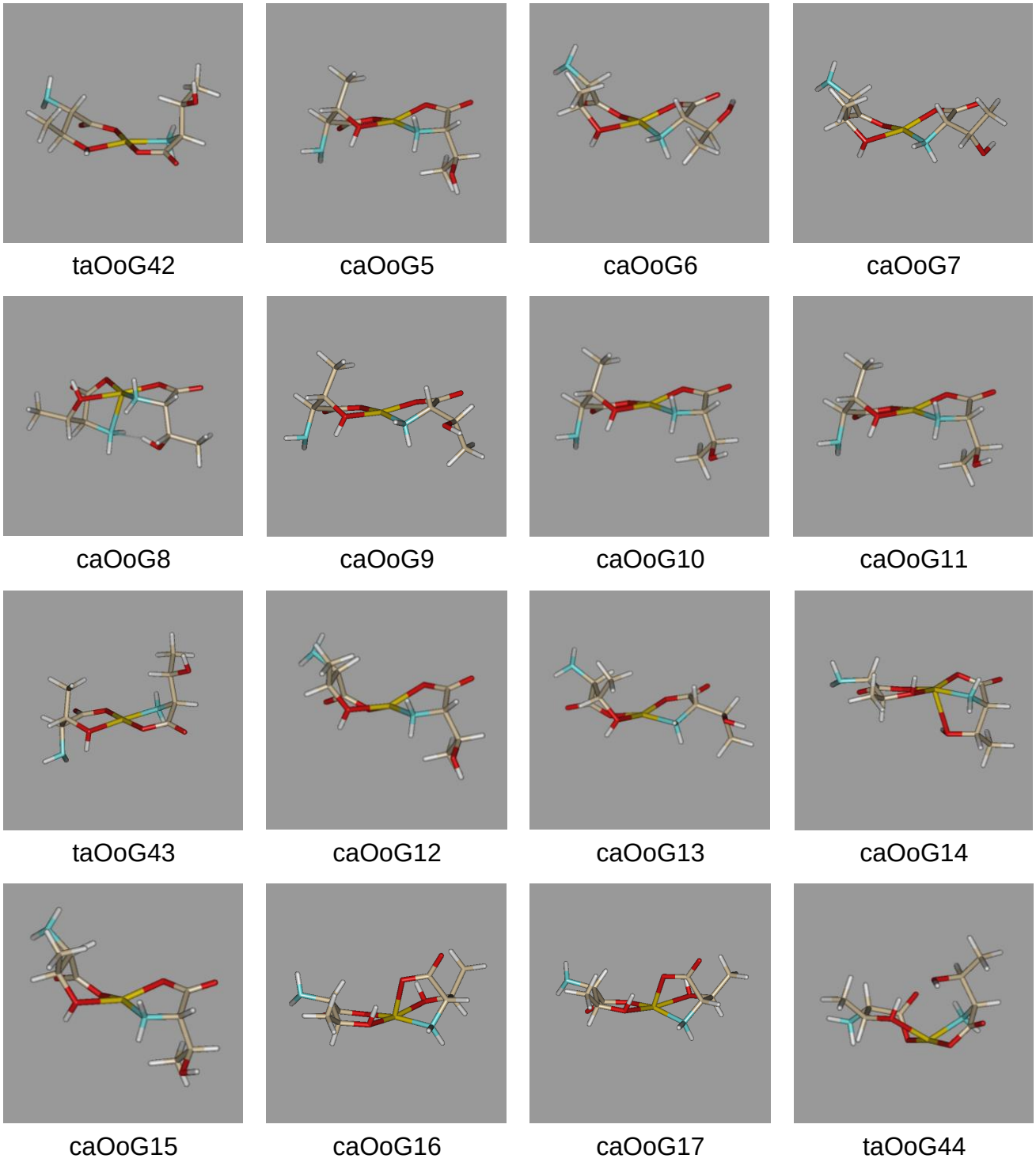


Figure S1. continued

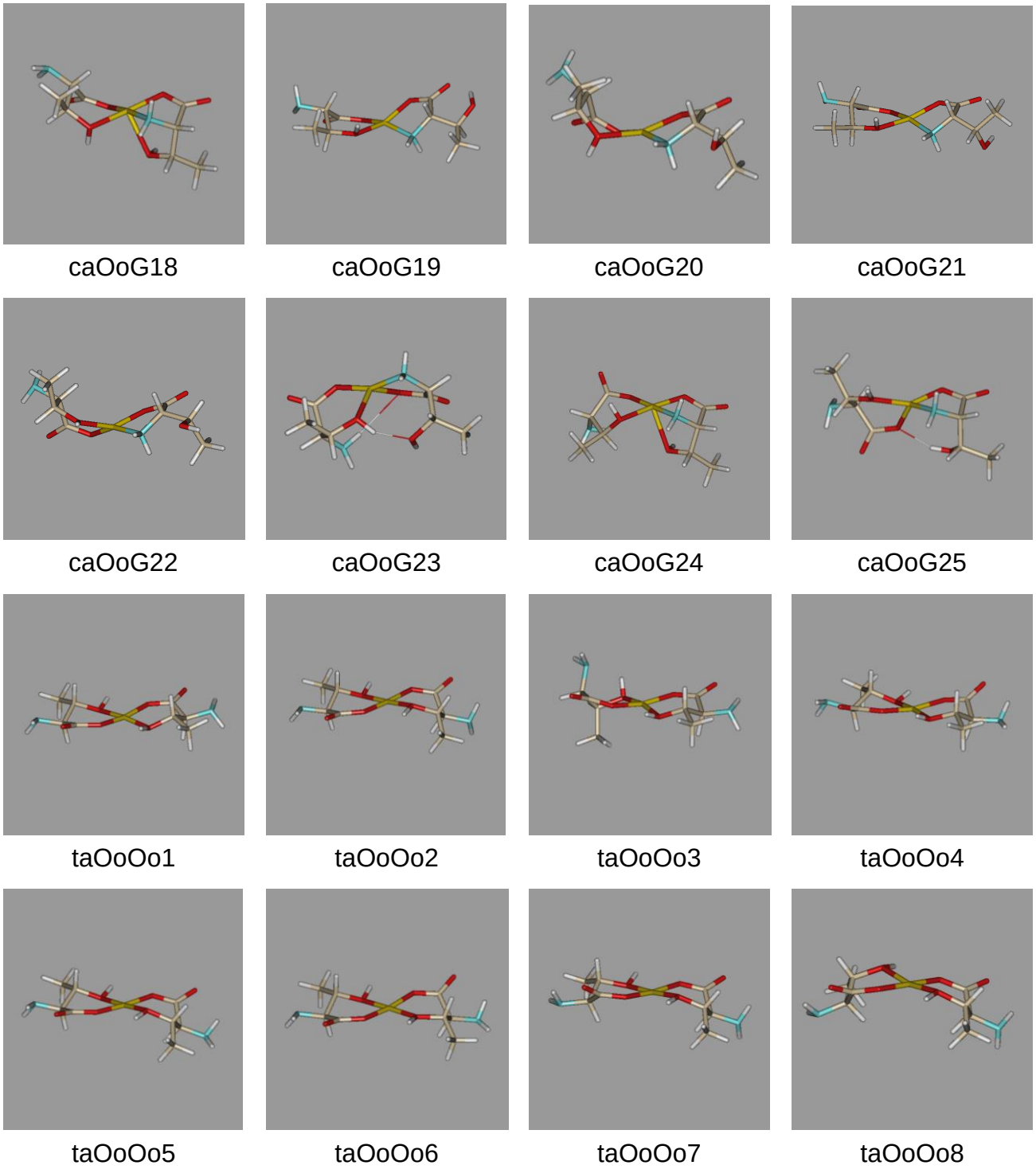
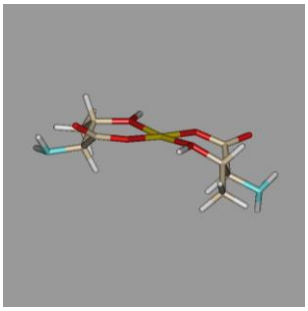
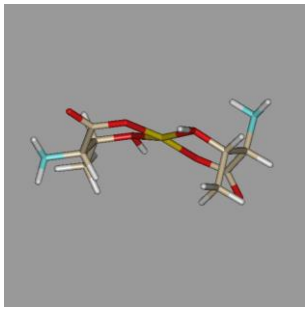


Figure S1. continued

taOoOo9



taOoOo10



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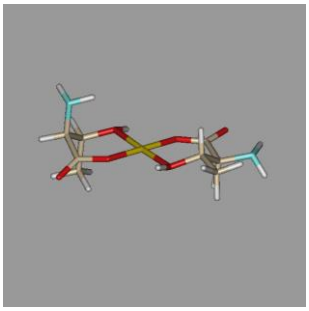

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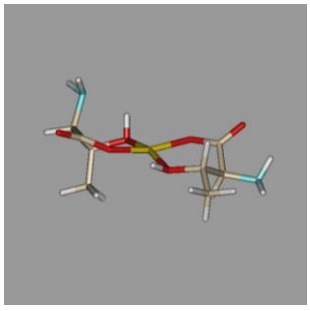

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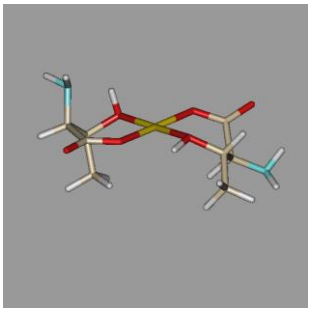

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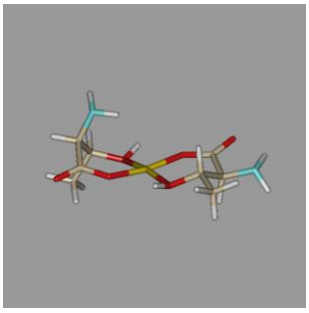

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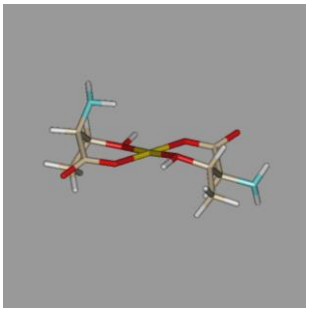

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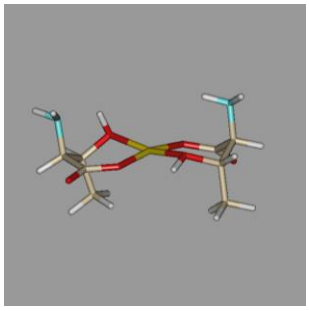
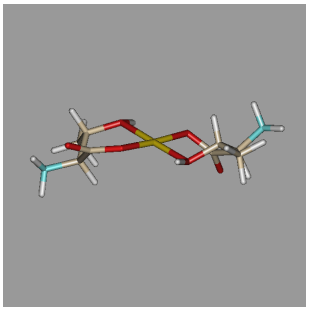


taOoOo17

taOoOo18



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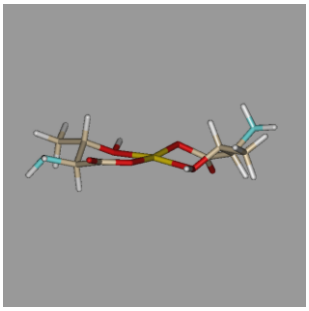
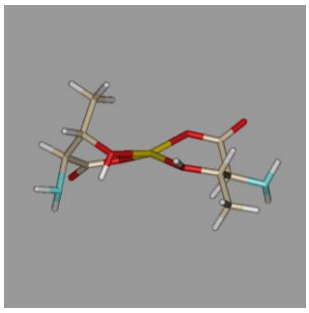


taOoOo20



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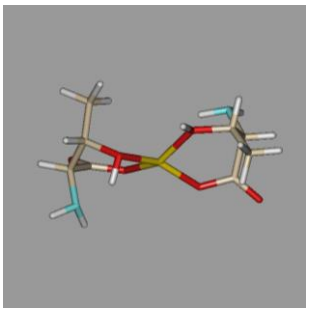

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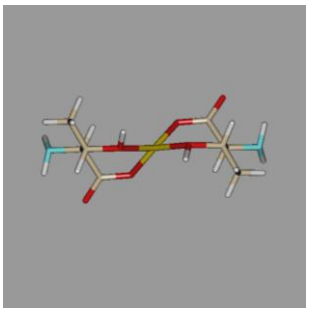
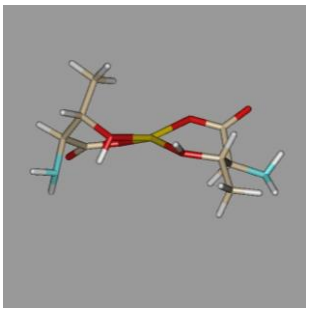


caOoOo3



caOoOo4

Figure S1. continued

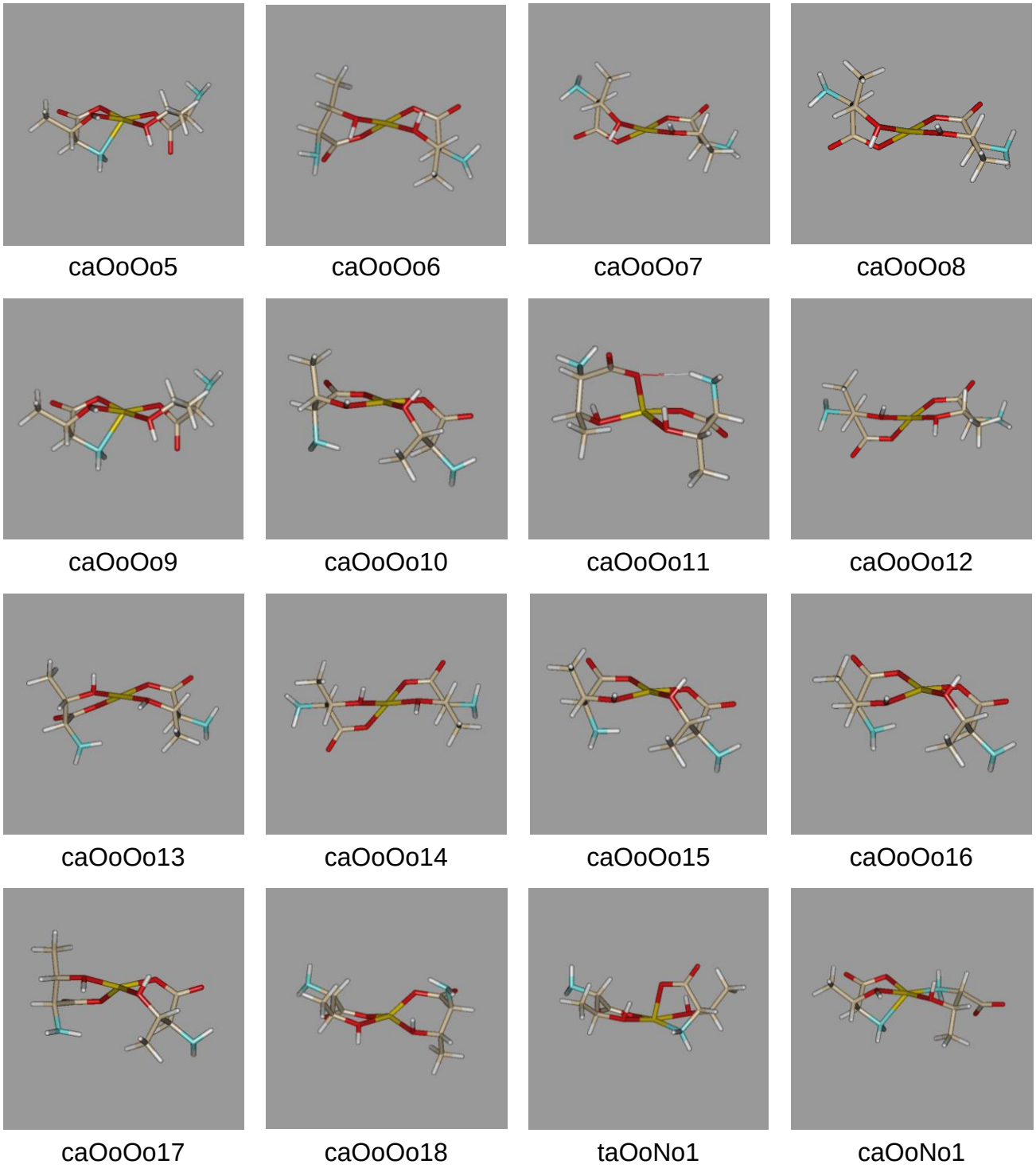


Figure S1. continued

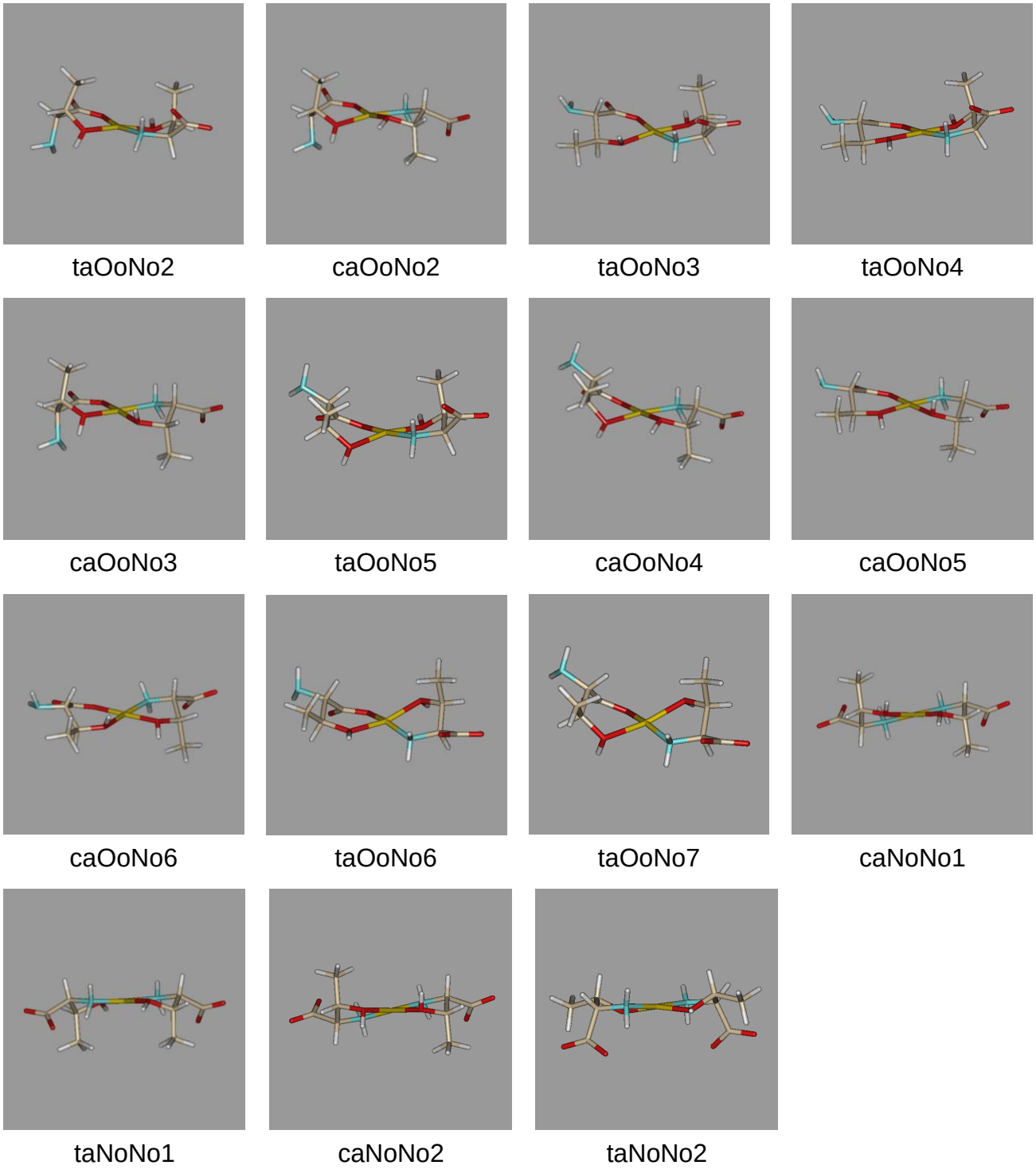


Figure S1. continued

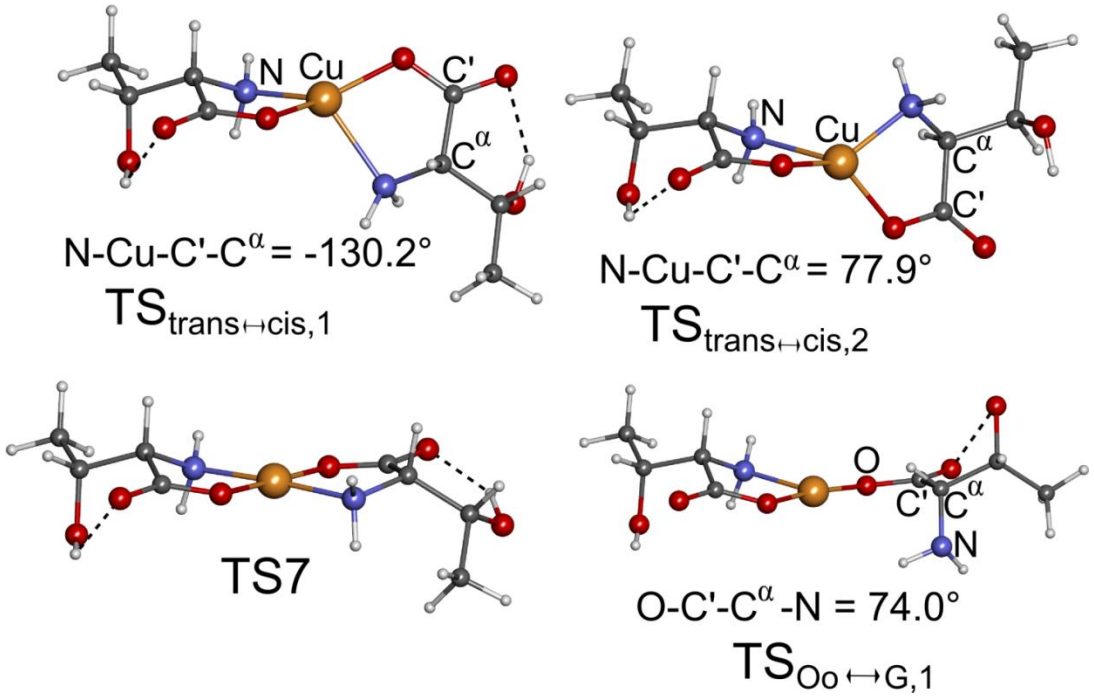


Figure S2. Illustrations of the B3LYP/BS0 TS structures calculated for Cu(L-Thr)$_2$. The hydrogen bonds are denoted by the broken lines.

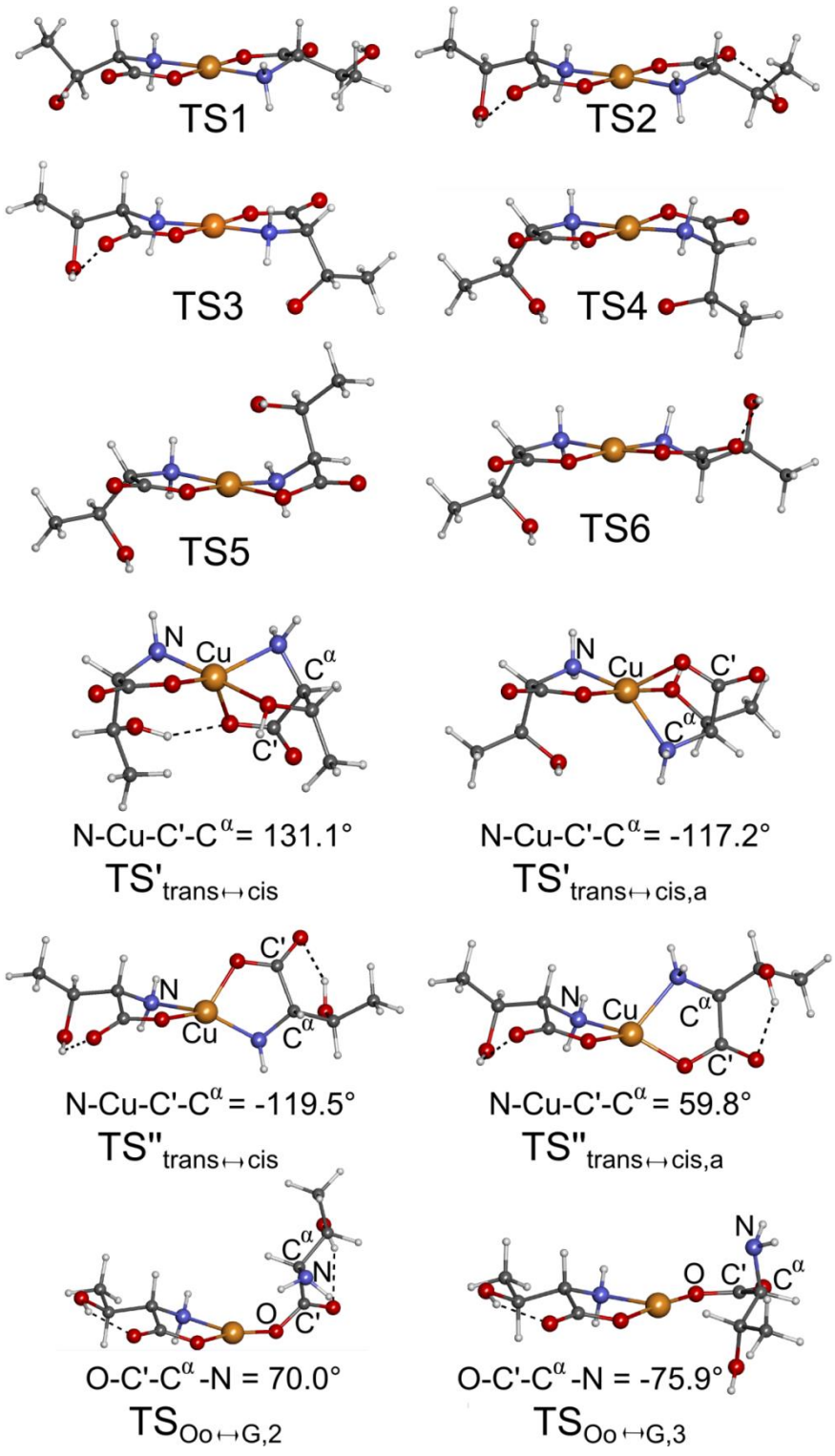


Figure S3. Illustrations of the B3LYP/BS0 TS structures calculated for Cu(L-*a*Thr)$_2$. The hydrogen bonds are denoted by the broken lines.

Table S1. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 57 Cu(L-Thr)$_2$ conformers in the G-G coordination mode[a]

name	conformer	ΔV	φ_1[b]	φ_2	φ_3	φ_4	φ_5	φ_6
tGG1	te1-te1	0.0	−154.4	60.8	74.0	−154.5	60.7	74.1
tGG2	te1-te8	7.0	−153.8	60.2	74.9	−148.5	−169.0	−52.6
tGG3	ta6-te1	10.5	−95.4	−47.5	179.2	−154.6	61.2	73.3
tGG4	ta5-te1	10.9	−95.6	−44.4	−89.4	−154.6	60.9	73.4
tGG5	te1-te6	13.8	−154.7	61.0	73.6	−157.2	−41.2	−170.4
tGG6	ta1-te1	14.4	−78.7	59.5	77.3	−154.7	60.5	73.3
tGG7	te8-te8	15.0	−150.2	−169.3	−53.3	−150.2	−169.3	−53.3
tGG8	ta3-te1	17.5	−85.4	49.4	175.5	−155.2	62.3	72.1
tGG9	ta6-te8	18.2	−95.4	−47.3	−179.9	−148.8	−169.4	−52.2
tGG10	ta2-te1	18.3	−73.2	51.6	−109.3	−156.4	62.8	72.3
tGG11	ta5-te8	18.4	−95.5	−44.1	−89.8	−149.5	−169.2	−52.4
tGG12	te6-te8	20.8	−157.8	−40.8	−170.1	−150.9	−169.4	−52.8
tGG13	ta1-te8	21.6	−81.3	60.8	77.2	−152.3	−169.6	−52.8
tGG14	ta5-ta5	22.0	−95.3	−44.6	−89.1	−95.4	−44.9	−89.0
tGG15	ta5-ta6	22.1	−95.4	−44.5	−88.9	−95.3	−47.6	−179.1
tGG16	ta6-ta6	22.5	−96.3	−47.3	−178.2	−96.3	−47.3	−178.2
tGG17	ta1-ta1	23.1	−76.7	57.1	82.9	−101.0	43.0	68.0
tGG18	ta1-ta5	23.6	−76.2	59.1	80.0	−89.0	−45.2	−89.7
tGG19	ta1-ta6	24.0	−78.7	59.9	74.3	−91.3	−47.7	−179.8
tGG20	ta3-te8	24.1	−86.2	49.9	176.8	−149.6	−169.4	−51.9
tGG21	ta2-te8	24.3	−73.3	51.6	−109.3	−152.2	−169.5	−53.3
tGG22	ta6-te6	25.4	−95.1	−48.0	179.4	−157.4	−41.1	−169.9
tGG23	ta5-te6	25.6	−95.4	−44.8	−88.7	−157.2	−41.1	−170.0
tGG24	te6-te6	28.0	−158.1	−41.2	−170.1	−158.1	−41.2	−170.2
tGG25	ta1-te6	28.6	−80.6	60.5	74.5	−157.9	−40.7	−169.6
tGG26	ta1-ta3	28.6	−100.1	84.2	69.5	−70.3	60.6	−139.4
tGG27	ta3-ta5	29.5	−88.5	49.1	166.3	−94.4	−45.8	−87.1
tGG28	ta3-te3	30.2	−80.0	52.0	−176.2	−145.9	46.1	163.0
tGG29	ta2-ta6	30.7	−74.7	50.5	−99.0	−93.1	−49.6	170.9
tGG30	ta2-te6	31.9	−73.5	51.6	−102.5	−158.4	−42.1	−171.0

tGG31	ta1-ta2	32.0	−106.0	30.9	66.7	−75.5	48.8	−88.3
tGG32	ta2-ta5	32.4	−74.2	50.0	−102.2	−95.6	−46.9	−87.4
tGG33	ta2-ta3	39.3	−96.8	63.6	−77.4	−73.8	56.8	−121.0
tGG34	ta2-ta2	39.4	−74.0	56.3	−118.9	−96.6	64.1	−77.0
tGG35	ta9-te1	43.7	−96.1	−156.2	−160.8	−153.5	60.8	74.3
cGG1	ce1-ce1	43.8	−156.6	59.7	73.5	−156.6	59.7	73.5
cGG2	ca1-ce1	49.5	−72.5	55.4	82.5	−158.3	60.5	72.5
cGG3	ca5-ce1	51.0	−87.7	−44.5	−95.2	−157.0	60.3	73.0
cGG4	ca6-ce1	51.9	−87.7	−45.3	−168.0	−157.1	60.3	73.0
cGG5	ce1-ce8	54.6	−155.4	58.9	74.6	−156.8	−170.6	−53.0
cGG6	ca1-ca5	55.3	−72.0	54.5	83.6	−90.3	−46.0	−93.5
cGG7	ce1-ce6	55.6	−156.9	60.5	73.0	−164.0	−42.0	−167.6
cGG8	ca1-ca6	55.8	−71.9	54.0	84.0	−90.4	−46.9	−172.4
cGG9	ca1-ca1	55.9	−73.2	54.5	80.1	−73.2	54.5	80.2
cGG10	ca5-ca5	58.3	−88.5	−45.1	−94.4	−88.4	−45.0	−94.3
cGG11	ca1-ce8	58.7	−71.9	54.8	84.9	−156.9	−170.5	−52.3
cGG12	ca5-ca6	59.0	−88.7	−44.9	−94.2	−88.7	−45.8	−170.3
cGG13	ca6-ca6	59.5	−87.8	−47.0	−173.3	−87.8	−47.0	−173.3
cGG14	ce1-ca8	59.8	−156.8	59.2	74.3	−108.7	−169.6	−44.9
cGG15	ca5-ce8	60.8	−87.4	−44.8	−96.1	−155.5	−170.4	−52.6
cGG16	ca6-ce8	61.1	−87.3	−46.1	−170.7	−156.1	−170.4	−52.7
cGG17	ca1-ce6	61.3	−72.1	55.0	81.8	−165.6	−41.7	−168.4
cGG18	ca5-ce6	63.5	−89.0	−45.2	−94.1	−162.9	−41.6	−167.9
cGG19	ca6-ce6	63.8	−88.9	−46.3	−173.3	−163.2	−41.9	−168.7
cGG20	ce8-ce8	65.0	−156.0	−170.3	−53.3	−156.0	−170.3	−53.3
cGG21	ce6-ce8	65.2	−164.1	−42.2	−168.0	−155.4	−170.6	−52.7
cGG22	ce6-ce6	67.2	−163.8	−42.1	−168.2	−163.9	−42.1	−168.2

[a] The conformers are depicted in Figure S1. The electronic energy of the most stable conformer (te1-te1) is used as the reference value (V_0 = −1071.76257129 a.u.). The torsion angles φ_1,φ_2, φ_3, φ_4, φ_5, and φ_6 are: Cu−N11−C12−C13, N11−C12−C13−O13, C12−C13−O13−HO13, Cu−N21−C22−C23, N21−C22−C23−O23, C22−C23−O23−HO23. The atom labels are defined in Figure 5.

Table S2. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 32 Cu(L-Thr)$_2$ conformers in the No-G coordination mode[a]

name	conformer	ΔV	φ_{11}	φ_{12}	φ_{13}	φ_4	φ_5	φ_6
tNoG1	tap-te1	41.3	86.5	−87.9	−71.9	−154.6	61.1	73.3
tNoG2	tap-ta1	56.1	86.5	−87.7	−71.9	−81.0	61.7	74.8
tNoG3	tap-ta2	61.4	83.5	−89.8	−74.4	−73.8	52.0	−92.5
cNoG1	cap-ca4	62.8	55.9	−26.6	−146.2	−81.7	−25.8	97.3
cNoG2	cap-ca2-A	75.0	70.2	28.6	−124.4	−84.7	55.7	−116.9
cNoG3	cap-ca3-A	82.8	75.6	20.7	−111.9	−69.6	54.8	−123.8
cNoG4	cap-ce6	84.1	54.4	−26.2	−140.7	−155.0	−44.1	−173.1
cNoG5	cap-ca2-B	85.2	69.7	3.9	−120.1	−78.2	49.0	−93.4
cNoG6	cap-ca3-B	89.7	102.4	−12.7	−165.7	−70.2	53.8	−123.7
cNoG7	cap-ca3-C	91.7	75.7	−99.2	−87.9	−70.4	38.5	143.7
cNoG8	cep-ce1	106.9	138.3	−11.0	−156.2	−153.9	58.8	76.7
cNoG9	cep-ca6	113.2	135.3	−10.3	−156.8	−90.9	−47.1	175.9
cNoG10	cep-ca5	115.5	139.7	−12.0	−155.6	−93.6	−44.1	−95.6
cNoG11	cep-ce8	116.1	135.4	−9.8	−157.5	−151.7	−168.9	−54.5
tNoG4	tem-te1	116.7	145.8	−17.1	104.7	−155.1	58.2	76.3
cNoG12	cep-ce6	117.0	137.2	−10.9	−156.3	−160.4	−42.2	−170.4
tNoG5	tep-te1	117.1	148.5	−18.2	−155.6	−154.7	58.6	76.1
cNoG13	cep-ca1	118.4	140.4	−11.4	−157.4	−74.1	58.2	90.9
tNoG6	tem-ta1	122.1	146.7	−17.2	102.3	−75.5	57.3	88.4
cNoG14	cem-ca6	123.0	151.6	−16.4	130.7	−91.2	−46.8	−179.6
cNoG15	cem-ca1	123.1	151.3	−16.0	119.6	−71.2	56.1	88.7
cNoG16	cem-ca5	124.1	153.4	−16.8	131.1	−91.4	−44.2	−94.9
tNoG7	tem-ta5	124.5	148.3	−18.1	109.2	−90.9	−43.1	−95.5
tNoG8	tep-ta6	124.7	149.1	−18.5	−154.0	−92.0	−46.3	−175.1
tNoG9	tep-ta5	124.8	148.6	−18.3	−155.6	−91.3	−44.6	−95.6
tNoG10	tem-ta6	125.4	148.7	−18.2	109.5	−92.1	−44.3	−168.0
tNoG11	tep-te6	127.6	149.1	−18.3	−153.4	−162.3	−41.5	−168.2
tNoG12	tep-te8	128.4	149.7	−19.0	−153.9	−154.0	−169.0	−54.3
tNoG13	tem-te8	128.7	146.7	−17.9	105.2	−154.7	−169.5	−54.4
tNoG14	tem-te6	129.0	147.5	−18.0	107.4	−162.3	−40.9	−168.1

tNoG15	tep-ta1	129.8	149.9	−19.1	−153.2	−75.7	58.2	86.4
tNoG16	tep-ta3	132.6	150.2	−19.2	−153.1	−79.0	48.1	159.2

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. The φ_4, φ_5, and φ_6 torsions are defined in Table S1. The torsion angles φ_{11}, φ_{12}, and φ_{13} are: Cu–N11–C12–C11, N11–C12–C11–O11, HO13–O13–Cu–N11. The atom labels are defined in Figure 5.

Table S3. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 62 Cu(L-Thr)$_2$ conformers in the Oo-G coordination mode[a]

name	conformer	ΔV	φ_7	φ_8	φ_9	φ_{10}	φ_4	φ_5	φ_6
tOoG1	te4dm-te1-A	49.4	−51.7	71.3	−8.7	150.7	−154.2	59.9	74.9
tOoG2	tbt2p-te1-A	53.5	−15.1	61.9	−9.0	−171.7	−154.4	60.1	74.9
tOoG3	ttw1m-te1	56.6	72.6	−66.3	−22.1	86.3	−154.8	60.4	73.9
tOoG4	te4dm-te8	57.2	−52.7	71.5	−8.1	151.1	−150.3	−169.2	−53.3
tOoG5	te4dm-ta5	60.1	−51.4	71.4	−8.9	149.1	−97.2	−43.5	−89.2
tOoG6	te4dm-ta6	60.4	−52.9	71.5	−9.0	150.6	−96.7	−47.4	−179.8
tOoG7	te3up-te1	60.7	62.3	−67.2	3.7	−160.1	−153.6	60.3	74.8
tOoG8	te4dm-te1-B	61.4	−45.0	73.5	−12.8	148.0	−154.4	59.9	75.1
tOoG9	tbt2p-te8	61.8	−17.0	63.2	−7.4	−167.0	−151.0	−169.4	−53.4
tOoG10	te4dm-ta1-A	63.1	−49.5	72.4	−6.8	145.6	−77.4	57.3	79.9
tOoG11	tbt2p-te3	63.3	−14.1	62.2	−8.0	−167.2	−145.4	45.5	165.1
tOoG12	te4dm-te6	63.8	−51.5	71.4	−8.4	151.0	−156.0	−40.6	−170.3
tOoG13	tbt2p-te1-B	63.8	−14.1	66.0	−7.2	−162.8	−154.3	60.3	74.7
tOoG14	ttw1m-te8	64.5	72.5	−66.8	−20.9	85.7	−150.4	−169.9	−52.7
tOoG15	tbt2p-ta6	65.1	−14.6	61.9	−8.7	−173.4	−96.9	−46.6	−178.7
tOoG16	te4dm-te5	66.7	−51.5	71.4	−8.5	150.9	−156.6	−40.1	−103.9
tOoG17	ttw1m-ta1	67.7	74.2	−67.3	−19.9	83.0	−73.1	58.3	77.7
tOoG18	tbt2p-ta1-A	67.7	−11.1	61.9	−6.8	−177.3	−77.5	60.3	79.0
tOoG19	tbt2p-te6	67.8	−14.6	62.5	−7.8	−166.0	−157.7	−40.9	−170.1
tOoG20	ttw1m-ta5	67.9	72.1	−65.9	−22.7	87.3	−96.3	−44.4	−88.5
tOoG21	ttw1m-ta6	68.3	71.6	−66.0	−23.2	88.2	−96.5	−47.2	−178.0
tOoG22	te3dm-ta2	70.4	−57.6	71.3	−7.7	155.2	−73.3	51.6	−114.0
tOoG23	te4dm-te3	71.2	−44.9	73.4	−13.0	147.6	−145.0	46.0	172.7
tOoG24	ttw1m-te6	71.7	71.8	−66.2	−22.6	87.5	−157.3	−40.8	−169.9

tOoG25	ttb2p-ta2	72.4	−23.6	67.2	−4.3	−149.5	−74.6	51.6	−100.1
tOoG26	te4up-te1	74.4	47.8	−69.0	18.6	−156.4	−153.5	60.3	74.9
tOoG27	ttw1m-te5	74.4	71.8	−65.9	−23.3	87.9	−157.0	−40.4	−100.6
tOoG28	ttw1m-ta3	75.2	73.4	−66.4	−21.6	85.2	−89.2	48.0	168.2
tOoG29	te4dm-ta1-B	75.2	−43.1	74.3	−11.3	142.0	−76.7	57.1	80.9
tOoG30	ttw1m-ta2	75.3	74.6	−68.1	−17.4	81.1	−72.6	50.5	−99.1
tOoG31	tch1p-ta2	75.7	51.9	−60.5	44.8	−166.1	−71.4	56.8	−119.1
tOoG32	te4um-te1	77.3	17.3	−61.2	16.2	161.0	−152.7	59.3	75.7
tOoG33	tbt2p-ta1-B	79.0	−13.3	65.7	−6.9	−167.6	−85.7	59.7	78.5
tOoG34	te4dm-ta3	79.1	−45.1	73.6	−12.4	146.9	−85.9	48.7	171.2
tOoG35	tbt2p-ta3	80.1	−14.4	68.0	−3.7	−159.2	−84.8	51.5	178.0
tOoG36	te4um-ta3-A	82.0	41.4	−72.0	4.0	127.3	−83.7	48.4	170.6
tOoG37	tbt2p-ta2	82.0	−19.2	68.4	−6.6	−153.3	−74.7	52.7	−112.7
cOoG1	ctw1m-ce1	86.5	78.8	−67.3	−17.8	72.8	−156.2	59.3	74.1
cOoG2	cbt1m-ca1	86.7	13.6	−69.8	8.3	141.8	−86.8	45.3	65.6
cOoG3	ctw1m-ca1	90.9	78.6	−65.8	−21.3	74.5	−70.8	51.6	87.2
tOoG38	ttb1m-ta1	91.7	22.4	−65.2	12.6	147.0	−78.1	57.4	79.8
cOoG4	ctw1m-ca6	94.2	78.4	−65.6	−21.8	75.4	−89.0	−47.4	−178.0
cOoG5	ctw1m-ca5	94.6	78.1	−66.5	−20.4	75.2	−89.4	−46.0	−93.1
tOoG39	te4um-ta3-B	94.7	14.2	−60.6	16.7	158.7	−81.5	50.2	−179.5
cOoG6	ctw1m-ce8	95.4	79.3	−67.1	−17.3	71.5	−154.5	−170.2	−52.8
cOoG7	ctb2m-ce1	95.9	10.8	55.6	−3.0	60.7	−154.9	58.6	75.1
cOoG8	cbt2m-ca1-A	98.5	8.3	57.0	−3.1	63.2	−71.0	51.8	88.7
cOoG9	ctw1m-ce6	99.1	79.5	−66.4	−18.7	72.5	−161.8	−41.8	−169.6
cOoG10	ctb2m-ca6	103.1	11.2	55.6	−3.2	60.3	−90.0	−47.2	−177.5
cOoG11	ctb2m-ca5	103.4	11.0	55.7	−3.1	60.5	−90.3	−45.8	−92.8
cOoG12	cbt2m-ca6	104.1	−9.4	66.4	−2.9	94.3	−89.7	−47.3	−177.7
cOoG13	ctb2m-ce8	105.3	12.2	54.8	−3.1	58.7	−152.8	−169.4	−53.0
cOoG14	ce4dp-ce1	105.7	−40.8	72.6	−6.4	−120.4	−153.9	58.6	75.2
cOoG15	ce4dp-ca1-A	107.9	−34.3	71.8	−7.4	−114.2	−65.9	47.0	107.3
cOoG16	ctb2m-ce6	108.3	12.8	54.4	−3.4	58.5	−160.8	−41.2	−169.2
cOoG17	ce4dp-ca1-B	108.4	−45.4	72.7	−8.0	−114.0	−70.9	50.3	87.1
cOoG18	cbt2m-ca1-B	110.7	−10.1	68.9	−1.9	81.1	−72.0	52.9	87.5

cOoG19	ce4dp-ca6	111.7	−33.9	72.0	−5.3	−131.4	−86.8	−48.3	179.3
cOoG20	ce4dp-ca5	112.9	−36.9	72.3	−5.7	−127.2	−87.2	−46.7	−93.3
cOoG21	ce4dp-ce8	113.6	−38.0	72.4	−6.2	−124.2	−154.2	−169.6	−53.1
cOoG22	ce4dp-ce6	116.0	−33.5	71.5	−4.8	−132.8	−161.3	−42.5	−170.2
cOoG23	ce4um-ca1	118.3	20.4	−66.5	17.3	133.9	−92.2	71.0	73.5

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. The φ_4, φ_5, and φ_6 torsions are defined in Table S1. The torsion angles φ_7, φ_8, φ_9, and φ_{10} are: Cu–O13–C13–C12, O13–C13–C12–C11, Cu–C12–C11–O11, HO13–O13–Cu–O11. The atom labels are defined in Figure 5.

Table S4. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 28 Cu(L-Thr)$_2$ conformers in the Oo-Oo coordination mode[a]

name	conformer	ΔV	φ_7	φ_8	φ_9	φ_{10}	φ_{14}	φ_{15}	φ_{16}	φ_{17}
tOoOo1	te4dm-te4dm-A	95.5	−54.7	71.9	−8.4	149.4	−54.1	71.8	−8.3	148.7
tOoOo2	te4dm-te4dm-B	107.7	−52.9	71.6	−8.8	147.8	−47.5	73.8	−13.2	146.0
tOoOo3	tbt2p-te3dm	112.4	−9.8	63.8	−7.3	−170.0	−57.4	71.3	−7.5	153.3
tOoOo4	tbt2p-tbt2p	117.3	−19.4	65.5	−3.4	−156.4	−15.8	67.5	−4.7	−157.6
tOoOo5	tbt4m-te4dm	117.3	68.3	−66.9	−23.3	92.8	−45.3	73.6	−12.9	142.2
tOoOo6	tbt2p-te3um	122.1	−7.6	63.7	−6.1	−167.2	71.0	−69.9	−14.9	84.4
tOoOo7	te3dm-te4up	122.9	−58.6	70.4	−8.0	157.3	54.8	−70.0	14.3	−160.5
tOoOo8	tbt1m-te4dm	123.3	19.2	−64.0	10.5	149.8	−53.4	71.4	−9.4	150.9
tOoOo9	te4up-ttb2p	124.0	−20.9	66.3	−3.5	−149.7	48.4	−69.2	20.1	−155.0
cOoOo1	ce3um-ctb1m	126.8	64.5	−80.7	14.5	73.9	−8.9	−62.2	7.8	177.0
tOoOo10	tbt2p-te4um	127.5	−13.8	62.9	−6.2	−160.9	9.8	−59.5	15.7	160.8
tOoOo11	te4dm-ttw1p	130.2	72.9	−47.4	−26.8	−164.0	−51.5	73.8	−12.5	150.7
tOoOo12	ttb1m-ttw1m	133.1	68.9	−65.6	−25.0	93.2	18.1	−63.7	10.8	147.5
tOoOo13	te3um-te4up	133.7	74.5	−68.3	−15.3	79.8	49.3	−68.5	18.9	−156.0
cOoOo2	ctb2m-ctw1m-A	137.7	−22.3	69.2	−5.1	118.0	79.3	−66.2	−20.1	73.0
cOoOo3	cbt2m-ctb1m	150.7	−7.5	−62.9	8.3	177.4	−0.4	64.3	−1.2	69.0
cOoOo4	ctb2m-ctw1m-B	151.4	−25.5	73.1	−5.6	119.2	79.2	−67.0	−18.4	72.3
cOoOo5	ce3um-ctb1p	154.2	63.9	−81.1	10.9	76.3	25.4	−66.3	14.3	−141.2
cOoOo6	ce4dp-ctb2m	155.2	−22.1	68.4	−7.1	133.1	−37.0	73.6	−7.0	−123.0
cOoOo7	cbt2p-ctb2p-A	155.8	−18.7	68.2	−3.5	−153.3	−23.7	69.9	−3.7	−145.8
cOoOo8	cch1m-ce4um	156.4	64.2	−71.4	46.1	59.7	32.9	−71.1	15.9	119.6

cOoOo9	cbt2m-ctb2m	158.3	9.3	57.3	−2.9	62.5	−25.0	73.0	−7.0	119.2
cOoOo10	ce4up-ctb2m	166.3	13.1	54.1	−3.3	58.0	42.2	−67.5	12.4	−155.2
cOoOo11	cbt2p-ctb2p-B	169.1	−15.3	66.5	−4.2	−159.2	−26.7	73.4	−4.9	−140.4
cOoOo12	cbt2p-ce4dp	169.1	−10.7	64.4	−5.0	−167.8	−29.4	74.3	−5.6	−135.8
cOoOo13	ctb2p-ctb2p	169.2	−21.6	68.9	−3.7	−149.7	−25.6	73.3	−3.7	−143.2
cOoOo14	cbt2m-ce4um	180.7	6.2	58.4	−4.1	68.5	42.9	−71.9	13.5	116.9
cOoOo15	cbt2m-ce4up	188.2	−9.7	66.3	−7.3	110.3	37.0	−73.4	8.8	−132.4

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. The φ_7, φ_8, φ_9, and φ_{10} torsions are defined in Table S2. The torsion angles φ_{14}, φ_{15}, φ_{16}, and φ_{17} are: Cu–O23–C23–C22, O23–C23–C22–C21, Cu–C22–C21–O21, HO23–O23–Cu–O21. The atom labels are defined in Figure 5.

Table S5. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 13 Cu(L-Thr)$_2$ conformers in the Oo-No coordination mode[a]

name	conformer	ΔV	φ_7	φ_8	φ_9	φ_{10}	φ_{18}	φ_{19}	φ_{20}
cOoNo1	ctb2p-cap	96.2	−21.4	66.1	−4.6	−152.5	87.9	−87.3	−71.2
cOoNo2	ctb1m-cem	151.2	−4.4	−65.7	7.8	174.1	138.2	−15.4	93.5
tOoNo1	te3um-tep	151.6	76.4	−70.6	−11.4	72.4	140.3	−13.4	−154.5
tOoNo2	ttw1m-tem	159.9	76.8	−68.0	−18.5	75.5	155.5	−18.1	131.5
tOoNo3	te4dp-tep	162.3	−43.2	71.8	−3.7	−124.3	134.2	−8.6	−157.4
cOoNo3	ctw1m-cem	162.7	74.3	−70.1	−17.2	78.7	155.5	−20.6	128.7
tOoNo4	te4dm-tep	163.4	−43.8	71.9	−4.8	146.9	136.5	−10.1	−157.7
tOoNo5	te4dm-tam	169.5	−37.6	69.8	−6.3	151.8	94.2	12.8	150.1
cOoNo4	ce4dm-cem	169.8	−39.6	72.6	−5.8	135.7	149.0	−19.6	108.7
tOoNo6	te4dm-tem	170.0	−37.8	71.3	−6.7	143.5	152.9	−16.5	124.1
tOoNo7	te4dp-tem	171.6	−34.1	70.6	−5.4	−137.0	151.8	−16.2	125.8
cOoNo5	ctb2m-cep	173.0	−24.8	71.5	−2.9	113.1	148.4	−19.0	−161.1
cOoNo6	ce4dp-cep	173.5	−48.6	72.9	−6.3	−112.6	152.4	−21.4	−144.5

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. [b] The φ_7, φ_8, φ_9, and φ_{10} torsions are defined in Table S2. The torsion angles φ_{18}, φ_{19}, and φ_{20} are: Cu–N21–C22–C21, N21–C22–C21–O21, HO23–O23–Cu–N21. The atom labels are defined in Figure 5.

Table S6. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 4 Cu(L–Thr)$_2$ conformers in the No-No coordination mode[a]

name	conformer	ΔV	φ_{11}[b]	φ_{12}	φ_{13}	φ_{18}	φ_{19}	φ_{20}
cNoNo1	cap-cap	99.7	53.9	−25.5	−137.2	86.6	−90.0	−72.6
cNoNo2	cep-cep	211.7	148.4	−18.4	−150.3	148.5	−18.2	−150.1
cNoNo3	cem-cem	212.8	146.6	−17.2	109.5	147.1	−17.2	110.3
tNoNo1	tep-tep	212.8	146.2	−15.5	−153.7	146.1	−15.4	−153.3

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. The φ_{11}, φ_{12}, and φ_{13} torsions are defined in Table S3. The φ_{18}, φ_{19}, and φ_{20} torsions are defined in Table S5.

Table S7. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 113 Cu(L-*a*Thr)$_2$ conformers in the G-G coordination mode[a]

name	conformer	ΔV	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6
taGG1	te8-te8	7.4	−153.8	−175.5	−51.0	−154.1	−175.5	−51.1
taGG2	te1-te8	8.6	−158.8	68.3	71.0	−153.9	−175.7	−50.7
taGG3	te1-te1	10.5	−159.4	68.8	70.4	−159.3	68.9	70.4
taGG4	ta1-te8	16.5	−77.8	59.9	83.7	−154.6	−176.0	−50.1
taGG5	te8-ta6	16.9	−153.7	−176.0	−50.4	−106.4	−55.3	178.0
taGG6	te6-te8	17.0	−154.9	−57.0	−176.4	−154.4	−175.9	−50.6
taGG7	te8-ta5	18.1	−154.0	−175.9	−50.5	−105.5	−55.5	−74.5
taGG8	ta1-te1	18.4	−77.0	58.8	84.8	−160.0	68.8	69.1
taGG9	te1-ta6	18.4	−158.7	69.1	69.8	−104.6	−55.9	177.3
taGG10	te1-te6	18.6	−158.7	68.9	69.8	−153.8	−56.9	−176.9
taGG11	ta3-te8	18.9	−78.1	57.0	−165.0	−153.2	−176.2	−49.6
taGG12	te1-ta5	19.6	−158.7	69.0	70.0	−104.0	−56.5	−74.0
taGG13	te5-te8	20.7	−147.5	−57.6	−83.5	−153.4	−175.8	−50.4
taGG14	ta3-te1	21.1	−77.9	56.3	−168.1	−158.3	70.4	68.5
taGG15	te3-te8	21.7	−144.6	54.9	173.7	−153.1	−175.7	−50.1
taGG16	te1-te5	22.3	−158.3	68.9	70.0	−147.9	−57.8	−83.0
taGG17	ta1-ta1	23.6	−80.5	52.3	84.1	−90.2	48.3	75.8
taGG18	te1-te3	23.8	−159.4	69.4	69.5	−145.2	54.8	173.1
taGG19	ta1-ta3	25.5	−99.2	93.5	65.5	−71.3	62.8	−143.8
taGG20	ta1-ta6	27.0	−78.8	59.9	78.9	−107.7	−53.1	177.4

taGG21	ta1-te6	27.4	−78.9	59.8	81.0	−154.0	−56.6	−176.3
taGG22	te6-ta6	27.7	−154.5	−57.1	−176.4	−106.0	−55.6	177.8
taGG23	te6-te6	27.7	−153.5	−57.1	−176.7	−153.9	−56.7	−176.6
taGG24	ta6-ta6	27.9	−107.1	−55.6	178.5	−107.2	−55.5	178.7
taGG25	ta1-ta5	28.2	−80.3	59.1	81.6	−107.4	−54.4	−74.0
taGG26	te6-ta5	28.6	−153.1	−57.2	−176.3	−104.3	−56.1	−73.8
taGG27	ta5-ta6	28.6	−105.3	−56.0	−73.9	−106.8	−55.8	178.2
taGG28	ta5-ta5	29.5	−105.1	−55.8	−74.3	−105.2	−55.5	−74.0
taGG29	te5-ta1	30.8	−151.6	−57.9	−82.2	−78.6	59.6	82.0
taGG30	te5-ta6	31.1	−148.1	−58.0	−81.7	−106.2	−55.5	177.8
taGG31	te5-te6	31.2	−148.6	−57.7	−82.5	−151.4	−56.9	−176.7
taGG32	ta3-te6	31.3	−79.2	56.7	−167.7	−153.7	−57.2	−176.4
taGG33	te6-ta2	31.6	−153.7	−57.9	−177.5	−73.9	54.3	−108.1
taGG34	ta3-ta6	32.0	−85.0	54.1	178.1	−108.0	−55.7	178.3
taGG35	te5-ta5	32.1	−149.1	−57.7	−82.4	−104.3	−55.8	−74.0
taGG36	ta3-ta5	32.4	−84.0	53.7	176.8	−108.5	−56.1	−72.6
taGG37	te3-ta6	32.6	−145.8	55.3	172.7	−106.0	−56.0	177.4
taGG38	te3-te6	32.8	−145.1	55.2	172.9	−151.4	−56.8	−177.3
taGG39	ta2-ta6	33.6	−74.6	54.8	−112.8	−113.5	−54.2	177.5
taGG40	ta1-te3	33.8	−79.1	59.0	81.8	−149.1	54.6	168.9
taGG41	ta3-te5	34.4	−80.3	55.5	−174.3	−146.7	−58.1	−80.3
taGG42	te5-te5	34.7	−149.0	−57.8	−82.8	−148.9	−57.7	−82.8
taGG43	ta2-te5	35.2	−73.9	55.0	−116.2	−153.5	−58.6	−83.0
taGG44	te3-te5	36.2	−145.3	55.1	173.0	−149.3	−57.9	−82.1
taGG45	ta3-te3	36.3	−76.3	58.3	−156.8	−144.9	56.1	173.9
taGG46	te3-te3	38.3	−145.8	55.4	172.6	−145.9	55.2	173.3
taGG47	ta1-ta2	38.4	−98.8	31.7	73.2	−76.8	50.5	−84.5
taGG48	ta3-ta2	39.8	−74.7	58.3	−132.1	−95.7	67.0	−70.3
taGG49	te8-ta9	49.0	−153.7	−176.0	−50.4	−82.8	177.9	−174.4
taGG50	te1-ta9	50.2	−158.9	69.2	69.9	−81.9	−179.7	−170.6
caGG1	ca1-ca1	51.1	−73.8	54.1	85.3	−73.7	54.4	84.7
caGG2	ca1-ce1	51.7	−72.9	56.0	85.9	−163.0	68.2	68.2
caGG3	ca1-ce8	52.0	−72.3	55.0	88.3	−159.0	−176.0	−50.5

taGG51	te7-te8	52.0	−165.0	−159.4	78.2	−153.7	−175.8	−50.6
caGG4	ce1-ce1	53.2	−160.8	67.1	69.7	−161.5	67.3	69.4
taGG52	te1-te7	54.0	−158.9	69.1	70.0	−165.1	−158.7	77.5
caGG5	ce8-ce1	55.2	−157.1	−176.4	−50.8	−161.0	66.7	70.2
caGG6	ce8-ce8	56.9	−157.7	−175.8	−51.4	−157.0	−175.7	−51.3
caGG7	ca1-ca6	57.8	−73.0	53.7	88.3	−99.3	−54.6	−179.8
caGG8	ca1-ca5	58.4	−72.8	54.2	88.3	−99.1	−55.5	−77.4
caGG9	ca1-ca8	59.1	−72.7	54.6	89.0	−100.5	−173.8	−41.0
taGG53	te6-ta9	59.5	−151.7	−56.6	−176.6	−81.7	−178.4	−170.0
caGG10	ca1-ce6	59.9	−72.3	54.6	87.1	−162.1	−56.0	−175.8
taGG54	ta6-ta9	60.0	−108.1	−55.7	178.7	−82.9	−179.6	−170.9
taGG55	ta5-ta9	60.6	−106.7	−55.8	−73.7	−83.0	−178.6	−168.0
caGG11	ce1-ca6	61.6	−161.3	67.6	69.2	−99.0	−53.7	−178.1
caGG12	ce8-ca6	61.8	−157.2	−175.9	−50.7	−98.0	−53.7	−179.2
caGG13	ce1-ce6	62.0	−161.0	67.5	69.1	−159.6	−55.8	−174.5
caGG14	ce1-ca5	62.2	−161.3	67.5	69.4	−97.6	−54.0	−78.7
taGG56	te6-te7	62.4	−153.8	−57.1	−176.9	−165.5	−159.0	76.7
taGG57	te7-ta6	62.5	−165.6	−159.2	76.9	−107.0	−55.6	177.6
caGG15	ce6-ce8	62.5	−159.1	−55.6	−175.3	−156.6	−175.8	−50.6
taGG58	te7-ta1	62.6	−166.0	−158.6	75.9	−78.0	60.4	81.3
taGG59	te5-ta9	62.9	−148.9	−57.5	−82.1	−82.0	−178.4	−169.7
caGG16	ce8-ca5	62.9	−156.7	−176.0	−50.6	−97.3	−54.3	−79.6
taGG60	ta2-ta9	63.4	−75.2	54.7	−101.0	−83.3	166.3	179.4
taGG61	te7-ta5	63.6	−165.5	−159.4	77.2	−105.7	−56.1	−73.9
caGG17	ca1-ce5	63.9	−72.5	55.1	86.4	−161.8	−58.0	−87.8
taGG62	te3-ta9	64.1	−144.9	55.3	173.4	−81.8	−179.4	−170.1
caGG18	ce1-ca8	64.4	−161.4	66.7	70.1	−99.0	−173.8	−41.2
taGG63	te7-ta2	65.0	−164.7	−159.9	76.3	−73.7	55.1	−112.7
taGG64	te7-ta3	65.2	−164.6	−159.1	75.3	−75.5	57.9	−145.9
caGG19	ce1-ce5	66.0	−161.1	67.4	69.3	−159.3	−57.4	−91.6
taGG65	te5-te7	66.2	−147.0	−57.8	−82.1	−165.3	−158.7	77.2
caGG20	ce8-ca8	66.2	−157.3	−176.0	−51.2	−98.0	−173.3	−41.7
caGG21	ce5-ce8	66.9	−159.0	−57.2	−95.1	−156.8	−175.9	−50.7

taGG66	te3-te7	67.4	−145.1	55.4	174.0	−165.5	−158.1	76.8
caGG22	ca6-ca6	69.0	−97.0	−54.2	−179.6	−98.7	−54.1	−179.8
caGG23	ce6-ca6	69.4	−160.4	−56.3	−175.9	−97.2	−54.0	179.7
caGG24	ce6-ce6	69.7	−159.0	−56.2	−175.5	−160.6	−55.8	−175.5
caGG25	ca5-ca6	69.9	−97.6	−54.7	−78.1	−98.5	−54.0	−179.0
caGG26	ce6-ca5	70.6	−160.4	−56.0	−175.3	−96.7	−55.1	−78.4
caGG27	ca5-ca5	70.7	−96.3	−54.4	−78.4	−97.6	−54.5	−78.2
caGG28	ca6-ca8	71.5	−98.5	−53.4	−178.4	−98.6	−173.5	−41.4
caGG29	ce6-ca8	72.2	−161.9	−56.0	−174.9	−98.0	−173.6	−41.3
caGG30	ca5-ca8	72.3	−97.7	−54.2	−79.3	−98.0	−173.5	−41.3
caGG31	ce5-ca6	73.8	−158.8	−57.8	−91.7	−97.6	−53.8	−179.3
caGG32	ce5-ce6	74.2	−158.4	−57.8	−91.6	−159.2	−55.8	−175.1
caGG33	ce5-ca5	74.6	−159.1	−57.6	−90.4	−96.7	−54.8	−78.4
caGG34	ca8-ca8	75.4	−100.7	−173.3	−41.8	−99.5	−173.6	−41.6
caGG35	ce5-ca8	76.4	−161.0	−57.3	−93.3	−97.9	−173.7	−41.1
caGG36	ce5-ce5	78.3	−158.7	−57.7	−91.8	−159.6	−57.6	−91.5
taGG67	te7-ta9	94.0	−165.5	−160.3	77.0	−82.4	178.6	−174.1
taGG68	te7-te7	97.3	−165.5	−158.8	78.1	−165.4	−158.8	77.8
caGG37	ce7-ca1	100.0	−170.1	−158.4	70.7	−72.6	55.7	86.4
caGG38	ce7-ce1	102.5	−168.7	−160.0	72.2	−161.4	67.1	69.3
caGG39	ce7-ce8	104.5	−168.2	−159.7	73.2	−158.0	−176.1	−51.0
caGG40	ce7-ca6	110.8	−167.7	−158.3	73.6	−97.5	−53.2	−177.8
caGG41	ce6-ce7	111.0	−161.3	−55.6	−175.0	−168.2	−159.5	72.2
caGG42	ce7-ca5	111.3	−168.1	−159.1	73.0	−97.0	−53.8	−79.2
caGG43	ce7-ca8	113.7	−168.4	−160.8	73.1	−97.2	−173.9	−40.8
caGG44	ce5-ce7	115.1	−160.2	−57.3	−92.5	−168.4	−159.7	72.2
caGG45	ce7-ce7	152.4	−168.8	−160.0	71.3	−169.0	−160.1	71.6

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. The φ_1, φ_2, φ_3, φ_4, φ_5, and φ_6 torsions are defined in Table S1.

Table S8. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 30 Cu(L-*a*Thr)$_2$ conformers in the No-G coordination mode[a]

name	conformer	ΔV	φ_{11}	φ_{12}	φ_{13}	φ_4	φ_5	φ_6
taNoG1	tap-ta1	54.1	86.6	−83.6	−72.0	−76.9	60.9	82.2
taNoG2	tap-ta3	59.2	86.9	−82.9	−71.7	−82.8	55.7	175.3
caNoG1	cap-ca3-A	81.4	68.0	31.1	−122.4	−81.9	58.8	−125.4
caNoG2	cap-ca3-B	85.6	70.7	36.0	−102.1	−69.9	59.6	−137.8
caNoG3	cam-ca3	94.8	80.5	4.7	149.8	−69.4	60.0	−127.2
caNoG4	cap-ca1	104.8	70.4	29.9	−118.3	−81.9	84.5	73.8
caNoG5	cep-ce1	119.0	142.5	−10.4	−154.8	−158.3	66.7	73.2
caNoG6	cep-ce8	119.4	140.0	−9.7	−156.4	−154.7	−174.6	−52.5
caNoG7	cep-ca1	122.6	145.7	−11.0	−155.6	−74.2	58.5	92.9
caNoG8	cep-ca3	123.0	134.3	−10.7	−156.4	−77.8	54.4	−169.9
caNoG9	cep-ce6	124.4	141.3	−10.2	−155.5	−157.5	−56.2	−176.8
caNoG10	cep-ca6	124.5	141.8	−10.6	−155.2	−103.0	−53.7	177.5
caNoG11	cep-ca5	127.4	143.6	−11.0	−154.8	−103.0	−53.9	−79.3
taNoG3	tem-ta1	127.5	149.5	−13.7	94.4	−74.6	57.3	92.8
caNoG12	cep-ce5	129.3	141.9	−10.4	−155.3	−156.8	−57.3	−96.0
taNoG4	tep-te1	130.0	151.7	−14.8	−152.2	−159.3	66.8	71.9
caNoG13	cem-ca1	130.4	155.9	−13.7	113.3	−72.0	55.8	92.1
taNoG5	tem-te1	130.4	147.5	−13.5	94.0	−159.5	66.4	72.2
caNoG14	cep-ce3	130.5	141.6	−9.8	−155.3	−145.8	54.1	172.0
taNoG6	tep-te8	131.9	152.8	−15.1	−150.6	−155.8	−174.8	−52.5
taNoG7	tem-te8	133.1	148.2	−13.8	94.1	−155.6	−175.5	−52.3
taNoG8	tep-ta1	134.5	154.6	−15.0	−148.2	−74.9	57.5	92.7
taNoG9	tep-te6	135.9	153.2	−15.0	−149.5	−158.1	−55.4	−175.1
taNoG10	tep-ta6	136.0	153.6	−15.0	−149.6	−101.4	−53.0	179.8
taNoG11	tep-ta3	137.4	155.5	−15.0	−146.9	−77.9	50.9	164.2
taNoG12	tep-ta5	137.5	152.7	−14.9	−150.9	−99.6	−53.9	−80.2
taNoG13	tem-ta5	139.2	148.0	−13.6	94.7	−102.3	−53.5	−78.2
taNoG14	tep-te5	140.4	152.6	−14.9	−150.2	−157.2	−56.6	−97.7
taNoG15	tep-te3	143.7	152.3	−14.5	−151.0	−147.8	53.7	162.8
caNoG15	cep-ca9	158.7	138.7	−9.4	−156.8	−81.4	−176.8	−167.9

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. The φ_4, φ_5, and φ_6 torsions are defined in Table S1. The torsion angles φ_{11}, φ_{12}, and φ_{13} are: Cu–N11–C12–C11, N11–C12–C11–O11, HO13–O13–Cu–N11. The atom labels are defined in Figure 5.

Table S9. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 69 Cu(L-*a*Thr)$_2$ conformers in the Oo-G coordination mode[a]

name	conformer	ΔV	φ_7	φ_8	φ_9	φ_{10}	φ_4	φ_5	φ_6
taOoG1	te4dm-te8	55.6	−53.1	67.7	−6.6	155.8	−153.5	−175.8	−50.7
taOoG2	ttb2p-te8	56.8	−1.8	53.6	−14.0	−171.6	−153.7	−176.0	−50.9
taOoG3	te4dm-te1	57.1	−52.4	68.0	−7.0	155.5	−159.4	68.5	71.1
taOoG4	ttb2p-te1	57.3	1.2	52.4	−14.5	−172.3	−158.9	68.5	71.0
taOoG5	ttb2m-te8	57.5	−20.3	58.8	−13.4	172.3	−153.6	−175.8	−50.7
taOoG6	te3um-te8	62.2	67.3	−69.5	−3.0	79.3	−154.7	−176.5	−50.4
taOoG7	te3um-te1	63.5	68.5	−67.5	−6.9	79.6	−159.2	68.4	70.1
taOoG8	te3dm-ta1	64.0	−51.6	70.0	−4.2	149.0	−75.6	57.3	87.0
taOoG9	te3dm-ta6	65.1	−54.9	68.0	−6.6	155.2	−105.5	−56.2	177.9
taOoG10	ttb2p-ta1-A	65.4	1.3	54.1	−11.4	−176.6	−77.5	59.5	84.4
taOoG11	te3dm-te6	65.8	−55.1	68.3	−6.2	155.5	−153.2	−56.7	−176.5
taOoG12	te4dm-ta5	65.9	−53.8	68.0	−7.3	154.7	−104.7	−56.1	−74.1
taOoG13	ttb2p-ta6	66.4	1.5	51.8	−15.1	−172.6	−108.1	−55.6	179.0
taOoG14	ttb2p-te6	66.6	1.7	52.2	−14.4	−171.9	−152.3	−56.8	−176.3
taOoG15	ttb2p-ta5	67.1	−1.2	53.5	−14.1	−171.9	−106.1	−55.9	−74.2
taOoG16	te4dm-ta6	67.2	−19.6	58.1	−14.8	171.2	−107.0	−55.9	178.6
taOoG17	te3um-ta1	68.8	64.3	−69.0	−7.8	85.6	−75.0	57.0	82.4
taOoG18	te3dm-ta3	68.9	−56.8	68.9	−5.0	154.1	−80.8	54.4	177.7
taOoG19	te4dm-te3	69.7	−53.6	68.2	−6.8	155.0	−144.5	54.6	173.8
taOoG20	ttb2p-ta3-A	69.7	3.6	52.4	−12.8	−172.2	−83.7	55.1	174.7
taOoG21	ttb2p-te3	70.4	1.2	52.5	−14.3	−172.1	−146.5	55.1	172.4
taOoG22	ttb2p-a2	72.6	−7.1	56.8	−11.6	−162.3	−74.7	54.0	−107.1
taOoG23	te3um-ta6	73.5	66.6	−67.8	−7.7	83.0	−109.1	−55.3	178.8
taOoG24	te3um-te6	73.7	67.6	−67.9	−6.2	80.8	−149.8	−56.7	−176.4
taOoG25	te3um-ta5	74.0	66.9	−67.6	−7.8	82.4	−105.5	−56.3	−73.5

taOoG26	te3up-ta1	74.4	60.2	−66.0	8.0	−163.6	−79.6	60.2	84.0
taOoG27	tch1p-ta3	76.0	46.0	−55.4	44.9	−166.0	−72.7	59.7	−122.6
taOoG28	te3um-ta3	76.4	66.1	−68.0	−8.7	83.9	−81.9	51.5	164.3
taOoG29	te3um-te5	76.7	66.9	−67.8	−7.3	82.3	−144.4	−57.2	−79.1
taOoG30	te3um-ta2	77.0	65.1	−73.1	9.2	75.1	−73.7	52.7	−98.2
taOoG31	te3um-te3	77.7	67.7	−67.6	−6.8	80.8	−146.7	54.7	172.2
taOoG32	te4dm-ta1	77.8	−38.9	72.6	−13.4	142.6	−75.4	57.3	86.3
taOoG33	ttb2p-ta1-B	78.7	−0.6	56.9	−13.0	−177.8	−78.1	59.2	85.6
taOoG34	ttb2p-ta3-B	80.7	0.7	57.0	−11.8	−170.6	−82.2	56.0	−176.8
taOoG35	te4dm-ta3	82.7	−41.4	71.5	−15.1	148.3	−80.8	53.8	177.1
taOoG36	te4up-ta1	87.9	49.2	−68.7	17.6	−159.2	−79.9	60.4	84.3
taOoG37	ttb1m-ta1	89.1	20.2	−64.2	11.0	148.8	−75.9	56.5	88.0
caOoG1	ce3um-ca1	89.6	74.4	−64.6	−9.8	70.4	−71.5	51.8	89.6
taOoG38	ttw1m-ta3	89.9	−64.0	33.4	48.1	158.6	−71.3	59.5	−124.4
taOoG39	ttw1p-ta3	90.3	−54.6	30.2	48.3	−121.8	−71.2	60.0	−122.6
caOoG2	ce3um-ce8	92.2	73.8	−67.4	−5.1	69.0	−156.8	−176.2	−50.5
caOoG3	ce3um-ce1	92.5	72.6	−68.4	−3.9	70.1	−160.4	67.3	69.8
caOoG4	ctb2m-ca1-A	95.5	22.0	45.5	−8.3	55.0	−71.6	51.1	92.5
taOoG40	te3dm-ta9	96.6	−57.4	68.1	−6.2	156.0	−83.2	179.0	−170.8
taOoG41	ttb2m-ta3	97.7	19.3	48.8	−8.3	57.4	−83.4	54.3	177.5
taOoG42	ttb2p-ta9	98.5	0.7	52.4	−14.7	−170.6	−82.9	−179.5	−171.7
caOoG5	ce3um-ca6	99.8	75.1	−64.6	−9.7	69.4	−98.3	−55.2	177.7
caOoG6	ctb2m-ce8	100.5	25.1	43.5	−8.2	50.9	−156.5	−175.3	−51.2
caOoG7	ctb2m-ce1	100.7	24.3	44.1	−8.4	51.9	−159.9	67.4	71.0
caOoG8	ctb1p-ca2	101.0	−17.7	−54.4	5.9	−49.2	−94.3	68.1	−35.5
caOoG9	ce3um-ce6	101.0	74.7	−65.8	−7.3	68.9	−156.8	−56.3	−176.0
caOoG10	ce3um-ca5	101.4	74.8	−65.9	−7.6	68.8	−98.6	−55.8	−76.9
caOoG11	ce3um-ce5	105.1	74.2	−66.5	−6.5	69.2	−155.0	−58.0	−87.5
taOoG43	te3um-ta9	105.3	66.6	−68.9	−4.4	81.2	−82.7	−176.3	−163.4
caOoG12	ctb2m-ca6	106.3	24.9	43.6	−8.8	51.4	−98.0	−54.6	177.8
caOoG13	ctb2m-ce6-A	107.6	25.4	43.4	–8.0	50.5	–156.3	–55.7	–175.5
caOoG14	ce4dp-ca1-A	107.6	−45.2	70.1	−5.4	−118.7	−71.6	50.1	91.7

caOoG15	ctb2m-ca5	108.0	24.3	44.2	−8.4	51.7	−98.0	−55.3	−77.7
caOoG16	ce4dp-ca1-B	108.4	−29.9	68.3	−9.2	−117.7	−65.9	48.4	104.2
caOoG17	ce4dp-ca1-C	108.6	−22.3	63.3	−19.2	−116.6	−72.2	51.4	95.6
taOoG44	ttw1p-ta1	109.1	−48.0	22.5	50.3	−113.5	−87.9	80.1	75.0
caOoG18	ctb2m-ca1-B	109.6	17.5	50.2	−7.7	55.9	−71.6	52.0	91.8
caOoG19	ctb2p-ce8	111.1	−26.4	67.3	−6.9	−140.3	−155.8	−174.4	−51.1
caOoG20	ctb2m-ce5	112.0	24.9	43.7	−8.4	51.3	−152.5	−57.6	−88.8
caOoG21	ce4dp-ce1	112.7	−37.8	69.6	−4.2	−128.7	−158.8	67.6	70.7
caOoG22	ctb2m-ce6-B	113.7	6.2	53.7	–11.8	156.8	–159.4	–56.1	–176.7
caOoG23	ce4um-ca1	117.8	22.1	−66.6	15.1	129.9	−89.6	69.4	76.8
caOoG24	ctw1p-ca1	135.2	−65.3	16.3	46.1	−74.8	−73.2	55.8	85.0
caOoG25	ce4dm-ca2	141.3	4.9	51.4	−19.0	165.1	−80.1	89.6	−68.4

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. The φ_4, φ_5, and φ_6 torsions are defined in Table S1. The torsion angles φ_7, φ_8, φ_9, and φ_{10} are: Cu–O13–C13–C12, O13–C13–C12–C11, Cu–C12–C11–O11, HO13–O13–Cu–O11. The atom labels are defined in Figure 5-

Table S10. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 38 Cu(L-*a*Thr)$_2$ conformers in the Oo-Oo coordination mode[a]

name	conformer	ΔV	φ_7	φ_8	φ_9	φ_{10}	φ_{14}	φ_{15}	φ_{16}	φ_{17}
taOoOo1	te3dm-te3dm	99.7	−56.2	68.3	−6.8	153.7	−56.1	68.2	−6.8	153.7
taOoOo2	te3dm-ttb2p-A	102.6	2.2	51.9	−13.3	−173.1	−59.3	68.3	−5.2	155.7
taOoOo3	te3um-te4dm-A	109.0	63.1	−69.3	−7.2	87.9	−52.8	68.2	−8.4	150.5
taOoOo4	te3dm-te4dm-A	114.1	−56.7	68.8	−6.5	152.2	−46.3	71.5	−16.8	149.9
taOoOo5	te3dm-ttb2p-B	114.8	−59.8	68.3	−5.3	156.4	2.3	54.6	−13.9	−173.2
taOoOo6	te3dm-te4dm-B	116.2	−58.0	68.4	−5.9	154.1	−18.5	61.3	−15.8	167.6
taOoOo7	te4dm-tbt2p-A	117.9	3.7	51.2	−13.5	−176.4	−46.8	72.0	−15.5	150.5
taOoOo8	ttb2p-ttb2p	118.2	−3.7	54.8	−11.2	−168.7	−1.7	57.8	−11.9	−170.0
taOoOo9	te4dm-ttb2m	118.5	−13.1	56.4	−13.9	171.1	−47.0	72.2	−15.6	149.3
taOoOo10	te4dm-ttb2p-B	119.8	0.9	53.2	−11.8	−172.1	−20.1	61.7	−15.5	171.0
taOoOo11	tbt2p-te4up	122.1	−8.7	58.1	−7.8	−158.1	48.9	−68.5	19.0	−156.6
taOoOo12	te3dm-te4up	122.5	−60.2	66.8	−5.9	161.0	52.1	−68.7	16.4	−159.9
taOoOo13	te3um-te4dm-B	122.7	62.2	−69.7	−7.3	89.1	−42.8	70.7	−17.0	145.8
taOoOo14	te3um-ttb2p	122.8	63.6	−72.0	−0.2	82.9	3.8	54.8	−12.7	−172.6

taOoOo15	tbt1m-te4dm	124.5	−54.9	67.8	−8.1	154.8	19.1	−63.4	9.6	151.7
taOoOo16	ttb1m-ttb2p	125.5	0.9	53.0	−12.7	−168.0	10.7	−58.9	14.1	163.1
taOoOo17	te3um-te4up	132.0	71.6	−68.7	1.3	70.7	47.6	−68.1	18.4	−153.0
taOoOo18	tbt1m-te3um	134.1	66.8	−67.3	−9.0	83.8	16.8	−62.7	9.5	150.7
taOoOo19	ttb2p-ttw1m	137.8	0.1	53.7	−12.0	−165.2	−71.8	39.3	34.1	160.3
taOoOo20	te3dm-ttw1m	138.0	−55.9	67.7	−7.6	156.7	−72.2	43.9	30.8	158.0
caOoOo1	ce3um-ctb2m-A	141.1	−13.8	62.6	−11.2	129.1	75.8	−65.3	−8.2	67.4
caOoOo2	ce3um-ctb1p	152.8	61.8	−77.9	13.0	74.8	27.6	−66.2	11.8	−139.5
caOoOo3	ctb2p-ctb2p-A	154.4	1.5	55.7	−12.6	−170.2	−0.3	56.7	−12.4	−167.5
caOoOo4	ce3um-ctb2m-B	156.1	75.5	−66.0	−6.8	67.3	−20.0	68.7	−11.2	125.1
caOoOo5	ctb1p-ctw1p-A	156.8	−14.0	−58.7	1.2	−49.7	−59.7	29.2	49.8	−110.2
caOoOo6	ce3um-ctb2m-C	158.6	74.0	−64.8	−10.8	72.7	16.0	50.6	−11.7	64.0
caOoOo7	ctb2m-ctb2m-A	161.9	24.6	44.6	−8.1	50.6	−20.3	68.3	−12.8	127.9
caOoOo8	ctb2m-ctb2m-B	163.5	−10.4	60.6	−12.4	136.3	22.5	46.9	−9.5	51.7
caOoOo9	ctb1p-ctw1p-B	164.0	−13.8	−58.6	5.9	−173.4	−63.3	20.7	50.3	−84.2
caOoOo10	ce4up-ctb2m-A	164.5	25.3	43.8	−7.4	49.9	45.8	−67.4	9.8	−155.7
caOoOo11	ce4um-ce4um	165.8	59.0	−77.3	17.4	77.0	35.0	−69.8	19.1	104.3
caOoOo12	ctb2p-ctb2p-B	170.2	6.9	53.3	−12.4	−179.7	−25.9	72.3	−9.2	−138.8
caOoOo13	ce4up-ctb2p	170.7	3.4	54.1	−12.7	−176.5	31.6	−69.8	6.8	−125.3
caOoOo14	ctb2p-ctb2p-C	170.9	3.6	55.0	−12.5	−171.9	−2.8	59.8	−14.0	−167.6
caOoOo15	ce4up-ctb2m-B	177.7	23.6	44.9	−7.7	52.1	29.2	−66.4	17.2	−141.7
caOoOo16	ce4up-ctb2m-C	178.0	21.9	46.2	−7.5	53.8	21.3	−65.6	16.7	−133.3
caOoOo17	ce4um-ctb2m	179.7	21.0	46.5	−9.5	56.6	44.3	−70.6	14.3	112.8
caOoOo18	cbt2m-ce4um	182.9	−4.6	61.3	−9.8	105.6	60.0	−71.1	21.9	80.4

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. The φ_7, φ_8, φ_9, and φ_{10} torsions are defined in Table S2. The torsion angles φ_{14}, φ_{15}, φ_{16}, and φ_{17} are: Cu–O23–C23–C22, O23–C23–C22–C21, Cu–C22–C21–O21, HO23–O23–Cu–O21. The atom labels are defined in Figure 5.

Table S11. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 13 Cu(L-*a*Thr)$_2$ conformers in the Oo-No coordination mode[a]

name	conformer	ΔV	φ_7	φ_8	φ_9	φ_{10}	φ_{18}	φ_{19}	φ_{20}
taOoNo1	te4dp-tap	108.5	−31.2	68.3	−8.1	−117.4	55.1	−31.1	−140.6
caOoNo1	ctb1p-cem	157.9	−9.8	−61.5	7.0	−176.3	145.3	−13.1	89.8

taOoNo2	te3um-tep	158.9	69.5	−72.9	5.9	68.9	144.7	−12.4	−152.5
caOoNo2	ce3um-cep	165.4	66.2	−76.0	11.1	70.2	150.9	−15.1	−151.5
taOoNo3	te4dp-tep	170.3	−43.2	68.9	−0.6	−129.2	140.1	−9.7	−156.0
taOoNo4	te4dm-tep	172.4	−48.7	68.4	−3.6	159.7	140.6	−9.8	−156.7
caOoNo3	ce3um-cem	173.7	62.8	−75.3	4.7	79.3	156.3	−15.5	112.0
taOoNo5	ttb2m-tep	177.6	21.7	44.6	−9.3	57.6	144.1	−12.5	−154.6
caOoNo4	ctb2m-cep	180.3	23.0	44.4	−10.7	55.9	152.1	−15.2	−150.5
caOoNo5	ce4dm-cem	181.3	−43.2	69.8	−5.0	145.5	150.7	−14.4	96.6
caOoNo6	ce4dp-cep	181.4	−44.8	70.0	−3.1	−121.9	156.7	−15.9	−142.3
taOoNo6	ttb2m-tem-A	182.4	−8.3	56.6	−14.2	178.3	153.6	−13.8	111.8
taOoNo7	ttb2m-tem-B	187.8	22.8	43.9	−10.4	57.3	157.5	−15.3	116.9

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. The φ_7, φ_8, φ_9, and φ_{10} torsions are defined in Table S2. The torsion angles φ_{18}, φ_{19}, and φ_{20} are: Cu−N21−C22−C21, N21−C22−C21−O21, HO23−O23−Cu−N21. The atom labels are defined in Figure 5.

Table S12. Characteristic torsion angles (°) and B3LYP/BS0 relative electronic energy ΔV (kJ mol^{-1}) of 4 Cu(L-*a*Thr)$_2$ conformers in the No-No coordination mode[a]

name	conformer	ΔV	φ_{11}	φ_{12}	φ_{13}	φ_{18}	φ_{19}	φ_{20}
caNoNo1	cep-cep	223.9	153.4	−15.3	−146.8	153.7	−15.4	−146.8
taNoNo1	tep-tep	227.1	150.5	−14.4	−152.0	150.5	−14.4	−151.7
caNoNo2	cem-cem	229.8	150.9	−14.5	100.5	152.0	−14.7	101.7
taNoNo2	tam-tam	257.0	108.0	1.4	171.2	104.3	3.7	170.7

[a] The conformers are depicted in Figure S1. The reference energy value V_0 is given in Table S1. The φ_{11}, φ_{12}, and φ_{13} torsions are defined in Table S3. The φ_{18}, φ_{19}, and φ_{20} torsions are defined in Table S5.

Table S13. Means and standard deviations (in parentheses) of B3LYP/BS0 Cu–donor in-plane bond lengths (in Å) and six valence angles (in degree) around the copper atom in a number of conformers (*n*) of *trans*- and *cis*-Cu(L-Thr)$_2$ conformers in six possible coordination modes.

Internal	G-G		No-G		Oo-G		Oo-Oo		Oo-No		No-No	
coordinate	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*
n	35	22	16	16	39	23	13	15	7	6	1	3
Cu–N_{am}	2.04(1)	2.068(9)	2.00(3)	2.02(4)							2.000	2.04(3)
Cu–N_{am}'	2.033(5)	2.064(7)	2.05(1)	2.06(2)	2.03(1)	2.034(8)			1.992(3)	2.01(2)	1.998	2.04(4)
Cu–O	1.94(1)	1.942(1)			1.91(1)	1.90(2)	1.90(1)	1.92(4)	1.90(1)	1.92(1)		
Cu–O'	1.932(7)	1.936(7)			1.924(9)	1.95(2)	1.889(6)	1.90(3)				
Cu–O_h			1.94(1)	1.92(2)	2.03(1)	2.11(3)	2.02(2)	2.09(6)	2.04(1)	2.08(5)	2.087	2.11(4)
Cu–O_h'			2.05(6)	2.06(3)			2.022(7)	2.08(5)	2.03(1)	2.04(6)	2.087	2.03(8)
N_{am}–Cu–O	83.6(9)	82.3(8)										
N_{am}'–Cu–O'	84.2(6)	82.7(4)	83.7(9)	83(1)	83.9(8)	83.2(9)						
N_{am}–Cu–N_{am}'	177(3)	100(1)	175(3)	104(2)							177.1	104.3(8)
N_{am}–Cu–O'	96.1(6)	176(2)	95.3(9)	170(3)								
N_{am}'–Cu–O	96(1)	176(2)			94(1)	167(5)			166(3)	94.2(9)		
N_{am}'–Cu–O_h'									82.5(7)	83(1)	81.7	83(1)
N_{am}'–Cu–O_h			99(2)	169(11)	171(2)	93(1)			96(1)	170(1)	98.7	172.2(9)
N_{am}–Cu–O_h			83(1)	82(1)							81.5	82(1)
N_{am}–Cu–O_h'											98.1	170(3)
O–Cu–O'	177(2)	95.5(4)			174(3)	98(3)	172(5)	100(4)				
O_h–Cu–O					93(1)	91(3)	93(1)	91(3)	93.9(8)	94(2)		
O_h–Cu–O'			173(3)	92(2)	90(2)	160(10)	89(3)	154(13)				
O'–Cu–O_h'							94(1)	94(2)				
O–Cu–O_h'							85(1)	150(17)	89.5(8)	173(5)		
O_h–Cu–O_h'							172(5)	87(5)	169(6)	89(2)	179.4	91(2)

Table S14. Means and standard deviations (in parentheses) of B3LYP/BS0 Cu–donor in-plane bond lengths (in Å) and six valence angles (in degree) around the copper atom in a number of conformers (*n*) of *trans*- and *cis*-Cu(L-*a*Thr)$_2$ conformers in six possible coordination modes

	G-G		No-G		Oo-G		Oo-Oo		Oo-No		No-No	
	Trans	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*
n	68	45	15	15	44	25	20	18	7	6	2	2
Cu–N_{am}	2.04(1)	2.07(1)	2.00(3)	2.01(2)							2.002(1)	2.024(2)
Cu–N_{am}'	2.037(9)	2.068(9)	2.05(1)	2.06(2)	2.04(1)	2.04(1)			2.00(2)	2.007(2)	2.003(1)	2.025(3)
Cu–O	1.93(1)	1.94(1)			1.91(2)	1.90(2)	1.89(1)	1.91(2)	1.89(2)	1.92(2)		
Cu–O'	1.930(8)	1.935(8)	1.94(1)	1.92(2)	1.92(1)	1.96(5)	1.888(4)	1.91(2)	2.200			
Cu–O_h				2.06(3)	2.03(4)	2.12(6)	2.01(2)	2.09(5)	2.06(4)	2.08(5)	2.08(4)	2.126(7)
Cu–O_h'							2.02(1)	2.09(8)	2.07(5)	2.08(3)	2.08(4)	2.126(6)
N_{am}–Cu–O	84.0(8)	82.4(6)	83.8(8)	83(1)								
N_{am}'–Cu–O'	84.2(8)	82.7(5)			83.8(8)	83(1)						
N_{am}–Cu–N_{am}'	177(2)	99.7(8)	177(2)	103(1)							175(1)	106.5(1)
N_{am}–Cu–O'	96.0(8)	176(2)	95.3(8)	171(2)	94(2)	165(9)						
N_{am}'–Cu–O	95.9(6)	176(2)							167(4)	95(2)		
N_{am}'–Cu–O_h'					171(8)	94(3)			82(2)	83.1(6)	81.6(1)	83(1)
N_{am}'–Cu–O_h			98(1)	167(13)					97.3(7)	170(2)	98.8(4)	166.6(7)
N_{am}–Cu–O_h			83(1)	82.4(6)							81.4(3)	83(1)
N_{am}–Cu–O_h'											98.8(6)	167.0(7)
O–Cu–O'	177(2)	95.5(4)			174(3)	100(6)	172(4)	101(4)				
O_h–Cu–O					92(2)	89(4)	92.9(8)	90(4)	92(3)	92(3)		
O_h–Cu–O'			172(3)	93(3)	90(3)	156(25)	89(2)	155(9)				
O'–Cu–O_h'							93(1)	92(3)				
O–Cu–O_h'							86(2)	152(18)	91(2)	173(6)		
O_h–Cu–O_h'							173(4)	89(7)	170(5)	89(1)	174(6)	89(1)

Table S15. The most stable vacuum *trans* and *cis* Cu(L-Thr)$_2$ and Cu(L-*a*Thr)$_2$ conformers in the six coordination modes, which were the starting structures for B3LYP/BS0 geometry optimization using PCM, their corresponding aqueous minima, and their relative vacuum electronic energies, and relative aqueous electronic and Gibbs free energies (ΔV and ΔG, in kJ mol^{-1})[a,b]

Cu(L-Thr)$_2$					Cu(L-*a*Thr)$_2$				
vacuum conformer	ΔV_{vacuum}	aqueous conformer / mode[c]	ΔV_{water}	ΔG_{water}	vacuum conformer	ΔV_{vacuum}	aqueous conformer / mode[c]	ΔV_{water}	ΔG_{water}
G-G					**G-G**				
te1-te1	0.0		0.0	0.0	te8-te8	7.4		–6.4	–0.3
te1-te8	7.0		1.5	3.1	te1-te8	8.6		2.2	6.0
te1-ta6	10.5		6.1	3.9	te1-te1	10.5		11.0	12.2
ta5-te1	10.9		4.3	4.6	te8-ta1	16.5		2.7	7.6
te3-ta5 (X-ray)[d]			6.4	2.9	te8-ta6	16.9		4.8	6.5
te1-te6	13.8		12.5	11.0	ca1-ca1	51.1		16.6	14.8
ce1-ce1	43.8		5.5	3.7	ce1-ca1	51.7		15.2	19.1
ce1-ca1	49.5		11.4	13.3	ce8-ca1	52.0		6.5	10.7
ce1-ca5	51.0		8.8	10.8	ce1-ce1	53.2		15.5	16.9
ce1-ca6	51.9		10.8	10.8	ce1-ce8	55.2		7.1	12.0
ce1-ce8	54.6		6.8	9.6	ce8-ce8	56.9		–1.1	4.4
ce8-ce8	65.0		8.7	13.9					
No-G					**No-G**				
tap-te1	*41.3*		*44.8*	*41.1*	*tap-ta1*	*54.1*		*50.0*	*52.9*
tap-ta1	*56.1*		*53.5*	*55.3*	*tap-ta3*	*59.2*		*50.2*	*51.5*
tap-ta2	*61.4*	*tap-ta3*	*55.0*	*52.2*	cap-ca3-A	81.4		50.3	54.8
cap-ca4	62.8		36.9	44.5	cap-ca3-B	85.6		52.4	60.2
cap-ca2-A	75.0	cap-ca2	65.8	76.0	cam-ca3	94.8		46.6	53.8
cap-ca3A	82.8	cap-ca3	44.8	55.6	cap-ca1	104.8		80.7	87.0
cap-ce6	84.1	ca1-ce6 / G-G	23.7	21.2	cep-ce1	119.0		57.2	60.3
cap-ca2-B	85.2	cap-ca3	44.8	55.6	cep-ce8	119.4		49.6	53.4
cap-ca3-B	89.7		54.5	64.1	cep-ca1	122.6		55.7	58.4
cap-ca3-C	91.7		52.6	53.1	tem-ta1	127.5		58.6	61.9
tem-te1	116.7		51.6	49.8	tep-te1	130.0		59.5	60.1
tep-te1	117.1		50.2	48.5	tem-te1	130.4		61.1	63.9
Oo-G					**Oo-G**				

te4dm-te1-A	49.4	ttw2m-te1	54.8	48.8	te4dm-te8	55.6		52.9	54.0
tbt2p-te1-A	53.5	tbt2p-te1	56.8	47.9	ttb2p-te8	56.8	ttb2m-te8	55.5	53.0
ttw1m-te1	56.6		57.6	50.9	te4dm-te1	57.1	te3dm-te1	61.3	59.4
te4dm-te8	57.2	ttw2m-te8	56.7	57.4	ttb2p-te1	57.3	ttb2m-te1	63.7	59.3
te4dm-ta5	60.1	ttw2m-ta5	59.1	56.2	ttb2m-te8	57.5	te4dm-te8	52.9	54.0
ctw1m-ce1	86.5		60.3	59.1	ce3um-ca1	89.6		64.7	64.6
cbt1m-ca1	86.7		69.3	75.9	ce3um-ce8	92.2		58.7	58.7
ctw1m-ca1	90.9		65.9	61.5	ce3um-ce1	92.5		66.9	64.3
ctw1m-ca6	94.2		66.0	62.9	ctb2m-ca1-A	95.5	ctb2m-ca1	71.9	67.9
ctw1m-ca5	94.6		64.1	62.2	ce3um-ca6	99.8		69.1	68.9
Oo-Oo					**Oo-Oo**				
te4dm-te4dm-A	95.5	te3dm-te3dm	109.4	104.1	te3dm-te3dm	99.7		110.8	104.5
te4dm-te4dm-B	107.7	te3dm-te4dm	113.6	106.0	te3dm-ttb2p-A	102.6		114.0	105.4
tbt2p-te3dm	112.4	tbt2p-ttw1m	115.4	109.4	te3um-te4dm-A	109.0	te3dm-te3um	114.3	111.9
tbt2p-tbt2p	117.3	tbt2p-tbt2p	117.1	108.7	te3dm-te4dm-A	114.1		116.8	110.8
tbt4m-te4dm	117.3		116.6	113.9	te3dm-ttb2p-B	114.8		117.8	111.0
tbt2p-te3um	122.1	tbt2p-te3um	118.3	110.5	te3dm-te4dm-B	116.2		116.8	110.8
ce3um-ctb1m	126.8	ce3um-ca3 / Oo-G	65.7	63.7	ce3um-ctb2m-A	141.1	ce3um-ce4dm	123.3	112.7
ctb2m-ctw1m-A	137.7	ce3um-ce4dm	118.6	111.5	ce3um-ctb1p	152.8	ce3um-ce4up	123.1	120.1
cbt2m-ctb1m	150.7	ce4dm-ca3 / Oo-G	72.7	69.1	ctb2p-ctb2p-A	154.4	cbt2m-ctb2m	129.8	119.5
ctb2m-ctw1m-B	151.4	ce3um-ce3up	123.9	121.1	ce3um-ctb2m-B	156.1	ce3um-ce4dm	125.9	120.8
ce3um-ctb1p	154.2	ce3um-ce3up	123.9	121.1	ctb1p-ctw1p-A	156.8	ce4dp-ca1 / Oo-G	75.9	74.0
					ce3um-ctb2m-C	158.6	ce3um-ce4dm	125.9	120.7
					cbt2m-ce4um	182.9	ce4um-ctb2m	135.3	125.0
Oo-No					**Oo-No**				
cbt2p-cap	*96.2*		*98.9*	*98.2*	te4dp-tap	108.5	ce3dp-ca1 / Oo-G	68.9	69.3
cbt1m-cem	151.2	tem-ta3 / No-G	56.0	56.5	ctb1p-cem	157.9	tem-ta3 / No-G	58.4	59.5
te3um-tep	151.5		104.9	102.4	te3um-tep	158.9		110.0	109.1
ttw1m-tem	159.9		109.4	109.4	ce3um-cep	165.4		111.2	110.3
te4dp-tep	162.3	ttw2p-tep	109.5	107.9	te4dp-tep	170.3	te3dp-tep	114.1	111.7
ctw1m-cem	162.7		108.9	107.1	te4dm-tep	172.4		114.3	113.3
te4dm-tep	163.4	ttw2m-tep	109.4	107.8	ce3um-cem	173.7		114.5	114.7
te4dm-tam	169.5		109.8	106.7	ttb2m-tep	177.6		116.8	112.8
ce4dm-cem	169.8		110.4	107.5	ctb2m-cep	180.3	cbt2m-cep	117.7	112.5
ctb2m-cep	173.0	ctb2m-cep	111.3	105.8	ce4dm-cem	181.3	ctw2m-cem	115.8	113.2

No-No					**No-No**				
cap-cap	*99.7*	*cap-ca1 / No-G*	*57.6*	*58.3*	cep-cep	223.9		109.7	112.9
cep-cep	211.7		101.9	101.2	tep-tep	227.1		112.6	113.4
cem-cem	212.8		105.5	105.1	cem-cem	229.8		113.9	112.4
tep-tep	212.8		104.0	103.7	tam-tam	257.0	ta3-ta3 / G-G	19.0	25.4

[a] The conformers are defined in Figure S1 and Tables S1-S12. The reference energy values are those of the Cu(L-Thr)$_2$ te1-te1 conformer: V_{vacuum}= –1071.76257129 a.u., V_{water}= –1071.80072926 a.u., G_{water}= –1071.586956 a.u.

[b] The conformers with H_h in the carboxylate group are denoted in italics.

[c] The names of the PCM optimized aqueous conformer and coordination mode are written only if the starting conformation and/or coordination mode changed during geometry optimization.

[d] The starting conformer from the X-ray crystal and molecular structure (Ref. 17).

Table S16. The most stable B3LYP/BS0 vacuum *trans* and *cis* Cu(L-Thr)$_2$ and Cu(L-*a*Thr)$_2$ conformers in the six coordination modes, which were the starting structures for the B3LYP/BS1 geometry optimization in the gas phase and in aqueous solution using PCM, and their corresponding B3LYP/BS1 relative electronic and Gibbs free energies (ΔV and ΔG, in kJ mol^{-1})[a,b,c]

Cu(L-Thr)$_2$				Cu(L-*a*Thr)$_2$			
starting conformer	ΔV_{vacuum}	ΔV_{water}	ΔG_{water}	starting conformer	ΔV_{vacuum}	ΔV_{water}	ΔG_{water}
G-G				**G-G**			
te1-te1	0.0	0.0	0.0	te8-te8	6.0	–5.7	0.8
te3-ta5 (X-ray)[d]	-	6.4	5.2	ca1-ca1	55.1	20.8	22.9
ce1-ce1	41.0	5.0	4.3	**No-G**			
No-G				*tap-ta1*	*56.3*	*53.3*	*57.1*
tap-te1	*41.8*	*45.5*	*47.1*	tem-ta1	134.7	67.6	73.0
cap-ca4	70.5	44.4	54.5	cap-ca3-A	84.4	57.5	62.6
Oo-G				**Oo-G**			
te4dm-te1-A	46.9	52.3	47.4	te4dm-te8	52.4	51.0	50.4
		ttw2m-te1					
ctw1m-ce1	84.5	60.4	59.9	ce3um-ca1	93.1	68.9	70.2
Oo-Oo				**Oo-Oo**			
te4dm-te4dm-A	90.7	104.3	99.6	te3dm-te3dm	95.3	106.7	100.8
		te3dm-te3dm		ce3um-ctb2m-A	139.2	120.0	114.2
ce3um-ctb1m	131.8	68.6	65.7			ce3um-ce4dm	

		ce3um-ca3/Oo-G					
Oo-No				**Oo-No**			
ctb2p-cap	*93.9*	*98.0*	*98.1*	te4dp-tap	114.3	70.7	72.4
						ce3dp-ca1/Oo-G	
te3um-tep	155.1	110.2	110.4	ctb1p-cem	134.7	67.1	70.2
					tem-ta1/No-G	tem-ta3/No-G	
No-No				te3um-tep	164.2	116.2	115.7
cap-cap	*89.9*	*59.8*	*60.7*	ce3um-cep	172.9	118.0	117.6
		cap-ca1/No-G					
cep-cep	222.2	113.7	113.1	**No-No**			
tep-tep	220.8	114.3	116.5	cep-cep	237.1	122.4	125.1
				tep-tep	237.8	123.8	126.2

[a] The conformers are defined in Figure S1 and Tables S1-S12. The reference B3LYP/BS1 energy values are of the Cu(L-Thr)$_2$ te1-te1 conformer: V_{vacuum}= –2516.37645582 a.u., V_{water}= –2516.41165205 a.u., G_{water}= – 2516.199097 a.u.

[b] The conformers with H_h in the carboxylate group are denoted in italics.

[c] The names of the B3LYP/BS1 vacuum and/or PCM optimized aqueous conformers and coordination mode are written under the relative energy value only if the starting conformation and/or coordination mode changed during geometry optimization.

[d] The starting conformer from the X-ray crystal and molecular structure (Ref. 17).

Table S17. Imaginary frequencies, ν (cm^{-1}), of the TS structures calculated by DFT/B3LYP and MP2 with the BS0, BS1, and BS2 basis sets, and the Q_{tunnel} factor calculated using Eq. 2.[a]

	B3LYP/BS0		B3LYP/BS1		B3LYP/BS2		MP2/BS2	
TS	ν	Q_{tunnel}	ν	Q_{tunnel}	ν	Q_{tunnel}	ν	Q_{tunnel}
				Cu(L-*a*Thr)$_2$				
TS1	78.9i	1.006	71.9i	1.005	78.2i	1.006		
TS2	78.1i	1.006	75.7i	1.006	76.8i	1.006		
TS3	31.9i	1.001	25.4i	1.001	23.7i	1.001		
TS4	35.0i	1.001	30.5i	1.001	35.7i	1.001		
TS'$_{trans\leftrightarrow cis}$	46.6i	1.002	67.8i	1.005	52.1i	1.003	43.7i	1.002
TS'$_{trans\leftrightarrow cis,a}$	68.9i	1.005	88.5i	1.008	71.9i	1.005		
TS6	39.6i	1.002	40.7i	1.002	34.0i	1.001		
TS5	43.9i	1.002	47.0i	1.002	46.0i	1.002		
TS"$_{trans\leftrightarrow cis}$	192.7i	1.037	177.3i	1.031	217.7i	1.048	222.5i	1.050
TS"$_{trans\leftrightarrow cis,a}$	213.7i	1.046	207.5i	1.043	238.8i	1.058		
TS$_{Oo\leftrightarrow G,2}$	76.2i	1.006	63.6i	1.004	65.2i	1.004	97.3i	1.009
TS$_{Oo\leftrightarrow G,3}$	80.8i	1.006	60.7i	1.004	67.5i	1.004		
				Cu(L-Thr)$_2$				
TS$_{trans\leftrightarrow cis,1}$	229.0i	1.053	210.2i	1.044	210.1i	1.044	230.1i	1.053
TS$_{trans\leftrightarrow cis,2}$	181.1i	1.033	179.8i	1.032	252.7i	1.065	225.7i	1.051
TS7	87.0i	1.007	83.4i	1.007	82.8i	1.007	87.0i	1.007
TS$_{Oo\leftrightarrow G,1}$	43.9i	1.002	33.3i	1.001	39.1i	1.002	61.4i	1.004

[a] The TS structures are illustrated in Figures S2 and S3, and their corresponding minimum structures are given in Table 6.