Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information for

Cu(I)/sucrose-catalyzed hydroxylation of arenes in water: the dual role of sucrose

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Contents

1. General

NMR spectra were obtained on a Bruker AVANCE HD 400 spectrometer. Chemical shifts are expressed in δ (ppm) values, and coupling constants are expressed in hertz (Hz). ^{1}H NMR spectra were referenced to the solvent residual signals. The following abbreviations are used: s = singlet, d = doublet, t = triplet, m = multiplet, and br-s = broad singlet. EI mass spectra were recorded on an Agilent 5977B MSD with an Agilent Intuvo 9000GC system. The major signals are quoted in m/z with the relative intensity in parentheses. ESI mass spectra were measured on a Bruker micrOTOF-II. Melting points were measured on a Yamato Melting Point Apparatus MP21-N.

Cu_2O (≥ 99.99%, trace metals basis, anhydrous) was purchased from Sigma-Aldrich, Inc. Other chemicals were of reagent grade and used as received. Unless otherwise noted, all the reactions were performed in a 10 mL screw cap tube. Thin-layer chromatography was carried out on 0.25 mm Merck silica gel plates (60F-254). Normal-phase column chromatography was performed on a Yamazen Automated Flash system, or performed manually with silica gel 60 (230-400 mesh) from Merck.

2. Supplementary results of experiments

2-1. Solubility of aryl iodide in water

Procedure for measuring the solubility of aryl iodides in water: *para*-Iodoacetophenone (**1a**, 24.6 mg, 0.1 mmol) and additive (0.05 mmol) were charged in a 10 mL sample tube, and 5 mL of distilled water was added via a syringe. After the mixture was stirred at 80 °C, 1 mL of solution was collected by syringe, quickly transferred to the flask, and evaporated in vacuo. The amount of the 4'-iodoacetophenone in 1 mL of solution was determined by ^{1}H NMR with dimethylsulfone as an internal standard. All data of solubility were summarized in **Table S1**.

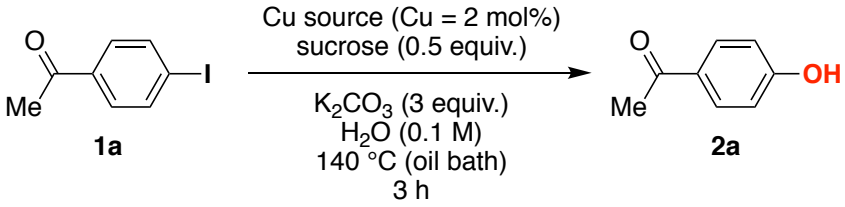
Table S1. Solubility of *para*-iodoacetophenone (**1a**) in water

Entry	Additive (0.5 equiv.)	Solubility in water (μmol/mL)
1	w/o additive	n.d.
2	w/o additive[a]	6.8
3	DME	0.52
4	Diglyme	0.35
5	TMEDA	0.46
6	SDS	6.8
7	Glucose	1.4
8	Fructose	1.1
9	Mannose	0.79
10	α-Methylglucoside	0.79
11	β-Methylglucoside hemihydrate	0.40
12	α-Methylgalactoside hydrate	1.07
13	Sucrose	0.93
14	Trehalose	1.1
15	Octa-*O*-methylsucrose[S1]	0.25

[a] Aqueous ammonia was used as a solvent instead of distilled water.

2-2. Screening of Cu sources

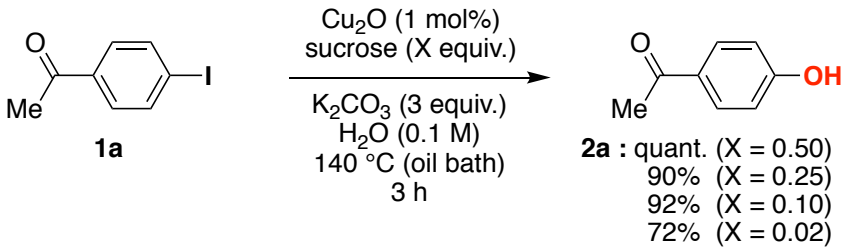
Table S2. Screening of Cu sources



Entry	Cu source	Yield (%)[a]
1	Cu_2O	quant.
2	CuI	98
3	CuBr	86
4	CuCl	76

[a] NMR yield.

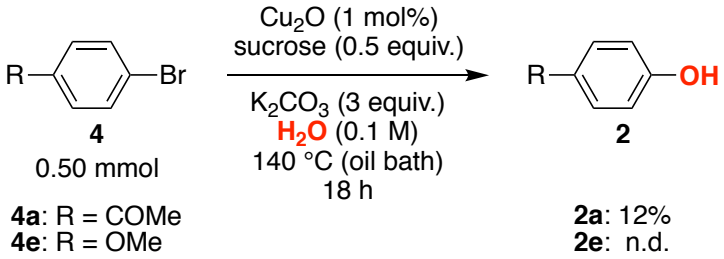
2-3. Amount of sucrose



Scheme S1. Cu-catalyzed hydroxylation reaction with various amounts of sucrose.

The hydroxylation reaction of **1a** afforded the product **2a** in 92% yield when the amount of sucrose was reduced to 0.1 equivalent. However, the yield was lowered when 0.02 equivalent of sucrose was used. Given the reactivity, in particular with poor solubility of substrates, and low cost of sucrose, we decided to use 0.5 equivalents of sucrose as the standard conditions for the present hydroxylation reaction.

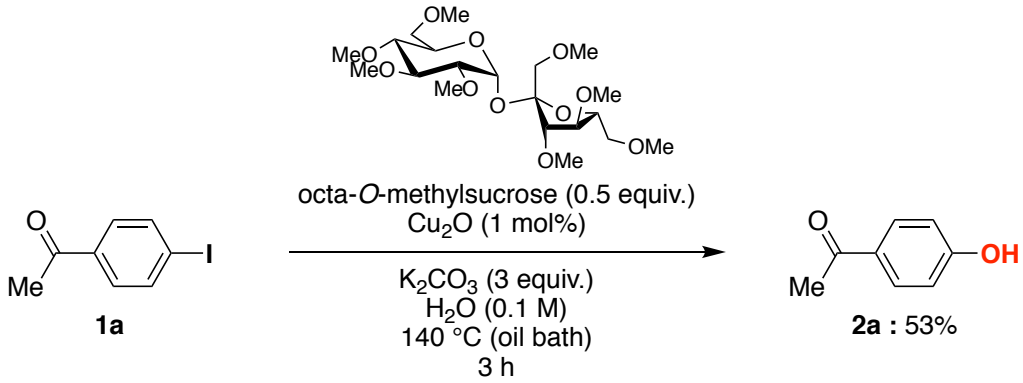
2-4. The hydroxylation reaction of aryl bromides



Scheme S2. Cu-catalyzed hydroxylation reaction of aryl bromides.

The reactions of aryl bromides did not proceed well, and the starting materials were recovered.

2-5. The reaction in the presence of octa-*O*-methylsucrose

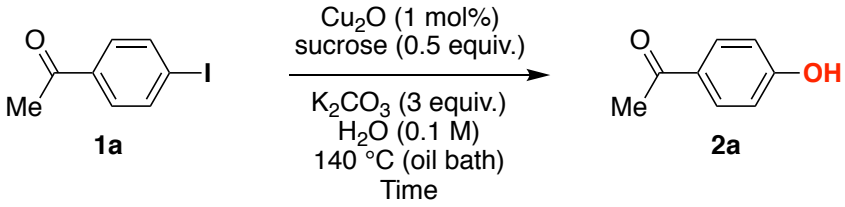


Scheme S3. Cu-catalyzed hydroxylation reaction in the presence of octa-*O*-methylsucrose.

Although octa-*O*-methylsucrose enhanced the solubility of the substrate (**Table S1**, Entry 15), the reaction of **1a** in the presence of octa-*O*-methylsucrose afforded **2a** in 53% yield with **1a** remained. This result indicated that alkoxide groups of sucrose are necessary for the high reactivity of catalyst.

2-6. The reaction profile

The reaction profile of the hydroxylation reaction of **1a** under the optimized conditions was monitored. The yields of the product and the remained starting material were determined by ^{1}H NMR analysis with dimethylsulfone as an internal standard (**Figure S1**).



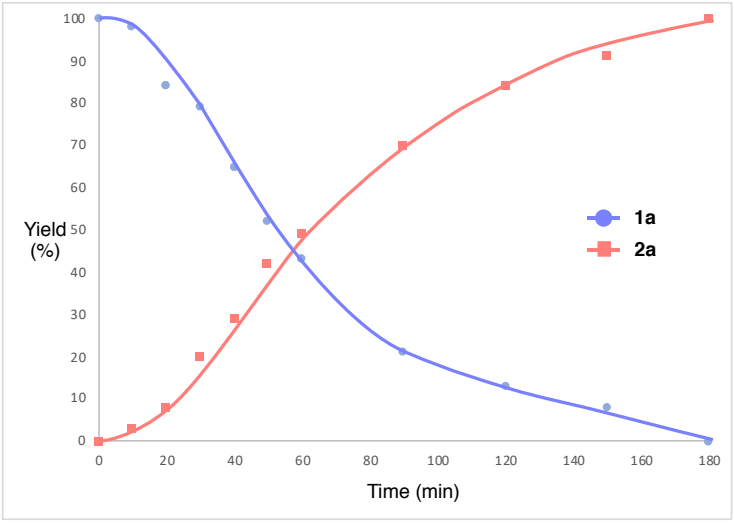


Figure S1. The reaction profile of the hydroxylation reaction of **1a** catalyzed by Cu/sucrose system.

3. Supplementary results of DFT calculations

3-1. Stability of the Cu-complexes with methylglucoside

Firstly, stable Cu-complexes coordinated by the alkoxide group of methylglucoside and water molecule were searched by GRRM search at a low level of theory (@HF/LanL2DZ). This search was initiated from the structures with the coordination of oxygen atom to the copper center at the 2, 3, 4, and 6-positions of methylglucoside, respectively. Subsequently, the stable structures, which were extracted from 181 conformers obtained by GRRM search, were re-optimized at the M06-2X/SDD&6-311+G*/SMD(water) //M06-2X/SDD&6-31+G*/SMD(water) level of theory (**Figure S2**).

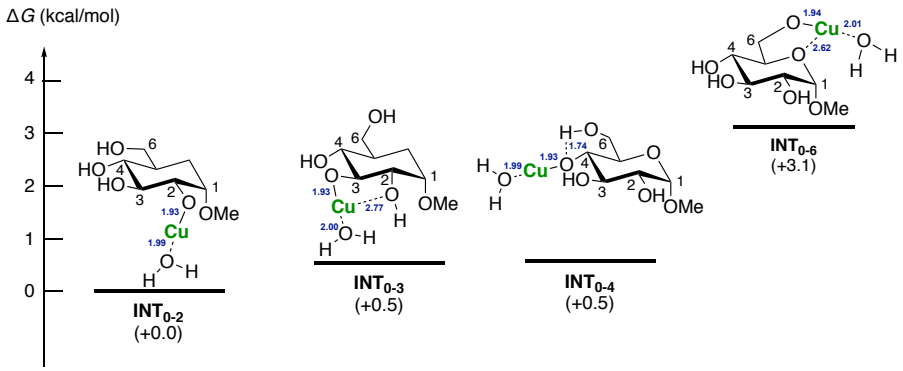


Figure S2. Optimized Cu-complexes coordinated by the alkoxide group of methylglucoside and water.

As a result, the 2-position complex **INT$_{0\text{-}2}$** is the most stable among them. **INT$_{0\text{-}3}$** and **INT$_{0\text{-}4}$** are also nearly stable (+0.5 kcal/mol). While **INT$_{0\text{-}6}$** is rather unstable (+3.1 kcal/mol) compared with **INT$_{0\text{-}2}$**, all of these complexes should exist in an equilibrium in the reaction mixture.

3-2. Reaction pathways with the neutral Cu-complex bearing a methylglucoside

To track the reaction pathway of iodobenzene as a model substrate, we set the Cu-complexes bearing iodobenzene and alkoxide group of methylglucoside as the model starting complex based on the previous research.[S2] We compared the stability among those Cu-complexes, which were similarly re-optimized structures after GRRM search. The 2-position complex **INT$_1$** is the most stable and the 3-, 4-, and 6-position complexes are less stable (>3 kcal/mol) (**Figure S3**). These values are reflected in the following calculations.

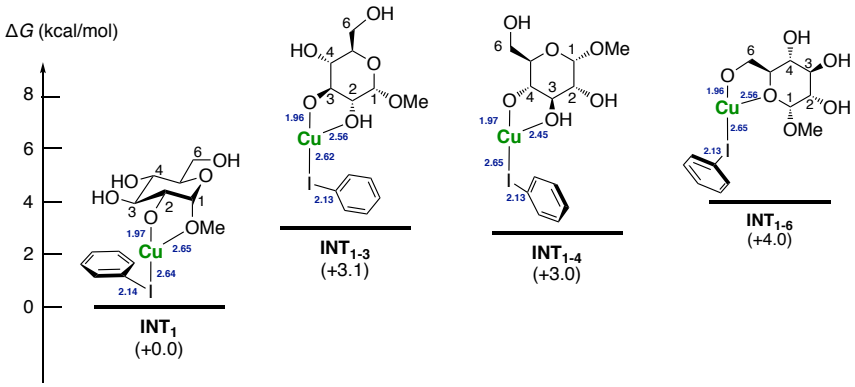


Figure S3. Stability of the neutral Cu-complexes bearing methylglucoside and iodobenzene.

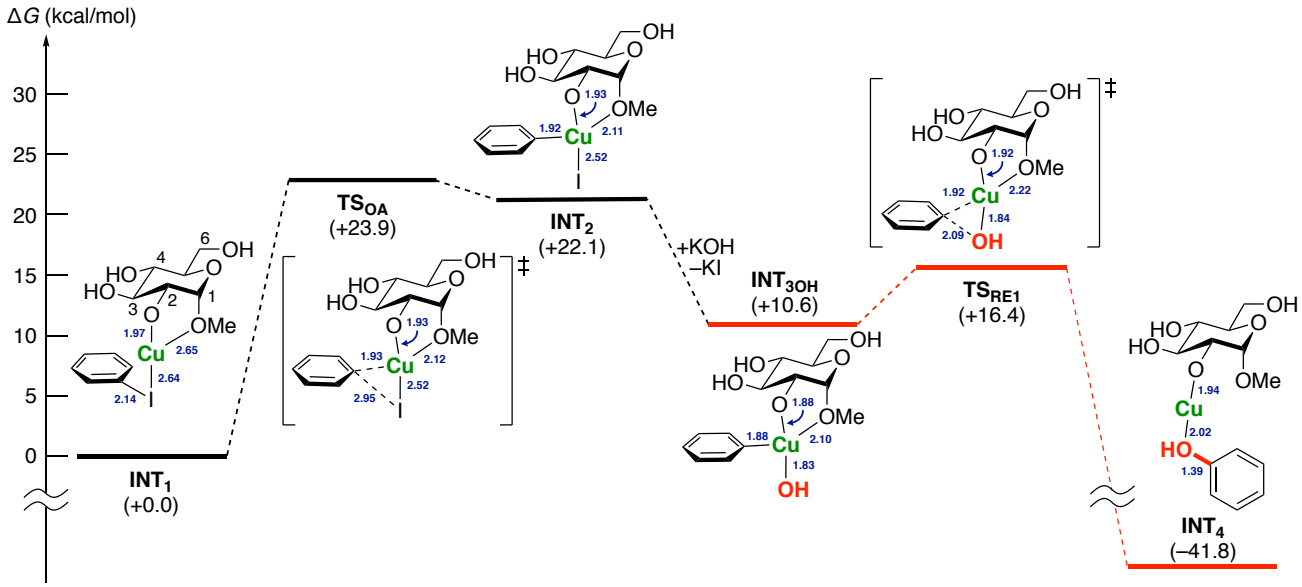


Figure S4. Modeled reaction pathway with the neutral 2-position Cu-complex. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD (water) level of theory are shown in kcal/mol and Å, respectively.

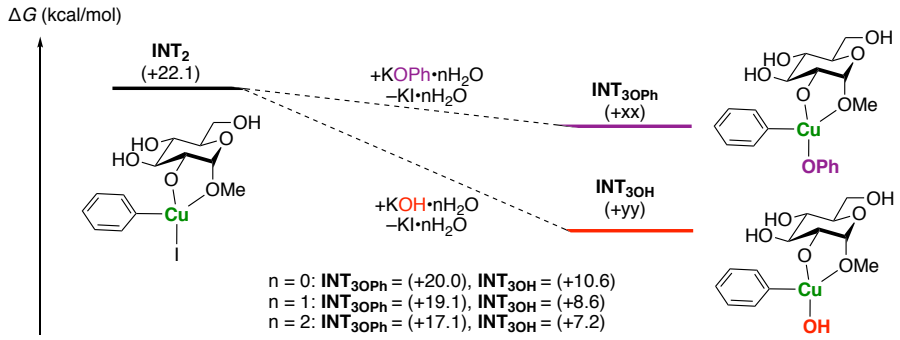


Figure S5. Comparison of energy changes in the ligand exchange events between iodide and HO^- /PhO^-.

In Figure 1 in the manuscript, we discussed the reaction pathways for the desired hydroxylation as well as the diphenyl ether formation. Before the C–O bond formation to afford phenol (desired) or diphenyl ether (a possible byproduct), the ligand exchange between iodide and HO^- or PhO^- should be occurred. This event was modeled as the following isodesmic reactions: LCu(Ph)I + KOH•nH2O -> LCu(Ph)OH + KI•nH2O and LCu(Ph)I + KOPh•nH2O -> LCu(Ph)OPh + KI•nH2O. Irrespective of the number of coordinating water molecules (n = 0-2), the energy changes of these reactions were similar as summarized in **Figure S5**. The discussion on Figure 1 is described with the results of n = 0.

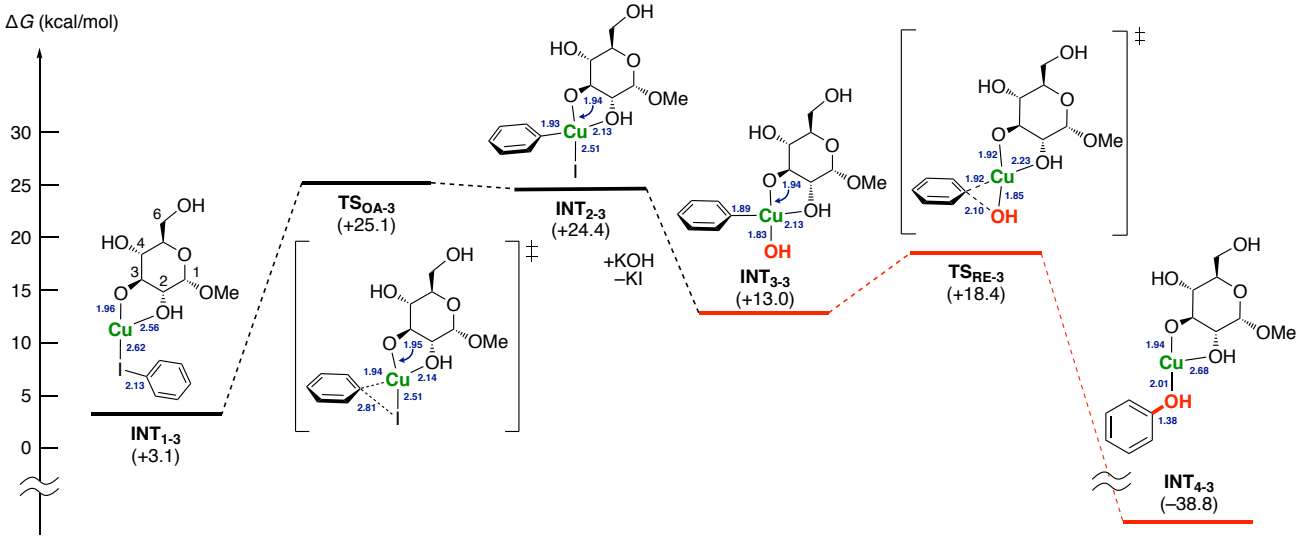


Figure S6. Modeled reaction pathway with the neutral 3-position Cu-complex. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD (water) level of theory are shown in kcal/mol and Å, respectively.

In the reaction pathway with the 3-position complex, a higher activation barrier is observed for the oxidative addition via **TS_{OA-3}** ($\Delta G^{‡}$ +25.1 kcal/mol) than that of the 2-position complex ($\Delta G^{‡}$ +23.9 kcal/mol). Since the energy changes including the following reductive elimination are similar and not very high, the possibility of the reaction with the 3-position complex is not excluded at this time.

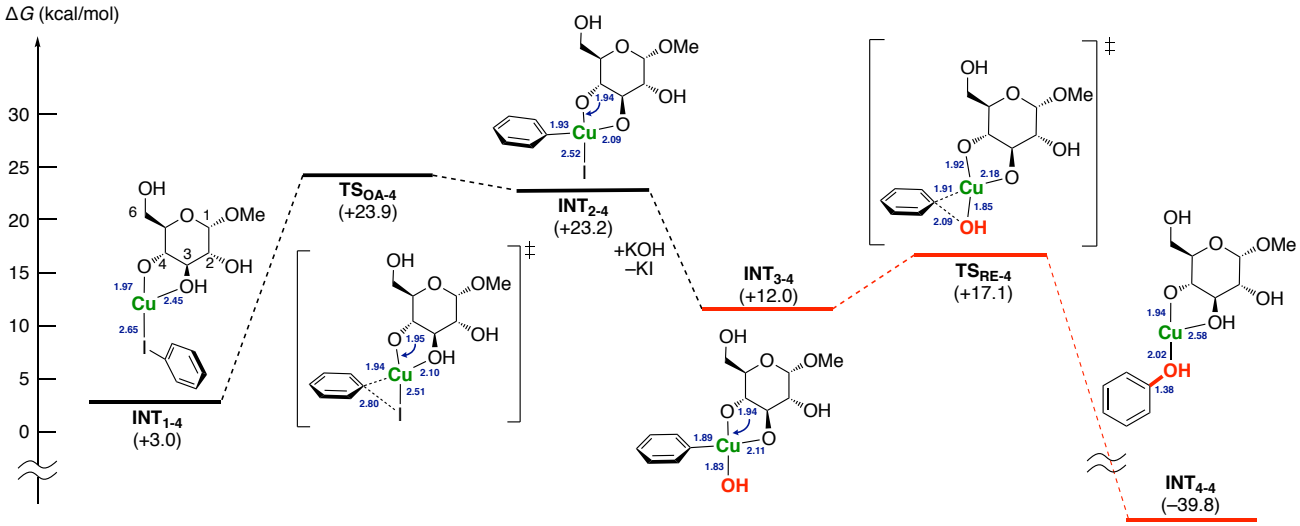


Figure S7. Modeled reaction pathway with the neutral 4-position Cu-complex. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD (water) level of theory are shown in kcal/mol and Å, respectively.

In the reaction pathway with the 4-position complex, similar activation barriers as the case of the 2-position complex were observed, and this is also a feasible pathway.

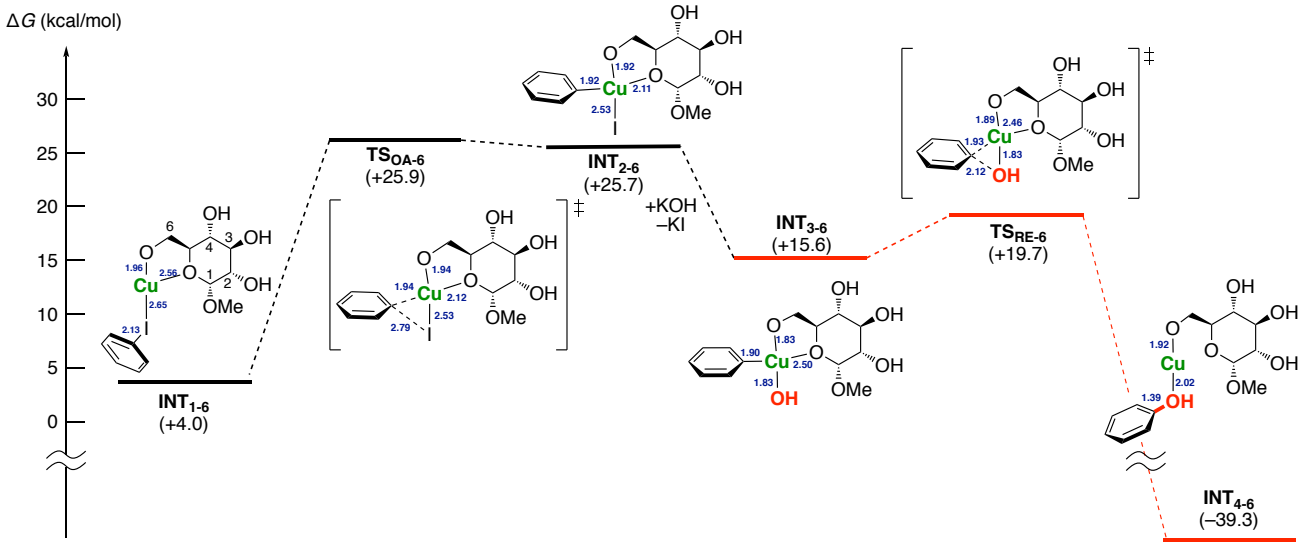


Figure S8. Modeled reaction pathway with the neutral 6-position Cu-complex. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD (water) level of theory are shown in kcal/mol and Å, respectively.

In the reaction pathway with the 6-position complex, a higher activation barrier is observed for the oxidative addition via **TS_{OA-6}** ($\Delta G^{\ddagger}$ +25.9 kcal/mol) than that of the 2-position complex ($\Delta G^{\ddagger}$ +23.9 kcal/mol). In addition, the 6-position complex **INT_{1-6}** is unstable compared with the 2-position complex **INT_{1-2}** (4.0 kcal/mol) and should not exist as in a substantial amount as described in **Figure S2**. Therefore, the pathway with the 6-position complex should be unlikely as the major pathway.

3-3. Reaction pathways with the anionic Cu-complex bearing a methylglucoside

The pathway with the anionic Cu-complexes generated from Cu(I) with the bidentate anionic ligand, namely an "anionic pathway," was proposed in the Ullmann-type coupling reaction of aryl halides with phenols.[S2g] To check the possibility of the anionic pathway, we set the Cu-complexes coordinated by iodobenzene, hydroxide, and the alkoxide group of methylglucoside as the model starting complex. We compared the stability among those Cu-complexes, which were similarly re-optimized structures after GRRM search. As a result, 2- and 4-position complexes **INT$_{1\text{-}2_anion}$** and **INT$_{1\text{-}4_anion}$** are stable while **INT$_{1\text{-}3_anion}$** and **INT$_{1\text{-}6_anion}$** are less stable (**Figure S9**). These values are reflected in the following calculations.

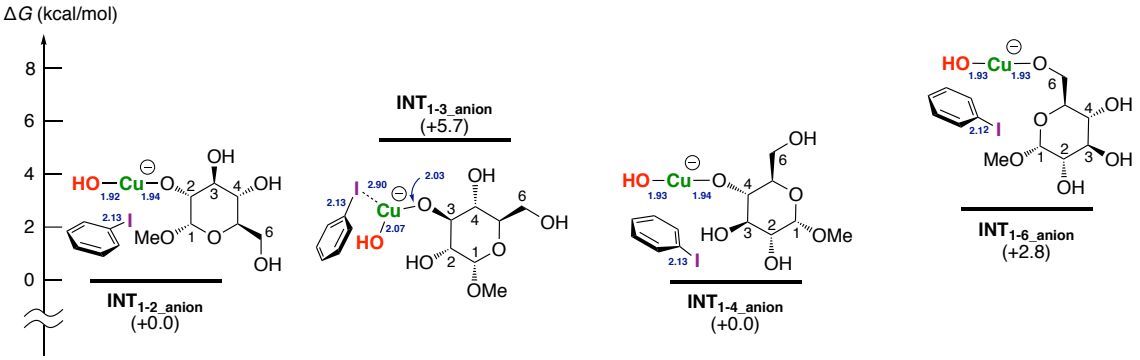


Figure S9. Stability of the anionic Cu-complexes bearing iodobenzene, hydroxide, and methylglucoside

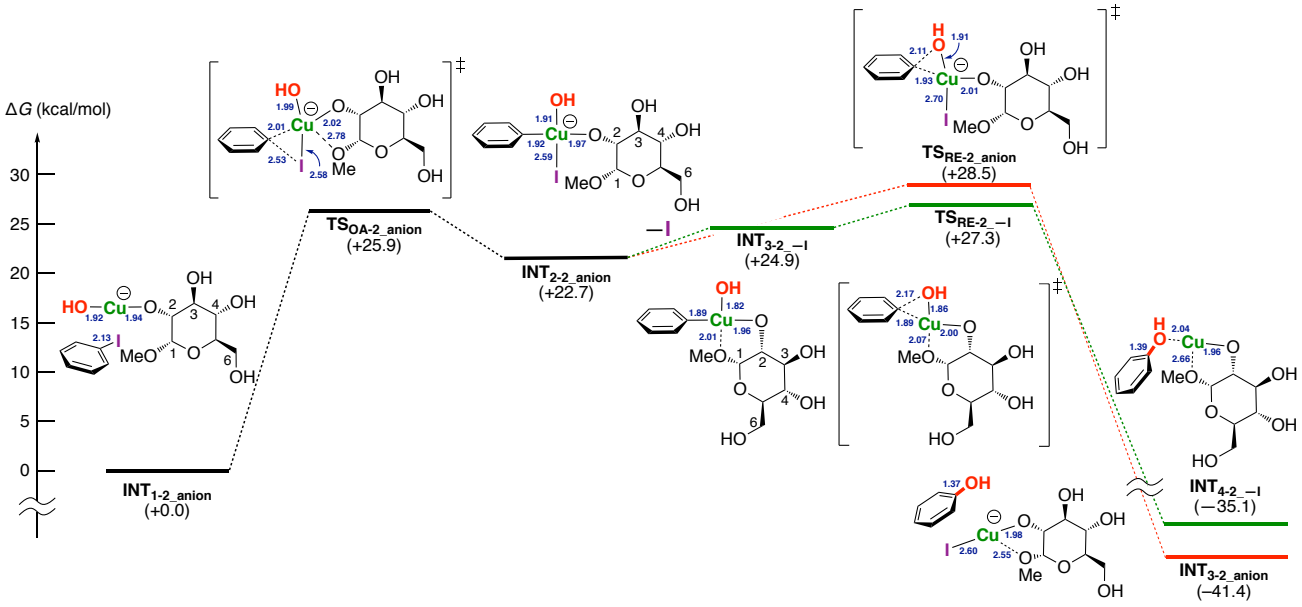


Figure S10. Modeled reaction pathways with the anionic 2-position Cu-complex. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD (water) level of theory are shown in kcal/mol and Å, respectively.

In the case of the pathway with the anionic 2-position Cu-complex, the higher energy barrier for the oxidative addition via **$TS_{OA\text{-}2\_anion}$** than the neutral pathway ($\Delta G^{\ddagger}$ +23.9 kcal/mol in **Figure S4**) is observed. Transition state **$TS_{RE\text{-}2\_anion}$** for the direct reductive elimination from anionic pentacoordinate species **$INT_{2\text{-}2\_anion}$** lies 2.6 kcal/mol above the **$TS_{OA\text{-}2\_anion}$**. Moreover, transition state **$TS_{RE\_2\_-I}$** for the reductive elimination via the dissociation of iodide anion also lies 1.6 kcal/mol above **$TS_{OA\text{-}2\_anion}$**. These results indicate the anionic pathway with the 2-position complex is less likely compared with the corresponding neutral pathway.

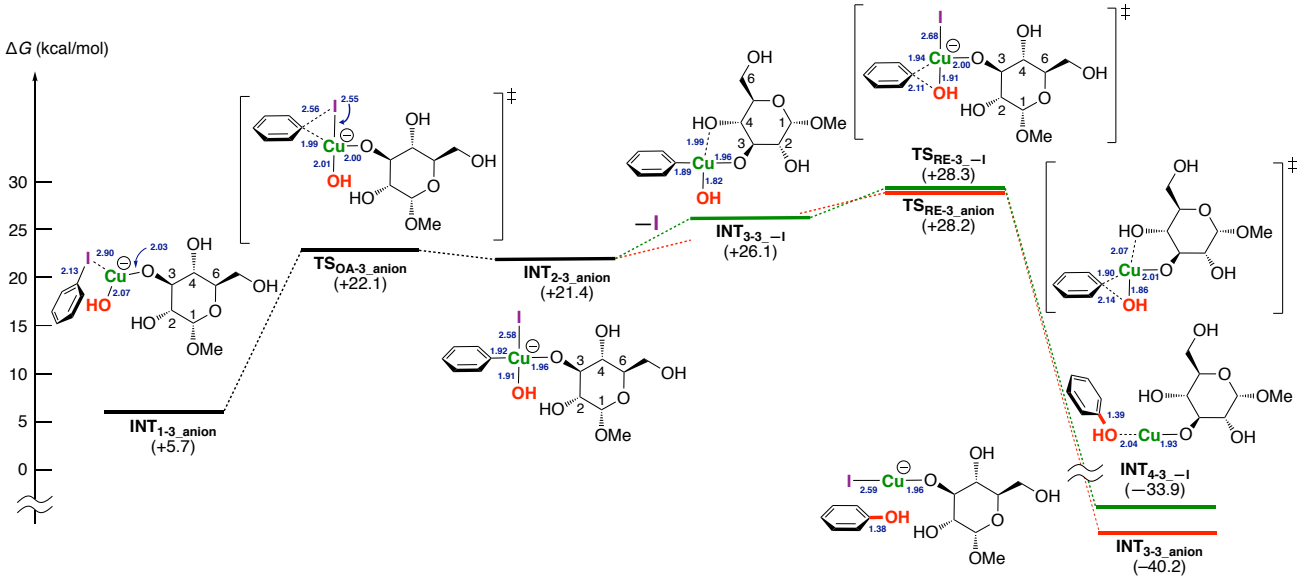


Figure S11. Modeled reaction pathways with the anionic 3-position Cu-complex. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD (water) level of theory are shown in kcal/mol and Å, respectively.

In the pathway with the anionic 3-position Cu-complex, the low barrier ($\Delta G^{\ddagger}$ +22.1 kcal/mol) for the oxidative addition **$TS_{OA\text{-}3\_anion}$** is observed. However, the following reductive elimination events with or without the dissociation of iodide anion lies at +28.2 and +28.3 kcal/mol, respectively. Moreover, **$INT_{1\text{-}3\_anion}$** is unstable compared with **$INT_{1\text{-}2\_anion}$** (+5.7 kcal/mol) and unlikely to participate in this catalytic cycle.

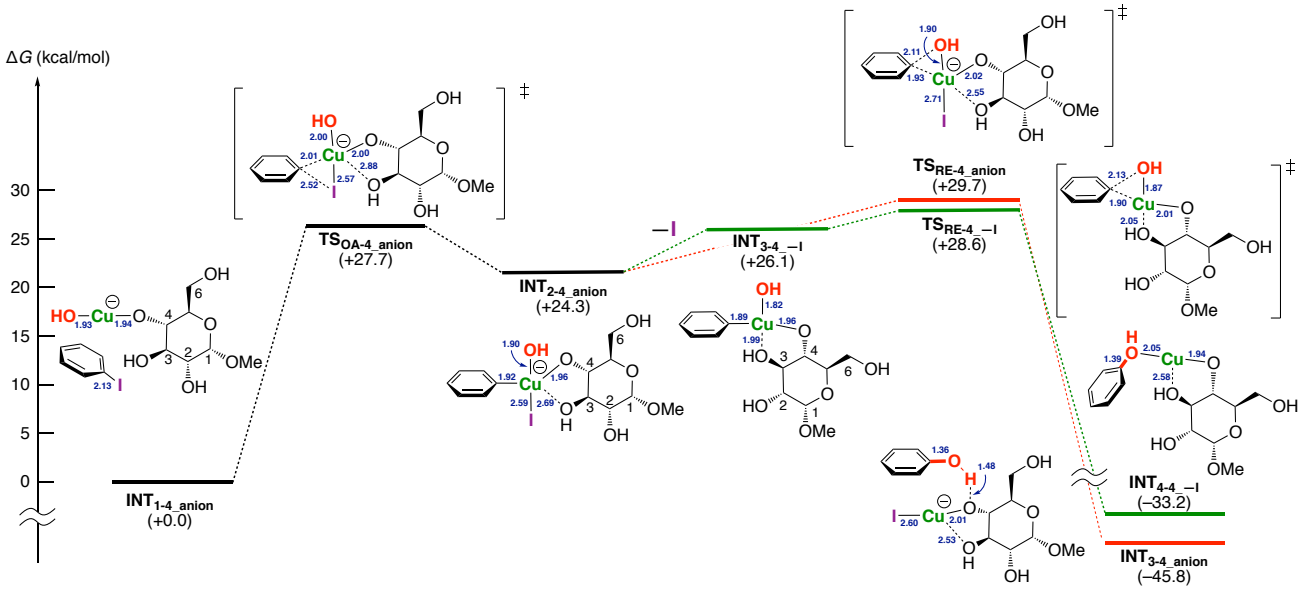


Figure S12. Modeled reaction pathways with the anionic 4-position Cu-complex. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD (water) level of theory are shown in kcal/mol and Å, respectively.

The pathway with the anionic 4-position complex should be unlikely, due to the high energy barriers for the oxidative addition $\mathbf{TS_{OA\text{-}4\_anion}}$ ($\Delta G^{\ddagger}$ +27.7 kcal/mol), reductive eliminations $\mathbf{TS_{RE\text{-}4\_anion}}$ and $\mathbf{TS_{RE\text{-}4\_\text{-}I}}$ ($\Delta G^{\ddagger}$ +29.7 and +28.6 kcal/mol, respectively).

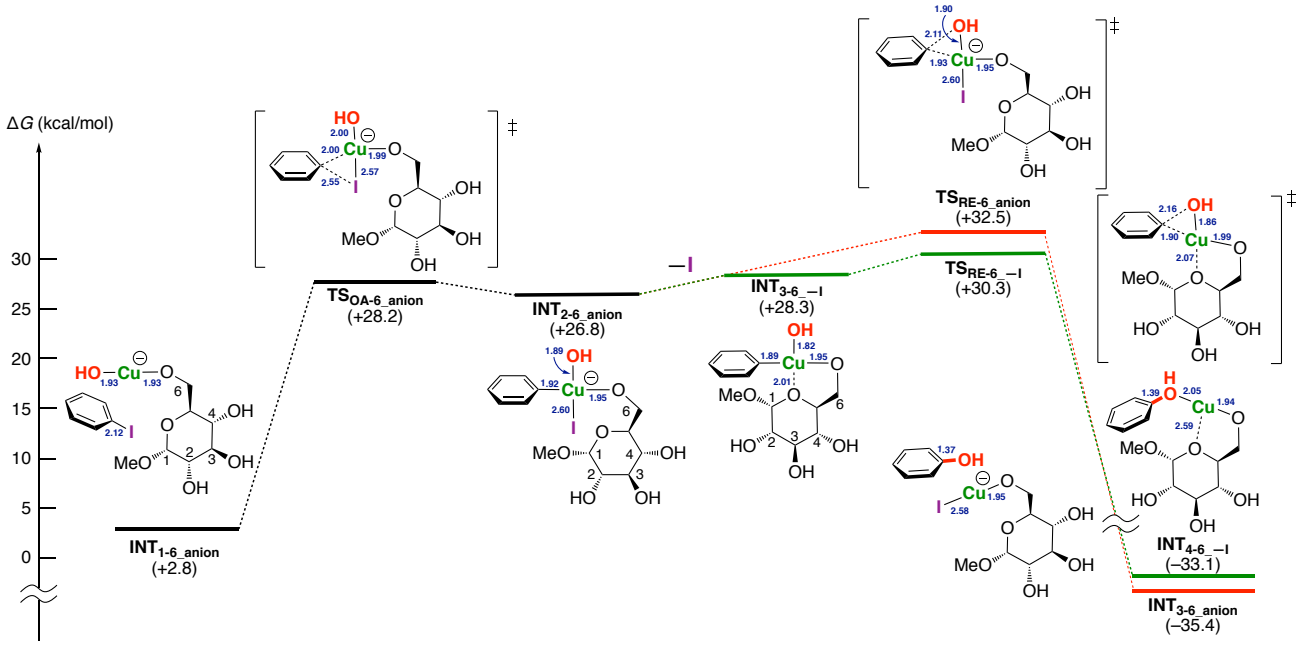


Figure S13. Modeled reaction pathways with the anionic 6-position Cu-complex. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD (water) level of theory are shown in kcal/mol and Å, respectively.

In the pathways with the anionic 6-position complex, transition states for both reductive elimination events with and without the dissociation of iodide anion lie above +30 kcal/mol. Therefore, these pathways are also unlikely.

Given the comparison of overall free energy barriers among the neutral and anionic pathways, the neutral pathway is likely to be favorable in this Cu-catalyzed hydroxylation reaction although the anionic pathways, especially with the anionic 2-position complex, are not be completely excluded at this time.

3-4. *σ*-Bond metathesis pathway

We examined the possibility of the pathway via *σ*-bond metathesis mechanism by DFT calculation with the 2-position Cu-complex (**Figure S14**). The activation barrier for *σ*-bond metathesis is +32.1 kcal/mol. Therefore, this pathway is excluded as the feasible pathway to produce phenol product.

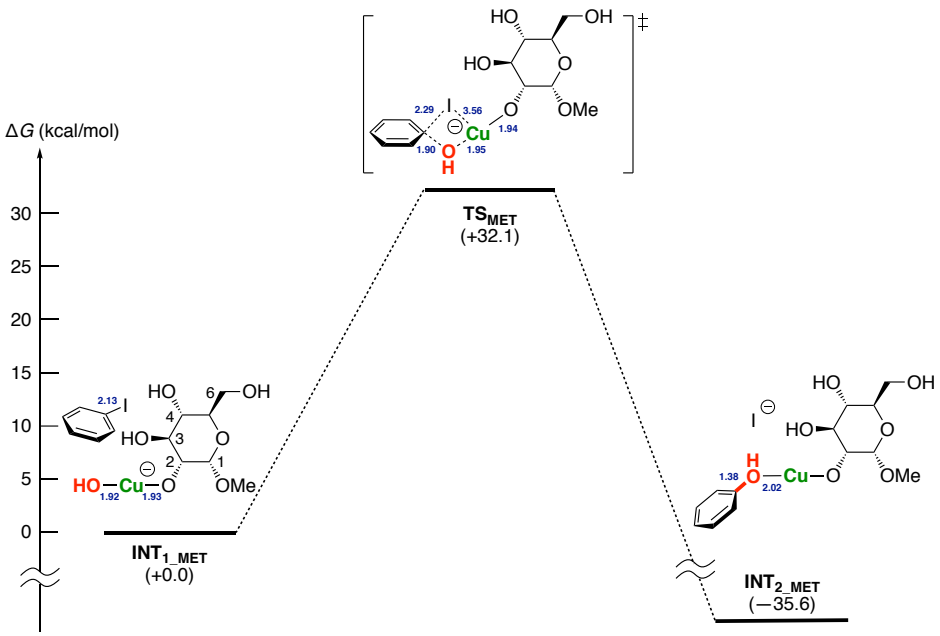


Figure S14. Modeled reaction pathway via *σ*-Bond metathesis mechanism. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD(water) level of theory are shown in kcal/mol and Å, respectively.

3-5. Other ligands: Cu-TMEDA and Cu-DME complexes

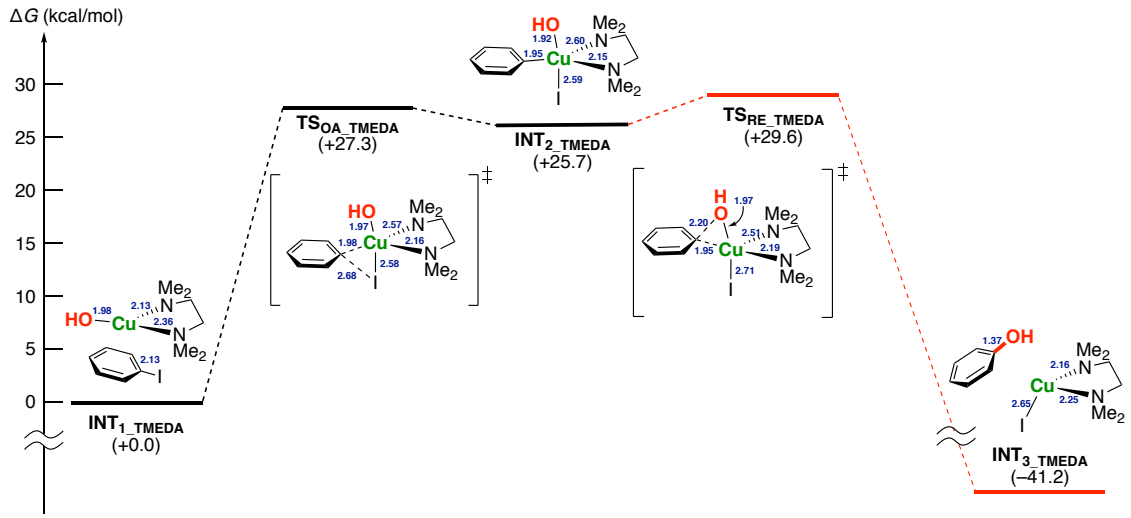


Figure S15. Modeled reaction pathway of the Cu-TMEDA -complex. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD(water) level of theory are shown in kcal/mol and Å, respectively.

In the case of Cu-TMEDA-complex, the activation barrier was higher than that observed with Cu-complex bearing a methylglucoside and the barrier for the reductive elimination is also high (**Figure 15**).

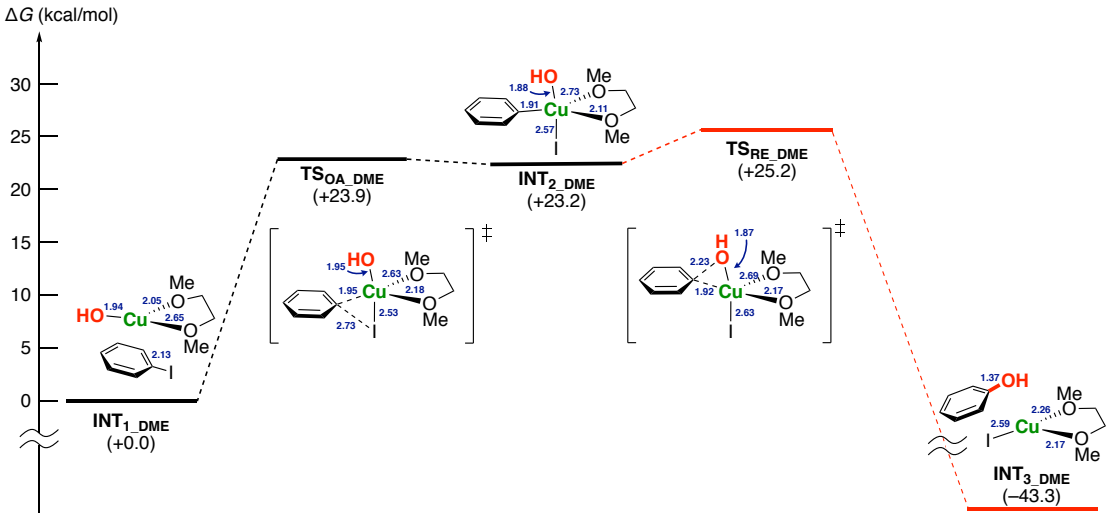


Figure S16. Modeled reaction pathway of the Cu-DME-complex. Energy changes and bond lengths at the M06-2X/SDD and 6-311+G*/SMD(water)//M06-2X/SDD and 6-31+G*/SMD (water) level of theory are shown in kcal/mol and Å, respectively.

Given that the transition states for the oxidative addition and reductive elimination are located at +23.9 kcal/mol and +25.2 kcal/mol, the reaction with the Cu-DME-complex should proceed rather smoothly (**Figure S16**). So, intrinsically, the coordination of DME would improve the catalytic activity. But, as discussed in Table 1 in the manuscript, the solubility of substrate is poor in the presence of 0.5 equivalents of DME. In total, the moderate yield was observed in the presence of DME in Table 2.

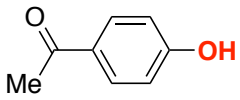
4. Experimental section

4-1. General procedure for Cu-catalyzed hydroxylation in water

Copper(I) oxide (0.7 mg, 0.005 mmol), K_2CO_3 (207 mg, 1.5 mmol), and iodo(hetero)arene **1** (0.50 mmol) were charged in a 10 mL screw cap tube under air, and 5.0 mL of distilled water was added via a syringe. The tube was closed after roughly purged with N_2 gas flow or without purging. The reaction mixture was heated (oil bath temp: 140 °C) and stirred. After stirring, the tube was cooled in an ice bath before the screw cap was opened. (otherwise, the mixture may spout out under high pressure.) The reaction mixture was diluted with AcOEt (*ca*. 30 mL, generally TLC check at this stage) and transferred to a separation funnel. The solution was washed with saturated ammonium chloride aqueous solution (20 mL), and then, the aqueous layer was re-extracted with AcOEt (20 mL × 2). The combined organic layer was dried over Na_2SO_4, and evaporated in vacuo. The chemical yield was determined by ^{1}H NMR analysis using dimethylsulfone as an internal standard. The obtained material was purified by silica gel flash column chromatography (eluent: AcOEt/n-hexane) to give the corresponding phenol products **2**.

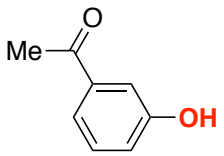
4-2. Characterization of the products

4-Acetylphenol (2a): CAS# 99-93-4[S3]



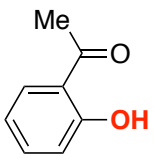
2a was obtained as a cream solid in 94% yield (64.2 mg, 0.472 mmol).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.8 Hz, 2H), 7.51 (br-s, 1H), 6.95 (d, *J* = 8.8 Hz, 2H), 2.59 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 198.4, 161.2, 131.2, 129.7, 115.5, 26.3; **EI-MS** *m/z* (rel intensity) 136 (M^+, 36); **mp** 106-108 °C.

3-Acetylphenol (2b): CAS# 121-71-1[S4]



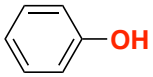
2b was obtained as a cream solid in 90% yield (61.4 mg, 0.451 mmol).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 2.3, 1.6 Hz, 1H), 7.52 (ddd, *J* = 7.9, 1.6, 0.8 Hz, 1H), 7.34 (dd, *J* = 7.9, 7.9 Hz, 1H), 7.12 (ddd, *J* = 7.9, 2.3, 0.8 Hz, 1H), 6.60 (br-s, 1H), 2.61 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 199.2, 156.3, 138.3, 129.9, 121.1, 120.8, 114.7, 26.8; **EI-MS** *m/z* (rel intensity) 136 (M^+, 61); **mp** 93-94 °C.

2-Acetylphenol (2c): CAS# 118-93-4[S5]



2c was obtained as a brown oil in 91% yield (61.8 mg, 0.454 mmol).
^{1}H NMR (400 MHz, $CDCl_3$) δ 12.27 (s, 1H), 7.74 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.48 (ddd, *J* = 7.8, 7.8, 1.6 Hz, 1H), 6.98 (dd, *J* = 7.8, 1.1 Hz, 1H), 6.91 (ddd, *J* = 7.8, 7.8, 1.1 Hz, 1H), 2.64 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 204.5, 162.4, 136.5, 130.7, 119.7, 118.9, 118.4, 26.6; **EI-MS** *m/z* (rel intensity) 136 (M^+, 55).

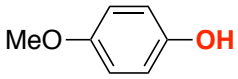
Phenol (2d): CAS# 108-95-2[S6]



2d was obtained as a white solid in 63% yield (29.6 mg, 0.315 mmol)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (dd, *J* = 8.6, 7.5 Hz, 2H), 6.93 (tt, *J* = 7.5, 0.8 Hz, 1H), 6.83 (dd, *J* = 8.6, 0.8 Hz, 2H), 4.89 (br-s,1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 155.4, 129.7, 120.9, 115.3; **EI-MS** *m/z* (rel intensity) 94 (M^+, 100); mp 38-40 °C.

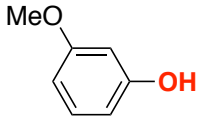
4-Methoxyphenol (2e): CAS# 150-76-5[S4]



2e was obtained as a white solid in 90% yield (55.9 mg, 0.450 mmol).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.81-6.75 (m, 4H), 4.66 (br-s, 1H), 3.76 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 153.7, 149.4, 116.0, 114.8, 55.8; **EI-MS** *m/z* (rel intensity) 124 (M^+, 94); **mp** 53-55 °C.

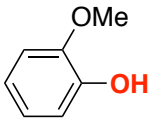
3-Methoxyphenol (2f): CAS# 150-19-6[S4]



2f was obtained as a brown oil in 92% yield (57.1 mg, 0.418 mmol).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (dd, *J* = 8.3, 8.3 Hz, 1H), 6.50 (dd, *J* = 8.3, 1.3 Hz, 1H), 6.44-6.42 (m, 1H), 6.42 (d, *J* = 1.3 Hz, 1H), 5.08 (br-s,1H), 3.78 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.9, 156.7, 130.1, 107.8, 106.4, 101.5, 55.3; **EI-MS** *m/z* (rel intensity) 124 (M^+, 100)**.**

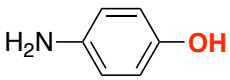
2-Methoxyphenol (2g): CAS# 90-05-1[S5]



2g was obtained as a yellow oil in 83% yield (51.5 mg, 0.415 mmol)

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92-6.94 (m, 1H), 6.85-6.90 (m, 3H), 5.61 (s,1H), 3.89 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 146.5, 145.6, 121.4, 120.1, 114.5, 110.7, 55.8; **EI-MS** *m/z* (rel intensity) 124 (M^+, 88).

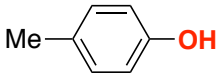
4-Aminophenoel (2h): CAS# 371-41-5[S7]



2h was obtained as a dark brown solid in 58% yield (31.4 mg, 0.288 mmol). Unsubstituted aniline (dehalogenation, 14% NMR yield), a trace amount of 4,4'-oxydianiline (detected on GC-MS analysis), and an insoluble purple material (probably due to the oxidation of **2h**) were also formed.

^{1}H NMR (400 MHz, CD_3OD) δ 6.65-6.58 (m, 4H), OH peak of phenol and NH_2 peak of aniline were diminished by CD_3OD; **^{13}C NMR (100 MHz, CD_3OD)** δ 152.2, 141.1, 119.4, 117.6; **EI-MS** *m/z* (rel intensity) 109 (M^+, 100); mp 183-185 °C.

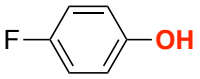
4-Methylphenol (2i): CAS# 106-44-5[S8]



2i was obtained as a brown oil in 58% yield (31.7 mg, 0.293 mmol).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 (d, *J* = 8.2 Hz, 2H), 6.73 (d, *J* = 8.2 Hz, 2H), 4.67 (s, 1H), 2.27 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 153.2, 130.1, 130.0, 115.0, 20.4; **EI-MS** *m/z* (rel intensity) 108 (M^+, 55).

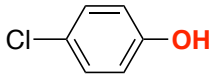
4-Fluorophenol (2j): CAS# 371-41-5[S6]



2i was obtained as a brown oil in 79% yield (44.3 mg, 0.395 mmol)

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (dd, *J* = 8.9, 8.8 Hz, 2H), 6.77 (dd, *J* = 8.8, 4.3 Hz, 2H), 4.65 (s, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.3 (d, *J* = 236.0 Hz), 151.4 (d, *J* = 2.1 Hz), 116.2 (d, *J* = 8.0 Hz), 116.0 (d, *J* = 23.2 Hz); **EI-MS** *m/z* (rel intensity) 112 (M^+, 100).

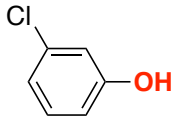
4-Chlorophenol (2k): CAS# 106-48-9[S6]



2k was obtained as a colorless oil in 59% yield (38.1 mg, 0.296 mmol).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 8.8 Hz, 2H), 6.76 (d, *J* = 8.8 Hz, 2H), 5.12 (s, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 154.0, 129.5, 125.7, 116.6; **EI-MS** *m/z* (rel intensity) 128 (M^+, 100).

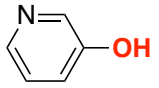
3-Chlorophenol (2l): CAS# 108-43-0[S4]



2l was obtained as a colorless oil in 52% yield (33.1 mg, 0.259 mmol).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (dd, *J* = 8.1, 8.1 Hz, 1H), 6.91 (d, *J* = 8.1 Hz, 1H), 6.86 (s, 1H), 6.71 (dd, *J* = 8.1, 1.8 Hz, 1H) 5.16 (br-s, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 156.2, 134.9, 130.5, 121.1, 115.9, 113.7; **EI-MS** *m/z* (rel intensity) 128 (M^+, 100).

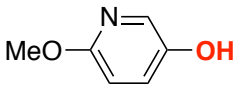
3-Hydroxypyridine (2m): CAS# 109-00-2[S4]



2m was obtained as a cream solid in 93% yield (44.1 mg, 0.464 mmol)

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.88 (s, 1H), 8.15 (br-s, 1H), 8.04 (br-s, 1H), 7.21-7.14 (m, 2H); **^{13}C NMR (100 MHz, DMSO-d_6)** δ 153.7, 140.3, 138.0, 124.2, 122.0; **EI-MS** *m/z* (rel intensity) 95 (M^+, 100); **mp** 122-123 °C.

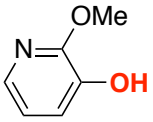
5-Hydroxy-2-methoxypyridine (2n): CAS# 51834-97-0[S9]



2n was obtained as a brown solid in 73% yield (45.7 mg, 0.365 mmol)

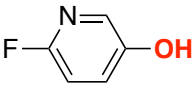
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.28 (s, 1H), 7.68 (d, *J* = 3.0 Hz, 1H), 7.17 (dd, *J* = 8.8, 3.0 Hz, 1H), 6.66 (d, *J* = 8.8 Hz, 1H), 3.75 (s, 3H); **^{13}C NMR (100 MHz, DMSO-d_6)** δ 156.9, 148.6, 132.3, 127.3, 110.5, 52.9; **EI-MS** *m/z* (rel intensity) 125 (M^+, 85); **mp** 72-74 °C.

3-Hydroxy-2-methoxypyridine (2o): CAS# 13472-83-8 (No data for the title compound is available)



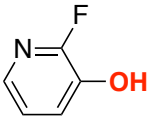
2o was obtained as a brown solid in 64% yield (40.0 mg, 0.320 mmol) **^{1}H NMR (400 MHz, DMSO-*d*$_6$)** δ. 9.45 (s, 1H), 7.58 (dd, *J* = 5.0, 1.6 Hz, 1H), 7.06 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.80 (dd, *J* = 7.6, 5.0 Hz, 1H), 3.85 (s, 3H); **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ.153.5, 141.4, 135.6, 121.6, 117.3, 52.8; **HRMS (ESI (+))** *m/z* calcd for $C_6H_8NO_2^+$ $[M+H]^+$ 126.0550, found 126.0556; **EI-MS** *m/z* (rel intensity) 125 (M^+, 100); **mp** 63-64 °C.

2-Fluoro-5-hydroxypyridine (2p): CAS# 55758-32-2 (No data for the title compound is available)



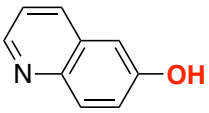
2p was obtained as a yellow solid in 71% yield (40.3 mg, 0.356 mmol) **^{1}H NMR (400 MHz, DMSO-*d*$_6$)** δ 9.93 (s, 1H), 7.69 (dd, *J* = 3.1, 2.2 Hz, 1H), 7.35 (ddd, *J* = 8.8, 6.8, 3.1 Hz, 1H), 6.99 (dd, *J* = 8.8, 3.4 Hz, 1H); **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 156.2 (d, *J* = 225.3 Hz), 152.0 (d, *J* = 3.8 Hz), 133.1 (d, *J* = 15.3 Hz), 128.4 (d, *J* = 7.7 Hz), 109.6 (d, *J* = 40.4 Hz); **HRMS (ESI (–))** *m/z* calcd for $C_5H_3FNO^-$ $[M–H]^–$ 112.0194, found 122.0193; **EI-MS** *m/z* (rel intensity) 113 (M^+, 100); **mp** 147-149 °C.

2-Fluoro-3-hydroxypyridine (2q): CAS# 174669-74-0[S10]



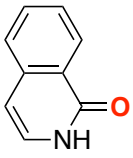
2q was obtained as a cream solid in 62% yield (35.1 mg, 0.310 mmol) **^{1}H NMR (400 MHz, DMSO-*d*$_6$)** δ 10.40 (s, 1H), 7.61 (ddd, *J* = 4.8, 1.8, 1.7 Hz, 1H), 7.38 (ddd, *J* = 10.8, 7.8, 1.7 Hz, 1H), 7.16 (ddd, *J* = 7.8, 4.8, 1.2 Hz, 1H); **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 152.4 (d, *J* = 231.8 Hz), 140.2 (d, *J* = 27.2 Hz), 135.6 (d, *J* = 13.1 Hz), 126.2 (d, *J* = 5.6 Hz), 122.6 (d, *J* = 3.9 Hz); **EI-MS** *m/z* (rel intensity) 113 (M^+, 100); **mp** 124-126 °C.

6-Hydroxyquinoline (2r): CAS# 580-16-5[S4]



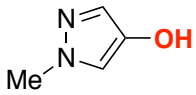
2r was obtained as a white solid in 82% yield (59.5 mg, 0.410mmol) **^{1}H NMR (400 MHz, DMSO-*d*$_6$)** δ 10.02 (br-s, 1H), 8.66 (dd, *J* = 4.1, 1.0 Hz, 1H), 8.14 (d, *J* = 8.3 Hz, 1H), 7.86 (d, *J* = 9.0 Hz, 1H), 7.39 (dd *J* = 8.3, 4.1 Hz, 1H), 7.31 (dd, *J* = 9.0, 2.6 Hz, 1H), 7.14 (d, *J* = 2.6 Hz, 1H); **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 155.5, 147.1, 143.1, 134.1, 130.4, 129.3, 122.0, 121.4, 108.3; **EI-MS** *m/z* (rel intensity) 145 (M^+, 100); **mp** 188-190 °C.

1(*2H*)-Isoquinolinone (2s): CAS# 491-30-5[S11]



2s was obtained as a cream solid in 72% yield (51.9 mg, 0.358 mmol) **^{1}H NMR (400 MHz, DMSO-*d*$_6$)** δ 11.25 (br-s, 1H), 8.19 (d, *J* = 7.1 Hz, 1H), 7.70 (ddd, *J* = 6.9, 6.8, 1.3 Hz, 1H), 7.65 (dd, *J* = 6.9, 1.3 Hz, 1H), 7.48 (ddd, *J* = 6.8, 6.7, 1.5 Hz, 1H), 7.18 (dd, *J* = 6.7, 1.5 Hz, 1H), 6.55 (d, *J* = 7.1 Hz, 1H); **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 161.8, 137.9, 132.3, 129.0, 126.6, 126.3, 126.2, 126.1, 104.6; **EI-MS** *m/z* (rel intensity) 145 (M^+, 100); **mp** 203-204 °C.

1-Methyl-1*H*-pyrazol-4-ol (2t): CAS# 491-30-5[S12]



2t was obtained as a yellow oil in 31% yield (15.2 mg, 0.155 mmol)

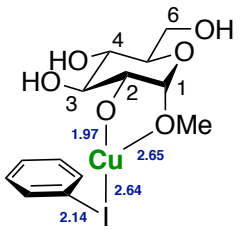
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (br-s, 1H), 7.11 (s, 1H), 7.04 (s, 1H), 3.78 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 141.6, 127.9, 117.5, 39.1; **EI-MS** *m/z* (rel intensity) 98 (M^+, 100).

5. Computational details

5-1. General information

All calculations were carried with the Gaussian 16 (revision B.01) program package.[S13] The molecular structures and harmonic vibrational frequencies were obtained using the hybrid density functional method based on the M06-2X function.[S14] We used SDD basis set[S15] for Cu and I atoms and 6-31+G* basis set[S16] for all other atoms. The self-consistent reaction field (SCRF) method based on the *solvation model based on density* (SMD)[S17] was employed to evaluate the solvent reaction field (water; ε = 78.39). Geometry optimization and vibrational analysis were performed at the same level. All stationary points were optimized without any symmetry assumptions, and characterized by normal coordinate analysis at the same level of theory (number of imaginary frequencies, NIMAG, 0 for minima and 1 for TSs). The intrinsic reaction coordinate (IRC) method was used to track minimum energy paths from transition structures to the corresponding local minima.[S18] Single point energies were calculated at the M06-2X/6-311+G*[S16] level of theory and the self-consistent reaction field (SCRF) method based on the SMD was employed to evaluate the solvent reaction field (water; ε = 78.39).

5.2 Cartesian Coordinates and Energies



INT_1

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.9982679999998 A.U.

Thermal correction to Gibbs Free Energy = 0.253816 A.U.

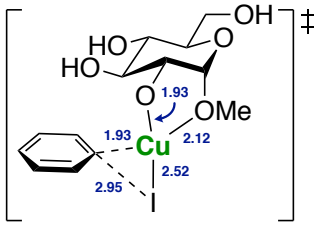
Sum of electronic and thermal Free Energies = -1165.744452 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.24631095

C	0.70332900	1.99027700	-1.00269700
C	-1.51599500	1.58188300	0.05016900
C	-1.29824600	2.00918800	1.35684900
C	-0.22851900	2.86978100	1.61024800
C	0.60322400	3.28719700	0.57096100
C	0.36495300	2.84840700	-0.73125300
H	-0.88875700	1.64704400	-2.01524400
H	-1.93975200	1.67486700	2.16582600
H	-0.04523100	3.20488300	2.62692700
H	1.43928400	3.94875500	0.77712400
H	1.01166100	3.16629800	-1.54458900
O	0.62672100	-1.02726500	-1.37216100
I	-3.11268500	0.21394100	-0.34283000
Cu	-1.35661500	-1.65734400	0.26913500
H	1.10596400	-1.55522000	-3.32375900
C	0.77804600	-0.68402700	-2.74322500
H	1.50430300	0.12852000	-2.86658700
H	-0.20008000	-0.35701600	-3.10104500
C	1.68158500	-1.79785700	-0.86169300
H	1.79553000	-2.71216700	-1.45808000
O	2.92382800	-1.12677600	-0.98308500
C	1.38936400	-2.12334600	0.60788500
C	2.99898400	0.10939700	-0.26971500

H	2.22706400	-2.76670200	0.93546700
C	1.47443600	-0.82974300	1.42872400
O	0.17361900	-2.76977200	0.81664800
H	2.19619200	0.78116000	-0.61366900
C	2.80955500	-0.13879300	1.23364900
C	4.34001800	0.73105100	-0.60517300
H	0.67683700	-0.14165300	1.09308200
O	1.28302300	-1.13376500	2.80352900
H	3.61866500	-0.78272200	1.60661700
O	2.78545500	1.08593000	1.95745600
H	4.48547400	1.63889300	-0.00845300
H	5.14343700	0.02515200	-0.37333800
O	4.45455800	1.02696200	-1.99229300
H	0.56159000	-1.79076600	2.81971600
H	3.69513500	1.35822300	2.15543000
H	3.78475200	1.69353000	-2.21945900



TS_{OA}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.963524 A.U.

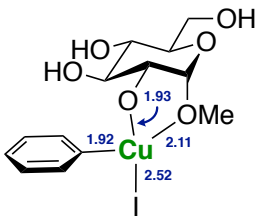
Thermal correction to Gibbs Free Energy = 0.256212 A.U.

Sum of electronic and thermal Free Energies = -1165.707312 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.21056562

C	-2.26811200	1.64325100	-0.98095800
C	-2.30507400	0.82766900	0.13641600
C	-3.20846700	0.96140700	1.17478300
C	-4.13814700	2.00403900	1.08243100
C	-4.13813600	2.85641600	-0.02224600
C	-3.20738100	2.67902100	-1.04688700
H	-1.54207600	1.49483900	-1.77461000
H	-3.20337000	0.29015600	2.02762400
H	-4.86303200	2.13833500	1.88020800
H	-4.86622400	3.65919400	-0.08611200
H	-3.20481400	3.34132200	-1.90788000
O	1.19691600	-1.07644000	0.68251000
I	-2.13538700	-2.01031900	-0.63938400
Cu	-0.72868000	-0.23009800	0.46110200
H	1.30181900	-2.66833200	2.00854200
C	1.46279300	-2.45507800	0.94644600
H	2.49258800	-2.69369300	0.66619700
H	0.76779600	-3.03289900	0.33740500
C	1.99442200	-0.17641200	1.44254200
H	1.93916800	-0.45492300	2.50039500
O	3.35026600	-0.26579600	1.09102000
C	1.42029400	1.21630100	1.19213100
C	3.65500100	0.09123400	-0.26178200
H	1.94259800	1.91201700	1.86869800
C	1.71660200	1.63951800	-0.25006600
O	0.04454600	1.24386200	1.43833900
H	3.13343400	-0.59498700	-0.94638100
C	3.19551000	1.52697700	-0.56269100
C	5.15340600	-0.08008000	-0.42170500
H	1.16712000	0.96639900	-0.93247300
O	1.28372300	2.97468600	-0.46001200
H	3.75908000	2.23463500	0.06153300
O	3.37805800	1.82983200	-1.93964600
H	5.46344200	0.28723500	-1.40617000
H	5.66935900	0.50061600	0.34899000
O	5.55733700	-1.43214000	-0.24669100
H	0.36158200	3.01405300	-0.14648000
H	4.27368800	2.17636300	-2.07625900
H	5.23204000	-1.94817400	-1.00243900



INT_2

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.963579 A.U.

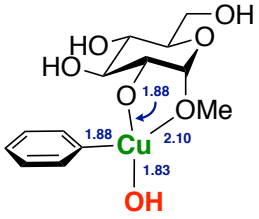
Thermal correction to Gibbs Free Energy = 0.253242 A.U.

Sum of electronic and thermal Free Energies = -1165.710337 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.21052346

C	-2.30758900	1.63705100	-0.97187600
C	-2.32882100	0.81481900	0.14075300
C	-3.24374200	0.91440300	1.17251300
C	-4.20485000	1.92844500	1.07784300
C	-4.22140800	2.78708400	-0.02165100
C	-3.27822200	2.64334200	-1.04036600
H	-1.56901500	1.51747500	-1.75885900
H	-3.22365800	0.24053400	2.02311100
H	-4.93903700	2.03690300	1.87109000
H	-4.97157700	3.56930800	-0.08568600
H	-3.28829600	3.31150200	-1.89677000
O	1.18488900	-1.03709300	0.73808600
I	-2.03562000	-2.05116700	-0.65697600
Cu	-0.73884000	-0.21394700	0.47204600
H	1.32245500	-2.59904600	2.09623400
C	1.47459500	-2.40555900	1.02910400
H	2.50680700	-2.63250600	0.74813700
H	0.78694600	-3.00731400	0.43526500
C	1.97627000	-0.10797200	1.46745600
H	1.92783700	-0.35496300	2.53338200
O	3.33123300	-0.19639000	1.11251400
C	1.38661200	1.27037400	1.17593600
C	3.62342900	0.11947700	-0.25320900
H	1.89680900	1.99032300	1.83604500
C	1.68335100	1.66218100	-0.27530800
O	0.00923500	1.28875400	1.41797500
H	3.09235700	-0.58415300	-0.91243800
C	3.16271700	1.54726100	-0.58590500
C	5.11887500	-0.06400200	-0.42569100
H	1.13593600	0.97270600	-0.94287000
O	1.24654700	2.99123700	-0.51351000
H	3.72501500	2.26857500	0.02365600
O	3.34373000	1.82237500	-1.96862600
H	5.41815900	0.27025100	-1.42512800
H	5.64804400	0.53702300	0.31999300
O	5.51702600	-1.41241600	-0.21352900
H	0.32508700	3.03585800	-0.19881900
H	4.24083300	2.16191300	-2.11313700
H	5.17094600	-1.95121900	-0.94369000



INT_{3OH}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.34568 A.U.

Thermal correction to Gibbs Free Energy = 0.268959 A.U.

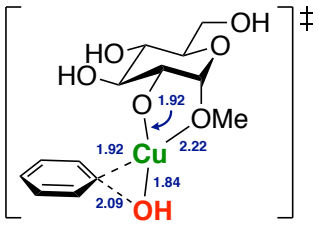
Sum of electronic and thermal Free Energies = -1230.076721 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.61635332

C	-2.86253700	1.04777500	-0.86742800
C	-2.77045800	-0.13186300	-0.14826700
C	-3.81256000	-0.68810800	0.57159200
C	-5.03434200	-0.00391500	0.56875900
C	-5.17189300	1.19011000	-0.13955000
C	-4.09360500	1.71343500	-0.85507500

H	-2.01570800	1.44982600	-1.41627300
H	-3.69460500	-1.61815800	1.11922500
H	-5.87388600	-0.41253900	1.12377000
H	-6.12226900	1.71499400	-0.13426400
H	-4.20045200	2.64410600	-1.40488600
O	0.94732900	-1.49321900	-0.00705400
Cu	-1.09064300	-0.98229800	-0.08260300
H	1.31319300	-3.43776100	0.61759200
C	1.45519000	-2.80380300	-0.26363500
H	2.51655300	-2.74516900	-0.52022000
H	0.89112200	-3.19928000	-1.10819900
C	1.52962000	-0.83788200	1.11058200
H	1.49895400	-1.50690300	1.97704900
O	2.88431900	-0.54962800	0.89271800
C	0.68761200	0.41711000	1.33218600
C	3.14881800	0.35641600	-0.18479300
H	1.00343400	0.86572800	2.28631400
C	0.94868100	1.43327600	0.21755000
O	-0.67497800	0.09099500	1.40024700
H	2.78186700	-0.07923600	-1.12651600
C	2.43358300	1.69505100	0.05157700
C	4.65662900	0.50696400	-0.25346900
H	0.56155500	1.02558400	-0.73182700
O	0.28697900	2.65418000	0.51117900
H	2.82800600	2.16830600	0.96181500
O	2.60008800	2.55708700	-1.06567900
H	4.91881400	1.27205900	-0.99225400
H	5.03536600	0.81796100	0.72495400
O	5.29876600	-0.72319100	-0.56245600
H	-0.64697000	2.43497100	0.67949800
H	3.42071300	3.06350300	-0.96172600
H	5.09763900	-0.94963400	-1.48510900
O	-1.57699900	-2.08956800	-1.45904300
H	-2.49715200	-1.96236000	-1.73293400



TS_{RE1}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.3369969999999 A.U.

Thermal correction to Gibbs Free Energy =

0.269901 A.U.

Sum of electronic and thermal Free Energies =

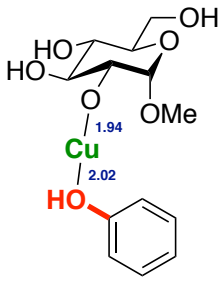
-1230.067096 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.60798551 A.U.

C	-2.88753000	0.94069400	-1.00932700
C	-2.88405900	-0.26962200	-0.33438600
C	-3.92554300	-0.73254000	0.45022600
C	-5.04526500	0.09794700	0.57692500
C	-5.09171500	1.33191000	-0.07187000
C	-4.01647400	1.75052600	-0.85921000
H	-2.04697200	1.25125800	-1.62263200
H	-3.87658500	-1.69322300	0.95311600
H	-5.87903300	-0.23101700	1.19045100
H	-5.96542700	1.96728100	0.03344900
H	-4.04835600	2.71145500	-1.36458300
O	1.01851400	-1.50379000	-0.04652500
Cu	-1.13902200	-0.99277000	-0.00855600
H	1.46926800	-3.44897400	0.51901200
C	1.53505800	-2.79471700	-0.35729500
H	2.57570100	-2.71812000	-0.68761600
H	0.92048300	-3.19226400	-1.16615000
C	1.60478500	-0.88920100	1.08195200
H	1.60040200	-1.59019500	1.92455700
O	2.95810200	-0.57389500	0.85652500
C	0.76818700	0.35705100	1.38037600
C	3.18906100	0.35384700	-0.20836500
H	1.15737000	0.78539500	2.31884800

C	0.98407700	1.38875400	0.26884900
O	-0.58873900	0.05064600	1.50859300
H	2.80919600	-0.06914700	-1.15096900
C	2.45890800	1.67781300	0.06507600
C	4.69279900	0.52637000	-0.30719800
H	0.57463800	0.98492600	-0.67287600
O	0.30562300	2.59362100	0.59523700
H	2.87012300	2.14476700	0.97120200
O	2.58443700	2.55997600	-1.04304100
H	4.92895200	1.30529400	-1.04050300
H	5.08964400	0.82794000	0.66698500
O	5.34529900	-0.69051600	-0.64785900
H	-0.59588000	2.33186600	0.85770300
H	3.40618100	3.06783700	-0.95610400
H	5.11217900	-0.91672800	-1.56309700
O	-1.97326800	-1.77186900	-1.45793400
H	-2.56371500	-2.47442000	-1.13718200



INT$_4$

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1230.430088 A.U.

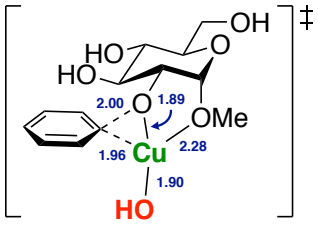
Thermal correction to Gibbs Free Energy = 0.270096 A.U.

Sum of electronic and thermal Free Energies = -1230.159992 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.70096939 A.U.

C	-2.14177900	1.08020700	-0.60659900
C	-3.19291700	0.29826300	-0.13369600
C	-4.31484300	0.86955100	0.45859300
C	-4.37662500	2.25783000	0.58368900
C	-3.33403300	3.06011600	0.11896800
C	-2.21921500	2.46535700	-0.47579700
H	-1.27793800	0.59619200	-1.05827900
H	-5.12317900	0.23701900	0.81586800
H	-5.24810800	2.70958100	1.04806100
H	-3.38871900	4.13929800	0.22088900
H	-1.40075300	3.07962200	-0.84021300
O	0.84250800	-0.34133300	-1.63471600
Cu	-1.27983800	-1.95824200	-0.23524500
H	1.65562000	-0.25866700	-3.54429400
C	1.14304400	0.38523200	-2.81866500
H	1.77138200	1.25595100	-2.59928500
H	0.19142400	0.72039400	-3.23528100
C	1.95077900	-0.99705000	-1.08111200
H	2.40341100	-1.66130400	-1.82870000
O	2.97821400	-0.08335300	-0.73443600
C	1.50039200	-1.77752000	0.15796300
C	2.59500200	0.89794700	0.23036300
H	2.41016200	-2.28629700	0.52640200
C	1.07617200	-0.78125300	1.24356500
O	0.49898200	-2.71300000	-0.09494100
H	1.74121100	1.47933200	-0.15330200
C	2.17179700	0.22262200	1.54310200
C	3.78587200	1.81997000	0.40976500
H	0.18939100	-0.22501500	0.89034100
O	0.73984500	-1.48894200	2.42976500
H	3.03443300	-0.29423400	1.98682200
O	1.64921500	1.17965800	2.45773100
H	3.58051900	2.53933900	1.21045200
H	4.66626200	1.23073100	0.68391700
O	4.11838800	2.49956300	-0.79490600
H	0.20029000	-2.24575400	2.13163900
H	2.37882200	1.57883900	2.95671000
H	3.38939400	3.10129400	-1.01819900
O	-3.09048300	-1.07497200	-0.29336300
H	-3.81355500	-1.53591300	0.16665400



TS_{RE2}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1230.328143 A.U.

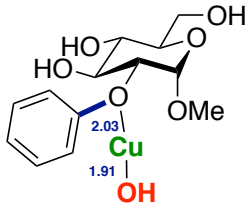
Thermal correction to Gibbs Free Energy = 0.269401 A.U.

Sum of electronic and thermal Free Energies = -1230.058742 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.59922519

C	2.44469300	-0.91756200	-0.97877200
C	2.41247300	-0.09158400	0.13188700
C	3.45092100	0.04447100	1.03884800
C	4.61045500	-0.69170200	0.79775000
C	4.69373800	-1.54756100	-0.30508700
C	3.61991000	-1.65598200	-1.18397000
H	1.62376100	-0.97950400	-1.68499800
H	3.35906800	0.69215800	1.90452600
H	5.44520700	-0.60174300	1.48665600
H	5.59583700	-2.12625700	-0.47592700
H	3.67924300	-2.30860000	-2.05010100
O	-1.09013400	1.55504200	-0.12992600
Cu	1.18239700	1.42379800	-0.08656200
H	-1.63809200	3.43351900	0.56270000
C	-1.76205200	2.79854500	-0.32151300
H	-2.82648900	2.63109700	-0.51392300
H	-1.30084300	3.27326000	-1.18843000
C	-1.48265000	0.86115900	1.02956500
H	-1.47276200	1.53792000	1.89123500
O	-2.80213100	0.38339000	0.93440900
C	-0.48977200	-0.28916900	1.22283200
C	-3.01964700	-0.53421300	-0.14090600
H	-0.71500300	-0.76112100	2.18952800
C	-0.67086700	-1.34604700	0.13468500
O	0.83341300	0.20193800	1.31880000
H	-2.76863000	-0.04758300	-1.09536900
C	-2.12863800	-1.77062000	0.03353400
C	-4.49740600	-0.87676700	-0.12695400
H	-0.37946900	-0.92235400	-0.83810300
O	0.10029700	-2.50073800	0.42288500
H	-2.41507200	-2.30273400	0.95149500
O	-2.24066100	-2.62950100	-1.09210100
H	-4.69881300	-1.66802600	-0.85767700
H	-4.77921000	-1.23631700	0.86732400
O	-5.30726300	0.26172700	-0.38856700
H	1.04120800	-2.25326600	0.41581700
H	-2.98198700	-3.23973600	-0.95602300
H	-5.16183100	0.53524600	-1.30919000
O	1.96522100	2.47176000	-1.46308300
H	1.34748800	3.20714700	-1.59997700



INT_5

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.422456 A.U.

Thermal correction to Gibbs Free Energy = 0.269591 A.U.

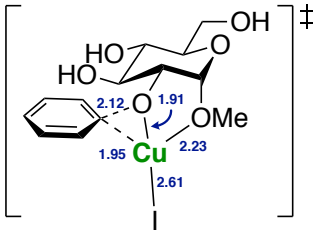
Sum of electronic and thermal Free Energies = -1230.152865 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.6930125 A.U.

C	-3.36909800	-0.30751700	0.52514800
C	-2.24284400	-0.83728000	-0.09796500
C	-2.26368400	-2.09835000	-0.68764000
C	-3.44370100	-2.84164100	-0.63827900
C	-4.58363700	-2.32652100	-0.02069000

C	-4.54367600	-1.05648800	0.55715200
H	-3.30944900	0.68292800	0.97189100
H	-1.38257000	-2.49081800	-1.18635300
H	-3.46909500	-3.82561700	-1.09656900
H	-5.49827500	-2.91029000	0.00819300
H	-5.42498700	-0.64649400	1.04091000
O	1.13687600	0.65762200	-1.59301500
Cu	-1.31612600	1.98816700	-0.15837500
H	1.47673600	0.05891400	-3.55316000
C	1.88118200	0.75057900	-2.80471200
H	2.93912500	0.52580100	-2.63149900
H	1.77886400	1.77711300	-3.15785300
C	1.03827100	-0.65219900	-1.11289900
H	0.62747800	-1.31395100	-1.88507000
O	2.29307500	-1.20101600	-0.77309800
C	0.16490600	-0.63477100	0.13572300
C	3.01055900	-0.46468900	0.22255800
H	0.00528500	-1.66571900	0.46669400
C	0.82379700	0.15457700	1.26020300
O	-1.10810600	-0.03552200	-0.14412700
H	3.17927500	0.56363600	-0.13035500
C	2.20928300	-0.40964300	1.53284300
C	4.34617100	-1.16333600	0.39542000
H	0.92232300	1.20818000	0.95506600
O	0.04501800	0.06733900	2.44048300
H	2.10731000	-1.42401900	1.94381700
O	2.84247700	0.44389500	2.47259900
H	4.89450100	-0.70942900	1.22864900
H	4.17768100	-2.22102000	0.61951400
O	5.12325300	-1.12232700	-0.79421200
H	-0.78863500	0.54449600	2.28004200
H	3.48606700	-0.06945200	2.98570200
H	5.37754000	-0.19978700	-0.96142500
O	-1.61110700	3.87814600	-0.14425200
H	-0.86856300	4.27724100	-0.62149900



TS_{RE4}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.954966 A.U.

Thermal correction to Gibbs Free Energy = 0.253873 A.U.

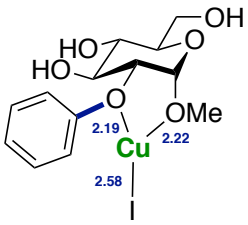
Sum of electronic and thermal Free Energies = -1165.701093 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.20141351 A.U.

C	1.77120800	1.92000900	0.93243300
C	1.78824400	1.39799100	-0.34543100
C	2.68064200	1.72669300	-1.34442600
C	3.67629300	2.64719500	-1.00633400
C	3.72054800	3.21023100	0.27206500
C	2.77698600	2.85065300	1.23208700
H	1.04708300	1.61386900	1.68151100
H	2.61244700	1.29610000	-2.33804500
H	4.40989900	2.92836900	-1.75595600
H	4.49129000	3.93404200	0.51669100
H	2.81045300	3.28065200	2.22874600
O	-1.18991800	-1.20582800	-0.62081400
I	2.33406000	-2.16225400	0.58890700
Cu	0.84318700	-0.30543800	-0.48405200
H	-1.30147600	-2.79855600	-1.94583800
C	1.47471200	-2.57872100	-0.88664900
H	-2.51144700	-2.80663700	-0.62134800
H	-0.79599000	-3.16565200	-0.26739700
C	-1.94315700	-0.30099000	-1.39692600
H	-1.89260700	-0.58768200	-2.45307400
O	-3.30747300	-0.33573400	-1.05688800
C	-1.34247100	1.09211400	-1.17374700

C	-3.59422800	0.01693100	0.29877700
H	-1.83347900	1.78311200	-1.87423300
C	-1.63718100	1.56798600	0.24777900
O	0.03341400	1.10158700	-1.48935600
H	-3.06960600	-0.67137600	0.97804400
C	-3.12217400	1.44596300	0.56050300
C	-5.09182600	-0.13607500	0.48347400
H	-1.07778400	0.93998100	0.96108300
O	-1.28837600	2.93259800	0.42085000
H	-3.68174400	2.13290500	-0.09287900
O	-3.37383800	1.75018900	1.92312300
H	-5.37707200	0.23192600	1.47414100
H	-5.61353800	0.45390900	-0.27609600
O	-5.51158500	-1.48321000	0.30748600
H	-0.32374200	3.02546900	0.33595300
H	-3.01500800	2.63635500	2.10077300
H	-5.18211700	-2.00631700	1.05651100



INT_5

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.059562 A.U.

Thermal correction to Gibbs Free Energy =

0.256807 A.U.

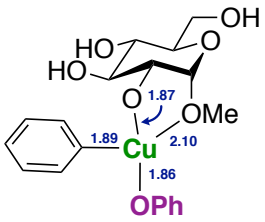
Sum of electronic and thermal Free Energies =

-1165.802755 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.30548572 A.U.

C	1.57036900	2.45315800	0.34867500
C	0.52634400	2.35029600	-0.56587200
C	0.07641900	3.45671900	-1.28239300
C	0.68134400	4.69283800	-1.05745800
C	1.72557200	4.81699400	-0.13872900
C	2.17115800	3.69429800	0.55958500
H	1.89597600	1.56041500	0.88003300
H	-0.72708100	3.35457600	-2.00562800
H	0.33757500	5.56127100	-1.61136300
H	2.19150700	5.78318600	0.02804800
H	2.98501500	3.78081100	1.27317500
O	-0.94261000	-1.40326900	-0.68329100
I	3.39706800	-1.77283600	0.33872800
Cu	1.10475100	-0.69964300	-0.18278100
H	-0.79733900	-2.59272600	-2.37940600
C	-1.03101900	-2.68289600	-1.31299700
H	-2.03331500	-3.10281500	-1.18332900
H	-0.29496300	-3.32040100	-0.82241800
C	-1.75907300	-0.42360100	-1.27701000
H	-1.58358200	-0.38999000	-2.35771600
O	-3.12391200	-0.71412500	-1.11330400
C	-1.42122900	0.91338000	-0.61825300
C	-3.54442000	-0.83394400	0.24954300
H	-1.96312600	1.70483100	-1.14632100
C	-1.82237900	0.88907000	0.85369800
O	-0.01073500	1.08715500	-0.78200600
H	-2.97688000	-1.63767400	0.74078700
C	-3.28874700	0.48379700	0.97787600
C	-5.01590400	-1.20006600	0.22092800
H	-1.20025500	0.15662500	1.38666800
O	-1.69764900	2.16625100	1.46429400
H	-3.90914200	1.27108600	0.52208000
O	-3.63963400	0.30867300	2.33952000
H	-5.41323200	-1.19216200	1.24101100
H	-5.56257900	-0.46458700	-0.37683400
O	-5.23286900	-2.46269700	-0.39494400
H	-0.78702100	2.28438600	1.78118600
H	-3.41286000	1.12921400	2.81007700
H	-4.86245400	-3.15222100	0.18029900



INT_{3OPh}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1461.307181 A.U.

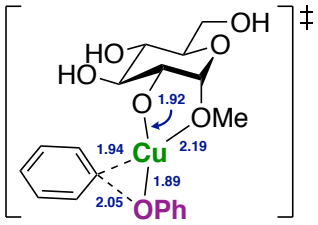
Thermal correction to Gibbs Free Energy = 0.345813 A.U.

Sum of electronic and thermal Free Energies = -1460.961368 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1461.62517189 A.U.

C	1.54890900	2.54990400	0.84234100
C	1.77919600	1.53665200	-0.07020200
C	2.84798900	1.48850500	-0.94327200
C	3.76285300	2.54854200	-0.88765600
C	3.57809700	3.59270800	0.01850000
C	2.47867500	3.59546500	0.87915100
H	0.68741900	2.54082700	1.50405100
H	2.98269100	0.66897200	-1.64377000
H	4.61678100	2.54843200	-1.55899300
H	4.29242000	4.40959900	0.05344100
H	2.33509400	4.40977900	1.58346100
O	-1.10650000	-1.20031900	-0.26639900
Cu	0.50675200	0.14454000	-0.15691000
H	-0.58641900	-2.93126600	-1.28692500
C	-0.91605600	-2.61643900	-0.29137500
H	-1.85092000	-3.11917000	-0.02749900
H	-0.15010200	-2.84403900	0.45059500
C	-2.00877000	-0.70339300	-1.24436700
H	-1.76552200	-1.14254800	-2.21751400
O	-3.32976300	-1.08114300	-0.96576200
C	-1.81852400	0.81248500	-1.24342600
C	-3.85467700	-0.57725000	0.26816000
H	-2.39162600	1.22069200	-2.08971800
C	-2.38234400	1.41096800	0.04807400
O	-0.46407300	1.14684800	-1.40251700
H	-3.24639100	-0.95442700	1.10412700
C	-3.81210900	0.95829000	0.28096000
C	-5.26416900	-1.12361300	0.38812700
H	-1.76758200	1.06453200	0.89672700
O	-2.34355900	2.82803400	-0.01517600
H	-4.45638600	1.35120700	-0.51818100
O	-4.22756400	1.46169500	1.54308900
H	-5.75757900	-0.68107800	1.26044000
H	-5.83400800	-0.86308900	-0.50893400
O	-5.27645700	-2.54270700	0.47584900
H	-1.43002500	3.07359300	-0.24679500
H	-5.19227000	1.56377800	1.54530300
H	-4.87953100	-2.79973300	1.32441600
O	1.51407700	-0.78589300	1.10088500
C	2.60473800	-1.46056200	0.70592700
C	3.65432700	-1.66663400	1.61994200
C	2.72682700	-1.99419700	-0.59065800
C	4.78109100	-2.39632000	1.24705900
H	3.56538200	-1.25026900	2.61989600
C	3.86234400	-2.71380600	-0.95691300
H	1.91860000	-1.82407300	-1.30164800
C	4.89638500	-2.92412600	-0.04161700
H	5.57931700	-2.54789900	1.96890900
H	3.93771100	-3.11360800	-1.96467300
H	5.77917400	-3.48705900	-0.32859200



TS_{RE3}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1461.2978859999998 A.U.

Thermal correction to Gibbs Free Energy = 0.34469 A.U.

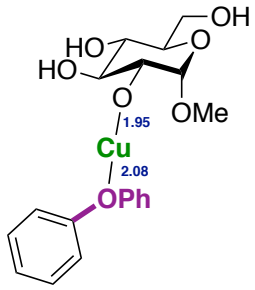
Sum of electronic and thermal Free Energies =

-1460.953196 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1461.61603848 A.U.

C	-1.49152900	2.33503000	-0.99468200
C	-1.89573800	1.32882700	-0.13545200
C	-2.91625900	1.43173000	0.78852900
C	-3.56554800	2.66955000	0.87367500
C	-3.19068800	3.72545400	0.04287600
C	-2.15954500	3.55841800	-0.88503900
H	-0.69328100	2.18507800	-1.71534600
H	-3.19962500	0.59801700	1.42552000
H	-4.36583300	2.79638700	1.59700900
H	-3.70469500	4.67872300	0.11447500
H	-1.86833400	4.37835600	-1.53511600
O	1.22589200	-1.32310500	0.12799200
Cu	-0.52465800	-0.00544900	0.21505100
H	0.81224000	-3.19144700	0.93320800
C	1.10568700	-2.73600200	-0.01907000
H	2.05397800	-3.16351500	-0.35959000
H	0.33307300	-2.90882400	-0.76989900
C	2.10047000	-0.90654000	1.15743700
H	1.88372200	-1.47090800	2.07160900
O	3.44294400	-1.18929800	0.84325800
C	1.86243100	0.59322700	1.35426200
C	3.94249900	-0.52415100	-0.32149000
H	2.46912700	0.89938000	2.22281700
C	2.38046300	1.35274300	0.12958100
O	0.51277500	0.87821500	1.57463700
H	3.35511500	-0.83342600	-1.19946200
C	3.82508600	0.99999800	-0.16677600
C	5.37867300	-0.98117000	-0.49301000
H	1.76766000	1.07383100	-0.74471900
O	2.27137300	2.75171200	0.35073400
H	4.46254100	1.33730700	0.66270200
O	4.19893800	1.65523500	-1.37261800
H	5.85511000	-0.41162800	-1.29871100
H	5.92983400	-0.80452700	0.43567200
O	5.46362200	-2.37655300	-0.75397600
H	1.36887000	2.90203400	0.68662300
H	5.15724100	1.80474400	-1.37189500
H	5.10036900	-2.54329500	-1.63919800
O	-1.82699000	-0.49432900	-1.06268900
C	-2.89125900	-1.23455100	-0.66062800
C	-4.09650600	-1.10932200	-1.36545700
C	-2.80851200	-2.12168500	0.42174700
C	-5.19510400	-1.88686600	-1.00523800
H	-4.15168600	-0.40546500	-2.19158100
C	-3.91538600	-2.88897800	0.77984100
H	-1.86877400	-2.19518200	0.96781300
C	-5.11141700	-2.77841700	0.06717500
H	-6.12360300	-1.79071100	-1.56095900
H	-3.84177400	-3.57670400	1.61745600
H	-5.97153500	-3.37898400	0.34670800



INT$_7$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1461.378656 A.U.

Thermal correction to Gibbs Free Energy =

0.346054 A.U.

Sum of electronic and thermal Free Energies =

-1461.032602 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1461.69639014 A.U.

C	-0.47780300	1.51298500	-1.50574500
C	-1.36833200	1.18606400	-0.49134900
C	-1.36732500	1.84262400	0.73540200

C	-0.43211400	2.85556500	0.94400600
C	0.48578200	3.19114400	-0.05384300
C	0.46068300	2.51888200	-1.27671600
H	-0.50709400	0.96204900	-2.44131400
H	-2.06775900	1.55543500	1.51432800
H	-0.41149800	3.37137500	1.89925100
H	1.21964100	3.97143000	0.12340400
H	1.17380600	2.77130500	-2.05662500
O	1.70063100	-0.76691200	-1.61945500
Cu	-0.99551000	-1.60198200	-0.46564700
H	2.84829400	-1.10274600	-3.31797000
C	2.36877900	-0.27881300	-2.77426500
H	3.12646800	0.46746700	-2.50808000
H	1.61114900	0.18426900	-3.40931500
C	2.49868600	-1.58758400	-0.81059100
H	2.86836000	-2.44145400	-1.39333500
O	3.66691400	-0.91327900	-0.37322600
C	1.67035900	-2.04934400	0.39389300
C	3.41947200	0.25614300	0.40945500
H	2.34101900	-2.71107600	0.97259900
C	1.37399000	-0.83080400	1.27878000
O	0.50683400	-2.73576800	0.04667000
H	2.81242500	0.96990400	-0.17212700
C	2.64197900	-0.10537800	1.68281900
C	4.77111700	0.87841400	0.70046800
H	0.74730300	-0.12184400	0.70939500
O	0.66931000	-1.24490800	2.44240600
H	3.25546000	-0.75392300	2.32412200
O	2.26168800	1.06995400	2.39118800
H	4.65233900	1.71187800	1.40214400
H	5.42956400	0.13043400	1.15249800
O	5.41860900	1.31896600	-0.48726600
H	-0.01399900	-1.86428400	2.12343200
H	2.98616400	1.34320200	2.97523500
H	4.89245100	2.04026600	-0.87100100
O	-2.19606900	0.07945300	-0.71999700
C	-3.51817900	0.13143200	-0.27577200
C	-4.30440100	1.25051700	-0.53341800
C	-4.02523400	-0.98941400	0.36879700
C	-5.63663300	1.23716300	-0.12379800
H	-3.88213800	2.11120400	-1.04391400
C	-5.36261700	-0.99194100	0.76575200
H	-3.37096500	-1.84081500	0.54825200
C	-6.16918400	0.12009500	0.52354700
H	-6.26124500	2.10337800	-0.31986400
H	-5.76894200	-1.86388600	1.26899800
H	-7.20849000	0.11737200	0.83656500

KI

at M06-2X/6-31+G*&SDD (for I)/SMD(water)

Energy = -611.366752 A.U.

Thermal correction to Gibbs Free Energy = -0.025597 A.U.

Sum of electronic and thermal Free Energies = -611.392349 A.U.

at M06-2X/6-311+G*&SDD (for I)/SMD(water)

Energy = -611.410443256 A.U.

I	0.00000000	0.00000000	0.88066000
K	0.00000000	0.00000000	-2.45657800

KI•H_2O

at M06-2X/6-31+G*&SDD (for I)/SMD(water)

Energy = -687.778039 A.U.

Thermal correction to Gibbs Free Energy = -0.009155 A.U.

Sum of electronic and thermal Free Energies = -687.787194 A.U.

at M06-2X/6-311+G*& SDD (for I)/SMD(water)

Energy = -687.847549640 A.U.

I	-1.51604400	0.03773300	0.00032500
K	1.85113200	-0.24021500	-0.00046300
O	4.40227400	0.23635100	-0.01773200
H	5.11042600	-0.42072500	0.07605300
H	4.85022600	1.09414600	0.05736200

KI•2H$_2$O

at M06-2X/6-31+G*& SDD (for I)/SMD(water)

Energy = -764.1874339999999 A.U.

Thermal correction to Gibbs Free Energy = 0.00577 A.U.

Sum of electronic and thermal Free Energies = -764.181664 A.U.

at M06-2X/6-311+G*&SDD SDD (for I)/SMD(water)

Energy = -764.282533028 A.U.

I	1.77954200	0.00884300	0.00547400
K	-1.63192600	0.00489900	-0.03767500
O	-3.04633500	-2.20272200	-0.02130500
H	-4.01343800	-2.26390800	-0.07234900
H	-2.76417000	-3.05614800	0.34444700
O	-3.18256900	2.12887500	-0.00000600
H	-2.96855300	2.96916800	-0.43584900
H	-3.73173900	2.37991300	0.75994900

KOH

at M06-2X/6-31+G*/SMD(water)

Energy = -675.725548 A.U.

Thermal correction to Gibbs Free Energy = -0.014186 A.U.

Sum of electronic and thermal Free Energies = -675.739734 A.U.

at M06-2X/6-311+G*/SMD(water)

Energy = -675.793621185 A.U.

K	0.03225100	-0.83433700	0.00000000
O	0.03225100	1.72235400	0.00000000
H	-0.87077400	2.07357700	0.00000000

KOH•H$_2$O

at M06-2X/6-31+G*/SMD(water)

Energy = -752.1355560000001 A.U.

Thermal correction to Gibbs Free Energy = 0.003093 A.U.

Sum of electronic and thermal Free Energies = -752.132463 A.U.

at M06-2X/6-311+G*/SMD(water)

Energy = -752.228356213 A.U.

K	-0.11051000	-0.28395400	-0.03707100
O	-2.60486900	0.22641100	0.11434400
H	-2.93565200	0.91295500	-0.48335600
O	2.47737200	0.24453200	-0.01051300
H	3.16551300	-0.39680200	0.22682600
H	2.88979800	1.11142300	0.13023200

KOH•2H$_2$O

at M06-2X/6-31+G*/SMD(water)

Energy = -828.5436639999999 A.U.

Thermal correction to Gibbs Free Energy = 0.017851 A.U.

Sum of electronic and thermal Free Energies = -828.525813 A.U.

at M06-2X/6-311+G*/SMD(water)

Energy = -828.660928036 A.U.

K	-3.75092744	1.14525132	-0.01023680
O	-1.06092744	1.14525132	-0.01023680
H	-0.74047285	1.17683313	0.89414777
O	-5.28652589	2.07709465	1.28071223
H	-5.49620981	1.69992191	2.13825137
H	-5.96841764	2.70519795	1.03149365
O	-5.19203250	1.02738368	-1.68268051
H	-5.16582003	0.71756452	-2.59093432
H	-6.10415666	1.07829406	-1.38765905

KOPh

at M06-2X/6-31+G*/SMD(water)

Energy = -906.701068 A.U.

Thermal correction to Gibbs Free Energy = 0.05977 A.U.

Sum of electronic and thermal Free Energies =

-906.641298 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -906.814544911 A.U.

C	0.39275500	0.76606800	0.83516800
C	1.55728400	1.36425300	0.35298000
C	2.47336200	0.63863800	-0.41041400
C	2.19900700	-0.70735400	-0.68175600
C	1.04015800	-1.31468800	-0.20999100
C	0.08952300	-0.59837900	0.56931100
H	-0.29388400	1.33879800	1.45917000
H	1.75037000	2.40983600	0.58280800
H	3.37886100	1.10647100	-0.78451100
H	2.90008300	-1.29145100	-1.27413400
H	0.83750000	-2.36056200	-0.43142100
O	-1.02955200	-1.14676700	0.98429800
K	-2.46574000	0.37262200	-0.53463600

KOPh•H_2O

at M06-2X/6-31+G*/SMD(water)

Energy = -983.111765 A.U.

Thermal correction to Gibbs Free Energy =

0.076114 A.U.

Sum of electronic and thermal Free Energies =

-983.035651 A.U.

at M06-2X/6-311+G*/SMD(water)

Energy = -983.250148834 A.U.

K	-1.87035200	-0.48361100	0.32426700
O	0.09222900	-1.73716400	-0.88819900
O	-3.98114700	1.06428200	0.24724400
H	-4.82849300	0.90112400	0.69085000
H	-4.19053600	1.69465400	-0.46006300
C	0.92715800	-0.80085300	-0.50293800
C	0.87937300	0.51170400	-1.05117100
C	1.89215900	-1.02014100	0.51985300
C	1.73393700	1.52129200	-0.60915100
H	0.16701200	0.71101200	-1.85144600
C	2.74035900	-0.00454900	0.95039000
H	1.95300500	-2.01200600	0.96332900
C	2.67393800	1.27856200	0.39478000
H	1.66403300	2.50939800	-1.05885700
H	3.46396200	-0.21534100	1.73500200
H	3.33751500	2.06673000	0.73716700

KOPh•2H_2O

at M06-2X/6-31+G*/SMD(water)

Energy = -1059.524642 A.U.

Thermal correction to Gibbs Free Energy =

0.097222 A.U.

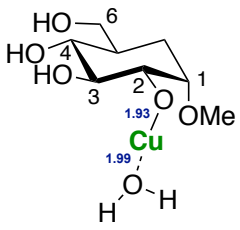
Sum of electronic and thermal Free Energies =

-1059.42742 A.U.

at M06-2X/6-311+G*/SMD(water)

Energy = -1059.68803324 A.U.

K	1.74669100	-0.04644100	0.34753700
O	0.10084800	-2.09588200	-0.20315300
O	0.21025200	2.08982400	-0.11136800
H	-0.73533400	1.85307200	-0.14543000
H	0.24648000	2.87817100	0.45293100
O	4.31817100	0.27878700	-0.20937200
H	4.89094900	-0.46769700	-0.44680700
H	4.58609900	0.99124000	-0.81125900
C	-0.87195500	-1.22184200	-0.12989900
C	-1.38299600	-0.77706700	1.12283600
C	-1.42986000	-0.61292300	-1.28934000
C	-2.35942700	0.21235000	1.20466600
H	-0.98340600	-1.22892500	2.02953600
C	-2.40879100	0.37245300	-1.19524900
H	-1.06198600	-0.92944600	-2.26329300
C	-2.88170300	0.80623600	0.04999300
H	-2.71377300	0.52966100	2.18303900
H	-2.80179500	0.81911000	-2.10604700
H	-3.64013700	1.58012700	0.11722500



INT_{0-2}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -999.480285 A.U.

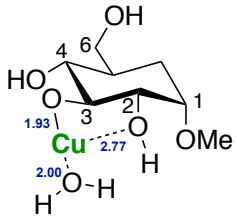
Thermal correction to Gibbs Free Energy = 0.194706 A.U.

Sum of electronic and thermal Free Energies = -999.285579 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy =-999.704285455 A.U.

O	-0.25978600	1.70670700	0.17423300
Cu	-2.67863900	-0.12768000	0.08285800
H	-0.02937000	3.71226900	-0.31360800
C	0.12933800	3.02805600	0.52913000
H	1.18172700	3.06174200	0.83130700
H	-0.49918800	3.32909700	1.36848500
C	0.33713400	1.25319300	-1.00996400
H	0.15941700	1.97417900	-1.81798900
O	1.75216000	1.19111200	-0.88652800
C	-0.23010000	-0.12633100	-1.36553800
C	2.21595000	0.29978600	0.12598300
H	0.26331000	-0.40411200	-2.31515900
C	0.23642400	-1.13535700	-0.31153800
O	-1.61194100	-0.14355600	-1.52547100
H	1.81825700	0.60197700	1.10618700
C	1.74742900	-1.12150500	-0.19267600
C	3.73422700	0.43099100	0.14547500
H	-0.20114200	-0.86525800	0.66424400
O	-0.19120800	-2.44341300	-0.66933300
H	2.19350300	-1.43723800	-1.14724800
O	2.20892900	-1.97078200	0.85629600
H	4.15162200	0.01755300	-0.78284700
H	3.99728300	1.49045300	0.20321300
O	4.30882400	-0.19948300	1.28236600
H	-1.12256800	-2.34889800	-0.94411100
H	2.03122600	-2.89264500	0.60617000
H	3.95772800	-1.10795700	1.31833600
O	-3.84545400	-0.13240000	1.69879100
H	-3.44510300	-0.70663300	2.37421300
H	-4.69077600	-0.56027100	1.47787800



INT_{0-3}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -999.4803099999999 A.U.

Thermal correction to Gibbs Free Energy = 0.195489 A.U.

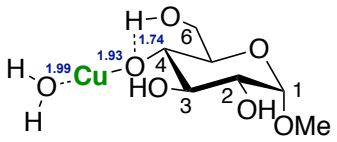
Sum of electronic and thermal Free Energies = -999.284821 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -999.704302671 A.U.

O	1.29371600	1.96431900	0.68593500
Cu	-3.06122800	-0.36514600	0.04670500
H	2.37284200	3.23963400	1.83676400
C	2.47494800	2.73524100	0.87514800
H	2.57597400	3.48013700	0.07622700
H	3.36308700	2.09413500	0.89072800
C	1.21157900	1.38512600	-0.58964700
H	1.32416700	2.15948700	-1.35873500
O	2.26729100	0.47606600	-0.82376400
C	-0.14894300	0.68971400	-0.69747000
C	2.29470000	-0.63841000	0.07671400
H	-0.28611600	0.37556300	-1.73817500
C	-0.21686800	-0.54628600	0.20742300
O	-1.18901700	1.61783800	-0.42723000
H	2.38506700	-0.27375200	1.11009000

C	1.00206600	-1.42357100	-0.08865200
C	3.53091900	-1.43523300	-0.28605900
H	-0.11742500	-0.19546500	1.25470700
O	-1.37487600	-1.30718200	0.04295500
H	0.93442400	-1.77558900	-1.13130000
O	1.01513300	-2.53807000	0.79331300
H	3.62034400	-2.30172400	0.37225100
H	3.45034400	-1.78425700	-1.32440100
O	4.71233100	-0.66203000	-0.11135900
H	-5.50702000	-0.07288100	-0.35010300
H	0.08355000	-2.81683600	0.86804100
H	4.62705700	0.13356300	-0.66353100
O	-4.85295200	0.51288500	0.06816400
H	-1.08943600	1.91548500	0.49404700
H	-4.82466100	1.30163500	-0.49990500



$INT_{0\text{-}4}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -999.481997 A.U.

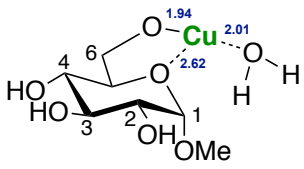
Thermal correction to Gibbs Free Energy = 0.196681 A.U.

Sum of electronic and thermal Free Energies = -999.285316 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -999.705544487 A.U.

O	-3.06250300	-0.65198400	0.85154800
C	-2.66846200	-0.57311400	-0.49254000
H	-3.50855700	-0.83837900	-1.14591100
O	-2.30215000	0.73726600	-0.86600900
C	-1.18792600	1.25858100	-0.13465400
H	-1.42588900	1.27942800	0.93946200
C	0.06832900	0.39905900	-0.35606100
H	0.26565400	0.38708800	-1.44647300
C	-1.49547800	-1.53284100	-0.67991900
H	-1.27118900	-1.58511100	-1.75022100
C	-0.25411300	-1.03610900	0.05773000
H	-0.43644300	-1.05881000	1.14353100
C	-0.98579900	2.68544100	-0.62726900
H	-0.72133200	2.66343300	-1.69475400
H	-1.91569200	3.25148500	-0.51452100
O	0.02534900	3.33943000	0.12817100
O	1.14304600	0.95081500	0.35176400
O	0.85700300	-1.86994500	-0.25289900
O	-1.84193400	-2.85119600	-0.28508000
C	-4.22111800	0.12108200	1.14471500
H	-4.00276200	1.19223900	1.08062600
H	-5.03249200	-0.12957400	0.45062600
H	-4.51872300	-0.12968300	2.16352200
H	0.70368800	2.63568800	0.29456800
H	-2.13237900	-2.81891100	0.64369100
H	0.61320700	-2.78356700	-0.02660400
Cu	2.84105100	0.04427500	0.21261800
O	4.63105900	-0.83094300	0.18068100
H	4.58888200	-1.62300900	-0.38193300
H	5.27200000	-0.24642800	-0.25897200



$INT_{0\text{-}6}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -999.4790200000001 A.U.

Thermal correction to Gibbs Free Energy = 0.198287 A.U.

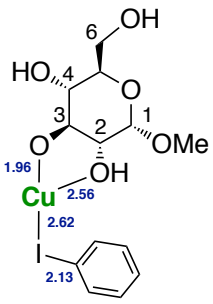
Sum of electronic and thermal Free Energies = -999.280733 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -999.702942425 A.U.

Cu	-2.27800900	0.88253300	0.56176600
O	1.95555800	-1.35331200	1.09231600

C	2.20564700	-1.02285900	-0.24754700
H	2.98956500	-1.67399700	-0.65358500
O	1.07728800	-1.24177600	-1.06652900
C	-0.08056800	-0.47048600	-0.70502700
H	-0.36162600	-0.71077000	0.33372800
C	0.21326400	1.03948000	-0.78692100
H	0.48164300	1.26725100	-1.83773400
C	2.61906600	0.44445600	-0.31593500
H	2.89748200	0.65586500	-1.35711800
C	1.44536900	1.32384000	0.07487600
H	1.17983300	1.12839800	1.12554800
C	-1.20229900	-0.91570600	-1.62886600
H	-1.93062700	-0.11007300	-1.75142000
H	-0.78749600	-1.16432800	-2.61308900
O	-1.93943100	-2.02425100	-1.10573400
O	-0.84811700	1.84469300	-0.36437300
H	-1.32284700	-2.75308200	-0.92197900
O	1.84123800	2.68364500	-0.06374200
H	1.02293100	3.20684900	0.01420000
O	3.74104100	0.62979500	0.53380600
H	4.07532900	1.53140800	0.39521700
O	-3.38108500	-0.76294200	0.97334800
H	-2.98870800	-1.36494700	0.29831100
H	-4.30583200	-0.63551000	0.70400700
C	1.62074900	-2.72461000	1.27281200
H	0.63598100	-2.94877500	0.84764400
H	2.37555800	-3.36766700	0.80375400
H	1.60178500	-2.90561100	2.34821700



INT_{1-3}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.9916070000002 A.U.

Thermal correction to Gibbs Free Energy = 0.251602 A.U.

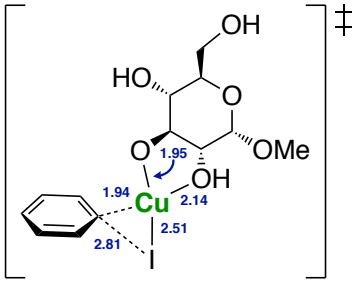
Sum of electronic and thermal Free Energies = -1165.740005 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.23919559 A.U.

O	2.89196300	0.94777200	1.93310700
H	3.86232400	1.46551100	3.63757200
C	3.84824400	1.77133000	2.59077600
H	3.55734500	2.82640400	2.51798800
H	4.84542600	1.63713100	2.15735500
C	2.64327100	1.33937300	0.60895600
H	2.35465000	2.39753200	0.58026700
O	3.79784100	1.24684600	-0.19764700
C	1.53569300	0.44482800	0.05634700
C	4.33457800	-0.07784700	-0.29339500
H	1.23605300	0.84525200	-0.91956000
C	1.99298800	-1.01185600	-0.13197400
O	0.38120000	0.52990600	0.88196000
H	4.58713000	-0.44334200	0.71261500
C	3.30254400	-1.01273300	-0.92798200
C	5.60484300	0.05900800	-1.10976700
H	2.23527100	-1.41144900	0.87466600
O	1.02244800	-1.78961600	-0.76146800
H	3.09044800	-0.67707100	-1.95431000
O	3.79299000	-2.35004800	-0.94543900
H	6.08580300	-0.91505700	-1.22522700
H	5.35928200	0.45440700	-2.10487400
O	6.54671600	0.90227300	-0.45804700
H	4.37981000	-2.46411900	-1.70909400
H	6.11464700	1.75950700	-0.30436400
H	0.61673500	0.18203900	1.76022500
Cu	-0.81005300	-1.48826900	-0.13620500
C	-3.30704900	0.88633500	-0.28765400
I	-3.34238000	-1.11816200	0.44084900
C	-4.31905800	1.76004200	0.09731700

C	-2.27681400	1.28453100	-1.13525300
C	-4.29121000	3.07188100	-0.38083700
H	-5.11612900	1.43242400	0.75685900
C	-2.26174200	2.60030200	-1.60147800
H	-1.49548600	0.58649100	-1.42659000
C	-3.26554800	3.49348300	-1.22658500
H	-5.07665100	3.76122900	-0.08581200
H	-1.46022700	2.92105900	-2.26042000
H	-3.24847700	4.51527300	-1.59290100



TS_{OA-3}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.960694 A.U.

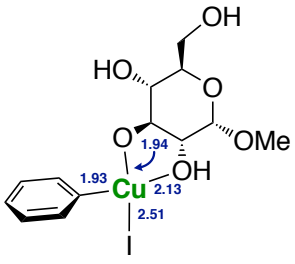
Thermal correction to Gibbs Free Energy = 0.255587 A.U.

Sum of electronic and thermal Free Energies = -1165.705107 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1166.20819504 A.U.

O	-3.02259000	-1.81390600	0.82816400
H	-4.00040900	-2.97327500	2.17615200
C	-4.18059500	-2.56416700	1.18154900
H	-4.33595800	-3.38173500	0.46748600
H	-5.06790500	-1.92250500	1.20374600
C	-3.05070600	-1.34912800	-0.49295900
H	-3.24115200	-2.18105600	-1.18140000
O	-4.09474400	-0.42758200	-0.72247200
C	-1.71876900	-0.66977800	-0.77427300
C	-4.02144400	0.76921500	0.06420800
H	-1.66317600	-0.44897000	-1.84478500
C	-1.53170100	0.62689400	0.01248800
O	-0.61341800	-1.53776000	-0.49859400
H	-4.03156900	0.50443500	1.13147200
C	-2.72927800	1.53670600	-0.24839800
C	-5.27789400	1.54772200	-0.27101600
H	-1.55493400	0.37489200	1.09084900
O	-0.30777600	1.21120900	-0.33453900
H	-2.72890700	1.84879100	-1.30286800
O	-2.60757200	2.67000600	0.60116500
H	-5.29697500	2.48616100	0.28772200
H	-5.29253600	1.77339200	-1.34586800
O	-6.44546600	0.82751900	0.10330800
H	-3.10828600	3.40954300	0.22268600
H	-6.42218300	-0.02983500	-0.35430400
H	-0.73674500	-1.91541300	0.39336200
Cu	1.04405300	-0.19937300	-0.28628800
C	2.51045800	1.03196100	0.03576800
I	2.99909700	-1.73166300	0.04645300
C	2.61198600	1.54879800	1.31753000
C	3.02690600	1.64783300	-1.09206900
C	3.25937300	2.77938200	1.46573000
H	2.20246900	1.02663200	2.17615300
C	3.66905200	2.87944200	-0.91626900
H	2.93834300	1.20070000	-2.07693800
C	3.78636100	3.44094700	0.35504300
H	3.34940700	3.21361500	2.45730000
H	4.07941600	3.39021000	-1.78263900
H	4.29150500	4.39351700	0.48198900



INT_{2-3}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.96074 A.U.

Thermal correction to Gibbs Free Energy =

0.254389 A.U.

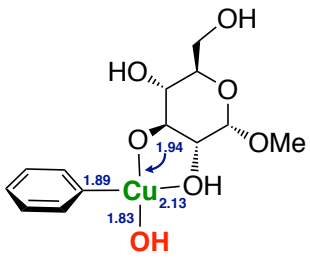
Sum of electronic and thermal Free Energies =

-1165.706351 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.20795173 A.U.

O	-2.99501600	-1.79718100	0.86546400
H	-3.96268700	-2.92042700	2.25065500
C	-4.15165000	-2.53532500	1.24814700
H	-4.31651400	-3.36947400	0.55582700
H	-5.03675300	-1.89042800	1.26355500
C	-3.03518700	-1.36220700	-0.46523300
H	-3.23029000	-2.20885600	-1.13405900
O	-4.08130500	-0.44590200	-0.70685700
C	-1.70814000	-0.68475900	-0.77173100
C	-4.00676100	0.76687800	0.05467100
H	-1.66507500	-0.47758100	-1.84536000
C	-1.51899600	0.62020900	-0.00154000
O	-0.59295200	-1.54170000	-0.49673300
H	-4.01742200	0.52459900	1.12723300
C	-2.71440800	1.52923800	-0.27180100
C	-5.26146900	1.54064100	-0.29813000
H	-1.53590200	0.38390300	1.07975500
O	-0.29596300	1.20091100	-0.36283000
H	-2.71562600	1.82693300	-1.33029700
O	-2.58952900	2.67272200	0.56281700
H	-5.27751900	2.49173400	0.23888100
H	-5.27513700	1.74177000	-1.37784300
O	-6.43105800	0.83275900	0.09236200
H	-3.08241700	3.41090200	0.17166900
H	-6.41353600	-0.03266900	-0.34996800
H	-0.70648800	-1.91655800	0.39795500
Cu	1.04629700	-0.19591000	-0.29656900
C	2.43754700	1.09950400	0.03832400
I	2.98436000	-1.75771500	0.03230100
C	2.55602300	1.58719500	1.32858100
C	2.97512500	1.71364400	-1.07905900
C	3.25361700	2.78780200	1.49876000
H	2.12442000	1.06708600	2.17768400
C	3.66785100	2.91453200	-0.88136400
H	2.86759800	1.28872300	-2.07197700
C	3.80748500	3.44722300	0.40000900
H	3.36076400	3.20020500	2.49793400
H	4.09910800	3.42361400	-1.73855500
H	4.35015900	4.37647900	0.54385400



INT_{3-3}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.342511 A.U.

Thermal correction to Gibbs Free Energy =

0.269814 A.U.

Sum of electronic and thermal Free Energies =

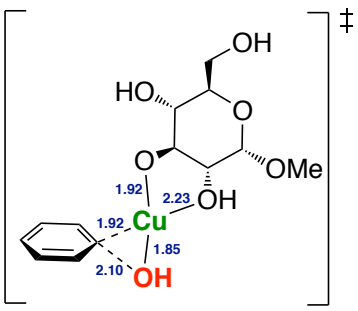
-1230.072697 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.61328015

O	-2.77327000	-1.67109000	0.85620000
H	-4.04449000	-2.53653600	2.17944300
C	-4.09175500	-2.10320800	1.17998600
H	-4.43102900	-2.86012800	0.46301100
H	-4.78865300	-1.25829500	1.17916200
C	-2.64980000	-1.22422500	-0.46483800
H	-3.00335700	-1.99381300	-1.16120400
O	-3.44072500	-0.08545700	-0.73102200
C	-1.19139000	-0.86371000	-0.70080700
C	-3.12786200	1.06602800	0.06441800
H	-1.06145600	-0.63081900	-1.76195700
C	-0.74663300	0.33296100	0.13516100
O	-0.30437200	-1.95708200	-0.43617700
H	-3.26510700	0.82318500	1.12795400

C	-1.67414300	1.50581300	-0.16437800
C	-4.13460900	2.12195000	-0.34651800
H	-0.86942800	0.07791900	1.20333900
O	0.59470000	0.63386300	-0.15211600
H	-1.54083300	1.81190900	-1.21202900
O	-1.33399900	2.57367500	0.70801400
H	-3.96084900	3.04336000	0.21394300
H	-4.02425500	2.33229600	-1.41898400
O	-5.46320400	1.71031300	-0.05317500
H	-1.62444200	3.41143100	0.31390400
H	-5.62005700	0.87008400	-0.51621700
H	-0.51297100	-2.31971200	0.44659300
Cu	1.57193800	-0.96990200	-0.19815800
C	3.14751000	0.04617200	0.02326200
C	3.63557400	0.22860500	1.30505800
C	3.71422000	0.59642300	-1.11268300
C	4.77441800	1.02948700	1.45077200
H	3.15918400	-0.22657500	2.16783700
C	4.85399300	1.39116600	-0.94165500
H	3.29719600	0.42304800	-2.10002600
C	5.37900600	1.60651700	0.33313700
H	5.18277600	1.19709600	2.44326300
H	5.32549300	1.83832700	-1.81203300
H	6.26294800	2.22486700	0.45592900
O	2.60262700	-2.48039900	-0.29591200
H	3.54790600	-2.29492900	-0.19734200



TS_{RE-3}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.334735 A.U.

Thermal correction to Gibbs Free Energy = 0.270857 A.U.

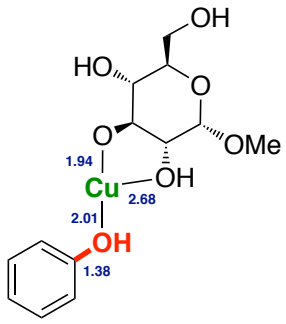
Sum of electronic and thermal Free Energies = -1230.063878 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.60582078

O	-2.80075700	-1.66788800	0.90637400
H	-4.05041100	-2.52873500	2.25289900
C	-4.10912800	-2.11697600	1.24483000
H	-4.43750200	-2.89509700	0.54542300
H	-4.82242900	-1.28585900	1.22957200
C	-2.68889100	-1.25138400	-0.42688100
H	-3.03340000	-2.04583700	-1.10002800
O	-3.50574800	-0.13686000	-0.71519100
C	-1.23381800	-0.88261600	-0.68011700
C	-3.20573500	1.03707600	0.05134000
H	-1.11347500	-0.68510000	-1.75026500
C	-0.79769600	0.35594500	0.10573100
O	-0.35423000	-1.96819600	-0.38678100
H	-3.32362300	0.81366600	1.12158700
C	-1.76481300	1.49478000	-0.20963300
C	-4.24147000	2.06258000	-0.36506600
H	-0.90675300	0.12989600	1.18414600
O	0.52817500	0.67883900	-0.20275800
H	-1.65408000	1.77824500	-1.26677300
O	-1.43320800	2.59362000	0.62983500
H	-4.08322200	2.99795400	0.17653600
H	-4.15059200	2.25607900	-1.44253500
O	-5.55663300	1.62609200	-0.04632500
H	-1.77680900	3.41113800	0.23641600
H	-5.69695100	0.77050700	-0.48593600
H	-0.52359700	-2.25735100	0.52951800
Cu	1.60498000	-0.90775400	-0.25586800
C	3.34676500	-0.14978600	0.00500600
C	3.71989200	0.08835900	1.31734700
C	3.92352300	0.46143400	-1.09511000
C	4.73033200	1.02951600	1.53271800
H	3.24717200	-0.43102600	2.14473500

C	4.93737500	1.39447100	-0.84919400
H	3.60175700	0.23392100	-2.10662900
C	5.33913500	1.67845500	0.45599800
H	5.04046800	1.24793600	2.55050700
H	5.40705500	1.89670500	-1.69002300
H	6.12762900	2.40265700	0.63492000
O	2.94441500	-2.18468000	-0.27120400
H	3.29540800	-2.22336300	-1.17731900



INT_{4-3}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.426137 A.U.

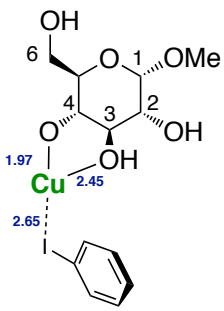
Thermal correction to Gibbs Free Energy = 0.271078 A.U.

Sum of electronic and thermal Free Energies = -1230.155059 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.69719468

O	-2.71767000	-1.82612400	0.99423300
H	-3.55170700	-2.88349900	2.51149100
C	-3.84097300	-2.52077800	1.52439200
H	-4.10289100	-3.36950900	0.88089300
H	-4.70511100	-1.85399900	1.61873900
C	-2.88933600	-1.43925500	-0.34381600
H	-3.15343200	-2.31233700	-0.95365500
O	-3.96273400	-0.53689200	-0.50130000
C	-1.58311800	-0.80448600	-0.81661000
C	-3.80350000	0.68653800	0.22594200
H	-1.66335400	-0.63822200	-1.89666100
C	-1.30782400	0.54642400	-0.13504600
O	-0.50890700	-1.71854400	-0.64032500
H	-3.69550500	0.46383500	1.29747400
C	-2.55646600	1.42562600	-0.26532100
C	-5.08731900	1.46096400	0.00397800
H	-1.17285100	0.34752400	0.94792000
O	-0.19214300	1.18684900	-0.67472200
H	-2.68687400	1.69737500	-1.32358300
O	-2.33998600	2.59741900	0.51517700
H	-5.04502600	2.41630300	0.53194400
H	-5.21720400	1.65403700	-1.06966700
O	-6.21071700	0.75958500	0.52269300
H	-2.89245000	3.31703800	0.17210000
H	-6.23702200	-0.11166100	0.09244200
H	-0.43984400	-1.91514400	0.31063100
Cu	1.43070100	0.12687900	-0.67995500
C	4.37039200	-0.33923100	-0.11749200
C	4.33274400	0.92709600	0.45877600
C	5.53200800	-1.10598400	-0.11215500
C	5.48755400	1.43537500	1.05016900
H	3.40326700	1.49227000	0.43414500
C	6.67971800	-0.58436900	0.48495000
H	5.53436200	-2.09256200	-0.56800200
C	6.66445300	0.68403500	1.06638600
H	5.46431500	2.42339500	1.50000300
H	7.58905900	-1.17786600	0.49247200
H	7.56148700	1.08398400	1.52830500
O	3.20931400	-0.80550700	-0.70088900
H	3.31321000	-1.70647600	-1.05214000



INT_{1-4}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.991789 A.U.

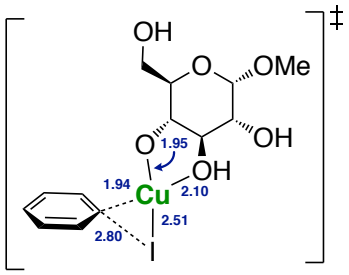
Thermal correction to Gibbs Free Energy = 0.251711 A.U.

Sum of electronic and thermal Free Energies = -1165.740078 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.23938465 A.U.

O	-4.45693100	0.90984200	-1.52205800
C	-4.05481200	1.46629600	-0.29677200
H	-4.66836500	2.34646000	-0.06805200
O	-4.24864600	0.58167700	0.78157400
C	-3.51196300	-0.64573100	0.68068900
H	-3.80594300	-1.17063600	-0.24216100
C	-1.99765200	-0.38096900	0.64274100
H	-1.73777500	0.15791400	1.57817100
C	-2.57945800	1.83672900	-0.42755500
H	-2.29325800	2.40251500	0.46481600
C	-1.71645500	0.58296700	-0.51587000
H	-1.92288700	0.05771200	-1.46069200
C	-3.91354200	-1.48453200	1.87614500
H	-3.30892200	-2.39622800	1.89843800
H	-3.73596800	-0.92045600	2.79734000
O	-5.30212300	-1.80494400	1.86635300
O	-1.28727300	-1.57430700	0.52040700
O	-0.33451700	0.93554200	-0.46743500
O	-2.36759600	2.70270900	-1.53217900
C	-5.84323900	0.59035200	-1.56281100
H	-6.07100900	-0.24901000	-0.89673200
H	-6.44389300	1.46089400	-1.27213200
H	-6.07370900	0.31205100	-2.59189500
H	-5.47573900	-2.37194600	1.09700200
H	-2.71448400	2.25953300	-2.32675900
H	-0.09547200	1.37027400	-1.30230700
Cu	0.59234300	-1.28453900	0.00311100
C	3.45386400	0.59271800	0.28990700
I	3.15633500	-1.28086800	-0.68385500
C	4.47867200	1.42944800	-0.14119200
C	2.61315300	0.94340800	1.34320300
C	4.66006100	2.65445700	0.50497300
H	5.12516700	1.14083500	-0.96363600
C	2.80636300	2.17232700	1.97628200
H	1.81842700	0.27357900	1.66248900
C	3.82718100	3.02705200	1.55978400
H	5.45640300	3.31556700	0.17627900
H	2.15433200	2.45585400	2.79712000
H	3.97306200	3.98142500	2.05637400



TS_{OA-4}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.962566 A.U.

Thermal correction to Gibbs Free Energy = 0.255847 A.U.

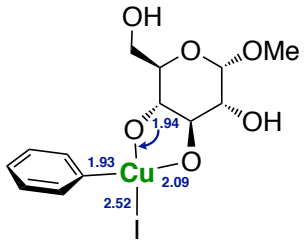
Sum of electronic and thermal Free Energies = -1165.706719 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.21023019 A.U.

O	-4.38708000	-0.77278700	1.20776500
C	-4.21299700	-0.87646600	-0.18079400
H	-5.10958400	-1.30871700	-0.64120900
O	-4.04800800	0.38342000	-0.79088200
C	-2.91249100	1.12883600	-0.32824200
H	-2.99398400	1.28490000	0.75854900
C	-1.62971900	0.34929400	-0.63786300
H	-1.60458000	0.18855100	-1.73369200
C	-2.98837600	-1.76677400	-0.41673700
H	-2.92531800	-1.98423600	-1.48728200
C	-1.73747500	-1.02282000	0.02028600
H	-1.73470600	-0.89734400	1.11165500

C	-2.95250200	2.46878000	-1.03254600
H	-2.04514300	3.03106200	-0.78878900
H	-2.99053200	2.31298800	-2.11523000
O	-4.11558800	3.21678400	-0.69383200
O	-0.48086700	1.00979100	-0.19221100
O	-0.54258700	-1.72491400	-0.36339000
O	-3.12739200	-3.01507800	0.23949600
C	-5.55165000	-0.03906700	1.57249900
H	-5.44086500	1.02092900	1.31953300
H	-6.43333600	-0.44622700	1.06311500
H	-5.66766900	-0.14643600	2.65154400
H	-4.06233300	3.45289200	0.24687700
H	-3.30051100	-2.84100500	1.18193400
H	-0.39994800	-2.48375100	0.22845000
Cu	0.97398200	-0.28844100	-0.15534500
C	2.30520900	1.08233200	0.18143400
I	3.12212800	-1.58830200	-0.07894400
C	2.37203700	1.51495900	1.49575100
C	2.74115100	1.82636400	-0.90292900
C	2.89552000	2.79214400	1.72749300
H	2.03248700	0.89388000	2.31853200
C	3.26077600	3.09893100	-0.64428300
H	2.68359900	1.44212900	-1.91616600
C	3.33916400	3.57887900	0.66399700
H	2.95681800	3.16189700	2.74699900
H	3.60715200	3.70785600	-1.47446000
H	3.75049100	4.56534500	0.85470000



INT_{2-4}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.9625839999999 A.U.

Thermal correction to Gibbs Free Energy = 0.254485 A.U.

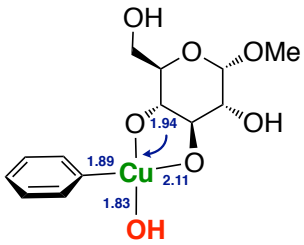
Sum of electronic and thermal Free Energies = -1165.708099 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.21000127 A.U.

O	-4.39846600	-0.77829400	1.17974700
C	-4.20593600	-0.86306100	-0.20751800
H	-5.09735600	-1.28562000	-0.68650500
O	-4.02882200	0.40505900	-0.79720300
C	-2.89830600	1.14033800	-0.30814900
H	-2.99424200	1.28171600	0.77936400
C	-1.61585100	0.35837400	-0.61111400
H	-1.57465900	0.21306200	-1.70810700
C	-2.98092900	-1.75501400	-0.43887400
H	-2.90264800	-1.95666800	-1.51147700
C	-1.73515500	-1.02071200	0.02794800
H	-1.74737900	-0.91085300	1.12071300
C	-2.92215500	2.49009500	-0.99425800
H	-2.01425200	3.04335300	-0.73246100
H	-2.94877500	2.34947700	-2.07931800
O	-4.08446100	3.23982700	-0.65765100
O	-0.47122700	1.01053500	-0.13997500
O	-0.53310600	-1.71586500	-0.34944600
O	-3.13440500	-3.01197600	0.19666300
C	-5.56412700	-0.04343400	1.53917900
H	-5.44378500	1.01954100	1.30376500
H	-6.44082300	-0.43771100	1.01143100
H	-5.69582000	-0.16631500	2.61474900
H	-4.03722600	3.46731800	0.28550400
H	-3.32246500	-2.85146700	1.13866300
H	-0.39231900	-2.47982700	0.23653200
Cu	0.97068700	-0.28202800	-0.13077800
C	2.25195800	1.12849400	0.16967400
I	3.09923400	-1.62420600	-0.07301500
C	2.35834800	1.56635800	1.47872700
C	2.70271700	1.84179400	-0.92781200
C	2.94769000	2.81803300	1.69220300

H	2.00203900	0.96843900	2.31165600
C	3.28798800	3.08973500	-0.68762700
H	2.61019200	1.45354000	-1.93700200
C	3.41154300	3.57434000	0.61535600
H	3.04395200	3.19143200	2.70769700
H	3.64987800	3.67513800	-1.52804500
H	3.87357000	4.54085500	0.79167400



INT_{3-4}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.3441930000001 A.U.

Thermal correction to Gibbs Free Energy =

0.270087 A.U.

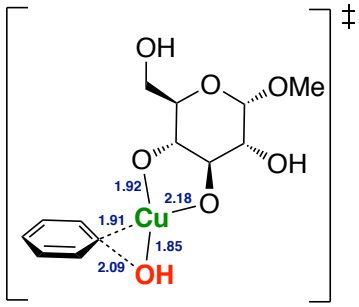
Sum of electronic and thermal Free Energies =

-1230.074106 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1230.61516798 A.U.

O	-3.86454400	-0.19478700	1.10845600
C	-3.66700300	-0.23984700	-0.27953700
H	-4.62701100	-0.36475600	-0.79448000
O	-3.12743600	0.96324400	-0.78066200
C	-1.84683000	1.31962200	-0.24275400
H	-1.91973000	1.40826400	0.85199900
C	-0.83463200	0.22509100	-0.59738600
H	-0.81190700	0.13429400	-1.69899400
C	-2.73244700	-1.42258200	-0.55944100
H	-2.67974600	-1.57071500	-1.64227500
C	-1.34864600	-1.08944200	-0.02748900
H	-1.36942800	-1.02337800	1.06852400
C	-1.47794500	2.66509100	-0.83083500
H	-0.45855800	2.92379500	-0.52561000
H	-1.51682200	2.61328700	-1.92319800
O	-2.39398900	3.68360900	-0.44440000
O	0.44096000	0.50706400	-0.08381300
O	-0.37360300	-2.07171800	-0.40788700
O	-3.24545000	-2.62362000	-0.01278900
C	-4.80200100	0.79797500	1.51218800
H	-4.39958400	1.80381400	1.35079500
H	-5.73991500	0.68449400	0.95544300
H	-4.98486800	0.64455200	2.57632600
H	-2.32782800	3.80485300	0.51729800
H	-3.40494000	-2.47708000	0.93650600
H	-0.46002200	-2.86123100	0.15442500
Cu	1.45695100	-1.07808600	-0.09211000
C	3.00936300	-0.02669400	0.11836000
C	3.29830300	0.43569300	1.39017400
C	3.76033600	0.26816500	-1.00611700
C	4.42236000	1.25677000	1.53690000
H	2.68108200	0.17680900	2.24511100
C	4.87718400	1.09494300	-0.83532000
H	3.49927700	-0.12171100	-1.98510700
C	5.20536100	1.58491500	0.42929000
H	4.67883800	1.63623900	2.52181500
H	5.48657500	1.34970200	-1.69764000
H	6.07495600	2.22325200	0.55235000
O	2.49085600	-2.58329700	0.04825000
H	3.43329900	-2.38212900	0.14246900



TS_{RE-4}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.335871 A.U.

Thermal correction to Gibbs Free Energy =

0.270204 A.U.

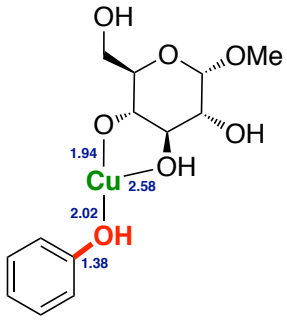
Sum of electronic and thermal Free Energies =

-1230.065667 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.60717253 A.U.

O	-3.88018700	-0.25680900	1.15349300
C	-3.71898900	-0.28624300	-0.24038400
H	-4.69086200	-0.42772400	-0.72861700
O	-3.21960100	0.93177300	-0.74499100
C	-1.92957400	1.30579200	-0.23964400
H	-1.97607900	1.38586300	0.85768400
C	-0.89503300	0.24167800	-0.62642100
H	-0.90358100	0.16113100	-1.73112900
C	-2.76666900	-1.44315500	-0.55638100
H	-2.74354500	-1.58139200	-1.64176200
C	-1.37112900	-1.09451100	-0.06308700
H	-1.36647300	-1.03685900	1.03456800
C	-1.60613700	2.66436700	-0.82415400
H	-0.58585500	2.94382800	-0.54162900
H	-1.67063300	2.62133800	-1.91584000
O	-2.53433300	3.66100300	-0.40793100
O	0.38233600	0.54960800	-0.14752800
O	-0.40684400	-2.07012400	-0.47432500
O	-3.24022800	-2.66071500	-0.00721900
C	-4.82281100	0.71628900	1.59044600
H	-4.44020400	1.73026200	1.43140100
H	-5.77190000	0.59467200	1.05457300
H	-4.97849500	0.54829200	2.65677100
H	-2.45496400	3.76836200	0.55436300
H	-3.36975700	-2.52702400	0.94852600
H	-0.50161200	-2.86833500	0.07213500
Cu	1.48188700	-1.02722200	-0.13042800
C	3.19583200	-0.21343300	0.12824600
C	3.50014900	0.16774200	1.42489200
C	3.82247500	0.28849100	-1.00000500
C	4.49099200	1.13908500	1.59088500
H	2.99302100	-0.27232900	2.27770100
C	4.81325600	1.25715700	-0.80315600
H	3.55445500	-0.04720600	-1.99696000
C	5.14695300	1.68114900	0.48337800
H	4.74961200	1.46405600	2.59456800
H	5.31908100	1.67741400	-1.66768100
H	5.91978100	2.43028600	0.62401000
O	2.84359700	-2.26781900	0.06892200
H	3.22946600	-2.41698300	-0.81134900



INT$_{4\text{-}4}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.426389 A.U.

Thermal correction to Gibbs Free Energy =

0.269669 A.U.

Sum of electronic and thermal Free Energies =

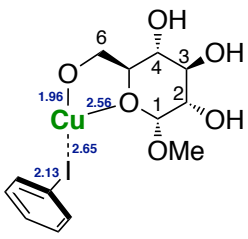
-1230.15672 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.69738294 A.U.

O	-4.07490200	-0.70969800	1.38748000
C	-4.07134800	-0.77730500	-0.01508000
H	-5.03617800	-1.15720400	-0.37343300
O	-3.91943000	0.48977300	-0.61098300
C	-2.70303000	1.16361000	-0.25756800
H	-2.66824200	1.29811200	0.83503500
C	-1.46794100	0.36002200	-0.69865000
H	-1.52263100	0.25486000	-1.80213100
C	-2.92444100	-1.69553300	-0.42738700
H	-2.99804900	-1.86033800	-1.50708900
C	-1.57733100	-1.05221800	-0.11467900
H	-1.44922400	-0.98425600	0.97694400

C	-2.76015400	2.52250900	-0.92454000
H	-1.81234700	3.04556200	-0.76535300
H	-2.91640700	2.39558900	-2.00063400
O	-3.85230100	3.30821600	-0.45471200
O	-0.30123900	1.01168700	-0.29887500
O	-0.52327100	-1.84011200	-0.66381100
O	-3.04480600	-2.97447200	0.17703000
C	-5.14701700	0.06826300	1.90788100
H	-5.01052100	1.12958600	1.67316800
H	-6.10354500	-0.27644100	1.49641600
H	-5.14158400	-0.06946700	2.98980500
H	-3.70028700	3.51047000	0.48297800
H	-3.06688400	-2.84852900	1.14224100
H	-0.53065800	-2.70507300	-0.22156400
Cu	1.31660400	-0.06722800	-0.30642400
C	4.28622600	-0.37936200	0.01263300
C	4.20808200	0.73029600	0.84891500
C	5.50859900	-0.85179300	-0.45681800
C	5.38353700	1.37932700	1.22178400
H	3.23158200	1.07059800	1.18701000
C	6.67637500	-0.18940600	-0.07819500
H	5.53978000	-1.72091600	-1.10887000
C	6.62069500	0.92417600	0.76070700
H	5.32938900	2.24654500	1.87302200
H	7.63296900	-0.55068000	-0.44373800
H	7.53327000	1.43501000	1.05114100
O	3.10050500	-1.00815100	-0.32094600
H	3.23810700	-1.69728700	-0.99414600



INT_{1-6}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.992748 A.U.

Thermal correction to Gibbs Free Energy = 0.254733 A.U.

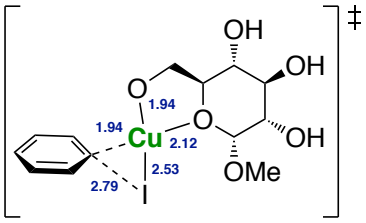
Sum of electronic and thermal Free Energies = -1165.738015 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.24082370 A.U.

Cu	1.00329200	1.09342700	-0.21034100
C	2.81736200	0.19827200	1.45326000
C	2.82067900	-0.08774600	0.07802800
C	3.42542300	0.79305500	-0.83397300
C	4.05952500	1.94372200	-0.35353400
C	4.08121200	2.21966500	1.01217300
C	3.45084400	1.35617800	1.90960700
H	2.34946800	-0.48603300	2.15414200
H	3.42978600	0.56412500	-1.89474100
H	4.53852300	2.61638200	-1.05829700
H	4.58150700	3.11071700	1.37810400
H	3.45508000	1.57201300	2.97362900
C	-2.17503200	1.29463200	-0.19668400
O	-1.45227300	0.06503300	-0.36386700
C	-1.94020600	-1.01762000	0.39770500
C	-3.37408900	-1.32679600	-0.01843200
H	-3.34958800	-1.61497900	-1.07846300
C	-3.62577100	1.08345800	-0.62934600
H	-3.65123200	0.85882200	-1.70654300
C	-4.24162600	-0.08650800	0.13317000
H	-4.31637800	0.17995000	1.19555900
I	2.00903300	-1.92956400	-0.62866700
C	-1.44570600	2.34521600	-1.02583000
H	-1.42649000	1.97441900	-2.06890800
H	-2.07040300	3.25282000	-1.02180400
O	-0.16281700	2.62833400	-0.54449200
O	-3.85115300	-2.40175800	0.77025700
H	-4.75277600	-2.60718100	0.47160400
O	-5.53321100	-0.41229300	-0.37057300
H	-6.19318100	0.15155400	0.06309300
O	-4.33630300	2.28604200	-0.36456000
H	-5.23326900	2.20053400	-0.72714000

H	-2.14917600	1.58872800	0.86332200
O	-1.92569500	-0.74836200	1.77338100
C	-0.61421000	-0.52696500	2.27983300
H	-0.70020100	-0.46782500	3.36599100
H	0.04584800	-1.35924600	2.00525600
H	-0.19821400	0.41359000	1.89572900
H	-1.27230500	-1.85821500	0.17170100



TS_{OA-6}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.9613080000001 A.U.

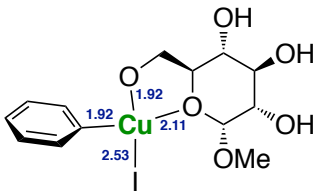
Thermal correction to Gibbs Free Energy = 0.257749 A.U.

Sum of electronic and thermal Free Energies = -1165.703559 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.20898919 A.U.

Cu	0.72301300	0.32524400	-0.20305400
C	3.01824500	0.73401600	1.36646300
C	2.62551800	0.62650300	0.04211900
C	3.33794900	1.15375400	-1.02266400
C	4.51313900	1.85222700	-0.72815000
C	4.94179500	1.99303400	0.59303200
C	4.19720900	1.43915800	1.63445500
H	2.44007900	0.28781500	2.16994500
H	3.00046600	1.03478100	-2.04713500
H	5.09116500	2.28176300	-1.54134800
H	5.85965000	2.53069700	0.81010700
H	4.52932100	1.54258300	2.66348300
C	-1.94876000	1.42138700	0.03095600
O	-1.38645200	0.12136800	-0.26301900
C	-2.07514500	-0.97511700	0.32919000
C	-3.49196000	-1.00726300	-0.23414400
H	-3.40799600	-1.16292800	-1.31848300
C	-3.36001300	1.47206700	-0.54137100
H	-3.30727900	1.37337000	-1.63566300
C	-4.19312200	0.32152900	0.01934500
H	-4.32307100	0.46713900	1.09980000
I	1.74725300	-1.96261200	-0.51411900
C	-0.98095700	2.42290600	-0.58101200
H	-1.03066500	2.31684800	-1.67971900
H	-1.33338000	3.43442100	-0.33159600
O	0.32185800	2.22132200	-0.09664600
O	-4.18316500	-2.08665500	0.36516400
H	-5.07755000	-2.10990100	-0.01522300
O	-5.46528200	0.24806500	-0.61189300
H	-6.06512500	0.87922100	-0.18281700
O	-3.91707600	2.72938100	-0.18905700
H	-4.75369100	2.84056400	-0.67015000
H	-1.97640700	1.55218800	1.12109300
O	-2.14709900	-0.85701800	1.71603700
C	-0.88253200	-0.94329000	2.36676900
H	-1.08428000	-0.94182000	3.43861500
H	-0.37068000	-1.87042500	2.08539100
H	-0.24990100	-0.08236900	2.11525000
H	-1.50292800	-1.86474000	0.04069600



INT_{2-6}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1165.961403 A.U.

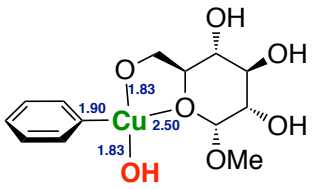
Thermal correction to Gibbs Free Energy = 0.257125 A.U.

Sum of electronic and thermal Free Energies = -1165.704278 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1166.20868312 A.U.

Cu	0.73308000	0.32797700	-0.20040500
C	3.00071000	0.81016300	1.37785700
C	2.60083300	0.71585100	0.05655600
C	3.34344100	1.17426300	-1.01739400
C	4.57185200	1.78142600	-0.73553200
C	5.01480300	1.90457800	0.58261000
C	4.23309700	1.42427600	1.63337000
H	2.39138900	0.42259100	2.18897400
H	2.99345500	1.06835800	-2.03917900
H	5.17916000	2.15314100	-1.55593400
H	5.97222000	2.37263700	0.79018900
H	4.57602100	1.51538600	2.66002200
C	-1.92229800	1.43172700	0.01422900
O	-1.36437700	0.12198900	-0.25066700
C	-2.06206000	-0.95746900	0.36646600
C	-3.47766300	-0.99235300	-0.20037600
H	-3.39155600	-1.17716300	-1.27993500
C	-3.32804800	1.47795600	-0.57036300
H	-3.26812000	1.35087800	-1.66129800
C	-4.17112300	0.34729800	0.01523400
H	-4.30504000	0.52168600	1.09096500
I	1.67945500	-1.99867900	-0.52604800
C	-0.94162800	2.41165900	-0.60770500
H	-0.97390400	2.28358500	-1.70397200
H	-1.28056100	3.43266300	-0.38230400
O	0.35284600	2.20884800	-0.09713400
O	-4.17851000	-2.05035400	0.42525600
H	-5.07263100	-2.07595500	0.04429700
O	-5.44046900	0.26563600	-0.62020000
H	-6.03832000	0.91143500	-0.21049900
O	-3.87799500	2.74761600	-0.25346900
H	-4.71125300	2.85300300	-0.74177600
H	-1.95726800	1.58341000	1.10119300
O	-2.13527600	-0.80481600	1.74913000
C	-0.87226200	-0.88549000	2.40414700
H	-1.07561200	-0.85193900	3.47513900
H	-0.36900700	-1.82487600	2.14932500
H	-0.23149400	-0.03782300	2.12963900
H	-1.49556400	-1.85702200	0.09952400



INT$_{3\text{-}6}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.339072 A.U.

Thermal correction to Gibbs Free Energy = 0.270529 A.U.

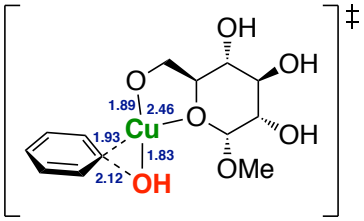
Sum of electronic and thermal Free Energies = -1230.068543 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.6099395 A.U.

Cu	1.39435900	1.02194200	-0.56975100
C	4.03611900	0.05305000	-0.38368600
C	2.76630400	-0.07374300	0.14856900
C	2.41999400	-0.94158900	1.16594500
C	3.43832300	-1.75232800	1.68356600
C	4.73558300	-1.66627100	1.17797200
C	5.03473900	-0.76860300	0.15205300
H	4.25447300	0.75113700	-1.18548800
H	1.40646800	-1.00059900	1.55142900
H	3.20585400	-2.44790600	2.48467300
H	5.51689500	-2.30094400	1.58469900
H	6.04455100	-0.70175700	-0.24230800
C	-1.19407600	-0.59464900	-0.90143300
O	-0.81973700	0.19567500	0.23519900
C	-1.86112900	0.97076500	0.79413900
C	-2.98059400	0.04665500	1.26455300
H	-2.56560300	-0.58863600	2.05799900
C	-2.26892700	-1.59141300	-0.48314200
H	-1.85358700	-2.27368600	0.27488900
C	-3.45093000	-0.84418400	0.11814700

H	-3.91544800	-0.22669800	-0.66187100
C	0.08867000	-1.24885400	-1.38986000
H	0.48137500	-1.89256300	-0.58346600
H	-0.14813300	-1.89604500	-2.24462200
O	1.03897800	-0.29615000	-1.79474000
O	-4.03382200	0.84437700	1.77602100
H	-4.63532200	0.26835100	2.27546400
O	-4.38275500	-1.81625700	0.57788800
H	-5.26839400	-1.41940000	0.59675900
O	-2.66282000	-2.32101700	-1.63427000
H	-3.41449700	-2.88447700	-1.38299600
H	-1.59009600	0.06405000	-1.68783000
O	-2.38920600	1.88184200	-0.12734700
C	-1.43180100	2.83546900	-0.57387900
H	-1.97931400	3.59143900	-1.13839700
H	-0.92945200	3.30247200	0.28140900
H	-0.68580900	2.36656300	-1.22818200
H	-1.40278000	1.50439300	1.63582500
O	1.79046200	2.41171400	0.55131200
H	2.71996100	2.40068200	0.82463200



TS_{RE-6}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.3322 A.U.

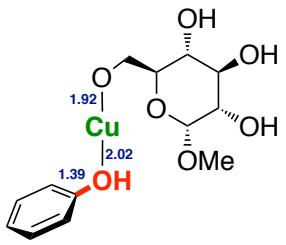
Thermal correction to Gibbs Free Energy = 0.270248 A.U.

Sum of electronic and thermal Free Energies = -1230.061952 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/ SMD(water)

Energy = -1230.60318610 A.U.

Cu	1.38261200	0.94747700	-0.64864800
C	4.09328800	0.15199400	-0.26237100
C	2.83202100	0.09838100	0.30282300
C	2.43629800	-0.80768800	1.27050100
C	3.38353400	-1.75223100	1.67883300
C	4.66865900	-1.74936500	1.13375200
C	5.02001100	-0.80348600	0.16966000
H	4.35354500	0.89239400	-1.01180900
H	1.43741900	-0.78729600	1.69537900
H	3.10802100	-2.48429400	2.43237000
H	5.39816900	-2.48202100	1.46420900
H	6.01884900	-0.79953100	-0.25695100
C	-1.27120600	-0.56966100	-0.96474700
O	-0.80793800	0.18009200	0.16793000
C	-1.78857100	0.97975100	0.79427400
C	-2.90636200	0.08278300	1.31739700
H	-2.46569000	-0.56949300	2.08253900
C	-2.33619300	-1.55193100	-0.49083900
H	-1.88642700	-2.25071600	0.23169000
C	-3.46198800	-0.78746300	0.19267900
H	-3.96081900	-0.15192500	-0.55113200
C	-0.03439600	-1.22180400	-1.56726900
H	0.40400200	-1.88805100	-0.79962600
H	-0.35413400	-1.85598200	-2.40655200
O	0.89074700	-0.26405800	-2.00950100
O	-3.90977300	0.90261000	1.89174500
H	-4.48059500	0.34488000	2.44514200
O	-4.38414600	-1.74621700	0.69827400
H	-5.25028800	-1.32221900	0.81052600
O	-2.82238900	-2.26225500	-1.61896600
H	-3.56460600	-2.81481500	-1.31973800
H	-1.70912900	0.11949200	-1.70145000
O	-2.33849000	1.92029300	-0.08493500
C	-1.37094400	2.83240200	-0.59357500
H	-1.92051400	3.61157400	-1.12356200
H	-0.79540800	3.27695100	0.22732800
H	-0.68682000	2.33208700	-1.29071100
H	-1.26688900	1.48831000	1.61474200
O	2.01387300	2.01492200	0.70308100
H	2.80559400	2.49064400	0.40068100



INT_{4-6}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.429038 A.U.

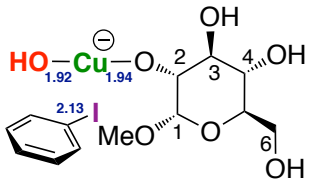
Thermal correction to Gibbs Free Energy = 0.273672 A.U.

Sum of electronic and thermal Free Energies = -1230.155366 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/ SMD(water)

Energy = -1230.70050210 A.U.

Cu	1.18841500	2.17575100	-0.01121300
C	4.07516000	-0.65243900	0.70315800
C	3.25994800	0.10733000	-0.12932200
C	2.58928200	-0.45867000	-1.20880600
C	2.73177200	-1.82349600	-1.45030800
C	3.53664200	-2.60912100	-0.62204800
C	4.20669800	-2.01824500	0.44992600
H	4.58581500	-0.18266100	1.53980200
H	1.95406200	0.16866300	-1.83000600
H	2.20504800	-2.27397500	-2.28651900
H	3.64077900	-3.67275300	-0.81164000
H	4.83574000	-2.62016600	1.09898300
C	-1.84277700	1.01276700	0.06486600
O	-0.81631800	0.17376200	-0.48739400
C	-0.83433300	-1.16702400	-0.04366400
C	-2.16030000	-1.81771700	-0.42347600
H	-2.22666000	-1.80850800	-1.51925600
C	-3.21281900	0.43845300	-0.29822800
H	-3.34156200	0.48353000	-1.39143200
C	-3.31873800	-1.01144800	0.14746000
H	-3.29033400	-1.05051400	1.24462300
C	-1.63664900	2.41425700	-0.50112100
H	-1.59916400	2.30806600	-1.60221800
H	-2.54768400	2.98892900	-0.26884300
O	-0.51120200	3.07540400	0.00299300
O	-2.15789400	-3.15243000	0.05560700
H	-2.88042000	-3.63479900	-0.37863400
O	-4.56991000	-1.50719300	-0.31682900
H	-4.80852900	-2.29411300	0.19938800
O	-4.20872300	1.22447700	0.34045000
H	-5.06439300	0.78700100	0.19181400
H	-1.73934500	1.04240600	1.15970900
O	-0.67038000	-1.26750900	1.34418500
C	0.64190100	-0.91708400	1.77169700
H	0.66757500	-1.04930300	2.85438200
H	1.38056700	-1.57781000	1.30013600
H	0.87033200	0.12903200	1.52540700
H	0.00151900	-1.65682900	-0.55848900
O	3.07658300	1.46325900	0.08662100
H	3.54066900	1.75346600	0.89207800



INT_{1-2_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.935354 A.U.

Thermal correction to Gibbs Free Energy = 0.261459 A.U.

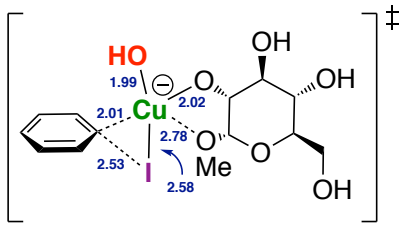
Sum of electronic and thermal Free Energies = -1241.673895 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.20863135 A.U.

C	2.52473900	-0.12574800	1.61611000
C	2.83535100	-0.29692300	0.26913700
C	3.45328400	0.71260600	-0.46634700
C	3.78615700	1.90868000	0.17257800
C	3.49947900	2.08944600	1.52592700

C	2.85858300	1.07787500	2.24117800
H	2.04139500	-0.91917000	2.17760300
H	3.68056300	0.57139600	-1.51824100
H	4.27205400	2.69774700	-0.39397300
H	3.76688500	3.01966700	2.01952600
H	2.62145300	1.21562700	3.29220200
O	-0.90619100	-0.52818000	1.02872200
I	2.39362800	-2.15244600	-0.67019800
Cu	0.36670100	2.20849900	-0.26415600
H	-0.20720000	-2.38616800	1.64263200
C	-0.80429400	-1.54433300	2.01726800
H	-1.79543200	-1.90688700	2.31348500
H	-0.31072000	-1.09894200	2.88263500
C	-1.39311700	-0.99898700	-0.20022700
H	-0.77582000	-1.83694300	-0.54724900
O	-2.69789700	-1.54037400	-0.07542100
C	-1.38697600	0.14943900	-1.21439800
C	-3.68621600	-0.61164100	0.36978300
H	-1.74392000	-0.30151700	-2.15960800
C	-2.43929200	1.18635600	-0.79924900
O	-0.13220600	0.72032100	-1.39904600
H	-3.39638400	-0.20623800	1.35202200
C	-3.80664500	0.55510200	-0.62122000
C	-4.97975200	-1.39077300	0.51525000
H	-2.13656000	1.63515600	0.16203400
O	-2.51971900	2.20840100	-1.78485900
H	-4.16852300	0.18064300	-1.58924600
O	-4.68996300	1.55338100	-0.12096600
H	-5.80059200	-0.70604600	0.75684000
H	-5.20977200	-1.89634000	-0.42761700
O	-4.87765000	-2.41056300	1.50196200
H	-1.59789200	2.48315900	-1.95070600
H	-5.60115700	1.32525100	-0.36286900
H	-4.75664500	-1.98773000	2.36815300
O	0.74052100	3.78542800	0.76310300
H	1.51871400	3.57660700	1.30067900



TS_{OA-2_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.8956369999999 A.U.

Thermal correction to Gibbs Free Energy = 0.263346 A.U.

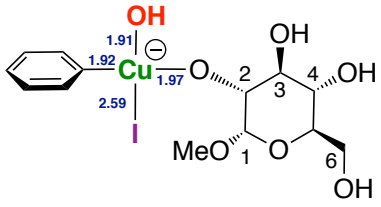
Sum of electronic and thermal Free Energies = -1241.632291 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.16926554 A.U.

C	2.38957400	0.56352100	1.80881100
C	2.66171000	0.48519900	0.44587400
C	3.74740100	1.13763200	-0.13417700
C	4.56039100	1.92755300	0.68158100
C	4.29771600	2.04047800	2.04846900
C	3.21507100	1.35946700	2.60722300
H	1.55046900	0.02844600	2.24206900
H	3.95240700	1.04446900	-1.19613200
H	5.40390400	2.45159700	0.24098500
H	4.93854600	2.65161400	2.67657400
H	3.00656400	1.44003600	3.67037300
O	-1.09264300	-0.62052700	0.78925400
I	2.18231300	-1.77523900	-0.58671800
Cu	0.99065400	0.51231900	-0.66662100
H	-0.66081200	-2.54698200	1.43759700
C	-1.00945000	-1.58383000	1.83138000
H	-1.98278900	-1.72124500	2.31635300
H	-0.29394400	-1.20751700	2.56398000
C	-1.87962600	-1.04944900	-0.29043200
H	-1.53842400	-2.03591700	-0.63222400
O	-3.23000000	-1.23967500	0.10180900
C	-1.80817000	-0.01528700	-1.41698700
C	-3.86582300	-0.06417700	0.60806400

H	-2.48382900	-0.40673200	-2.20165200
C	-2.43505700	1.28939500	-0.91004700
O	-0.53949300	0.19087900	-1.93950300
H	-3.32424400	0.29221700	1.49806500
C	-3.85934100	1.05708400	-0.44415300
C	-5.26954700	-0.47293000	1.01177100
H	-1.84928800	1.67245900	-0.06067800
O	-2.42230700	2.25073900	-1.95801100
H	-4.47986200	0.76103400	-1.30191600
O	-4.34787400	2.27226300	0.11500600
H	-5.84162800	0.41149900	1.31432300
H	-5.77260400	-0.94285400	0.16116700
O	-5.26234100	-1.43857700	2.05656600
H	-1.54905800	2.14357400	-2.38152800
H	-5.31575400	2.28567600	0.05360000
H	-4.88935000	-1.02370100	2.85181000
O	0.74213500	2.47365400	-0.41884700
H	1.48923800	2.77475300	0.12081800



INT$_{2\text{-}2_anion}$

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.904159 A.U.

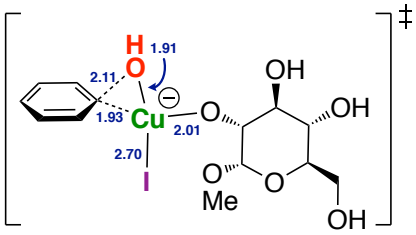
Thermal correction to Gibbs Free Energy = 0.265844 A.U.

Sum of electronic and thermal Free Energies = -1241.638315 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.1767782 A.U.

C	1.93174200	1.30487200	1.58888400
C	2.41629300	0.97682300	0.33086700
C	3.68588500	1.32958200	-0.10209100
C	4.50821700	2.04166200	0.77669700
C	4.05149200	2.38609100	2.05070600
C	2.76695100	2.02152200	2.45446900
H	0.93256600	1.01086800	1.90215600
H	4.03794900	1.05907300	-1.09324200
H	5.50788200	2.32515600	0.45924100
H	4.69697500	2.93760700	2.72762100
H	2.40650000	2.28763700	3.44423700
O	-1.27245900	-1.06727500	0.70947500
I	2.10295500	-1.97452400	-0.14586500
Cu	1.07272300	0.28993700	-0.85904100
H	-1.28676800	-3.07792100	1.22600000
C	-1.41992100	-2.08946600	1.68391000
H	-2.40539900	-2.03918100	2.16184700
H	-0.64415100	-1.92893800	2.43501400
C	-2.10962500	-1.22682400	-0.40306400
H	-2.02540500	-2.24965600	-0.79318000
O	-3.47472800	-1.07518300	-0.04740400
C	-1.71776100	-0.19434600	-1.46368500
C	-3.78253700	0.19329000	0.53107700
H	-2.44107700	-0.33294900	-2.28852000
C	-1.97246200	1.20601300	-0.88200000
O	-0.42425400	-0.38005100	-1.94652700
H	-3.20628500	0.32324400	1.46025100
C	-3.41806400	1.33943400	-0.42589000
C	-5.26269200	0.16937200	0.86367500
H	-1.32145000	1.35032900	-0.00300000
O	-1.68360700	2.21049600	-1.83752800
H	-4.07595900	1.30615900	-1.30658700
O	-3.55666200	2.59246900	0.23686800
H	-5.58070600	1.15641600	1.21803600
H	-5.83458600	-0.08156400	-0.03497500
O	-5.57608400	-0.82743100	1.82932000
H	-0.68647600	2.27078900	-1.83892400
H	-4.47763500	2.88903500	0.17134500
H	-5.15941000	-0.57892700	2.67075000
O	0.93554400	2.06643700	-1.56030600
H	1.35074800	2.71056200	-0.96756600



TS_{RE-2_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.8943290000002 A.U.

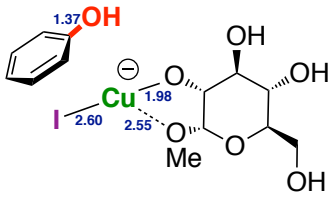
Thermal correction to Gibbs Free Energy = 0.26455 A.U.

Sum of electronic and thermal Free Energies = -1241.629779 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.16636544

C	1.72345000	1.59747900	1.49817000
C	2.21960000	1.41056700	0.21880800
C	3.53701800	1.62769400	-0.14642700
C	4.42458700	2.01276600	0.86307900
C	3.97863800	2.18197300	2.17553700
C	2.63404100	1.97442800	2.49005100
H	0.67174500	1.44305600	1.72583000
H	3.87490200	1.48202400	-1.16805400
H	5.46947000	2.17511900	0.61414900
H	4.67649600	2.48267300	2.95065900
H	2.28144700	2.11110900	3.50835800
O	-1.22078500	-1.08112400	0.68404500
I	2.20961200	-1.99196300	-0.16071300
Cu	1.04867300	0.33991000	-0.87929100
H	-1.18824300	-3.07953300	1.24531000
C	-1.32426800	-2.08313100	1.68477900
H	-2.29634000	-2.03705100	2.18997200
H	-0.52975200	-1.89369700	2.40906700
C	-2.08339100	-1.27979800	-0.40277400
H	-1.98898300	-2.30902800	-0.77319500
O	-3.44207700	-1.14771000	-0.01414300
C	-1.73658300	-0.26344800	-1.49526800
C	-3.76050000	0.12788000	0.54148000
H	-2.47518900	-0.43846400	-2.30060400
C	-2.01601000	1.14183300	-0.93733500
O	-0.44481400	-0.42108300	-1.98495100
H	-3.15420500	0.29683600	1.44505600
C	-3.45520300	1.25531800	-0.45817700
C	-5.22607300	0.07976800	0.92984500
H	-1.35373700	1.32348300	-0.07488600
O	-1.76554200	2.13338300	-1.92183900
H	-4.13166700	1.17520400	-1.32150600
O	-3.61514800	2.52347800	0.16902700
H	-5.54980000	1.06646700	1.27999100
H	-5.82695800	-0.19862800	0.05866900
O	-5.48164000	-0.90596900	1.92383600
H	-0.78966000	2.25617400	-1.91360700
H	-4.54703300	2.78792700	0.12070500
H	-5.02938300	-0.64077100	2.74164000
O	0.88048800	2.21669800	-1.19182000
H	1.59023700	2.47239100	-1.80413900



INT_{3-2_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.0056980000002 A.U.

Thermal correction to Gibbs Free Energy = 0.263779 A.U.

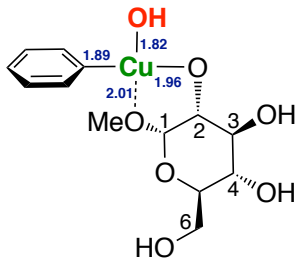
Sum of electronic and thermal Free Energies = -1241.741919 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.27693361

C	1.00212200	2.67776600	1.18140500
C	1.49199800	3.01472300	-0.08139800
C	2.79781400	2.68967500	-0.44964500
C	3.62274400	2.03718600	0.46669900

C	3.15019200	1.70212800	1.73575800
C	1.83598800	2.01997000	2.08439400
H	-0.02100700	2.93620100	1.44144200
H	3.15985200	2.95171400	-1.44067500
H	4.63937500	1.78477700	0.17901900
H	3.79505800	1.18800800	2.44162800
H	1.45346700	1.75709600	3.06646400
O	-1.13861900	-1.36515700	0.10505900
I	2.89293800	-1.94836700	0.08323200
Cu	1.04028400	-0.26953900	-0.64488600
H	-0.79590000	-3.32944900	-0.47129700
C	-1.13774900	-2.75562900	0.39929500
H	-2.13814300	-3.09451800	0.69197900
H	-0.44578200	-2.90498800	1.22975500
C	-1.92788600	-1.02436800	-1.00410400
H	-1.69501000	-1.68855800	-1.84656100
O	-3.30421500	-1.22819000	-0.73676200
C	-1.65994700	0.43998000	-1.36930900
C	-3.80171700	-0.46285900	0.36209500
H	-2.31466000	0.64373100	-2.23844700
C	-2.15916200	1.33066000	-0.22546100
O	-0.33350000	0.70089100	-1.68701400
H	-3.25329300	-0.73376600	1.27730000
C	-3.61287800	1.03949000	0.10552100
C	-5.26198400	-0.83981500	0.52672700
H	-1.54824500	1.13594800	0.67176700
O	-2.04835700	2.70105100	-0.58421300
H	-4.24098900	1.34625100	-0.74324600
O	-3.96055600	1.79017700	1.26479200
H	-5.72745100	-0.19965600	1.28479200
H	-5.78527400	-0.69560500	-0.42351800
O	-5.42260700	-2.21114200	0.86923500
H	-1.11891400	2.86431700	-0.84268000
H	-4.91515900	1.96108100	1.26158200
H	-5.06174700	-2.34759200	1.76068500
O	0.63714800	3.67510300	-0.93064300
H	1.04831900	3.78976500	-1.80507300



$INT_{3\text{-}2\_-I}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.332157 A.U.

Thermal correction to Gibbs Free Energy = 0.270863 A.U.

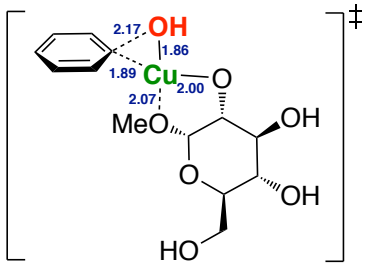
Sum of electronic and thermal Free Energies = -1230.061294 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.60334915 A.U.

C	3.69641800	0.46151300	-1.01997900
C	3.07847400	-0.06204000	0.10322900
C	3.48338100	0.19904600	1.40191600
C	4.57430400	1.05730200	1.58027300
C	5.21930700	1.61339000	0.47440000
C	4.78512900	1.31871900	-0.81863300
H	3.35397600	0.22086400	-2.02226000
H	2.97510900	-0.24102100	2.25514900
H	4.91467500	1.28564100	2.58619000
H	6.06628500	2.27672000	0.62123300
H	5.28999900	1.75032700	-1.67802600
O	2.54862400	-2.53279200	-0.24039500
H	3.49205100	-2.32525100	-0.16730900
Cu	1.48506500	-1.05893400	-0.11847100
O	-0.22698800	-1.97667200	-0.37936600
C	-1.23696200	-1.08123400	-0.01885600
C	-2.60917500	-1.46909300	-0.57398600
C	-0.89520300	0.31261300	-0.53426100
H	-1.32851500	-1.00732100	1.08246900
C	-3.64141700	-0.37535800	-0.27542900
H	-2.53478700	-1.57796000	-1.66121400
O	-3.05423700	-2.71971900	-0.07998400

C	-1.95976800	1.33016700	-0.14558100
H	-0.78278000	0.28755800	-1.62588100
O	0.39740300	0.60135700	0.05241400
O	-3.87879800	-0.38020800	1.10558800
H	-4.57651000	-0.55590700	-0.81944500
O	-3.19190900	0.88686300	-0.72755700
H	-3.16811300	-2.63681500	0.88298900
H	-2.05857800	1.37809300	0.94771200
C	-1.71871800	2.72043100	-0.69955200
H	0.83184400	1.33568400	-0.42012500
C	-4.91242400	0.51723600	1.49767500
H	-0.77690600	3.11786100	-0.31220000
H	-1.66010900	2.67251200	-1.79500700
O	-2.74004400	3.61896000	-0.29061400
H	-5.10309200	0.33673300	2.55611500
H	-5.82383900	0.32348300	0.91923800
H	-4.60228900	1.55786900	1.35360900
H	-3.58781600	3.27156800	-0.61556900



TS_{RE-2_-I}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.3269360000002 A.U.

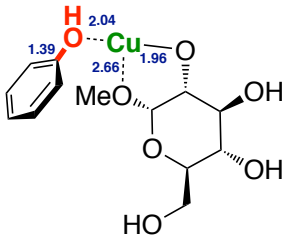
Thermal correction to Gibbs Free Energy = 0.269557 A.U.

Sum of electronic and thermal Free Energies = -1230.057379 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.59849575 A.U.

C	3.68442600	0.39228000	-1.06403500
C	3.20239400	-0.20909900	0.08598500
C	3.61637500	0.10311700	1.36931300
C	4.57348200	1.11593000	1.50137500
C	5.07960700	1.76196800	0.37309300
C	4.63558700	1.40414400	-0.90201700
H	3.34140400	0.09011300	-2.04889000
H	3.21288900	-0.40835200	2.23826200
H	4.91700600	1.39353900	2.49368600
H	5.82536700	2.54262500	0.48638300
H	5.03216900	1.90473700	-1.78050100
O	2.90713000	-2.30124400	-0.25591100
H	3.25237600	-2.52009900	0.62581600
Cu	1.51971700	-1.07655000	-0.06030900
O	-0.24152200	-1.98666000	-0.37159100
C	-1.25277800	-1.09302200	-0.02153200
C	-2.61231600	-1.46575900	-0.62090400
C	-0.90380700	0.32015300	-0.49033900
H	-1.37771300	-1.04235000	1.07925400
C	-3.66146900	-0.38868800	-0.32644000
H	-2.50874000	-1.54804400	-1.70837100
O	-3.06592500	-2.73155300	-0.17129600
C	-1.99322000	1.31564900	-0.10960800
H	-0.76565600	0.32040800	-1.58023000
O	0.35652300	0.62252800	0.13715700
O	-3.93925500	-0.42710200	1.04738400
H	-4.58034900	-0.56265900	-0.89971000
O	-3.20867000	0.88656300	-0.73558100
H	-3.18924400	-2.67771800	0.79255300
H	-2.12349500	1.33237000	0.98170800
C	-1.74728700	2.72395600	-0.61306000
H	0.79964700	1.35422600	-0.32827700
C	-4.98667500	0.45748400	1.43078300
H	-0.82131200	3.11682100	-0.18537600
H	-1.65582300	2.71123700	-1.70741000
O	-2.78894700	3.60171300	-0.20784000
H	-5.20922500	0.24908800	2.47788600
H	-5.87981000	0.27747600	0.82016500
H	-4.67552500	1.50235000	1.32372300
H	-3.62634700	3.24153400	-0.54595300



$INT_{4\text{-}2\_I}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.429318 A.U.

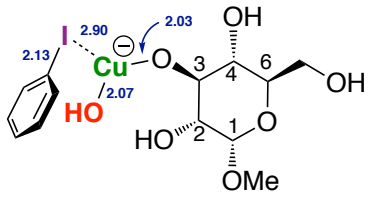
Thermal correction to Gibbs Free Energy = 0.272501 A.U.

Sum of electronic and thermal Free Energies = -1230.156817 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.70061611 A.U.

C	2.77352100	0.55073000	-1.23170000
C	3.39109900	-0.15456300	-0.20141300
C	3.99135400	0.49817100	0.87127000
C	3.95745000	1.89295900	0.91382100
C	3.33392600	2.61918900	-0.10139200
C	2.74705700	1.94338000	-1.17407300
H	2.31181000	0.00683800	-2.05103400
H	4.46138300	-0.07846700	1.66352200
H	4.41781200	2.40891300	1.75098800
H	3.30549800	3.70341100	-0.05823400
H	2.26124200	2.49973400	-1.97016000
O	3.34961500	-1.54234500	-0.27506700
H	3.90341800	-1.93625900	0.42323000
Cu	1.42090300	-2.15361700	-0.00952500
O	-0.47614200	-2.39999500	0.27247400
C	-1.28463200	-1.26652700	0.38750700
C	-2.43190000	-1.31842600	-0.63380800
C	-0.52497400	0.05508500	0.20171100
H	-1.74204300	-1.22229500	1.39681000
C	-3.28704500	-0.05321600	-0.62085900
H	-1.99923800	-1.41618400	-1.63585800
O	-3.25139100	-2.46337000	-0.44873400
C	-1.47284800	1.25602700	0.19720400
H	0.01567900	0.01229300	-0.75821400
O	0.40404500	0.18574200	1.27527300
O	-3.98153300	-0.01525300	0.59799100
H	-3.99859100	-0.04337500	-1.45617700
O	-2.47963700	1.08954300	-0.80651800
H	-3.66756200	-2.39255200	0.42809700
H	-1.95011600	1.34518100	1.18390200
C	-0.77329800	2.55776900	-0.14147100
H	1.17278000	0.69863600	0.97381300
C	-4.88647800	1.07887900	0.69266300
H	0.03146000	2.74928100	0.57290900
H	-0.34300300	2.48800400	-1.15022900
O	-1.66538100	3.66236300	-0.05586600
H	-5.46300200	0.93466600	1.60720200
H	-5.56171600	1.09123100	-0.17165800
H	-4.34636800	2.03053200	0.74715800
H	-2.41163000	3.48507500	-0.65301900



$INT_{1\text{-}3\_anion}$

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.927892 A.U.

Thermal correction to Gibbs Free Energy = 0.261276 A.U.

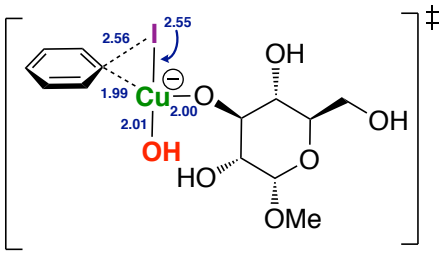
Sum of electronic and thermal Free Energies = -1241.666616 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.20089953 A.U.

C	-2.66786800	1.20821900	-1.20888400
C	-3.48880700	0.67207300	-0.21896800
C	-4.23039100	1.48452400	0.63339300
C	-4.13932700	2.87143400	0.48926500

C	-3.31830500	3.42740200	-0.49136400
C	-2.58610000	2.59525800	-1.33919200
H	-2.08544000	0.55922400	-1.85619000
H	-4.86215700	1.05276100	1.40278500
H	-4.71162300	3.51336100	1.15247400
H	-3.24764300	4.50591300	-0.59410400
H	-1.94088700	3.02062900	-2.10238300
I	-3.53154000	-1.44288300	0.03845600
O	-0.53213400	0.89936600	1.43688400
H	-1.36481500	1.38369100	1.32065700
Cu	-0.70971400	-0.88038100	0.40264000
O	0.92197700	-1.56472400	-0.59258300
C	1.95916100	-0.71197600	-0.20446800
C	1.97926300	0.63851400	-0.93958100
C	3.30887800	-1.39292000	-0.44955500
H	1.90987700	-0.50087800	0.88288300
C	3.19378500	1.46168500	-0.49454000
H	2.11116500	0.44134200	-2.01268400
O	0.79359700	1.39531300	-0.80094300
C	4.45613200	-0.50746600	0.01522700
H	3.42011600	-1.58325500	-1.53011800
O	3.34853800	-2.62497300	0.25878600
O	3.02070100	1.82275100	0.85029800
H	3.30559500	2.36433700	-1.10906300
O	4.39518300	0.73746800	-0.69070300
H	0.35573600	1.23782600	0.09867000
H	4.36846100	-0.32202900	1.09589400
C	5.82111100	-1.09088200	-0.28559400
H	2.44086200	-2.97818100	0.18881800
C	4.05315000	2.67102600	1.33681200
H	5.93490200	-2.05049600	0.22307500
H	5.92135200	-1.24876600	-1.36800600
O	6.86257000	-0.24735800	0.19236900
H	3.74959000	3.00204000	2.33096500
H	4.17461000	3.54155700	0.68010200
H	5.00534200	2.13328900	1.40673900
H	6.74073300	0.62740300	-0.21338900



TS_{OA-3_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.903933 A.U.

Thermal correction to Gibbs Free Energy = 0.265785 A.U.

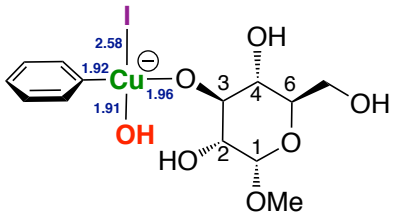
Sum of electronic and thermal Free Energies = -1241.638148 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.17737097 A.U.

C	-3.28881300	1.45930800	-0.89336800
C	-2.99792000	0.65269800	0.20326300
C	-3.50000600	0.91244200	1.47518100
C	-4.29339800	2.04811800	1.65436600
C	-4.58667400	2.88567700	0.57616700
C	-4.08425300	2.59051700	-0.69215700
H	-2.90138300	1.22300900	-1.87982000
H	-3.27373000	0.25746700	2.31081300
H	-4.68402800	2.27183000	2.64310200
H	-5.20979900	3.76247600	0.72317600
H	-4.31145400	3.23619600	-1.53578800
I	-2.87848100	-1.84360800	-0.36683400
O	-0.35267000	1.71322200	0.70951100
H	-1.06880200	2.36094200	0.61962300
Cu	-1.13609800	-0.05369200	0.16912700
O	0.57171300	-1.07207700	-0.03144800
C	1.75940700	-0.34685800	0.05652900
C	2.06155400	0.49668700	-1.19071100
C	2.92959600	-1.31061200	0.26943000
H	1.74547900	0.33081000	0.93077000
C	3.42863600	1.17553900	-1.05449200
H	2.13316400	-0.18054100	-2.05385500

O	1.06031500	1.45451700	-1.47315400
C	4.24491000	-0.55270300	0.38274200
H	2.98676800	-1.99528100	-0.59285700
O	2.72064400	-2.05861400	1.46048200
O	3.35891600	2.12614500	-0.02507300
H	3.72337000	1.66499300	-1.99185500
O	4.44108400	0.21508900	-0.81056200
H	0.53354900	1.63994700	-0.62934800
H	4.21315500	0.12081100	1.25158300
C	5.45084600	-1.46260200	0.49667300
H	1.76586800	-2.25862600	1.47035000
C	4.55474600	2.88269500	0.11698500
H	5.37172300	-2.07245200	1.39902200
H	5.49371400	-2.12599800	-0.37773700
O	6.65485200	-0.71303200	0.61161700
H	4.34529500	3.67515100	0.83680700
H	4.84396900	3.32579500	-0.84420900
H	5.37448400	2.25871900	0.49040100
H	6.71440200	-0.13443400	-0.16727600



$INT_{2\text{-}3\_anion}$

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.907201 A.U.

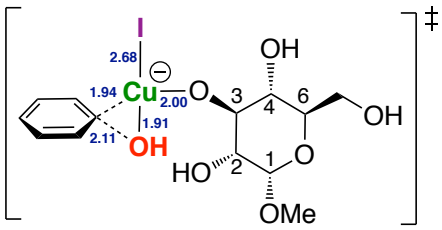
Thermal correction to Gibbs Free Energy = 0.266265 A.U.

Sum of electronic and thermal Free Energies = -1241.640936 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.1793275 A.U.

C	-3.27551400	1.65451600	-0.79616200
C	-2.87201200	0.94111700	0.32409600
C	-3.53299000	1.02124900	1.54141000
C	-4.65400200	1.85402400	1.63321200
C	-5.08607000	2.58127500	0.52305900
C	-4.39807900	2.48243300	-0.68732900
H	-2.73904500	1.57343500	-1.73756100
H	-3.19577800	0.45431500	2.40447600
H	-5.18544500	1.93003600	2.57781900
H	-5.95738500	3.22457700	0.60092100
H	-4.73021100	3.04704500	-1.55413300
I	-2.60446700	-1.98965300	-0.48929400
O	-0.39150400	1.67223000	0.79284800
H	-1.05843400	2.37486800	0.80539400
Cu	-1.18210600	0.02697700	0.24666800
O	0.50982900	-0.95453600	0.14503300
C	1.70726400	-0.23993900	0.15540300
C	1.99023400	0.48836600	-1.16499200
C	2.86204600	-1.20815200	0.42159300
H	1.72172700	0.50506600	0.97121800
C	3.37330600	1.14578300	-1.12961400
H	2.01543100	-0.25671000	-1.97200700
O	0.99775500	1.44470500	-1.49100200
C	4.19221500	-0.46725200	0.43481200
H	2.88402000	-1.96460300	-0.37970500
O	2.67579300	-1.84557300	1.67796700
O	3.35356200	2.18802800	-0.19168200
H	3.64989600	1.53937000	-2.11617600
O	4.37082200	0.18751200	-0.82646500
H	0.50607100	1.67923000	-0.65827600
H	4.19327800	0.28081200	1.24093200
C	5.38507100	-1.38611800	0.60067900
H	1.72355600	-2.04922200	1.72774500
C	4.56726100	2.92919600	-0.16028000
H	5.31047000	-1.92359200	1.54825200
H	5.40322300	-2.11488600	-0.22087600
O	6.60229500	-0.65056400	0.64117600
H	4.39369500	3.79563200	0.47928400
H	4.83608300	3.26442400	-1.16984600
H	5.38547800	2.32872000	0.25273400
H	6.66041700	-0.13266700	-0.17932400



TS_{RE-3_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.896634 A.U.

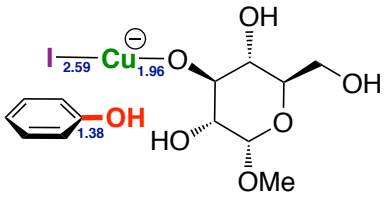
Thermal correction to Gibbs Free Energy = 0.266038 A.U.

Sum of electronic and thermal Free Energies = -1241.630596 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.16847365 A.U.

C	-3.27779600	1.87462900	-0.72277900
C	-2.57451700	1.35331700	0.35002300
C	-2.99866300	1.41763600	1.66588800
C	-4.24405500	2.00821000	1.90875700
C	-5.00244900	2.52359000	0.85668600
C	-4.51966200	2.45544000	-0.45274800
H	-2.88748100	1.82223000	-1.73460900
H	-2.39986100	1.01396200	2.47684400
H	-4.61322700	2.06272400	2.92896700
H	-5.96465800	2.98475500	1.05641400
H	-5.10528200	2.85876900	-1.27406100
I	-2.78512000	-2.03407200	-0.34033300
O	-0.54707500	1.88132400	0.13382100
H	-0.21532800	1.89409600	1.04978300
Cu	-1.16120100	0.08012000	-0.03601400
O	0.51117200	-0.99177000	-0.29165200
C	1.70913200	-0.30555900	-0.11569200
C	2.19547400	0.40556500	-1.38310800
C	2.80291600	-1.27550900	0.33560900
H	1.61662700	0.45941800	0.68136400
C	3.55646500	1.06432200	-1.13829600
H	2.34160000	-0.34365100	-2.17263900
O	1.26008700	1.35506800	-1.86243200
C	4.11946800	-0.54056200	0.54675900
H	2.94269400	-2.04067500	-0.44552200
O	2.41541500	-1.89847600	1.55276200
O	3.39039000	2.11172300	-0.22009300
H	3.98612800	1.45239400	-2.07071500
O	4.49135300	0.10591500	-0.67669900
H	0.66973600	1.61614900	-1.11543400
H	4.00197700	0.21296000	1.33921700
C	5.26949900	-1.46227100	0.89660000
H	1.46217700	-2.08093400	1.45243200
C	4.58700400	2.84603700	0.00849200
H	5.05339100	-1.98785900	1.82910900
H	5.40352800	-2.20141200	0.09528700
O	6.47210600	-0.73142700	1.10599200
H	4.31729600	3.71093000	0.61603600
H	5.01609900	3.18399700	-0.94303000
H	5.32526300	2.23959400	0.54495100
H	6.65104300	-0.22304100	0.29694500



INT_{3-3_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.0055220000002 A.U.

Thermal correction to Gibbs Free Energy = 0.265458 A.U.

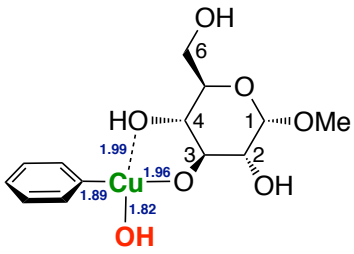
Sum of electronic and thermal Free Energies = -1241.740064 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.27662899 A.U.

C	-2.18052000	2.59231600	-0.37144700
C	-1.69923800	2.02859800	0.80972900
C	-2.55646800	1.75065600	1.87335200
C	-3.91522400	2.03658100	1.74424200

C	-4.41428900	2.59660600	0.56762600
C	-3.54063200	2.87260100	-0.48645300
H	-1.49006300	2.79380900	-1.18577900
H	-2.16032300	1.30755900	2.78369100
H	-4.58523300	1.81407100	2.56964800
H	-5.47355800	2.81327000	0.47113300
H	-3.91874500	3.30471800	-1.40839700
I	-3.42402300	-1.37025900	-0.54749900
O	-0.35085500	1.76749300	0.87769100
H	-0.15365900	1.21457600	1.65495600
Cu	-0.92395900	-1.31651500	0.14567900
O	0.91794900	-1.67956600	0.72432900
C	1.88273800	-0.72879000	0.39739200
C	1.82689100	-0.25325200	-1.06013500
C	3.27969000	-1.30091400	0.65118100
H	1.79254500	0.16660900	1.04470800
C	2.97205100	0.72173100	-1.35162700
H	1.95628600	-1.11907100	-1.72073300
O	0.58033100	0.32963100	-1.40106900
C	4.34842100	-0.26170700	0.34206600
H	3.43135800	-2.17486700	-0.00348100
O	3.39004200	-1.69688100	2.01202500
O	2.74289300	1.89795200	-0.62283500
H	3.03599000	0.95325900	-2.42231700
O	4.22005300	0.13771800	-1.02820000
H	0.30252200	0.91262700	-0.66456700
H	4.21534300	0.61417700	0.99378500
C	5.76056900	-0.78841500	0.49136000
H	2.52557400	-2.09272400	2.23108900
C	3.70387500	2.91351500	-0.88531400
H	5.92718700	-1.11745500	1.51915200
H	5.90672100	-1.64253000	-0.18350300
O	6.72106700	0.22698300	0.22481800
H	3.35551600	3.81654600	-0.38226000
H	3.77973300	3.09843200	-1.96400400
H	4.68841700	2.63433800	-0.49386800
H	6.55338100	0.56151900	-0.67237300



$INT_{3\text{-}3\_-I}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.332157 A.U.

Thermal correction to Gibbs Free Energy = 0.270863 A.U.

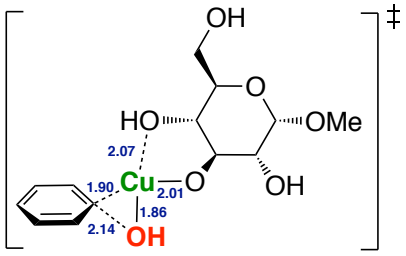
Sum of electronic and thermal Free Energies = -1230.061294 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.60334915 A.U.

C	3.69641800	0.46151300	-1.01997900
C	3.07847400	-0.06204000	0.10322900
C	3.48338100	0.19904600	1.40191600
C	4.57430400	1.05730200	1.58027300
C	5.21930700	1.61339000	0.47440000
C	4.78512900	1.31871900	-0.81863300
H	3.35397600	0.22086400	-2.02226000
H	2.97510900	-0.24102100	2.25514900
H	4.91467500	1.28564100	2.58619000
H	6.06628500	2.27672000	0.62123300
H	5.28999900	1.75032700	-1.67802600
O	2.54862400	-2.53279200	-0.24039500
H	3.49205100	-2.32525100	-0.16730900
Cu	1.48506500	-1.05893400	-0.11847100
O	-0.22698800	-1.97667200	-0.37936600
C	-1.23696200	-1.08123400	-0.01885600
C	-2.60917500	-1.46909300	-0.57398600
C	-0.89520300	0.31261300	-0.53426100
H	-1.32851500	-1.00732100	1.08246900
C	-3.64141700	-0.37535800	-0.27542900
H	-2.53478700	-1.57796000	-1.66121400
O	-3.05423700	-2.71971900	-0.07998400

C	-1.95976800	1.33016700	-0.14558100
H	-0.78278000	0.28755800	-1.62588100
O	0.39740300	0.60135700	0.05241400
O	-3.87879800	-0.38020800	1.10558800
H	-4.57651000	-0.55590700	-0.81944500
O	-3.19190900	0.88686300	-0.72755700
H	-3.16811300	-2.63681500	0.88298900
H	-2.05857800	1.37809300	0.94771200
C	-1.71871800	2.72043100	-0.69955200
H	0.83184400	1.33568400	-0.42012500
C	-4.91242400	0.51723600	1.49767500
H	-0.77690600	3.11786100	-0.31220000
H	-1.66010900	2.67251200	-1.79500700
O	-2.74004400	3.61896000	-0.29061400
H	-5.10309200	0.33673300	2.55611500
H	-5.82383900	0.32348300	0.91923800
H	-4.60228900	1.55786900	1.35360900
H	-3.58781600	3.27156800	-0.61556900



TS_{RE-3_I}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.3269360000002 A.U.

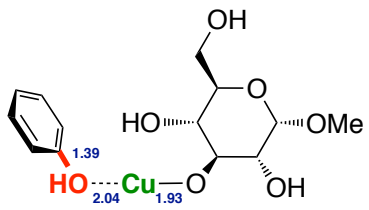
Thermal correction to Gibbs Free Energy = 0.269557 A.U.

Sum of electronic and thermal Free Energies = -1230.057379 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.59849575 A.U.

C	3.68442600	0.39228000	-1.06403500
C	3.20239400	-0.20909900	0.08598500
C	3.61637500	0.10311700	1.36931300
C	4.57348200	1.11593000	1.50137500
C	5.07960700	1.76196800	0.37309300
C	4.63558700	1.40414400	-0.90201700
H	3.34140400	0.09011300	-2.04889000
H	3.21288900	-0.40835200	2.23826200
H	4.91700600	1.39353900	2.49368600
H	5.82536700	2.54262500	0.48638300
H	5.03216900	1.90473700	-1.78050100
O	2.90713000	-2.30124400	-0.25591100
H	3.25237600	-2.52009900	0.62581600
Cu	1.51971700	-1.07655000	-0.06030900
O	-0.24152200	-1.98666000	-0.37159100
C	-1.25277800	-1.09302200	-0.02153200
C	-2.61231600	-1.46575900	-0.62090400
C	-0.90380700	0.32015300	-0.49033900
H	-1.37771300	-1.04235000	1.07925400
C	-3.66146900	-0.38868800	-0.32644000
H	-2.50874000	-1.54804400	-1.70837100
O	-3.06592500	-2.73155300	-0.17129600
C	-1.99322000	1.31564900	-0.10960800
H	-0.76565600	0.32040800	-1.58023000
O	0.35652300	0.62252800	0.13715700
O	-3.93925500	-0.42710200	1.04738400
H	-4.58034900	-0.56265900	-0.89971000
O	-3.20867000	0.88656300	-0.73558100
H	-3.18924400	-2.67771800	0.79255300
H	-2.12349500	1.33237000	0.98170800
C	-1.74728700	2.72395600	-0.61306000
H	0.79964700	1.35422600	-0.32827700
C	-4.98667500	0.45748400	1.43078300
H	-0.82131200	3.11682100	-0.18537600
H	-1.65582300	2.71123700	-1.70741000
O	-2.78894700	3.60171300	-0.20784000
H	-5.20922500	0.24908800	2.47788600
H	-5.87981000	0.27747600	0.82016500
H	-4.67552500	1.50235000	1.32372300
H	-3.62634700	3.24153400	-0.54595300



$INT_{4\text{-}3\_I}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.429318 A.U.

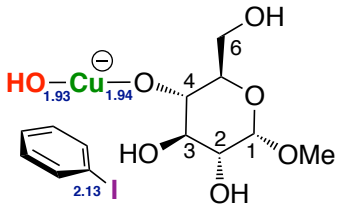
Thermal correction to Gibbs Free Energy = 0.272501 A.U.

Sum of electronic and thermal Free Energies = -1230.156817 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.70061611 A.U.

C	2.77352100	0.55073000	-1.23170000
C	3.39109900	-0.15456300	-0.20141300
C	3.99135400	0.49817100	0.87127000
C	3.95745000	1.89295900	0.91382100
C	3.33392600	2.61918900	-0.10139200
C	2.74705700	1.94338000	-1.17407300
H	2.31181000	0.00683800	-2.05103400
H	4.46138300	-0.07846700	1.66352200
H	4.41781200	2.40891300	1.75098800
H	3.30549800	3.70341100	-0.05823400
H	2.26124200	2.49973400	-1.97016000
O	3.34961500	-1.54234500	-0.27506700
H	3.90341800	-1.93625900	0.42323000
Cu	1.42090300	-2.15361700	-0.00952500
O	-0.47614200	-2.39999500	0.27247400
C	-1.28463200	-1.26652700	0.38750700
C	-2.43190000	-1.31842600	-0.63380800
C	-0.52497400	0.05508500	0.20171100
H	-1.74204300	-1.22229500	1.39681000
C	-3.28704500	-0.05321600	-0.62085900
H	-1.99923800	-1.41618400	-1.63585800
O	-3.25139100	-2.46337000	-0.44873400
C	-1.47284800	1.25602700	0.19720400
H	0.01567900	0.01229300	-0.75821400
O	0.40404500	0.18574200	1.27527300
O	-3.98153300	-0.01525300	0.59799100
H	-3.99859100	-0.04337500	-1.45617700
O	-2.47963700	1.08954300	-0.80651800
H	-3.66756200	-2.39255200	0.42809700
H	-1.95011600	1.34518100	1.18390200
C	-0.77329800	2.55776900	-0.14147100
H	1.17278000	0.69863600	0.97381300
C	-4.88647800	1.07887900	0.69266300
H	0.03146000	2.74928100	0.57290900
H	-0.34300300	2.48800400	-1.15022900
O	-1.66538100	3.66236300	-0.05586600
H	-5.46300200	0.93466600	1.60720200
H	-5.56171600	1.09123100	-0.17165800
H	-4.34636800	2.03053200	0.74715800
H	-2.41163000	3.48507500	-0.65301900



$INT_{1\text{-}4\_anion}$

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.935504 A.U.

Thermal correction to Gibbs Free Energy = 0.261503 A.U.

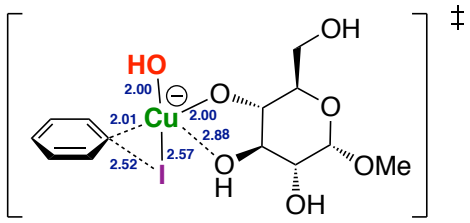
Sum of electronic and thermal Free Energies = -1241.674001 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.20864754 A.U.

C	-1.62852400	1.49314200	-0.44986700
C	-2.75572900	0.93172900	0.14475400
C	-3.35035900	1.51067200	1.26381300
C	-2.78989400	2.67178300	1.80213800
C	-1.65583500	3.24350800	1.22386800

C	-1.08009800	2.65485900	0.09776000
H	-1.17039400	1.02695900	-1.31736200
H	-4.22596300	1.06134000	1.72164200
H	-3.24370800	3.12382900	2.67920200
H	-1.22263400	4.14295300	1.65056900
H	-0.19410200	3.09042200	-0.35856700
I	-3.53868300	-0.88242900	-0.63885500
O	-0.95251900	-0.61550000	2.58046900
H	-1.51916700	0.15336500	2.41115100
Cu	-0.19272600	-1.07641900	0.86888300
O	0.60659600	-1.62010200	-0.81492300
C	1.82303600	-1.01113800	-1.12115800
C	2.84579900	-1.15635000	0.02116100
H	2.27100900	-1.47594200	-2.02191200
C	1.65675600	0.48173100	-1.41713000
O	4.07911200	-0.49285600	-0.29156700
H	2.41564700	-0.71098600	0.93435400
C	3.19085900	-2.60505600	0.29482500
C	2.99371900	1.18024000	-1.63898000
H	1.15008400	0.93787000	-0.54979800
O	0.83850400	0.62398900	-2.57276700
C	3.95065300	0.89697800	-0.48529400
H	2.26800700	-3.17074900	0.45764000
H	3.71770900	-3.02808800	-0.56658200
O	4.06878600	-2.74887700	1.40866800
H	3.45091800	0.79707100	-2.55684100
O	2.81951900	2.57600500	-1.83622000
H	0.68760700	1.57383900	-2.71530600
O	3.44741900	1.55076900	0.65128000
H	4.96299300	1.25781800	-0.70586900
H	3.59956700	-2.44620300	2.20364100
H	2.46403400	2.95014200	-1.01040000
C	4.29319600	1.42519100	1.78909900
H	4.30230300	0.39368500	2.15799600
H	5.31618400	1.73285700	1.54009300
H	3.88833100	2.08354200	2.55862600



TS_{OA-4_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.894113 A.U.

Thermal correction to Gibbs Free Energy = 0.264643 A.U.

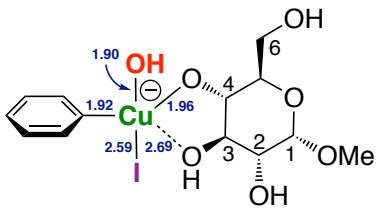
Sum of electronic and thermal Free Energies = -1241.62947 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.16759729 A.U.

C	-3.21792100	1.48737000	-0.46779600
C	-3.06035400	0.26927000	0.19040200
C	-4.03290800	-0.24342100	1.04565100
C	-5.18333800	0.51531300	1.27425700
C	-5.35752600	1.74813500	0.64230700
C	-4.37547400	2.23016200	-0.22512800
H	-2.45589400	1.85574300	-1.14801700
H	-3.89802900	-1.20483500	1.53142100
H	-5.94539700	0.13329000	1.94775700
H	-6.25829800	2.32756500	0.81979600
H	-4.50643200	3.18650700	-0.72370700
I	-1.86779800	-1.47014700	-1.18358100
O	-1.36669900	1.29431200	2.31428700
H	-2.28496200	1.60404400	2.28557800
Cu	-1.17136900	-0.01501800	0.81477900
O	0.74404800	-0.45268100	1.20281800
C	1.65241900	-0.30496300	0.16316000
C	3.04096400	-0.80953100	0.59576200
H	1.35752900	-0.88947400	-0.73534000
C	1.79530500	1.15535700	-0.28629800
O	4.01677800	-0.62662000	-0.44089000
H	3.35771500	-0.25133500	1.49105500
C	3.03137500	-2.29046400	0.91429000

C	2.90176900	1.31611100	-1.32422300
H	2.03274200	1.76628200	0.59887300
O	0.55389700	1.58963200	-0.83739700
C	4.21056500	0.71508700	-0.82196100
H	2.23500500	-2.50116800	1.63402400
H	2.84138800	-2.86164400	-0.00017600
O	4.28875700	-2.74214100	1.41218300
H	2.61441200	0.78047800	-2.23490700
O	3.07062100	2.67460000	-1.70261300
H	0.65455700	2.52001000	-1.09964500
O	4.65940900	1.51392200	0.24251600
H	4.96919300	0.68904100	-1.61431200
H	4.44649300	-2.31309400	2.26941700
H	3.41448100	3.15778000	-0.93059000
C	5.91744500	1.09956300	0.76252600
H	5.82836300	0.14121600	1.28571800
H	6.65315000	1.00728900	-0.04581000
H	6.23860300	1.86952600	1.46512200



INT$_{2\text{-}4_anion}$

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.900418 A.U.

Thermal correction to Gibbs Free Energy =

0.264 A.U.

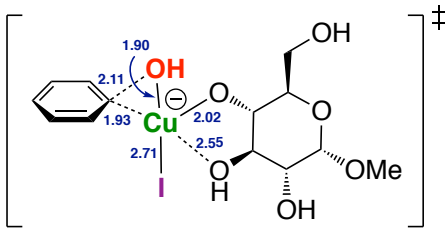
Sum of electronic and thermal Free Energies =

-1241.636418 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.17236900 A.U.

C	3.16869400	-1.66023500	-0.44034000
C	2.96606300	-0.64119500	0.48073000
C	3.98147300	-0.16608300	1.29989400
C	5.25465000	-0.73400500	1.18175400
C	5.48831400	-1.75584600	0.26012700
C	4.44777100	-2.21753500	-0.54731500
H	2.35880700	-2.01822100	-1.07028300
H	3.79909700	0.62991200	2.01635900
H	6.06088000	-0.37216900	1.81397900
H	6.47888600	-2.19190300	0.17203200
H	4.62376000	-3.01377600	-1.26536500
I	1.73064400	1.75679600	-1.01634000
O	1.07488600	-1.35723000	2.12584700
H	1.92816000	-1.80477300	2.22319700
Cu	1.16378000	-0.03868300	0.76554500
O	-0.67818400	0.54652800	1.11964400
C	-1.60172000	0.33896900	0.10029700
C	-3.00630500	0.75985900	0.56195200
H	-1.36188100	0.93855400	-0.80255000
C	-1.65514500	-1.12840100	-0.33919700
O	-3.97971100	0.51563000	-0.46314100
H	-3.27696400	0.18607300	1.46218500
C	-3.07550500	2.24080500	0.87360800
C	-2.76434600	-1.36471800	-1.35934700
H	-1.83243700	-1.75180200	0.55058700
O	-0.39051400	-1.46318700	-0.90595700
C	-4.09888700	-0.83625100	-0.84059000
H	-2.28998400	2.49756200	1.59065100
H	-2.91615100	2.81578000	-0.04433900
O	-4.35391700	2.62812300	1.36973200
H	-2.52147400	-0.81933500	-2.27711200
O	-2.86267300	-2.73232100	-1.72616600
H	-0.35269300	-2.42618400	-1.02523800
O	-4.48816400	-1.65679300	0.23039000
H	-4.86720100	-0.85509200	-1.62367200
H	-4.48907400	2.19525800	2.22865500
H	-3.16099300	-3.22870500	-0.94385700
C	-5.76437800	-1.31679600	0.76037700
H	-5.72806600	-0.35431000	1.28223100
H	-6.51026000	-1.26894100	-0.04246500
H	-6.03399300	-2.10374500	1.46574700



TS_{RE-4_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.891094 A.U.

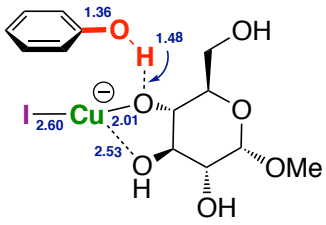
Thermal correction to Gibbs Free Energy = 0.263124 A.U.

Sum of electronic and thermal Free Energies = -1241.62797 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.16290203 A.U.

C	2.99679400	-1.90568500	-0.37934500
C	2.80923600	-1.02023000	0.67012600
C	3.84251300	-0.50759300	1.43938500
C	5.14767900	-0.87691700	1.09926200
C	5.38368100	-1.74424400	0.03127800
C	4.31098900	-2.25505500	-0.70285300
H	2.15664000	-2.30725400	-0.93780800
H	3.65009400	0.17317200	2.26353900
H	5.97763000	-0.47787600	1.67562100
H	6.40012500	-2.02748000	-0.22373900
H	4.48891400	-2.93571600	-1.53060800
I	1.89485600	1.92286500	-0.88551600
O	1.17558200	-1.64229100	1.85867200
H	1.67912400	-1.44398900	2.66466800
Cu	1.11376200	-0.10622400	0.73821500
O	-0.73959000	0.59605000	1.13224300
C	-1.64562300	0.39447000	0.09789400
C	-3.06833000	0.78508900	0.52875000
H	-1.39747400	1.00894200	-0.79504500
C	-1.65559500	-1.06675500	-0.36660800
O	-4.02164400	0.51231600	-0.50927900
H	-3.34069200	0.21235400	1.42927800
C	-3.17575200	2.26660700	0.82543000
C	-2.74673300	-1.33203000	-1.39748900
H	-1.81457200	-1.70908900	0.51259800
O	-0.37185400	-1.34287800	-0.92586400
C	-4.09885500	-0.84266600	-0.88554000
H	-2.40328300	2.54894800	1.54722300
H	-3.02030000	2.83546200	-0.09698100
O	-4.46759700	2.63108800	1.30440700
H	-2.51342600	-0.77750600	-2.31212300
O	-2.80604600	-2.70094400	-1.76868500
H	-0.24204200	-2.30441900	-0.95483700
O	-4.46822000	-1.67326700	0.18529200
H	-4.86284100	-0.88605900	-1.67189600
H	-4.60408200	2.20110300	2.16451900
H	-3.09068000	-3.20781500	-0.98805400
C	-5.75638100	-1.37102800	0.70906000
H	-5.75425600	-0.40205600	1.22012600
H	-6.50168200	-1.35776600	-0.09563700
H	-6.00045700	-2.15869600	1.42289900



INT_{3-4_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.012751 A.U.

Thermal correction to Gibbs Free Energy = 0.262923 A.U.

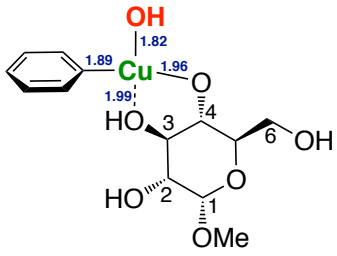
Sum of electronic and thermal Free Energies = -1241.749828 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.28312352 A.U.

C	-1.79999100	2.40770100	-1.94774100
C	-1.09859600	2.26755700	-0.74428100
C	-1.76936100	2.46289600	0.47255300
C	-3.12844300	2.77395200	0.47652400

C	-3.83174300	2.90646000	-0.72220100
C	-3.15732200	2.72631200	-1.93189300
H	-1.27251400	2.25487700	-2.88534400
H	-1.21941100	2.36493500	1.40524400
H	-3.63950200	2.91325200	1.42534300
H	-4.89019100	3.14785000	-0.71436000
H	-3.69145400	2.82811700	-2.87266600
I	-3.45593500	-1.45119200	0.16858900
O	0.22567600	1.95136600	-0.78112400
H	0.45735600	1.34474900	0.04101400
Cu	-1.06512600	-0.57352200	0.68989100
O	0.64110400	0.38272600	1.14977000
C	1.80762100	-0.36846200	0.97838700
C	3.03423300	0.55455200	0.91394600
H	1.95332500	-1.06352000	1.82694600
C	1.75948000	-1.21274700	-0.29853800
O	4.23259600	-0.19842400	0.68779900
H	2.89721700	1.27346100	0.09023700
C	3.24045500	1.31672200	2.20721900
C	3.08742500	-1.91820600	-0.55475400
H	1.52782500	-0.54938300	-1.14560300
O	0.71220000	-2.16718500	-0.14860000
C	4.24140900	-0.91909200	-0.52332000
H	2.31462300	1.83587100	2.47434900
H	3.49681500	0.61706700	3.00900600
O	4.32405700	2.23700400	2.11865800
H	3.25734800	-2.65460700	0.23719600
O	3.07004800	-2.64309300	-1.77427000
H	0.51847600	-2.55300900	-1.01838700
O	4.10306300	-0.08155600	-1.64150900
H	5.21249600	-1.42846800	-0.55453300
H	4.08947400	2.91838700	1.46738700
H	2.99503800	-2.00086000	-2.50218800
C	5.16288500	0.85963000	-1.77000700
H	5.12088600	1.60755500	-0.97061800
H	6.13258000	0.34808400	-1.74087100
H	5.03458900	1.35060000	-2.73535900



$INT_{3\text{-}4\_I}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.3332859999998 A.U.

Thermal correction to Gibbs Free Energy = 0.272008 A.U.

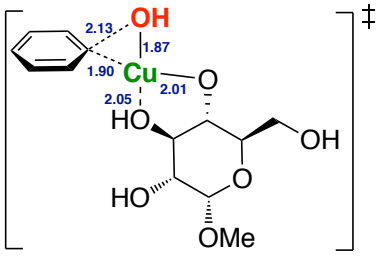
Sum of electronic and thermal Free Energies = -1230.061278 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.60446116 A.U.

C	-3.59107800	0.57747200	1.18573000
C	-3.15203700	-0.16230600	0.10018300
C	-3.84607100	-0.27359600	-1.09299800
C	-5.05800300	0.41781400	-1.20333000
C	-5.53286200	1.18006200	-0.13484400
C	-4.80579200	1.26116100	1.05355200
H	-3.01845500	0.63058300	2.10724600
H	-3.46870800	-0.87312000	-1.91637200
H	-5.62635900	0.35442600	-2.12677400
H	-6.47543400	1.71093900	-0.22799400
H	-5.17773800	1.85372100	1.88445100
O	-2.26183300	-2.45531000	0.72334800
H	-3.22464700	-2.36326400	0.77534600
Cu	-1.42232200	-0.92420100	0.19514000
O	0.40548700	-1.63389300	0.29553100
C	1.22878500	-0.74663300	-0.40002600
C	2.71672700	-0.88893000	-0.05996000
H	1.13471100	-0.87766100	-1.49610100
C	0.81783500	0.68300100	-0.07328100
O	3.46506500	0.08477000	-0.80397000
H	2.86777800	-0.72397000	1.01800900
C	3.26065200	-2.24882500	-0.44391900

C	1.65153300	1.70453500	-0.82314400
H	0.89204400	0.84620800	1.00936800
O	-0.57943400	0.76012200	-0.44137400
C	3.13235300	1.42689800	-0.53099800
H	2.64986100	-3.02606900	0.02716700
H	3.20834700	-2.37053300	-1.53033600
O	4.63076500	-2.40167000	-0.08984600
H	1.48600200	1.59467800	-1.89892300
O	1.30345600	3.03682500	-0.49378000
H	-0.98620100	1.55499100	-0.04909100
O	3.35265200	1.76541100	0.81262900
H	3.77968700	2.02600600	-1.18256000
H	4.69770000	-2.40945400	0.87900400
H	1.55142000	3.19119200	0.43536900
C	4.71805100	1.65663600	1.20214500
H	5.03929400	0.60962300	1.21093200
H	5.35571800	2.23001700	0.51858300
H	4.79251900	2.06974100	2.20865000



TS_{RE-4_I}

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.327584 A.U.

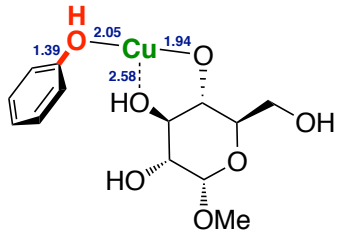
Thermal correction to Gibbs Free Energy = 0.270564 A.U.

Sum of electronic and thermal Free Energies = -1230.05702 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.59914157 A.U.

C	-3.60924000	0.53549500	1.18836300
C	-3.23104800	-0.32129400	0.16863200
C	-3.86678100	-0.41316600	-1.05761700
C	-4.94683700	0.44597600	-1.28066000
C	-5.36201400	1.33516200	-0.28681000
C	-4.69783800	1.37948100	0.93952000
H	-3.08285500	0.55818900	2.13800500
H	-3.54152800	-1.12164700	-1.81331300
H	-5.46553600	0.40887300	-2.23415100
H	-6.20803300	1.99084900	-0.46747500
H	-5.01957800	2.07030500	1.71341300
O	-2.64338000	-2.25355800	0.83301800
H	-2.88061000	-2.03761100	1.75038400
Cu	-1.44501900	-0.96310300	0.21783900
O	0.43360600	-1.66825700	0.25946400
C	1.23910000	-0.75652400	-0.42111300
C	2.73100000	-0.89481900	-0.09139900
H	1.14435100	-0.86857000	-1.52074400
C	0.81911800	0.67164200	-0.07947700
O	3.48130200	0.09727100	-0.80973900
H	2.88388000	-0.75713200	0.99049200
C	3.28173600	-2.24193200	-0.51004400
C	1.66481700	1.70601100	-0.80040500
H	0.88831700	0.81649200	1.00708100
O	-0.56696400	0.76645500	-0.46009800
C	3.14300300	1.43073200	-0.50542800
H	2.67794800	-3.03480800	-0.05674200
H	3.22682000	-2.33694200	-1.59913400
O	4.65461700	-2.39674500	-0.16516200
H	1.50816700	1.61734500	-1.87968000
O	1.31036900	3.03257300	-0.44997900
H	-0.97122000	1.54835000	-0.04318700
O	3.35493900	1.73644000	0.84815500
H	3.79308700	2.04858900	-1.13675100
H	4.72643700	-2.41301900	0.80322100
H	1.54706900	3.16865600	0.48477000
C	4.71779500	1.61852300	1.24262500
H	5.04107100	0.57218800	1.22329400
H	5.35899100	2.21205100	0.57977400
H	4.78596800	2.00268800	2.26101900



$INT_{4\text{-}4\_-I}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.4267129999998 A.U.

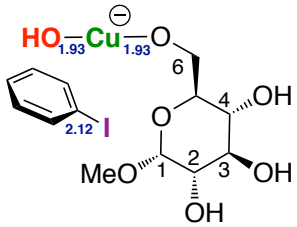
Thermal correction to Gibbs Free Energy = 0.270523 A.U.

Sum of electronic and thermal Free Energies = -1230.15619 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.69756515 A.U.

C	-3.76531700	0.48633000	1.37084500
C	-3.60662700	-0.49575300	0.39837100
C	-3.87429800	-0.24450200	-0.94407900
C	-4.30141700	1.02788700	-1.31829000
C	-4.46507700	2.03100700	-0.35983600
C	-4.20007100	1.75419700	0.98166000
H	-3.54269900	0.26050100	2.41053900
H	-3.73139000	-1.03448500	-1.67563200
H	-4.50692100	1.23419300	-2.36442300
H	-4.79755100	3.02050900	-0.65735200
H	-4.32523300	2.52714400	1.73407300
O	-3.13798100	-1.76466400	0.72383600
H	-3.18759700	-1.90082400	1.68720800
Cu	-1.15002300	-1.90743900	0.26108800
O	0.76963900	-1.96843000	-0.02570100
C	1.35090300	-0.84701000	-0.61729900
C	2.79825100	-0.67368700	-0.12587900
H	1.39061100	-0.94502900	-1.72213900
C	0.58532800	0.44848100	-0.31832000
O	3.40836500	0.49068300	-0.70115700
H	2.79255500	-0.57420700	0.97116400
C	3.67231500	-1.84846100	-0.51458900
C	1.31459300	1.67531400	-0.85700100
H	0.46996300	0.53714000	0.77308200
O	-0.70279000	0.34689300	-0.92075200
C	2.76335600	1.70052000	-0.37849600
H	3.20748000	-2.77673600	-0.16903700
H	3.77080500	-1.88714100	-1.60419900
O	4.99612800	-1.72828700	-0.00043200
H	1.32256700	1.62951200	-1.95071900
O	0.64384300	2.87858900	-0.51517900
H	-1.29569000	1.00159500	-0.51547100
O	2.74482100	1.94249100	1.00467500
H	3.33794700	2.48450700	-0.88709400
H	4.94939900	-1.76822100	0.96880800
H	0.70114700	2.98596200	0.45064600
C	4.04537600	2.08151100	1.56564600
H	4.58559400	1.12876900	1.54288100
H	4.61812700	2.83930100	1.01724400
H	3.91147000	2.40003400	2.60014100



$INT_{1\text{-}6\_anion}$

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.930948 A.U.

Thermal correction to Gibbs Free Energy = 0.261836 A.U.

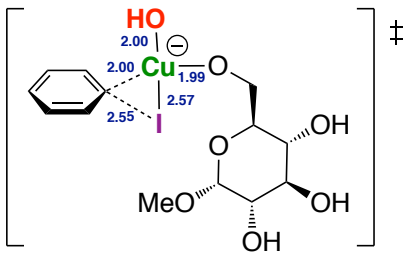
Sum of electronic and thermal Free Energies = -1241.669112 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.20447664 A.U.

Cu	-0.79549000	-0.19589500	2.02272100
C	-1.49683700	1.24559300	-1.26541300
C	-2.59035500	0.46405800	-0.89984700
C	-3.78176900	1.04284800	-0.46688100
C	-3.86908900	2.43536600	-0.38989500

C	-2.77826300	3.23246200	-0.73867500
C	-1.59599000	2.63568500	-1.17713300
H	-0.57817100	0.78150400	-1.60991300
H	-4.62780300	0.42515400	-0.18295100
H	-4.79339100	2.89164000	-0.04801600
H	-2.84993900	4.31350800	-0.66925300
H	-0.74205500	3.24851400	-1.45263800
C	2.14540000	-0.87705100	0.64974500
O	1.35388300	0.12309800	-0.01032500
C	2.04115800	1.30978200	-0.33042800
C	3.19151500	1.00363800	-1.28316000
H	2.74988700	0.60322400	-2.20584400
C	3.30455200	-1.27721300	-0.27046300
H	2.90108300	-1.75850100	-1.17334500
C	4.10737600	-0.05047600	-0.68203200
H	4.60250900	0.36206600	0.20882600
I	-2.42158200	-1.65279600	-0.97502700
C	1.21397600	-2.04266800	0.96844300
H	0.71278500	-2.31190600	0.01786000
H	1.85222500	-2.90145600	1.24018600
O	0.29961300	-1.78858600	1.99341400
O	3.87939200	2.21207800	-1.55473700
H	4.52072900	2.04082400	-2.26354900
O	5.08154400	-0.37268000	-1.66547000
H	5.71247500	-0.99658600	-1.26931900
O	4.21697800	-2.15160500	0.38330800
H	3.88655500	-3.06141800	0.32134100
H	2.55089400	-0.46521900	1.58622900
O	2.56079500	1.94911600	0.80372600
C	1.55065700	2.33086300	1.73180800
H	2.01523200	3.01744200	2.44140100
H	0.72507500	2.83612100	1.21337600
H	1.15835000	1.45716800	2.26579600
H	1.29896800	1.95838500	-0.81345400
O	-1.88067900	1.35328100	2.39069400
H	-2.42855900	1.52373600	1.60951200



TS_{OA-6_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.8924439999998 A.U.

Thermal correction to Gibbs Free Energy = 0.264027 A.U.

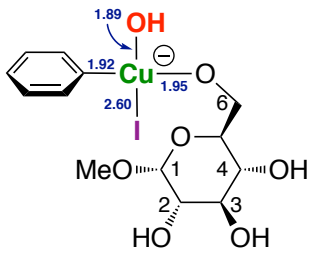
Sum of electronic and thermal Free Energies = -1241.628417 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.16628836 A.U.

Cu	-1.26576700	-0.48739500	1.05189600
C	-2.02039700	1.61462700	-0.64859300
C	-2.58310800	0.45852600	-0.11543800
C	-3.92397900	0.38745000	0.25578100
C	-4.71010100	1.53341600	0.12252700
C	-4.16395200	2.71483900	-0.38613900
C	-2.82268400	2.75301600	-0.76831900
H	-0.98048000	1.63513500	-0.96122800
H	-4.34540400	-0.53109800	0.65242300
H	-5.75480000	1.49733000	0.41855500
H	-4.78487900	3.59920300	-0.49075900
H	-2.39210000	3.66566300	-1.17125100
C	2.18568600	-0.57631600	0.86297200
O	1.42191000	0.15979100	-0.10643300
C	2.01868100	1.35874300	-0.54476200
C	3.35641800	1.05860100	-1.21253600
H	3.14697700	0.43587200	-2.09280800
C	3.53602500	-0.95907900	0.24768400
H	3.37085600	-1.65024600	-0.59159500
C	4.25682800	0.27957200	-0.26731000
H	4.52392900	0.91452900	0.58967900
I	-1.68527700	-1.66871000	-1.19023600

C	1.34615900	-1.78654300	1.26578800
H	1.11006900	-2.33700700	0.33309400
H	1.99714900	-2.44813100	1.86384900
O	0.20218900	-1.44804200	1.98713500
O	3.94037800	2.28653300	-1.61052100
H	4.72587700	2.08685700	-2.14560800
O	5.42935900	-0.06219300	-0.99425500
H	6.05177500	-0.48587400	-0.38047900
O	4.39926200	-1.55575800	1.20955500
H	4.19284400	-2.50079800	1.28156700
H	2.35690100	0.05590200	1.74693900
O	2.23866800	2.25722900	0.50789200
C	1.02894600	2.71546700	1.10282700
H	1.31106500	3.41419000	1.89162300
H	0.41040900	3.23139800	0.35765800
H	0.46232200	1.88314800	1.53631800
H	1.31510800	1.79081800	-1.26783900
O	-1.78336500	0.59156000	2.65105400
H	-2.50503200	1.17231000	2.36509500



$INT_{2\text{-}6\_anion}$

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.897452 A.U.

Thermal correction to Gibbs Free Energy = 0.265298 A.U.

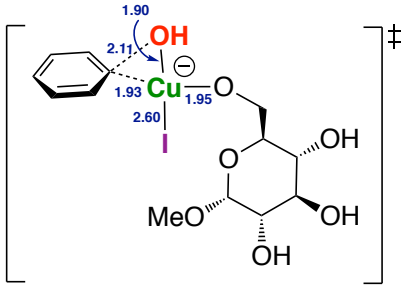
Sum of electronic and thermal Free Energies = -1241.632154 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.16973505 A.U.

Cu	-1.24901100	-0.38887200	1.00766800
C	-2.06065200	1.79931800	-0.56754300
C	-2.55904500	0.75549700	0.20044900
C	-3.90859500	0.63585000	0.50425800
C	-4.79167200	1.60134300	0.00979200
C	-4.31749100	2.66106500	-0.76588600
C	-2.95553700	2.76001100	-1.05241500
H	-1.00097800	1.86975500	-0.79974100
H	-4.27664400	-0.18803900	1.10925100
H	-5.85148900	1.52021400	0.23522200
H	-5.00836800	3.40729000	-1.14667800
H	-2.58043400	3.58171300	-1.65651800
C	2.14086700	-0.54581200	0.84413300
O	1.37766400	0.23173200	-0.09250800
C	2.00140700	1.42206300	-0.52242800
C	3.31487500	1.09729900	-1.22584100
H	3.07230200	0.48800200	-2.10689500
C	3.47776600	-0.93879100	0.20426000
H	3.28743900	-1.61303500	-0.64340200
C	4.21640000	0.29061200	-0.30576800
H	4.51190800	0.90987500	0.55313400
I	-1.63362200	-1.88291200	-1.08595200
C	1.29706100	-1.76421100	1.20973700
H	1.09894400	-2.31565900	0.27185000
H	1.92857500	-2.41785000	1.83481900
O	0.12451000	-1.44769200	1.89656800
O	3.91677200	2.31636200	-1.62471600
H	4.68765400	2.10568200	-2.17654500
O	5.36827400	-0.06877100	-1.05671700
H	5.99240300	-0.51150300	-0.45833200
O	4.34095100	-1.56851400	1.14471300
H	4.12954000	-2.51410100	1.19028600
H	2.32959400	0.05562200	1.74567300
O	2.27743500	2.29212300	0.54002900
C	1.10146500	2.81255600	1.15052600
H	1.42983900	3.46683400	1.95943000
H	0.52019900	3.39144800	0.42208300
H	0.48113500	2.00784300	1.55955500
H	1.29391500	1.88887500	-1.21945900
O	-1.50888400	0.63027800	2.58360000

H	-2.15714200	1.33371300	2.43195300



TS_{RE-6_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.888264 A.U.

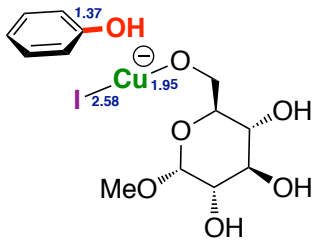
Thermal correction to Gibbs Free Energy = 0.264772 A.U.

Sum of electronic and thermal Free Energies = -1241.623492 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy =-1242.16012343 A.U.

Cu	-1.20801300	-0.20741200	1.02080800
C	-1.95122500	1.97202000	-0.55396500
C	-2.47730200	1.09417600	0.38079300
C	-3.83680100	0.91344900	0.58333200
C	-4.71422700	1.62971700	-0.23575500
C	-4.22540600	2.50374900	-1.20924700
C	-2.84850700	2.67208100	-1.36605600
H	-0.87808400	2.10162300	-0.66272700
H	-4.21009700	0.22369500	1.33471500
H	-5.78477100	1.49515600	-0.10870600
H	-4.91566900	3.05669900	-1.83867800
H	-2.46114600	3.35368800	-2.11815000
C	2.19947700	-0.57567900	0.83207600
O	1.42642300	0.26994400	-0.03469800
C	2.10293600	1.42552500	-0.47610800
C	3.33492100	1.02991300	-1.28360100
H	2.98322100	0.47546200	-2.16408700
C	3.43777000	-1.06280200	0.07247400
H	3.11963300	-1.68701600	-0.77536600
C	4.23435400	0.12078600	-0.45997700
H	4.64264800	0.68450400	0.39083200
I	-1.85284000	-1.99844900	-0.89254700
C	1.28524400	-1.71352100	1.27685300
H	1.00103900	-2.27658400	0.36698800
H	1.89753200	-2.39570100	1.89228300
O	0.17217700	-1.27139500	1.99218400
O	4.00142600	2.21413200	-1.68487000
H	4.71238900	1.96734900	-2.29873000
O	5.29470200	-0.30076800	-1.30728000
H	5.93533600	-0.79184600	-0.76673300
O	4.31709300	-1.79685500	0.91670500
H	3.99173100	-2.70707400	1.00027400
H	2.51692400	0.00250800	1.71266000
O	2.51894300	2.23789300	0.58855900
C	1.43776200	2.68272500	1.40084400
H	1.84997400	3.41106400	2.10081100
H	0.66596600	3.16109600	0.78461200
H	0.99625400	1.84869200	1.95578000
H	1.38283100	1.96685500	-1.10275500
O	-1.45667500	1.24729700	2.21917500
H	-2.27950100	1.08772400	2.71036800



INT_{3-6_anion}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.995838 A.U.

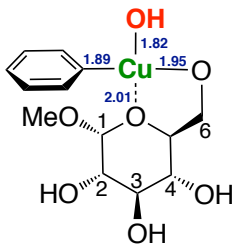
Thermal correction to Gibbs Free Energy = 0.263612 A.U.

Sum of electronic and thermal Free Energies = -1241.732226 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/ SMD(water)

Energy = -1242.26715799 A.U.

Cu	-1.38579200	-1.29423500	0.53064700
C	-0.95020500	1.79101900	-0.14169200
C	-1.73492000	1.98519400	0.99738300
C	-2.96088000	2.64564500	0.91217000
C	-3.40374000	3.10833700	-0.32759600
C	-2.63091300	2.92122900	-1.47417400
C	-1.40301600	2.26276900	-1.37178200
H	-0.00721700	1.25782500	-0.05335700
H	-3.56284500	2.78382300	1.80698100
H	-4.36154400	3.61663100	-0.39255900
H	-2.98151200	3.28208900	-2.43607200
H	-0.79341700	2.10499400	-2.25738500
C	2.53013300	-0.98442900	0.50744000
O	1.99576500	0.12289400	-0.23263100
C	2.86596400	1.22364300	-0.35606100
C	4.12143300	0.80010400	-1.11084600
H	3.80720100	0.49418100	-2.11802900
C	3.76825000	-1.51313100	-0.22307700
H	3.47169600	-1.90643100	-1.20628100
C	4.77628300	-0.38840300	-0.42250200
H	5.15408700	-0.07622200	0.56163200
I	-3.71069200	-1.19548300	-0.59261900
C	1.40490600	-2.00369400	0.63451800
H	1.09704800	-2.27673500	-0.39149400
H	1.83914200	-2.91393000	1.08602300
O	0.34241300	-1.51747300	1.40590300
O	4.99591600	1.91181100	-1.18869600
H	5.75351300	1.65773600	-1.74107500
O	5.86210200	-0.79662900	-1.24381800
H	6.35607800	-1.48628800	-0.77033900
O	4.43443300	-2.52177600	0.52728200
H	3.98808200	-3.37155900	0.38667700
H	2.82145700	-0.64438800	1.51258200
O	3.25194300	1.73932400	0.88961200
C	2.15005300	2.20372800	1.66279500
H	2.56820300	2.66866100	2.55666200
H	1.57038400	2.94473800	1.09780300
H	1.49786300	1.37246800	1.95133100
H	2.30309900	1.98071000	-0.91821800
O	-1.25490100	1.48978100	2.18327300
H	-1.88813200	1.66959600	2.89826600



INT$_{3\text{-}6_\text{I}}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.330189 A.U.

Thermal correction to Gibbs Free Energy = 0.27276 A.U.

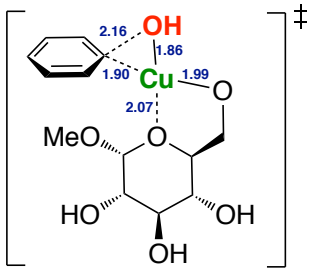
Sum of electronic and thermal Free Energies = -1230.057429 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/SMD(water)

Energy = -1230.60172474 A.U.

Cu	-1.12630900	-1.44309300	-0.04271900
C	-3.09263300	0.48255500	0.75259500
C	-2.31622300	0.01016700	-0.29226000
C	-2.23905800	0.62299900	-1.53332300
C	-2.96333200	1.80541600	-1.72124100
C	-3.73885500	2.32574300	-0.68383900
C	-3.80649600	1.66868000	0.54572000
H	-3.14115300	-0.03813500	1.70476800
H	-1.62754500	0.21242200	-2.33235700
H	-2.91756000	2.31332600	-2.68027600
H	-4.29858900	3.24345500	-0.83700700
H	-4.41620500	2.07179600	1.34927500
C	1.71063300	-1.10833900	0.13593900
O	0.52265000	-0.28897800	-0.08689100
C	0.62618100	1.03896600	0.45579700
C	1.75345700	1.75455600	-0.27781700
H	1.48267500	1.78408600	-1.34192200
C	2.89214200	-0.44834500	-0.57365100

H	2.71564200	-0.46149500	-1.65838500
C	3.06365700	0.99537400	-0.12125200
H	3.36698300	1.00520200	0.93477500
C	1.35100300	-2.48558400	-0.39810500
H	1.30220900	-2.42348800	-1.50086200
H	2.17210000	-3.17388200	-0.14462600
O	0.13617700	-2.91380400	0.15349700
O	1.83703400	3.06561000	0.24646600
H	2.45347800	3.57124200	-0.30857700
O	4.03053800	1.67268000	-0.90872000
H	4.90108400	1.28270600	-0.72527400
O	4.10036400	-1.12539600	-0.26012800
H	4.17097700	-1.92579700	-0.80475400
H	1.88935600	-1.15594600	1.21671100
O	0.90969300	1.00842800	1.81385900
C	-0.18027300	0.54855300	2.61168000
H	0.18108700	0.51232200	3.63972500
H	-1.02117400	1.24614100	2.53579200
H	-0.49864300	-0.45396000	2.29830300
H	-0.33794100	1.51838000	0.25908600
O	-2.61606600	-2.48862300	-0.15029200
H	-3.43816300	-1.98246400	-0.22932500



$TS_{RE\text{-}6\_I}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.325599 A.U.

Thermal correction to Gibbs Free Energy = 0.271651 A.U.

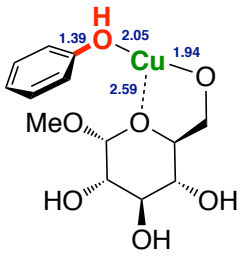
Sum of electronic and thermal Free Energies = -1230.053948 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/ SMD(water)

Energy = -1230.59746069 A.U.

Cu	-1.19425700	-1.44607900	0.00461100
C	-3.05153200	0.57248000	0.78763200
C	-2.46093900	-0.06000600	-0.29181200
C	-2.38230700	0.47136900	-1.56790200
C	-2.89378400	1.76170300	-1.75369000
C	-3.46716700	2.45369900	-0.68667800
C	-3.54749000	1.86189700	0.57658900
H	-3.11863800	0.09141500	1.75853000
H	-1.92501600	-0.07603100	-2.38717500
H	-2.83651400	2.21816700	-2.73760800
H	-3.86165700	3.45327600	-0.84070100
H	-4.00442600	2.39706700	1.40398200
C	1.69475600	-1.13344000	0.13554300
O	0.53067000	-0.29703700	-0.09321100
C	0.64987800	1.02694800	0.43190000
C	1.78761200	1.72495000	-0.30355900
H	1.51797700	1.75677700	-1.36779400
C	2.88735200	-0.50507600	-0.58427500
H	2.70809300	-0.52510100	-1.66869000
C	3.08361700	0.94036800	-0.14501100
H	3.38917000	0.95265800	0.91042200
C	1.30871500	-2.51565000	-0.37457000
H	1.23305800	-2.45688500	-1.47744500
H	2.14234000	-3.19946800	-0.14470500
O	0.10999100	-2.94158500	0.20923100
O	1.89888000	3.03636200	0.21579600
H	2.53422700	3.52355900	-0.33432400
O	4.06275300	1.59477900	-0.93794600
H	4.92600600	1.19071900	-0.75074600
O	4.08842700	-1.19594200	-0.26940700
H	4.14297000	-2.00477800	-0.80303900
H	1.88255600	-1.17413000	1.21597700
O	0.93736900	1.01368900	1.79346400
C	-0.13849100	0.54223600	2.60113800
H	0.23595600	0.50127700	3.62458500
H	-0.98486600	1.23463900	2.54186200
H	-0.45564600	-0.46078400	2.28775000
H	-0.31294500	1.51325200	0.23209500

O	-2.90762200	-2.16639800	-0.10611700
H	-3.16426500	-2.19917900	-1.04299900



$INT_{4\text{-}6\_I}$

at M06-2X/6-31+G*&SDD (for Cu)/SMD(water)

Energy = -1230.4261769999998 A.U.

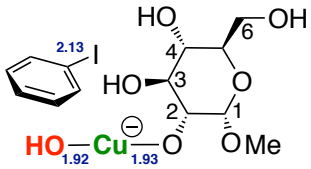
Thermal correction to Gibbs Free Energy = 0.270351 A.U.

Sum of electronic and thermal Free Energies = -1230.155826 A.U.

at M06-2X/6-311+G*&SDD (for Cu)/ SMD(water)

Energy = -1230.69728731 A.U.

Cu	-1.28498500	-2.17147300	0.07128300
C	-3.24904300	0.85887000	0.66323200
C	-2.94156600	0.12094200	-0.47401200
C	-2.50225200	0.73375500	-1.64448900
C	-2.37579100	2.12247400	-1.67178800
C	-2.67744600	2.88268900	-0.53974900
C	-3.11179500	2.24667900	0.62430200
H	-3.58283000	0.34670000	1.56089500
H	-2.25854500	0.12763800	-2.51327300
H	-2.03345600	2.60810800	-2.58078500
H	-2.57157700	3.96274400	-0.56449500
H	-3.34580600	2.82983400	1.51012100
C	1.69980400	-1.10268100	0.06086300
O	0.51642400	-0.31793200	-0.15755000
C	0.55718600	0.96272200	0.43512600
C	1.68335700	1.77149700	-0.19866500
H	1.44346100	1.87835200	-1.26576800
C	2.88122200	-0.39026400	-0.60365500
H	2.71613200	-0.34824100	-1.69008400
C	3.00608400	1.03027300	-0.06562500
H	3.28882600	0.97984100	0.99558000
C	1.42250500	-2.49285300	-0.49959800
H	1.20745300	-2.37487300	-1.57905700
H	2.36182000	-3.06702000	-0.42283000
O	0.38891000	-3.15606200	0.17518700
O	1.72441300	3.04326100	0.42351000
H	2.37542400	3.58867400	-0.04764700
O	3.97692600	1.77886800	-0.78426300
H	4.84850200	1.38423700	-0.61621200
O	4.11602000	-1.03734100	-0.31969600
H	4.21967600	-1.80090000	-0.90915900
H	1.88497300	-1.18568200	1.14150600
O	0.78149500	0.89269600	1.81653400
C	-0.30246300	0.30460000	2.52915200
H	0.04194800	0.14526800	3.55208500
H	-1.16501000	0.98010500	2.53021500
H	-0.59010800	-0.65878200	2.08622100
H	-0.41832100	1.42032100	0.22828100
O	-3.06204000	-1.26629500	-0.39066700
H	-3.23399500	-1.63337000	-1.27779900



INT_{1_MET}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.9350670000001 A.U.

Thermal correction to Gibbs Free Energy = 0.261287 A.U.

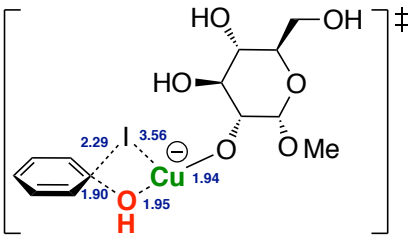
Sum of electronic and thermal Free Energies = -1241.67378 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.20824267 A.U.

C	-3.98063900	-1.13411400	-0.38125400
C	-2.69356900	-0.95110400	0.12036100

C	-2.46210700	-0.18850800	1.26356500
C	-3.54823300	0.40050500	1.91464900
C	-4.84285800	0.23197400	1.42389100
C	-5.05622800	-0.53514200	0.27846400
H	-4.14794100	-1.72649500	-1.27515100
H	-1.45344000	-0.03734400	1.63544500
H	-3.37249500	0.99980200	2.80327400
H	-5.68238000	0.69777000	1.93084600
H	-6.06096900	-0.67049300	-0.11091400
O	0.91572600	-0.06880200	1.58884200
I	-1.04688600	-1.81583500	-0.91353300
Cu	-0.88763600	2.25314000	-0.24628800
H	1.13003600	-0.76455600	3.53359500
C	0.95542300	-1.14241900	2.51815800
H	1.74070400	-1.86196500	2.25908100
H	-0.01596600	-1.64012700	2.47547900
C	2.02452000	0.78370200	1.66615200
H	2.11499100	1.18739400	2.68322700
O	3.23565300	0.08179600	1.44348500
C	1.85765200	1.90831200	0.63825400
C	3.31725600	-0.54641000	0.16430600
H	2.73828200	2.56237400	0.78396600
C	1.97727900	1.32487800	-0.77530700
O	0.68295200	2.63375100	0.81570200
H	2.47367800	-1.24483800	0.03931800
C	3.24367400	0.50685600	-0.94837000
C	4.61716900	-1.32711300	0.14277700
H	1.11218300	0.66660400	-0.96152100
O	1.98269900	2.37437900	-1.73688800
H	4.11962100	1.16824500	-0.88795300
O	3.18738300	-0.11736400	-2.22699200
H	4.78127200	-1.74557800	-0.85675500
H	5.44938600	-0.65905000	0.38496400
O	4.63386600	-2.35929900	1.12132800
H	1.19610200	2.91996000	-1.55065000
H	4.08887900	-0.29048100	-2.53996600
H	3.95421400	-3.01235600	0.88649100
O	-2.44198000	2.08133100	-1.36016400
H	-2.96619300	1.35450300	-0.98954300



TS_{MET}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.885935 A.U.

Thermal correction to Gibbs Free Energy = 0.26336 A.U.

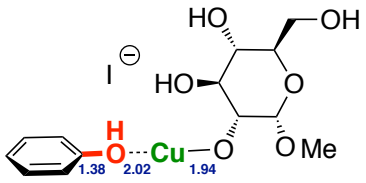
Sum of electronic and thermal Free Energies = -1241.622575 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.15961511 A.U.

C	-4.22243900	-0.45471900	-0.58201500
C	-2.92357100	-0.21791600	-0.08957300
C	-2.72487600	-0.10653700	1.30247700
C	-3.82126400	-0.13841800	2.16040000
C	-5.12138900	-0.31829400	1.67718000
C	-5.30077500	-0.48003600	0.30072600
H	-4.38002000	-0.60147500	-1.64594400
H	-1.72048000	0.02879400	1.69435500
H	-3.64634000	-0.03142300	3.22843800
H	-5.96714700	-0.35256300	2.35628200
H	-6.29685800	-0.64488800	-0.10343300
O	0.93139300	-0.14650700	1.48264200
I	-1.25839900	-1.32233800	-1.21765200
Cu	-0.64678700	1.97992600	-0.04508200
H	0.86357200	-0.89710200	3.41790700
C	0.80245500	-1.24229300	2.37790500
H	1.58068100	-1.99296900	2.19842900
H	-0.17716200	-1.68955200	2.19669300
C	2.08975800	0.61352900	1.68991400
H	2.12463500	0.96655100	2.72893100

O	3.26212100	-0.16847600	1.53085300
C	2.10161900	1.78642400	0.70422300
C	3.41207200	-0.74652400	0.23333800
H	3.01778700	2.35642400	0.94751300
C	2.28106700	1.24445000	-0.71825700
O	0.98463200	2.61317700	0.79639700
H	2.53791200	-1.37834100	0.00688400
C	3.50102400	0.35283200	-0.83577900
C	4.65469300	-1.61440800	0.28569600
H	1.39127800	0.64887300	-0.98440700
O	2.40093600	2.33327700	-1.62626200
H	4.41200900	0.94798700	-0.67965700
O	3.50016900	-0.21159000	-2.14313100
H	4.89087400	-1.98415100	-0.71854700
H	5.49959800	-1.02135100	0.64871600
O	4.50726500	-2.70067000	1.19246100
H	1.69351200	2.95599100	-1.37353600
H	4.40302800	-0.47180500	-2.38372500
H	3.81173900	-3.28944800	0.85487900
O	-2.32770100	1.41279800	-0.86636200
H	-3.02745100	1.99188000	-0.51705100



INT$_{2\text{-MET}}$

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -1241.99592 A.U.

Thermal correction to Gibbs Free Energy =

0.265464 A.U.

Sum of electronic and thermal Free Energies =

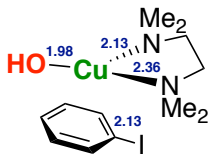
-1241.730456 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -1242.26724487 A.U.

C	-4.30633800	0.06329600	-0.59187000
C	-3.27555400	0.82838900	-0.05472800
C	-2.95941400	0.77247500	1.29920100
C	-3.68759300	-0.07765800	2.12955700
C	-4.71975400	-0.86130400	1.60997300
C	-5.02465000	-0.78525700	0.25008200
H	-4.52839300	0.12167300	-1.65427300
H	-2.13853300	1.37748300	1.68013000
H	-3.43876700	-0.13119200	3.18547500
H	-5.28036100	-1.52653900	2.25904000
H	-5.82410600	-1.39199800	-0.16462500
O	0.63371900	0.45834600	1.41339600
I	-0.82370600	-1.94031300	-1.09106300
Cu	-0.64420600	2.20162800	-0.34859000
H	0.41084100	0.13660900	3.45263800
C	0.31950100	-0.40121300	2.50004600
H	0.97773400	-1.27792300	2.51319600
H	-0.71267900	-0.72849200	2.36043500
C	1.87088800	1.10324500	1.54374000
H	1.89891000	1.67368300	2.48151000
O	2.93539600	0.17336100	1.64996900
C	2.08467100	2.01635800	0.33129800
C	3.06836700	-0.69701600	0.52402300
H	3.05034500	2.52280100	0.51503700
C	2.26296100	1.15185900	-0.92109800
O	1.07427700	2.95822500	0.15131800
H	2.12916000	-1.25359700	0.37411800
C	3.35560800	0.11565900	-0.74605400
C	4.17805600	-1.67523100	0.85814600
H	1.31474000	0.62373600	-1.12147600
O	2.57929300	1.98379400	-2.03115700
H	4.32895100	0.61809500	-0.65160200
O	3.34575300	-0.72284700	-1.89705700
H	4.40202300	-2.29517700	-0.01740300
H	5.08115700	-1.12462000	1.13894600
O	3.84434500	-2.49407100	1.97314400
H	1.95788700	2.73330600	-1.97890800
H	4.22242400	-1.12114300	-2.01267700
H	3.08881200	-3.05347500	1.72658700

O	-2.52698900	1.67606800	-0.85306600
H	-2.68862000	1.50152100	-1.79698700



INT_{1_TMEDA}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -863.7552900000001 A.U.

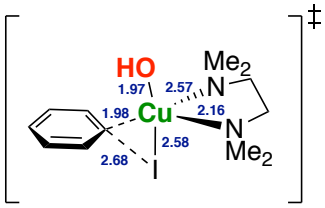
Thermal correction to Gibbs Free Energy = 0.277326 A.U.

Sum of electronic and thermal Free Energies = -863.477964 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -863.912497164 A.U.

Cu	-0.80961000	0.80111000	-0.53267000
N	-1.94854300	1.16415400	1.22497200
N	-2.65761900	-0.55696600	-1.09462900
C	-1.20540200	1.15971100	2.49065300
H	-0.69351700	0.20222300	2.61901100
H	-0.46469500	1.96336800	2.48417000
C	-2.56982900	2.48649700	1.05197200
H	-3.29668200	2.68621800	1.85620900
H	-1.79178300	3.25349900	1.08005500
H	-3.07902600	2.55336500	0.08837700
C	-2.97542400	0.10452500	1.26875400
H	-2.48304500	-0.81371400	1.60851000
H	-3.74752300	0.36210200	2.01244600
C	-3.63274500	-0.12896100	-0.08497400
H	-4.10719100	0.79364400	-0.43228400
H	-4.43568700	-0.87631200	0.02973800
C	-2.42626300	-1.99748100	-1.01499300
H	-3.33771500	-2.56224400	-1.27828200
H	-1.62619300	-2.28257600	-1.70478000
H	-2.12321100	-2.28207000	-0.00397800
C	-3.10426500	-0.20499000	-2.44003500
H	-4.06510400	-0.68604100	-2.69317200
H	-3.22299600	0.87968100	-2.51984400
H	-2.35484500	-0.52717500	-3.16941000
H	-1.88463500	1.31753700	3.34430700
O	0.30540000	1.21603600	-2.11751500
H	1.20049800	1.40018100	-1.79373300
C	3.31869100	-0.27149400	-0.90162800
C	2.38663500	-0.11861000	0.12144000
C	2.25158400	1.08698400	0.80662600
C	3.06377400	2.16444100	0.44822200
C	3.99722300	2.03211900	-0.58051100
C	4.12518600	0.81478100	-1.24939700
H	3.41232500	-1.21485400	-1.43005000
H	1.52035800	1.19171000	1.60202600
H	2.95900600	3.10834800	0.97515900
H	4.62345000	2.87428200	-0.85862900
H	4.85073000	0.70356200	-2.04984300
I	1.09530400	-1.73623800	0.60778100



TS_{OA_TMEDA}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -863.718668 A.U.

Thermal correction to Gibbs Free Energy = 0.284313 A.U.

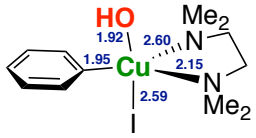
Sum of electronic and thermal Free Energies = -863.434355 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -863.875984275 A.U.

Cu	-0.21635200	0.25384400	-0.55985500
N	-1.49334300	1.21961400	1.45107300
N	-2.27457700	0.01787500	-1.17964300
C	-1.25948500	0.62416200	2.76329100

H	-1.44910300	-0.45220200	2.72565700
H	-0.21912200	0.78194100	3.06504500
C	-1.19062000	2.64809900	1.50720000
H	-1.78029100	3.14980500	2.29458300
H	-0.12743600	2.79528300	1.72179100
H	-1.41337900	3.12664100	0.55072200
C	-2.88263000	0.99963300	1.03414000
H	-3.20273900	0.02079200	1.40349200
H	-3.55318400	1.74531500	1.49485600
C	-3.04797100	1.06127400	-0.47654500
H	-2.70843700	2.03096300	-0.85431500
H	-4.11582300	0.96073100	-0.72942300
C	-2.83202400	-1.31450600	-0.90957500
H	-3.89899200	-1.34450800	-1.17919300
H	-2.29515400	-2.05650800	-1.50583600
H	-2.72129700	-1.58203400	0.14238700
C	-2.34870700	0.26242000	-2.62816700
H	-3.38794200	0.17887300	-2.98153700
H	-1.97318600	1.26140000	-2.85308400
H	-1.73711500	-0.47564600	-3.15460100
H	-1.91228400	1.06988500	3.53455700
O	-0.01986900	1.93743600	-1.55753200
H	0.86153400	2.27964200	-1.34488300
C	2.54777200	0.04851600	-1.32558800
C	1.73804400	0.26344600	-0.21591900
C	2.15232000	1.00669000	0.88086100
C	3.42429700	1.58863100	0.84356800
C	4.25401000	1.40593400	-0.26263200
C	3.81464900	0.63711100	-1.34261000
H	2.20451200	-0.55068700	-2.16337100
H	1.51151300	1.13775500	1.74693900
H	3.76071300	2.18034800	1.69035000
H	5.24204900	1.85552400	-0.28172000
H	4.45669300	0.48755800	-2.20617100
I	0.47262600	-1.99080600	0.49946500



INT_{2_TMEDA}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -863.718833 A.U.

Thermal correction to Gibbs Free Energy = 0.281236 A.U.

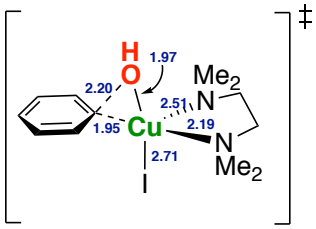
Sum of electronic and thermal Free Energies = -863.437597 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -863.875441988

Cu	0.20691000	-0.17697400	-0.55690300
N	1.46260700	-1.53036300	1.26759900
N	2.26721800	0.15348500	-1.07570100
C	1.22777200	-1.17428100	2.66377700
H	1.40061500	-0.10402200	2.81126600
H	0.19264200	-1.40045400	2.93729700
C	1.15057200	-2.94440500	1.06567200
H	1.73073000	-3.58196000	1.75549200
H	0.08509700	-3.12222500	1.24107500
H	1.38203400	-3.24592900	0.04148000
C	2.85588600	-1.25483500	0.89914000
H	3.19107400	-0.37203300	1.45109900
H	3.51367400	-2.08623300	1.20469900
C	3.01930000	-1.02570000	-0.59508900
H	2.65947900	-1.89384000	-1.15545200
H	4.08748000	-0.89499900	-0.82925700
C	2.85697200	1.38976400	-0.53605400
H	3.92949800	1.43145500	-0.77770100
H	2.35860500	2.25257700	-0.98268200
H	2.72989700	1.44723200	0.54557500
C	2.35855800	0.21366600	-2.54387400
H	3.40329900	0.36008800	-2.85594400
H	1.98045700	-0.71268300	-2.97600400
H	1.75964600	1.05218700	-2.91043400
H	1.89133100	-1.73590200	3.34468400

O	0.10722200	-1.63602800	-1.80490800
H	-0.76715800	-2.04782200	-1.74298000
C	-2.55245200	-0.05116600	-1.36165300
C	-1.71279400	-0.41972700	-0.31916700
C	-2.13360000	-1.19949300	0.74549900
C	-3.46226100	-1.64304700	0.75463600
C	-4.33075200	-1.29473000	-0.27881500
C	-3.87584900	-0.49924800	-1.33291500
H	-2.19615700	0.56815100	-2.17941500
H	-1.46373400	-1.45604900	1.55965800
H	-3.80968900	-2.25832600	1.57993200
H	-5.36027700	-1.63912500	-0.26328000
H	-4.54780900	-0.22119300	-2.14005900
I	-0.44388200	2.01771500	0.65321100



TS_{RE_TMEDA}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -863.7147470000001 A.U.

Thermal correction to Gibbs Free Energy =

0.282897 A.U.

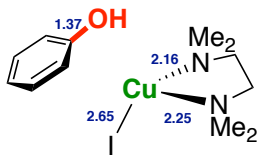
Sum of electronic and thermal Free Energies =

-863.43185 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -863.870894618 A.U.

Cu	-0.20984800	-0.30940500	0.50354200
N	-1.50192200	-1.28759300	-1.41369500
N	-2.26034100	0.05698200	1.17784100
C	-1.17352100	-0.78609600	-2.74573800
H	-1.24112200	0.30508000	-2.76172900
H	-0.15074700	-1.07489800	-3.00800200
C	-1.36785400	-2.74395100	-1.40315800
H	-2.00606700	-3.20602800	-2.17605400
H	-0.32923600	-3.02631400	-1.60025900
H	-1.65519800	-3.15446600	-0.43225600
C	-2.86800600	-0.89535100	-1.04332400
H	-3.04466500	0.11688700	-1.42010400
H	-3.60781200	-1.55239600	-1.53173500
C	-3.08837200	-0.93357600	0.46232200
H	-2.83243600	-1.92238200	0.85657700
H	-4.15300900	-0.75757700	0.68382900
C	-2.79076200	1.41246400	0.97646500
H	-3.82937200	1.47133300	1.33690900
H	-2.18087400	2.12728400	1.53360800
H	-2.76298100	1.69133800	-0.07756400
C	-2.28559200	-0.23561000	2.61809500
H	-3.31229700	-0.17486700	3.01053900
H	-1.89429400	-1.23848800	2.79895800
H	-1.66343300	0.49176600	3.14748500
H	-1.85580500	-1.19391500	-3.51177400
O	0.01571900	-1.95545400	1.42800900
H	0.24543700	-2.66664500	0.80830100
C	2.48043400	-0.42872200	1.51149600
C	1.66627300	-0.85503700	0.47646300
C	2.13006300	-1.40386100	-0.70407700
C	3.51895700	-1.49102600	-0.86843100
C	4.38005400	-1.04866700	0.13444700
C	3.86101100	-0.51915600	1.31933800
H	2.06513800	-0.02767300	2.43078500
H	1.45608100	-1.73063500	-1.48974000
H	3.91563300	-1.90387400	-1.79161700
H	5.45452900	-1.12131300	-0.00214600
H	4.52820400	-0.17851200	2.10598500
I	0.45988400	2.10431100	-0.52243800



INT_{3_TMEDA}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -863.829736 A.U.

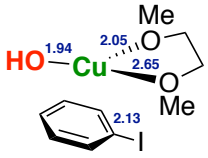
Thermal correction to Gibbs Free Energy = 0.283848 A.U.

Sum of electronic and thermal Free Energies = -863.545888 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -863.984682712 A.U.

Cu	-0.67264400	0.09469700	-0.15641400
N	-2.14145700	-0.93544600	-1.36493600
N	-2.30907200	0.21134300	1.37648500
C	-2.11340900	-0.49358700	-2.76386500
H	-2.19026400	0.59609700	-2.80694100
H	-1.16937400	-0.79793400	-3.22367900
C	-2.00749700	-2.39614100	-1.31778900
H	-2.88773200	-2.88462600	-1.76696200
H	-1.12105800	-2.69685200	-1.88121400
H	-1.89809000	-2.74597600	-0.28772600
C	-3.40689800	-0.50771900	-0.73848400
H	-3.59171600	0.52840400	-1.03844600
H	-4.24366600	-1.11411600	-1.12215100
C	-3.37303500	-0.61187100	0.78085300
H	-3.20042200	-1.65045900	1.08016500
H	-4.35836600	-0.31825800	1.18024800
C	-2.67371100	1.63222100	1.36218800
H	-3.60622700	1.80710800	1.92466800
H	-1.87069300	2.21611100	1.82074800
H	-2.80835900	1.98736900	0.33721100
C	-2.06885300	-0.20706100	2.75829600
H	-2.96292400	-0.04822200	3.38449700
H	-1.80672300	-1.26757800	2.78693700
H	-1.24132600	0.37186600	3.17867500
H	-2.94524900	-0.93316600	-3.33826700
O	0.57835100	-1.82463000	1.74175800
H	-0.18836200	-2.03750100	1.17805000
C	2.86204800	-1.22762200	1.58386500
C	1.70819500	-1.71438400	0.96958600
C	1.71443600	-2.06127700	-0.38202000
C	2.88088700	-1.89388400	-1.12758900
C	4.03790600	-1.39229100	-0.53014100
C	4.02169900	-1.06646600	0.82808300
H	2.83360200	-0.96256600	2.63676000
H	0.80890300	-2.44974100	-0.84108400
H	2.87954300	-2.15566700	-2.18182400
H	4.94295800	-1.25945100	-1.11448400
H	4.91670900	-0.67675300	1.30445300
I	1.17456200	1.98211200	-0.36276300



INT_{1_DME}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -824.887853 A.U.

Thermal correction to Gibbs Free Energy = 0.197285 A.U.

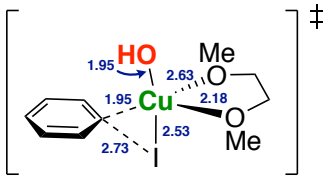
Sum of electronic and thermal Free Energies = -824.690568 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -825.044271115 A.U.

Cu	0.74507900	-1.23227100	0.01607000
C	2.97984700	0.28895900	1.28739500
H	2.60377800	1.31147900	1.14528000
H	3.67742200	0.27661000	2.13327200
C	3.66878800	-0.20800400	0.04263900
H	3.87698700	-1.28322200	0.14203000
H	4.62109400	0.32202200	-0.09311600
C	-2.78830800	-0.06389400	-1.11153100

C	-2.02037700	0.32204500	-0.01579200
C	-2.17500200	-0.28455200	1.22898200
C	-3.11456200	-1.30768100	1.37166300
C	-3.88781200	-1.71167300	0.28326200
C	-3.72502700	-1.08732000	-0.95335200
H	-2.65558300	0.41355100	-2.07704000
H	-1.57682200	0.03137000	2.07757700
H	-3.23744200	-1.78599500	2.33901700
H	-4.61572000	-2.50891400	0.39891800
H	-4.32402000	-1.39602200	-1.80510200
I	-0.55761000	1.84733700	-0.25370100
O	1.88534400	-0.58128200	1.58508100
O	2.81689900	0.01863600	-1.06757700
C	3.17575000	-0.75685600	-2.19767100
H	2.46456500	-0.52099300	-2.99165100
H	4.19254800	-0.51305000	-2.53234300
H	3.12077700	-1.82835800	-1.96337600
C	1.19936000	-0.19876800	2.77429300
H	0.43040600	-0.94987700	2.95831200
H	1.90454500	-0.17521600	3.61284600
H	0.74070200	0.78915400	2.64970600
O	-0.16262100	-2.14545800	-1.43940600
H	0.52989100	-2.64427000	-1.89829400



TS_{OA_DME}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -824.854112 A.U.

Thermal correction to Gibbs Free Energy =

0.201554 A.U.

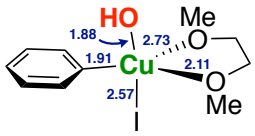
Sum of electronic and thermal Free Energies =

-824.652558 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -825.010388206 A.U.

Cu	0.25798000	-0.57123500	-0.36329000
C	3.02048900	-0.32760800	1.25993500
H	2.97726900	0.76369700	1.12799500
H	3.82865400	-0.56427100	1.96539400
C	3.29311400	-0.99915500	-0.06088800
H	3.21748500	-2.09149400	0.03517700
H	4.30017900	-0.73974300	-0.40985200
C	-2.47045900	-0.47922900	-1.15207500
C	-1.65300300	-0.32353600	-0.04253500
C	-2.07657300	-0.54195900	1.25899200
C	-3.39510000	-0.96886600	1.44998000
C	-4.24609300	-1.14885500	0.35919000
C	-3.78436400	-0.90565500	-0.93529100
H	-2.10724200	-0.28292700	-2.15576200
H	-1.41443200	-0.38842400	2.10488100
H	-3.74984300	-1.15303200	2.46003800
H	-5.26987800	-1.47347100	0.51764100
H	-4.44368500	-1.04149100	-1.78783700
I	-0.12290000	1.92911100	-0.23798600
O	1.78236100	-0.80099400	1.76505000
O	2.33672700	-0.54061400	-1.01329400
C	2.54187100	-1.11364100	-2.30138100
H	1.75511500	-0.72935700	-2.95274200
H	3.52394300	-0.81630500	-2.68559400
H	2.48160800	-2.20710400	-2.25094600
C	1.41032600	-0.12567500	2.95522400
H	0.50518000	-0.60265600	3.33403400
H	2.20476200	-0.20957300	3.70814900
H	1.21443200	0.93576300	2.75427800
O	0.03375900	-2.48914000	-0.59803200
H	0.94469700	-2.82563700	-0.59287800



INT_{2_DME}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -824.854442 A.U.

Thermal correction to Gibbs Free Energy =

0.201685 A.U.

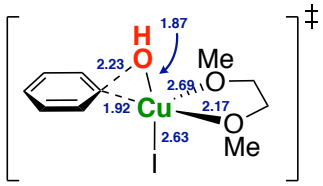
Sum of electronic and thermal Free Energies =

-824.652757 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -825.010022038 A.U.

Cu	0.22503700	-0.58321600	-0.36060400
C	2.99823400	-0.37907600	1.26407000
H	2.98517800	0.71059500	1.11434300
H	3.80262200	-0.62764900	1.96969300
C	3.24527200	-1.07929400	-0.04639800
H	3.15171200	-2.16833400	0.06850300
H	4.25148300	-0.84279000	-0.41245000
C	-2.49420700	-0.56912400	-1.15556100
C	-1.66889200	-0.47895200	-0.04849900
C	-2.10607700	-0.60600000	1.25758300
C	-3.46994900	-0.84811800	1.46006300
C	-4.33945400	-0.94829700	0.37361800
C	-3.85362200	-0.81067000	-0.92735200
H	-2.10977300	-0.45578000	-2.16430300
H	-1.42543100	-0.51778300	2.09834900
H	-3.84352200	-0.95297300	2.47467700
H	-5.39649000	-1.13134300	0.54063500
H	-4.52729000	-0.88628200	-1.77618100
I	-0.02059900	1.95654100	-0.25979500
O	1.74894000	-0.80899800	1.78059500
O	2.28578200	-0.61984300	-0.99777400
C	2.48192600	-1.19947400	-2.28616900
H	1.69737800	-0.80893000	-2.93623200
H	3.46605600	-0.91178300	-2.67122600
H	2.41116400	-2.29202900	-2.23158900
C	1.39909400	-0.09914100	2.95766100
H	0.47745800	-0.53656800	3.34449900
H	2.18972900	-0.19637400	3.71294300
H	1.24042200	0.96427700	2.73618700
O	-0.01655700	-2.47303300	-0.56051000
H	0.89568400	-2.80577300	-0.51378900



TS_{RE_DME}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -824.851813 A.U.

Thermal correction to Gibbs Free Energy =

0.199931 A.U.

Sum of electronic and thermal Free Energies =

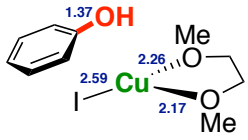
-824.651882 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -825.006833789 A.U.

Cu	0.22405600	-0.51043900	-0.55196300
C	2.86070100	-0.79297700	1.37612700
H	3.11003800	0.27829600	1.38001800
H	3.52351700	-1.30880500	2.08465100
C	3.06588400	-1.35764400	-0.00485300
H	2.70087500	-2.39244100	-0.06821000
H	4.13426200	-1.34068500	-0.25221400
C	-2.53232500	-0.52390900	-1.24048300
C	-1.64177500	-0.85422800	-0.23598600
C	-1.99613000	-1.17838300	1.05887300
C	-3.35847500	-1.11406500	1.37813400
C	-4.29662000	-0.75614300	0.41028000
C	-3.88513400	-0.46660000	-0.89289000
H	-2.19887200	-0.30012700	-2.24866800
H	-1.25706600	-1.46360400	1.80095500
H	-3.67430400	-1.34835200	2.39062300
H	-5.35007400	-0.70956600	0.66793000
H	-4.61372000	-0.19306900	-1.65059500
I	0.06396300	2.07240800	-0.06372800
O	1.50711700	-0.96956400	1.76274800
O	2.35991300	-0.54695800	-0.94305200
C	2.62477500	-0.93562700	-2.28871900
H	2.02747900	-0.28812700	-2.93300700
H	3.68980500	-0.80295600	-2.50778200

H	2.34279900	-1.98265700	-2.44904000
C	1.22425300	-0.29175500	2.97591900
H	0.16548000	-0.43459400	3.19919000
H	1.82901700	-0.70217500	3.79507300
H	1.43259500	0.78135700	2.87732800
O	-0.12439100	-2.28448400	-1.03410100
H	-0.08153400	-2.79136900	-0.20489700



INT_{3_DME}

at M06-2X/6-31+G*&SDD (for Cu & I)/SMD(water)

Energy = -824.964148 A.U.

Thermal correction to Gibbs Free Energy =

0.202519 A.U.

Sum of electronic and thermal Free Energies =

-824.761629 A.U.

at M06-2X/6-311+G*&SDD (for Cu & I)/SMD(water)

Energy = -825.118493765 A.U.

Cu	0.83459700	0.65678100	0.00786300
C	3.40947000	-0.55303300	0.95700900
H	3.72440000	0.42119100	1.35328300
H	4.03098300	-1.34082300	1.39956500
C	3.53023700	-0.57609000	-0.54592000
H	3.19919400	-1.54205200	-0.95077800
H	4.57345400	-0.40833700	-0.84070200
C	-1.59105200	-2.00781900	-1.52137400
C	-0.70870800	-2.12428300	-0.44628800
C	-1.19157800	-2.19525100	0.86233500
C	-2.56473400	-2.12294600	1.09270900
C	-3.45671100	-1.99529600	0.02687500
C	-2.96201800	-1.94379100	-1.27826400
H	-1.19468600	-1.95200900	-2.53129200
H	-0.49137700	-2.30616600	1.68648000
H	-2.93578700	-2.16958000	2.11263000
H	-4.52504500	-1.93823900	0.21066700
H	-3.64690700	-1.84487700	-2.11559200
I	-1.45048900	1.86488600	0.12403000
O	2.03912700	-0.76907900	1.28977900
O	2.70828300	0.46513900	-1.06302700
C	2.57583900	0.40764100	-2.47933900
H	1.95388900	1.25306200	-2.77689700
H	3.56133300	0.48522500	-2.95303500
H	2.09539700	-0.53127100	-2.77903000
C	1.78971600	-0.63490800	2.68537400
H	0.71437900	-0.73819400	2.83607300
H	2.32365000	-1.41455500	3.24056800
H	2.11466000	0.35301400	3.03082600
O	0.63456300	-2.17342800	-0.71785000
H	1.13651500	-1.91839400	0.08570700

6. Reference

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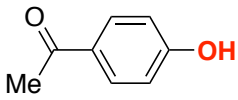
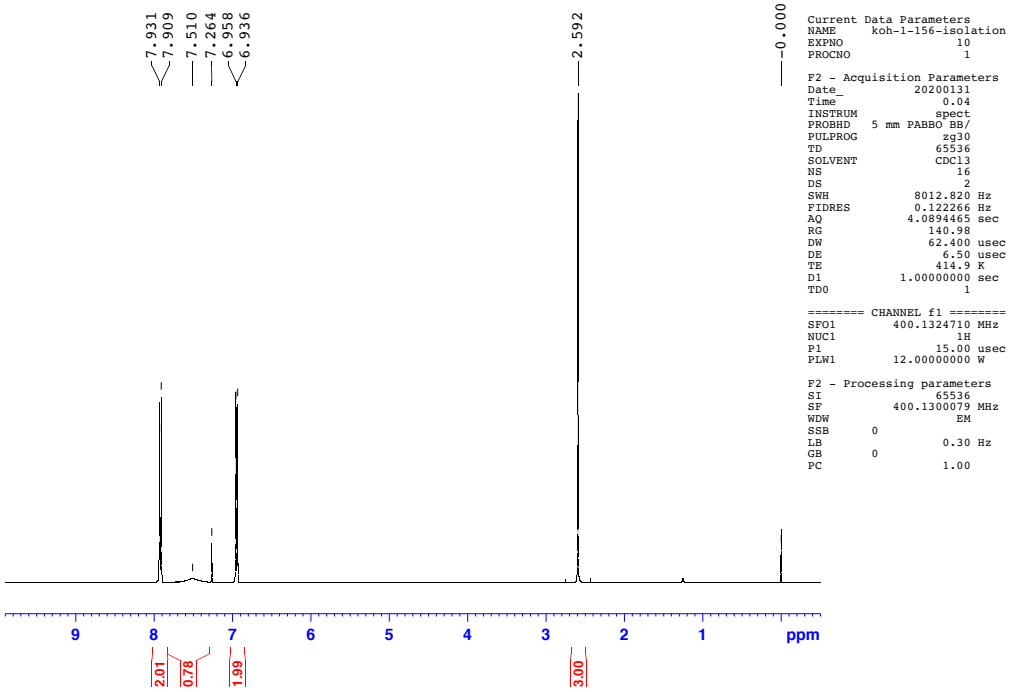
7. Copies for NMR spectra

4-Acetylphenol (2a)



^{1}H NMR

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PROCNO                      1

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PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                    140.98
DW                  62.400 usec
DE                   6.50 usec
TE                   414.9 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
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NUC1                      1H
P1                     15.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
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WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
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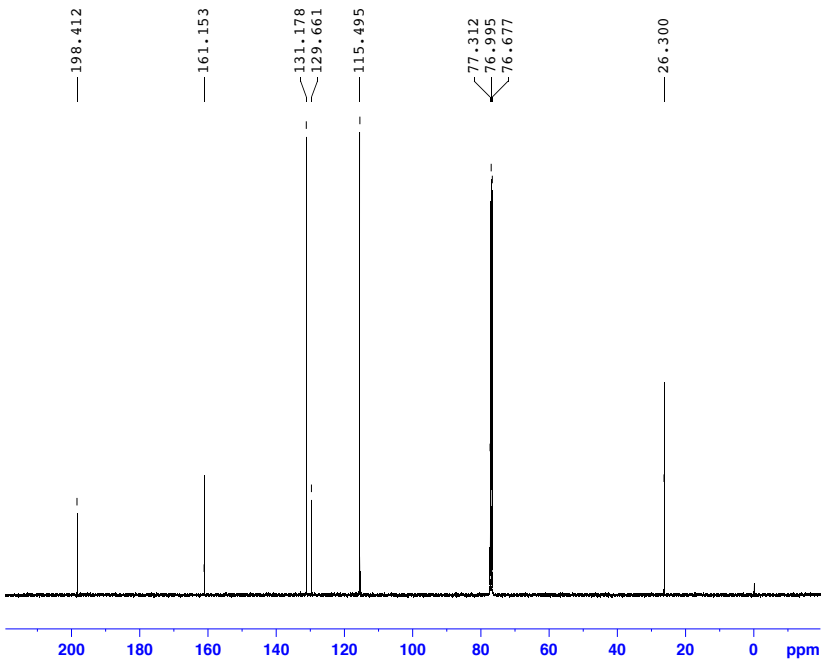
^{13}C NMR

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EXPNO                      11
PROCNO                      1

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INSTRUM               spect
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PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    196.64
DW                  20.800 usec
DE                   6.50 usec
TE                   426.1 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                     13C
P1                     10.00 usec
PLW1          52.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                      1H
CPDPRG[2           waltz16
PCPD2                  90.00 usec
PLW2          12.00000000 W
PLW12          0.33333001 W
PLW13          0.27000001 W

F2 - Processing parameters
SI                       32768
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WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
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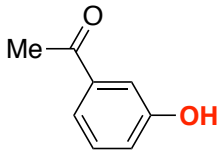
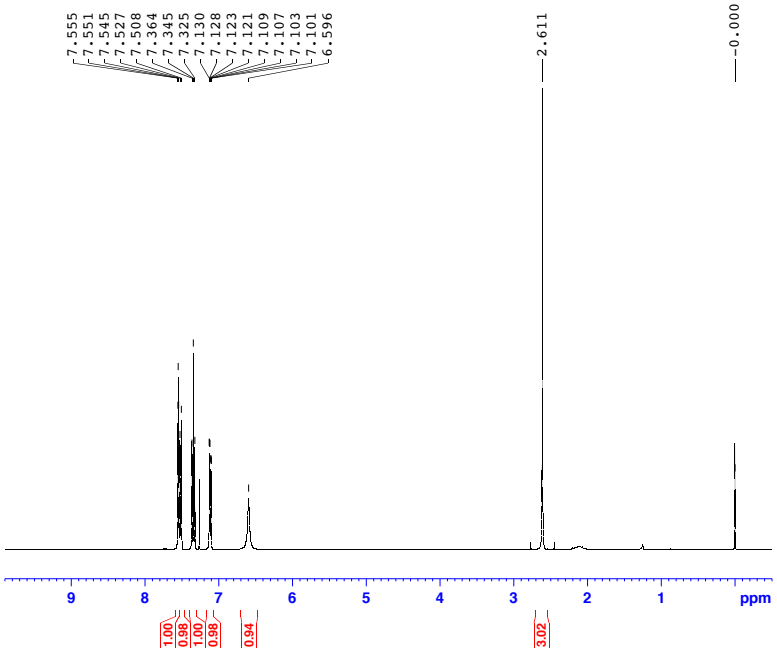
3-Acetylphenol (2b)



^{1}H NMR



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EXPNO 10
PROCNO 1

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INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 154.67
DW 62.400 usec
DE 6.50 usec
TE 427.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W

F2 - Processing parameters
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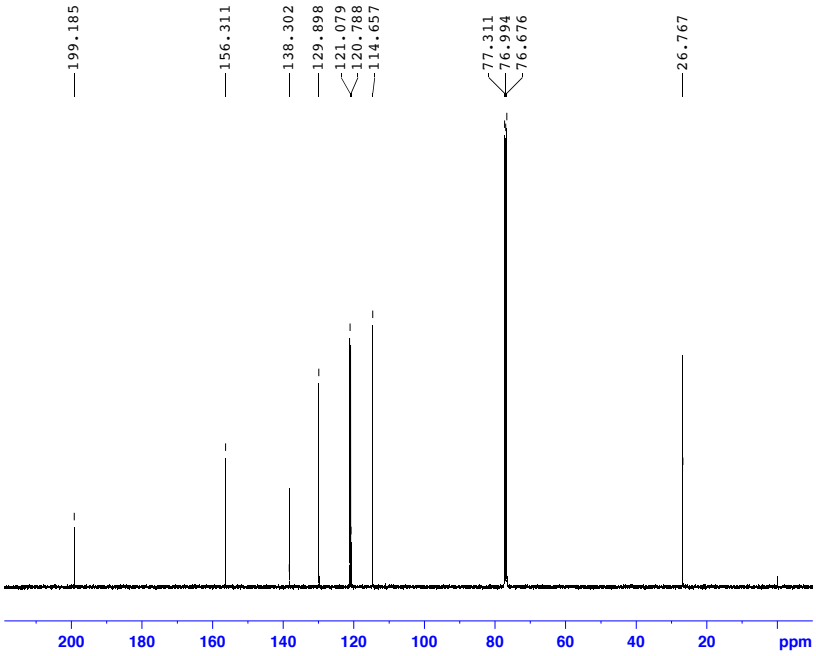
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR



Current Data Parameters
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PROCNO 1

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INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.64
DW 20.800 usec
DE 6.50 usec
TE 429.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.33333001 W
PLW13 0.27000001 W

F2 - Processing parameters
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WDW EM
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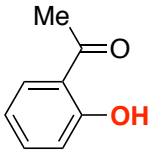
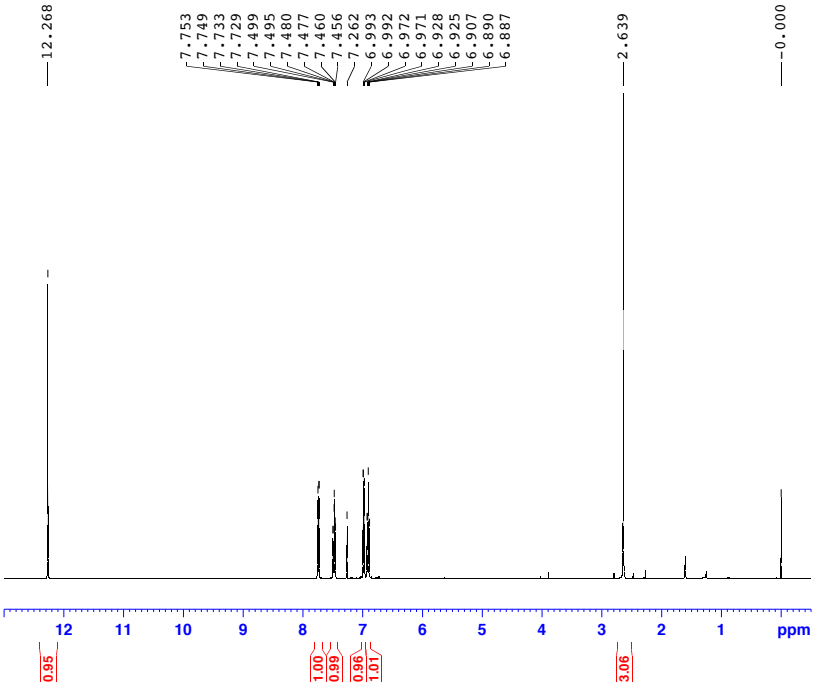
GB 0
PC 1.40

2-Acetylphenol (2c)



^{1}H NMR

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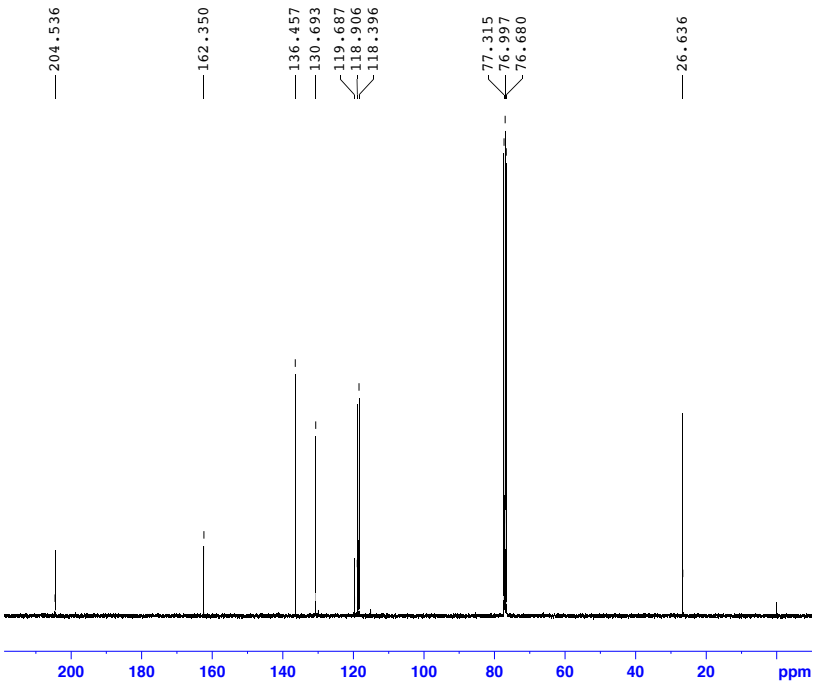
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                     154.67
DW                    62.400 usec
DE                     6.50 usec
TE                     427.8 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                      1H
P1                     15.00 usec
PLW1           12.00000000 W

F2 - Processing parameters
SI                      65536
SF             400.1300088 MHz
WDW                        EM
SSB       0
LB                      0.30 Hz
GB        0
PC                      1.00
```

^{13}C NMR

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EXPNO                        11
PROCNO                        1

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Time                      3.10
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     196.64
DW                    20.800 usec
DE                     6.50 usec
TE                     423.7 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1           100.6228293 MHz
NUC1                      13C
P1                     10.00 usec
PLW1           52.00000000 W

======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2           12.00000000 W
PLW12           0.33333001 W
PLW13           0.27000001 W

F2 - Processing parameters
SI                      32768
SF             100.6127728 MHz
WDW                        EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
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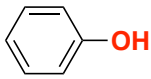
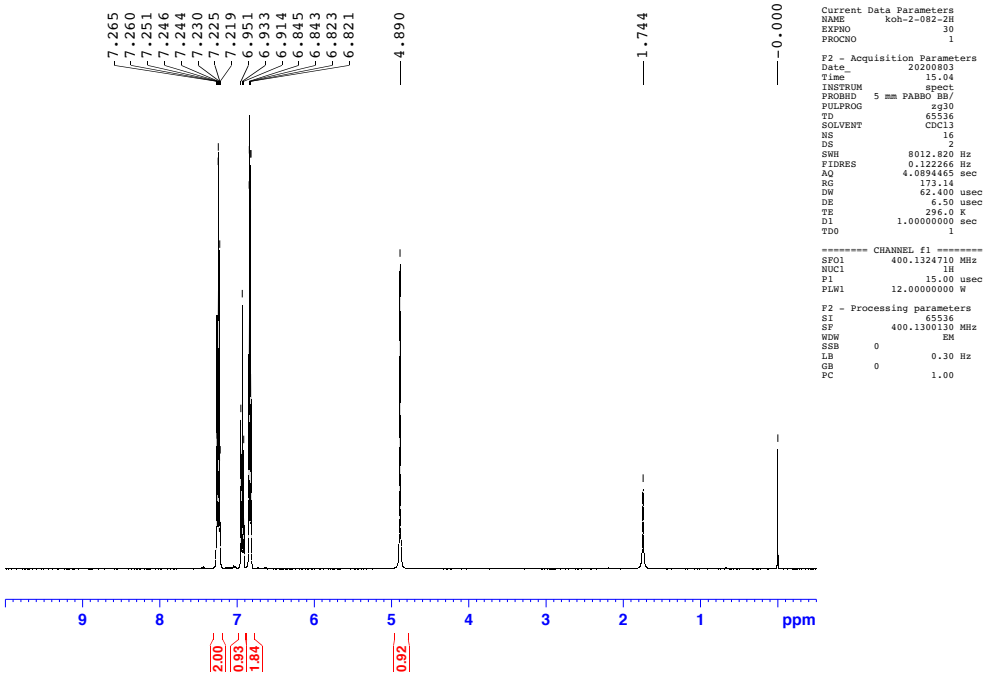
Phenol (2d)



^{1}H NMR

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EXPNO                 30
PROCNO                 1

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INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                173.14
DW              62.400 usec
DE               6.50 usec
TE              296.0 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
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NUC1               1H
P1                15.00 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                65536
SF           400.1300130 MHz
WDW                  EM
SSB       0
LB              0.30 Hz
GB        0
PC                1.00
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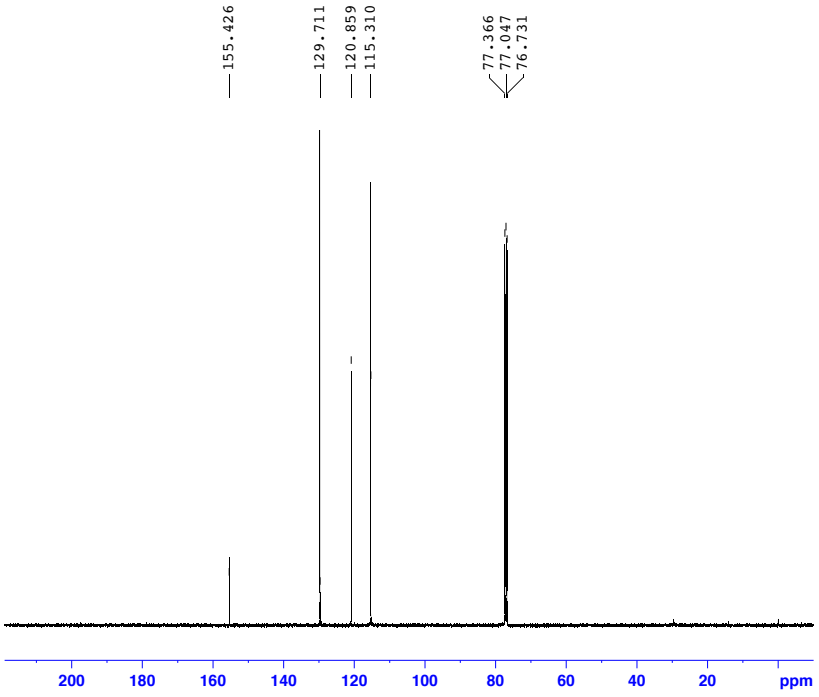
^{13}C NMR

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TD               65536
SOLVENT          CDCl3
NS                1024
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG                196.64
DW              20.800 usec
DE               6.50 usec
TE          0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1               13C
P1                10.00 usec
PLW1         52.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.33333001 W
PLW13         0.27000001 W

F2 - Processing parameters
SI                32768
SF           100.6127685 MHz
WDW                  EM
SSB       0
LB              1.00 Hz
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PC                1.40
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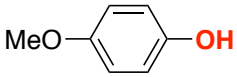
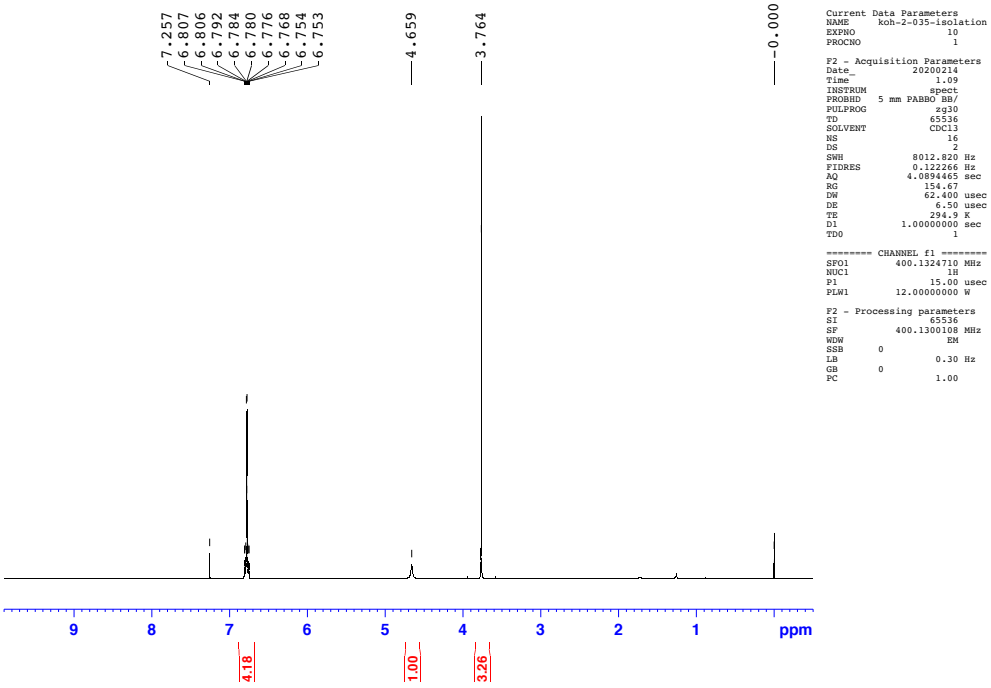
4-Methoxyphenol (2e)



^{1}H NMR

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EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
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Time                   1.09
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PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894465 sec
RG                    154.67
DW                  62.400 usec
DE                   6.50 usec
TE                   294.9 K
D1              1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
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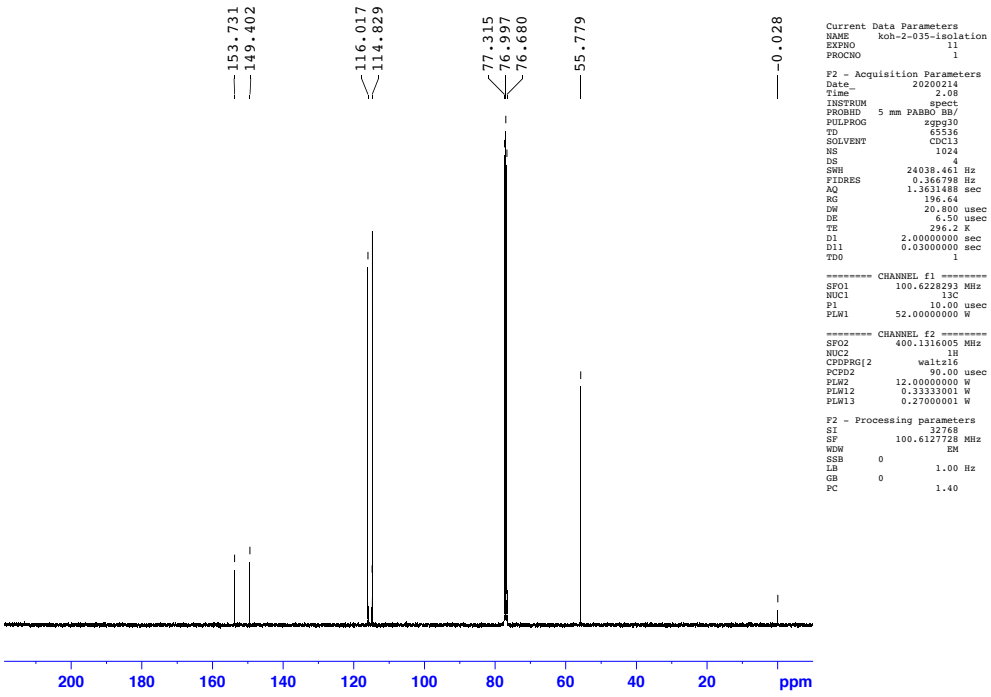
NUC1                     1H
P1                    15.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                       65536
SF            400.1300108 MHz
WDW                         EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```

^{13}C NMR

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PROCNO                      1

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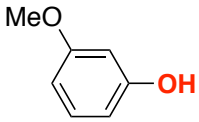
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES               0.366798 Hz
AQ                1.3631488 sec
RG                    196.64
DW                  20.800 usec
DE                   6.50 usec
TE                   296.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                    13C
P1                    10.00 usec
PLW1          52.00000000 W

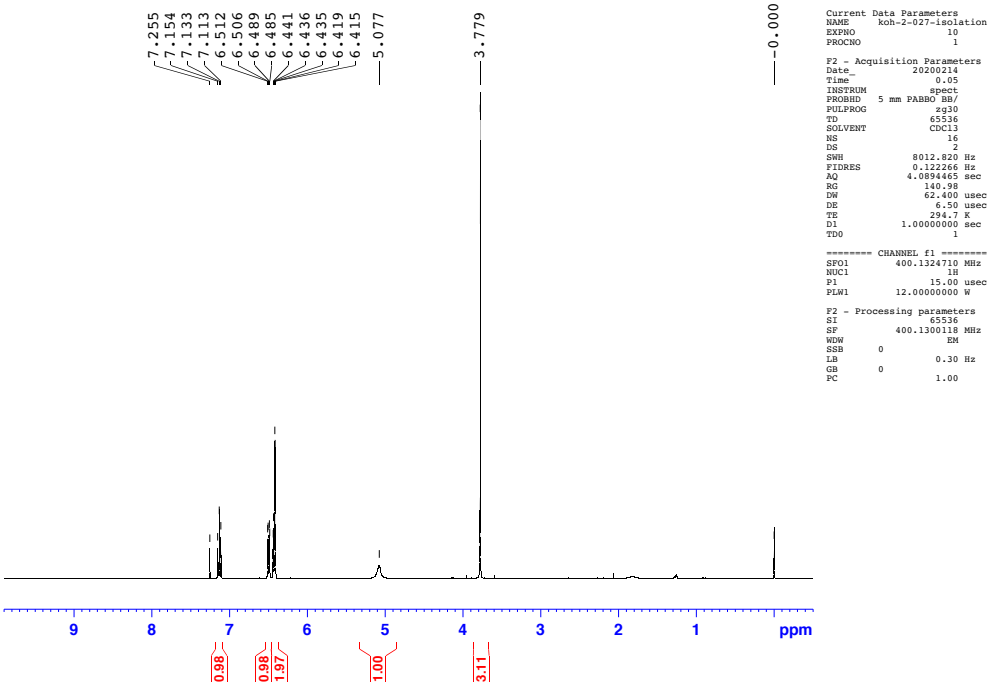
======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                 90.00 usec
PLW2          12.00000000 W
PLW12          0.33333001 W
PLW13          0.27000001 W

F2 - Processing parameters
SI                       32768
SF            100.6127728 MHz
WDW                         EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

3-Methoxyphenol (2f)



^{1}H NMR



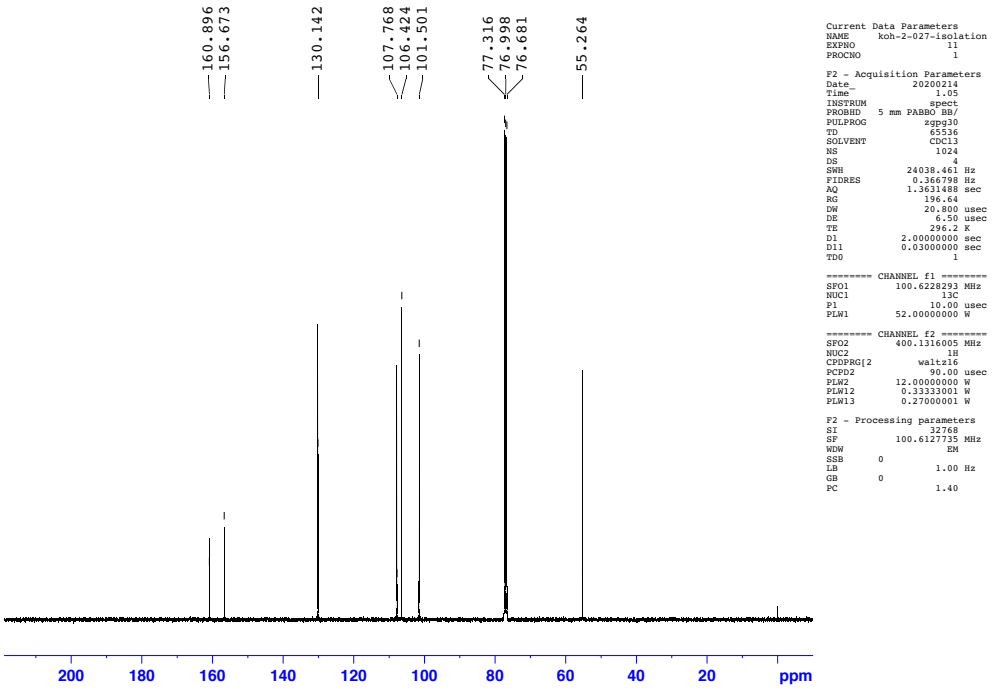

```
Current Data Parameters
NAME      koh-2-027-isolation
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_              20200214
Time                   0.05
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894465 sec
RG                   140.98
DW                  62.400 usec
DE                   6.50 usec
TE                  294.7 K
D1              1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                    15.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                       65536
SF             400.1300118 MHz
WDW                         EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

^{13}C NMR




```
Current Data Parameters
NAME      koh-2-027-isolation
EXPNO                      11
PROCNO                      1

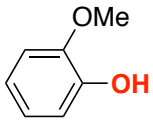
F2 - Acquisition Parameters
Date_              20200214
Time                   1.05
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES               0.366798 Hz
AQ                1.3631488 sec
RG                   196.64
DW                  20.800 usec
DE                   6.50 usec
TE                  296.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1           100.6228293 MHz
NUC1                    13C
P1                    10.00 usec
PLW1          52.00000000 W

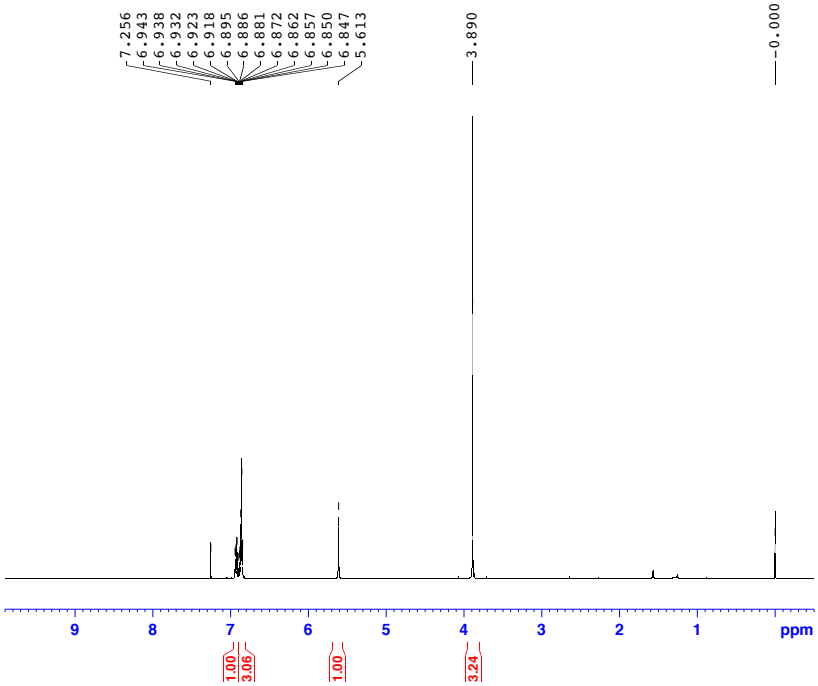
======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                90.00 usec
PLW2          12.00000000 W
PLW12          0.33333001 W
PLW13          0.27000001 W

F2 - Processing parameters
SI                       32768
SF             100.6127735 MHz
WDW                         EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

2-Methoxyphenol (2g)



^{1}H NMR



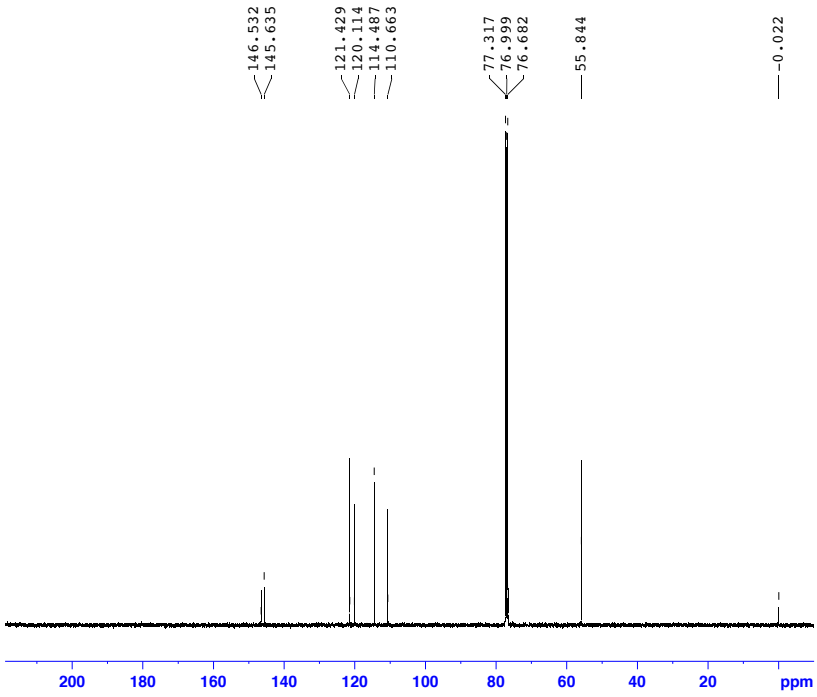

```
Current Data Parameters
NAME      koh-2-045-isolation
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_            20200214
Time               2.13
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES            0.122266 Hz
AQ             4.0894465 sec
RG                 196.64
DW                62.400 usec
DE                 6.50 usec
TE                294.8 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                65536
SF            400.1300115 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C NMR




```
Current Data Parameters
NAME      koh-2-045-isolation
EXPNO                      11
PROCNO                      1

F2 - Acquisition Parameters
Date_            20200214
Time               3.12
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES            0.366798 Hz
AQ             1.3631488 sec
RG                 196.64
DW                20.800 usec
DE                 6.50 usec
TE                296.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

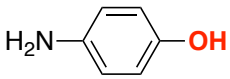
======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          52.00000000 W

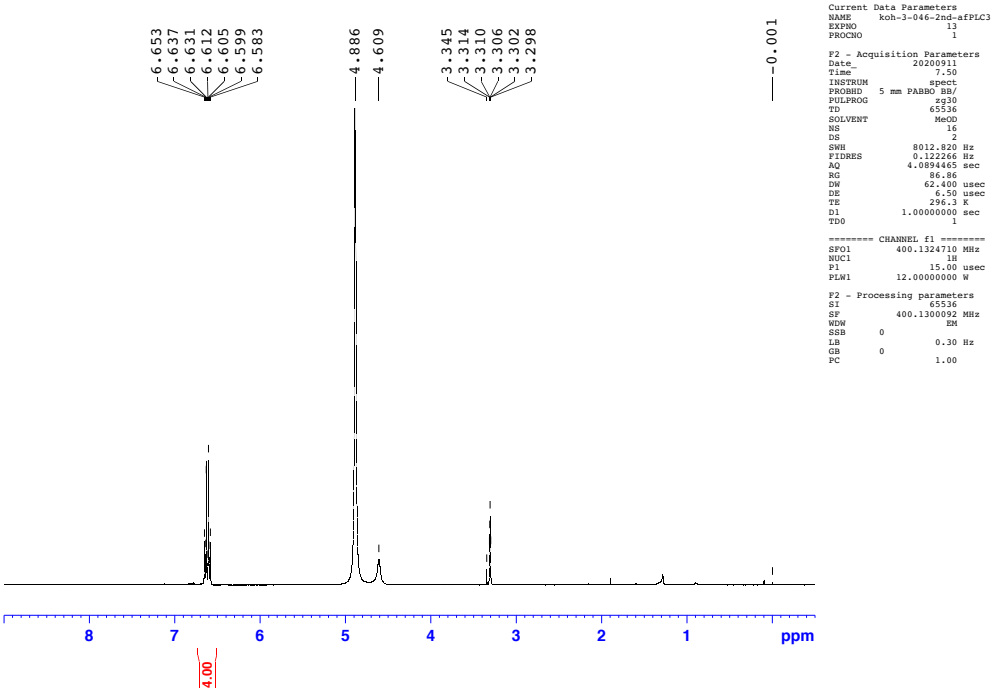
======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.33333001 W
PLW13          0.27000001 W

F2 - Processing parameters
SI                32768
SF            100.6127721 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

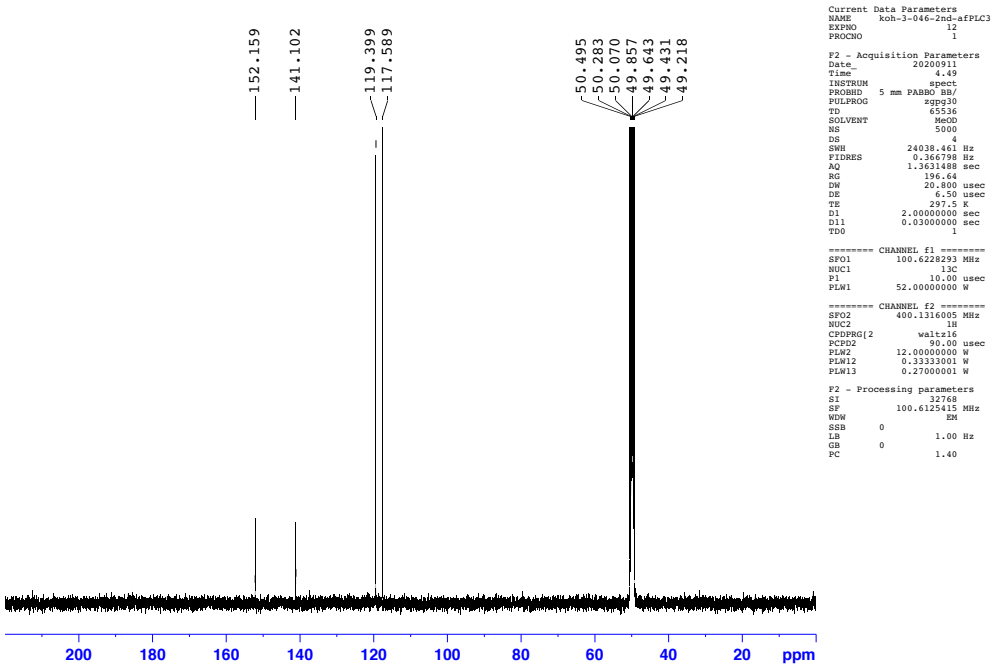
4-Aminophenol (2h)

^{1}H NMR

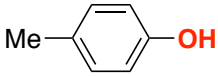




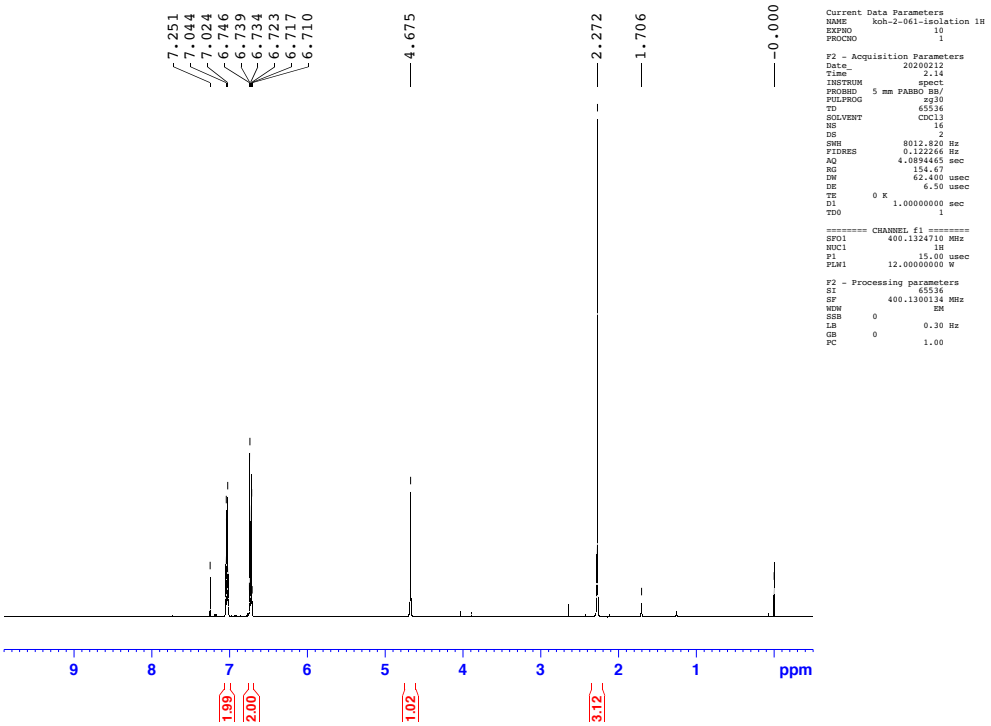
^{13}C NMR



4-Methylphenol (2i)



^{1}H NMR



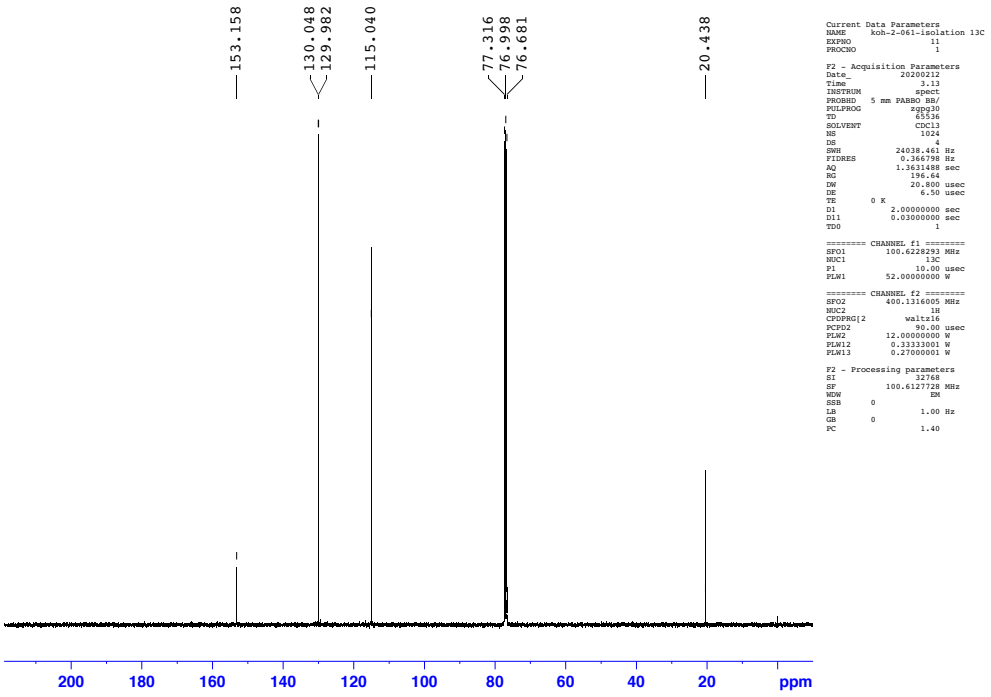
Current Data Parameters
NAME koh-2-061-isolation 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200212
Time 2.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 154.67
DW 62.400 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR



Current Data Parameters
NAME koh-2-061-isolation 13C
EXPNO 11
PROCNO 1

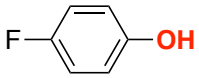
F2 - Acquisition Parameters
Date_ 20200212
Time 3.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.64
DW 20.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

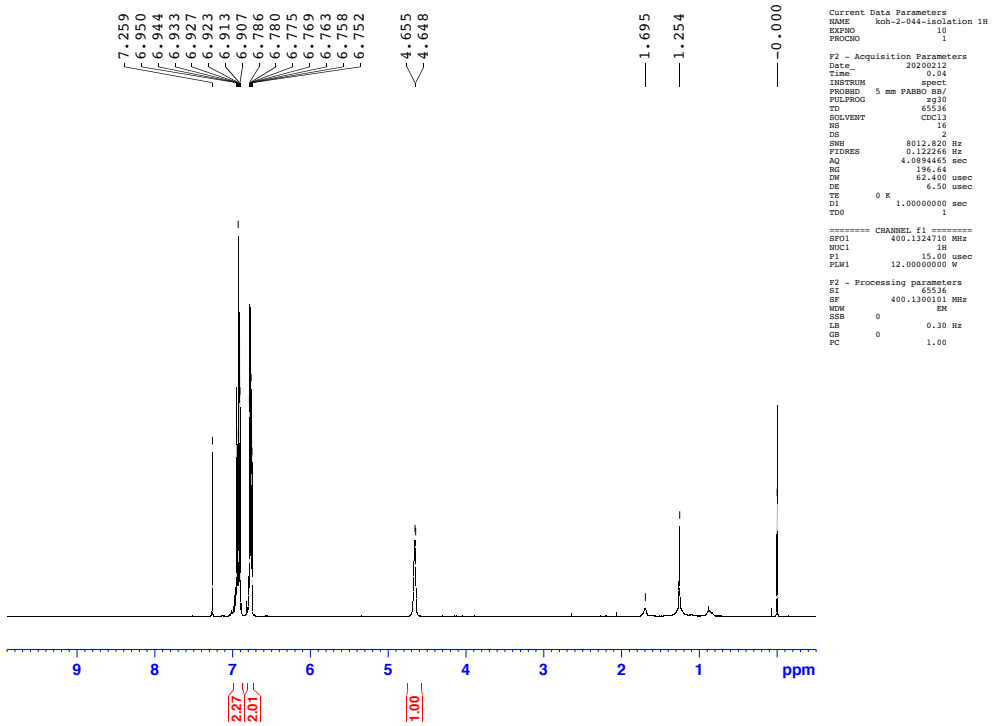
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.33333001 W
PLW13 0.27000001 W

F2 - Processing parameters
SI 32768
SF 100.6127728 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Fluorophenol (2j)



^{1}H NMR



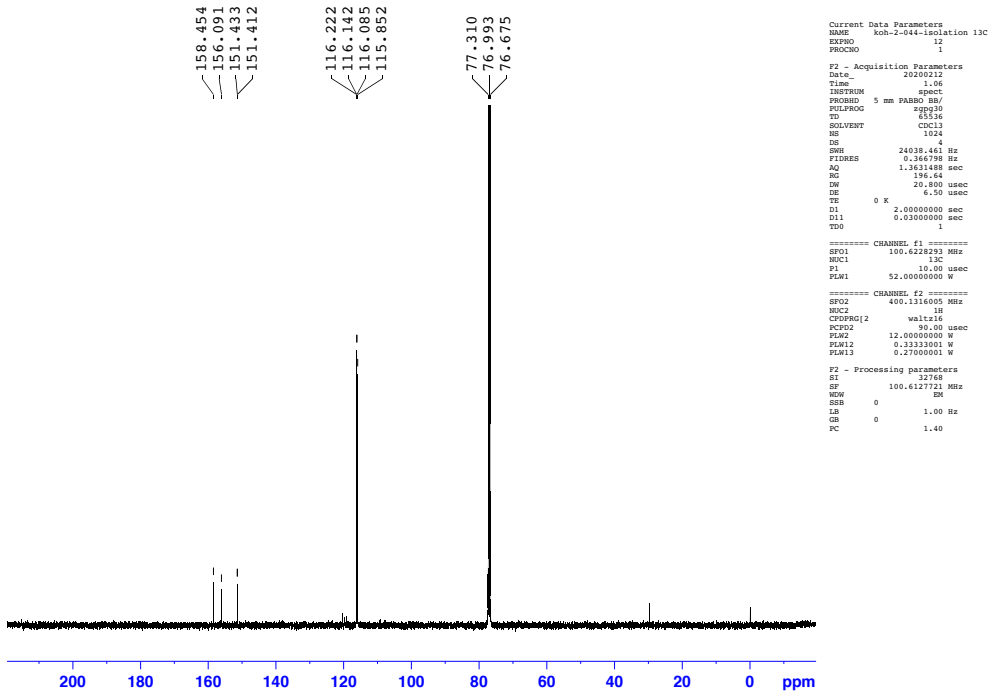
Current Data Parameters
NAME koh-2-044-isolation 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200212
Time 0.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 196.64
DW 62.400 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR



Current Data Parameters
NAME koh-2-044-isolation 13C
EXPNO 12
PROCNO 1

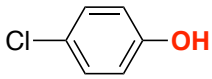
F2 - Acquisition Parameters
Date_ 20200212
Time 1.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.64
DW 20.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

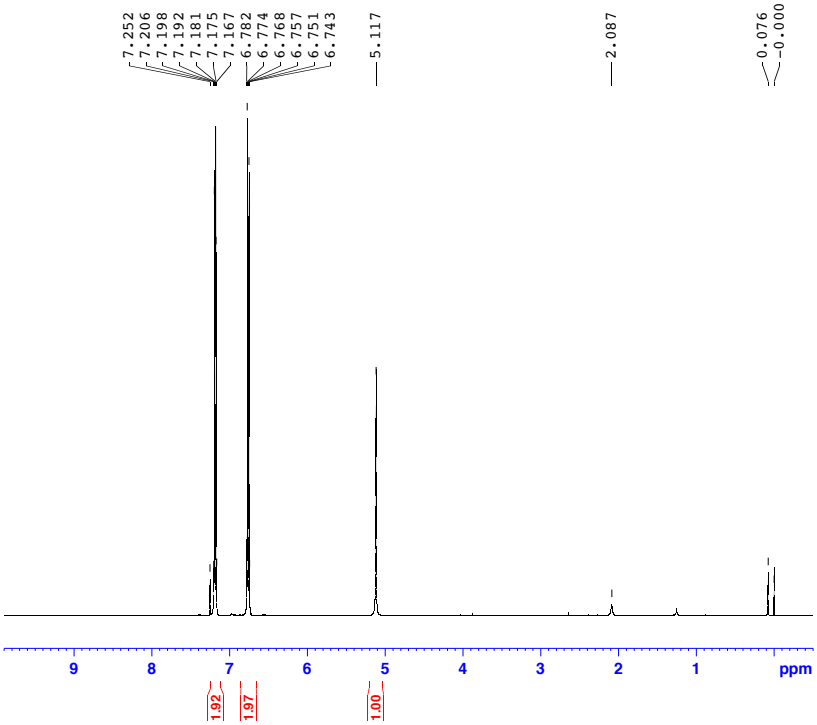
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.33333001 W
PLW13 0.27000001 W

F2 - Processing parameters
SI 32768
SF 100.6127721 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Chlorophenol (2k)



^{1}H NMR



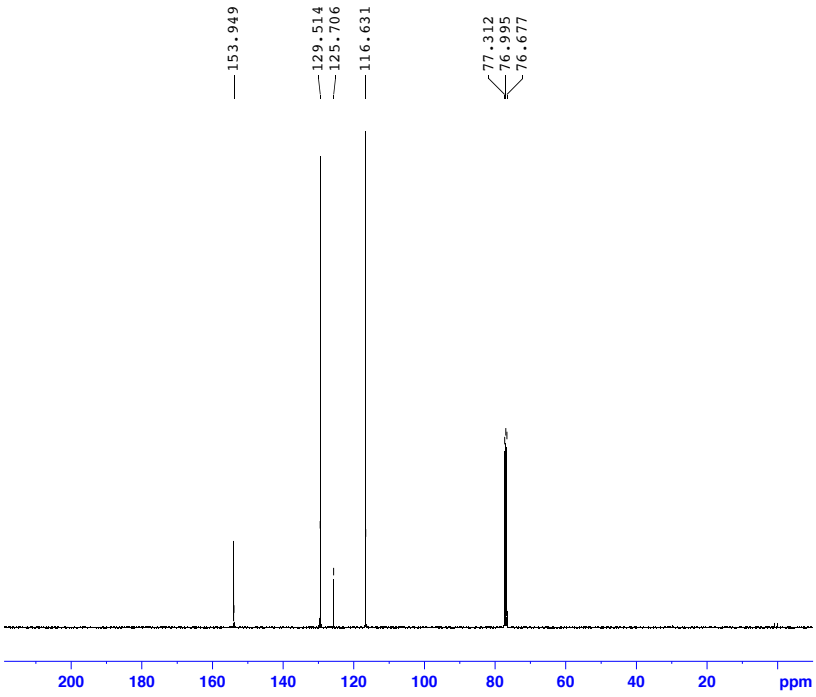
Current Data Parameters
NAME koh-2-047-isolation 1H
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200212
Time 1.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 110.61
DW 62.400 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR



Current Data Parameters
NAME koh-2-047-isolation 13C
EXPNO 22
PROCNO 1

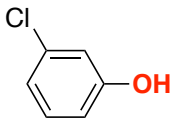
F2 - Acquisition Parameters
Date_ 20200212
Time 2.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.64
DW 20.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

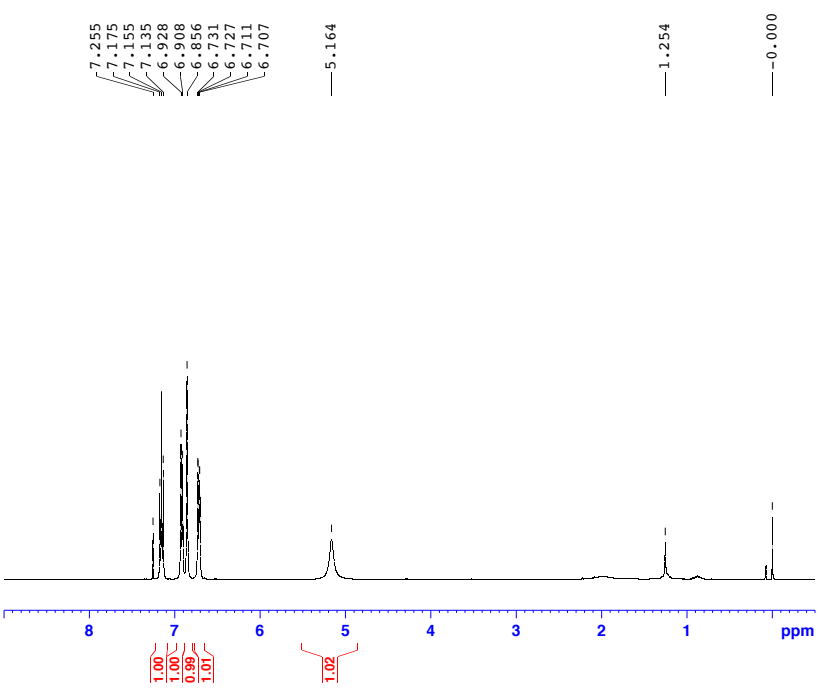
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.33333001 W
PLW13 0.27000001 W

F2 - Processing parameters
SI 32768
SF 100.6127750 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3-Chlorophenol (2l)



^{1}H NMR



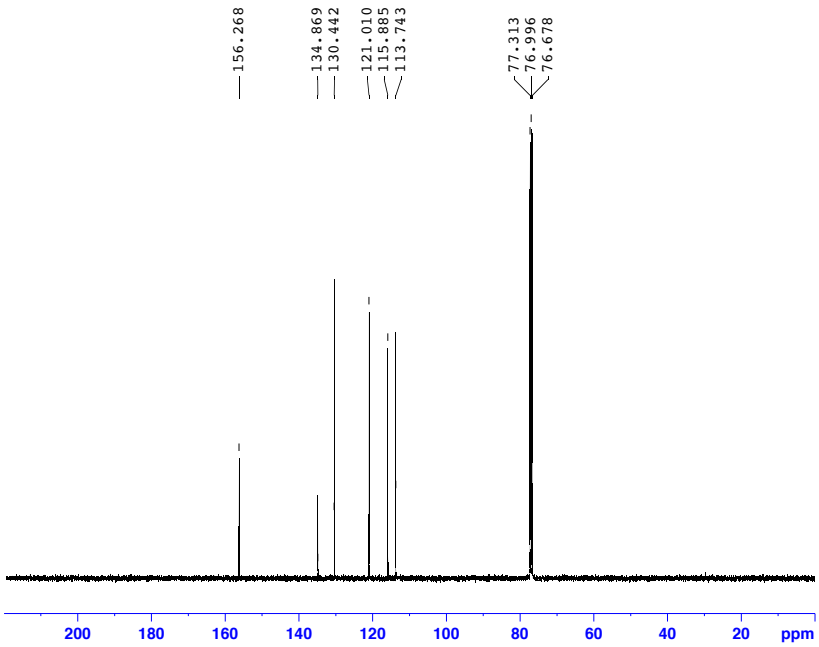

```
Current Data Parameters
NAME       koh-3-047-2nd-Fr11-14
EXPNO                         30
PROCNO                         1

F2 - Acquisition Parameters
Date_               20200911
Time                   21.26
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                    140.98
DW                   62.400 usec
DE                    6.50 usec
TE                   296.4 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                    15.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.1300118 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

^{13}C NMR




```
Current Data Parameters
NAME       koh-3-047-1st-afcolumn
EXPNO                         20
PROCNO                         1

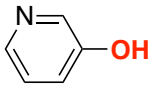
F2 - Acquisition Parameters
Date_               20200911
Time                   16.36
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG             zgpg30
TD                  65536
SOLVENT              CDCl3
NS                     512
DS                       4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    196.64
DW                   20.800 usec
DE                    6.50 usec
TE                   297.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           100.6228293 MHz
NUC1                     13C
P1                    10.00 usec
PLW1          52.00000000 W

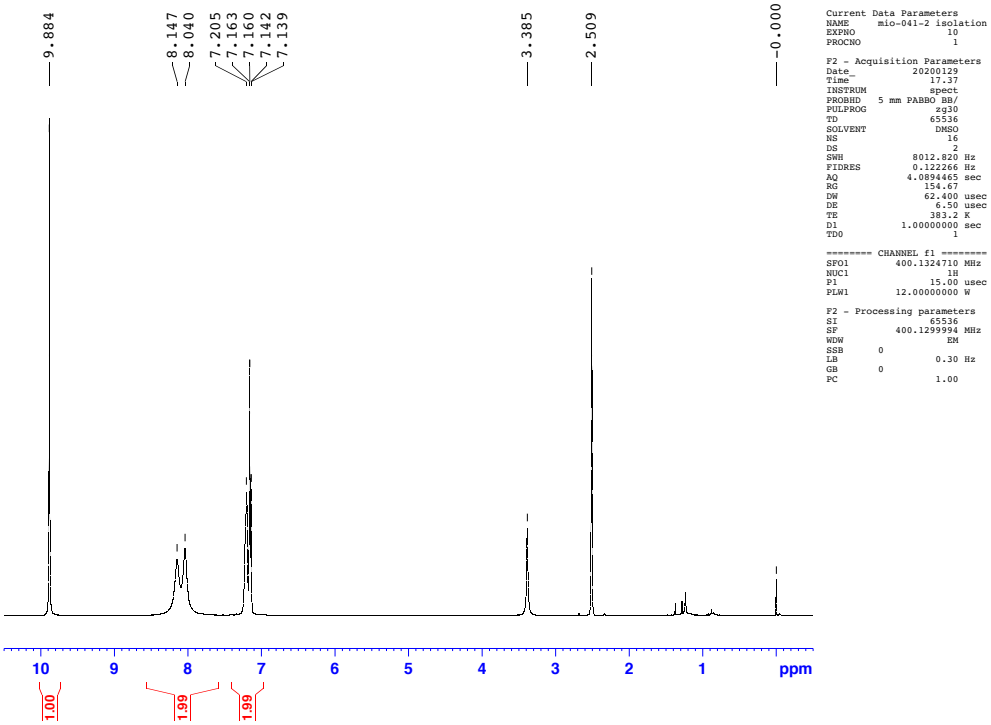
======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                     1H
CPDPRG[2            waltz16
PCPD2                 90.00 usec
PLW2          12.00000000 W
PLW12          0.33333001 W
PLW13          0.27000001 W

F2 - Processing parameters
SI                    32768
SF             100.6127734 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

3-Hydroxypyridine (2m)



^{1}H NMR



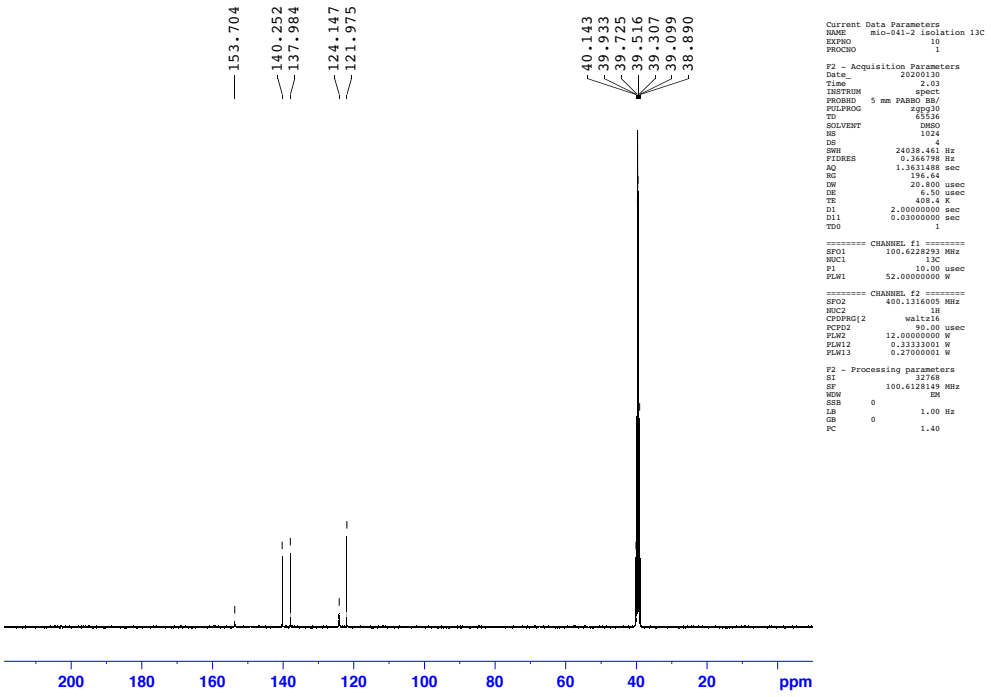

```
Current Data Parameters
NAME       mio-041-2 isolation
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_              20200129
Time               17.37
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  154.67
DW                62.400 usec
DE                 6.50 usec
TE                 383.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                     1H
P1                   15.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                   65536
SF            400.1299994 MHz
WDW                     EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   1.00
```

^{13}C NMR




```
Current Data Parameters
NAME      mio-041-2 isolation 13C
EXPNO                       10
PROCNO                       1

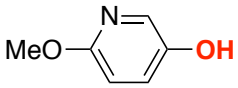
F2 - Acquisition Parameters
Date_              20200130
Time               2.03
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                  65536
SOLVENT              DMSO
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                  196.64
DW                20.800 usec
DE                 6.50 usec
TE                 408.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                    13C
P1                   10.00 usec
PLW1          52.00000000 W

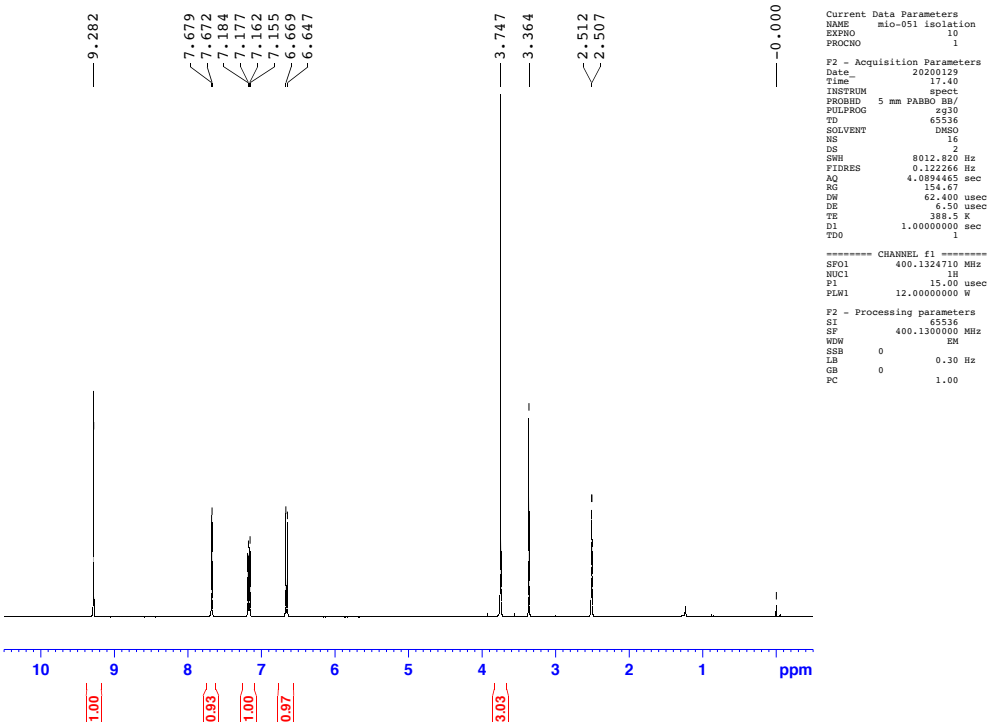
======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                90.00 usec
PLW2          12.00000000 W
PLW12          0.33333001 W
PLW13          0.27000001 W

F2 - Processing parameters
SI                   32768
SF            100.6128149 MHz
WDW                     EM
SSB                  0
LB                   1.00 Hz
GB                   0
PC                   1.40
```

5-Hydroxy-2-methoxypyridine (2n)



^{1}H NMR



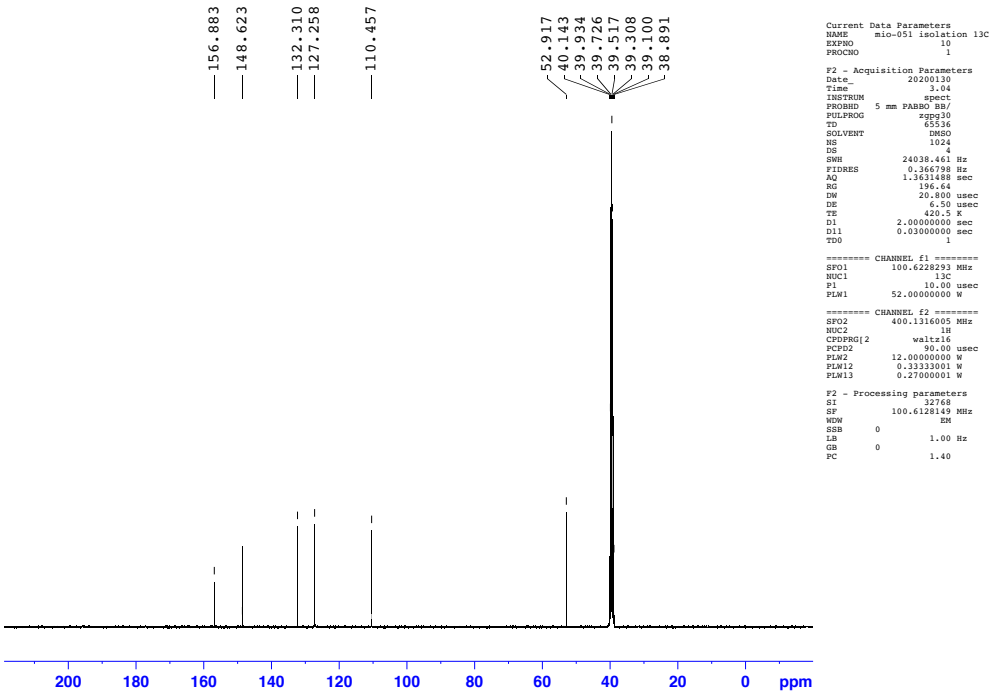
Current Data Parameters
NAME mio-051 isolation
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200129
Time 17.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 154.67
DW 62.400 usec
DE 6.50 usec
TE 388.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR



Current Data Parameters
NAME mio-051 isolation 13C
EXPNO 10
PROCNO 1

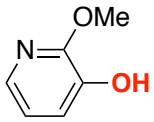
F2 - Acquisition Parameters
Date_ 20200130
Time 3.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.64
DW 20.800 usec
DE 6.50 usec
TE 420.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

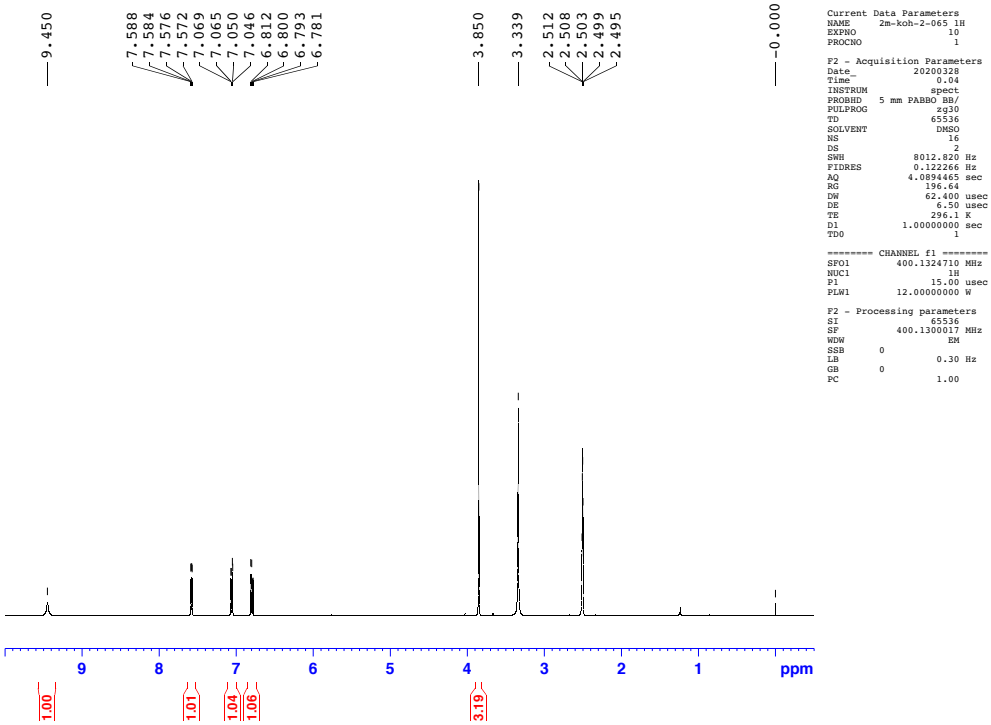
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.33333001 W
PLW13 0.27000001 W

F2 - Processing parameters
SI 32768
SF 100.6128149 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3-Hydroxy-2-methoxypyridine (2o)



^{1}H NMR



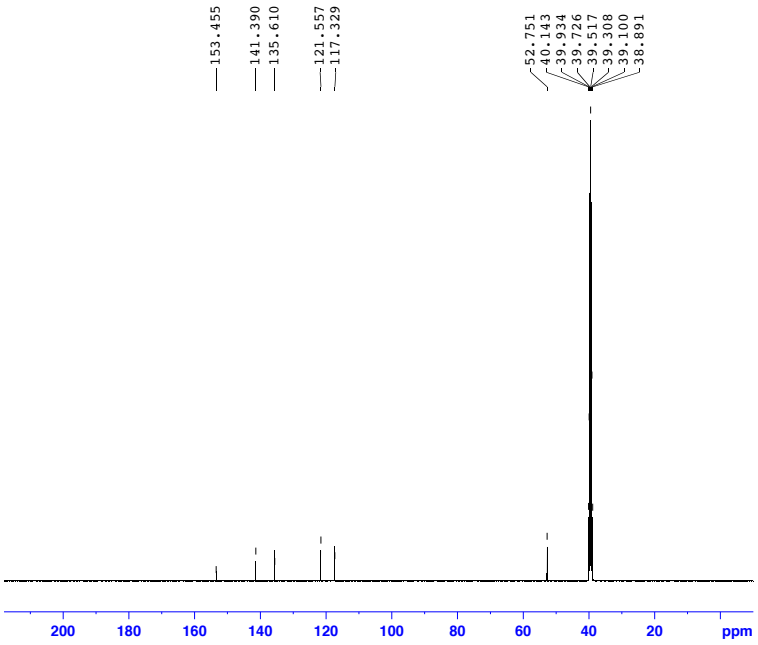

```
Current Data Parameters
NAME      2m-koh-2-065 1H
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200328
Time               0.04
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                  16
DS                   2
SWH           8012.820 Hz
FIDRES           0.122266 Hz
AQ            4.0894465 sec
RG                196.64
DW              62.400 usec
DE               6.50 usec
TE               296.1 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1               1H
P1                15.00 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI                 65536
SF          400.1300017 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C NMR




```
Current Data Parameters
NAME      2m-koh-2-065 13C
EXPNO                 11
PROCNO                 1

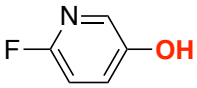
F2 - Acquisition Parameters
Date_           20200328
Time               3.01
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD               65536
SOLVENT           DMSO
NS                3072
DS                   4
SWH          24038.461 Hz
FIDRES           0.366798 Hz
AQ            1.3631488 sec
RG                196.64
DW              20.800 usec
DE               6.50 usec
TE               297.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1               13C
P1                10.00 usec
PLW1        52.00000000 W

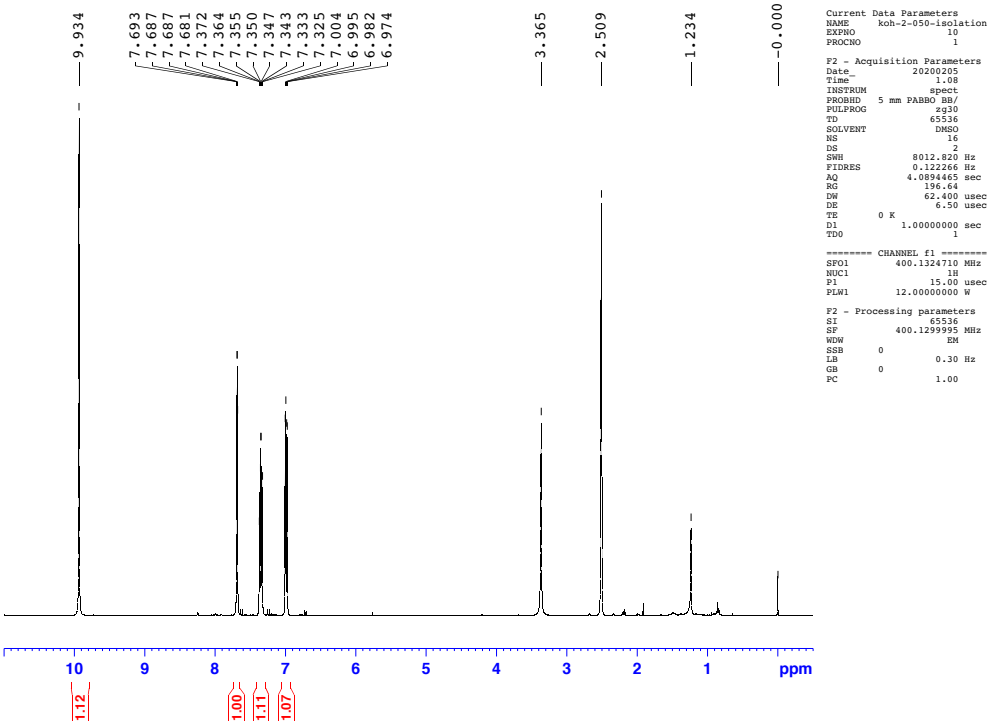
======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.00000000 W
PLW12        0.33333001 W
PLW13        0.27000001 W

F2 - Processing parameters
SI                 32768
SF          100.6128164 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

2-Fluoro-5-hydroxypyridine (2p)



^{1}H NMR



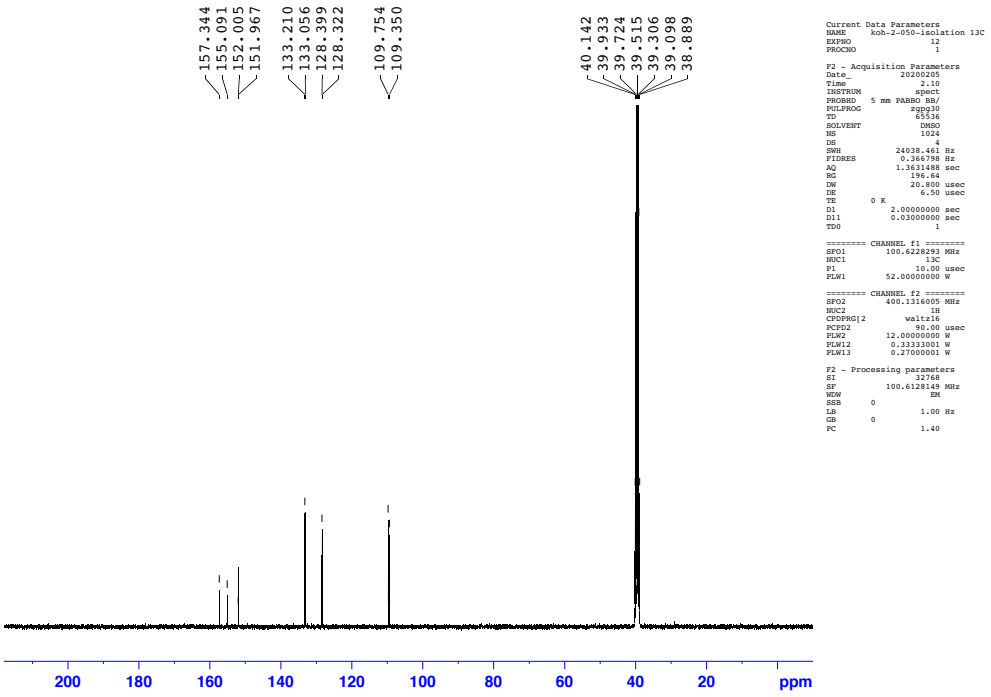
Current Data Parameters
NAME koh-2-050-isolation
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200205
Time 1.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 196.64
DW 62.400 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1299995 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR



Current Data Parameters
NAME koh-2-050-isolation 13C
EXPNO 12
PROCNO 1

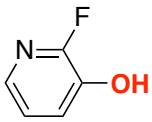
F2 - Acquisition Parameters
Date_ 20200205
Time 2.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.64
DW 20.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

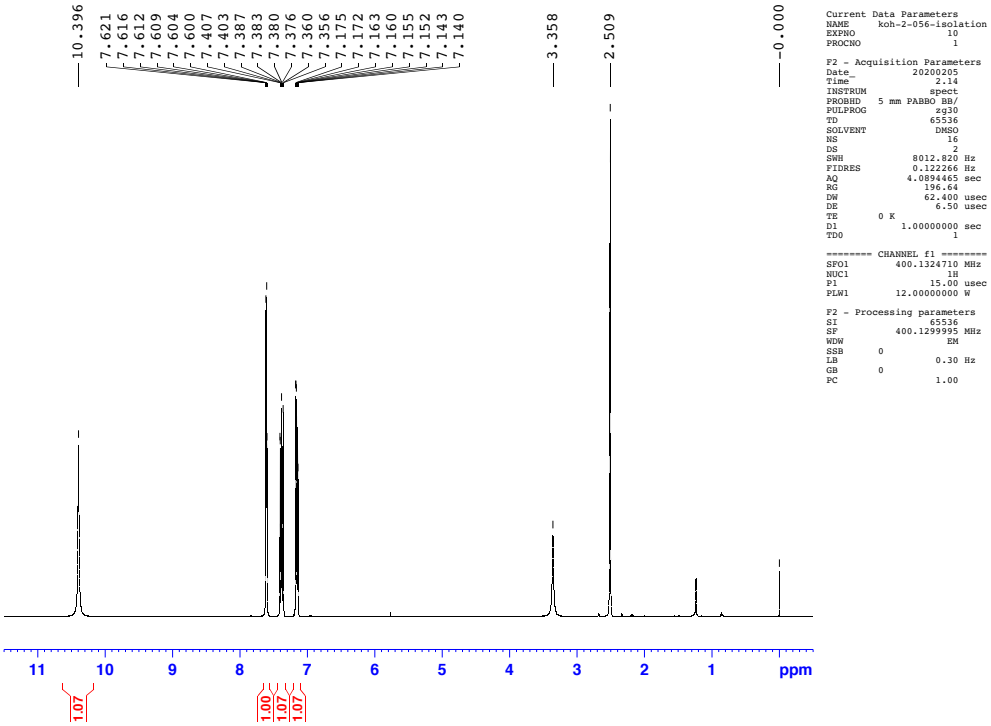
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.33333001 W
PLW13 0.27000001 W

F2 - Processing parameters
SI 32768
SF 100.6128149 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-Fluoro-3-hydroxypyridine (2q)



^{1}H NMR



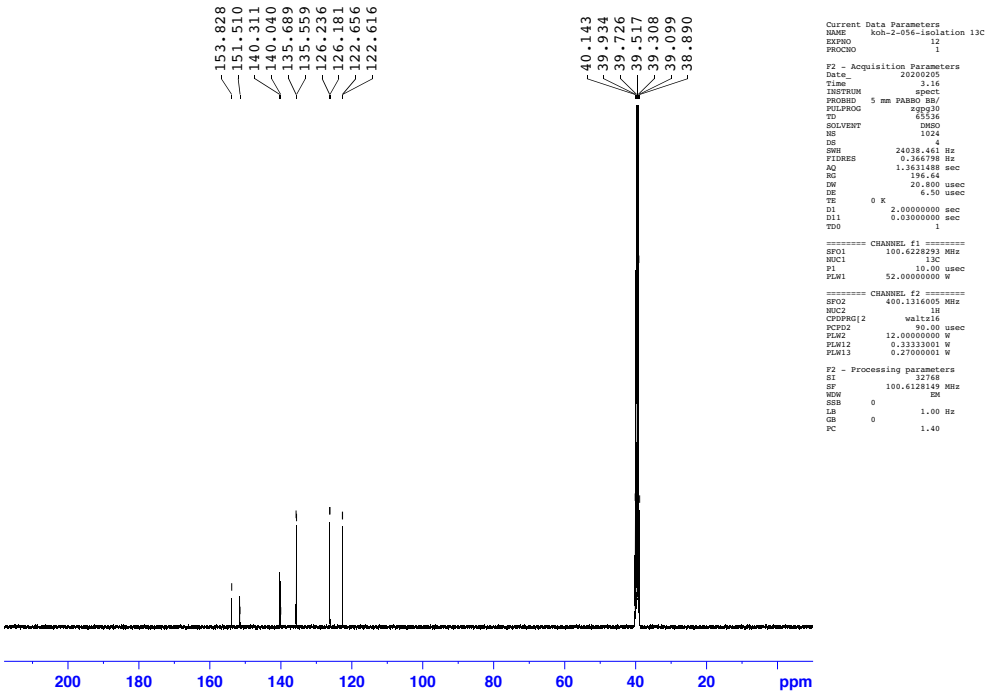

```
Current Data Parameters
NAME      koh-2-056-isolation
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_            20200205
Time_                2.14
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                  196.64
DW                62.400 usec
DE                 6.50 usec
TE         0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                     1H
P1                   15.00 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                     65536
SF            400.1299995 MHz
WDW                      EM
SSB        0
LB                    0.30 Hz
GB         0
PC                    1.00
```


^{13}C NMR




```
Current Data Parameters
NAME      koh-2-056-isolation 13C
EXPNO                      12
PROCNO                      1

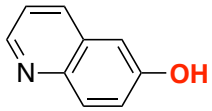
F2 - Acquisition Parameters
Date_            20200205
Time_                3.16
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631488 sec
RG                  196.64
DW                20.800 usec
DE                 6.50 usec
TE         0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                    13C
P1                   10.00 usec
PLW1         52.00000000 W

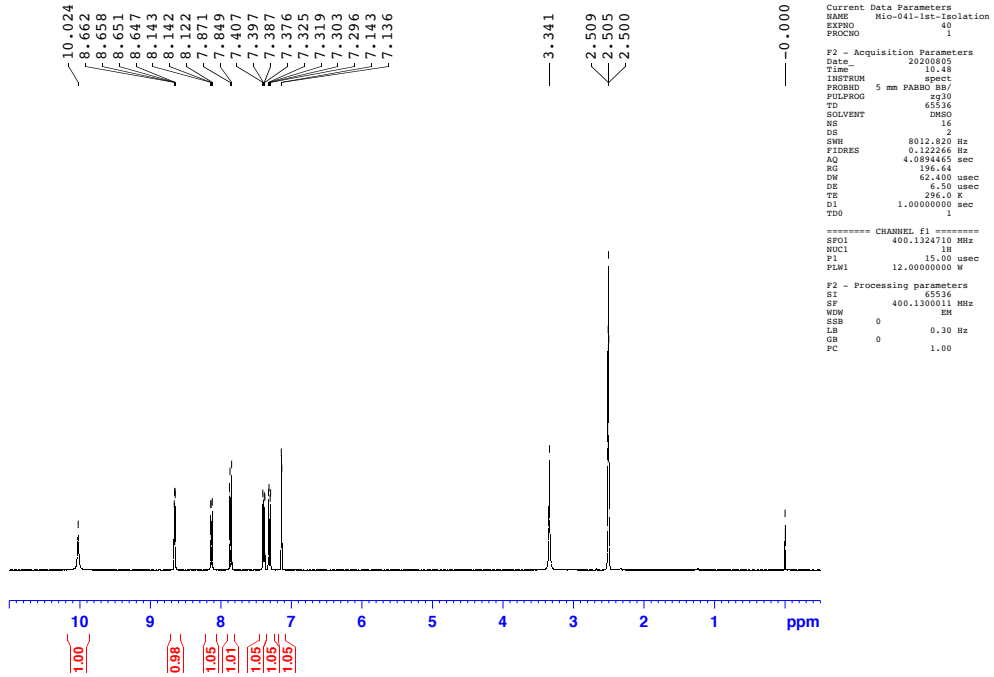
======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                90.00 usec
PLW2         12.00000000 W
PLW12         0.33333001 W
PLW13         0.27000001 W

F2 - Processing parameters
SI                     32768
SF            100.6128149 MHz
WDW                      EM
SSB        0
LB                    1.00 Hz
GB         0
PC                    1.40
```

6-Hydroxyquinoline (2r)



^{1}H NMR



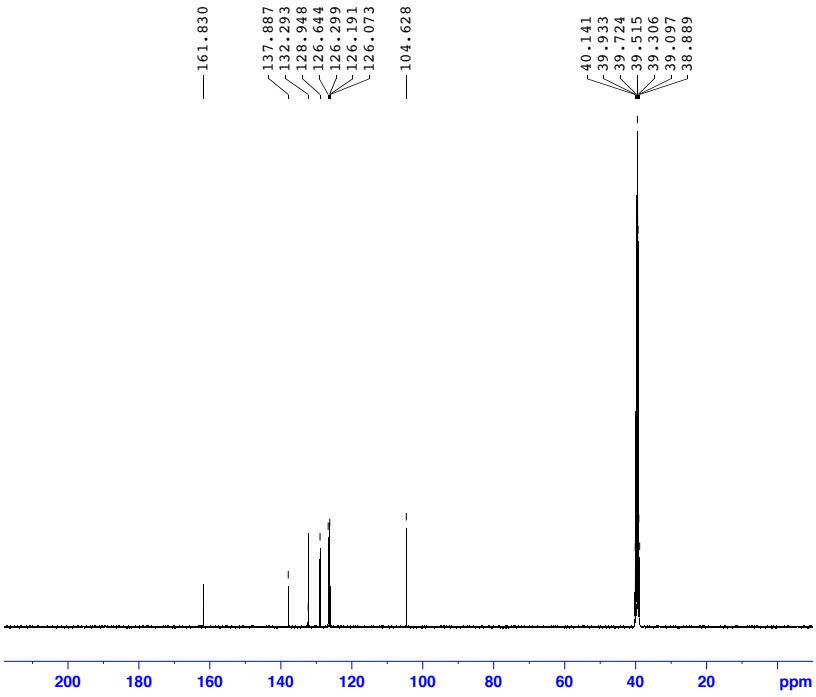

```
Current Data Parameters
NAME      Mio-041-1st-Isolation
EXPNO                    40
PROCNO                    1

F2 - Acquisition Parameters
Date_           20200805
Time_             10.48
INSTRUM           spect
PROBHD  5 mm PABBO BB/
PULPROG          zg30
TD              65536
SOLVENT          DMSO
NS                 16
DS                  2
SWH          8012.820 Hz
FIDRES       0.122266 Hz
AQ           4.0894465 sec
RG              196.64
DW              62.400 usec
DE               6.50 usec
TE              296.0 K
D1         1.00000000 sec
TD0                 1

======== CHANNEL f1 ========
SFO1       400.1324710 MHz
NUC1              1H
P1               15.00 usec
PLW1      12.00000000 W

F2 - Processing parameters
SI              65536
SF         400.1300011 MHz
WDW               EM
SSB        0
LB                0.30 Hz
GB         0
PC                1.00
```

^{13}C NMR




```
Current Data Parameters
NAME      koh-2-017-isolation 13C
EXPNO                    12
PROCNO                    1

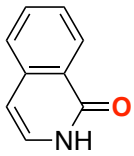
F2 - Acquisition Parameters
Date_           20200205
Time_             1.05
INSTRUM           spect
PROBHD  5 mm PABBO BB/
PULPROG          zgpg30
TD              65536
SOLVENT          DMSO
NS                1024
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ           1.3631488 sec
RG              196.64
DW              20.800 usec
DE               6.50 usec
TE         0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
SFO1       100.6228293 MHz
NUC1              13C
P1               10.00 usec
PLW1      52.00000000 W

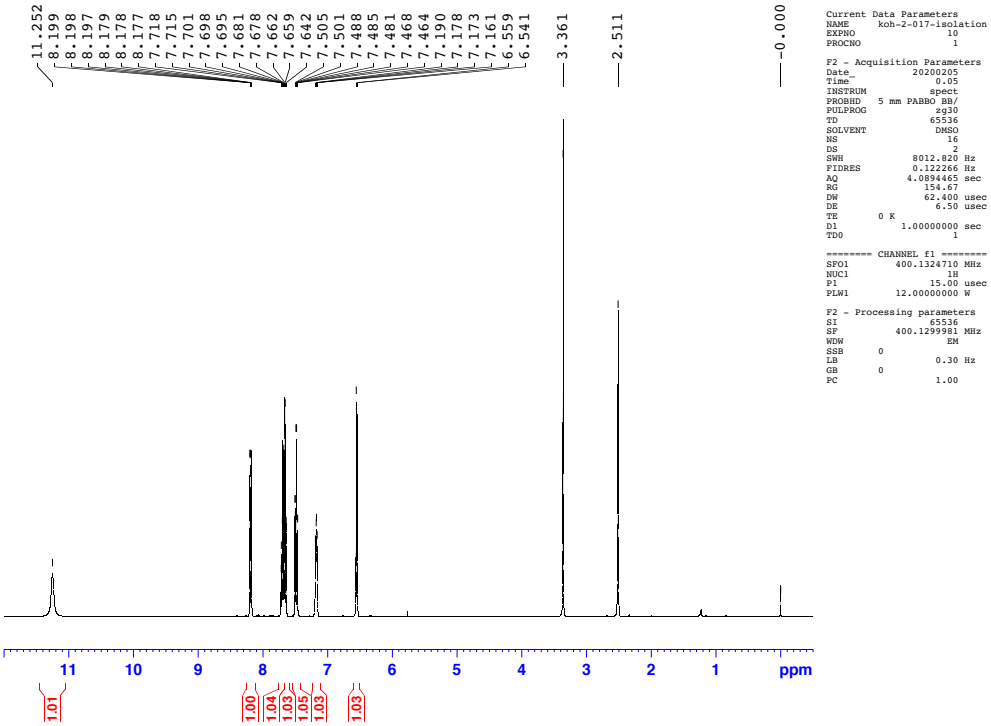
======== CHANNEL f2 ========
SFO2       400.1316005 MHz
NUC2              1H
CPDPRG[2          waltz16
PCPD2            90.00 usec
PLW2      12.00000000 W
PLW12      0.33333001 W
PLW13      0.27000001 W

F2 - Processing parameters
SI              32768
SF         100.6128154 MHz
WDW               EM
SSB        0
LB                1.00 Hz
GB         0
PC                1.40
```

1(*2H*)-Isoquinolinone (2s)



^{1}H NMR



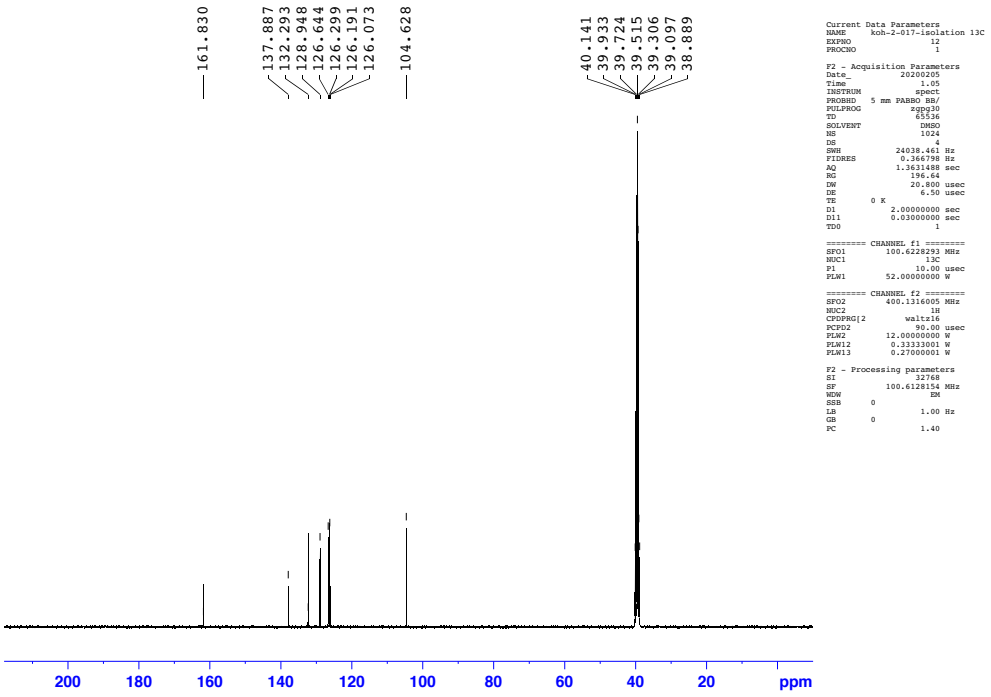
Current Data Parameters
NAME koh-2-017-isolation
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200205
Time 0.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 154.67
DW 62.400 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1299981 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR



Current Data Parameters
NAME koh-2-017-isolation 13C
EXPNO 12
PROCNO 1

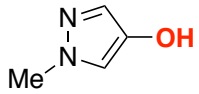
F2 - Acquisition Parameters
Date_ 20200205
Time 1.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.64
DW 20.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

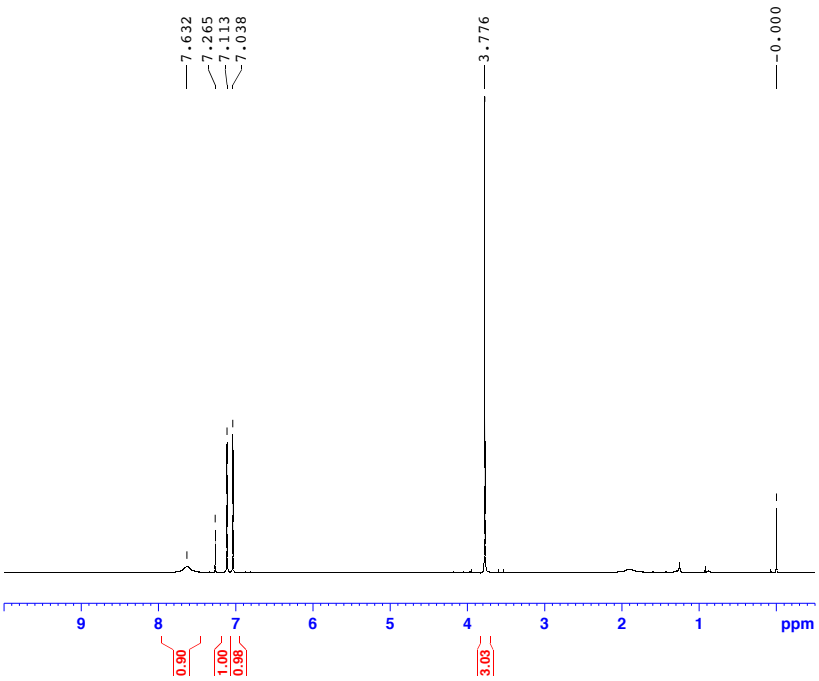
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.33333001 W
PLW13 0.27000001 W

F2 - Processing parameters
SI 32768
SF 100.6128154 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1-Methyl-1*H*-pyrazol-4-ol (2t)



^{1}H NMR



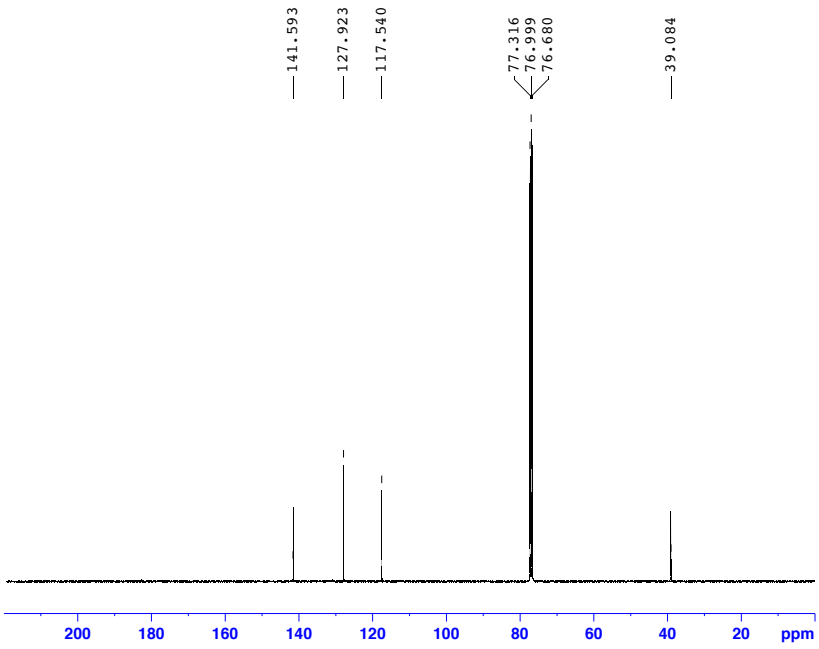

```
Current Data Parameters
NAME      koh-3-043-Fr9-11
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_            20200909
Time               21.19
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 196.64
DW                62.400 usec
DE                 6.50 usec
TE                 296.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300075 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C NMR




```
Current Data Parameters
NAME      koh-3-043-Fr9-11
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_            20200910
Time               2.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  3072
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                 196.64
DW                20.800 usec
DE                 6.50 usec
TE                 297.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          52.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.33333001 W
PLW13          0.27000001 W

F2 - Processing parameters
SI                 32768
SF            100.6127717 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```