Supporting Information

β-Cyclodextrin-NHC-Gold(I) Complex (β-ICyD)AuCl: a Chiral Nanoreactor for Enantio- and Substrate-Selective Alkoxycyclization Reactions

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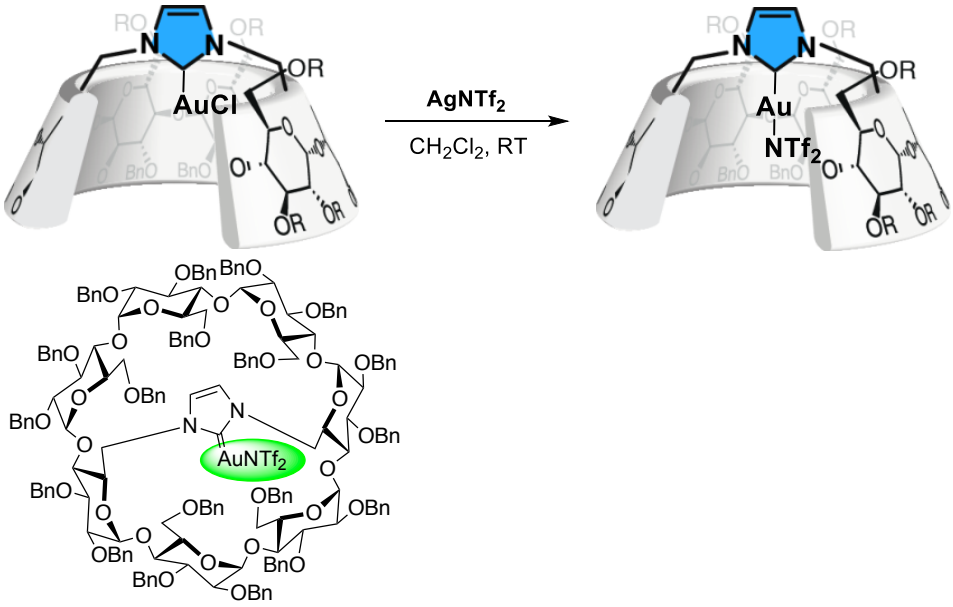
1. General information

All reactions were performed under argon atmosphere. All solvents were freshly distilled prior to use: tetrahydrofuran over sodium and benzophenone, dichloromethane over calcium hydride. Silica gel (35–70 mm) was used for column chromatography. Thin-layer chromatography (TLC) was performed on silica gel and visualized with a UV lamp (254 nm). ^{1}H NMR and ^{13}C NMR spectra were recorded at room temperature unless otherwise required on 300 and 400 MHz spectrometers with solvent resonance as the internal standard (^{1}H NMR: $CDCl_3$ at 7.26 ppm, THF-d_8 at 1.72 and 3.58, ^{13}C NMR: $CDCl_3$ at 77.16 ppm, THF-d_8 at 25.31 and 67.21, ^{31}P NMR: H_3PO_4 at 0.00 ppm and ^{19}F: NMR $CFCl_3$ at 0.00 ppm). Chemical Shifts (δ) are given in parts per million (ppm) and coupling constants (*J*) are given in Hertz (Hz). The letters m, s, d, t, q and sept, stand for multiplet, singlet, doublet, triplet, quartet and septuplet respectively. The letters bs indicated that the signal is broad. Referenced High Resolution Mass Spectra were obtained at Sorbonne Université using a mass spectrometer with an electrospray ion source (ESI) and an Orbitrap analyzer. Melting points (m.p.) were recorded with a melting point apparatus. IR data are reported as characteristic bands (cm^{-1}).

2. Synthesis of perbenzylated gold(I)-NTf_2 complex, (β-ICyD)AuNTf_2



Chemical Formula: $C_{180}H_{184}AuF_6N_3O_{37}S_2$
Molecular Weight: 3356,5130

In a flame-dried Schlenk under argon, (β-ICyD)AuCl complex (100 mg, 0.032 mmol) and $AgNTf_2$ (12 mg, 0.032 mmol, 1.0 equiv.) were dissolved in 8 mL of dichloromethane previously degassed. The reaction was protected from the light and stirred 30 minutes at room temperature. After that, the mixture was filtered over Millipore (0.20 µm), washing with dichloromethane, and concentrated under reduced pressure to afford the (β-ICyD)AuNTf_2 complex as a white solid (93.8 mg, 87 %).

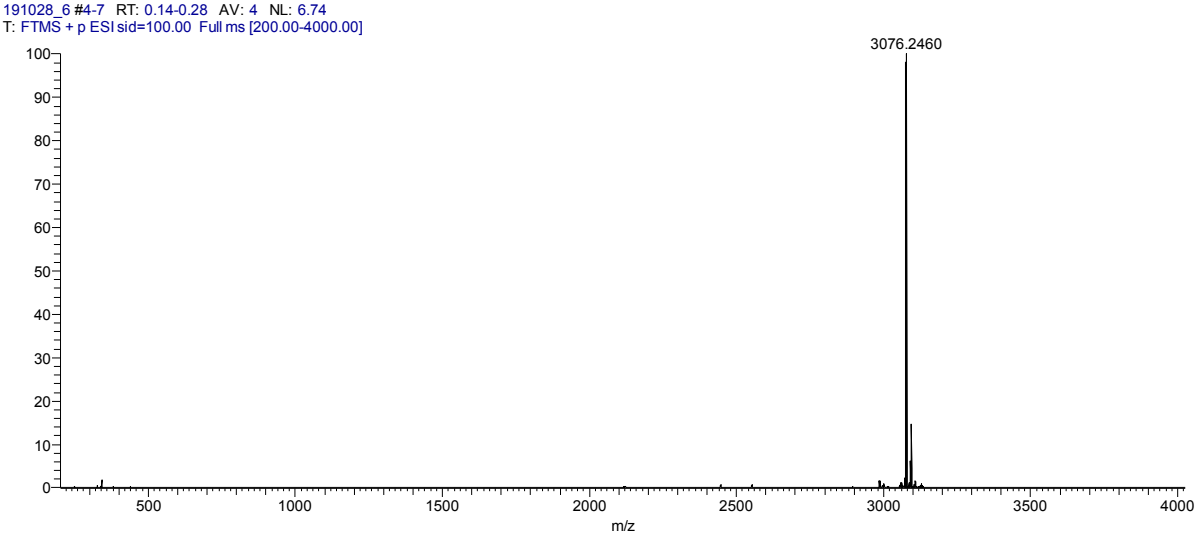
^{1}H NMR (600 MHz, 300 K, THF-d_8) δ 7.41 – 6.90 (m, 96H, H_{Ar}, 1 x N-C<u>H</u>=CH-N), 6.74 (d, ^{3}J = 1.0 Hz, 1H, N-C<u>H</u>=CH-N), 5.90 (d, ^{3}J = 3.8 Hz, 1H, H_1), 5.90 (d, ^{3}J = 3.8 Hz, 1H, H_1), 5.63 (d, ^{2}J = 11.1 Hz, 1H, <u>CH</u>Ph), 5.62 (d, ^{2}J = 11.3 Hz, 1H, <u>CH</u>Ph), 5.63 (d, ^{2}J = 12.4 Hz, 1H, C<u>H</u>Ph), 5.62 (d, ^{2}J = 11.3 Hz, 1H, C<u>H</u>Ph), 5.46 (d, ^{2}J = 11.0 Hz, 1H, C<u>H</u>Ph), 5.38 (d, ^{2}J = 11.1 Hz, 1H, C<u>H</u>Ph), 5.30 (d, ^{2}J = 11.6 Hz, 1H, C<u>H</u>Ph), 5.08 (1H, H_5), 5.07 (1H, H_1), 5.03 (1H, H_5), 5.08 – 5.00 (m, 2H, 2 x C<u>H</u>Ph), 4.98 (d, ^{2}J = 11.4 Hz, 1H, C<u>H</u>Ph), 4.87 (d, ^{3}J = 3.7 Hz, 1H, H_1), 4.93 – 4.80 (m, 9H, 9 x C<u>H</u>Ph), 4.84 (1H, H_6), 4.80

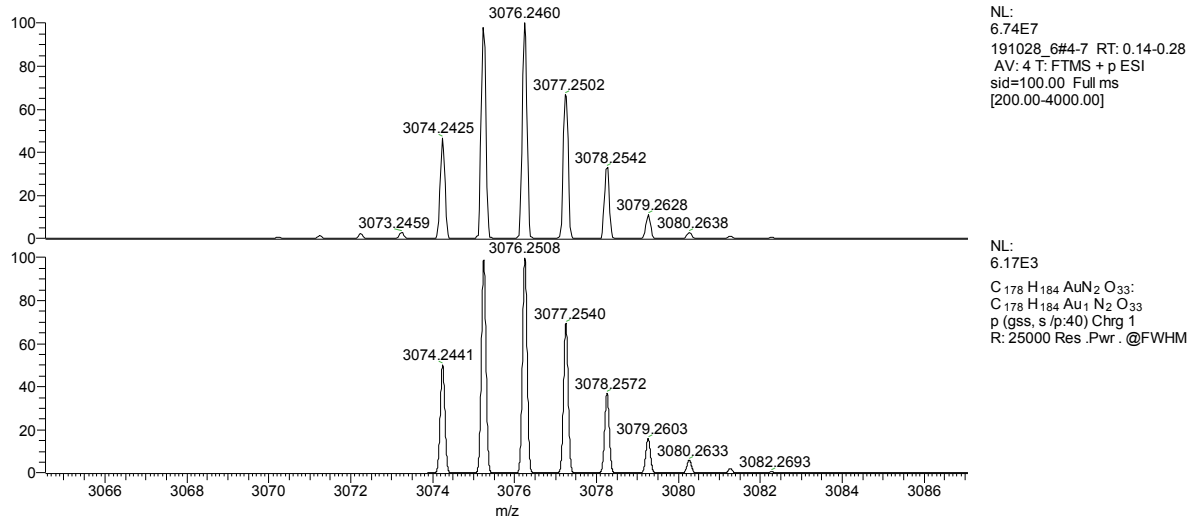
(d, ^3J = 3.4 Hz, 1H, H_1), 4.74 – 4.69 (m, 3H, 3 x C<u>H</u>Ph), 4.74 (1H, H_6), 4.72 (1H, H_1), 4.71 (1H, H_1), 4.66 (d, ^2J = 11.3 Hz, 1H, C<u>H</u>Ph), 4.63 (d, ^2J = 11.7 Hz, 1H, C<u>H</u>Ph), 4.52 – 4.41 (m, 6H, 6 x CHPh), 4.43 (1H, H_3), 4.39 – 4.16 (m, 8H, 8 x CHPh), 4.27 (1H, H_3), 4.26 (1H, H_3), 4.17 (1H, H_3), 4.06(1H, H_3), 4.03 (1H, H_6), 4.00 (1H, H_3), 3.98 (1H, H_4), 3.95 (1H, H_3), 3.95 (1H, H_6), 3.87 (1H, H_6), 3.86 (1H, H_5), 3.86 (1H, H_6), 3.85 (1H, H_6), 3.84 (1H, H_4), 3.80 (1H, H_6), 3.80 (1H, H_5), 3.78 (1H, H_6), 3.75 (1H, H_4), 3.75 (1H, H_5), 3.74 (1H, H_4), 3.71 (1H, H_6), 3.70 (1H, H_4), 3.67 (1H, H_4), 3.66 (1H, H_4), 3.63 (1H, H_5), 3.61 (1H, H_5), 3.55 (dd, 1H, H_2, ^2J = 11.9 Hz, ^3J = 3.8 Hz, 1H, H_2), 3.45 (dd, ^2J = 10.4 Hz, ^3J = 3.5 Hz, 1H, H_2), 3.44 (dd, ^2J = 10.1 Hz, ^3J = 3.3 Hz, 1H, H_2), 3.36 (dd, ^2J = 10.6 Hz, ^3J = 3.2 Hz, 1H, H_2), 3.34 (dd, ^2J = 10.1 Hz, ^3J = 3.1 Hz, 1H, H_2), 3.33 (dd, ^2J = 9.9 Hz, ^3J = 3.2 Hz, 1H, H_2), 3.29 (dd, ^2J = 11.2 Hz, ^3J = 2.8 Hz, 1H, H_6), 3.21 (dd, ^2J = 10.0 Hz, ^3J = 3.3 Hz, 1H, H_2), 3.01 (dd, ^2J = 10.7 Hz, ^3J = 5.4 Hz, 2H, 2 x H_6), 2.78 (dd, ^2J = 11.0 Hz, ^3J = 2.6 Hz, 1H, H_6).

^{13}C NMR (151 MHz, 300 K, THF-d_8) δ 162.7 (<u>C</u>-Au), 141.8, 141.7, 141.6, 141.3, 141.2, 140.5, 140.4, 140.3, 140.2, 140.2, 140.1, 140.1, 139.9, 139.8, 139.6, 139.4, 139.2, 139.0 (19 x C_{ArQuat}), 129.1, 129.1, 129.0, 129.0, 128.9, 128.9, 128.9, 128.8, 128.7, 128.7, 128.6, 128.6, 128.5, 128.5, 128,4, 128.4, 128.4, 128.3, 128.3, 128.2, 128.2, 128.1, 128.1, 128.0, 128.0, 128.0, 127.9, 127.9, 127.9, 127.6, 127.5, 127.4, 127.3, 127.2, 127.1, 127.0, 126.9, 126.6 121.9, 120.1, 119.7 (95 x C_{Ar}), 124.6 (N-<u>C</u>H=CH-N), 124.3 (N-<u>C</u>H=CH-N), 102.0 (C_1), 100.2 (C_1), 99.9 (C_1), 98.9 (C_1), 98.8 (C_1), 98.5 (C_1), 97.9 (C_1), 83.9 (C_4), 83.4 (2 x C_4) , 82.8 (C_3), 82.5 (C_4), 82.4 (C_3), 81.4 (C_4,C_2), 81.3 (C_3), 81.2 (C_3), 81.0 (C_2), 81.0 (C_3), 80.6 (C_3), 80.6 (C_3), 80.1 (C_2), 80.1 (C_2), 80.0 (C_2), 79.4 (C_2), 79.0 (C_2), 77.3 (<u>C</u>H_2Ph), 76.9 (<u>C</u>H_2Ph), 76.6 (<u>C</u>H_2Ph), 76.5 (<u>C</u>H_2Ph), 76.5 (<u>C</u>H_2Ph), 76.4 (C_4), 75.5 (<u>C</u>H_2Ph), 75.3 (<u>C</u>H_2Ph), 75.2 (C_4), 75.1 (<u>C</u>H_2Ph), 74.9 (C_5), 74.7 (<u>C</u>H_2Ph), 74.4 (C_5), 74.3 (<u>C</u>H_2Ph), 74.1 (<u>C</u>H_2Ph), 74.0 (<u>C</u>H_2Ph), 73.9 (<u>C</u>H_2Ph), 73.8 (<u>C</u>H_2Ph), 73.7 (<u>C</u>H_2Ph), 73.5 (C_5) , 73.3 (<u>C</u>H_2Ph), 73.2 (<u>C</u>H_2Ph), 73.1(<u>C</u>H_2Ph), 73.0 (<u>C</u>H_2Ph), 72.8 (C_5), 72.5 (C_5), 72.0 (C_6), 71.7 (C_5), 71.6 (C_5), 71.0 (C_6) , 70.8 (C_6) , 69.3 (C_6), 69.2 (C_6), 55.9 (C_6) , 54.8 (C_6).

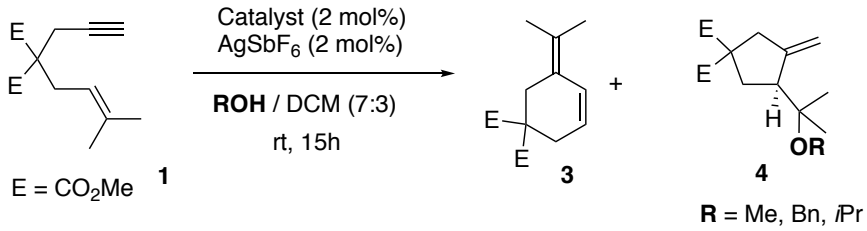
^{19}F{^{1}H}-NMR (565 MHz, CD_2Cl_2): δ = -74.4 (s, Au-NTf_2).

HRMS (ESI) calcd for ([$C_{178}H_{184}AuN_2O_{33}]^+$): 3076.2508; **found**: 3076.2460.





3. Alkoxycyclization reaction of dimethyl 2-(3-methylbut-2-en-1-yl)-2-(prop-2-yn-1-yl) malonate 1 in the presence of R-OH (R = Me, *i*Pr, Bn, H)



3.1. **General procedure A**: Generation of the cationic gold catalyst by adding the silver salt before the substrate **1**

The gold catalyst (0.004 mmol, 2 mol %, 13 mg) was dissolved in 1.5 mL of alcohol, followed by the addition of the $AgSbF_6$ solution in alcohol (1.44 mg, 0.004 mmol, 2 mol%, 1.45 mL). The substrate **1** (50 mg, 0.210 mmol) was added also in a solution of dichloromethane (1.25 mL). The final concentration of **1** was 0.05 M. The reaction was monitored by TLC (pentane/EtOAc 90:10). After completion, the mixture was filtered over a short pad of silica, washed with ethyl acetate, and concentrated under reduced pressure. The crude mixture was purified by column chromatography on silica gel (pentane/EtOAc 99:1) affording the desired product.

3.2. **General procedure B**: Adding the silver salt to the mixture of (β-ICyD)AuCl and dimethyl 2-(3-methylbut-2-en-1-yl)-2-(prop-2-yn-1-yl) malonate **1** at the end

(β-ICyD)AuCl (0.004 mmol, 2 mol%, 13 mg) was dissolved in 0.6 mL of alcohol. Then, the substrate **1** was added (50 mg, 0.210 mmol) in alcohol (2.35 mL), followed by the addition of the $AgSbF_6$ solution in dichloromethane (0.004 mmol, 2 mol%, 1.25 mL). The final concentration of **1** was 0.05 M. The reaction mixture was stirred at room temperature for 15 hours. The reaction was monitored by TLC (pentane/EtOAc, 90:10). After completion, the mixture was filtered over a short pad of silica, washed with ethyl acetate, and concentrated under reduced pressure. The crude mixture was purified by column chromatography on silica gel (pentane/EtOAc, 99:1) affording the desired products.

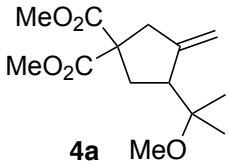
3.3. **General procedure C**: Using (β-ICyD)AuNTf$_2$ as catalyst

(β-ICyD)AuNTf$_2$ (0.004 mmol, 2 mol%, 14 mg) catalyst was dissolved in 2.2 mL of a solution of alcohol/DCM (7:3). Then dimethyl 2-(3-methylbut-2-en-1-yl)-2-(prop-2-yn-1-yl) malonate **1** was added in 2 mL of the same mixture. The final concentration of **1** was 0.05 M. The reaction mixture was stirred at room temperature for 15 hours. The reaction was monitored by TLC (pentane/EtOAc, 90:10). After completion, the mixture was filtered over a short pad of silica, washed with ethyl acetate, and concentrated under reduced pressure. The crude mixture was purified by column chromatography on silica gel (pentane/EtOAc, 99:1) affording the desired products.

3.4. Reaction with methanol as nucleophile

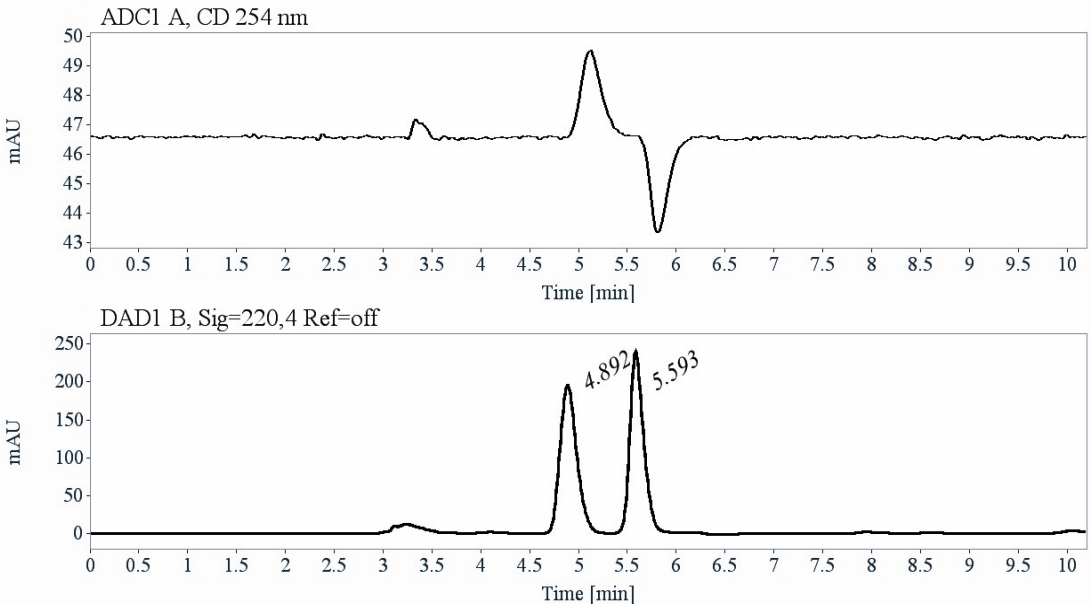
3.4.1. (IPr)AuCl-catalyzed cycloisomerization

Following procedure A: Using (IPr)AuCl (2.6 mg) as catalyst, and methanol as alcohol, dimethyl-3-(2-methoxypropane-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** was obtained as a yellow oil. (55.6 mg, 0.206 mmol, 98%). The spectral data correspond to those previously reported.[1]



^{1}H-NMR (400 MHz, $CDCl_3$): δ = 5.05 (m, 1H), 4.99 (m, 1H), 3.72 (s, 3H), 3.71 (s, 3H), 3.18 (s, 3H), 2.95-2.79 (m, 3H), 2.55 (ddd, J = 13.5, 8.5, 1.8 Hz, 1H), 2.01 (dd, J = 13.5, 9.3 Hz), 1.18 (s, 3H), 1.12 (s, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ = 172.2, 172.1, 148.4, 110.7, 76.9, 58.7, 52.9, 52.8, 49.3, 49.2, 43.5, 36.2, 22.8, 22.3.

Chromatogram recorded using a Chiralpak AD-H column, with a debit of 1 mL/min and heptane/isopropanol (95:5) as the eluent at λ = 254 nm. (±)-dimethyl 3-(2-methoxypropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** was obtained.



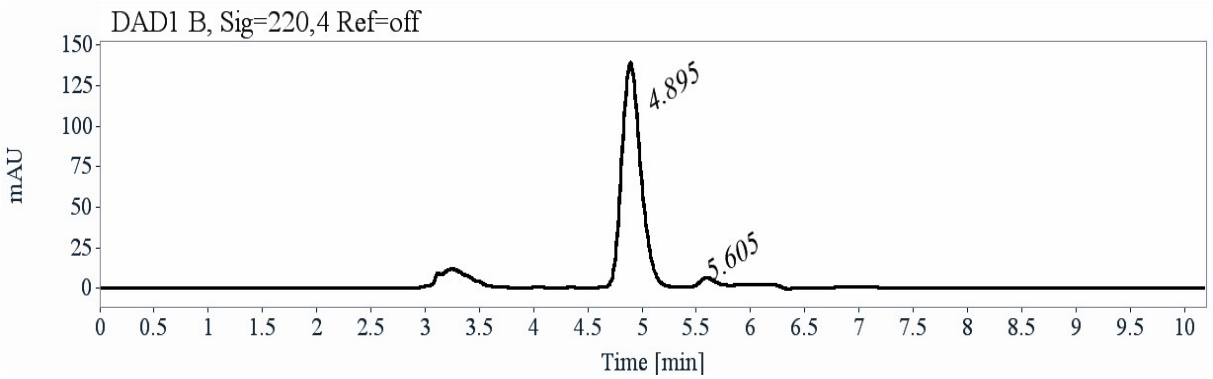
Signal: DAD1 B, Sig=220,4 Ref=off

RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
4.89	2351	50.20	0.66		
5.59	2332	49.80	0.90	1.36	2.44

3.4.2. (β-ICyD)AuCl-catalyzed cycloisomerization

Following procedure A: Using (β-ICyD)AuCl (13 mg) as catalyst and **methanol** as alcohol, dimethyl (-)-(*S*)-3-(2-methoxypropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** (53.9 mg, 0.199 mmol, 95%, er 97:3) was obtained as a yellow oil. $[\alpha]^{20}_D$ = - 27.5 (*c*=1, $CHCl_3$). (litt[2] $[\alpha]^{20}_D$ = + 18.5 (c= 0.14, $CHCl_3$) for the antipode with er 40:60)

Chromatogram recorded using a Chiralpak AD-H column, with a debit of 1 mL/min and heptane/isopropanol (95:5) as the eluent at λ = 254 nm. (-)-(*S*)-dimethyl 3-(2-methoxypropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** was obtained as the major enantiomer (er 97:3).

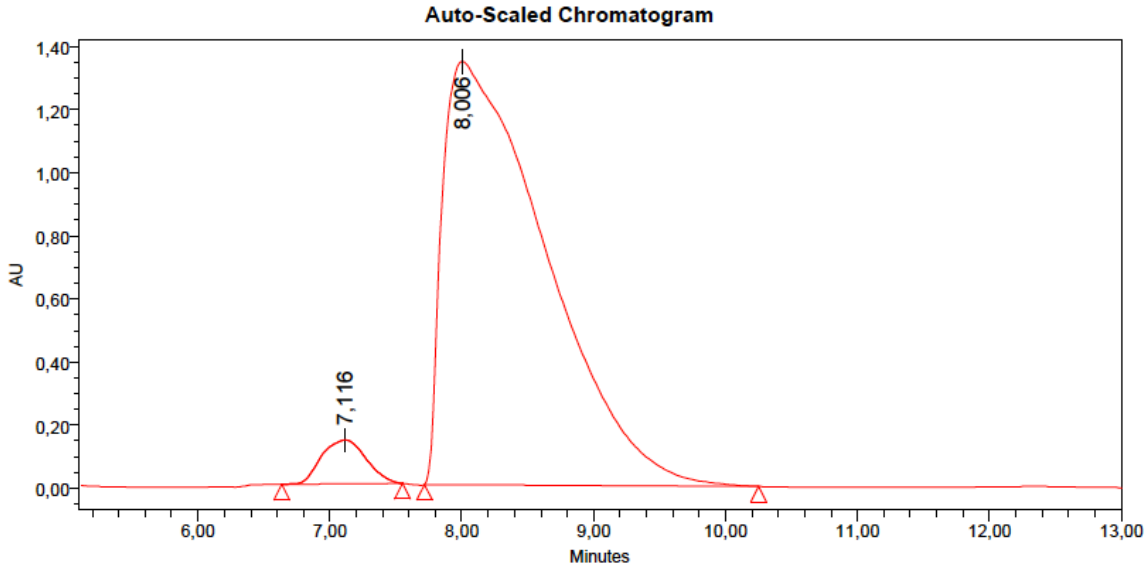


Signal: DAD1 B, Sig=220,4 Ref=off

RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
4.90	1683	97.20	0.66		
5.60	48	2.80	0.90	1.36	2.54

Following procedure B: Using (β-ICyD)AuCl (13 mg) and **methanol** as alcohol, dimethyl-3-(2-methoxypropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate (32.4 mg, 0.199 mmol, 57%, er 96:4) was obtained as a yellow oil.

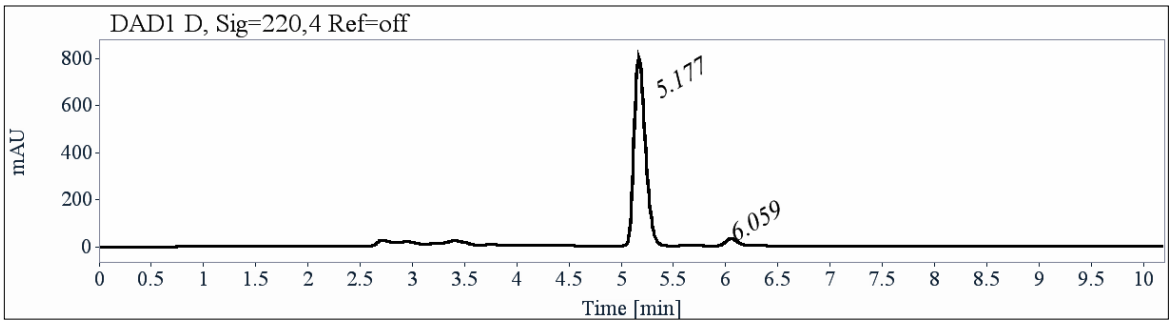
Chromatogram recorded using an OJ column, with a debit of 1 mL/min and heptane/isopropanol (95:5) as the eluent at λ = 254 nm. (-)-(*S*)-dimethyl-3-(2-methoxypropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate was obtained as the major enantiomer (er 96:4).



Peak Results

	Name	RT	Area	% Area
1		7,116	3253289	4,26
2		8,006	73089073	95,74

Chromatogram recorded using a Lux-Amylose-1[a] column, with a debit of 1 mL/min and heptane/isopropanol (95:5) as the eluent at λ = 254 nm. (-)-(*S*)-dimethyl-3-(2-methoxypropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate was obtained as the major enantiomer (er 96:4) by comparing HPLC spectra.



Signal: DAD1 D, Sig=220,4 Ref=off

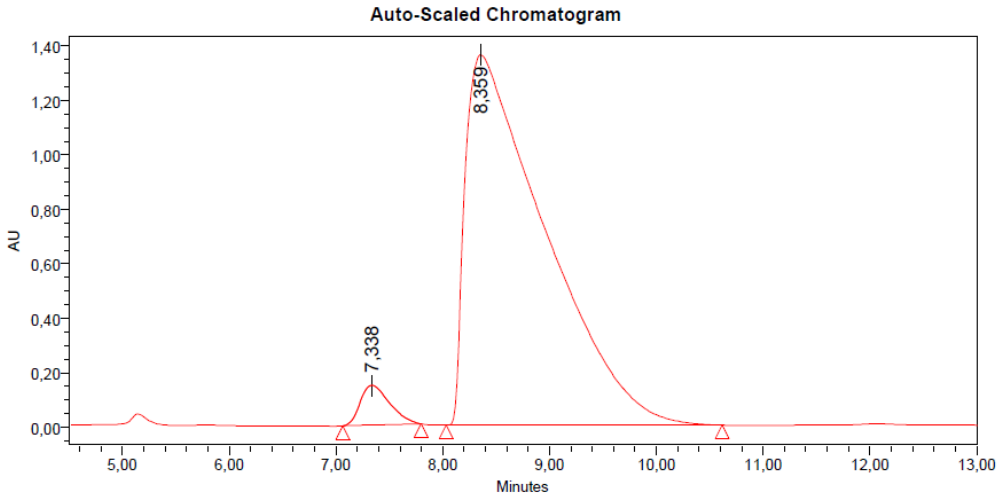
RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
5.18	6059	95.42	0.75		
6.06	291	4.58	1.05	1.40	4.23
Sum	6350	100.00			

[a] It is important to note that depending on the chiral column that is used, the retention time of the two enantiomers is reversed.

3.4.3. (β-ICyD)AuNTf$_2$-catalyzed cycloisomerization

Following procedure C: Using (β-ICyD)AuNTf$_2$ (14 mg) as catalyst and **methanol** as alcohol, (-)-(*S*)-dimethyl-3-(2-methoxypropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** (43.7 mg, 0.162 mmol, 77%, er 96:4) was obtained as a yellow oil.

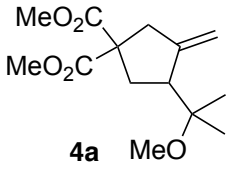
Chromatogram recorded using a Chiralpak OJ column (99: 1 hexane: isopropanol, 1 mL/min, 215 nm). (-)-(*S*)-dimethyl-3-(2-methoxypropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate was obtained as the major enantiomer (er 96:4) by comparing HPLC spectra.



Peak Results

	Name	RT	Area	% Area
1		7,338	2768694	3,77
2		8,359	70696706	96,23

3.4.3. Relative TON between IPrAuCl and (β-ICyD)AuCl following procedure A



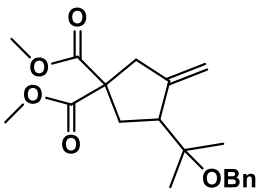
4a

0.2 mol% IPrAuCl
0.2 mol% AgSbF6
CH_2Cl_2/MeOH (3:7)
TON = 180
0.2 mol% (β-ICyD)AuCl
0.2 mol% AgSbF6
CH_2Cl_2/MeOH (3:7)
TON = 190

3.5. Reaction with benzylic alcohol as nucleophile

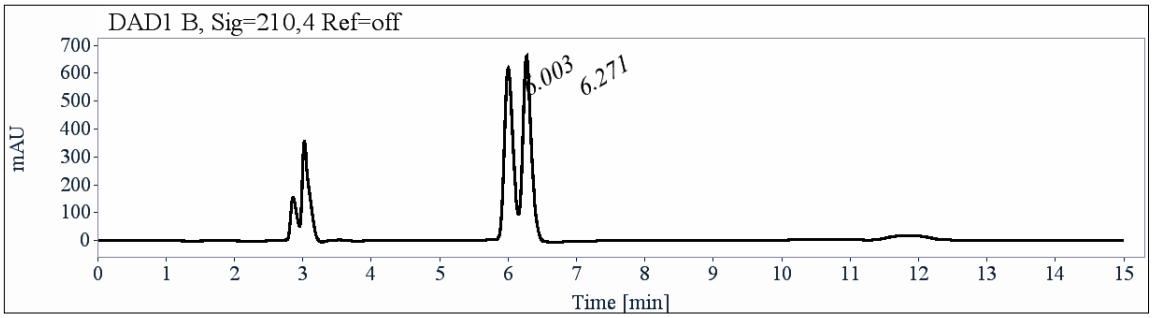
3.5.1. (IPr)AuCl-catalyzed cycloisomerization

Following procedure A: Using (IPr)AuCl (2.6 mg) as catalyst, and **benzylic alcohol**, (±)dimethyl-3-(2-(benzyloxy)propan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4b** was obtained as a yellow oil. (65.5 mg, 0.189 mmol, 90%).



^{1}H-NMR (300 MHz, $CDCl_3$,) δ = 7.38-7.16 (m, 5H), 5.05 (m, 2H), 4.46 (s, 2H), 3.73 (s, 3H), 3.72 (s, 3H), 3.03-2.80 (m, 3H), 2.63 (ddd, *J* = 13.4, 8.5, 1.9 Hz, 1H), 2.12 (dd, *J* = 13.5, 9.3 Hz, 1H), 1.30 (s, 3H), 1.24 (s, 3H). **^{13}C-NMR** (75 MHz, $CDCl_3$) δ = 172.2, 172.1, 148.3, 139.7, 128.4, 127.3, 127.2, 110.9, 77.5, 63.6, 58.8, 50.2, 43.6, 36.2, 23.4, 22.8. **HRMS (ESI) calcd for** $[C_{20}H_{26}O_5 + Na]^+$:369.1672; **found**: 369.1660.

HPLC of the racemic mixture of (±)-dimethyl-3-(2-(benzyloxy)propan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate. Chromatogram recorded using a Lux-Cellulose-2 column, with a debit of 1 mL/min and heptane/isopropanol (95:5) as the eluent at λ = 254 nm.



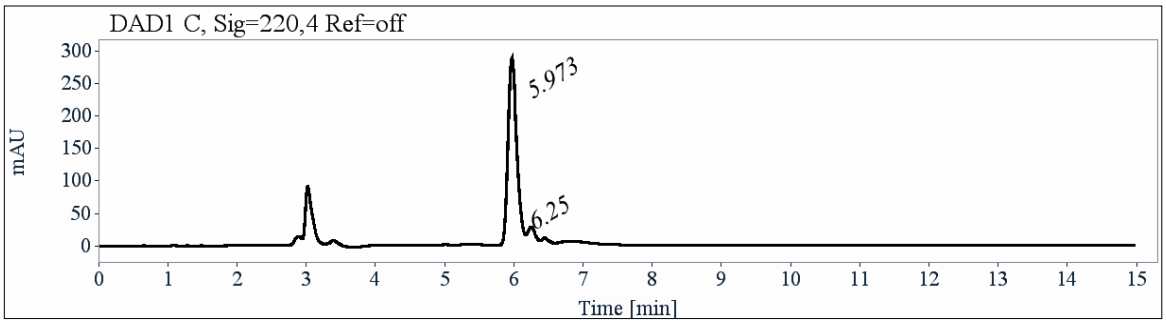
Signal: DAD1 B, Sig=210,4 Ref=off

RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
6.00	5358	48.46	1.03		
6.27	5699	51.54	1.13	1.09	1.19

3.5.2. (β-ICyD)AuCl-catalyzed cycloisomerization

Following procedure A: Using (β-ICyD)AuCl (13 mg) as catalyst and **benzylic alcohol**, (-)-dimethyl-3-(2-(benzyloxy)propan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4b** (65.5 mg, 0.189 mmol, 90%, 84% ee) was obtained as a yellow oil.

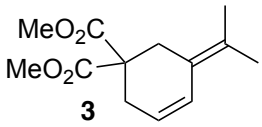
Chromatogram recorded using a Lux-Cellulose-2 column, with a debit of 1 mL/min and heptane/isopropanol (95/5) as the eluent at λ = 254 nm. (-)-dimethyl-3-(2-(benzyloxy)propan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate was obtained as the major enantiomer (er 92:8).



Signal: DAD1 C, Sig=220,4 Ref=off

RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
5.97	2558	92.42	1.02		
6.25	210	7.58	1.12	1.09	1.16

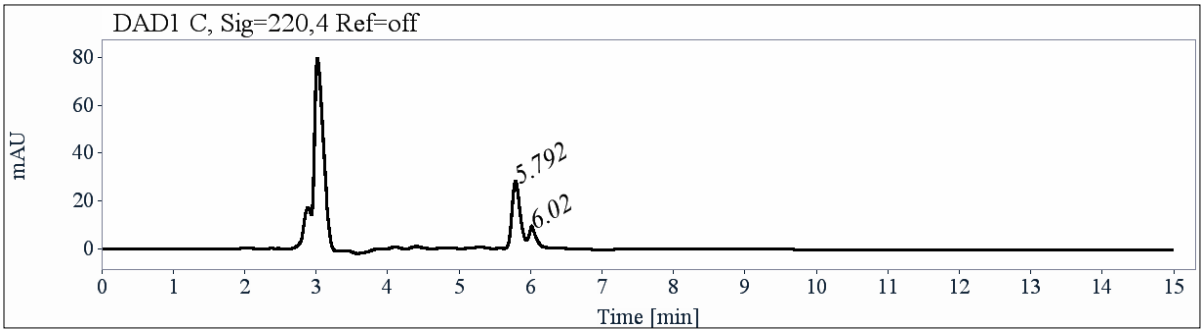
Following procedure B: Using (β-ICyD)AuCl (13 mg) as catalyst and **benzylic alcohol**, dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (12.6 mg, 0.053 mmol, 25%) and (-)-dimethyl-3-(2-(benzyloxy)-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4b** (43.6 mg, 0.126 mmol, 60%, er 75:25) were obtained as yellow oils.
The spectral data for **3** correspond to those previously reported.[3]



3

^{1}H-NMR (300 MHz, $CDCl_3$,) δ = 6.44 (dt, J = 10.2, 2.0 Hz, 1H), 5.62 (dt, J = 9.6, 4.2 Hz, 1H), 3.70 (bs, 6H), 2.87–2.81 (m, 2H), 2.70–2.64 (m, 2H), 1.78 (s, 3H), 1.77 (s, 3H).

Chromatogram recorded using a Lux-Cellulose-2 column, with a debit of 1 mL/min and heptane/isopropanol (95:5) as the eluent at λ = 254 nm. (-)-dimethyl-3-(2-(benzyloxy)-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4b** was obtained as the major enantiomer (er 75:25).



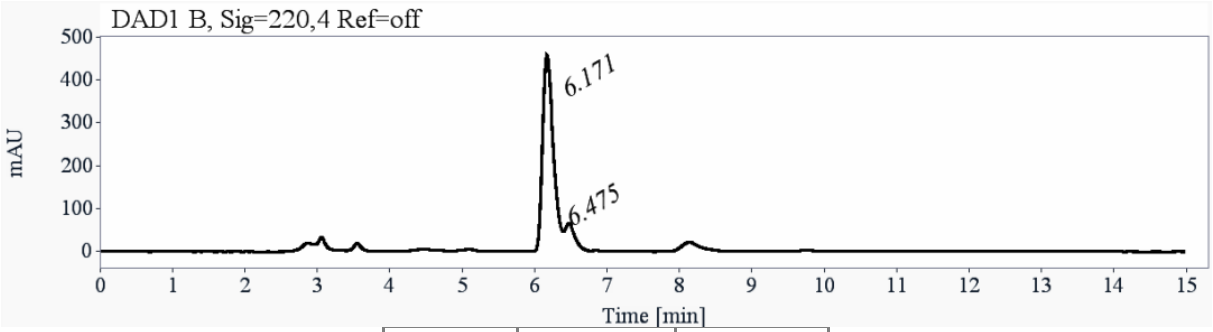
Signal: DAD1 C, Sig=220,4 Ref=off

RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
5.79	217	75.28	0.96		
6.02	71	24.72	1.04	1.08	1.20

3.5.3. (β-ICyD)AuNTf$_2$-catalyzed cycloisomerization

Following procedure C: Using (β-ICyD)AuNTf$_2$ (14 mg) as catalyst and **benzylic alcohol,** dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (8.7 mg, 0.025 mmol, 12%) and (-)-dimethyl-3-(2-(benzyloxy)-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4b** (50.2 mg, 0.144 mmol, 69%, er 88:12) were obtained as yellow oils.

Chromatogram recorded using a Lux-Cellulose-2 column, with a debit of 1 mL/min and heptane/isopropanol (95:5) as the eluent at λ = 220 nm. (-)-dimethyl-3-(2-(benzyloxy)-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4b** was obtained as the major enantiomer (er 88:12). $[\alpha]_{\lambda}^{25} = -15$ (CH_2Cl_2, *c* =0.41) (sodium lamp)



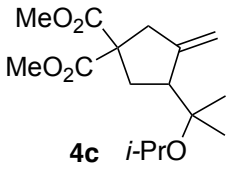
RT [min]	Area	Area%
6.17	4777	87.83
6.47	662	12.17

The sign of the derivative **4b** was determined by rotary power measurement of the mixture of enantiomers, which was obtained in the experiment using (β-ICyD)AuNTf$_2$ as catalyst and attributed for all the compound **4b** by comparing chiral HPLC.

3.6. Reaction with isopropanol as nucleophile

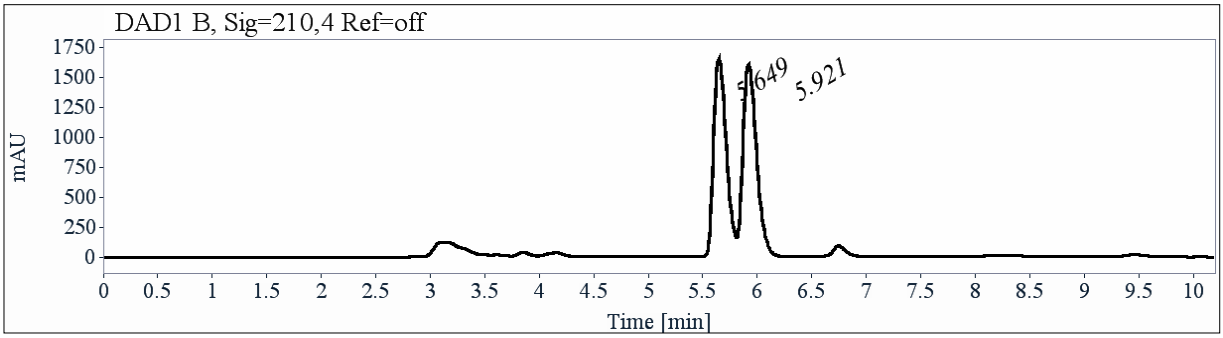
3.6.1. (IPr)AuCl-catalyzed cycloisomerization

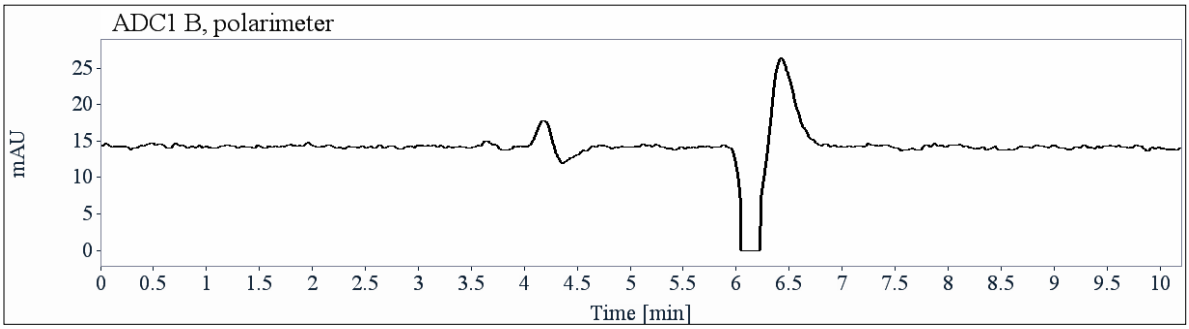
Following procedure A: Using (IPr)AuCl (2.6 mg) as catalyst, and **isopropanol** as alcohol, (±)-dimethyl-3-(2-isopropylpropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4c** was obtained a as yellow oil. (54.0 mg, 0.181 mmol, 86%).



^{1}H-NMR (300 MHz, $CDCl_3$) δ = 5.07 (m, 1H), 4.99 (m, 1H), 3.81 (sept, *J* = 6.1 Hz, 1H), 3.72 (s, 3H), 3.71 (s, 3H), 2.98-2.86 (m, 1H), 2.70 (tq, *J* = 8.8, 2.0 Hz, 1H), 2.56 (ddd, *J* = 13.2, 8.4, 1.8 Hz, 1H), 2.03 (dd, *J* = 13.2, 9.0 Hz, 1H), 1.16 (s, 3H), 1.13 (s, 3H), 1.09 (d, *J* = 6.1 Hz, 6H). **^{13}C-NMR** (75 MHz, $CDCl_3$) δ = 172.3, 172.3, 148.6, 110.8, 63.4, 58.7, 52.8, 51.8, 43.5, 36.3, 25.2, 25.0, 24.2, 22.8. **HRMS (ESI) calcd for** ($[C_{16}H_{26}O_5 + Na]^+$):321.1672; **found**:321.1685.

Chromatogram recorded using a Lux-Cellulose-4 column, with a debit of 1 mL/min and heptane/isopropanol (98:2) as the eluent at λ = 254 nm. (±)-dimethyl-3-(2-isopropylpropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4c** was obtained.





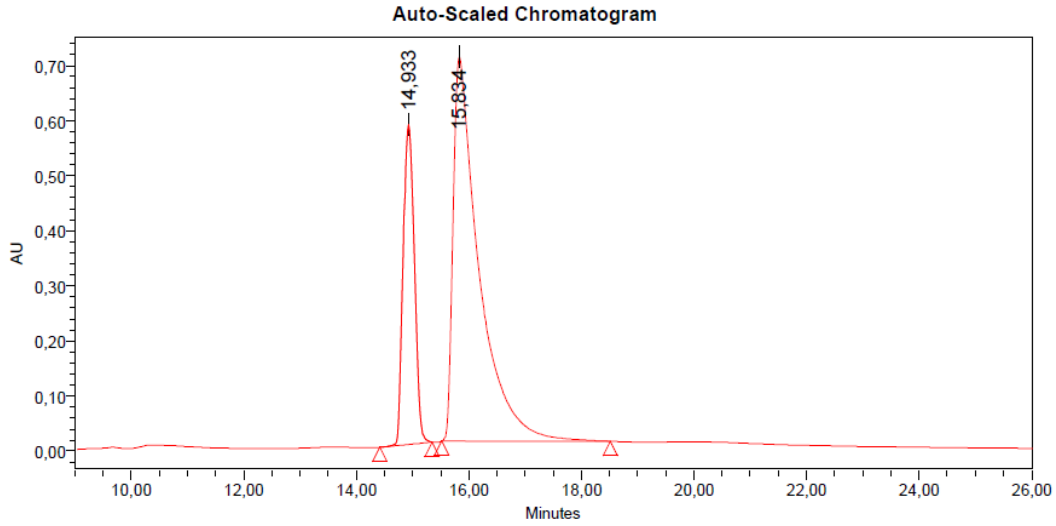
Signal: DAD1 B, Sig=220,4 Ref=off

RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
5.65	13519	48.83	0.92		
5.92	14169	51.17	1.01	1.10	1.26

3.6.2. (β-ICyD)AuCl-catalyzed cycloisomerization

Following procedure A: Using (β-ICyD)AuCl (13 mg) as catalyst and **isopropanol** as alcohol, dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (15.0 mg, 0.638 mmol, 30%) and dimethyl-3-(2-isopropylpropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4c** (33.2 mg, 0.111 mmol, 53%, er 73:27) were obtained as yellow oils.

Chromatogram recorded using an OJ column, with a debit of 0.5 mL/min and heptane/isopropanol (95:5) as the eluent at λ = 254 nm. (-)-dimethyl-3-(2-isopropylpropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4c** was obtained as the major enantiomer (er 73:27).



Peak Results

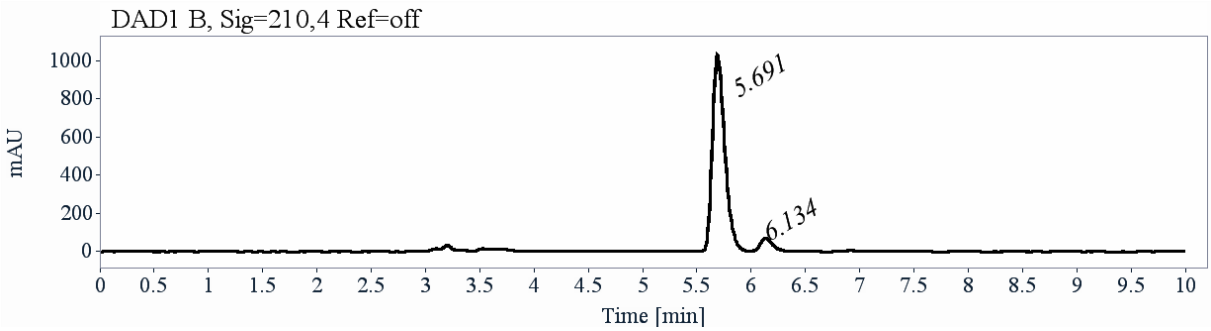
	Name	RT	Area	Height	% Area
1		14,933	8124288	579992	26,79
2		15,834	22201943	697633	73,21

Following procedure B: Using (β-ICyD)AuCl (13 mg) as catalyst and **isopropanol** as alcohol, dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (48.3 mg, 0.162 mmol, 77%) and dimethyl-3-(2-isopropylpropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4c** (4.4 mg, 0.015 mmol, 7%) were obtained as yellow oils.

3.6.3. (β-ICyD)AuNTf$_2$-catalyzed cycloisomerization

Following procedure C: (β-ICyD)AuNTf$_2$ (14 mg) as catalyst and **isopropanol**, dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (4.5 mg, 0.017 mmol, 8%) and (-)-dimethyl-3-(2-isopropylpropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4c** (31.9 mg, 0.107 mmol, 51%, er 93:7) were obtained as yellow oils.

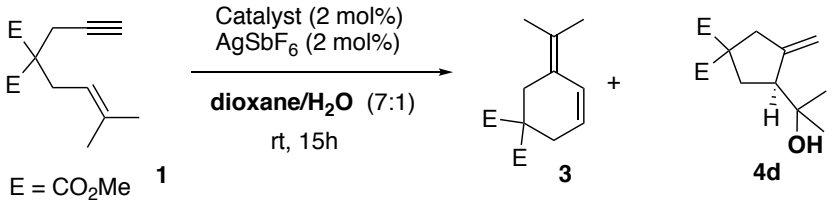
Chromatogram recorded using a Lux-Cellulose-4 column, with a debit of 1 mL/min and heptane/isopropanol (98:2) as the eluent at λ = 210 nm. (-)-dimethyl-3-(2-isopropylpropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4c** was obtained as the major enantiomer (er 93:7). $[\alpha]_D^{25}$ = – 19 (CH_2Cl_2, c = 0.28) (sodium lamp).



RT [min]	Area	Area%
5.69	8239	93.35
6.13	587	6.65

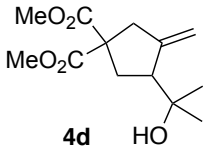
The sign of the derivative **4c** was determinate by rotary power measurement of the mixture of enantiomers, which was obtained in the experiment using (β-ICyD)AuNTf$_2$ as catalyst and attributed for all the compounds **4c** by comparing chiral HPLC.

3.7. Reaction with water as nucleophile



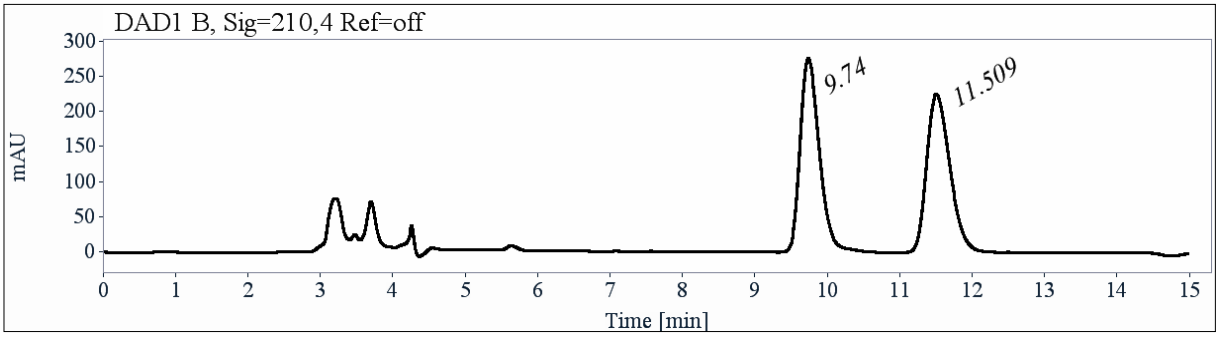
3.7.1. (IPr)AuCl-catalyzed cycloisomerization

(IPr)AuCl (2.6 mg, 0.004 mmol, 2 mol%, 14 mg) was dissolved in 2.5 mL of a solution of dioxane/H_2O (7:1), followed by the addition of the $AgSbF_6$ (1.44 mg, 0.004 mmol, 2 mol%). **1** (50 mg, 0.210 mmol) was added in solution in 1.5 mL of dioxane. The final concentration was 0.05M. The reaction was monitored by TLC (pentane/EtOAc, 90:10). After 15h at room temperature, the reaction was filtered over a short pad of silica, washing with ethyl acetate, and concentrated under reduced pressure. The crude mixture was purified by column chromatography on silica gel (pentane/EtOAc, 95:5) affording (±)-dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate **4d** (108 mg, 0.420 mmol, quant.) as a yellow oil.



^{1}H-NMR (400 MHz, $CDCl_3$) δ = 5.08 (m, 1H, C=CH_2), 4.99 (m, 1H, C=CH_2), 3.70 (s, 3H, CH_3O), 3.69 (s, 3H, CH_3O), 2.90 - 2.81 (m, 2H, CH_2), 2.72 - 2.52 (m, 2H, CH_2), 2.00 - 1.94 (m, 1H, CH), 1.21 (s, 3H, CH_3), 1.17 (s, 3H, CH_3). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ = 172.0, 171.9, 148.6, 111.2, 72.6, 58.8, 52.8, 52.7, 43.5, 36.2, 28.1, 26.2. The spectral data for **4d** correspond to those previously reported.[1]

Chromatogram recorded using a Chiralpak AZ-H column, with a debit of 1 mL/min and heptane/isopropanol (90:10) as the eluent at λ = 210 nm. (±)-Dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate was obtained.



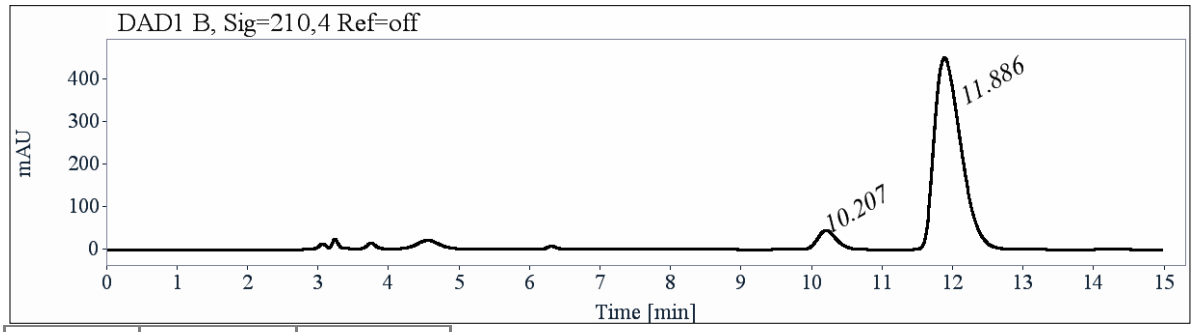
Signal: DAD1 B, Sig=210,4 Ref=off

RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
9.74	5007	49.89	2.30		
11.51	5029	50.11	2.90	1.26	3.33
Sum	10036	100.00			

3.7.2. (β-ICyD)AuCl-catalyzed cycloisomerization

Adding the silver salt before the substrate: (β-ICyD)AuCl (0.004 mmol, 2 mol%, 13 mg) was dissolved in 2.5 mL of a solution of dioxane/H_2O (7:1). Then $AgSbF_6$ was added (0.004 mmol, 2 mol%, 1.4 mg). **1** (50 mg, 0.210 mmol, 1 equiv.) was added in a solution of dioxane (7:1, 1.5 mL). The concentration of the reaction was 0.05 M. The reaction mixture was stirred at room temperature for 15 hours. The reaction was followed by TLC (pentane/EtOAc, 90:10). After completion, the mixture was filtered over silica, washed with ethyl acetate, and concentrated under reduced pressure. The crude mixture was purified by column chromatography on silica gel (pentane/EtOAc 95:5 to 80:20) affording dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (5.0 mg, 0.021 mmol, 10 %) and (-)-dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate **4d** (27.5 mg, 0.107 mmol, 51%, er 93:7) as yellow oils.

Chromatogram recorded using a Chiralpak AZ-H column, with a debit of 1 mL/min and heptane/isopropanol (90/10) as the eluent at λ = 210 nm. (-)-Dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate was obtained as the major enantiomer (er 93:7).



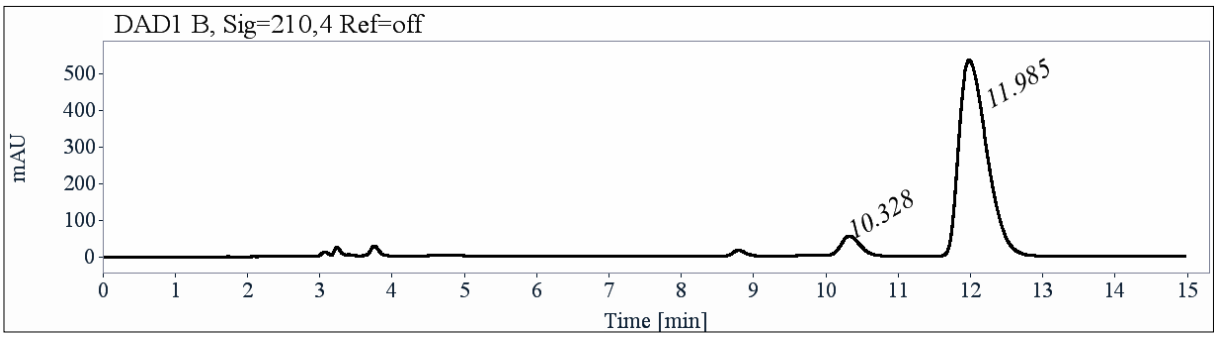
RT [min]	Area	Area%
10.21	834	6.63
11.89	11740	93.37
Sum	12574	100.00

Optical rotations were measured on a Jasco P-2000 polarimeter with a halogen lamp (589, 578, 546, 436, 405 and 365 nm), in a 10 cm cell, thermostated at 25°C with a Peltier controlled cell holder.

λ (nm)	second eluted on Chiralpak AZ-H $[\alpha]_\lambda^{25}$ (CH_2Cl_2, c =0.76)
589	- 15
578	- 15
546	- 18
436	- 30
405	- 37

Adding the silver salt after the substrate: (β-ICyD)AuCl (0.004 mmol, 2 mol%, 13 mg) was dissolved in 2.5 mL of a solution of dioxane/H_2O (7:1). **1** (50 mg, 0.210 mmol, 50 mg) was added in a solution of dioxane/H_2O (7:1, 1.5 mL) then $AgSbF_6$ was added (0.004 mmol, 2 mol%, 1.4 mg), the concentration of the reaction was 0.05 M. The reaction was followed by TLC (pentane/EtOAc, 90:10). After 15h the mixture was filtered over silica, washed with ethyl acetate, and concentrated under reduced pressure. The crude mixture was purified by column chromatography on silica gel (pentane/ EtOAc 95: 5 to 80: 20) affording dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (6.0 mg, 0.025 mmol, 12%) and (-)-dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate **4d** (22.6 mg, 0.088 mmol, 42%, er 94:6) as yellow oils.

Chromatogram recorded using a Chiralpak AZ-H column, with a debit of 1 mL/min and heptane/isopropanol (90/10) as the eluent at λ = 210 nm. (-)-Dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate was obtained as the major enantiomer (er 94:6).



RT [min]	Area	Area%
10.33	984	6.43
11.98	14329	93.57
Sum	15313	100.00

Optical rotations were measured on a Jasco P-2000 polarimeter with a halogen lamp (589, 578, 546, 436, 405 and 365 nm), in a 10 cm cell, thermostated at 25°C with a Peltier controlled cell holder.

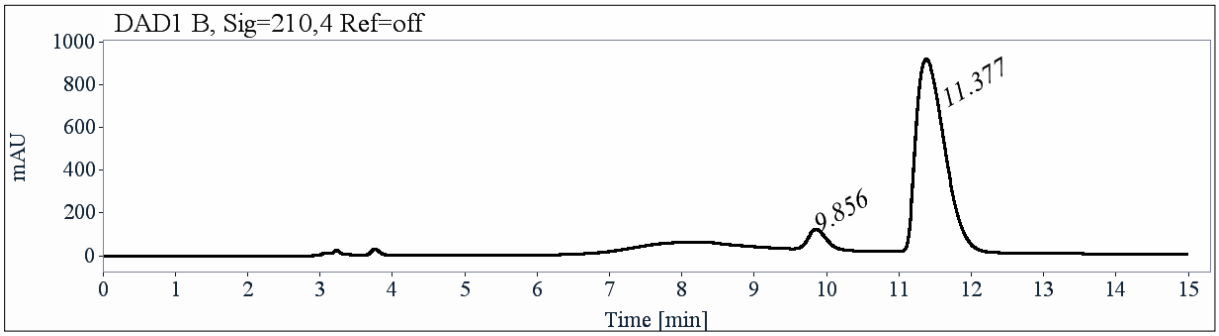
λ (nm)	second eluted on Chiralpak AZ-H $[\alpha]_{\lambda}^{25}$ (CH_2Cl_2, c =0.72)
589	- 16
578	- 16
546	- 19
436	- 31
405	- 37

3.7.3. (β-ICyD)AuNTf$_2$-catalyzed cycloisomerization

(β-ICyD)AuNTf$_2$ (0.004 mmol, 2 mol%, 14 mg) as catalyst was dissolved in 2.5 mL of a solution of dioxane/H_2O (7:1). Then dimethyl 2-(3-methylbut-2-en-1-yl)-2-(prop-2-yn-1-yl) malonate **1** was added in 1 mL of a solution of dioxane/H_2O (7:1). The final concentration was 0.05 M. The reaction was monitored by TLC (pentane/ EtOAc 90:10). After completion, the mixture was filtered over a short pad of silica, washing with ethyl acetate, and concentrated under reduced pressure. The crude mixture was purified by column chromatography on silica gel

(pentane/EtOAc, 95:5 to 80:20) affording dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (16.0 mg, 0.067 mmol, 32%) and (-)-dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate **4d** (32.8 mg, 0.128 mmol, 61%, er 94:6) as yellow oils.

Chromatogram recorded using a Chiralpak AZ-H column, with a debit of 1 mL/min and heptane/isopropanol (90:10) as the eluent at λ = 210 nm. (-)-Dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate was obtained as the major enantiomer (er 94:6).



RT [min]	Area	Area%
9.86	1642	6.23
11.38	24717	93.77
Sum	26359	100.00

Optical rotations were measured on a Jasco P-2000 polarimeter with a halogen lamp (589, 578, 546, 436, 405 and 365 nm), in a 10 cm cell, thermostated at 25°C with a Peltier controlled cell holder.

λ (nm)	second eluted on Chiralpak AZ-H $[\alpha]_{\lambda}^{25}$ (CH_2Cl_2, c =0.74)
589	- 14
578	- 15
546	- 17
436	- 30
405	- 36

4. Competitive alkoxycyclization

4.1. Reaction with a mixture of methanol and isopropanol as nucleophile

Following procedure A: Using (IPr)AuCl (2.6 mg) as catalyst, and a mixture of alcohols MeOH (0.82 mL)/BnOH (2.11 mL), mol/mol, dimethyl-3-(2-methoxypropane-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** (30.1 mg, 0.111 mmol, 53%) and dimethyl-3-(2-(benzyloxy)-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4b** (19.6 mg, 0.057 mmol, 27%) were obtained as yellow oils.

Following procedure A: Using (β-ICyD)AuCl (13 mg) as catalyst and a mixture of MeOH (0.82 mL)/BnOH (2.11 mL), mol/mol, dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (14.5 mg, 0.061 mmol, 29%), dimethyl-3-(2-methoxypropane-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** (22.1 mg, 0.0.082 mmol, 39 %) and dimethyl-3-(2-(benzyloxy)-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4b** (23.3 mg, 0.067 mmol, 32%) were obtained as yellow oils.

Following procedure B: Using (β-ICyD)AuCl (13 mg) and a mixture of MeOH (0.82 mL)/BnOH (2.11 mL), mol/mol, dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (15.0 mg, 0.063 mmol, 30%), dimethyl-3-(2-methoxypropane-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** (15.9 mg, 0.059 mmol, 28%) and dimethyl-3-(2-(benzyloxy)-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4b** (24.5 mg, 0.074 mmol, 35%) were obtained as yellow oils.

4.2. Reaction with a mixture of methanol and benzylic alcohol as nucleophile

Following procedure A: Using (IPr)AuCl (2.6 mg) as catalyst, and a mixture of MeOH (1.02 mL)/*i*PrOH (1.92 mL), mol/mol, dimethyl-3-(2-methoxypropane-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** (30.1 mg, 0.122 mmol, 58%) and dimethyl-3-(2-isopropylpropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4c** (19.6 mg, 0.088 mmol, 42%) were obtained as yellow oils.

Following procedure A: Using (β-ICyD)AuCl (13 mg) as catalyst and a mixture of MeOH (1.02 mL)/*i*PrOH (1.92 mL), mol/mol, dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (6.0 mg, 0.025 mmol, 12%), dimethyl-3-(2-methoxypropane-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** (44.8 mg, 0.166 mmol, 79%) and dimethyl-3-(2-isopropylpropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4c** (6.2 mg, 0.017 mmol, 8%) were obtained as yellow oils.

Following procedure B: Using (β-ICyD)AuCl (13 mg) and a mixture of MeOH (1.02 mL)/*i*PrOH (1.92 mL), mol/mol, dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (15.0 mg, 0.063 mmol, 30%), dimethyl-3-(2-methoxypropane-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** (28.4 mg, 0.105 mmol, 50%) and dimethyl-3-(2-isopropylpropan-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4c** (7.3 mg, 0.021 mmol, 10%) were obtained as yellow oils.

4.3. Reaction with a mixture of methanol and water as nucleophile

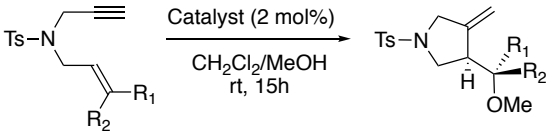
Following procedure A: Using (IPr)AuCl (2.6 mg) as catalyst, and a mixture of MeOH (0.90 mL)/H_2O (2.04 mL), mol/mol, dimethyl-3-(2-methoxypropane-2-yl)-4-methylenecyclopentane-1,1-dicarboxylates **4a** (11.9 mg, 0.044 mmol, 41%) and dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate **4d** (9.1 mg, 0.036 mmol, 17%) were obtained as yellow oils.

Following procedure A: Using (β-ICyD)AuCl (13 mg) as catalyst and a mixture of MeOH (0.90 mL)/H_2O (2.04 mL), mol/mol, dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (15.0 mg, 0.063 mmol, 30%), dimethyl-3-(2-methoxypropane-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** (30.1 mg, 0.118 mmol, 56%) and dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate **4d** (2.7 mg, 0.011 mmol, 5%) were obtained as yellow oils.

Following procedure B: Using (β-ICyD)AuCl (13 mg) and a mixture of MeOH (0.90 mL)/H_2O (2.04 mL), mol/mol, dimethyl-5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate **3** (10.0 mg,

0.042 mmol, 20%), dimethyl-3-(2-methoxypropane-2-yl)-4-methylenecyclopentane-1,1-dicarboxylate **4a** (12.4 mg, 0.048 mmol, 23%) and dimethyl-3-(2-hydroxypropan-2-yl)-4-methylenecyclopentane-1-1-dicarboxylate **4d** (2.7 mg, 0.011 mmol, 5%) were obtained as yellow oils.

5. Methoxycyclizations with N-tethered enynes



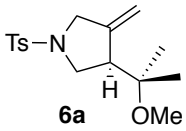
5a, R_1=R_2=Me
5b, R_1= Ph, R_2=H

6a, R_1=R_2=Me
6b, R_1= Ph, R_2=H

5.1 Reaction with 4-methyl-N-(3-methylbut-2-en-1-yl)-N-(prop-2-yn-1-yl)benzenesulfonamide **5a**

5.1.1 (IPr)AuCl-catalyzed methoxycyclization

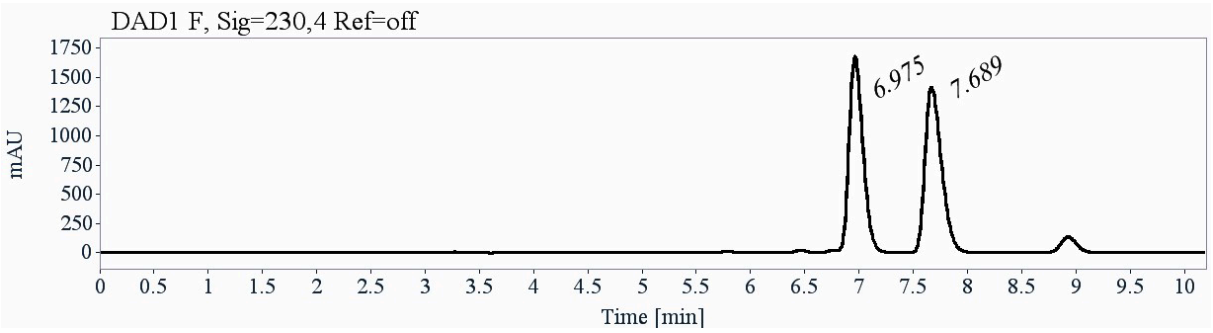
Following procedure A: Using (IPr)AuCl (2.2 mg) as catalyst, $AgSbF_6$ (1.2 mg), **5a** (50 mg, 0.180 mmol) as substrate and **methanol** as alcohol, (±)-3-(2-methoxypropan-2-yl)-4-methylene-1-tosylpyrrolidine **6a** (33.4 mg, 0.108 mmol, 60%) was obtained as a yellow oil. The spectral data correspond to those previously reported.[4]



6a

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.3 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 5.02 (s, 2H), 3.76 (s, 2H), 3.39 (dd, J = 10.1, 4.4 Hz, 1H), 3.27 (dd, J = 10.1, 8.1 Hz, 1H), 3.07 (s, 3H), 2.82 – 2.74 (m, 2H), 2.41 (s, 3H), 1.10 (s, 3H), 0.98 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.8, 143.7, 133.0, 129.7, 128.0, 110.8, 76.3, 53.5, 51.0, 49.8, 49.2, 22.4, 21.9, 21.7.

Chromatogram recorded using a Lux-Cellulose-3 column, with a debit of 1 mL/min and Heptane/Ethanol (80:20) as the eluent at λ = 230 nm. (±)-3-(2-methoxypropan-2-yl)-4-methylene-1-tosylpyrrolidine **6a** was obtained.



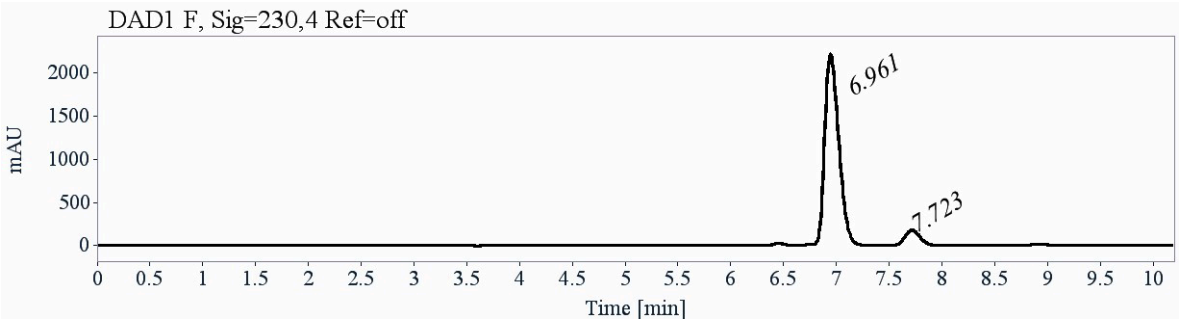
Signal: DAD1 F, Sig=230,4 Ref=off

RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
6.97	15056	50.09	1.36		
7.69	15002	49.91	1.61	1.18	2.76
Sum	30058	100.00			

5.1.2. (β-ICyD)AuCl-catalyzed methoxycyclization

Following procedure A: Using (β-ICyD)AuCl (11.2 mg) as catalyst, $AgSbF_6$ (1.2 mg), **5a** (50 mg, 0.180 mmol) as substrate and **methanol** as alcohol, (-)-3-(2-methoxypropan-2-yl)-4-methylene-1-tosylpyrrolidine **6a** (44.0 mg, 0.142 mmol, 79%, er 92:8) was obtained as a yellow oil.

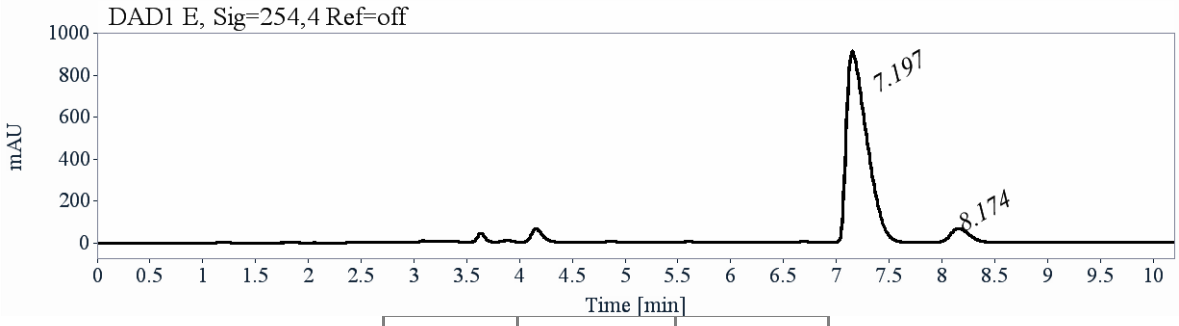
Chromatogram recorded using a Lux-Cellulose-3 column, with a debit of 1 mL/min and Heptane/Ethanol (80:20) as the eluent at λ = 230 nm. (-)-3-(2-methoxypropan-2-yl)-4-methylene-1-tosylpyrrolidine was obtained with an er of 92:8.



5.1.3. (β-ICyD)AuNTf$_2$-catalyzed methoxycyclization

Following procedure C: Using (β-ICyD)AuNTf$_2$ (12.0 mg) as catalyst, **5a** (50 mg, 0.180 mmol) as substrate and **methanol** as alcohol, (-)-3-(2-methoxypropan-2-yl)-4-methylene-1-tosylpyrrolidine **6a** (39.5 mg, 0.128 mmol, 71%, er 94:6) was obtained as a yellow oil.

Chromatogram recorded using a Lux-Cellulose-3 column, with a debit of 1 mL/min and Heptane/Ethanol (80:20) as the eluent at λ = 254 nm. (-)-3-(2-methoxypropan-2-yl)-4-methylene-1-tosylpyrrolidine was obtained with an er of 94:6.



RT [min]	Area	Area%
7.20	12308	93.70
8.17	828	6.30
Sum	13136	100.00

Optical rotations were measured on a Jasco P-2000 polarimeter with a halogen lamp (589, 578, 546, 436, 405 and 365 nm), in a 10 cm cell, thermostated at 25°C with a Peltier controlled cell holder.

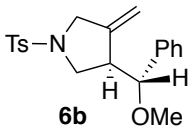
λ (nm)	first eluted on Lux-Cellulose-3 $[\alpha]_{\lambda}^{25}$ (CH_2Cl_2, c =1.05)
589	- 18
578	- 19
546	- 22
436	- 41
405	- 52
365	- 75

The sign of the derivative **6a** was determined by rotary power measurement of the mixture of enantiomers, which was obtained in the experiment using (IPr)AuCl as catalyst and attributed for all the compounds **6a** by comparing chiral HPLC.

5.2. Reaction with N-cinnamyl-4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide **5b**

5.2.1. (IPr)AuCl-catalyzed methoxycyclization

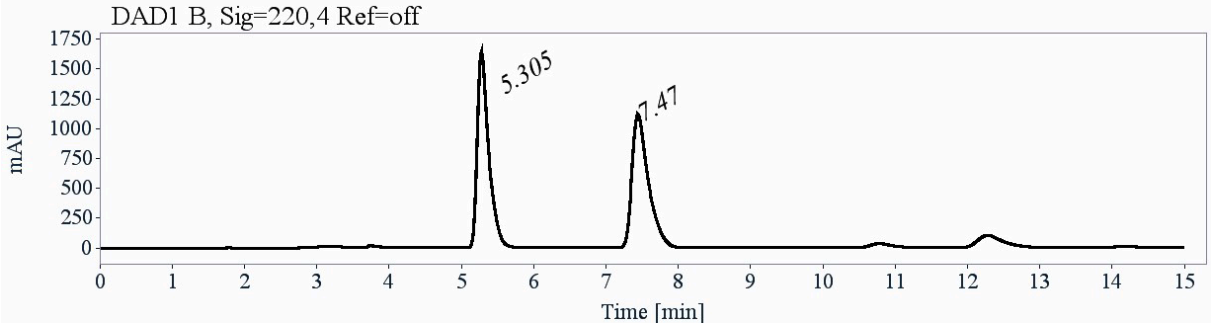
Following procedure A: Using (IPr)AuCl (1.9 mg) as catalyst, $AgSbF_6$ (1.1 mg), **5b** (50 mg, 0.154 mmol) as substrate and **methanol** as alcohol, (±)-3-(methoxy(phenyl)methyl)-4-methylene-1-tosylpyrrolidine **6b** (30.3 mg, 0.085 mmol, 55%) was obtained as a yellow oil. The spectral data correspond to those previously reported.[5]



6b

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76–7.69 (m, 2H), 7.38–7.24 (m, 5H), 7.20–7.12 (m, 2H), 4.79–4.73 (m, 1H), 4.23–4.17 (m, 1H), 3.94–3.81 (m, 2H), 3.76–3.64 (m, 2H), 3.29–3.17 (m, 1H), 3.10 (s, 3H), 2.90–2.80 (m, 1H), 2.44 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.7, 143.6, 139.5, 133.0, 129.8, 128.3, 128.1, 128.0, 127.7, 110.1, 83.9, 57.0, 52.4, 50.6, 50.6, 21.7.

Chromatogram recorded using a Chiralpak AD-H column, with a debit of 1 mL/min and Heptane/Ethanol (50:50) as the eluent at λ = 220 nm. (±)-3-(methoxy(phenyl)methyl)-4-methylene-1-tosylpyrrolidine was obtained **6b**.

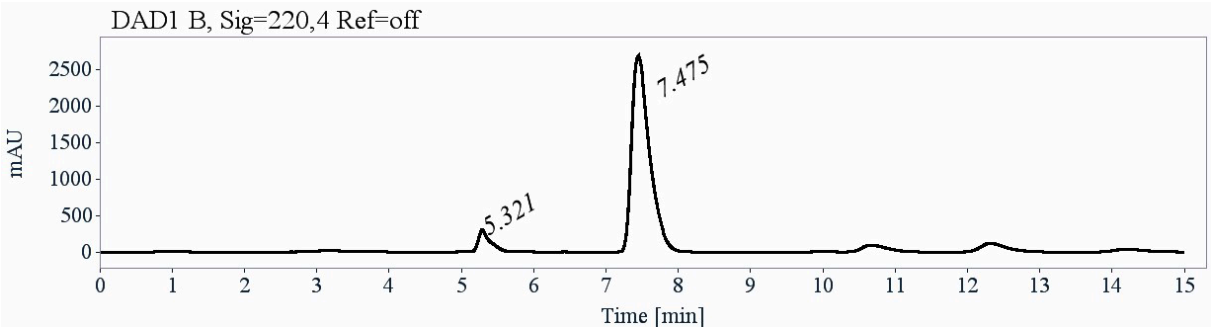


RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
5.30	17940	50.33	0.80		
7.47	17706	49.67	1.53	1.92	6.51
Sum	35646	100.00			

5.2.2. (β-ICyD)AuCl-catalyzed methoxycyclization

Following procedure A: Using (β-ICyD)AuCl (9.6 mg) as catalyst, $AgSbF_6$ (1.1 mg), **5b** (50 mg, 0.154 mmol) as substrate and methanol as alcohol. The mixture was heated at 40 °C. (-)-3-(2-methoxypropan-2-yl)-4-methylene-1-tosylpyrrolidine **6b** (31.9 mg, 0.089 mmol, 58%, er 93:7) was obtained as a yellow oil.

Chromatogram recorded using a Chiralpak AD-H column, with a debit of 1 mL/min and Heptane/Ethanol (50/50) as the eluent at λ = 220 nm. (-)-3-(methoxy(phenyl)methyl)-4-methylene-1-tosylpyrrolidine was obtained with an er of 93:7.



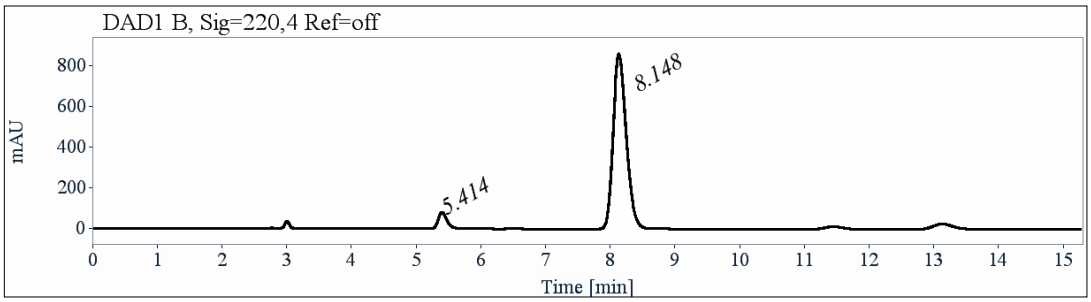
Signal: DAD1 B, Sig=220,4 Ref=off

RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
5.32	3522	7.08	0.80		
7.47	46218	92.92	1.53	1.91	6.20
Sum	49741	100.00			

5.2.3. (β-ICyD)AuNTf$_2$-catalyzed methoxycyclization

Following procedure C: Using (β-ICyD)AuNTf$_2$ (10.3 mg) as catalyst, **5b** (50 mg, 0.154 mmol) as substrate and methanol as alcohol, (-)-3-(2-methoxypropan-2-yl)-4-methylene-1-tosylpyrrolidine **6b** (40.2 mg, 0.112 mmol, 73%, er 94:6) was obtained as a yellow oil.

Chromatogram recorded using a Lux-Amylose-1column, with a debit of 1 mL/min and Heptane/Ethanol (50/50) as the eluent at λ = 220 nm. (-)-3-(methoxy(phenyl)methyl)-4-methylene-1-tosylpyrrolidine was obtained with an er of 94:6.



Signal: DAD1 B, Sig=220,4 Ref=off

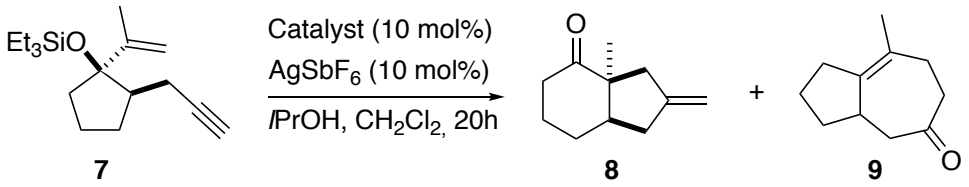
RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
5.41	758	5.91	0.84		
8.15	12063	94.09	1.76	2.11	8.94
Sum	12821	100.00			

Optical rotations

λ (nm)	second eluted on Lux-Amylose-1 $[\alpha]_{\lambda}^{25}$ (CH_2Cl_2, c =1.05)
589	- 62
578	- 64
546	- 75
436	- 133
405	- 166
365	- 235

6. Diagnostic cycloisomerization

6.1. Cycloisomerization of triethyl((1-(prop-1-en-2-yl)-2-(prop-2-yn-1-yl)cyclopentyl)oxy)silane **7**

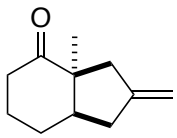


7 **8** **9**

General procedure D: The catalyst (0.011 mmol, 10 mol%) and $AgSbF_6$ (0.011 mmol, 10 mol%) were introduced. Then, isopropanol (9 µL, 0.119 mmol, 1.1 equiv.) was added. Finally, triethyl((1-(prop-1-en-2-yl)-2-(prop-2-yn-1-yl)cyclopentyl)oxy)silane **7**[6] (30 mg, 0.108 mmol, 1.0 equiv.) is added in solution in dichloromethane (1.2 mL). The final concentration was 0.05 M. The reaction mixture was stirred in the dark at room temperature for 20 h. The reaction was monitored by TLC (EtOAc). After completion, the solution was filtered through a pad of silica and the pad was washed with EtOAc. The crude mixture was purified by flash chromatography on silica gel (pentane/EtOAc 98:2 to 95:5).

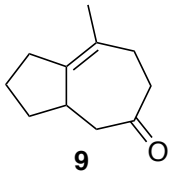
6.1.1. (IPr)AuCl-catalyzed cycloisomerization

Following procedure D: Using (IPr)AuCl (7 mg), 3a-methyl-2-methylenehexahydro-1H-inden-4(2H)-one **8** (6 mg, 0.036 mmol, 33%) as a yellow oil and 8-methyl-2,3,3a,4,6,7-hexahydroazulen-5(1H)-one **9** (3 mg, 0.018 mmol, 17%) were obtained as yellow oils.



8

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 5.01-4.80 (m, 2H), 2.99 (dd, $^3J_{HH}$ = 16.5, 2.0 Hz, 1H), 2.59-2.28 (m, 3H), 2.26-2.08 (m, 2H), 2.07-1.69 (m, 4H), 1.67-1.47 (m, 1H), 1.19 (s, 2H). The spectral data for 3amethyl- 2-methylenehexahydro-1H-inden-4(2H)-one **8** correspond to those previously reported.[6]



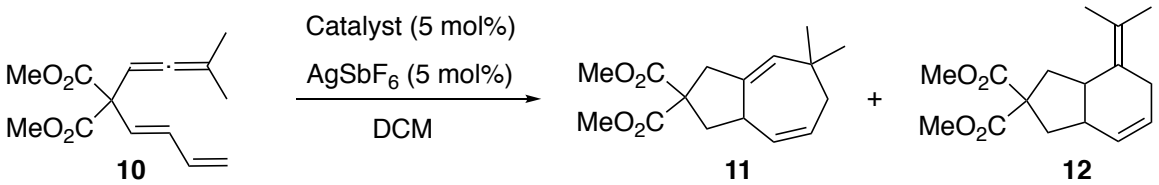
9

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 3.00-2.71 (m, 2H), 2.56 (dd, $^3J_{HH}$ = 15.7, 3.1 Hz, 1H), 2.47-2.25 (m, 6H), 2.04-1.89 (m, 1H), 1.80-1.63 (m, 4H), 1.60-1.42 (m, 1H), 1.38-1.23 (m, 1H). The spectral data for 8-methyl-2,3,3a,4,6,7-hexahydroazulen-5(1H)-one **9** correspond to those previously reported.[6]

6.1.2. (β-ICyD)AuCl-catalyzed cycloisomerization

Following procedure D: Using (β-ICyD)AuCl (34 mg), 3a-methyl-2-methylenehexahydro-1H-inden-4(2H)-one **8** was obtained (5 mg, 0.030 mmol, 28%) as a yellow oil and 8-methyl-2,3,3a,4,6,7-hexahydroazulen-5(1H)-one **9** was obtained (7 mg, 0.042 mmol, 39%) as yellow oils.

6.2. cycloisomerization of (E)-dimethyl 2-(4-methylpenta-2,3-dien-1-yl)-2-(penta-2,4-dien-1-yl)malonate **10**

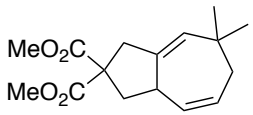


10 **11** **12**

General procedure E: Catalyst (0.018 mmol, 5 mol%) and $AgSbF_6$ (3 mg, 0.018 mmol, 5 mol%) were dissolved in dichloromethane (11.4 mL). Then, (*E*)-dimethyl 2-(4-methylpenta-2,3-dien-1-yl)-2-(penta-2,4-dien-1-yl)malonate **10** (100 mg, 0.360 mmol, 1.0 equiv.) was added in dichloromethane (3 mL). The reaction was monitored by TLC (PE/EtOAc, 9:1). After completion, the solution was filtered through a pad of silica. The latter was washed with diethyl ether. The solvent was removed under reduced pressure to give an inseparable mixture of dimethyl 7,7-dimethyl-3,3a,6,7-tetrahydroazulene-2,2(1H)-dicarboxylate **11** and dimethyl 7-(propan-2-ylidene)-3,3a,7,7a-tetrahydro-1H-indene-2,2(6H)-dicarboxylate **12**.

6.2.1. (IPr)AuCl-catalyzed cycloisomerization

(IPr)AuCl (22.4 mg, 0.036 mmol, 10 mol%) and $AgSbF_6$ (12 mg, 0.036 mmol, 10 mol%) were dissolved in dichloromethane (11.4 mL). Then, (*E*)-dimethyl 2-(4-methylpenta-2,3-dien-1-yl)-2-(penta-2,4-dien-1-yl)malonate **10** (100 mg, 0.360 mmol, 1.0 equiv.) was added in dichloromethane (3 mL). After 30 min at room temperature the solution was filtered through a pad of silica and the pad was washed with diethyl ether. The solvent was removed under reduced pressure to give dimethyl 7,7-dimethyl-3,3a,6,7-tetrahydroazulene-2,2(1H)-dicarboxylate **11** (91 mg, 0.328 mmol, 91%). The spectral data correspond to those previously reported.[7]

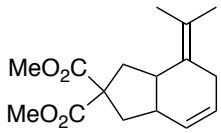


11

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 5.71 (s, 2H), 5.17 (s, 1H), 3.74 (s, 3H), 3.71 (s, 3H), 3.54 (dd, $^3J_{HH}$ = 10.3 / 8.8 Hz, 1H), 2.96 (dd, $^3J_{HH}$ = 16.5, 1.4 Hz, 1H), 2.88 (dt, $^3J_{HH}$ = 16.5, 2.3 Hz, 1H), 2.62-2.58 (m, 1H), 2.50-2.46 (m, 1H), 2.08 (dd, $^3J_{HH}$ = 12.6, 11.3 Hz, 1H), 1.88-1.83 (m, 1H), 1.00 (s, 3H), 0.95 (s, 3H).

6.2.2. (β-ICyD)AuCl-catalyzed cycloisomerization

(β-ICyD)AuCl (56 mg, 0.018 mmol, 5 mol%) and $AgSbF_6$ (6 mg, 0.018 mmol, 2 mol%) were dissolved in dichloromethane (11.4 mL). Then, (*E*)-dimethyl 2-(4-methylpenta-2,3-dien-1-yl)-2-(penta-2,4-dien-1-yl)malonate **10** (100 mg, 0.360 mmol, 1.0 equiv.) was added in dichloromethane (3 mL). The reaction was stirred 15h at 40°C. Then the solution was filtered through a pad of silica. The latter was washed with diethyl ether. The solvent was removed under reduced pressure. Dimethyl 7,7-dimethyl-3,3a,6,7-tetrahydroazulene-2,2(1H)-dicarboxylate **11** and dimethyl 7-(propan-2-ylidene)-3,3a,7,7a-tetrahydro-1H-indene-2,2(6H)-dicarboxylate **12** were obtained in 79% global yield as a yellow oil in an inseparable mixture and in a 1:2.3 ratio.



12

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 5.85 (d, $^3J_{HH}$ = 9.6 Hz, 1H), 5.75 - 5.71 (m, 1H), 3.74 (s, 3H), 3.73 (s, 3H), 3.00 (dd, $^3J_{HH}$ = 19.2 Hz / 11.6 Hz, 1H), 2.86 (d, $^3J_{HH}$ = 20.0 Hz, 1H), 2.73 (d, $^3J_{HH}$ = 20.0 Hz, 1H), 2.66 (dd, $^3J_{HH}$ = 13.2 / 6.8 Hz, 1H), 2.20 - 2.15 (m, 2H), 1.81 (s, 3H), 1.64 (s, 3H). The spectral data for dimethyl-7-(propan-2-ylidene)-3,3a,7,7a-tetrahydro-1H-indene-2,2(6H)-dicarboxylate **12** correspond to those previously reported.[8]

7. Computational details

The xtb program (version 6.2)[9] was used to simulate the various cyclodextrin species, in conjunction with the GFN2-xTB method.[10] For all calculations, default values were used. In order to maintain solvent molecules around the modified cyclodextrin, the system was confined with a spherical logfermi potential automatically determined on the basis of the starting structure and centered around the center of mass. To determine the number of solvent molecules inside the cavity, model systems were built by adding manually solvent molecules around the cyclodextrins and then equilibrated by molecular dynamics during 50 ps. To determine the barrier associated to methanol extrusion from the cavity, a relaxed scan was performed by slowly decreasing the distance between the oxygen's methanol and the gold atom.

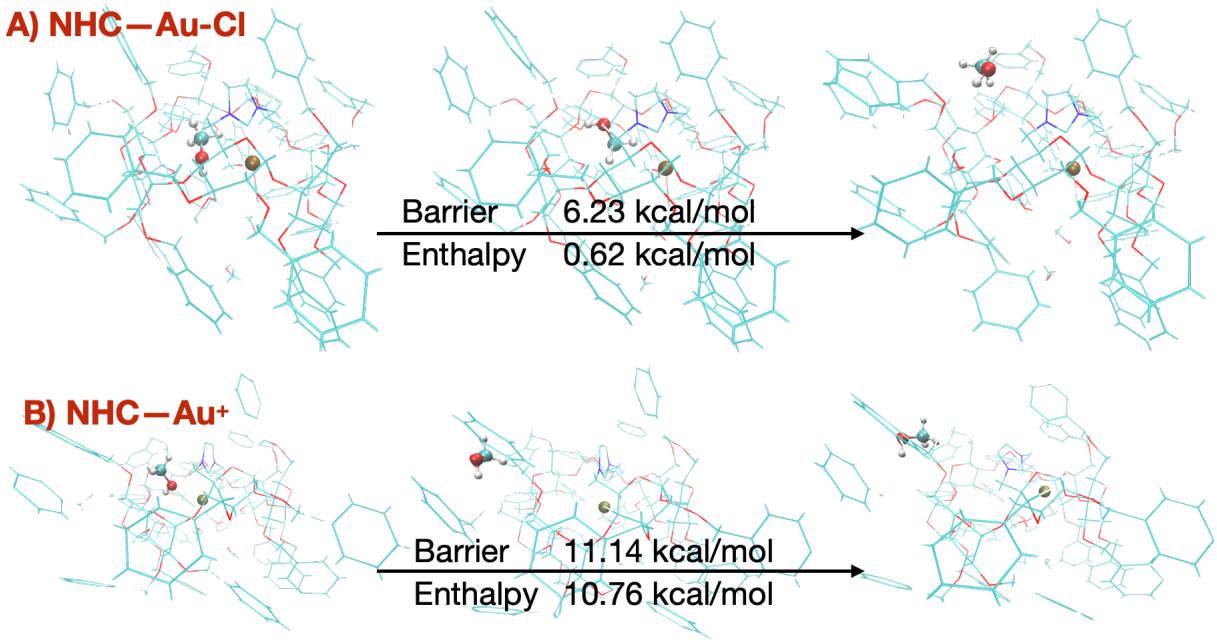


Figure S1: Methanol extrusion from CD cavity for two different systems: A) (β-ICyD)AuCl, B) (β-ICyD)Au+

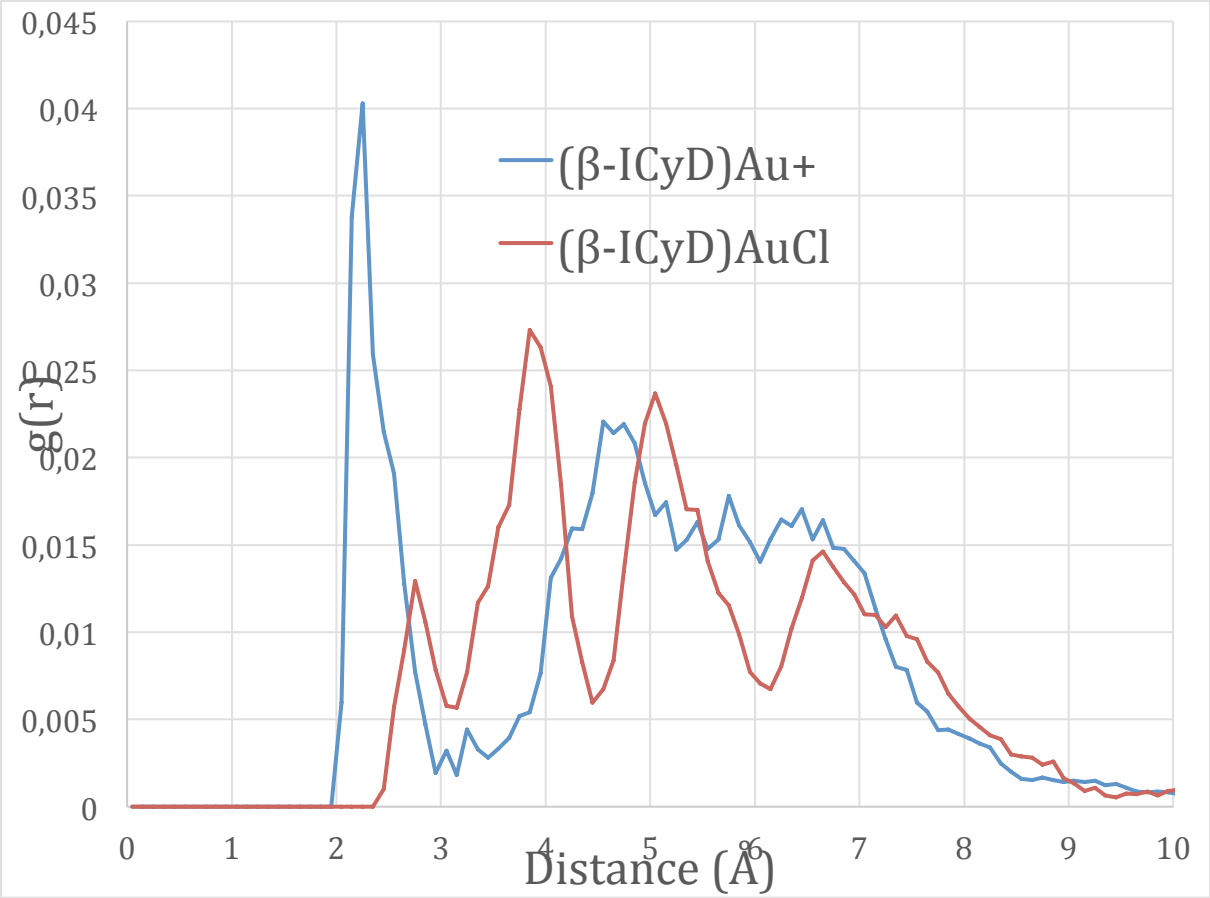


Figure S2: Radial pair distribution function between gold and oxygens in (β-ICyD)AuCl and (β-ICyD)Au+, both solvated by iPrOH.

7.1. XYZ Coordinates

7.1.1. (β-ICyD)AuCl methanol inside

```
  429
FINAL HEAT OF FORMATION =  -664.738067
 C    -1.220395    -5.027098    -3.141440
 H    -1.723844    -5.161280    -4.105993
 C     0.597954    -3.898381    -2.217330
 H    -0.099463    -3.414205    -1.526101
 O    -0.077779    -4.275959    -3.407982
 C    -0.792048    -6.412343    -2.605727
 H    -0.280700    -6.928798    -3.439002
 O    -1.979846    -7.088796    -2.293555
 C    -1.857931    -8.472870    -2.013020
 H    -1.270389    -8.956530    -2.813031
 H    -1.341354    -8.633868    -1.059413
 C    -3.243242    -9.060039    -1.971273
 C    -3.622767    -9.921800    -0.952376
 H    -2.911124   -10.179674    -0.183255
 C    -4.903856   -10.444010    -0.916570
 H    -5.190801   -11.111006    -0.117143
 C    -5.820347   -10.105402    -1.897196
 H    -6.822145   -10.508301    -1.865910
 C    -5.448036    -9.246810    -2.918340
 H    -6.159355    -8.979910    -3.686889
 C    -4.165479    -8.730395    -2.956854
 H    -3.871183    -8.057579    -3.748777
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C	0.181356	-6.298233	-1.410187
H	-0.430615	-6.138526	-0.514369
O	0.841531	-7.528629	-1.159683
C	1.744854	-8.036946	-2.139675
H	1.440744	-9.076104	-2.326075
H	1.676410	-7.482235	-3.080765
C	3.167952	-8.014509	-1.632009
C	3.497339	-8.739561	-0.491669
H	2.738580	-9.342645	-0.016123
C	4.772422	-8.667280	0.038879
H	5.015925	-9.230908	0.927810
C	5.732407	-7.873144	-0.566427
H	6.725753	-7.809738	-0.147550
C	5.419518	-7.165023	-1.713109
H	6.163487	-6.542650	-2.186922
C	4.144589	-7.240592	-2.245830
H	3.903592	-6.685172	-3.142041
C	1.189193	-5.121182	-1.500369
H	2.086310	-5.451075	-2.038916
O	1.560716	-4.717079	-0.183305
C	1.677047	-2.906931	-2.630604
H	2.272060	-2.651521	-1.754366
H	2.320678	-3.373958	-3.380844
C	-5.655171	-2.586279	-1.907513
H	-6.726259	-2.334410	-1.963118
C	-3.951965	-3.328998	-3.361988
H	-3.396203	-2.405377	-3.149484
O	-5.341344	-3.070931	-3.193535
C	-5.424146	-3.737947	-0.896226
H	-6.033845	-4.591948	-1.242672
O	-5.761234	-3.383352	0.408394
C	-7.137689	-3.403901	0.705475
H	-7.690331	-2.710078	0.047329
H	-7.547169	-4.414126	0.538706
C	-7.339934	-2.987612	2.138576
C	-8.486311	-3.366753	2.824287
H	-9.224337	-3.986195	2.333625
C	-8.680006	-2.959610	4.132422
H	-9.573294	-3.260350	4.661150
C	-7.730621	-2.172430	4.763732
H	-7.884321	-1.858817	5.786099
C	-6.587488	-1.791777	4.082149
H	-5.842104	-1.176856	4.562060
C	-6.392253	-2.196442	2.772809
H	-5.509274	-1.902610	2.230838
C	-3.931687	-4.100315	-0.926370
H	-3.387103	-3.226515	-0.561897
O	-3.546371	-5.115451	-0.042392
C	-4.235075	-6.348456	-0.089135
H	-4.589914	-6.583750	-1.099194
H	-3.483427	-7.102170	0.178360
C	-5.370170	-6.443007	0.900538
C	-5.306256	-5.745422	2.099761
H	-4.463735	-5.097094	2.277028
C	-6.320130	-5.865834	3.032343
H	-6.265678	-5.317575	3.961209
C	-7.406089	-6.686582	2.776069
H	-8.198076	-6.780641	3.504801
C	-7.476250	-7.382529	1.581019
H	-8.323654	-8.021264	1.374746
C	-6.462295	-7.260844	0.645505
H	-6.514076	-7.808553	-0.286269
C	-3.432750	-4.386875	-2.364896
H	-3.739019	-5.392407	-2.676937
O	-2.022912	-4.319005	-2.240944
C	-3.811710	-3.685246	-4.854636

H	-4.072821	-4.735365	-5.012249
H	-4.542868	-3.060493	-5.390117
O	-2.539106	-3.515304	-5.409895
C	-2.069192	-2.174117	-5.381157
H	-2.892758	-1.485907	-5.613236
H	-1.689548	-1.944741	-4.372664
C	-0.943927	-2.000675	-6.362158
C	-0.957393	-0.953848	-7.272674
H	-1.805805	-0.284672	-7.298321
C	0.101058	-0.768727	-8.145600
H	0.082223	0.049818	-8.850874
C	1.178216	-1.637227	-8.121207
H	2.002375	-1.496657	-8.805283
C	1.192200	-2.689507	-7.220383
H	2.031223	-3.370485	-7.203651
C	0.139623	-2.869733	-6.341343
H	0.142553	-3.674796	-5.624127
C	-4.316921	2.535319	-2.113780
H	-4.482102	3.584739	-2.389563
C	-4.750742	0.396994	-3.109650
H	-3.703053	0.069099	-3.117322
O	-4.817694	1.810132	-3.208736
C	-5.156035	2.172289	-0.866008
H	-6.209215	2.365778	-1.137845
O	-4.809060	2.916419	0.264213
C	-5.438104	4.180528	0.332525
H	-6.532450	4.052485	0.330013
H	-5.174897	4.790930	-0.544099
C	-5.028813	4.905732	1.583676
C	-3.925340	4.496527	2.316868
H	-3.365678	3.641100	1.977999
C	-3.560398	5.167023	3.470915
H	-2.709730	4.821752	4.041160
C	-4.285681	6.268445	3.890858
H	-4.004079	6.793295	4.792475
C	-5.377480	6.693470	3.152056
H	-5.945616	7.554325	3.473224
C	-5.750397	6.014468	2.006579
H	-6.606992	6.342895	1.436221
C	-4.972361	0.674524	-0.575117
H	-3.910815	0.495105	-0.378367
O	-5.617406	0.217359	0.578983
C	-6.998853	0.485876	0.743920
H	-7.505849	0.645865	-0.216236
H	-7.416419	-0.419539	1.204170
C	-7.257959	1.647304	1.672245
C	-8.293119	2.541234	1.439057
H	-8.925123	2.420733	0.567963
C	-8.526692	3.585820	2.319194
H	-9.336849	4.276178	2.130740
C	-7.719042	3.748824	3.430487
H	-7.894556	4.569836	4.110016
C	-6.685964	2.856894	3.666693
H	-6.055270	2.983295	4.534031
C	-6.460999	1.805984	2.798151
H	-5.669104	1.096819	2.970969
C	-5.374491	-0.168694	-1.812674
H	-6.471082	-0.183838	-1.912813
O	-4.898131	-1.479532	-1.547629
C	-5.455218	-0.146049	-4.362250
H	-5.638208	-1.215634	-4.223111
H	-6.413821	0.374116	-4.470375
O	-4.687385	-0.023725	-5.538190
C	-5.054986	1.005097	-6.442060
H	-4.622089	0.689209	-7.398045
H	-6.148231	1.032748	-6.547425

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C	-3.200517	2.687980	-6.274421
H	-2.533165	1.934117	-6.667830
C	-2.717519	3.948941	-5.970408
H	-1.670695	4.173572	-6.122117
C	-3.574785	4.919916	-5.477821
H	-3.202068	5.905604	-5.239783
C	-4.912838	4.619240	-5.290614
H	-5.588212	5.373022	-4.912731
C	-5.393003	3.357682	-5.594783
H	-6.439606	3.133725	-5.449594
C	0.669331	4.163880	-2.765084
H	1.430347	4.606992	-3.421795
C	-0.753791	2.243355	-2.781858
H	-0.468264	1.898566	-1.782195
O	0.310894	2.965074	-3.393895
C	-0.564889	5.091829	-2.695895
H	-0.922562	5.238951	-3.730640
O	-0.267520	6.327636	-2.109861
C	0.496580	7.227842	-2.891076
H	1.558021	7.146645	-2.620693
H	0.393623	6.980110	-3.959597
C	0.009899	8.637121	-2.658855
C	-1.351036	8.895887	-2.564346
H	-2.055114	8.084884	-2.658846
C	-1.807102	10.181554	-2.339061
H	-2.868182	10.361931	-2.249015
C	-0.907354	11.228163	-2.233127
H	-1.261554	12.233879	-2.061304
C	0.450065	10.981217	-2.350273
H	1.156766	11.795301	-2.275312
C	0.906548	9.690915	-2.554292
H	1.967543	9.501798	-2.636127
C	-1.691542	4.399212	-1.903875
H	-1.343679	4.159324	-0.892114
O	-2.838221	5.212772	-1.848572
C	-2.843536	6.131782	-0.763238
H	-2.947653	5.584454	0.185636
H	-1.895825	6.680547	-0.722972
C	-3.968938	7.115454	-0.910122
C	-4.150709	8.080819	0.073550
H	-3.483441	8.098938	0.921505
C	-5.167325	9.009649	-0.039592
H	-5.299285	9.756247	0.729607
C	-6.015315	8.986754	-1.135501
H	-6.809790	9.713404	-1.223326
C	-5.836663	8.030239	-2.118968
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C	-4.817803	7.099045	-2.007616
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C	-2.039647	3.080212	-2.620478
H	-2.467366	3.313833	-3.604152
O	-2.959647	2.299813	-1.871859
C	-1.031765	1.041603	-3.689408
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H	-1.170203	1.398470	-4.712095
C	4.814943	3.441026	0.295751
H	5.872621	3.470170	0.589118
C	3.475434	3.110010	-1.601950
H	3.032391	2.213128	-1.156918
O	4.799369	3.263430	-1.091753
C	4.144330	4.789648	0.640307
H	4.622508	5.583713	0.052221
O	4.244008	5.060056	2.017727
C	5.404597	5.760365	2.414356
H	5.476363	5.590031	3.496546

H	6.301816	5.329436	1.945225
C	5.365921	7.250140	2.161810
C	6.539619	7.988011	2.261338
H	7.470891	7.485631	2.484439
C	6.519950	9.359147	2.081647
H	7.436622	9.925458	2.161547
C	5.326614	10.004529	1.797291
H	5.313428	11.075509	1.656041
C	4.156847	9.272060	1.695052
H	3.221408	9.765788	1.477096
C	4.173656	7.900039	1.880907
H	3.264170	7.327665	1.793318
C	2.668334	4.680118	0.246776
H	2.223997	3.887890	0.861014
O	2.043221	5.913083	0.493117
C	0.735391	5.810588	1.027768
H	0.084283	5.300184	0.305889
H	0.757884	5.213543	1.952339
C	0.168433	7.172928	1.308867
C	-0.902532	7.295414	2.186526
H	-1.302362	6.414851	2.667439
C	-1.459629	8.534884	2.442610
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C	-0.954588	9.666049	1.822163
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C	0.110720	9.548592	0.947080
H	0.504371	10.427212	0.457042
C	0.669197	8.308726	0.689971
H	1.499668	8.208447	0.010564
C	2.554734	4.294671	-1.245813
H	2.837429	5.173609	-1.840215
O	1.192832	3.961990	-1.479017
C	3.588088	2.868181	-3.115381
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H	2.630983	2.481817	-3.473812
O	3.855799	3.999564	-3.900493
C	5.198519	4.461767	-3.893340
H	5.881975	3.632274	-3.681839
H	5.384101	4.819893	-4.915200
C	5.447434	5.595769	-2.931352
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H	7.205546	4.738402	-2.069931
C	6.764574	6.655134	-1.221838
H	7.619176	6.646911	-0.560786
C	5.901864	7.738067	-1.214558
H	6.080653	8.569955	-0.551509
C	4.807369	7.748051	-2.062314
H	4.133357	8.591878	-2.054613
C	4.588405	6.688312	-2.923489
H	3.752306	6.698662	-3.609090
C	4.955433	-1.162207	2.885143
H	5.476826	-1.875258	3.537528
C	5.564391	0.393801	1.172904
H	4.879764	-0.086223	0.462449
O	5.995902	-0.560763	2.139183
C	4.265231	-0.048840	3.716601
H	5.063097	0.440854	4.308513
O	3.228149	-0.473131	4.537217
C	3.577719	-1.234230	5.684816
H	3.840489	-2.255712	5.389001
H	4.433012	-0.764567	6.197335
C	2.351935	-1.241165	6.559459
C	2.081924	-0.169678	7.399610
H	2.791017	0.642554	7.480074
C	0.903342	-0.130645	8.124318
H	0.699671	0.710559	8.771290

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C	0.248186	-2.230756	7.172180
H	-0.478991	-3.020316	7.066513
C	1.428981	-2.273069	6.452352
H	1.635960	-3.095277	5.784169
C	3.650810	0.922416	2.692127
H	3.027707	0.303545	2.040647
O	2.742052	1.843526	3.201926
C	3.189415	2.768537	4.179244
H	3.660796	2.239324	5.020338
H	3.906072	3.475206	3.743585
C	1.968034	3.504330	4.662585
C	1.838852	4.874049	4.481164
H	2.622526	5.422599	3.979571
C	0.706913	5.533033	4.932847
H	0.614135	6.600418	4.790660
C	-0.304975	4.823397	5.557147
H	-1.180698	5.341912	5.921746
C	-0.191419	3.451069	5.715739
H	-0.984606	2.891824	6.190200
C	0.941127	2.792851	5.271569
H	1.035599	1.723601	5.386447
C	4.787582	1.547368	1.846170
H	5.467382	2.130024	2.486970
O	4.132957	2.391008	0.922553
C	6.814233	0.876996	0.413555
H	6.486804	1.564046	-0.371124
H	7.487069	1.397051	1.108935
O	7.498488	-0.148275	-0.258047
C	8.460482	-0.869953	0.512841
H	9.430028	-0.352006	0.435371
H	8.154370	-0.904269	1.560493
C	8.558925	-2.265173	-0.043870
C	8.111512	-3.354022	0.691669
H	7.731227	-3.204739	1.692099
C	8.140129	-4.626979	0.149103
H	7.774162	-5.460142	0.730035
C	8.623947	-4.823479	-1.132787
H	8.649117	-5.816090	-1.558106
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H	9.389584	-1.626363	-1.905376
C	2.752111	-5.283928	0.285192
H	2.838937	-6.315497	-0.072577
C	3.990284	-3.273332	0.218579
H	3.064949	-2.722622	0.001009
O	3.878099	-4.620447	-0.224158
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C	0.565176	-5.664484	2.484383
H	0.418153	-5.119761	3.428579
H	0.373794	-4.976924	1.654064
C	-0.401516	-6.818423	2.409563
C	-0.023173	-8.036218	1.862032
H	0.978977	-8.149559	1.481532
C	-0.921061	-9.088006	1.808298
H	-0.610485	-10.035715	1.389164
C	-2.207195	-8.932459	2.296759
H	-2.907999	-9.754759	2.269525
C	-2.595571	-7.714458	2.829144
H	-3.600439	-7.584002	3.202260
C	-1.698043	-6.664018	2.885295
H	-2.005144	-5.716619	3.300749

C	3.041935	-3.955347	2.451861
H	2.129073	-3.365967	2.310672
O	3.232984	-3.982376	3.856701
C	3.880124	-5.092265	4.469832
H	3.737422	-4.897691	5.539434
H	3.365644	-6.025821	4.219969
C	5.358398	-5.212567	4.185022
C	6.234961	-4.227300	4.627212
H	5.847064	-3.393128	5.194948
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C	8.093002	-5.405161	3.672276
H	9.150824	-5.476080	3.467382
C	7.232962	-6.406559	3.255127
H	7.622037	-7.272017	2.738316
C	5.874910	-6.309428	3.506320
H	5.213349	-7.102654	3.187431
C	4.171209	-3.165822	1.744210
H	5.155827	-3.540556	2.050710
O	4.014298	-1.791512	2.086103
C	5.138333	-2.669078	-0.586643
H	5.739078	-1.993614	0.028110
H	5.786846	-3.486744	-0.926156
O	4.588699	-1.971966	-1.685727
C	5.553669	-1.454011	-2.574304
H	5.019196	-0.698763	-3.165367
H	6.353253	-0.949962	-2.014751
C	6.160075	-2.473504	-3.508549
C	7.262687	-2.118163	-4.276316
H	7.675784	-1.124480	-4.178938
C	7.827428	-3.022368	-5.156114
H	8.683773	-2.735149	-5.749094
C	7.298086	-4.297087	-5.275580
H	7.740964	-5.006477	-5.959208
C	6.198866	-4.655854	-4.516028
H	5.782344	-5.648407	-4.611997
C	5.628340	-3.748468	-3.639121
H	4.771489	-4.027195	-3.043513
C	1.808345	-1.044657	-4.220682
H	2.715293	-1.419752	-4.647090
C	1.091722	0.064959	-4.514286
H	1.250856	0.839265	-5.234255
N	1.150775	-1.696642	-3.213859
N	0.012641	0.059418	-3.676826
C	0.045328	-1.018775	-2.866789
Au	-1.133070	-1.221480	-1.198579
Cl	-2.462231	-1.411130	0.692419
C	-0.216806	2.135644	1.068386
O	-0.990120	1.303033	0.231112
H	-1.605742	0.794874	0.779119
H	0.459598	2.689099	0.419277
H	-0.851788	2.847340	1.609223
H	0.364840	1.558361	1.791005
C	2.027441	-0.009791	-0.581388
O	1.449443	-1.184950	-0.064627
H	1.043086	-0.985510	0.809457
H	1.271644	0.614675	-1.067701
H	2.510265	0.578385	0.198247
H	2.776800	-0.307340	-1.318376
C	-2.933315	0.998943	3.277620
O	-3.629298	-0.221972	3.378441
H	-1.850050	0.844254	3.278583
H	-3.230117	1.532369	2.371304
H	-3.204516	1.597777	4.147511
H	-3.476614	-0.712283	2.550869
C	0.252870	-1.521147	3.443605

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O     0.070783    -0.763259     2.268066
H    -0.792186    -1.007339     1.873500
H     1.239562    -1.274109     3.828972
H     0.195190    -2.593568     3.232783
H    -0.501108    -1.276419     4.197151
C    -3.057891    -3.279417     4.502775
O    -2.751493    -2.112506     5.220002
H    -3.077402    -1.358062     4.692056
H    -4.141074    -3.423034     4.411020
H    -2.624841    -3.260201     3.496622
H    -2.637631    -4.117604     5.061128
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7.1.2. (β-ICyD)AuCl methanol extraction transition state

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 429
FINAL HEAT OF FORMATION =  -664.728142
C    -1.208378    -4.902691    -2.895127
H    -1.622029    -5.001399    -3.906092
C     0.474533    -3.824420    -1.735602
H    -0.333656    -3.546755    -1.052256
O    -0.072300    -4.102126    -3.017326
C    -0.788784    -6.305533    -2.386621
H    -0.250534    -6.789496    -3.222686
O    -1.984672    -6.994817    -2.140181
C    -1.871108    -8.390511    -1.922394
H    -1.257561    -8.836444    -2.724816
H    -1.385766    -8.596805    -0.961176
C    -3.256016    -8.979104    -1.954855
C    -3.661445    -9.904599    -1.004021
H    -2.968692   -10.215156    -0.236557
C    -4.942791   -10.426594    -1.034961
H    -5.250013   -11.143627    -0.288088
C    -5.833777   -10.024350    -2.015106
H    -6.835982   -10.426944    -2.035360
C    -5.434890    -9.104067    -2.970309
H    -6.125627    -8.788454    -3.739204
C    -4.151900    -8.588111    -2.942396
H    -3.836272    -7.868659    -3.683560
C     0.155254    -6.260923    -1.156824
H    -0.471118    -6.149805    -0.263242
O     0.806021    -7.505735    -0.964240
C     1.718763    -7.966959    -1.958670
H     1.371326    -8.964477    -2.264340
H     1.722085    -7.318325    -2.840028
C     3.117438    -8.076669    -1.398820
C     3.343152    -8.871218    -0.279542
H     2.517869    -9.421475     0.146650
C     4.600550    -8.932241     0.291976
H     4.764147    -9.545655     1.166122
C     5.646954    -8.206961    -0.254601
H     6.627864    -8.252332     0.196244
C     5.435684    -7.431595    -1.380703
H     6.248459    -6.866284    -1.812214
C     4.176025    -7.368683    -1.950835
H     4.013767    -6.759893    -2.829122
C     1.154764    -5.076125    -1.171321
H     2.027982    -5.325946    -1.788720
O     1.590333    -4.762612     0.148063
C     1.441876    -2.648867    -1.857228
H     1.577989    -2.257691    -0.847430
H     2.405501    -2.967086    -2.259673
C    -5.769671    -2.599210    -1.869731
H    -6.840668    -2.357973    -1.962768
C    -4.015149    -3.341046    -3.268215
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H	-3.474690	-2.405782	-3.066711
O	-5.410954	-3.094773	-3.139403
C	-5.563869	-3.740116	-0.842128
H	-6.160414	-4.598448	-1.200913
O	-5.941900	-3.378324	0.449161
C	-7.327855	-3.390512	0.698750
H	-7.853005	-2.694896	0.019949
H	-7.736799	-4.398810	0.519597
C	-7.579624	-2.967775	2.121977
C	-8.732304	-3.376315	2.779465
H	-9.434837	-4.025601	2.275411
C	-8.977738	-2.960165	4.076037
H	-9.875387	-3.284863	4.582782
C	-8.074145	-2.133062	4.722898
H	-8.266622	-1.811840	5.736098
C	-6.924745	-1.722832	4.069903
H	-6.216037	-1.079372	4.566617
C	-6.675963	-2.138521	2.772800
H	-5.785258	-1.825123	2.253479
C	-4.070596	-4.097685	-0.820858
H	-3.543750	-3.226123	-0.424228
O	-3.719707	-5.124103	0.063756
C	-4.405764	-6.355811	-0.032456
H	-4.725254	-6.570659	-1.058869
H	-3.663295	-7.114618	0.245636
C	-5.576716	-6.465273	0.912960
C	-5.562714	-5.771307	2.115900
H	-4.731346	-5.117042	2.323444
C	-6.610021	-5.900572	3.009663
H	-6.593697	-5.354883	3.941462
C	-7.680438	-6.726637	2.708886
H	-8.499120	-6.828009	3.406459
C	-7.701070	-7.419083	1.509764
H	-8.536486	-8.061725	1.269444
C	-6.653034	-7.289072	0.613814
H	-6.665702	-7.833631	-0.321220
C	-3.503546	-4.370166	-2.237556
H	-3.755770	-5.388539	-2.554080
O	-2.105490	-4.248250	-2.041108
C	-3.841442	-3.735114	-4.747599
H	-4.078550	-4.794276	-4.879974
H	-4.573623	-3.139504	-5.313624
O	-2.561928	-3.556923	-5.283601
C	-2.115905	-2.205460	-5.286792
H	-2.948665	-1.540472	-5.551204
H	-1.754638	-1.942664	-4.281588
C	-0.984300	-2.056456	-6.265128
C	-1.078832	-1.175610	-7.332665
H	-1.986188	-0.605184	-7.473280
C	-0.022665	-1.028796	-8.216151
H	-0.104160	-0.339524	-9.044360
C	1.132826	-1.770353	-8.042764
H	1.955286	-1.659653	-8.734348
C	1.229218	-2.656816	-6.982466
H	2.130295	-3.237413	-6.847809
C	0.178472	-2.797821	-6.094354
H	0.244896	-3.475624	-5.257582
C	-4.479692	2.529904	-2.112660
H	-4.648804	3.573959	-2.406495
C	-4.888684	0.372177	-3.084961
H	-3.841598	0.041640	-3.073885
O	-4.952780	1.784382	-3.206082
C	-5.337168	2.178300	-0.874934
H	-6.386732	2.359664	-1.166949
O	-5.011949	2.940903	0.248948
C	-5.676508	4.185410	0.312040

H	-6.767379	4.026421	0.315781
H	-5.434480	4.799797	-0.567825
C	-5.285311	4.928953	1.558575
C	-4.296542	4.444385	2.401723
H	-3.825113	3.507477	2.154142
C	-3.941055	5.146914	3.539358
H	-3.173691	4.757688	4.192276
C	-4.570194	6.341838	3.842576
H	-4.297620	6.888218	4.734216
C	-5.557751	6.830323	3.003406
H	-6.054141	7.761143	3.235661
C	-5.914132	6.128396	1.866732
H	-6.684944	6.510101	1.213114
C	-5.142911	0.687554	-0.558749
H	-4.080697	0.525207	-0.350737
O	-5.793695	0.239799	0.594373
C	-7.170677	0.527519	0.761025
H	-7.669512	0.728461	-0.195721
H	-7.611582	-0.382490	1.190054
C	-7.406702	1.663433	1.726819
C	-8.457559	2.552131	1.548750
H	-9.116892	2.444348	0.696398
C	-8.671050	3.575201	2.458374
H	-9.491006	4.263726	2.310335
C	-7.832051	3.718050	3.549035
H	-7.993047	4.521597	4.252728
C	-6.786212	2.828925	3.732460
H	-6.132893	2.936686	4.585418
C	-6.574916	1.803837	2.829763
H	-5.765469	1.103884	2.959965
C	-5.523559	-0.178142	-1.787170
H	-6.619230	-0.205482	-1.896619
O	-5.036260	-1.479803	-1.497986
C	-5.576116	-0.193126	-4.337461
H	-5.752801	-1.261675	-4.183368
H	-6.536998	0.319181	-4.463679
O	-4.798862	-0.088187	-5.508217
C	-5.147513	0.938880	-6.421330
H	-4.732160	0.601160	-7.377788
H	-6.240389	0.994783	-6.517457
C	-4.593296	2.302458	-6.090412
C	-3.238784	2.558513	-6.260270
H	-2.593748	1.770049	-6.621857
C	-2.716866	3.809410	-5.979813
H	-1.660054	3.994016	-6.113696
C	-3.549051	4.822027	-5.528998
H	-3.147814	5.800986	-5.310329
C	-4.899665	4.573406	-5.356361
H	-5.552702	5.360882	-5.009182
C	-5.418452	3.321315	-5.635509
H	-6.474170	3.136402	-5.501770
C	0.517380	4.193517	-2.748989
H	1.222514	4.672555	-3.439623
C	-0.911125	2.278663	-2.745618
H	-0.597136	1.952523	-1.747970
O	0.127186	3.009659	-3.388454
C	-0.715809	5.117526	-2.589830
H	-1.086787	5.321398	-3.610484
O	-0.402545	6.322613	-1.947950
C	0.336206	7.259535	-2.710304
H	1.412104	7.072863	-2.597916
H	0.079699	7.155092	-3.777095
C	0.001461	8.654752	-2.248889
C	-1.324887	9.026648	-2.073494
H	-2.109022	8.312535	-2.268680
C	-1.645030	10.301904	-1.646502

H	-2.681127	10.569551	-1.500815
C	-0.642776	11.228408	-1.415822
H	-0.891478	12.227272	-1.088966
C	0.680409	10.871043	-1.610039
H	1.466481	11.592804	-1.440150
C	1.001366	9.587763	-2.016202
H	2.035820	9.311201	-2.159643
C	-1.852777	4.409903	-1.826469
H	-1.527148	4.157752	-0.811077
O	-2.997972	5.226817	-1.782874
C	-3.028167	6.121056	-0.678106
H	-3.215644	5.555564	0.247576
H	-2.061244	6.623287	-0.565777
C	-4.102555	7.153799	-0.865223
C	-4.195655	8.201179	0.044531
H	-3.486512	8.255856	0.856422
C	-5.175865	9.164707	-0.097788
H	-5.239595	9.974774	0.613981
C	-6.073897	9.096598	-1.151175
H	-6.839826	9.850138	-1.262015
C	-5.980090	8.061566	-2.064337
H	-6.673301	8.007411	-2.891647
C	-4.998959	7.094507	-1.922751
H	-4.912246	6.290091	-2.637271
C	-2.199172	3.106364	-2.570420
H	-2.619646	3.359862	-3.551696
O	-3.124198	2.313807	-1.841196
C	-1.190412	1.055755	-3.626877
H	-2.154040	0.650246	-3.325467
H	-1.228294	1.376751	-4.669026
C	4.968482	3.324149	-0.219141
H	6.055004	3.380494	-0.047633
C	3.439508	3.266827	-2.026163
H	3.058680	2.275489	-1.776052
O	4.802353	3.362825	-1.596303
C	4.292190	4.568025	0.399869
H	4.690689	5.452438	-0.116034
O	4.546081	4.649053	1.781373
C	5.745841	5.302134	2.141156
H	5.995643	4.912328	3.137463
H	6.563980	5.023797	1.460313
C	5.655222	6.808616	2.226406
C	6.817180	7.540526	2.444509
H	7.765982	7.027630	2.523104
C	6.763667	8.917384	2.559710
H	7.671208	9.479098	2.727121
C	5.547377	9.574585	2.458770
H	5.507185	10.650328	2.548290
C	4.389634	8.847895	2.244844
H	3.437032	9.351327	2.171861
C	4.440025	7.468261	2.130903
H	3.540087	6.900569	1.955206
C	2.782142	4.495390	0.141516
H	2.376288	3.640854	0.699195
O	2.217734	5.698587	0.602115
C	0.860012	5.596555	0.995580
H	0.260209	5.232590	0.153267
H	0.770724	4.875880	1.821752
C	0.308123	6.928247	1.413858
C	-0.888154	6.966506	2.121442
H	-1.388347	6.043277	2.375566
C	-1.439017	8.175504	2.502339
H	-2.364190	8.187705	3.061396
C	-0.803439	9.362442	2.175269
H	-1.231616	10.308250	2.473305
C	0.382120	9.329662	1.463276

H	0.876619	10.253453	1.200303
C	0.933260	8.119338	1.079352
H	1.852956	8.085733	0.518112
C	2.515206	4.315419	-1.374877
H	2.687262	5.292685	-1.847408
O	1.143957	3.946457	-1.513881
C	3.463007	3.344047	-3.562418
H	4.305654	2.728086	-3.901257
H	2.535009	2.909543	-3.941706
O	3.542854	4.633466	-4.116009
C	4.844308	5.185896	-4.234407
H	5.575893	4.387063	-4.403238
H	4.800782	5.817879	-5.131195
C	5.272686	6.037275	-3.065403
C	6.465971	5.797922	-2.399523
H	7.083654	4.963092	-2.695802
C	6.868826	6.628764	-1.367362
H	7.808044	6.447062	-0.864603
C	6.077257	7.696987	-0.980991
H	6.394624	8.348723	-0.182012
C	4.874120	7.927734	-1.626577
H	4.253967	8.756635	-1.318564
C	4.481757	7.109521	-2.670017
H	3.561308	7.302336	-3.203520
C	5.024871	-1.128239	2.745698
H	5.435526	-1.796362	3.511484
C	5.845329	0.257678	1.005505
H	5.239324	-0.316513	0.290999
O	6.162317	-0.582328	2.106560
C	4.253598	0.044672	3.395697
H	4.969116	0.551611	4.069090
O	3.095959	-0.333682	4.071755
C	3.254272	-0.927031	5.354964
H	3.735549	-1.906101	5.263518
H	3.871160	-0.272524	5.992878
C	1.859810	-1.077466	5.902152
C	1.201819	0.009382	6.462197
H	1.722610	0.949183	6.583631
C	-0.122369	-0.100899	6.851576
H	-0.628182	0.755823	7.273225
C	-0.797725	-1.299391	6.692832
H	-1.838547	-1.387454	6.964198
C	-0.137239	-2.390901	6.153276
H	-0.665524	-3.324312	6.029476
C	1.183541	-2.281259	5.754521
H	1.695911	-3.118286	5.305412
C	3.794608	0.978185	2.262229
H	3.185538	0.352109	1.606379
O	2.918635	1.995001	2.661724
C	3.245073	2.737831	3.828053
H	3.427679	2.057973	4.670342
H	4.134193	3.354683	3.660137
C	2.064536	3.605935	4.169098
C	2.181625	4.986596	4.242941
H	3.128499	5.455186	4.022177
C	1.088155	5.761268	4.591682
H	1.184874	6.835609	4.645358
C	-0.129746	5.161219	4.863244
H	-0.977010	5.770824	5.141600
C	-0.255099	3.784002	4.776686
H	-1.201178	3.305431	4.985365
C	0.837848	3.008546	4.433447
H	0.752460	1.933622	4.374381
C	4.998211	1.484672	1.426655
H	5.600034	2.195795	2.002905
O	4.458419	2.099914	0.263379

C	7.160059	0.650412	0.313220
H	6.924159	1.360612	-0.483830
H	7.832291	1.119153	1.044466
O	7.793449	-0.426743	-0.325500
C	8.631028	-1.220779	0.512929
H	9.524725	-0.633280	0.778586
H	8.101281	-1.488322	1.432336
C	9.021586	-2.458028	-0.249373
C	8.505430	-3.697474	0.101808
H	7.843932	-3.780427	0.951956
C	8.838447	-4.827556	-0.624802
H	8.422069	-5.784290	-0.345267
C	9.698569	-4.731288	-1.703887
H	9.958751	-5.611896	-2.271944
C	10.225908	-3.499609	-2.052905
H	10.905267	-3.421668	-2.888329
C	9.885361	-2.368900	-1.333357
H	10.288217	-1.406188	-1.610704
C	2.761015	-5.406659	0.554351
H	2.737942	-6.462463	0.261362
C	4.134468	-3.510033	0.222595
H	3.263545	-2.917852	-0.072933
O	3.906020	-4.878174	-0.071209
C	2.991678	-5.355989	2.077784
H	3.918621	-5.931004	2.208156
O	2.046702	-6.051536	2.836006
C	0.712216	-5.545097	2.875665
H	0.543037	-5.109508	3.870345
H	0.569375	-4.756863	2.130717
C	-0.285629	-6.649395	2.636198
C	0.098539	-7.868298	2.096195
H	1.134163	-8.024441	1.839665
C	-0.833461	-8.871917	1.895890
H	-0.518869	-9.818972	1.478576
C	-2.158569	-8.669759	2.239978
H	-2.888614	-9.454901	2.102227
C	-2.550777	-7.452896	2.773557
H	-3.583880	-7.290666	3.042306
C	-1.621577	-6.447821	2.965283
H	-1.933560	-5.499216	3.375335
C	3.239296	-3.919080	2.563112
H	2.321057	-3.335030	2.433164
O	3.510604	-3.836086	3.951804
C	4.309762	-4.828654	4.588254
H	4.164632	-4.614806	5.653277
H	3.920652	-5.830736	4.385051
C	5.780614	-4.740571	4.259076
C	6.535398	-3.685834	4.763351
H	6.068173	-2.973080	5.429145
C	7.872042	-3.550091	4.431901
H	8.442085	-2.720211	4.822951
C	8.478926	-4.481311	3.605982
H	9.520639	-4.376676	3.341529
C	7.744916	-5.552917	3.125547
H	8.219425	-6.290404	2.495433
C	6.404488	-5.680452	3.447043
H	5.841722	-6.521681	3.067507
C	4.335596	-3.224263	1.722063
H	5.330756	-3.548650	2.049792
O	4.197005	-1.809211	1.860834
C	5.324997	-3.076270	-0.630911
H	5.930795	-2.333477	-0.100346
H	5.952866	-3.955242	-0.828527
O	4.832572	-2.524977	-1.830002
C	5.840274	-1.999526	-2.666636
H	5.312334	-1.336489	-3.362739

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 H     6.545227    -1.391400    -2.081630
 C     6.606663    -3.040300    -3.447071
 C     7.789751    -2.691076    -4.085144
 H     8.160682    -1.680514    -3.995409
 C     8.485677    -3.625581    -4.829124
 H     9.399673    -3.342439    -5.330454
 C     8.014902    -4.923972    -4.931804
 H     8.562471    -5.655326    -5.508064
 C     6.837920    -5.278753    -4.296750
 H     6.464011    -6.289588    -4.379055
 C     6.133085    -4.339082    -3.564719
 H     5.208119    -4.604949    -3.075009
 C     1.644350    -1.099360    -3.760132
 H     2.586805    -1.504376    -4.060455
 C     0.930354    -0.061186    -4.252224
 H     1.119271     0.603767    -5.067611
 N     0.942791    -1.601026    -2.703558
 N    -0.195962     0.035218    -3.483158
 C    -0.195012    -0.911631    -2.523519
Au    -1.505610    -1.108924    -0.960444
Cl    -2.827482    -1.346587     0.944728
 C    -0.604323     2.301999     1.138321
 O    -1.269490     1.270778     0.449506
 H    -1.891496     0.818096     1.041766
 H     0.042685     2.798975     0.417107
 H    -1.313189     3.033139     1.543988
 H     0.015642     1.919515     1.955716
 C     1.931281     0.462329    -0.539438
 O     2.988464     0.211997    -1.448748
 H     3.817076     0.360925    -0.979766
 H     1.798599    -0.371780     0.156095
 H     2.095854     1.378039     0.028315
 H     1.019619     0.578059    -1.117774
 C    -2.868864     0.822753     3.905165
 O    -3.843656    -0.156827     3.658215
 H    -1.860687     0.396434     3.926727
 H    -2.907409     1.618176     3.153773
 H    -3.091059     1.251611     4.883015
 H    -3.652900    -0.577365     2.796999
 C     0.322534    -1.318159     2.533489
 O     0.124826    -2.366817     1.609726
 H    -0.830522    -2.402838     1.441316
 H     1.386666    -1.254238     2.754918
 H    -0.218247    -1.505931     3.466139
 H    -0.009962    -0.366480     2.113358
 C    -3.610934    -3.337474     4.666184
 O    -3.699384    -2.233875     5.529224
 H    -3.812984    -1.443890     4.967791
 H    -4.534880    -3.471242     4.093668
 H    -2.778313    -3.228931     3.961845
 H    -3.446200    -4.220312     5.285690
```

7.1.3. (β-ICyD)AuCl methanol outside

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  429
FINAL HEAT OF FORMATION =  -664.737717
 C    -1.121666    -4.406958    -3.199501
 H    -1.512295    -4.449265    -4.224667
 C     0.540023    -3.370605    -1.942682
 H    -0.268512    -3.109632    -1.251453
 O    -0.000493    -3.576686    -3.242477
 C    -0.691506    -5.832390    -2.762983
 H    -0.038171    -6.233232    -3.559740
 O    -1.878830    -6.578553    -2.688495
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C	-1.748555	-7.987895	-2.580599
H	-1.141616	-8.361766	-3.423603
H	-1.260818	-8.263626	-1.639384
C	-3.126694	-8.588858	-2.643252
C	-3.563155	-9.471612	-1.664791
H	-2.903870	-9.737472	-0.851023
C	-4.837772	-10.007480	-1.724998
H	-5.169886	-10.691087	-0.958059
C	-5.690173	-9.658918	-2.758820
H	-6.686711	-10.073489	-2.802578
C	-5.262633	-8.774363	-3.735333
H	-5.925485	-8.497577	-4.542531
C	-3.985772	-8.245206	-3.679633
H	-3.647840	-7.552477	-4.436407
C	0.101302	-5.782916	-1.436203
H	-0.610690	-5.544126	-0.636565
O	0.629522	-7.034367	-1.048565
C	1.561351	-7.685091	-1.897837
H	1.029908	-8.375618	-2.573662
H	2.115400	-6.974150	-2.521968
C	2.527544	-8.486044	-1.057696
C	2.142235	-8.954844	0.191414
H	1.160168	-8.713082	0.564748
C	3.021337	-9.701116	0.955163
H	2.713132	-10.055729	1.927087
C	4.284645	-9.998003	0.473405
H	4.969308	-10.586529	1.066641
C	4.669479	-9.538679	-0.775063
H	5.652304	-9.776154	-1.156737
C	3.798412	-8.779468	-1.536212
H	4.105538	-8.414313	-2.506636
C	1.185199	-4.670703	-1.450025
H	2.010331	-4.936494	-2.125850
O	1.692164	-4.450722	-0.141565
C	1.512612	-2.188694	-2.024133
H	1.726652	-1.863692	-1.002174
H	2.434048	-2.485060	-2.530034
C	-5.807310	-2.487749	-1.909612
H	-6.894159	-2.310648	-1.940662
C	-4.077444	-3.016723	-3.427733
H	-3.598456	-2.052196	-3.210392
O	-5.478540	-2.884171	-3.221878
C	-5.482241	-3.670169	-0.965890
H	-6.047346	-4.538871	-1.349317
O	-5.803500	-3.415164	0.365180
C	-7.174527	-3.466863	0.683884
H	-7.737522	-2.710824	0.108335
H	-7.588117	-4.455634	0.425807
C	-7.343374	-3.191835	2.154860
C	-8.441443	-3.691097	2.841871
H	-9.166756	-4.301918	2.322043
C	-8.603722	-3.412885	4.187670
H	-9.459704	-3.806779	4.717222
C	-7.669962	-2.636681	4.854270
H	-7.797331	-2.425799	5.906091
C	-6.575118	-2.135395	4.171586
H	-5.842027	-1.530449	4.680696
C	-6.412402	-2.409684	2.824878
H	-5.568601	-2.019581	2.280311
C	-3.972452	-3.937425	-1.030539
H	-3.480991	-3.077652	-0.566286
O	-3.546551	-5.027252	-0.258437
C	-4.197556	-6.267098	-0.461323
H	-4.515382	-6.395370	-1.502458
H	-3.428973	-7.022219	-0.259350
C	-5.363571	-6.499820	0.468241

C	-5.320149	-6.019349	1.770524
H	-4.466881	-5.440949	2.084306
C	-6.366332	-6.260801	2.641625
H	-6.324673	-5.874658	3.648763
C	-7.464400	-6.992163	2.220059
H	-8.281861	-7.183795	2.899885
C	-7.514891	-7.473231	0.922333
H	-8.372078	-8.040245	0.586865
C	-6.469948	-7.225524	0.047828
H	-6.509458	-7.601844	-0.965983
C	-3.437164	-4.053298	-2.480133
H	-3.605615	-5.066137	-2.859475
O	-2.045730	-3.812978	-2.328273
C	-3.954413	-3.335970	-4.929180
H	-4.183488	-4.391088	-5.100380
H	-4.713025	-2.722942	-5.438567
O	-2.696992	-3.117786	-5.501200
C	-2.262180	-1.763279	-5.446839
H	-3.115254	-1.094794	-5.624369
H	-1.848058	-1.560345	-4.449178
C	-1.190790	-1.550285	-6.480186
C	-1.405400	-0.716319	-7.567947
H	-2.360576	-0.222999	-7.681634
C	-0.406938	-0.517438	-8.506632
H	-0.582014	0.135305	-9.349731
C	0.811567	-1.158744	-8.367325
H	1.589695	-1.005454	-9.100698
C	1.028164	-1.999366	-7.287656
H	1.978009	-2.501323	-7.177528
C	0.033634	-2.193748	-6.346415
H	0.195435	-2.839279	-5.496935
C	-4.801174	2.693038	-1.867809
H	-5.010701	3.751308	-2.069208
C	-5.185927	0.604018	-2.964135
H	-4.121637	0.348881	-3.034642
O	-5.343276	2.013850	-2.973739
C	-5.543224	2.227551	-0.592605
H	-6.618187	2.405035	-0.771633
O	-5.122698	2.897722	0.556644
C	-5.753965	4.140757	0.778780
H	-6.841304	3.996887	0.884980
H	-5.589555	4.818680	-0.071878
C	-5.207557	4.773410	2.028162
C	-4.087285	4.247134	2.655268
H	-3.636848	3.360849	2.238879
C	-3.570525	4.848456	3.788752
H	-2.697857	4.428744	4.268035
C	-4.170281	5.984971	4.303704
H	-3.769250	6.455216	5.190059
C	-5.288849	6.514319	3.682031
H	-5.761536	7.400054	4.080700
C	-5.805949	5.912823	2.548946
H	-6.676979	6.328157	2.063360
C	-5.281890	0.725760	-0.410044
H	-4.202265	0.595864	-0.283574
O	-5.834186	0.161576	0.743648
C	-7.198742	0.397981	1.039683
H	-7.782932	0.627792	0.138977
H	-7.572492	-0.545892	1.458679
C	-7.379442	1.477961	2.078738
C	-8.449937	2.359069	2.027383
H	-9.171354	2.285891	1.223114
C	-8.603165	3.331167	3.003181
H	-9.440325	4.013312	2.955281
C	-7.681438	3.433223	4.029769
H	-7.794613	4.199015	4.783122

C	-6.614625	2.551536	4.086412
H	-5.895693	2.628146	4.888439
C	-6.466827	1.573857	3.121161
H	-5.646766	0.875312	3.154981
C	-5.703844	-0.067603	-1.671877
H	-6.801140	-0.152087	-1.711908
O	-5.123834	-1.351386	-1.502091
C	-5.896412	0.071185	-4.217385
H	-6.050302	-1.005273	-4.097373
H	-6.868097	0.570595	-4.305423
O	-5.145610	0.223490	-5.400275
C	-5.513970	1.284228	-6.265788
H	-5.146324	0.970625	-7.249729
H	-6.608484	1.362264	-6.312464
C	-4.921200	2.627926	-5.919499
C	-3.578954	2.879925	-6.175219
H	-2.967543	2.100529	-6.608550
C	-3.027718	4.118448	-5.895970
H	-1.981339	4.299876	-6.096019
C	-3.819223	5.121854	-5.359407
H	-3.398840	6.094801	-5.149621
C	-5.154977	4.875221	-5.092394
H	-5.773233	5.655197	-4.672691
C	-5.702566	3.635179	-5.370674
H	-6.746512	3.451152	-5.164940
C	0.090268	4.480518	-2.826265
H	0.743204	4.994484	-3.544138
C	-1.271968	2.547442	-2.752865
H	-0.840461	2.259226	-1.786871
O	-0.350318	3.332109	-3.496281
C	-1.124749	5.377492	-2.495229
H	-1.590089	5.654103	-3.457914
O	-0.754823	6.530107	-1.790545
C	0.000107	7.487834	-2.509858
H	1.073417	7.282578	-2.396827
H	-0.251650	7.433023	-3.581664
C	-0.314470	8.870366	-1.995955
C	-1.619108	9.217598	-1.672705
H	-2.408227	8.491949	-1.787221
C	-1.910832	10.483623	-1.199110
H	-2.928779	10.731272	-0.936551
C	-0.905223	11.425749	-1.069766
H	-1.132473	12.416818	-0.705630
C	0.394491	11.093381	-1.412286
H	1.182801	11.826864	-1.320940
C	0.689118	9.819700	-1.864784
H	1.706332	9.560692	-2.121379
C	-2.175997	4.595791	-1.678322
H	-1.744758	4.283079	-0.719659
O	-3.317368	5.387384	-1.460750
C	-3.229444	6.198875	-0.295326
H	-3.310568	5.564081	0.599778
H	-2.256743	6.700486	-0.253183
C	-4.316471	7.234164	-0.281042
C	-4.316678	8.191088	0.727963
H	-3.531971	8.172464	1.469169
C	-5.302670	9.157866	0.772966
H	-5.294023	9.897360	1.560293
C	-6.299410	9.183163	-0.189753
H	-7.069985	9.939284	-0.154202
C	-6.299097	8.238542	-1.200440
H	-7.070179	8.257506	-1.957326
C	-5.311889	7.268351	-1.246734
H	-5.298739	6.534223	-2.038005
C	-2.567990	3.326301	-2.463105
H	-3.053155	3.615383	-3.403288

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O    -3.426743     2.484053    -1.713820
C    -1.524862     1.288202    -3.581290
H    -2.397559     0.791221    -3.161467
H    -1.705913     1.567645    -4.619970
C     4.674915     3.260635    -0.739099
H     5.774356     3.233450    -0.698772
C     2.935785     3.182812    -2.319161
H     2.524086     2.257210    -1.894844
O     4.342659     3.216926    -2.087561
C     4.169799     4.592346    -0.136875
H     4.536254     5.411801    -0.769600
O     4.624395     4.757196     1.185870
C     5.887897     5.374667     1.327483
H     6.243912     5.057469     2.316345
H     6.594460     4.993748     0.575787
C     5.864085     6.884880     1.284690
C     7.067443     7.579518     1.244636
H     8.000163     7.033280     1.214436
C     7.075309     8.962256     1.247603
H     8.014538     9.495199     1.216667
C     5.879645     9.662265     1.289357
H     5.887307    10.742457     1.291506
C     4.680524     8.972767     1.329065
H     3.745567     9.511820     1.367784
C     4.670248     7.587791     1.330340
H     3.737903     7.046009     1.356668
C     2.637106     4.568362    -0.186972
H     2.283804     3.720809     0.415834
O     2.143582     5.779521     0.327737
C     0.870865     5.660929     0.946290
H     0.140548     5.301512     0.211701
H     0.928580     4.925553     1.762342
C     0.379871     6.974617     1.480567
C    -0.705933     6.973499     2.349990
H    -1.155731     6.035872     2.643290
C    -1.211818     8.162491     2.839964
H    -2.052302     8.144910     3.519409
C    -0.638764     9.367792     2.467434
H    -1.032192    10.298006     2.850275
C     0.440142     9.373619     1.601978
H     0.886599    10.311723     1.306213
C     0.943759     8.183636     1.105381
H     1.776809     8.181126     0.421440
C     2.203448     4.368677    -1.659168
H     2.448927     5.290443    -2.205294
O     0.797571     4.167389    -1.657323
C     2.749273     3.134957    -3.845247
H     3.419288     2.356019    -4.231148
H     1.716849     2.857568    -4.061898
O     2.963317     4.346047    -4.520579
C     4.317503     4.719554    -4.726570
H     4.961871     3.834616    -4.706453
H     4.348700     5.155940    -5.734751
C     4.819644     5.747152    -3.744380
C     6.060455     5.614833    -3.137754
H     6.663567     4.743174    -3.345426
C     6.525130     6.594470    -2.276315
H     7.497590     6.492706    -1.816509
C     5.749943     7.708717    -2.003235
H     6.114349     8.472848    -1.334662
C     4.504381     7.838064    -2.593470
H     3.899265     8.706761    -2.380110
C     4.046400     6.868283    -3.466769
H     3.086893     6.974830    -3.953460
C     4.717516    -0.914774     2.558532
H     5.143541    -1.510943     3.377006
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C	5.540095	0.368463	0.735756
H	4.962361	-0.247527	0.032830
O	5.849315	-0.409398	1.882845
C	3.936519	0.294369	3.119613
H	4.676412	0.848731	3.730894
O	2.807969	-0.013939	3.869255
C	3.023211	-0.744681	5.073865
H	3.263070	-1.786323	4.834413
H	3.852657	-0.288273	5.637332
C	1.737859	-0.680493	5.854740
C	1.514224	0.337976	6.770933
H	2.285420	1.071818	6.960058
C	0.304314	0.422156	7.438535
H	0.140901	1.217961	8.151332
C	-0.691147	-0.506153	7.186441
H	-1.638242	-0.439040	7.701474
C	-0.475802	-1.525771	6.272796
H	-1.260053	-2.240915	6.073909
C	0.736976	-1.613249	5.611077
H	0.915992	-2.401052	4.895181
C	3.457952	1.151909	1.932299
H	2.827827	0.511929	1.304664
O	2.601787	2.195891	2.295134
C	3.028548	3.122653	3.290237
H	3.704182	2.641487	4.006656
H	3.557652	3.957683	2.818914
C	1.829241	3.630132	4.048098
C	1.689080	4.984790	4.320913
H	2.423374	5.686401	3.951116
C	0.616191	5.438726	5.068653
H	0.516419	6.493769	5.277212
C	-0.324973	4.541751	5.545367
H	-1.151223	4.896188	6.145003
C	-0.200104	3.191647	5.258869
H	-0.931099	2.486191	5.625473
C	0.872974	2.736728	4.513953
H	0.989533	1.686190	4.297499
C	4.663516	1.599781	1.069532
H	5.244157	2.362002	1.600832
O	4.117274	2.120190	-0.132095
C	6.872931	0.770341	0.076543
H	6.646565	1.221930	-0.893140
H	7.384944	1.504760	0.713817
O	7.723583	-0.313854	-0.190776
C	8.623435	-0.627671	0.870480
H	9.316605	0.217645	1.007883
H	8.064215	-0.782167	1.798691
C	9.387272	-1.872550	0.510856
C	8.978251	-3.108504	0.993909
H	8.114545	-3.166832	1.640046
C	9.678554	-4.255942	0.667355
H	9.348661	-5.212220	1.044198
C	10.801036	-4.178483	-0.138174
H	11.353435	-5.072882	-0.382903
C	11.211309	-2.950750	-0.629271
H	12.086236	-2.885593	-1.259436
C	10.504753	-1.804329	-0.311041
H	10.824167	-0.846804	-0.696036
C	2.807791	-5.208667	0.226817
H	2.753463	-6.231546	-0.160379
C	4.313752	-3.365295	0.110982
H	3.642808	-2.665559	-0.402453
O	4.005890	-4.688432	-0.295710
C	2.959601	-5.286303	1.758994
H	3.934014	-5.771127	1.911412
O	2.051736	-6.139698	2.385909

C	0.689655	-5.713252	2.475559
H	0.563048	-5.104232	3.383271
H	0.416895	-5.093830	1.619962
C	-0.196743	-6.926004	2.557333
C	0.292500	-8.118337	3.075862
H	1.320377	-8.161325	3.400222
C	-0.519888	-9.234954	3.162859
H	-0.125845	-10.159898	3.560188
C	-1.839275	-9.164574	2.750406
H	-2.479586	-10.031901	2.825938
C	-2.337432	-7.975403	2.244731
H	-3.371594	-7.914969	1.938344
C	-1.519849	-6.862908	2.137237
H	-1.911831	-5.942814	1.729328
C	3.008973	-3.853542	2.300539
H	2.068851	-3.355643	2.040820
O	3.090597	-3.747769	3.709438
C	3.817826	-4.721377	4.450333
H	3.521471	-4.516158	5.485115
H	3.487266	-5.731104	4.189595
C	5.318617	-4.607446	4.330608
C	5.976277	-3.506756	4.871482
H	5.403106	-2.759551	5.402391
C	7.347833	-3.373090	4.748551
H	7.845162	-2.510560	5.167871
C	8.085335	-4.350048	4.099731
H	9.156506	-4.249161	4.006935
C	7.442755	-5.460983	3.580222
H	8.012975	-6.235867	3.089380
C	6.068615	-5.587070	3.691585
H	5.576828	-6.462128	3.290388
C	4.167017	-3.080036	1.622335
H	5.105309	-3.329088	2.134868
O	3.897560	-1.682137	1.745420
C	5.752078	-3.121481	-0.346911
H	6.147943	-2.194579	0.082269
H	6.371110	-3.961448	-0.009895
O	5.765590	-3.039029	-1.757153
C	7.059751	-3.120557	-2.322450
H	6.940620	-2.780520	-3.357939
H	7.739258	-2.427419	-1.805249
C	7.650914	-4.509103	-2.334919
C	8.978982	-4.673578	-2.708595
H	9.568628	-3.805308	-2.965197
C	9.542058	-5.934937	-2.754368
H	10.573274	-6.052760	-3.053744
C	8.785768	-7.045424	-2.416305
H	9.228186	-8.030538	-2.445127
C	7.461394	-6.886641	-2.049244
H	6.862322	-7.745843	-1.787288
C	6.890047	-5.625605	-2.017982
H	5.852000	-5.508115	-1.743891
C	1.482634	-0.607865	-3.929958
H	2.423062	-0.955016	-4.305097
C	0.634620	0.342910	-4.387602
H	0.675645	0.963042	-5.257506
N	0.936027	-1.106394	-2.779770
N	-0.412794	0.387160	-3.509143
C	-0.233811	-0.501404	-2.516312
Au	-1.466899	-0.775527	-0.926856
Cl	-2.752132	-1.221161	0.930496
C	-0.534394	2.333631	1.169439
O	-1.486694	1.563029	0.474072
H	-2.061127	1.105725	1.106363
H	0.090516	2.815216	0.418303
H	-1.019078	3.106062	1.777319

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 H     0.103034     1.724712     1.815331
 C     5.110664    -0.052051    -3.255173
 O     4.489567    -1.286428    -3.521569
 H     4.796970    -1.930108    -2.859894
 H     4.639323     0.460827    -2.409095
 H     6.177277    -0.173805    -3.048397
 H     4.993962     0.565994    -4.145972
 C    -2.804551     0.598330     4.170313
 O    -3.654116    -0.463137     3.824306
 H    -1.748816     0.317832     4.089959
 H    -2.989581     1.479853     3.547340
 H    -3.020158     0.851978     5.208675
 H    -3.469307    -0.727801     2.901795
 C     0.414604    -1.210963     2.143361
 O    -0.072427    -2.508688     1.907656
 H    -1.009450    -2.410513     1.662882
 H     1.464350    -1.286688     2.414259
 H    -0.123054    -0.729037     2.965954
 H     0.319405    -0.585309     1.247593
 C    -2.851608    -3.739888     3.953541
 O    -3.196428    -2.954893     5.070040
 H    -3.389166    -2.056440     4.744297
 H    -3.581426    -3.627639     3.147470
 H    -1.859617    -3.475425     3.569839
 H    -2.833225    -4.780227     4.281714
```

7.1.4. (β-ICyD)Au+ methanol inside

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  428
FINAL HEAT OF FORMATION =  -659.826147
 C     3.064185    -4.797448    -1.076406
 H     3.998530    -4.902671    -1.638445
 C     2.203971    -3.691454     0.784179
 H     1.477167    -3.228265     0.105632
 O     3.370976    -4.037286     0.052636
 C     2.576113    -6.192079    -0.623982
 H     3.415566    -6.678456    -0.097980
 O     2.268050    -6.891186    -1.802813
 C     2.025020    -8.288414    -1.669827
 H     2.885755    -8.755714    -1.165374
 H     1.121097    -8.465217    -1.077655
 C     1.868342    -8.869344    -3.049180
 C     0.726436    -9.576722    -3.399032
 H    -0.071531    -9.693020    -2.681559
 C     0.605482   -10.128184    -4.663124
 H    -0.283818   -10.681737    -4.923545
 C     1.617593    -9.963051    -5.593246
 H     1.523987   -10.393877    -6.578743
 C     2.750691    -9.239965    -5.257094
 H     3.540503    -9.104050    -5.981153
 C     2.877470    -8.699829    -3.989782
 H     3.761860    -8.140840    -3.720733
 C     1.374374    -6.058116     0.335895
 H     0.502283    -5.809479    -0.281740
 O     1.013341    -7.273274     0.954519
 C     1.962630    -7.947062     1.783608
 H     2.483870    -8.710672     1.189340
 H     2.707188    -7.255440     2.190701
 C     1.182066    -8.601806     2.895121
 C     0.353195    -9.677374     2.601349
 H     0.324268   -10.062178     1.592946
 C    -0.430734   -10.246965     3.587707
 H    -1.071613   -11.082523     3.349999
 C    -0.395237    -9.744037     4.877739
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H	-1.008748	-10.187445	5.647652
C	0.429490	-8.673892	5.177680
H	0.457405	-8.275455	6.181005
C	1.216115	-8.103843	4.190965
H	1.855755	-7.267141	4.433579
C	1.521331	-4.923171	1.386294
H	2.095568	-5.275690	2.252031
O	0.221761	-4.519294	1.810444
C	2.632650	-2.648549	1.820250
H	1.762334	-2.332149	2.393536
H	3.386874	-3.065417	2.488681
C	1.377336	-2.608920	-5.529019
H	1.318586	-2.463734	-6.617763
C	3.017695	-3.298934	-3.948135
H	2.999926	-2.332121	-3.424633
O	2.675308	-3.095798	-5.313863
C	0.372086	-3.690567	-5.063334
H	0.660290	-4.634436	-5.555890
O	-0.953878	-3.367087	-5.359978
C	-1.314929	-3.611633	-6.707174
H	-0.695278	-3.002078	-7.386658
H	-1.128191	-4.667029	-6.955622
C	-2.764848	-3.278865	-6.937047
C	-3.468775	-3.933074	-7.940058
H	-2.973017	-4.684264	-8.537796
C	-4.796462	-3.625762	-8.175249
H	-5.334702	-4.136340	-8.959861
C	-5.435475	-2.670994	-7.401874
H	-6.474304	-2.437509	-7.579923
C	-4.735404	-2.012235	-6.407237
H	-5.225122	-1.256509	-5.812130
C	-3.400734	-2.303585	-6.184003
H	-2.839159	-1.772531	-5.434301
C	0.558747	-3.815661	-3.543378
H	0.397339	-2.820753	-3.111675
O	-0.394951	-4.614383	-2.890190
C	-0.480826	-6.003477	-3.212531
H	0.513276	-6.450935	-3.273440
H	-0.998653	-6.436331	-2.349113
C	-1.271713	-6.323509	-4.453804
C	-2.592779	-5.910525	-4.567891
H	-3.024706	-5.315648	-3.779770
C	-3.346867	-6.263774	-5.670921
H	-4.372707	-5.936513	-5.750962
C	-2.789195	-7.043936	-6.670719
H	-3.382801	-7.335858	-7.524021
C	-1.468201	-7.446200	-6.572911
H	-1.023887	-8.047965	-7.352136
C	-0.710130	-7.080550	-5.472747
H	0.320146	-7.399134	-5.399776
C	2.017664	-4.227321	-3.219349
H	2.199530	-5.265984	-3.514809
O	2.098440	-4.085070	-1.812708
C	4.464734	-3.831570	-4.016845
H	4.448727	-4.910356	-4.194048
H	4.934309	-3.343652	-4.883294
O	5.237018	-3.636846	-2.870462
C	5.615778	-2.290396	-2.622121
H	5.900008	-1.803177	-3.564417
H	4.765284	-1.737304	-2.190353
C	6.759185	-2.290422	-1.643181
C	7.948074	-1.633572	-1.926331
H	8.070065	-1.120739	-2.869730
C	8.986396	-1.639998	-1.009898
H	9.907266	-1.124754	-1.238401
C	8.849113	-2.316852	0.189235

H	9.662489	-2.330063	0.899135
C	7.668804	-2.985634	0.469946
H	7.565347	-3.525886	1.399994
C	6.625208	-2.969471	-0.437910
H	5.702050	-3.488244	-0.229560
C	1.807094	2.576243	-4.662765
H	2.086908	3.615079	-4.873352
C	2.733071	0.400414	-5.025558
H	2.855836	0.141895	-3.967695
O	2.853292	1.805811	-5.186913
C	0.506249	2.205682	-5.399591
H	0.720096	2.302241	-6.473934
O	-0.567529	3.038796	-5.043649
C	-0.817374	4.089336	-5.976587
H	-1.209545	3.648897	-6.908670
H	0.119739	4.612169	-6.207959
C	-1.815607	5.080039	-5.437249
C	-2.927780	4.671209	-4.714746
H	-3.101121	3.626224	-4.525148
C	-3.837334	5.601175	-4.242713
H	-4.696147	5.256941	-3.688273
C	-3.651650	6.949189	-4.494570
H	-4.363416	7.674266	-4.128264
C	-2.556221	7.362043	-5.234649
H	-2.406655	8.408909	-5.452156
C	-1.644758	6.433605	-5.704717
H	-0.796400	6.764164	-6.285543
C	0.183619	0.735565	-5.070365
H	0.053911	0.647949	-3.986363
O	-1.042198	0.305376	-5.592890
C	-1.185020	0.236093	-7.002230
H	-0.528399	0.961676	-7.503845
H	-0.908393	-0.766191	-7.357840
C	-2.612341	0.528459	-7.394069
C	-3.139338	-0.003101	-8.563231
H	-2.535114	-0.653626	-9.179607
C	-4.438289	0.290309	-8.936272
H	-4.841234	-0.129993	-9.845386
C	-5.221004	1.114911	-8.145057
H	-6.235020	1.340464	-8.439384
C	-4.699757	1.646126	-6.978248
H	-5.299405	2.288240	-6.351065
C	-3.399763	1.354370	-6.607035
H	-2.987563	1.753287	-5.695207
C	1.367891	-0.172509	-5.479130
H	1.373790	-0.294455	-6.571873
O	1.117763	-1.421278	-4.847626
C	3.886476	-0.229822	-5.826896
H	3.735682	-1.310933	-5.865836
H	3.857420	0.177307	-6.846833
O	5.151960	-0.046023	-5.256430
C	5.802947	1.183590	-5.547463
H	6.834316	0.917112	-5.821434
H	5.332731	1.667734	-6.408416
C	5.864679	2.147230	-4.389809
C	6.234010	1.699509	-3.126508
H	6.406661	0.643882	-2.973375
C	6.404741	2.597331	-2.086514
H	6.715255	2.247661	-1.112911
C	6.206758	3.951256	-2.297324
H	6.370619	4.648343	-1.488999
C	5.811243	4.401956	-3.546242
H	5.644111	5.455187	-3.717667
C	5.639726	3.503211	-4.586087
H	5.343351	3.859552	-5.561298
C	3.067022	4.251854	0.137786

H	3.816183	4.650727	0.829281
C	2.652081	2.317894	-1.120804
H	1.659991	2.239411	-0.654504
O	3.534655	2.974227	-0.231566
C	2.982466	5.158552	-1.113248
H	3.990066	5.214784	-1.555053
O	2.510439	6.439755	-0.805020
C	3.449542	7.305645	-0.189386
H	3.580945	7.040251	0.868007
H	4.425551	7.200836	-0.691228
C	2.963830	8.725158	-0.320537
C	2.600259	9.213795	-1.568627
H	2.662230	8.568162	-2.430750
C	2.164397	10.517950	-1.710067
H	1.881292	10.882436	-2.686153
C	2.106346	11.354072	-0.608268
H	1.776422	12.376123	-0.719526
C	2.477727	10.876291	0.636469
H	2.440832	11.525834	1.498850
C	2.896719	9.565217	0.781162
H	3.184927	9.198428	1.755403
C	2.043224	4.524626	-2.154420
H	1.030029	4.476431	-1.738755
O	2.039434	5.270771	-3.345723
C	1.018022	6.260348	-3.397599
H	0.049864	5.768296	-3.591944
H	0.945153	6.779960	-2.436691
C	1.299490	7.258100	-4.484605
C	0.678999	8.501962	-4.435721
H	0.029433	8.734582	-3.604383
C	0.896115	9.428705	-5.438459
H	0.409053	10.391737	-5.395519
C	1.740029	9.127735	-6.495724
H	1.910538	9.852708	-7.277244
C	2.368509	7.895769	-6.542268
H	3.032483	7.659117	-7.360889
C	2.147533	6.963312	-5.542202
H	2.641610	6.003753	-5.568038
C	2.526549	3.094711	-2.447179
H	3.508538	3.147042	-2.933775
O	1.615911	2.393049	-3.283740
C	3.187938	0.917686	-1.424817
H	2.432682	0.434143	-2.048731
H	4.129453	1.022776	-1.971697
C	0.477654	3.403723	4.515555
H	0.322933	3.418617	5.603511
C	2.256181	3.294861	2.963796
H	1.886089	2.372018	2.501154
O	1.851095	3.339424	4.332589
C	-0.075528	4.709397	3.906874
H	0.471663	5.548201	4.358278
O	-1.455369	4.831096	4.151266
C	-1.805971	5.435195	5.382252
H	-2.849534	5.137165	5.549924
H	-1.203300	5.022802	6.205277
C	-1.729828	6.944317	5.408392
C	-1.832881	7.600109	6.630076
H	-1.929502	7.024713	7.540329
C	-1.815416	8.981745	6.684588
H	-1.895899	9.483379	7.637575
C	-1.693696	9.720122	5.517751
H	-1.680475	10.798986	5.561748
C	-1.590104	9.069613	4.300976
H	-1.500353	9.636912	3.386630
C	-1.610910	7.685803	4.243240
H	-1.518713	7.179308	3.295781

C	0.191266	4.714048	2.396994
H	-0.401310	3.913993	1.929695
O	-0.198367	5.971748	1.911988
C	-0.510737	6.006301	0.529591
H	0.357777	5.674136	-0.049523
H	-1.347754	5.322635	0.323897
C	-0.852397	7.399217	0.084219
C	-1.550967	7.580031	-1.104186
H	-1.876293	6.719626	-1.672362
C	-1.837659	8.853512	-1.560496
H	-2.383097	8.978728	-2.484669
C	-1.436655	9.960383	-0.830669
H	-1.666080	10.954993	-1.182815
C	-0.742637	9.784885	0.353398
H	-0.428373	10.645680	0.924696
C	-0.441849	8.511370	0.803616
H	0.109358	8.365496	1.718547
C	1.695844	4.459559	2.129426
H	2.236256	5.385733	2.364836
O	1.805228	4.167844	0.740880
C	3.796978	3.225195	2.978903
H	4.082556	2.587902	3.825496
H	4.133868	2.753480	2.052080
O	4.464090	4.456888	3.051451
C	4.659787	4.993930	4.353492
H	4.815552	4.180693	5.072167
H	5.586070	5.576267	4.275806
C	3.551488	5.899485	4.828128
C	2.887045	5.661760	6.022368
H	3.144444	4.795411	6.613653
C	1.908290	6.537382	6.462453
H	1.407178	6.356871	7.402394
C	1.574859	7.649410	5.707790
H	0.819593	8.335814	6.056484
C	2.218886	7.880800	4.503714
H	1.954652	8.744449	3.911867
C	3.208507	7.015923	4.074283
H	3.741707	7.206093	3.152941
C	-2.685856	-0.858210	4.666002
H	-3.496126	-1.467533	5.084863
C	-0.938132	0.517583	5.459187
H	-0.227914	-0.138046	4.939232
O	-2.090950	-0.244158	5.787395
C	-3.254583	0.264429	3.769549
H	-3.931245	0.848450	4.420770
O	-3.914544	-0.176429	2.624855
C	-5.185776	-0.778483	2.830856
H	-5.064413	-1.750945	3.319156
H	-5.809319	-0.125651	3.462315
C	-5.807404	-0.966645	1.473313
C	-6.587075	0.028463	0.899063
H	-6.777662	0.943607	1.440970
C	-7.127087	-0.149142	-0.363459
H	-7.734319	0.628141	-0.802028
C	-6.888280	-1.321039	-1.062090
H	-7.314936	-1.461704	-2.044167
C	-6.100636	-2.311964	-0.498519
H	-5.913167	-3.226276	-1.042134
C	-5.559404	-2.134739	0.762789
H	-4.941260	-2.896796	1.212049
C	-2.082483	1.139265	3.292861
H	-1.415698	0.483344	2.719210
O	-2.453911	2.136878	2.378636
C	-3.584920	2.938890	2.715919
H	-4.458949	2.296360	2.879163
H	-3.381801	3.520278	3.621097

C	-3.891189	3.867265	1.572034
C	-3.712280	5.237357	1.702853
H	-3.310131	5.635402	2.621240
C	-4.043324	6.087010	0.660609
H	-3.904394	7.152173	0.772066
C	-4.544057	5.571281	-0.522814
H	-4.801012	6.238980	-1.331512
C	-4.717239	4.203849	-0.664288
H	-5.099585	3.790235	-1.585311
C	-4.396249	3.356021	0.382194
H	-4.540767	2.289718	0.282208
C	-1.280977	1.684445	4.500706
H	-1.860260	2.452280	5.023262
O	-0.092902	2.238214	3.950538
C	-0.295443	0.982539	6.778673
H	0.647881	1.482407	6.540961
H	-0.969042	1.684910	7.288087
O	0.041711	-0.079925	7.629144
C	-0.983393	-0.458365	8.547931
H	-1.147848	0.368716	9.255858
H	-1.915004	-0.653840	8.007347
C	-0.534162	-1.693102	9.280520
C	-0.974517	-2.946528	8.877682
H	-1.663031	-3.027803	8.048729
C	-0.551441	-4.084987	9.540568
H	-0.897951	-5.054783	9.216229
C	0.308661	-3.981259	10.619308
H	0.631259	-4.868905	11.141557
C	0.752094	-2.734548	11.026864
H	1.420245	-2.648590	11.870761
C	0.337801	-1.596963	10.357307
H	0.686582	-0.624822	10.673570
C	-0.280770	-5.209591	2.926514
H	0.054708	-6.252756	2.923120
C	-0.171177	-3.315194	4.344737
H	0.313317	-2.681312	3.590196
O	0.193210	-4.667982	4.129752
C	-1.821028	-5.220654	2.984666
H	-2.038935	-5.729486	3.932794
O	-2.428984	-6.025777	2.016127
C	-2.509066	-5.518050	0.687624
H	-3.339080	-4.804603	0.605688
H	-1.582193	-4.994670	0.424642
C	-2.728783	-6.679114	-0.244024
C	-2.003447	-7.852691	-0.074415
H	-1.292169	-7.917105	0.733833
C	-2.199998	-8.922334	-0.929338
H	-1.647512	-9.838812	-0.776408
C	-3.111138	-8.829051	-1.968623
H	-3.262434	-9.663274	-2.637280
C	-3.837843	-7.663821	-2.140050
H	-4.557026	-7.591669	-2.942044
C	-3.652157	-6.596628	-1.277563
H	-4.227705	-5.690995	-1.404089
C	-2.349681	-3.784626	3.060379
H	-2.079688	-3.244159	2.144257
O	-3.759493	-3.693143	3.115640
C	-4.506970	-4.656975	3.857742
H	-5.540694	-4.439747	3.566745
H	-4.262984	-5.671016	3.526528
C	-4.374328	-4.537217	5.356333
C	-4.923650	-3.442008	6.016117
H	-5.476728	-2.705638	5.449297
C	-4.785683	-3.299721	7.385461
H	-5.212845	-2.441968	7.883497
C	-4.112611	-4.263242	8.118651

H	-4.006813	-4.155685	9.187511
C	-3.588104	-5.371284	7.475060
H	-3.082653	-6.137460	8.043523
C	-3.714878	-5.506057	6.103081
H	-3.312582	-6.381257	5.612233
C	-1.680505	-3.021997	4.228065
H	-2.187123	-3.267708	5.168901
O	-1.783318	-1.628735	3.945444
C	0.369518	-2.952413	5.726147
H	-0.122593	-2.053375	6.114638
H	0.168305	-3.786527	6.409742
O	1.756902	-2.726216	5.610199
C	2.407766	-2.590001	6.857898
H	3.378370	-2.137518	6.621850
H	1.850252	-1.892240	7.498949
C	2.635218	-3.892942	7.586186
C	3.070415	-3.869572	8.904919
H	3.216830	-2.919488	9.397393
C	3.315873	-5.049666	9.581718
H	3.657869	-5.021021	10.605520
C	3.125358	-6.266617	8.948209
H	3.315647	-7.188681	9.477042
C	2.696377	-6.295565	7.633117
H	2.557645	-7.243023	7.132537
C	2.456027	-5.114342	6.951990
H	2.123919	-5.131866	5.924154
C	4.508518	-1.153556	1.157569
H	5.231437	-1.636194	1.780870
C	4.656104	-0.145710	0.264140
H	5.520389	0.412234	-0.026487
N	3.193992	-1.515174	1.133852
N	3.423794	0.075929	-0.285458
C	2.519519	-0.753609	0.260684
Au	0.530937	-0.792706	0.102522
C	-2.508683	-0.018173	-0.200108
O	-1.594784	-1.080938	0.070085
H	-1.859549	-1.855594	-0.488549
H	-2.316253	0.779635	0.512971
H	-2.388259	0.359069	-1.217428
H	-3.525778	-0.379482	-0.047615
C	2.382130	-0.004701	3.888073
O	1.464540	0.110278	2.809337
H	0.744062	0.690270	3.095862
H	3.380627	-0.119170	3.464106
H	2.369392	0.888706	4.512096
H	2.151658	-0.879922	4.501543
C	-1.541948	3.094147	-1.721777
O	-1.916243	2.113353	-2.662465
H	-2.142249	2.937366	-0.826914
H	-0.483392	2.996860	-1.466306
H	-1.733528	4.100447	-2.105840
H	-1.463341	2.314521	-3.498161
C	-2.985432	-2.402384	-2.650543
O	-2.330030	-3.062397	-1.580884
H	-1.655218	-3.650141	-1.965378
H	-3.834115	-1.866091	-2.227535
H	-3.347469	-3.114903	-3.392545
H	-2.314065	-1.696775	-3.147939
C	-5.106100	0.810005	-3.375510
O	-4.657528	2.134496	-3.277775
H	-3.738417	2.120687	-2.953682
H	-4.456756	0.211368	-4.023315
H	-5.163716	0.333229	-2.390031
H	-6.105932	0.841971	-3.807879

7.1.5. (β-ICyD)Au+ methanol extraction transition state

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  428
FINAL HEAT OF FORMATION =  -659.808399
 C     2.643975    -4.527208    -0.950055
 H     3.648172    -4.559593    -1.388153
 C     1.455339    -3.445307     0.738588
 H     0.724637    -3.171270    -0.025419
 O     2.725934    -3.669571     0.135796
 C     2.235915    -5.944106    -0.487944
 H     3.072641    -6.339505     0.112076
 O     2.073517    -6.695792    -1.664609
 C     1.952688    -8.108206    -1.513770
 H     2.843044    -8.492225    -0.991165
 H     1.057184    -8.356589    -0.935219
 C     1.867441    -8.702150    -2.893345
 C     0.768158    -9.459192    -3.274114
 H    -0.031621    -9.626526    -2.568567
 C     0.696494    -9.995761    -4.548078
 H    -0.159991   -10.586575    -4.835333
 C     1.717763    -9.769920    -5.455660
 H     1.661644   -10.188437    -6.449352
 C     2.812478    -9.005480    -5.085527
 H     3.611314    -8.826901    -5.790232
 C     2.888425    -8.477195    -3.809093
 H     3.743621    -7.886346    -3.513924
 C     0.959757    -5.900134     0.380876
 H     0.108162    -5.746770    -0.295561
 O     0.665400    -7.131612     1.003957
 C     1.604091    -7.698323     1.918726
 H     2.449457    -8.140761     1.374492
 H     1.992977    -6.946976     2.615650
 C     0.860942    -8.771695     2.671214
 C     0.621086    -9.998830     2.066656
 H     1.005296   -10.185710     1.074340
 C    -0.101770   -10.975315     2.728220
 H    -0.281608   -11.927765     2.252185
 C    -0.591199   -10.734159     4.001066
 H    -1.153684   -11.496815     4.517942
 C    -0.354822    -9.513398     4.608904
 H    -0.731704    -9.321474     5.602590
 C     0.365571    -8.533941     3.946530
 H     0.543522    -7.581935     4.426130
 C     0.942590    -4.729323     1.399619
 H     1.562755    -4.964525     2.273787
 O    -0.401932    -4.502963     1.809354
 C     1.630793    -2.258190     1.695254
 H     0.648291    -1.800421     1.843514
 H     2.036954    -2.595117     2.653254
 C     1.478144    -2.588464    -5.552821
 H     1.513661    -2.342524    -6.623676
 C     2.948272    -3.399799    -3.888535
 H     2.960727    -2.443497    -3.336458
 O     2.736813    -3.138636    -5.266565
 C     0.417358    -3.684234    -5.283981
 H     0.763225    -4.599358    -5.791984
 O    -0.861999    -3.331992    -5.715726
 C    -1.116052    -3.596308    -7.083324
 H    -0.471475    -2.972694    -7.726237
 H    -0.878116    -4.647157    -7.307974
 C    -2.562186    -3.329110    -7.411406
 C    -3.061425    -3.716748    -8.648339
 H    -2.408412    -4.200505    -9.360677
 C    -4.387976    -3.490538    -8.965254
 H    -4.768335    -3.793703    -9.929136
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C	-5.228674	-2.882763	-8.047250
H	-6.265758	-2.713299	-8.293834
C	-4.733384	-2.492438	-6.816401
H	-5.380734	-2.010746	-6.099176
C	-3.402650	-2.706543	-6.502919
H	-3.003184	-2.393756	-5.554063
C	0.411503	-3.894090	-3.766490
H	0.128759	-2.933114	-3.310820
O	-0.558116	-4.786088	-3.285461
C	-0.541054	-6.143063	-3.730051
H	0.480869	-6.512983	-3.844580
H	-1.009113	-6.696341	-2.907091
C	-1.326909	-6.383030	-4.992790
C	-2.632277	-5.920221	-5.101276
H	-3.060345	-5.361124	-4.284719
C	-3.374209	-6.169228	-6.240834
H	-4.385852	-5.800542	-6.318160
C	-2.821051	-6.895088	-7.282695
H	-3.402237	-7.095702	-8.169660
C	-1.521014	-7.360649	-7.182625
H	-1.084175	-7.926948	-7.991890
C	-0.774207	-7.100455	-6.045013
H	0.239959	-7.468081	-5.968433
C	1.823981	-4.241641	-3.245303
H	2.024122	-5.306374	-3.396532
O	1.713152	-3.966248	-1.859929
C	4.350154	-4.043295	-3.805868
H	4.260406	-5.130325	-3.727379
H	4.872170	-3.803956	-4.741871
O	5.095262	-3.623542	-2.699182
C	5.738225	-2.368229	-2.869484
H	6.426662	-2.420924	-3.724317
H	5.000192	-1.582965	-3.094284
C	6.485136	-2.007867	-1.614802
C	7.754860	-1.449635	-1.692951
H	8.219201	-1.305074	-2.657895
C	8.434200	-1.087024	-0.543008
H	9.418916	-0.650614	-0.616370
C	7.858885	-1.301504	0.697829
H	8.394269	-1.033752	1.596341
C	6.600912	-1.873787	0.781696
H	6.156117	-2.059525	1.747769
C	5.909183	-2.215121	-0.367810
H	4.928788	-2.661718	-0.300761
C	2.030271	2.547495	-4.480574
H	2.320184	3.579071	-4.705764
C	2.866922	0.351355	-4.902048
H	2.994286	0.091686	-3.840869
O	3.017549	1.747737	-5.076967
C	0.681675	2.219387	-5.147093
H	0.847907	2.318857	-6.230509
O	-0.310734	3.121672	-4.733358
C	-1.187026	3.569576	-5.779398
H	-1.866087	2.758377	-6.065207
H	-0.581348	3.855683	-6.649728
C	-1.983607	4.757488	-5.311761
C	-3.180043	4.581177	-4.627724
H	-3.548731	3.589495	-4.419329
C	-3.921283	5.680506	-4.231228
H	-4.858561	5.529521	-3.718606
C	-3.475974	6.961933	-4.507672
H	-4.063141	7.816374	-4.204550
C	-2.285252	7.142691	-5.190492
H	-1.932304	8.135685	-5.424697
C	-1.545013	6.045406	-5.593640
H	-0.625693	6.194744	-6.141050

C	0.346056	0.751419	-4.805498
H	0.311622	0.657931	-3.712370
O	-0.934309	0.361110	-5.220897
C	-1.143876	0.139424	-6.604504
H	-0.523578	0.814467	-7.212835
H	-0.869112	-0.893933	-6.854296
C	-2.591589	0.358451	-6.971471
C	-2.997016	0.136671	-8.281853
H	-2.280720	-0.209706	-9.013597
C	-4.311071	0.353645	-8.650538
H	-4.617144	0.175609	-9.670285
C	-5.230373	0.803026	-7.716343
H	-6.254032	0.980569	-8.009522
C	-4.831281	1.021763	-6.410421
H	-5.534539	1.376815	-5.673024
C	-3.517728	0.794126	-6.037484
H	-3.203928	0.953693	-5.018967
C	1.472798	-0.166441	-5.327434
H	1.434822	-0.209069	-6.425319
O	1.198222	-1.453877	-4.786484
C	3.991977	-0.299931	-5.729372
H	3.858286	-1.383723	-5.724583
H	3.908376	0.070402	-6.760728
O	5.276692	-0.077302	-5.225695
C	5.900132	1.150375	-5.587810
H	6.909536	0.881491	-5.930904
H	5.364875	1.618842	-6.418475
C	6.035078	2.126231	-4.447084
C	6.529700	1.693552	-3.223055
H	6.754156	0.646108	-3.087666
C	6.740333	2.594443	-2.193028
H	7.148748	2.250691	-1.253075
C	6.454248	3.937581	-2.375017
H	6.633938	4.639520	-1.574507
C	5.945109	4.373651	-3.587583
H	5.709953	5.417148	-3.735362
C	5.737837	3.471486	-4.618616
H	5.349150	3.817156	-5.564818
C	3.137928	4.399572	0.292887
H	3.812724	4.865534	1.019967
C	3.006144	2.404452	-0.969960
H	1.999111	2.195014	-0.579646
O	3.735801	3.163282	-0.025241
C	3.074542	5.266877	-0.985990
H	4.110125	5.379094	-1.351420
O	2.492180	6.518629	-0.769817
C	3.245728	7.418008	0.025185
H	3.033622	7.246009	1.088596
H	4.321710	7.247576	-0.143402
C	2.905125	8.839485	-0.341215
C	2.681016	9.187667	-1.665539
H	2.736487	8.429054	-2.429913
C	2.387669	10.495941	-2.004492
H	2.209911	10.750762	-3.038669
C	2.336190	11.473106	-1.025800
H	2.114263	12.496120	-1.290424
C	2.576684	11.134887	0.295055
H	2.546606	11.894767	1.062249
C	2.853458	9.823154	0.636537
H	3.039267	9.562903	1.668693
C	2.260927	4.544325	-2.073394
H	1.224388	4.440284	-1.730385
O	2.303758	5.268053	-3.277354
C	1.191747	6.138296	-3.467434
H	0.303213	5.531204	-3.709587
H	0.986595	6.695541	-2.547575

C	1.472496	7.097302	-4.589286
C	0.898243	8.363078	-4.568571
H	0.281760	8.649585	-3.728912
C	1.119853	9.247098	-5.609325
H	0.667216	10.227721	-5.587481
C	1.925183	8.881678	-6.675476
H	2.100993	9.573669	-7.485301
C	2.509003	7.626734	-6.694886
H	3.143011	7.339557	-7.521153
C	2.280505	6.737101	-5.659092
H	2.737176	5.758841	-5.666808
C	2.836754	3.137669	-2.311431
H	3.803609	3.228288	-2.819682
O	1.944151	2.351043	-3.095804
C	3.770787	1.087021	-1.155759
H	3.434624	0.620421	-2.080315
H	4.837817	1.309526	-1.212366
C	0.354942	3.556016	4.563698
H	0.139257	3.603553	5.640521
C	2.194431	3.394042	3.111191
H	1.839264	2.439527	2.697310
O	1.740608	3.510322	4.454743
C	-0.174869	4.841033	3.893446
H	0.356166	5.695953	4.333569
O	-1.561700	4.968946	4.088059
C	-1.949839	5.624452	5.280769
H	-2.989335	5.311026	5.446196
H	-1.353826	5.268143	6.133940
C	-1.907533	7.134785	5.231634
C	-2.081393	7.849063	6.411809
H	-2.208929	7.318322	7.345113
C	-2.095828	9.231602	6.395641
H	-2.231469	9.778796	7.316807
C	-1.936167	9.912808	5.198930
H	-1.948588	10.992580	5.187632
C	-1.761537	9.204255	4.023402
H	-1.640165	9.726252	3.085888
C	-1.749286	7.819136	4.036622
H	-1.602066	7.267896	3.121804
C	0.150843	4.788849	2.396530
H	-0.426204	3.975871	1.934928
O	-0.200695	6.032342	1.849405
C	-0.533140	6.010941	0.472574
H	0.294507	5.577072	-0.099963
H	-1.424116	5.384655	0.319133
C	-0.778759	7.402500	-0.038003
C	-1.411331	7.575850	-1.263763
H	-1.748089	6.713479	-1.822518
C	-1.616353	8.846082	-1.770451
H	-2.112556	8.966760	-2.722246
C	-1.197028	9.957160	-1.057561
H	-1.360358	10.949064	-1.451787
C	-0.569961	9.789078	0.163902
H	-0.241274	10.652619	0.722885
C	-0.353777	8.518302	0.667289
H	0.141391	8.378330	1.614564
C	1.665388	4.526406	2.209704
H	2.189415	5.457986	2.462264
O	1.859292	4.217200	0.833122
C	3.733803	3.349417	3.179883
H	4.002533	2.681471	4.007826
H	4.110811	2.931729	2.244180
O	4.369675	4.589397	3.326541
C	4.440385	5.110373	4.649527
H	4.453623	4.289925	5.374856
H	5.402622	5.636283	4.693586

C	3.338691	6.083065	4.985414
C	2.571205	5.934206	6.131472
H	2.745769	5.091495	6.783790
C	1.594860	6.865916	6.442991
H	1.011359	6.754826	7.345416
C	1.366055	7.945051	5.605966
H	0.608739	8.672366	5.852595
C	2.117589	8.089941	4.451941
H	1.937137	8.930218	3.797928
C	3.106277	7.170748	4.151555
H	3.723378	7.294298	3.272047
C	-2.745521	-0.752385	4.703361
H	-3.582058	-1.324577	5.120359
C	-1.001625	0.636921	5.472060
H	-0.286832	-0.013129	4.947756
O	-2.157053	-0.116761	5.811926
C	-3.274277	0.341293	3.748069
H	-3.965889	0.948290	4.359688
O	-3.922091	-0.154323	2.614083
C	-5.258899	-0.590494	2.838434
H	-5.254806	-1.492812	3.460139
H	-5.822487	0.201727	3.356130
C	-5.892435	-0.903792	1.510520
C	-6.754471	-0.006011	0.896372
H	-6.970247	0.942693	1.366595
C	-7.351482	-0.326063	-0.311444
H	-8.032769	0.372396	-0.773453
C	-7.079979	-1.538909	-0.921008
H	-7.550809	-1.789734	-1.859920
C	-6.207508	-2.431816	-0.320001
H	-5.999460	-3.382553	-0.788971
C	-5.617864	-2.116749	0.891096
H	-4.953612	-2.811892	1.380134
C	-2.103255	1.223887	3.280456
H	-1.399935	0.586185	2.733730
O	-2.474797	2.201530	2.347187
C	-3.613706	3.000000	2.663115
H	-4.497872	2.358438	2.775165
H	-3.446512	3.556896	3.590899
C	-3.870316	3.959015	1.532412
C	-3.750798	5.329276	1.716189
H	-3.438288	5.712851	2.673985
C	-4.020194	6.199826	0.673271
H	-3.920364	7.264704	0.823749
C	-4.406481	5.705764	-0.560959
H	-4.611785	6.389541	-1.371019
C	-4.529392	4.338844	-0.751452
H	-4.829577	3.941803	-1.709154
C	-4.267064	3.470710	0.293846
H	-4.371253	2.404122	0.158125
C	-1.345072	1.797027	4.506496
H	-1.959996	2.546077	5.017081
O	-0.159471	2.375733	3.991804
C	-0.364449	1.096313	6.791226
H	0.451833	1.785449	6.567954
H	-1.120854	1.599658	7.405886
O	0.226771	0.035648	7.500135
C	-0.646337	-0.680213	8.370724
H	-0.971097	-0.004965	9.178484
H	-1.532929	-1.017049	7.824018
C	0.100060	-1.852530	8.946873
C	-0.404612	-3.139954	8.824700
H	-1.342241	-3.297998	8.310619
C	0.279176	-4.214625	9.366922
H	-0.120981	-5.212703	9.267589
C	1.474918	-4.012497	10.033150

H	2.004021	-4.850744	10.459333
C	1.988585	-2.731635	10.148987
H	2.921141	-2.568042	10.667583
C	1.306340	-1.656440	9.608493
H	1.707955	-0.658377	9.696639
C	-0.805927	-5.251258	2.928025
H	-0.528987	-6.304825	2.815084
C	-0.380046	-3.409370	4.309254
H	0.030521	-2.860606	3.458580
O	-0.178704	-4.797001	4.097606
C	-2.323772	-5.170119	3.169849
H	-2.465315	-5.669271	4.137559
O	-3.111675	-5.913524	2.288647
C	-3.101391	-5.566326	0.908537
H	-4.063138	-5.096673	0.662370
H	-2.307228	-4.845848	0.691483
C	-2.907079	-6.792643	0.051822
C	-2.323426	-7.945994	0.555864
H	-2.010255	-7.977775	1.587053
C	-2.160162	-9.058517	-0.251197
H	-1.713079	-9.951590	0.160502
C	-2.577680	-9.030839	-1.570577
H	-2.471184	-9.904545	-2.197302
C	-3.154622	-7.880134	-2.084078
H	-3.484621	-7.855349	-3.113020
C	-3.318442	-6.769273	-1.275951
H	-3.775541	-5.873659	-1.669786
C	-2.726754	-3.694832	3.308413
H	-2.528380	-3.182302	2.358063
O	-4.107455	-3.493273	3.520375
C	-4.832067	-4.362800	4.389096
H	-5.875614	-4.112477	4.169860
H	-4.666056	-5.408650	4.115778
C	-4.557883	-4.133997	5.854945
C	-5.014345	-2.971426	6.468295
H	-5.599659	-2.265438	5.895271
C	-4.742023	-2.723054	7.801900
H	-5.098133	-1.814452	8.263800
C	-4.025516	-3.645578	8.546143
H	-3.816454	-3.456996	9.588463
C	-3.587747	-4.817198	7.950894
H	-3.043450	-5.546757	8.531882
C	-3.847727	-5.057452	6.612412
H	-3.507846	-5.976870	6.156811
C	-1.856424	-2.976485	4.373354
H	-2.269765	-3.142137	5.374814
O	-1.838170	-1.586191	4.053168
C	0.439297	-3.043591	5.543355
H	0.129462	-2.067744	5.936354
H	0.289957	-3.803339	6.317973
O	1.793069	-2.996001	5.138249
C	2.720420	-3.083412	6.205210
H	3.664643	-2.712120	5.791501
H	2.427743	-2.410241	7.021845
C	2.941199	-4.471678	6.755026
C	3.754152	-4.619969	7.872809
H	4.192710	-3.742988	8.325599
C	4.002953	-5.874326	8.396447
H	4.638935	-5.979508	9.262939
C	3.438800	-6.995946	7.810301
H	3.630345	-7.976389	8.220166
C	2.634063	-6.855020	6.694217
H	2.200412	-7.729709	6.230734
C	2.389174	-5.598418	6.164256
H	1.762376	-5.486345	5.292002
C	3.531054	-0.700371	1.918667

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 H     3.716468    -0.991268     2.931262
 C     4.145981     0.219337     1.136406
 H     4.967948     0.875144     1.328242
 N     2.535640    -1.263287     1.170642
 N     3.513512     0.185388    -0.072590
 C     2.525789    -0.721320    -0.056405
Au     1.303457    -1.357809    -1.638975
 C    -1.702775    -0.514184    -0.291116
 O    -0.934032    -1.659151    -0.635049
 H    -1.538506    -2.333105    -1.026853
 H    -1.039755     0.179850     0.222820
 H    -2.099073    -0.022991    -1.182050
 H    -2.520361    -0.784966     0.380214
 C     2.898969     0.311978     5.433223
 O     3.020033     0.117945     6.817775
 H     2.130478     0.056588     7.197585
 H     3.913444     0.324590     5.031967
 H     2.335286    -0.499723     4.960087
 H     2.413099     1.263373     5.192073
 C    -1.366340     2.912714    -1.500095
 O    -1.777921     2.026910    -2.516326
 H    -1.865262     2.615382    -0.578626
 H    -0.283370     2.858113    -1.355946
 H    -1.647581     3.942199    -1.741650
 H    -1.356024     2.315921    -3.344321
 C    -3.359606    -2.693691    -2.687069
 O    -2.548801    -3.463816    -1.820780
 H    -1.948576    -4.016606    -2.352232
 H    -4.027710    -2.107791    -2.055899
 H    -3.960626    -3.330710    -3.341325
 H    -2.755610    -2.021373    -3.304030
 C    -5.133085     0.798097    -2.666748
 O    -4.512030     1.993072    -3.054244
 H    -3.575233     1.966856    -2.778313
 H    -4.751640    -0.057773    -3.236939
 H    -5.003424     0.596886    -1.598579
 H    -6.197338     0.907355    -2.872892
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7.1.6. (β-ICyD)AuCl methanol outside

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  428
FINAL HEAT OF FORMATION =  -659.808993
 C     2.665947    -4.633285    -1.037957
 H     3.670304    -4.660000    -1.476336
 C     1.452853    -3.557449     0.626083
 H     0.735739    -3.305209    -0.157265
 O     2.737401    -3.776105     0.049798
 C     2.261164    -6.053886    -0.583983
 H     3.101115    -6.457855     0.005769
 O     2.090287    -6.794214    -1.766951
 C     1.958554    -8.206642    -1.627200
 H     2.850645    -8.603232    -1.117435
 H     1.067467    -8.452790    -1.040995
 C     1.853164    -8.784667    -3.012206
 C     0.737757    -9.516722    -3.394950
 H    -0.060561    -9.678825    -2.686781
 C     0.647613   -10.035339    -4.675179
 H    -0.221383   -10.606908    -4.963801
 C     1.666492    -9.816325    -5.587063
 H     1.596133   -10.221298    -6.585454
 C     2.777377    -9.076599    -5.214936
 H     3.574553    -8.903573    -5.922886
 C     2.871558    -8.566267    -3.932449
 H     3.739366    -7.994827    -3.635875
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C	0.990448	-6.023532	0.294082
H	0.129463	-5.899939	-0.376130
O	0.735212	-7.250589	0.940442
C	1.718037	-7.784879	1.829337
H	2.420359	-8.415605	1.265856
H	2.285115	-6.991561	2.327590
C	0.983301	-8.620649	2.845738
C	0.429259	-9.835446	2.462484
H	0.565837	-10.181425	1.448712
C	-0.291253	-10.592460	3.368252
H	-0.718874	-11.535439	3.062384
C	-0.461949	-10.142922	4.667306
H	-1.021525	-10.735723	5.375070
C	0.087149	-8.933046	5.054830
H	-0.041888	-8.576740	6.066065
C	0.803937	-8.171649	4.147286
H	1.219398	-7.223422	4.455285
C	0.950855	-4.840149	1.297494
H	1.566077	-5.058280	2.179510
O	-0.397729	-4.627305	1.696822
C	1.575716	-2.357079	1.571657
H	0.583348	-1.904883	1.656981
H	1.929158	-2.673277	2.556949
C	1.467483	-2.614453	-5.570912
H	1.485031	-2.327329	-6.631631
C	2.954539	-3.507820	-3.969048
H	2.999609	-2.571555	-3.382979
O	2.724543	-3.188260	-5.331203
C	0.398861	-3.710157	-5.331731
H	0.732859	-4.609437	-5.874444
O	-0.879588	-3.330390	-5.742010
C	-1.157607	-3.572187	-7.109353
H	-0.505996	-2.957557	-7.753773
H	-0.948629	-4.625871	-7.349019
C	-2.601367	-3.266680	-7.415183
C	-3.104915	-3.562271	-8.675604
H	-2.456662	-4.000777	-9.420864
C	-4.429573	-3.302761	-8.974237
H	-4.813227	-3.534652	-9.956393
C	-5.263835	-2.751757	-8.015449
H	-6.299124	-2.554938	-8.248747
C	-4.764492	-2.453475	-6.760757
H	-5.406934	-2.016853	-6.011036
C	-3.436113	-2.702968	-6.463933
H	-3.034373	-2.463647	-5.494756
C	0.406270	-3.970008	-3.823194
H	0.136465	-3.021338	-3.335498
O	-0.566264	-4.865500	-3.354912
C	-0.568415	-6.211498	-3.830667
H	0.448328	-6.592750	-3.956055
H	-1.042910	-6.776835	-3.019770
C	-1.361029	-6.412024	-5.096068
C	-2.656470	-5.919889	-5.192737
H	-3.069413	-5.365148	-4.365555
C	-3.406015	-6.133331	-6.334677
H	-4.410183	-5.743013	-6.402661
C	-2.869838	-6.850821	-7.391155
H	-3.456648	-7.022907	-8.280429
C	-1.579249	-7.344567	-7.303049
H	-1.155720	-7.904078	-8.123987
C	-0.825090	-7.121294	-6.162438
H	0.181436	-7.511026	-6.094749
C	1.822860	-4.341930	-3.329307
H	2.006009	-5.407893	-3.491941
O	1.730784	-4.073036	-1.942704
C	4.343599	-4.181672	-3.920290

H	4.234393	-5.265514	-3.825629
H	4.847537	-3.963586	-4.870905
O	5.119593	-3.761457	-2.834134
C	5.796596	-2.530377	-3.045522
H	6.529084	-2.651372	-3.856123
H	5.089959	-1.748116	-3.360901
C	6.486290	-2.091340	-1.783207
C	7.721596	-1.458772	-1.855625
H	8.196736	-1.321073	-2.816312
C	8.351725	-1.013985	-0.706815
H	9.309182	-0.520023	-0.776614
C	7.763546	-1.220610	0.529511
H	8.262318	-0.890472	1.428427
C	6.541036	-1.865436	0.608488
H	6.087752	-2.046541	1.571517
C	5.895305	-2.286652	-0.541698
H	4.939724	-2.783824	-0.475691
C	2.042419	2.507831	-4.440871
H	2.329575	3.540387	-4.665191
C	2.873090	0.314400	-4.884650
H	3.018615	0.045583	-3.827512
O	3.022278	1.710848	-5.053775
C	0.685967	2.180631	-5.091590
H	0.841478	2.276288	-6.176988
O	-0.300778	3.085996	-4.672423
C	-1.180146	3.535977	-5.715153
H	-1.854943	2.723296	-6.006217
H	-0.575937	3.831600	-6.583450
C	-1.983555	4.715577	-5.239151
C	-3.195265	4.528035	-4.585686
H	-3.569890	3.532956	-4.405037
C	-3.942762	5.621117	-4.183802
H	-4.892414	5.462114	-3.697395
C	-3.486701	6.906741	-4.420763
H	-4.077166	7.756595	-4.111282
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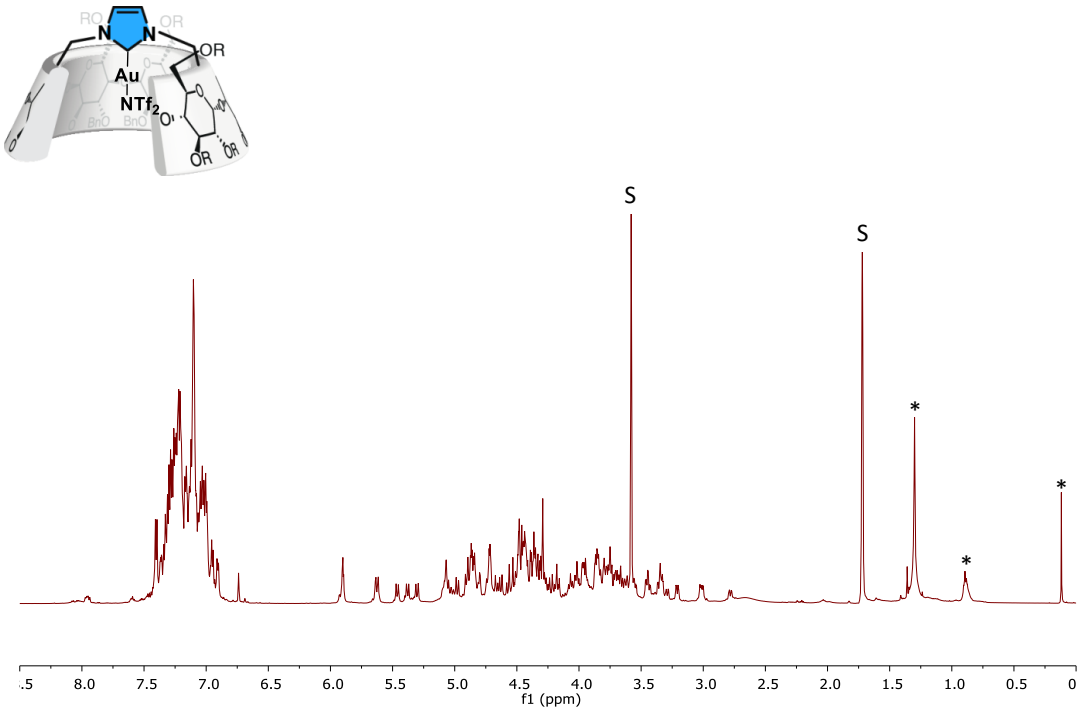
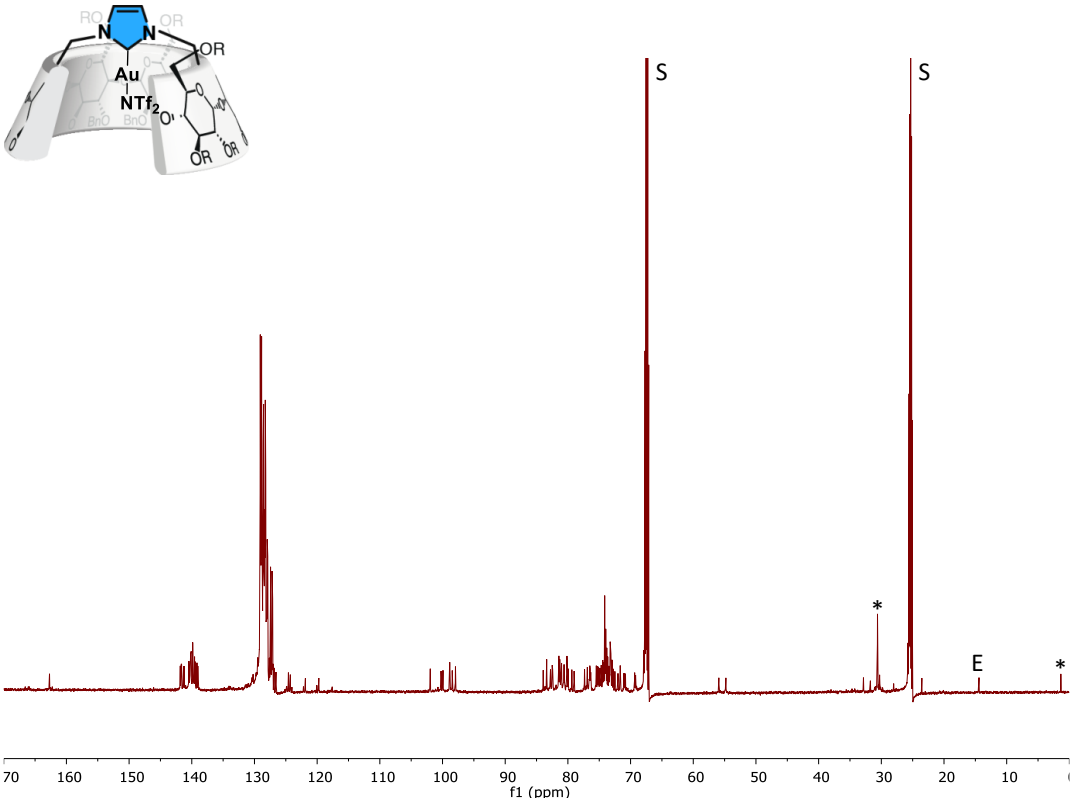
8. NMR spectrum



^{1}H NMR of (β-ICyD)AuNTf$_2$, THF-d$_8$, 600 MHz, 300 K ; S : solvent, * : grease



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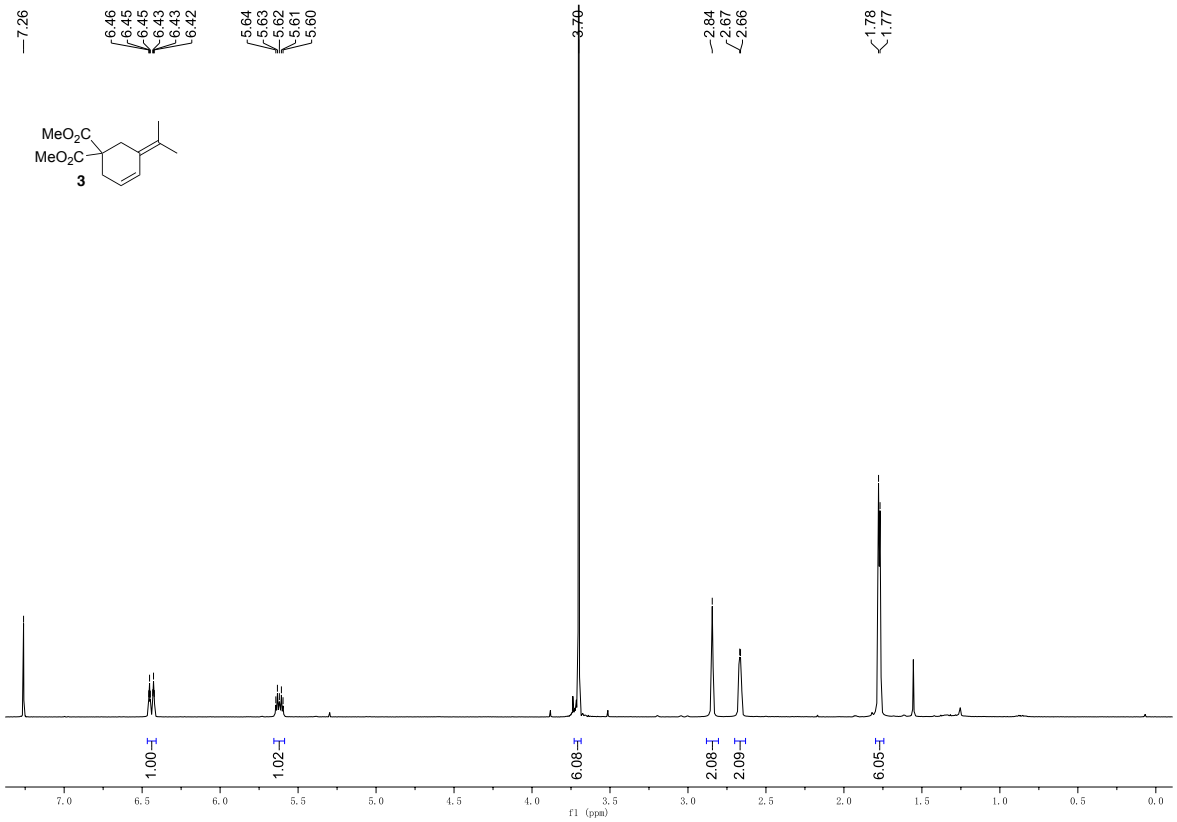

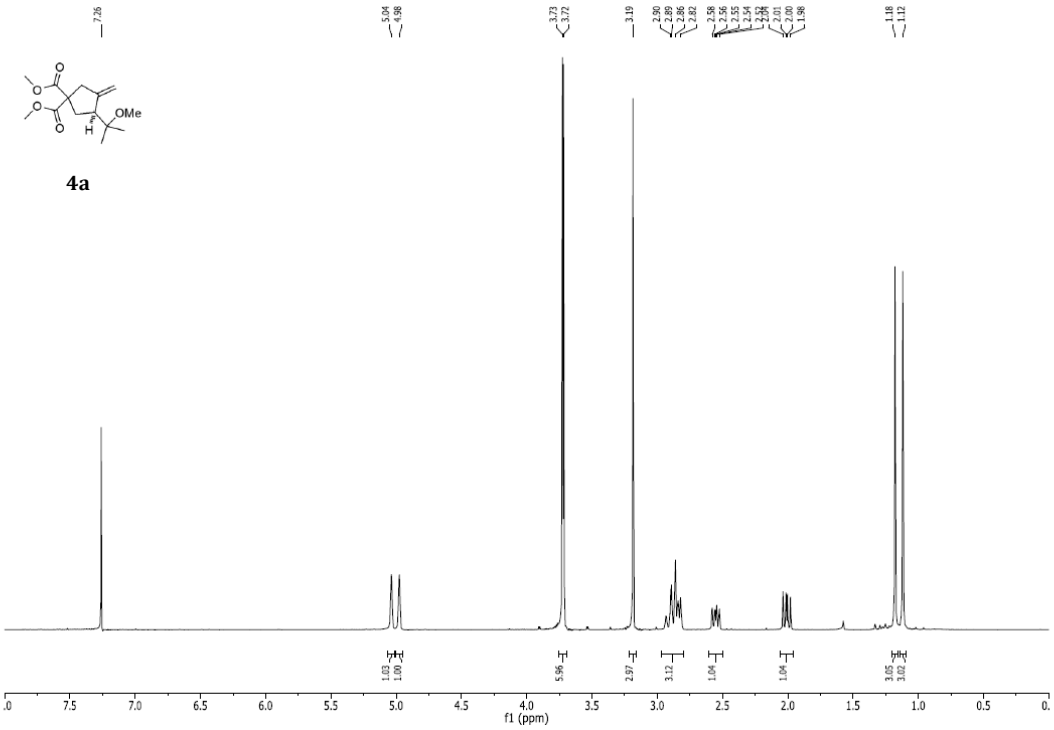
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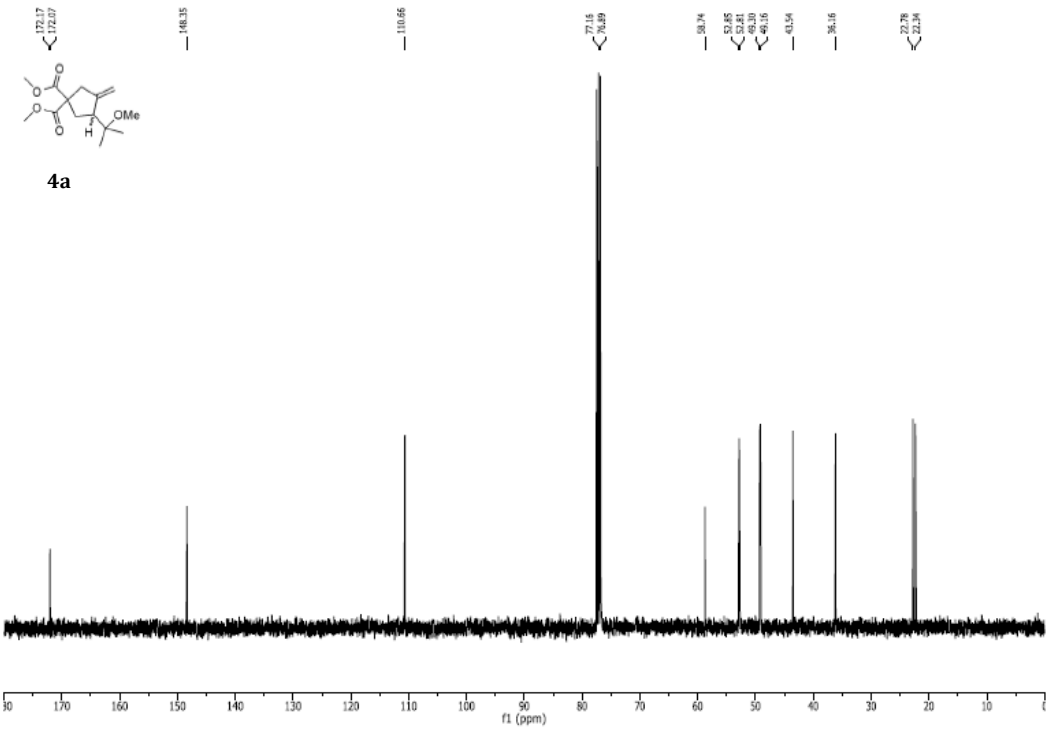
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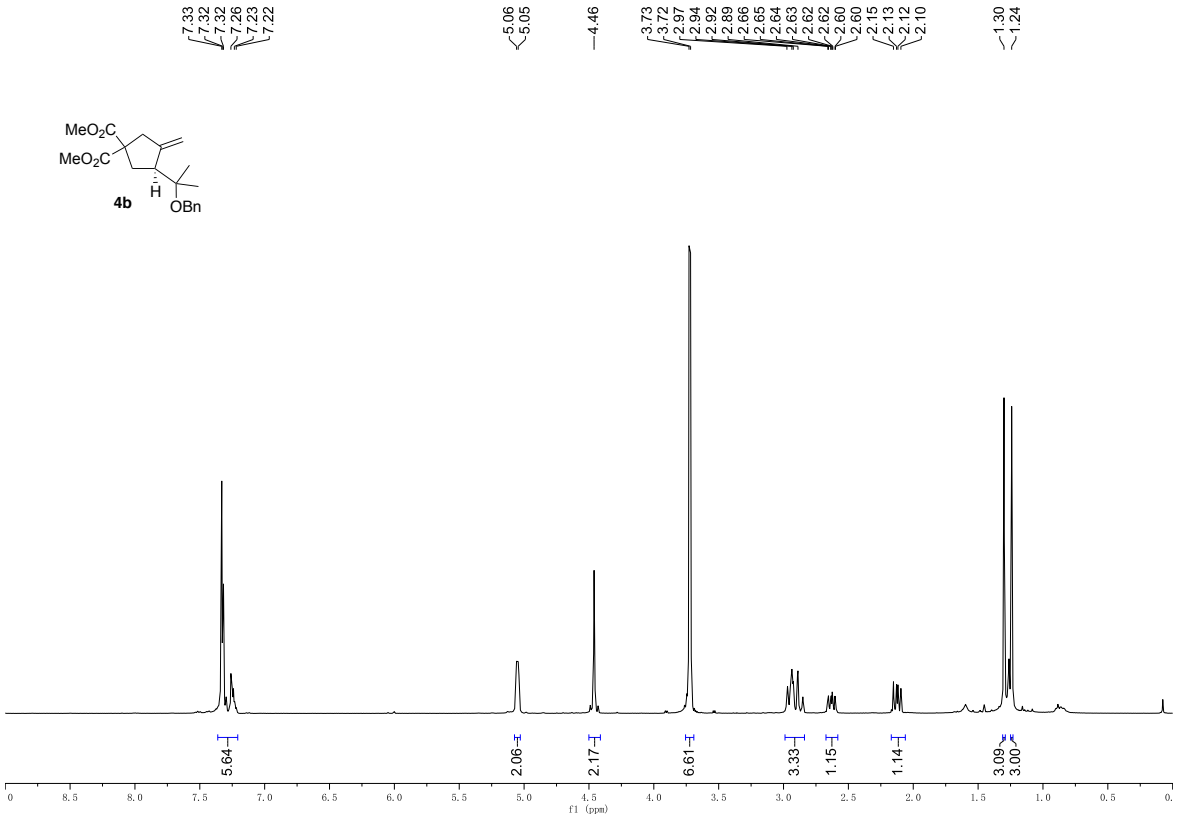
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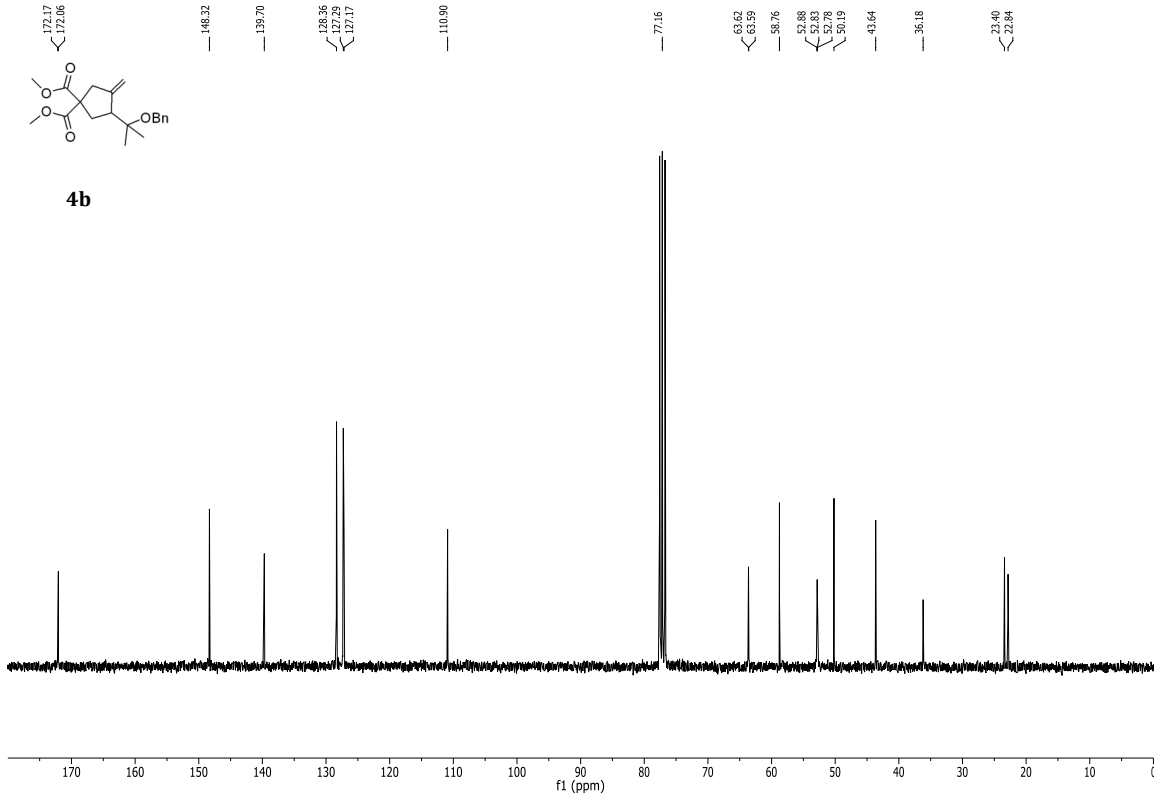
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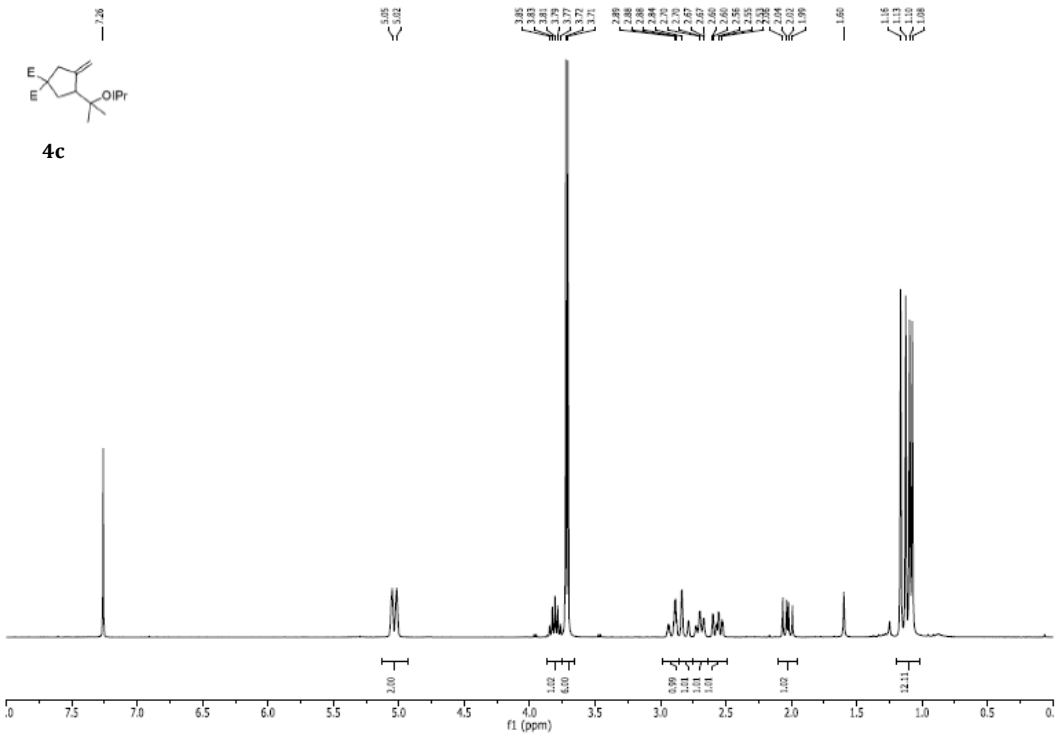
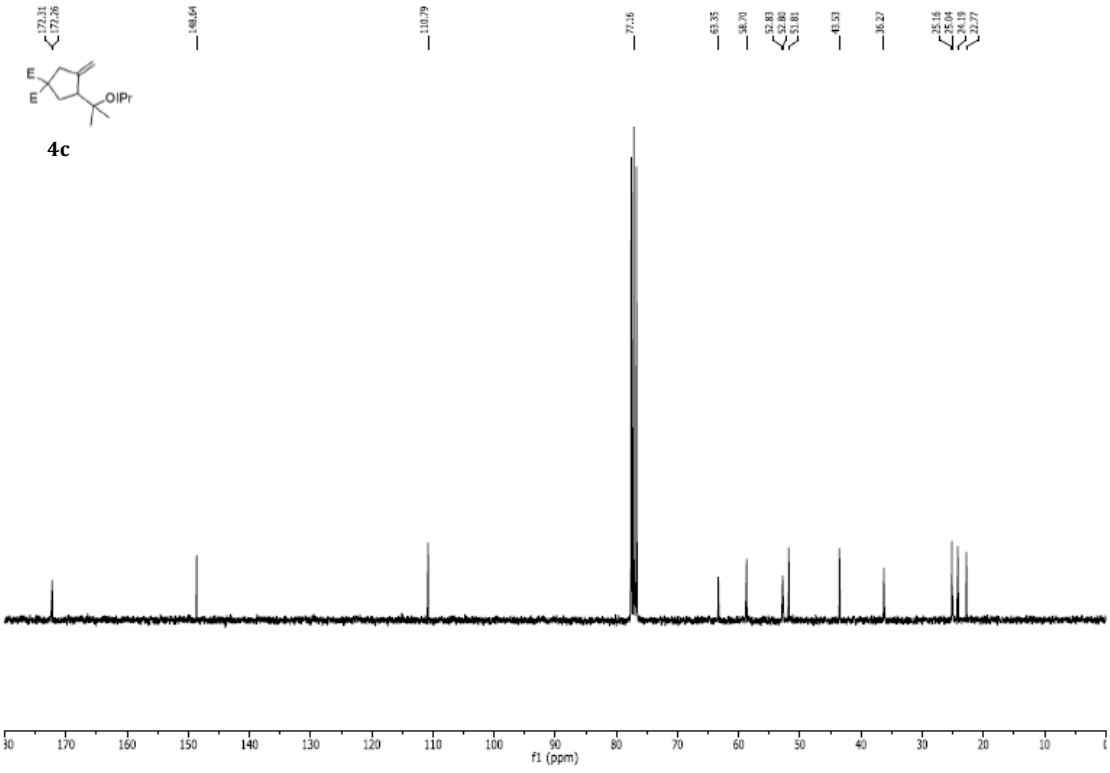
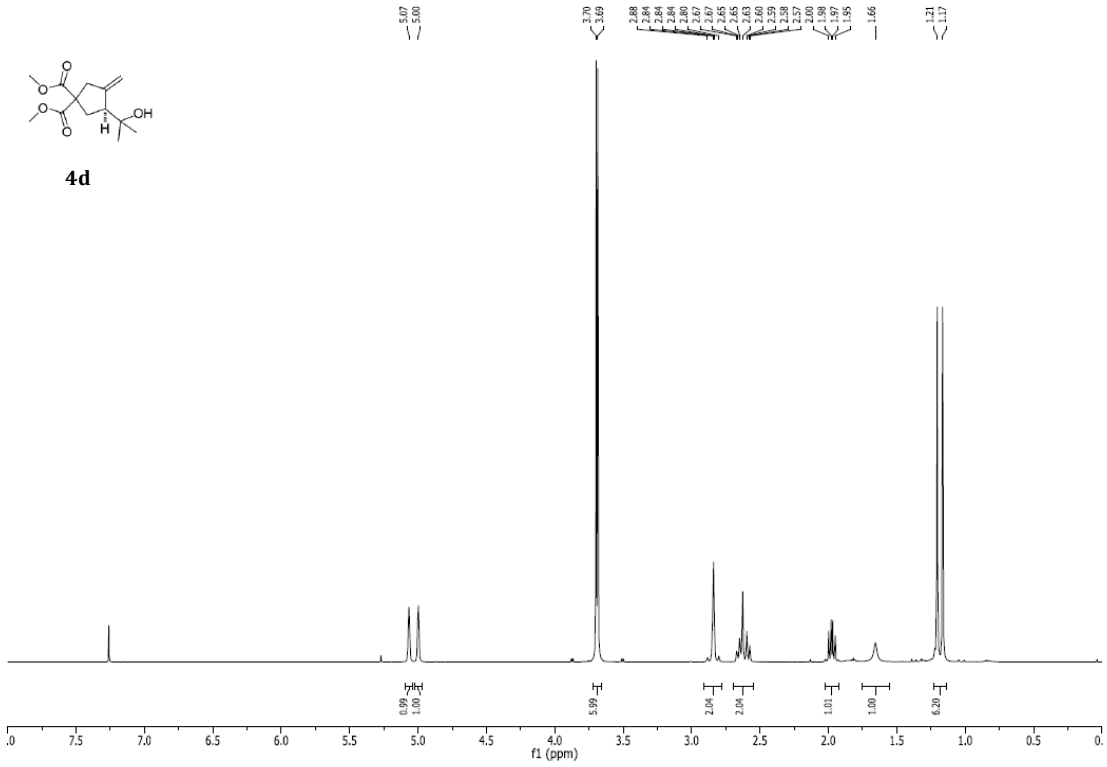
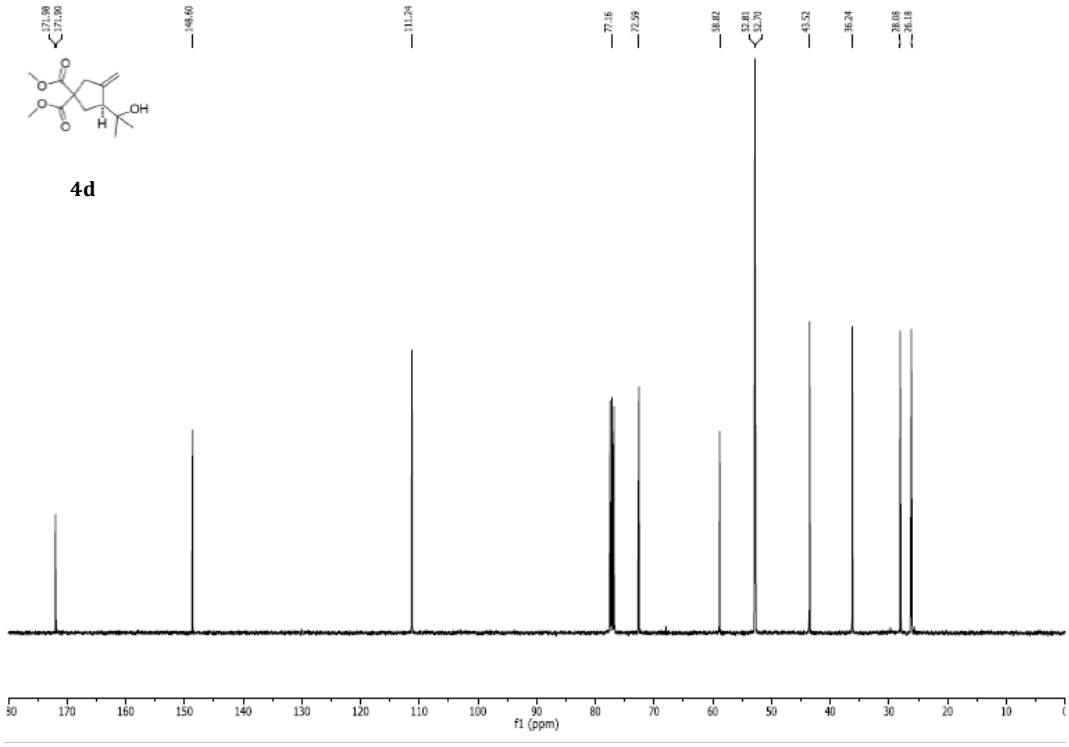

OIPr
4c
f1 (ppm)

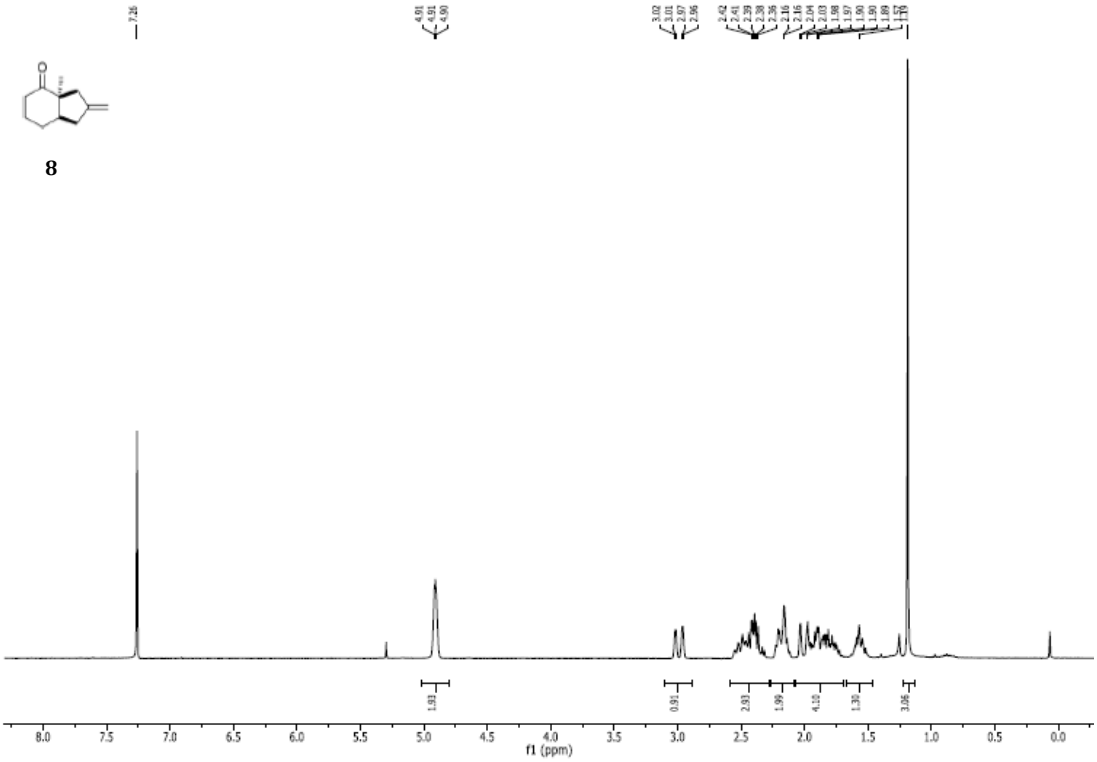

OIPr
4c
f1 (ppm)


5.07
5.00
3.70
3.69
2.68
2.64
2.64
2.64
2.60
2.67
2.67
2.65
2.65
2.63
2.60
2.59
2.58
2.57
2.00
1.98
1.97
1.95
1.66
1.21
1.17
OH
H
0.99
1.00
5.99
2.04
2.04
1.01
1.00
6.20
f1 (ppm)

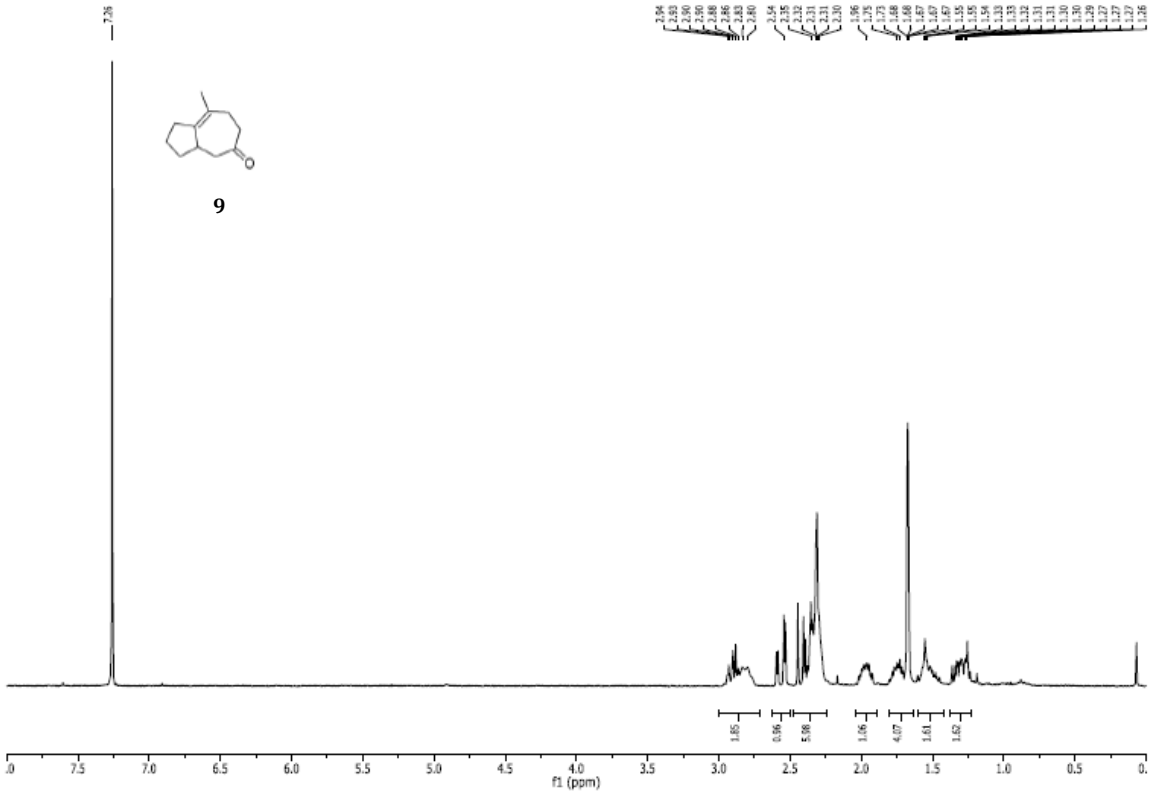
4d


171.98
171.90
148.60
111.24
77.16
72.99
58.82
52.81
52.70
43.52
36.24
28.08
26.18
OH
H
f1 (ppm)

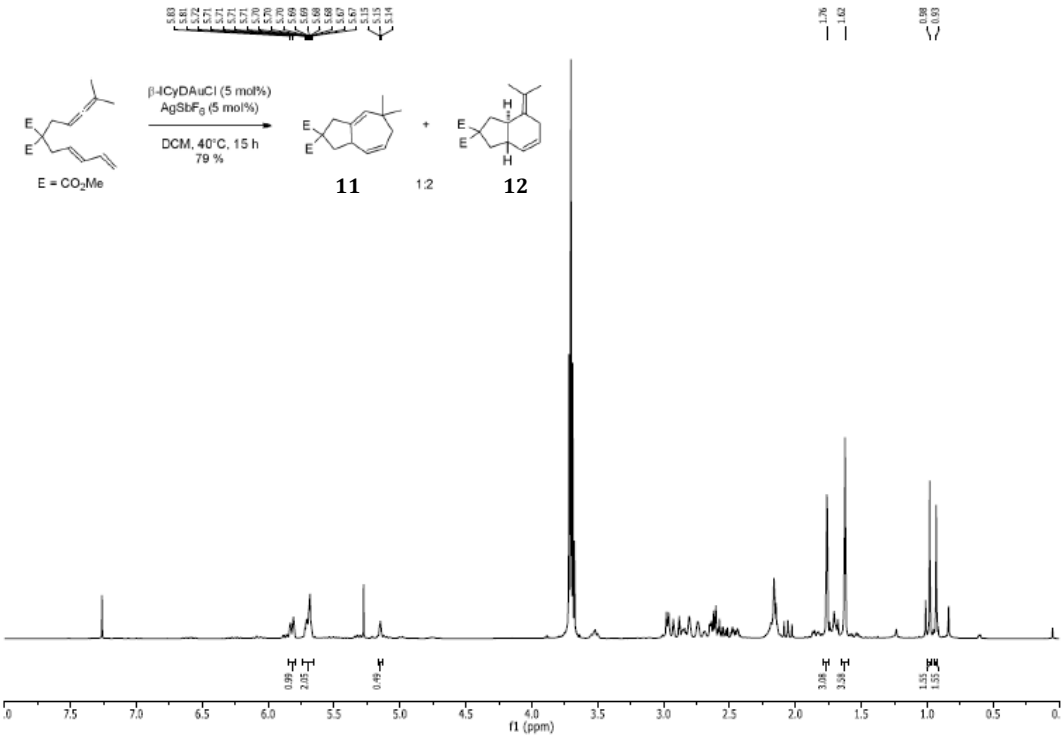
4d


7.26
4.91
4.91
4.90
3.02
3.01
2.97
2.96
2.42
2.41
2.39
2.38
2.36
2.16
2.16
2.04
2.03
1.98
1.97
1.90
1.90
1.89
1.78
1.78
1.93
0.91
2.03
1.99
4.10
1.36
3.06
f1 (ppm)

8


7.26
2.94
2.93
2.90
2.90
2.88
2.86
2.83
2.80
2.54
2.35
2.32
2.31
2.31
2.30
1.96
1.75
1.73
1.68
1.68
1.67
1.67
1.56
1.55
1.55
1.54
1.33
1.33
1.32
1.31
1.31
1.30
1.30
1.29
1.27
1.27
1.27
1.26
1.85
0.96
5.98
1.06
4.07
1.61
1.62
f1 (ppm)

9



9. References

[1] Méndez, M.; Muñoz, M. P.; Echavarren A. M. Platinum-Catalyzed Alkoxy- and Hydroxycyclization of Enynes. *J. Am. Chem. Soc.* **2000**, *122*, 11549-11550.

[2] Charruault, L.; Michelet, V.; Taras, R.; Gladiali, S.; Genêt, J.-P. Functionalized carbo- and heterocycles *via* Pt-catalyzed asymmetric alkoxycyclization of 1,6-enynes. *Chem. Commun*. **2004**, 850-851.

[3] Gryparis, C.; Efe, C.; Raptis, C.; Lykakis, I.N.; Stratakis, M. Cyclization of 1,6-Enynes Catalyzed by Gold Nanoparticles Supported on TiO_2: Significant Changes in Selectivity and Mechanism, as Compared to Homogeneous Au-Catalysis .*Org. Lett.* **2012**, *14*, 2956-2959

[4] Nieto-Oberhuber, C.; Munoz, M. P.; Lopez, S.; Jiménez-Nunez, E.; Nevado, C.; Herrero-Gomez, E.; Raducan, M.; Echavarren, A. M. Gold(I)-catalyzed cyclization of 1,6-enynes: alkoxycyclizations and exo/endo skeletal rearrangements. *Chem. Eur. J.* **2006**, *12*, 1677-1693.

[5] Nevado, C.; Charruault, L.; Michelet, V.; Nieto-Oberhuber, C.; Muñoz, M. P.; Méndez, M.; Rager, M.-N.; Genêt, J.-P.; Echavarren, A. M. On the mechanism of carbohydroxypalladation of enynes. Additional insights on the cyclization of enynes with electrophilic metal complexes. *Eur. J. Org. Chem.* **2003**, *4*, 706-713.

[6] (a) Baskar, B.; Bae, H. J.; Ar, S .E.; Cheong, J. Y.; Rhee, Y. H.; Duschek, A.; Kirsch, S. F. *Org. Lett.* **2008**, *10*, 2605-2607. (b) Alcarazo, M.; Stork, T.; Anoop, A.; Thiel, W.; Fürstner, A. Streering the surprisingly modular pi-acceptor properties of N-heterocyclic carbenes: implications for gold catalysis. *Angew. Chem. Int. Ed.* **2010**, *49*, 2542-2546

[7] Trillo, B.; López, F.; Montserrat, S.; Ujaque, G.; Castedo, L.; Lledós, A.; Mascareñas, J. L. Gold-Catalyzed [4C+3C] Intramolecular Cycloaddition of Allenedienes: Synthetic and Mechanistic Implication. *Chem. Eur. J.* **2009**, *15*, 3336-3339

[8] Mauleón, P.; Zeldin, R. M.; González, A. Z.; Toste, F. D. Ligand-Controlled Access to [4+2] and [4+3] Cycloadditions in Gold-Catalyzed Reactions of Allene-Dienes. *J. Am. Chem. Soc.* **2009**, *131*, 6348-6349.

[9] Bursch, M.; Neugebauer, H.; Grimme, S. Structure Optimisation of Large Transition-Metal Complexes with Extended Tight-Binding Methods. *Angew. Chem. Int. Ed. Engl.* **2019**, *58*, 11078-11087.

[10] Bannwarth, C.; Ehlert, S.; Grimme, S. GFN2-xTB-An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. *J. Chem. Theory Comput.* **2019**, *15*, 1652-1671.