Supporting Information

Electrochemical Oxidative Decarboxylation and 1,2-Aryl Migration towards the Synthesis of 1,2-Diaryl Ethers

Faxiang Bu¹, Lijun Lu¹, Xia Hu¹, Shengchun Wang¹ and Aiwen Lei¹,²,*

¹College of Chemistry and Molecular Sciences, The Institute for Advanced Studies (IAS), Wuhan University, Wuhan 430072, Hubei, P. R. China.

²National Research Center for Carbohydrate Synthesis, Jiangxi Normal University, Nanchang 330022, Jiangxi, P. R. China.

Correspondence to: aiwenlei@whu.edu.cn
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Materials and Methods

Unless otherwise stated, analytical grade solvents and commercially available reagents were used without further purification. All solvents were analytical reagent or better and were degassed prior to use. The instrument for electrolysis is dual display potentiostat (DJS-292B) (made in China). The anode electrode is carbon cloth (15 mm×15 mm×0.36 mm) and the cathode electrode is platinum plate electrodes (15 mm×15 mm×0.3 mm). Cyclic voltammograms were obtained on a CHI 605E potentiostat. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum ether (bp. 60–90 °C). Gradient flash chromatography was conducted eluting with a continuous gradient from petroleum ether to the ethyl acetate. Gas chromatographic analyses were performed on SHIMADZU GC-2014 gas chromatography instrument with a FID detector and biphenyl was added as internal standard. All new compounds were characterized by $^1$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS. The known compounds we characterized by $^1$H NMR, $^{13}$C NMR and $^{19}$F NMR. The $^1$H NMR, $^{13}$C NMR and $^{19}$F NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer. The chemical shifts (δ) were given in part per million relative to internal tetramethyl silane (TMS, 0 ppm for $^1$H), CDCl$_3$ (77.0 ppm for $^{13}$C). All chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument and Thermo Fisher Scientific LTQ FT Ultra. EPR spectra were recorded on a Bruker X-band A200 spectrometer.

Experimental Procedures

1. General Procedure for the Electrooxidation Decarboxylation 1,2 Aryl Migration Construct C-O Bond

The substrate (0.4 mmol, 1 equiv.) and $^7$Bu$_4$NOAc (0.6 mmol, 1.5 equiv.) were placed in an oven-dried undivided three-necked bottle (25 mL). The bottle was equipped with a stir bar, a carbon cloth (15 mm×15 mm×0.36 mm) anode and a platinum plate (15 mm×15 mm×0.3 mm) cathode. The bottle was flushed with nitrogen. Degased HFIP (700 μL), and degased ROH (12.0 mL) were added. The reaction mixture was stirred and electrolyzed at a constant current of 15 mA at room temperature for 3.5 h. After completion of the reaction, the products were determined by TLC and GC-MS. The solvent was removed under reduced pressure by an aspirator, then the pure product was obtained by flash column chromatography on silica gel (eluent: petroleum ether/ethyl acetate= 200:1).
2. Analysis of the product and side products

2.1 Analysis of the product and side products of electrochemical decarboxylation of 3,3-diarylpropionic acid to construct C-O bond reaction.

The substrates with ortho-substituent aryl group usually gave higher yields than para or meta substituted ones. Because they could inhibit the formation of side-product I and II.

![Diagram of the reaction scheme](image)

Scheme S1. Main and side products of the electrochemical decarboxylation of 3,3-diarylepropionic acid to construct C-O bond reaction.

2.2 Analysis of the product and side products of other substrates.

![Diagram of the reaction scheme](image)

Scheme S2. Main and side products of the electrochemical decarboxylation of 3,3-di(2-chlorophenyl)arylpropionic acid with Cyclohexanol.

Conversion = 89%
Mass balance = 73%
3. Procedure for Gram Scale Synthesis

The 3,3-diphenylpropionic acid (8.8 mmol, 1.99g, 1 equiv.), 4Bu₄NOAc (1.5 equiv.), 4Bu₄NBF₄ (0.72 equiv.) were placed in an oven-dried undivided three-necked bottle (250 mL). The bottle was equipped with a stir bar, a carbon cloth (15 mm×15 mm×0.36 mm) anode and a platinum plate (15 mm×15 mm×0.3 mm) cathode. The bottle was flushed with nitrogen. Degased DCE (36.0 mL), commercially available MeOH (72.0 mL) were added. The reaction mixture was stirred and electrolyzed at a constant current of 50 mA at room temperature for 23 h. After completion of the reaction, the products were determined by TLC and GC-MS. The solvent was removed under reduced pressure by an aspirator, then the pure
product was obtained by flash column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 200:1).

4. General Procedure for Substrates synthesis

The substrates was synthesised according to the method described in the reported literature.[1] The synthesis of 3,3-di(4-methylphenyl)-propanoic acid from 4-methylphenylboronic acid and 4-methylcinnamic acid was chosen as representative. To a Schlenk tube with a cooling finger were added 4-methylphenylboronic acid (543.8 mg, 4.0 mmol), 4-methylcinnamic acid (324.4 mg, 2.0 mmol), Pd(OAc)$_2$ (22.4 mg, 0.1 mmol), bpy (31.2 mg, 0.2 mmol), HOAc (2.0 mL), THF (4.0 mL) and H$_2$O (1.2 mL) under an air atmosphere. The mixture was stirred and heated at 80 °C for about 24 h until the substrate disappeared as monitored by TLC. After reaction, the solution was diluted with EA and washed with water two times, then, the oil phase was concentrated under reduced pressure by an aspirator. The crude product was obtained by flash column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10:1), and the pure product was obtained by crystallization using EtOH and H$_2$O.

5. DFT calculation of poor selectivity of substrates with different aryl group

In order to explain the problem about reaction selectivity, we did DFT calculation.

The calculated free energy barriers, -PhMe migration (16.1 kcal/mol) is nearly the same as -PhCl migration (15.7 kcal/mol) of 1,1-diarylethyl carbon radical.
The calculated free energy barriers, -PhMe migration (13.6 kcal/mol) is nearly the same as -Ph migration (13.4 kcal/mol) of 1,1-diarylethyl carbon radical.
The calculated free energy barriers, -PhCF₃ migration (11.2 kcal/mol) is relatively lower than -Ph migration (13.1 kcal/mol) of 1,1-diarylethyl carbon radical.

From the results of DFT calculation, the calculated free energy barriers of different aryl migration had no obvious difference. Hence, the selectivity of substrates with two different aryl rings is not good in current reaction system. Metall electrocatalysis or designing new electrodes with controllable pore channel might solve this problem. We will try them in the follow-up works.

6. General Procedure for Product derivatization

A. Synthesis of 1-Azido-1,2-diphenyl thane

The title compound was synthesized according to Sajiki’s procedure.[9] FeCl₃ (10 mol%) and TMSN₃ (1.5 equiv.) were placed in an oven-dried Schlenk tube. The Schlenk tube was equipped with a stir bar and
flushed with nitrogen. Ether 3ba (0.2 mmol, 1 equiv.) and CH₂Cl₂ (2.0 mL) were added. The reaction mixture was stirred at room temperature for 1 h. After completion of the reaction, the products were determined by TLC. The solvent was removed under reduced pressure by an aspirator, then the pure product was obtained by flash column chromatography on silica gel (eluent: petroleum ether/ethyl acetate= 200:1).

B. Synthesis of 1-allyl-1,2-diphenyl thane

![Scheme S10. Synthesis of 1-allyl-1,2-diphenyl thane](image)

The title compound was synthesized according to Sajiki's procedure. FeCl₃ (10 mol%) and Allyltrimethylsilane (1.5 equiv.) were placed in an oven-dried Schlenk tube. The Schlenk tube was equipped with a stir bar and flushed with nitrogen. Ether 3ba (0.2 mmol, 1 equiv.) and CH₂Cl₂ (2.0 mL) were added. The reaction mixture was stirred at room temperature for 1.5 h. After completion of the reaction, the products were determined by TLC. The solvent was removed under reduced pressure by an aspirator, then the pure product was obtained by flash column chromatography on silica gel (eluent: petroleum ether).

C. Synthesis of 1,2-diphenyl ethylene

![Scheme S11. Synthesis of 1,2-diphenyl ethylene](image)

The title compound was synthesized according to Ranu's procedure.⁷ Zn power (25 mol%) was placed in an oven-dried Schlenk tube. The Schlenk tube was equipped with a stir bar and flushed with nitrogen. Ether 3ba (0.8 mmol, 1 equiv.), AcCl (1.1 equiv.) and petroleum ether (2 mL) were added. The reaction mixture was stirred at room temperature for 5 h. After completion of the reaction, the products were determined by TLC. The solvent was removed under reduced pressure by an aspirator, then the pure product was obtained by flash column chromatography on silica gel (eluent: petroleum ether/ethyl acetate= 50:1).

D. Synthesis of 2-Propenoic acid, 3-(2-(2-methoxy-2phenyl ethyl)phenyl), ethyl ester

![Scheme S12. Synthesis of 2-Propenoic acid, 3-(2-(2-methoxy-2phenyl ethyl)phenyl), ethyl ester](image)
The title compound was synthesized according to Yu's procedure.\textsuperscript{[11]} To a sealed tube (with a Teflon cap) equipped with a magnetic stir bar was sequentially added Pd(OAc)\textsubscript{2} (4.5 mg, 0.02 mmol, 10 mol%), Ac-Gly-OH (4.7 mg, 0.040 mmol, 20 mol%), Ag\textsubscript{2}CO\textsubscript{3} (110 mg, 0.40 mmol, 2.0 equiv.) and ether 3ba (0.2 mmol). HFIP (1 mL) was added to the mixture, followed by olefin (0.3 mmol, 1.5 equiv.). Then an additional 1.0 mL of HFIP was added to rinse the residual chemical on the inner side wall of the tube. The tube was then capped and submerged into a pre-heated 80 °C oil bath. The reaction was stirred for 24 h and cooled down to room temperature. The crude reaction mixture was diluted with diethyl ether (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 20 mL of diethyl ether. The filtrate was concentrated in vacuo, and the resulting residue was purified by flash column chromatography or preparative TLC using petroleum ether/EtOAc as the eluent.

E. Synthesis of 9,10-dihydro-9-methoxy-phenanthrene

![Scheme S13. Synthesis of 9,10-dihydro-9-methoxy-phenanthrene](image)

The title compound was synthesized according to Fagnou's procedure.\textsuperscript{[12]} To a mixture of crushed K\textsubscript{2}CO\textsubscript{3} (2 equiv.), Pd(OAc)\textsubscript{2} (5 mol\%), ligand (10 mol\%) and bromo ether 5aa (0.5 mmol) under nitrogen atmosphere was added 3mL of N,N-Dimethylacetamide (DMA) in a sealing tube equipped with a mechanical stir bar. The reaction mixture is then heated overnight at 135°C. After the reaction was judged complete by TLC analysis, the heat source was removed and the reaction mixture was allowed to cool. The crude mixture was then loaded onto a silica gel flash chromatography column (eluent: petroleum ether/ethyl acetate = 200:1).

7. General Procedure for Cyclic Voltammetry (CV)

Cyclic voltammetry experiment was performed in a three-electrode cell connected to a schlenk line under nitrogen at room temperature. The working electrode was a glass carbon electrode, the counter electrode a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution, and separated from reaction by a salt bridge. Anhydrous degassed MeOH/DCE = 8/4 mL containing 0.4 mmol tBuNBF\textsubscript{4} were poured into the electrochemical cell in all experiments. The scan rate is 0.025 V/s, ranging from 0 V to 1.95 V). Data was analyzed using MATLAB by subtracting a background current prior to identifying the maximum current (C\textsubscript{p}) and determining the potential (E\textsubscript{p/2}) at half this value (C\textsubscript{p/2}). The obtained value was referenced to Ag/AgCl and converted to SCE by subtracting 0.03 V. An oxidation peak of tBu\textsubscript{4}NOAc was observed at 1.71 V (vs Ag/AgCl), the half-peak potential was measured as 1.60 V (vs Ag/AgCl). And the oxidation peak of 1b and 1.0 equivalent tBu\textsubscript{4}NOAc was observed at 1.68 V (vs Ag/AgCl), the half-peak potential was measured as 1.57 V (vs Ag/AgCl). An oxidation peak of 1b and Li\textsubscript{2}CO\textsubscript{3} was observed at 1.68 V (vs Ag/AgCl), the half-peak potential was measured as 1.55 V (vs Ag/AgCl). No oxidation peak of 1b or Li\textsubscript{2}CO\textsubscript{3} alone was found below 1.95V (vs Ag/AgCl).
8. Analysis of the oxidation of $^\text{tBu}_4\text{NOAc}$

We think the oxidation of acetate may go through following procedure. First, acetoxy radical is produced by oxidation of acetate. Then, a molecule of CO$_2$ is removed to form methyl radical. The generated methyl radicals may be involved in the following four reaction processes.

1) The methyl radical may capture a hydrogen atom in the reaction system to produce methane.

2) Two methyl radicals couple to produce ethane.

3) The methyl radical can react with the carbon radical generated from 3,3-diphenylpropionic acid decarboxylation forming 1,1-diphenylpropane or 1,2-diphenylpropane.

4) The methyl radical may be oxidated to produce methyl positive ion, which will be captured by alcohol forming ether.

To detected oxidation products of acetate, we used cyclohexanol as nucleophile making product easier to detect by GC-MS, but we didn’t detect the ether methoxycyclohexane.
Besides, we didn’t detect any crosscoupling products of 3,3-diphenyl propionic acid and acetate under standard reaction conditions. But when we used Pt as the anode, a small amount of 1,1-diphenylpropane was detected. This may be explained as

\[
\begin{align*}
&\text{Ph} & & \text{COOH} \\
&\text{Ph} & & \text{Ph} & & \text{COOH} \\
0.4 \text{ mmol} & & & & & 1.5 \text{ equiv.} & \text{Bu}_{4}\text{NOAc} \\
& & & & & \text{MeOH/HIFIP} \\
& & & & & \text{Pt} & \text{electrode} \\
& & & & & 15 \text{ mA, 1.5 equiv.} \\
& & & & & \text{Cu}^{2+} & \text{I}^- \\
& & & & & \text{N}_{2} & 3.5 \text{ h} \\
& & & & & \text{Ph} & \text{Ph} & \text{Ph} & \text{Ph} \\
\text{MeOH/HIFIP} & & & & & & & \text{N.D.} \\
& & & & & & & 1.5 \text{ equiv.} & \text{Bu}_{4}\text{NOAc} \\
& & & & & & & 12.0 \text{ mL} & \text{MeOH, 700 } \mu \text{L} & \text{HIFIP} \\
& & & & & & & \text{r.t., } & \text{N}_{2} & 3.5 \text{ h} \\
& & & & & & & \text{Ph} & \text{Ph} & \text{MeOH} & \text{Ph} & \text{MeOH} \\
& & & & & & & \text{OMe} & \text{MeOH} & \text{Ph} & \text{Ph} \\
& & & & & & & \text{OMe} & \text{MeOH} & \text{Ph} & \text{Ph} \\
& & & & & & & \text{OMe} & \text{MeOH} & \text{Ph} & \text{Ph} \\
& & & & & & & \text{OMe} & \text{MeOH} & \text{Ph} & \text{Ph} \\
\end{align*}
\]

Methane and ethane were obtained when we detected the gaseous products. In the first two hours, only a small mount of methane and ethane were formed, which indicated that the oxidation of 3,3-diphenylpropionic acid anion was more preferential than acetate anion at the beginning of the reaction. With the reaction proceeding, the oxidation of acetate anion became more.

To sum up, the oxidation products of acetate are methane and ethane under our reaction conditions, and the total yield is about 56% after eletrolysis 3.5 hours in the standard reaction system. In the first two hours, the main oxidized substrate is 3,3-diphenylpropionic acid, which indicated \text{Bu}_{4}\text{NOAc} can really act as a base to extract the hydrogen of 3,3-diphenylpropionic acid and 3,3-diphenylpropionic acid is prior to be oxidated compared with \text{Bu}_{4}\text{NOAc}.

9. NMR experiments

The active hydrogen peak of 3,3-diphenylpropionic acid shifted close to acetic acid after adding \text{Bu}_{4}\text{NOAc}. It indicated that 3,3-diphenylpropionic reacted with \text{Bu}_{4}\text{NOAc to partly afford 3,3-diphenylpropionate, which can promote the oxidation of carboxylic acids.}
10. EPR experiments

EPR spectra was recorded at 298 K on EPR spectrometer operated at 9.816 GHz. Typical spectrometer parameters are shown as follows, scan range: 100 G; center field set: 3503 G; time constant: 163.84 ms; S21 scan time: 30.72 s; modulation amplitude: 1.0 G; modulation frequency: 100 kHz; receiver gain: \(1.00 \times 10^4\); microwave power: 21.56 mW.

A. EPR studies of 1a in MeCN: Under constant current conditions, a dried three-necked flask equipped with a stir bar was loaded with 1a (0.4 mmol), \(^7\)BuNBF\(_4\) (0.4 mmol) and Li\(_2\)CO\(_3\) (0.6 mmol) in 12.0 mL MeCN was stirred under a N\(_2\) atmosphere at room temperature. After 30 mins, DMPO (80 \(\mu\)L) was added and stir 1min. Then, the solution sample was taken out into a small tube and analyzed by EPR. A mixture signal of carbon radicals \((g = 2.0062, A_N = 14.20 \text{ G}, A_H = 21.30 \text{ G})\) and oxidized DMPO \((g = 2.0062, A_N = 13.80 \text{ G})\) was identified. Meanwhile, the reaction system of EPR experiment was tested by high resolution electrospray ionization mass spectrometry. The molecular ion peak with molecular weight of 293.1774 was detected (Figure S3D). This indicated that the DMPO captured carbon radical was produced by the decarboxylation of the substrate (Figure S3E).

B. EPR studies of 1b in MeOH/DCE: Under constant current conditions, a dried three-necked flask equipped with a stir bar was loaded with 1b (0.4 mmol), \(^7\)BuNBF\(_4\) (0.4 mmol) and \(^7\)Bu4NOAc (0.6 mmol) in 8.0 mL MeOH and 4.0 mL DCE was stirred under a N\(_2\) atmosphere at room temperature. After 30 mins, DMPO (80 \(\mu\)L) was added and stir 1min. Then, the solution sample was taken out into a small tube and analyzed by EPR. A signal of hydrogenated DMPO \((g = 2.0067, A_N = 15.45 \text{ G}, A_{H1} = 20.60 \text{ G}, A_{H2} = 20.60 \text{ G})\) was identified.

C. EPR studies of 1b in MeOH/MeCN: Under constant current conditions, a dried three-necked flask equipped with a stir bar was loaded with 1b (0.4 mmol), \(^7\)BuNBF\(_4\) (0.4 mmol) and Li\(_2\)CO\(_3\) (0.3 mmol) in 12.0 mL MeCN was stirred under a N\(_2\) atmosphere at room temperature. After 30 mins, DMPO (80 \(\mu\)L) was added and stir 1min. Then, the solution sample was taken out into a small tube and analyzed by EPR. A mixture signal of carbon radicals \((g = 2.0068, A_N = 14.30 \text{ G}, A_{H1} = 21.30 \text{ G})\) and hydrogenated DMPO \((g = 2.0068, A_N = 14.65 \text{ G}, A_{H1} = 19.54 \text{ G}, A_{H2} = 19.54 \text{ G})\) was identified. Meanwhile, the reaction system of EPR experiment was tested by high resolution electrospray ionization mass spectrometry. The molecular ion peak with molecular weight of 293.1774 was detected (Figure S3D). This indicated that the DMPO captured carbon radical was produced by the decarboxylation of the substrate (Figure S3E).
HRMS (ESI) calcd for C_{20}H_{23}NO, [M-H], 293.1785, found: 293.1774. The experimental result provided strong evidence for the radical process of the reaction.

**Figure S3.** A. 1a (0.4 mmol), "BuNBF_4 (0.4 mmol), Li_2CO_3 (0.6 mmol), DMPO (80 μL), MeCN (12.0 mL), constant current, 30 min. B. 1b (0.4 mmol), "BuNOAc (0.6 mmol), "BuNBF_4 (0.4 mmol), DMPO (80 μL), MeOH (8.0 mL), DCE (4.0 mL), constant current, 30 min. C. 1b (0.4 mmol), "BuNOAc (0.6 mmol), "BuNBF_4 (0.4 mmol), DMPO (80 μL), MeOH (0.5 mL), MeCN (11.5 mL), constant current, 30 min. D. High resolution ESI spectrum. E. The possible molecular formula of the captured compound.

11. radical capture experiment

a) 22% yield of 1,1-diphenyl-2-bromoethane was obtained by using BrCCl_3 as the radical trapping agent. This result indicated the existence of primary carbon radical I.
b) 16% benzophenone was obtained by using oxygen as the radical trapping agent. We supposed the following process for the formation of benzophenone, which indicated the existence of primary carbon radical I.

**Scheme S15. BrCl capture experiment**

12. **Effect of the electrode material**

We screened different electrode materials when we optimized the reaction conditions. The yields had a big decrease by changing the anode from carbon cloth to Pt plate. For cathode, Ni plate and Fe plate had the similar effects to Pt plate, but carbon cloth and Pb plate gave poor performance.

**Scheme S16. O₂ capture experiment**

| Entry | Anode       | Cathode | Yield [%] |
|-------|-------------|---------|-----------|
| 1     | Carbon cloth| Pt plate| 66 (65)   |
| 2     | Pt plate    | Pt plate| 10        |
| 3     | Carbon cloth| Ni plate| 64        |
| 4     | Carbon cloth| Fe plate| 66        |
| 5     | Carbon cloth| Pb plate| Trace     |
| 6     | Carbon cloth| Carbon cloth| 41        |

*Yields were determined by gas chromatography analysis and calibrated with naphthalene as the internal standard (isolated yield in parentheses)
When using Pt plate as anode, the conversion and yield were relatively low. 1,1-diphenyl-propane was obtained after reaction.

We supposed that 1,1-diphenyl-propane was formed through the following path. 3,3-diphenylpropionic acid anion and acetate anion were oxidized at anode at the same time. Then, they underwent decarboxylation to produce carbon radicals, which coupled to form 1,1-diphenyl-propane.

Moreover, we used glassy carbon electrode and Pt electrode as working electrodes to conduct cyclic voltammetry experiments, respectively. We can saw the oxidation peaks of 3,3-diphenylpropionic acid anion (1.68 V) and acetate anion (1.71 V) by using glassy carbon electrode as working electrode. However, we couldn’t find obvious oxidation peaks of 3,3-diphenylpropionic acid anion and acetate anion by using Pt electrode as working electrode. So, the conversion and yield were low when Pt plate was used as anode.
13. DFT calculation

General Computational Calculation Details: DFT calculations were performed using the M06-2x method[13] with the Gaussian09 program[14]. The 6-31G(d) basis set was used for all the elements and methanol was employed as the solvent during the geometry optimization. For the integration grid in the calculations, the parameter int = ultrafine was used. Frequency calculations at the same level of theory have been performed to identify all of the stationary points as minima (zero imaginary frequencies) or transition state (one imaginary frequencies) and to provide free energies at 298.15 K. The transition states were checked through intrinsic reaction coordinate (IRC) calculations. The solvent effects were considered during the geometry optimization with SMD model[15]. For the single point energy calculations, 6-311+G(d,p) basis set was used for all the elements. Grimme's dispersion correction[16] was used during the calculations.

DFT calculation was performed to exclude the path that 1,2-aryl migration go through after the oxidation of radical intermediate produced from decarboxylation of 3,3-biarylpropionic acid: Apart from aryl migration through the radical intermediate produced from decarboxylation of 3,3-biarylpropionic acid, there is another possibility that the radical intermediate is oxidized to yield the corresponding carbon cation intermediate at the anode before rearrangement. The DFT calculation results indicate that the activation energy of two reaction paths are low and the difference is not significant (see below Figure S4B). And we didn’t detect 1,2-H migration product in our reaction system, so the pathway that the radical intermediate is oxidized to yield the corresponding carbon cation intermediate at the anode before rearrangement is impossible.

![Diagram](diagram.png)

**Figure S4 A.** Possible paths of 1,2-aryl migration  B. Free energy barriers for the 1,2-aryl migration vs. 1,2-H migration of carbon cation intermediate.
Characterization of Products

1-methoxy-1,2-di(2-chlorophenyl) thane (3aa). 84.3 mg (yield: 75%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – $d_6$) $\delta$ 7.49 – 7.18 (m, 8H), 4.93 (dd, $J = 5.6$, 8.0 Hz, 1H), 3.13 (dd, $J = 8.0$, 14.0 Hz, 1H), 3.08 (s, 3H), 3.01 (dd, $J = 5.6$, 14.0 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) $\delta$ 138.5, 135.1, 133.6, 132.5, 129.3, 129.1, 128.4, 127.8, 126.9, 78.3, 56.5, 39.9. HRMS (EI) calcd for C$_{15}$H$_{14}$Cl$_2$O$^+$, [M]$^+$, 280.0422, found: 280.0417.

(1-methoxy-2-phenylethyl)benzene (3ba).[2] 55.2 mg (yield: 65%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.33 – 7.09 (m, 10H), 4.32 (dd, $J = 5.6$, 7.6 Hz, 1H), 3.19 (s, 3H), 3.12 (dd, $J = 7.6$, 13.6 Hz, 1H), 2.89 (dd, $J = 5.6$, 13.6 Hz, 1H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 141.7, 138.5, 129.5, 128.4, 128.1, 127.7, 126.8, 126.2, 85.1, 56.8, 44.9.

1-ethoxy-1,2-di(2-chlorophenyl) thane (3ab). 81.5 mg (yield: 69%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.60 – 7.58 (m, 1H), 7.37 – 7.15 (m, 7H), 5.11 (dd, $J = 5.6$, 8.0 Hz, 1H), 3.44 – 3.29 (m, 2H), 3.22 – 3.10 (m, 2H), 1.13 (td, $J = 7.2$, 1.2 Hz, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 139.9, 135.8, 134.6, 133.2, 132.0, 129.3, 129.2, 128.5, 127.7, 127.7, 127.1, 126.2, 76.8, 64.6, 40.8, 15.2. HRMS (EI) calcd for C$_{16}$H$_{16}$Cl$_2$O$^+$, [M]$^+$, 294.0578, found: 294.0567.

(1-ethoxy-2-phenylethyl)benzene (3bb). 52.5 mg (yield: 58%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – $d_6$) $\delta$ 7.33 – 7.12 (m, 1H), 7.37 – 7.15 (m, 7H), 5.11 (dd, $J = 5.6$, 8.0 Hz, 1H), 3.44 – 3.29 (m, 2H), 3.22 – 3.10 (m, 2H), 1.13 (td, $J = 7.2$, 1.2 Hz, 3H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) $\delta$ 142.3, 138.6, 129.4, 128.3, 128.0, 127.5, 126.7, 126.1, 82.1, 63.5, 44.0, 15.3. HRMS (EI) calcd for C$_{16}$H$_{18}$O$^+$, [M]$^+$, 226.1358, found: 226.1362.

1-trifluoroethoxy-1,2-di(2-chlorophenyl) thane (3ac). 72.4 mg (yield: 52%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – $d_6$) $\delta$ 7.53 – 7.50 (m, 1H), 7.45 – 7.34 (m, 4H), 7.28 – 7.20 (m, 3H), 5.26 (dd, $J = 6.4$, 7.6 Hz, 1H), 3.95 – 2.85 (m, 2H), 3.22 (dd, $J = 8.0$, 13.6 Hz, 1H), 3.13 (dd, $J = 6.4$, 14.0 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) $\delta$ 137.7, 134.7, 134.1, 132.7, 132.6, 130.2, 129.8, 129.5,
129.0, 128.2, 128.2, 127.2, 126.0, 123.2, 78.5, 66.0 (q, \( J_{C,F} = 33.3 \) Hz). \(^{19}\)F NMR (377 MHz, DMSO – \( d_6 \)) \( \delta \) -73.0. HRMS (EI) calcd for C\(_{16}\)H\(_{13}\)Cl\(_2\)F\(_3\)O\(^+\), [M]\(^+\), 348.0296, found: 348.0301.

(1-trifluoroethoxy-2-phenylethyl)benzene (3bc),\(^{(3)}\) 58.3 mg (yield: 52%, 0.4 mmol scale), colorless liquid. \(^1\)H NMR (400 MHz, DMSO – \( d_6 \)) \( \delta \) 7.37 – 7.13 (m, 10H), 4.73 (dd, \( J = 6.0, 7.6 \) Hz, 1H), 3.92 – 3.71 (m, 2H), 3.12 (dd, \( J = 7.6, 13.6 \) Hz, 1H), 2.93 (dd, \( J = 6.0, 13.6 \) Hz, 1H); \(^{13}\)C NMR (101 MHz, DMSO – \( d_6 \)) \( \delta \) 140.2, 137.7, 129.5, 128.5, 128.1, 128.0, 126.9, 126.3, 124.38 (q, \( J_{C,F} = 279.8 \) Hz), 83.5, 65.3 (q, \( J_{C,F} = 33.3 \) Hz), 43.2. \(^{19}\)F NMR (377 MHz, DMSO – \( d_6 \)) \( \delta \) -72.9.

1-isopropoxy-1,2-di(2-chlorophenyl) thane (3ad), 64.4 mg (yield: 52%, 0.4 mmol scale), colorless liquid. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 7.67 – 7.65 (m, 1H), 7.38 – 7.30 (m, 3H), 7.25 – 7.15 (m, 4H), 5.19 (t, \( J = 6.8 \) Hz, 1H), 3.45 – 3.36 (m, 1H), 3.13 (\( J = 6.4 \) Hz, 2H), 1.06 (d, \( J = 6.0 \) Hz, 3H), 0.99 (d, \( J = 6.0 \) Hz, 3H); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 140.9, 136.0, 134.6, 132.9, 132.3, 129.1, 128.4, 128.1, 127.7, 126.1, 126.2, 74.4, 70.1, 41.4, 23.2, 21.3. HRMS (EI) calcd for C\(_{17}\)H\(_{18}\)Cl\(_2\)O\(^+\), [M]\(^+\), 308.0735, found: 308.0739.

(1-isopropoxy-2-phenylethyl)benzene (3bd),\(^{(2)}\) 52.9 mg (yield: 55%, 0.4 mmol scale), colorless liquid. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 7.31 – 7.30 (m, 4H), 7.26 – 7.15 (m, 6H), 7.16 – 7.05 (m, 3H), 5.01 (t, \( J = 6.8 \) Hz, 1H), 3.35 – 3.29 (m, 1H), 2.90 (dd, \( J = 8.4, 13.6 \) Hz, 1H), 2.80 (dd, \( J = 5.2, 13.6 \) Hz, 1H), 0.94 (d, \( J = 6.4 \) Hz, 3H), 0.90 (d, \( J = 6.0 \) Hz, 3H); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 143.2, 138.8, 129.5, 128.2, 127.9, 127.3, 126.6, 126.0, 79.5, 68.7, 44.7, 23.3, 21.2.

1-cyclohexyloxyl-1,2-di(2-chlorophenyl) thane (3ae), 19.6 mg (yield: 28%, 0.2 mmol scale), colorless liquid. \(^1\)H NMR (400 MHz, DMSO – \( d_6 \)) \( \delta \) 7.63 – 7.61 (m, 1H), 7.43 – 7.38 (m, 3H), 7.34 – 7.23 (m, 4H), 5.13 (dd, \( J = 6.0, 7.6 \) Hz, 1H), 3.05 – 3.01 (m, 3H), 1.54 – 1.52 (m, 2H), 1.36 – 0.98 (m, 8H); \(^{13}\)C NMR (101 MHz, DMSO – \( d_6 \)) \( \delta \) 140.6, 135.9, 133.9, 132.9, 132.2, 129.5, 129.4, 128.7, 128.5, 128.0, 127.1, 74.8, 73.9, 41.1, 33.0, 30.8, 25.7, 23.4, 23.0. HRMS (EI) calcd for C\(_{20}\)H\(_{22}\)Cl\(_2\)O\(^+\), [M]\(^+\), 249.0238, found: 249.0237.
(1-cyclohexyloxy-2-phenylethyl)benzene (3be), 46.0 mg (yield: 41%, 0.4 mmol scale), colorless liquid. 

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.33 – 7.16 (m, 10H), 4.58 (dd, $J = 5.2$, 8.4 Hz, 1H), 3.16 – 3.10 (m, 1H), 3.07 (dd, $J = 8.4$, 13.6 Hz, 1H), 2.87 (dd, $J = 5.2$, 13.6 Hz, 1H), 1.71 – 1.05 (m, 10H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 143.6, 139.1, 129.8, 128.3, 128.0, 127.3, 126.7, 126.1, 80.3, 75.2, 45.8, 33.6, 31.3, 25.9, 24.2, 23.9. HRMS (EI) calcd for C$_{14}$H$_{13}$O$^+$, [M-C$_6$H$_{11}$]$^+$, 197.0966, found: 197.0961.

1-tert-butoxy-1,2-di(2-chlorophenyl) thane (3af), 55.4 mg (yield: 43%, 0.4 mmol scale), colorless liquid. 

$^1$H NMR (400 MHz, DMSO – d$_6$) $\delta$ 7.69 – 7.66 (m, 1H), 7.43 – 7.35 (m, 3H), 7.30 – 7.17 (m, 4H), 5.12 (dd, $J = 4.4$, 8.8 Hz, 1H), 2.98 (dd, $J = 4.4$, 13.2 Hz, 1H), 2.85 (dd, $J = 9.2$, 13.2 Hz, 1H), 0.83 (s, 9H); $^{13}$C NMR (101 MHz, DMSO – d$_6$) $\delta$ 143.2, 136.1, 134.1, 133.5, 130.9, 129.3, 129.3, 129.1, 128.9, 128.7, 126.9, 74.2, 69.4, 42.4, 28.1. HRMS (EI) calcd for C$_{19}$H$_{22}$Cl$_2$O$^+$, [M]$^+$, 336.1048, found: 336.1040.

(1-tert-butoxy-2-phenylethyl)benzene (3bf), 36.6 mg (yield: 36%, 0.4 mmol scale), colorless liquid. 

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.36 – 7.17 (m, 10H), 4.66 (dd, $J = 4.8$, 8.4 Hz, 1H), 2.78 – 2.68 (m, 2H), 0.84 (s, 9H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 143.6, 139.1, 129.8, 128.3, 128.0, 127.3, 126.7, 126.1, 80.3, 75.0, 73.6, 46.5, 28.2. HRMS (EI) calcd for C$_{14}$H$_{13}$O$^+$, [M-C$_4$H$_9$]$^+$, 197.0966, found: 197.0970.

1-propoxy-1,2-di(2-chlorophenyl) thane (3ag), 79.1 mg (yield: 64%, 0.4 mmol scale), colorless liquid. 

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.60 – 7.57 (m, 1H), 7.38 – 7.15 (m, 7H), 5.10 (dd, $J = 6.0$, 7.2 Hz, 1H), 3.34 – 3.28 (m, 1H), 3.22 – 3.13 (m, 3H), 1.57 – 1.48 (m, 2H), 0.84 (t, $J = 7.6$ Hz, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 134.0, 135.9, 134.6, 133.2, 132.1, 129.3, 129.2, 128.5, 127.8, 127.7, 127.1, 126.2, 77.0, 70.9, 40.8, 23.0, 10.6. HRMS (EI) calcd for C$_{17}$H$_{18}$Cl$_2$O$^+$, [M]$^+$, 308.0735, found: 308.0736.

1-(2-methyl propoxy)-1,2-di(2-chlorophenyl) thane (3ah), 70.0 mg (yield: 54%, 0.4 mmol scale), colorless liquid. 

$^1$H NMR (400 MHz, DMSO – d$_6$) $\delta$ 7.53 – 7.51 (m, 1H), 7.43 – 7.39 (m, 3H), 7.35 – 7.30
(m, 1H), 7.27 – 7.24 (m, 3H), 4.99 (dd, J = 5.2, 8.0 Hz, 1H), 3.12 – 2.98 (m, 3H), 2.90 (dd, J = 6.0, 9.2 Hz, 1H), 1.74 – 1.64 (m, 1H), 0.73 (dd, J = 4.4, 6.8 Hz, 6H); \(^{13}\text{C}\) NMR (101 MHz, DMSO – d6) δ 139.5, 135.7, 134.0, 132.7, 132.6, 129.7, 129.6, 129.4, 128.7, 128.2, 128.0, 127.1, 77.2, 75.7, 40.6, 28.5, 19.5, 19.5. HRMS (EI) calcd for C\(_{18}\)H\(_{30}\)Cl\(_2\)O\(^+\), [M]+, 322.0891, found: 322.0887.

1-neopentyloxy-1,2-di(2-chlorophenyl) thane \((3\text{ai})\). 25.6 mg (yield: 38%, 0.2 mmol scale), white solid. \(^1\text{H}\) NMR (400 MHz, DMSO – d6) δ 7.54 (dd, J = 2.0, 8.0 Hz, 1H), 7.37 – 7.17 (m, 7H), 5.01 (dd, J = 4.0, 8.8 Hz, 1H), 3.18 (dd, J = 4.4, 14.0 Hz, 1H), 3.09 (dd, J = 8.8, 13.6 Hz, 1H), 3.01 (d, J = 8.4 Hz, 1H), 2.79 (d, J = 8.8 Hz, 1H), 1.74 – 1.64 (m, 1H), 0.83 (s, 9H); \(^{13}\text{C}\) NMR (101 MHz, DMSO – d6) δ 140.1, 136.2, 134.6, 133.0, 132.4, 129.3, 129.1, 128.4, 127.7, 127.6, 127.0, 126.1, 79.7, 78.0, 40.7, 32.2, 26.7. HRMS (EI) calcd for C\(_{18}\)H\(_{30}\)Cl\(_2\)O\(^+\), [M]+, 322.0891. found: 322.0899.

1-heptanoyloxy-1,2-di(2-chlorophenyl) thane \((3\text{aj})\). 22.6 mg (yield: 38%, 0.2 mmol scale), colorless liquid. \(^1\text{H}\) NMR (400 MHz, DMSO – d6) δ 7.55 – 7.52 (m, 1H), 7.43 – 7.39 (m, 3H), 7.35 – 7.30 (m, 1H), 7.27 – 7.21 (m, 3H), 5.00 (dd, J = 5.6, 8.0 Hz, 1H), 3.25 – 3.20 (m, 1H), 3.16 – 3.06 (m, 3H), 1.40 – 1.35 (m, 2H), 1.25 – 1.13 (m, 10H), 0.85 (t, J = 6.4, 3H); \(^{13}\text{C}\) NMR (101 MHz, DMSO – d6) δ 139.6, 135.7, 133.9, 132.7, 132.6, 129.6, 129.4, 128.7, 128.2, 128.0, 127.2, 76.8, 68.7, 31.7, 29.5, 28.8, 25.8, 22.5, 14.4. HRMS (EI) calcd for C\(_{22}\)H\(_{30}\)Cl\(_2\)O\(^+\), [M]+, 364.1361. found: 364.1352.

1-methoxy-1,2-di(2-methylphenyl) thane \((3\text{ca})\). 74.9mg (yield: 78%, 0.4 mmol scale), colorless liquid. \(^1\text{H}\) NMR (400 MHz, CDCl\(_3\)) δ 7.47 – 7.45 (m, 1H), 7.27–7.02 (m, 7H), 4.65 (dd, J = 6.0, 7.6 Hz, 1H), 3.18 – 3.12 (m, 4H), 2.87 (dd, J = 6.0, 14.0 Hz, 1H), 2.23 (m, 3H), 2.09 (m, 3H); \(^{13}\text{C}\) NMR (101 MHz, CDCl\(_3\)) δ 140.0, 136.7, 136.6, 135.8, 130.2, 130.0, 127.2, 126.3, 126.2, 125.7, 80.3, 56.6, 41.2, 19.6, 18.9. HRMS (EI) calcd for C\(_{17}\)H\(_{26}\)O\(^+\), [M]+, 240.1514. found: 240.1520.

1-methoxy-1,2-di(2-fluorophenyl) thane \((3\text{da})\). 62.5mg (yield: 63%, 0.4 mmol scale), colorless liquid. \(^1\text{H}\) NMR (400 MHz, DMSO – d6) δ 7.42 – 7.30 (m, 2H), 7.26 – 7.04 (m, 6H), 4.78 (dd, J = 6.0, 7.6 Hz, 1H), 3.15 – 3.07 (m, 4H), 2.97 (dd, J = 6.0, 13.6 Hz, 1H); \(^{13}\text{C}\) NMR (101 MHz, DMSO – d6) δ 162.4, 161.8, 160.0, 159.4, 132.4, 132.3, 130.0, 129.9, 128.9, 128.8, 128.3, 128.2, 128.1, 125.0, 125.0, 124.9,
124.8, 124.4, 124.4, 115.7, 115.5, 115.4, 115.2, 76.6, 56.8, 35.9. $^{19}$F NMR (377 MHz, DMSO – $d_6$) δ -118.4, -119.8. HRMS (EI) calcd for C$_{15}$H$_4$F$_2$O$^+$, [M$^+$], 248.1013, found: 248.1019.

![Chemical structure](image)

1-methoxy-1,2-di(2-bromphenyl) thane (3ea), 109.6mg (yield: 74%, 0.4 mmol scale), colorless liquid.

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.54 – 7.49 (m, 3H), 7.36 (t, J = 8.0 Hz, 1H), 7.21 – 7.05 (m, 4H), 4.98 (dd, J = 7.2, 8.0 Hz, 1H), 3.25 – 3.20 (m, 4H), 3.08 (dd, J = 7.2, 14.0 Hz, 1H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 140.7, 137.3, 132.7, 131.9, 129.1, 128.1, 127.9, 127.1, 125.4, 123.8, 81.2, 57.1, 43.2. HRMS (EI) calcd for C$_{15}$H$_4$Br$_2$O$^+$, [M$^+$], 367.9411, found: 367.9400.

![Chemical structure](image)

1-methoxy-1,2-di(3-chlorophenyl) thane (3fa), 54.0 mg (yield: 48%, 0.4 mmol scale), colorless liquid.

$^1$H NMR (400 MHz, DMSO – $d_6$) δ 7.38 – 7.33 (m, 3H), 7.28 – 7.22 (m, 4H), 7.13 – 7.11 (m, 1H), 4.47 (dd, J = 5.2, 8.0 Hz, 1H), 3.07 (s, 3H), 2.97 (dd, J = 8.0, 14.0 Hz, 1H), 2.88 (dd, J = 5.2, 14.0 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) δ 144.2, 140.9, 133.1, 132.7, 130.3, 139.8, 129.3, 128.3, 127.6, 126.6, 126.2, 125.4, 82.7, 56.4, 43.0. HRMS (EI) calcd for C$_{15}$H$_4$Cl$_2$O$^+$, [M$^+$], 280.0422, found: 280.0419.

![Chemical structure](image)

1-methoxy-1,2-di(4-tolyl) thane (3ga), 50.0 mg (yield: 52%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – $d_6$) δ 7.15 – 7.10 (m, 4H), 7.03 – 6.98 (m, 4H), 4.30 (dd, J = 6.0, 7.6 Hz, 1H), 3.02 (s, 3H), 2.95 (dd, J = 7.6, 13.6 Hz, 1H), 2.77 (dd, J = 6.0, 13.6 Hz, 1H), 2.27 (s, 3H), 2.23 (s, 3H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) δ 138.6, 136.6, 135.5, 134.9, 129.3, 128.9, 128.6, 83.9, 56.0, 43.4, 20.9, 20.7. HRMS (EI) calcd for C$_{17}$H$_{20}$O$^+$, [M$^+$], 240.1514, found: 240.1508.

![Chemical structure](image)

1-methoxy-1,2-di(4-fluorophenyl) thane (3ha), 62.6 mg (yield: 63%, 0.4 mmol scale), colorless liquid.

$^1$H NMR (400 MHz, DMSO – $d_6$) δ 7.29 – 7.26 (m, 2H), 7.17 – 7.12 (m, 4H), 7.06 – 7.01 (m, 2H), 4.39 (dd, J = 5.6, 7.6 Hz, 1H), 3.06 (s, 3H), 2.99 (dd, J = 7.6, 14.0 Hz, 1H), 2.83 (dd, J = 5.6, 13.6 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) δ 162.4 (d, J$_{C,F} = 72.8$ Hz), 160.0 (d, J$_{C,F} = 72.8$ Hz), 137.6 (d, J$_{C,F} = 3.0$ Hz), 134.4 (d, J$_{C,F} = 3.0$ Hz), 131.2 (d, J$_{C,F} = 8.0$ Hz), 128.8 (d, J$_{C,F} = 8.0$ Hz), 115.1 (d, J$_{C,F} = 21.2$ Hz), 114.7 (d, J$_{C,F} = 20.2$ Hz), 83.1, 56.1, 42.7. $^{19}$F NMR (377 MHz, DMSO – $d_6$) δ -115.1, -117.2. HRMS (EI) calcd for C$_{15}$H$_4$F$_2$O$^+$, [M$^+$], 248.1013, found: 248.1022.

![Chemical structure](image)

1-methoxy-1,2-di(4-chlorophenyl) thane (3ia), 70.9 mg (yield: 63%, 0.4 mmol scale), colorless liquid.

$^1$H NMR (400 MHz, DMSO – $d_6$) δ 7.39 – 7.37 (m, 2H), 7.29 – 7.25 (m, 4H), 7.15 – 7.13 (m, 2H), 4.42 (dd,
J = 5.6, 7.6 Hz, 1H), 3.06 (s, 3H), 2.98 (dd, J = 7.6, 13.6 Hz, 1H), 2.84 (dd, J = 5.6, 13.6 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO – d$_6$) δ 140.4, 137.2, 132.1, 131.3, 130.8, 128.7, 128.4, 128.0, 82.8, 56.2, 42.7. HRMS (EI) calcd for C$_{15}$H$_{14}$ClO$_2$", [M$^+$], 280.0422, found: 280.0429.

1-methoxy-1,2-di(4-bromophenyl) thane (3ja), 90.3 mg (yield: 61%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – d$_6$) δ 7.54 – 7.51 (m, 2H), 7.43 – 7.40 (m, 2H), 7.23 – 7.19 (m, 2H), 7.10 – 7.07 (m, 2H), 4.40 (dd, J = 5.6, 7.6 Hz, 1H), 3.06 (s, 3H), 2.96 (dd, J = 5.8, 13.8 Hz, 1H), 2.83 (dd, J = 5.6, 13.6 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO – d$_6$) δ 140.8, 137.6, 131.8, 131.3, 130.9, 129.1, 120.7, 119.4, 82.8, 56.3, 42.7. HRMS (EI) calcd for C$_{15}$H$_{14}$BrO$_2$", [M$^+$], 367.9411, found: 367.9414.

1-methoxy-1,2-di(4-tert-butyl phenyl) thane (3ka), 62.3 mg (yield: 48%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.43 – 7.41 (m, 2H), 7.35 – 7.33 (m, 2H), 7.29 – 7.27 (m, 2H), 7.19 – 7.17 (m, 2H), 4.38 (dd, J = 4.4, 8.4 Hz, 1H), 3.23 (s, 3H), 3.11 (dd, J = 8.4, 14.4 Hz, 1H), 2.91 (dd, J = 4.4, 14.4 Hz, 1H), 1.39 (s, 9H), 1.37 (s, 9H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 150.3, 148.6, 139.4, 136.4, 129.3, 126.8, 125.5, 125.2, 84.0 56.5, 43.9, 34.7, 34.5, 31.7, 31.7. HRMS (EI) calcd for C$_{22}$H$_{26}$O", [M$^+$], 324.2453, found: 324.2457.

1-methoxy-1,2-di(4-trifluoromethylphenyl) thane (3la), 66.9 mg (yield: 48%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – d$_6$) δ 7.72 (d, J = 8 Hz, 2H), 7.61 (d, J = 8 Hz, 2H), 7.53 (d, J = 8 Hz, 2H), 7.41 (d, J = 8 Hz, 2H), 4.61 (dd, J = 5.2, 8.0 Hz, 1H), 3.11 – 3.05 (m, 4H), 3.00 (dd, J = 5.2, 14.0 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO – d$_6$) δ 146.3, 143.2, 130.3, 128.3 (q, J$_{C\text{-}C}$ = 31.3 Hz), 127.6, 127.0 (q, J$_{C\text{-}C}$ = 31.3 Hz), 125.4 (q, J$_{C\text{-}C}$ = 4.0 Hz), 124.9 (q, J$_{C\text{-}C}$ = 4.0 Hz), 124.6 (q, J$_{C\text{-}C}$ = 272.7 Hz), 124.4 (q, J$_{C\text{-}C}$ = 272.7 Hz), 82.6, 56.5, 43.2. $^{19}$F NMR (377 MHz, CDCl$_3$) δ -62.1, -62.3. HRMS (EI) calcd for C$_{17}$H$_{14}$FeO$_2$", [M$^+$], 348.0949, found: 348.0941.

1-methoxy-1,2-di(4-trifluoromethoxyphenyl) thane (3ma), 73.0 mg (yield: 48%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – d$_6$) δ 7.43 – 7.41 (m, 2H), 7.35 – 7.28 (m, 4H), 7.24 – 7.22 (m, 2H), 4.51 (dd, J = 4.8, 8.0 Hz, 1H), 3.09 (s, 3H), 3.03 (dd, J = 8.0, 14.0 Hz, 1H), 2.91 (dd, J = 4.8, 14.0 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO- d$_6$) δ 148.1, 148.1, 147.3, 147.2, 141.3, 138.2, 131.5, 129.0, 121.3, 121.0, 120.6 (q, J$_{C\text{-}C}$ = 252.5), 120.6 (q, J$_{C\text{-}C}$ = 252.5), 83.0, 56.7, 43.1. $^{19}$F NMR (377 MHz, DMSO – d$_6$) δ -57.0, -57.0. HRMS (EI) calcd for C$_{17}$H$_{14}$FeO$_2$", [M$^+$], 380.0847, found: 380.0852.

S23
1-methoxy-1-(2-bromophenyl)-2-(4-tolyl) thane and 1-methoxy-1-(4-tolyl)-2-(2-bromophenyl) thane (3na, ratio = 3.5:1), 79.4 mg (yield: 65%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – $d_6$) δ 7.62 – 7.57 (m, 1.3H), 7.44 (d, $J = 4.4$ Hz, 2H), 7.27 – 7.06 (m, 7.7 H), 4.72 (dd, $J = 4.0$, 8.4 Hz, 1H), 4.43 (dd, $J = 5.2$, 8.0 Hz, 0.3H), 3.14 (dd, $J = 8.4$, 14.0 Hz, 0.4H), 3.08 (s, 3H), 3.05 (s, 0.9H), 2.98 – 2.86 (m, 1.4H), 2.79 (dd, $J = 8.4$, 14.0 Hz, 1.0H), 2.30 (s, 0.9H), 2.27 (s, 3.1H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) δ 140.8, 138.6, 138.0, 137.3, 135.6, 133.0, 132.8, 132.6, 129.9, 129.5, 129.4, 129.1, 128.8, 128.5, 128.0, 127.8, 127.0, 124.7, 123.1, 83.3, 82.5, 57.1, 56.5, 44.4, 42.5, 21.1. HRMS (EI) calcd for C$_{16}$H$_{17}$BrO$^+$, [M]$^+$, 304.0463, found: 304.0467.

1-methoxy-1-(2-chlorophenyl)-2-(4-tolyl) thane and 1-methoxy-1-(4-tolyl)-2-(2-chlorophenyl) thane (3oa, ratio = 2.6:1), 67.8 mg (yield: 65%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – $d_6$) δ 7.46 – 7.37 (m, 3.4H), 7.34 – 7.30 (m, 1.1H), 7.22 – 7.21 (m, 1.1 H), 7.16 (d, $J = 0.8$ Hz, 1.3H), 7.06 (s, 3.9H), 4.78 (dd, $J = 4.8$, 7.6 Hz, 1H), 4.42 (dd, $J = 5.2$, 8.0 Hz, 0.4H), 3.15 (dd, $J = 8.4$, 14.0 Hz, 0.4H), 3.09 (s, 3H), 3.05 (s, 1.2H), 2.97 – 2.81 (m, 2.5H), 2.26 (s, 3H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) δ 139.3, 138.7, 137.2, 136.4, 135.5, 135.5, 133.7, 132.6, 132.5, 129.8, 129.5, 129.5, 129.5, 129.4, 129.1, 128.5, 127.9, 127.9, 127.3, 127.0, 82.5, 80.9, 57.0, 56.5, 42.4, 41.8, 21.2, 21.1. HRMS (EI) calcd for C$_{16}$H$_{17}$ClO$^+$, [M]$^+$, 260.0968, found: 260.0979.

1-methoxy-1-phenyl-2-(4-tolyl) thane and 1-methoxy-1-(4-tolyl)-2-phenyl thane (3pa, ratio = 2:1), 72.4 mg (yield: 56%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – $d_6$) δ 7.34 – 7.00 (m, 9H), 4.37 – 4.33 (m, 1H), 3.05 (s, 2H), 3.03 (s, 1H), 3.01 – 2.94 (m, 1H), 2.84 – 2.77 (m, 1H), 2.28 (s, 1H), 2.23 (s, 2H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) δ 141.7, 138.6, 138.6, 136.7, 135.4, 134.9, 129.4, 129.3, 128.9, 128.6, 128.3, 128.0, 127.6, 126.8, 126.0, 84.1, 83.8, 56.1, 56.0, 43.8, 43.4, 20.9, 20.7.

1-methoxy-1-phenyl-2-(4-chlorophenyl) thane and 1-methoxy-1-(4-chlorophenyl)-2-phenyl thane (3qa, ratio = 1.5:1), 61.2 mg (yield: 62%, 0.4 mmol scale), colorless liquid. $^1$H NMR (400 MHz, DMSO – $d_6$) δ 7.47 – 7.17 (m, 16H), 4.82 (dd, $J = 5.2$, 8.0 Hz, 1H), 4.47 (dd, $J = 5.2$, 8.0 Hz, 0.7H), 3.16 (dd, $J = 8.0$, 14.0, 0.7H), 3.10 (s, 2.9H), 3.07 (s, 2H), 3.00 – 2.86 (m, 3.2H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) δ 141.7, 139.2, 138.6, 136.3, 133.8, 132.6, 132.5, 129.8, 129.7, 129.5, 129.5, 128.8, 128.6, 128.5, 128.1, 127.9, 127.9, 127.2, 127.0, 126.7, 82.7, 80.8, 57.0, 56.6, 42.8, 41.9. HRMS (EI) calcd for C$_{15}$H$_{15}$ClO$^+$, [M]$^+$, 246.0811, found: 246.0813.
1-methoxy-1-phenyl-2-(4-bromophenyl) thane and 1-methoxy-1-(4-bromophenyl)-2-phenyl thane (3ra, ratio = 1.5:1).\[1] 71.1 mg (yield: 61%, 0.4 mmol scale), colorless liquid. \[1]H NMR (400 MHz, DMSO – d6) δ 7.52 – 7.08 (m, 9H), 4.43 – 4.36 (m, 1H), 3.06 (s, 1.8H), 3.05 (s, 1.2H), 3.03 – 2.95 (m, 1H), 2.83 (dd, J = 5.6, 13.6 Hz, 1H); \[13]C NMR (101 MHz, DMSO – d6) δ 141.4, 141.1, 138.1, 138.0, 131.7, 131.2, 130.9, 129.4, 129.1, 128.4, 128.1, 127.7, 126.8, 126.2, 120.6, 119.2, 83.6, 83.2, 56.2, 56.2, 43.5, 43.0.

1-methoxy-1-phenyl-2-(4-trifluoromethylphenyl) thane and 1-methoxy-1-(4- trifluoromethylphenyl) -2-phenyl thane (3sa, ratio = 1.3:1).\[2] 65.0 mg (yield: 58%, 0.4 mmol scale), colorless liquid. \[1]H NMR (400 MHz, DMSO – d6) δ 7.69 – 7.67 (d, J = 8.0 Hz, 0.9H), 7.59 – 7.57 (d, J = 8.0 Hz, 1.2H), 7.49 – 7.47 (d, J = 8.0 Hz, 0.9H), 7.39 – 7.13 (m, 6.3H), 4.54 (dd, J = 5.6, 8.0 Hz, 0.4H), 4.45 (dd, J = 5.2, 8.4 Hz, 0.6H), 3.11 – 2.93 (m, 4.7H), 2.87 (dd, J = 5.6, 14.0 Hz, 0.5H); \[13]C NMR (101 MHz, DMSO – d6) δ 146.6, 143.6, 141.3, 138.0, 130.2, 129.5, 128.4, 128.2 (q, J_{CF} = 31.3 Hz), 128.1, 127.8, 127.6, 126.9 (q, J_{CF} = 31.3 Hz), 126.8, 126.2, 125.2 (q, J_{CF} = 4.0 Hz), 124.8 (q, J_{CF} = 4.0 Hz), 124.6 (q, J_{CF} = 272.7 Hz), 124.4 (q, J_{CF} = 272.7 Hz), 83.4, 83.3, 56.5, 56.2, 43.6, 43.5. \[19]F NMR (377 MHz, CDCl3) δ -60.8, -60.9.

1-methoxy-1-(4-cyanophenyl)-2-phenyl thane and 1-methoxy-1-phenyl-2-(4-cyanophenyl) thane (3ta, ratio = 1.2:1). 37.0 mg (yield: 39%, 0.4 mmol scale), colorless liquid. \[1]H NMR (400 MHz, DMSO – d6) δ 7.81 – 7.69 (m, 2H), 7.45 – 7.11 (m, 7H), 4.55 (dd, J = 5.6, 7.6 Hz, 0.5H), 4.46 (dd, J = 5.0, 8.0 Hz, 0.5H), 3.11 – 2.94 (m, 4.4H), 2.86 (dd, J = 5.6, 13.6 Hz, 0.5H); \[13]C NMR (101 MHz, DMSO – d6) δ 147.5, 144.8, 141.2, 137.8, 132.3, 131.9, 130.6, 129.5, 128.4, 128.1, 127.8, 126.8, 126.3, 110.3, 109.0, 83.2, 83.1, 56.6, 56.2, 43.7, 43.3. HRMS (EI) calcd for C_{18}H_{19}NO, [M]+, 237.1154, found: 237.1157.

1-methoxy-1-(2-bromophenyl)-2-phenyl thane and 1-methoxy-1-phenyl-2-(2-bromophenyl) thane (5aa, ratio = 2:1). 65.2 mg (yield: 56%, 0.4 mmol scale), colorless liquid. \[1]H NMR (400 MHz, DMSO – d6) δ 7.46 – 7.12 (m, 22.9H), 4.76 (dd, J = 4.0, 8.4 Hz, 1.7H), 4.47 (dd, J = 5.2, 8.0 Hz, 0.9H), 3.19 – 3.13 (dd, J = 8.4, 13.6 Hz, 1H), 3.09 (s, 5H), 3.07 (s, 2.9H), 3.00 – 2.82 (m, 4.9H); \[13]C NMR (101 MHz, DMSO – d6) δ 141.7, 140.7, 138.6, 138.0, 133.0, 132.8, 132.6, 129.9, 129.7, 128.8, 128.5, 128.5, 128.2, 128.0, 127.8, 127.0, 126.7, 124.7, 123.1, 83.2, 82.7, 57.1, 56.7, 44.4, 42.9. HRMS (EL) calcd for C_{18}H_{16}BrO, [M]+, 290.0306, found: 290.0313.

1-methoxy-1,2-diphenyl-2-methyl thane (3ua). 54.5 mg (yield: 60%, 0.4 mmol scale), colorless liquid. \[1]H NMR (400 MHz, CDCl3) δ 7.40 – 7.12 (m, 10H), 4.29 – 4.24 (m, 1H), 3.29 (s, 1.9H), 3.19 – 3.06 (m, 2.2H), 1.46 (d, J = 7.2 Hz, 1.9H), 1.12 (d, J = 7.2 Hz, 1.2H); \[13]C NMR (101 MHz, CDCl3) δ 144.5, 144.1, 140.8, 140.5, 128.2, 128.2, 128.1, 128.0, 127.9, 127.9, 127.7, 127.7, 127.3, 127.2, 126.2, 126.2, 88.8, 88.8, 57.2, 57.0, 47.3, 46.6, 18.4, 17.0. HRMS (EI) calcd for C_{18}H_{18}O, [M]+, 226.1358, found: 226.1364.
1-methoxy-1-phenyl-2-methyl-2-(4-trifluorophenyl) thane and 1-methoxy-1-(4-trifluorophenyl)-2-methyl-2-phenyl thane (3va, ratio = 1.8:1), 71.9 mg (yield: 61%, 0.4 mmol scale), colorless liquid. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.61 – 7.05 (m, 9H), 4.32 – 4.21 (m, 1H), 3.25 – 3.25 (m, 2.2H), 3.18 – 2.98 (m, 1.8H), 1.42 – 1.39 (m, 2.2H), 1.13 – 1.06 (m, 0.8H); \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 148.1, 145.0, 143.3, 140.0, 129.5, 129.2, 128.5, 128.3, 128.2, 128.1, 128.1, 128.0, 127.9, 127.5, 127.5, 127.5, 127.2, 126.4, 125.6, 125.0, 124.8, 124.8, 124.7, 122.9, 88.3, 88.3, 88.2, 57.4, 57.2, 57.0, 47.2, 47.0, 46.7, 18.46, 16.8, 16.5.

1-methoxy-1-methyl-1,2-diphenyl thane (3wa), 29.1 mg (yield: 32%, 0.4 mmol scale), colorless liquid. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.40 – 7.30 (m, 5H), 7.23 – 7.17 (m, 3H), 6.94 – 6.92 (m, 2H), 3.18 (s, 3H), 3.07 (dd, \(J = 13.2\) Hz, 2H), 1.56 (s, 3H); \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 144.3, 137.5, 130.8, 128.0, 127.6, 127.0, 126.8, 126.2, 79.8, 50.8, 50.6, 21.2. HRMS (EI) calcd for C\(_{16}\)H\(_{18}\)O\(^+\), [M\(^+\)], 226.1358, found: 226.1361.

1-methoxy-1,1,2-triphenyl thane (3xa), 87.7 mg (yield: 76%, 0.4 mmol scale), white solid. \(^1\)H NMR (400 MHz, DMSO – d\(_6\)) \(\delta\) 7.44 – 7.41 (m, 4H), 7.37 – 7.32 (m, 6H), 7.28 – 7.18 (m, 3H), 3.75 (s, 2H), 3.20 (s, 3H), 3.07 (dd, \(J = 13.2\) Hz, 2H), 1.56 (s, 3H); \(^13\)C NMR (101 MHz, DMSO – d\(_6\)) \(\delta\) 168.4, 150.6, 144.8, 129.8, 128.5, 128.0, 127.5, 127.0, 126.2, 121.9, 82.0, 51.1. HRMS (EI) calcd for C\(_{20}\)H\(_{17}\)O\(^+\), [M\(^-\)CH\(_3\)O\(^+\)], 257.1330, found: 257.1329.

1,1-dimethoxy-2-phenyl thane (3ya), 37.2 mg (yield: 56%, 0.4 mmol scale), colorless liquid. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.37 – 7.25 (m, 5H), 4.60 (t, \(J = 5.6\) Hz, 1H), 3.39 (s, 6H), 2.97 (d, \(J = 5.6\) Hz, 2H); \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 137.0, 129.5, 128.4, 126.4, 105.3, 53.4, 39.7. HRMS (EI) calcd for C\(_{10}\)H\(_{14}\)O\(_2\)^+\([M]^+\), 166.0994, found: 166.0992.

2-Methoxy-1,3-diphenylpropane (3za), 38.1 mg (yield: 42%, 0.4 mmol scale), colorless liquid. \(^1\)H NMR (400 MHz, DMSO – d\(_6\)) \(\delta\) 7.41 – 7.30 (m, 10H), 3.76 – 3.69 (m, 1H), 3.35 (s, 3H), 2.94 – 2.83 (m, 4H); \(^13\)C NMR (101 MHz, DMSO – d\(_6\)) \(\delta\) 139.1, 129.5, 128.4, 126.2, 83.7, 57.6, 40.3. HRMS (EI) calcd for C\(_{16}\)H\(_{16}\)O\(^+\), [M\(^+\)], 226.1358, found: 226.1354.
1-Azido-1,2-diphenyl thane (6a),[7] 31.6 mg (yield:71%, 0.2 mmol scale), colorless liquid. ^1H NMR (400 MHz, DMSO – d6) δ 7.44 – 7.20 (m, 10H), 5.00 (dd, J = 7.2, 8.0 Hz, 1H), 3.11 – 3.08 (m, 2H); ^13C NMR (101 MHz, DMSO – d6) δ 139.3, 137.5, 129.4, 128.8, 128.5, 128.4, 127.0, 126.8, 67.7, 43.1.

1-allyl-1,2-diphenyl thane (6b), 26.2 mg (yield:59%, 0.2 mmol scale), colorless liquid. ^1H NMR (400 MHz, DMSO – d6) δ 7.26 – 7.07 (m, 10H), 5.69 – 5.58 (m, 1H), 4.96 – 4.89 (m, 2H), 3.02 – 2.92 (m, 2H), 2.87 – 2.81 (m, 1H), 2.39 – 2.35 (m, 2H); ^13C NMR (101 MHz, DMSO – d6) δ 144.7, 140.7, 137.3, 129.4, 128.5, 128.5, 128.2, 126.4, 126.2, 116.7, 47.1, 42.3.

1,2-diphenyl ethylene (6c),[8] 68.2 mg (yield:47%, 0.8 mmol scale), colorless liquid. ^1H NMR (400 MHz, DMSO – d6) δ 7.59 – 7.56 (m, 4H), 7.42 (t, J = 7.6 Hz, 4H), 7.34 – 7.29 (m, 2H), 7.17 (m, 2H); ^13C NMR (101 MHz, DMSO – d6) δ 137.4, 128.8, 128.7, 127.7, 126.6.

2-Propenoic acid, 3-(2-(2-methoxy-2phenyl ethyl)phenyl), ethyl ester (6d), 24.7 mg (yield:40%, 0.2 mmol scale), colorless liquid. ^1H NMR (400 MHz, CDCl3) δ 7.97 (d, J = 15.6 Hz, 1H), 7.56 – 7.54 (m, 1H), 7.35 – 7.22 (m, 7H), 7.16 – 7.14 (m, 1H), 6.29 (d, J = 15.6 Hz, 1H), 4.34 – 4.29 (m, 3H), 3.30 – 3.22 (m, 4H), 3.09 (dd, J = 6.0, 14.0 Hz, 1H), 1.41 (t, J = 7.2 Hz, 3H); ^13C NMR (101 MHz, CDCl3) δ 166.9, 142.1, 141.2, 137.9, 133.8, 131.5, 129.7, 128.4, 127.7, 126.9, 126.6, 126.4, 119.4, 84.7, 60.5, 56.9, 42.1, 14.4. HRMS (ESI) calcd for C20H22O3, [M+Na]^+, 333.1461, found: 333.1462.

9,10-dihydro-9-methoxy-phenanthrene (6f), 74.7 mg (yield:71%, 0.5 mmol scale), colorless liquid. ^1H NMR (400 MHz, DMSO – d6) δ 7.93 – 7.88 (dd, J = 7.6, 14.8 Hz, 2H), 7.49 – 7.44 (m, 2H), 7.37 – 7.25 (m, 4H), 4.37 (t, J = 4.4 Hz, 1H), 3.19 (s, 1H), 3.14 – 3.03 (m, 2H); ^13C NMR (101 MHz, DMSO – d6) δ 135.2, 134.4, 133.7, 133.4, 129.6, 129.4, 129.2, 128.2, 127.7, 127.5, 124.5, 123.8, 76.0, 55.8, 34.4. HRMS (EI) calcd for C13H14O^+, [M]^+, 210.1045, found: 210.1041.
Characterization of Substrates

3,3-di(2-chlorophenyl)-propanoic acid (1a), white solid. $^1$H NMR (400 MHz, DMSO – $d_6$) δ 12.41 (s, 1H), 7.45 (dd, $J = 1.6, 7.6$ Hz, 2H), 7.33 – 7.23 (m, 6H), 5.20 (t, $J = 8.0$ Hz, 1H), 2.20 (d, $J = 8.0$ Hz, 2H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) δ 172.5, 139.9, 133.7, 130.1, 129.3, 128.9, 127.8, 40.59, 38.63. HRMS (ESI) calcd for C$_{15}$H$_{13}$Cl$_2$O$_2$+, [M+H]$^+$, 295.0287, found: 295.0284.

3,3-diphenylpropanoic acid (1b), white solid. $^1$H NMR (400 MHz, DMSO – $d_6$) δ 12.15 (s, 1H), 7.33 – 7.24 (m, 8H), 7.18 – 7.13 (m, 2H), 4.41 (t, $J = 8.0$ Hz, 1H), 3.02 (d, $J = 7.6$ Hz, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 178.0, 143.1, 128.5, 127.5, 126.5, 46.5, 40.3.

3,3-di(2-methylphenyl)-propanoic acid (1c), white solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.15 – 7.07 (m, 8H), 4.82 (t, $J = 8.0$ Hz, 1H), 3.92 (t, $J = 8.0$ Hz, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 177.8, 140.8, 136.1, 130.8, 126.7, 126.6, 126.3, 39.6, 39.5, 19.5. HRMS (ESI) calcd for C$_{17}$H$_{22}$O$_2$N$^+$, [M+NH$_4$]$^+$, 272.1645, found: 272.1644.

3,3-di(2-fluorophenyl)-propanoic acid (1d), white solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.31 – 7.01 (m, 8H), 5.07 (t, $J = 8.0$ Hz, 1H), 3.18 (d, $J = 8.0$ Hz, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 161.8, 159.4, 128.9, 128.9, 128.8, 128.8, 128.7, 128.6, 128.6, 124.2, 124.2, 115.9, 115.7, 37.9, 34.3. $^{19}$F NMR (377 MHz, CDCl$_3$) δ -116.5. HRMS (ESI) calcd for C$_{15}$H$_{11}$F$_2$O$_2$+, [M-HF]$^+$, 261.0733, found: 261.0740.

3,3-di(2-bromphenyl)-propanoic acid (1e), white solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 12.43 (s, 1H), 7.63 – 7.17 (m, 8H), 5.08 (t, $J = 8.0$ Hz, 1H), 2.89 (d, $J = 8.0$ Hz, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 172.4,
3,3-di(3-chlorophenyl)-propanoic acid (1f), white solid. $^1$H NMR (400 MHz, DMSO – d$_6$) δ 7.46 (s, 2H), 7.36 – 7.22 (m, 6H), 4.46 (t, $J = 8.0$ Hz, 1H), 3.02 (d, $J = 8.0$ Hz, 2H); $^{13}$C NMR (101 MHz, DMSO – d$_6$) δ 172.7, 146.3, 133.3, 130.5, 127.7, 126.7, 126.5, 46.0, 39.0. HRMS (ESI) calcd for C$_{15}$H$_{11}$Br$_2$O$_2^+$, [M-H]$^+$, 380.9131, found: 380.9133.

3,3-di(4-methylphenyl)-propanoic acid (1g), white solid. $^1$H NMR (400 MHz, DMSO – d$_6$) δ 12.17 (s, 1H), 7.18 – 7.16 (d, $J = 8.0$ Hz, 4H), 7.07 – 7.05 (d, $J = 8.0$ Hz, 4H), 4.34 (t, $J = 8.0$ Hz, 1H), 2.96 (d, $J = 8.0$ Hz, 2H), 2.22 (s, 6H); $^{13}$C NMR (101 MHz, DMSO – d$_6$) δ 173.0, 141.5, 135.3, 129.1, 127.5, 46.1, 40.1, 20.7.

3,3-di(4-fluorophenyl)-propanoic acid (1h), white solid. $^1$H NMR (400 MHz, DMSO – d$_6$) δ 7.38 – 7.34 (m, 4H), 7.11 – 7.06 (m, 4H), 4.46 (t, $J = 8.0$ Hz, 1H), 3.02 (d, $J = 8.0$ Hz, 2H); $^{13}$C NMR (101 MHz, DMSO – d$_6$) δ 172.8, 160.9 (d, J$_{C,F}$ = 242.4 Hz), 140.4 (d, J$_{C,F}$ = 3.0 Hz), 129.5 (d, J$_{C,F}$ = 8.1 Hz), 115.3 (d, J$_{C,F}$ = 21.2 Hz), 45.3, 40.1. $^{19}$F NMR (377 MHz, DMSO – d$_6$) δ -116.8.

3,3-di(4-chlorophenyl)-propanoic acid (1i), white solid. $^1$H NMR (400 MHz, DMSO – d$_6$) δ 12.26 (s, 1H), 7.36 – 7.31 (m, 8H), 4.44 (t, $J = 8.0$ Hz, 1H), 3.03 (d, $J = 8.0$ Hz, 2H); $^{13}$C NMR (101 MHz, DMSO – d$_6$) δ 173.0, 143.3, 131.5, 129.9, 128.9, 45.7, 39.7.
3,3-di(4-bromophenyl)-propanoic acid (1j), white solid. \(^1\)H NMR (400 MHz, DMSO – \(d_6\)) \(\delta\) 12.24 (s, 1H), 7.47 – 7.45 (m, 4H), 7.30 – 7.28 (m, 4H), 4.41 (t, \(J = 8.0\) Hz, 1H), 3.02 (d, \(J = 8.0\) Hz, 2H); \(^{13}\)C NMR (101 MHz, DMSO – \(d_6\)) \(\delta\) 172.6, 143.3, 131.4, 129.9, 119.7, 45.5, 39.2.

3,3-di(4-tertbutylphenyl)-propanoic acid (1k), white solid. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 12.17 (s, 1H), 7.33 – 7.31 (m, 4H), 7.20 – 7.18 (m, 4H), 4.50 (t, \(J = 8.0\) Hz, 1H), 3.10 (d, \(J = 8.0\) Hz, 2H), 1.31 (s, 9H); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 177.3, 149.2, 140.4, 127.2, 125.5, 45.7, 40.5, 34.4, 31.4. HRMS (ESI) calcd for C\(_{23}\)H\(_{34}\)NO\(_2\), [M+NH\(_4\)]\(^+\), 356.2584, found: 356.2584.

3,3-di(4-trifluoromethylphenyl)-propanoic acid (1l), white solid. \(^1\)H NMR (400 MHz, DMSO – \(d_6\)) \(\delta\) 12.36 (s, 1H), 7.65 – 7.59 (m, 8H), 4.67 (t, \(J = 8.0\) Hz, 1H), 3.16 (d, \(J = 7.6\) Hz, 2H); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 176.3, 146.1, 129.3 (q, \(J_{C-F} = 32.6\) Hz), 127.9, 125.8 (q, \(J_{C-F} = 3.8\) Hz), 123.9 (q, \(J_{C-F} = 273.0\) Hz), 46.1, 39.6. \(^{19}\)F NMR (377 MHz, DMSO – \(d_6\)) \(\delta\) -61.0. HRMS (EI) calcd for C\(_{17}\)H\(_{12}\)F\(_6\)O\(_2\), [M]\(^+\), 362.0741, found: 362.0735.

3,3-di(4-trifluoromethoxyphenyl)-propanoic acid (1m), white solid. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.27 – 7.17 (m, 8H), 4.58 (t, \(J = 8.0\) Hz, 1H), 3.10 (d, \(J = 8.0\) Hz, 2H); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 176.7, 148.0, 148.0, 141.3, 128.9, 121.3, 120.4, 45.3, 40.3. \(^{19}\)F NMR (377 MHz, CDCl\(_3\)) \(\delta\) -57.9. HRMS (EI) calcd for C\(_{18}\)H\(_{15}\)BrO\(_2\), [M]\(^+\), 393.0567, found: 393.0562.

3-(2-bromophenyl)-3-(4-tolyl)-propanoic acid (1n), white solid. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.57 (dd, \(J = 1.2, 8.0\) Hz, 1H), 7.30 - 7.07 (m, 7H), 5.02 (t, \(J = 8.0\) Hz, 1H), 3.13 – 3.02 (m, 2H), 2.33 (s, 3H); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 177.2, 142.4, 138.6, 136.4, 133.3, 129.3, 128.5, 128.1, 127.8, 127.7, 124.8, 44.9, 40.0, 21.1. HRMS (ESI) calcd for C\(_{16}\)H\(_{15}\)BrO\(_2\)Na\(^+\), [M+Na]\(^+\), 341.0148, found: 341.0144.
3-(2-chlorophenyl)-3-(4-tolyl)-propanoic acid (1o), white solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.39 - 7.37 (m, 1H), 7.27 – 7.12 (m, 7H), 5.03 (t, $J$ = 8.0 Hz, 1H), 3.14 – 3.03 (m, 2H), 2.34 (s, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 177.1, 140.8, 138.6, 134.0, 134.0, 130.0, 129.3, 128.2, 127.8, 127.8, 127.0, 42.4, 39.7, 21.1. HRMS (ESI) calcd for C$_{16}$H$_{15}$ClO$_2$Na$^+$, [M+Na]$^+$, 297.0653, found: 297.0652.

3-(4-methylphenyl)-3-phenylpropanoic acid (1p),$^{[1]}$ white solid. $^1$H NMR (400 MHz, DMSO – $d_6$) $\delta$ 12.10 (s, 1H), 7.31 – 7.06 (m, 9H), 4.39 (t, $J$ = 8.0 Hz, 1H), 3.00 (d, $J$ = 8.0 Hz, 2H), 2.22 (s, 3H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) $\delta$ 172.9, 144.6, 141.3, 135.4, 129.1, 128.5, 127.6, 127.5, 126.3, 46.5, 40.0, 20.7.

3-(4-chlorophenyl)-3-phenylpropanoic acid (1q), white solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.40 – 7.17 (m, 9H), 5.07 (t, $J$ = 8.0 Hz, 1H), 3.16 – 3.05 (m, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 177.2, 141.6, 140.5, 134.0, 130.0, 128.6, 128.2, 127.9, 127.1, 126.8, 42.8, 39.7. HRMS (ESI) calcd for C$_{16}$H$_{11}$ClO$_2$Na$^+$, [M-H]$^+$, 259.0531, found: 259.0533.

3-(4-bromophenyl)-3-phenylpropanoic acid (1r),$^{[6]}$ white solid. $^1$H NMR (400 MHz, DMSO – $d_6$) $\delta$ 12.27 (s, 1H), 7.47 – 7.15 (m, 9H), 4.45 (t, $J$ = 8.0 Hz, 1H), 3.05 (d, $J$ = 8.0 Hz, 2H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) $\delta$ 172.8, 143.8, 143.8, 131.4, 130.0, 128.7, 127.7, 126.6, 119.6, 46.3, 39.7.

3-(4-trifluoromethylphenyl)-3-phenylpropanoic acid (1s),$^{[6]}$ white solid. $^1$H NMR (400 MHz, DMSO – $d_6$) $\delta$ 12.32 (s, 1H), 7.64 – 7.56 (m, 4H), 7.37 – 7.16 (m, 5H), 4.56 (t, $J$ = 8.0 Hz, 1H), 3.17 – 3.05 (m, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 177.7, 147.1, 142.1, 128.9 (q, $J_{C,F} = 32.5$ Hz), 128.8, 127.9, 127.5, 127.0, 125.6 (q, $J_{C,F} = 4.0$ Hz), 124.0 (q, $J_{C,F} = 273.0$ Hz), 46.3, 40.0. $^{19}$F NMR (377 MHz, DMSO – $d_6$) $\delta$ -60.9.
3-(4-Cyanophenyl)-3-phenylpropanoic acid (1t), white solid. $^1$H NMR (400 MHz, DMSO – $d_6$) $\delta$ 12.26 (s, 1H), 7.74 (d, $J = 8.4$ Hz, 2H), 7.60 (d, $J = 8.0$ Hz, 2H), 7.35 (d, $J = 7.2$ Hz, 2H), 7.28 (t, $J = 7.6$ Hz, 2H), 7.18 (t, $J = 7.2$ Hz, 1H), 4.52 (t, $J = 8.0$ Hz, 1H), 3.15 – 3.02 (m, 2H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) $\delta$ 173.0, 150.5, 143.5, 132.8, 129.1, 129.1, 128.1, 127.1, 119.3, 109.6, 47.1, 39.4. HRMS (ESI) calcd for C$_{16}$H$_{14}$O$_2$N$^+$, [M+H]$^+$, 252.1019, found: 252.1017.

3-(2-bromophenyl)-3-phenylpropanoic acid (4a), white solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.58 (dd, $J = 1.2$, 7.6 Hz, 1H), 7.34 – 7.22 (m, 7H), 7.13 – 7.08 (m, 1H), 5.06 (t, $J = 8.0$ Hz, 1H), 3.15 – 3.04 (m, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 176.3, 142.2, 141.6, 133.4, 128.6, 128.5, 128.2, 128.0, 127.7, 126.8, 124.9, 45.3, 39.8. HRMS (ESI) calcd for C$_{15}$H$_{13}$BrO$_2$Na$^+$, [M+Na]$^+$, 328.9971, found: 328.9965.

2-methyl-3,3-diphenyl-propanoic acid (1u), white solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.35 – 7.17 (m, 10H), 4.11 (d, $J = 11.6$ Hz, 1H), 3.40 – 3.32 (m, 1H), 1.18 (d, $J = 6.8$ Hz, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 181.8, 142.9, 142.1, 128.7, 128.6, 128.2, 127.6, 126.6, 54.6, 44.3, 17.2. HRMS (ESI) calcd for C$_{16}$H$_{16}$O$_2$Na$^+$, [M+Na]$^+$, 263.1043, found: 263.1043.

2-methyl-3-phenyl-3(4-trifluorophenyl)-propanoic acid (1v), white solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.53 (d, $J = 8.0$ Hz, 2H), 7.45 (d, $J = 8.0$ Hz), 7.35 – 7.23 (m, 5H), 4.16 (d, $J = 11.2$ Hz, 1H), 3.41 – 3.33 (m, 1H), 1.18 (d, $J = 6.8$ Hz, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 181.2, 146.9, 141.0, 129.0, 128.1, 127.9, 127.1, 125.6, 125.6, 125.5, 54.4, 44.0, 17.1.

3,3-diphenyl-3-methyl-propanoic acid (1w), white solid. $^1$H NMR (400 MHz, DMSO – $d_6$) $\delta$ 11.95 (s, 1H), 7.30 – 7.16 (m, 10H), 3.13 (s, 2H), 1.84 (s, 3H); $^{13}$C NMR (101 MHz, DMSO – $d_6$) $\delta$ 172.7, 149.0, 128.4, 127.3, 126.2, 45.9, 45.1, 28.0. HRMS (ESI) calcd for C$_{16}$H$_{16}$O$_2$Na$^+$, [M+Na]$^+$, 263.1043, found: 263.1043.
3-phenyl-3methoxy-propanoic acid (1y), white solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.46 – 7.34 (m, 5H), 4.67 (dd, $J = 4.0$, 9.6 Hz, 1H), 3.28 (s, 3H), 2.88 (dd, $J = 9.2$, 15.6 Hz, 1H), 2.68 (dd, 4.0, 15.6 Hz, 1H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 176.4, 140.1, 128.7, 128.3, 126.6, 79.8, 56.9, 43.3. HRMS (ESI) calcd for C$_{10}$H$_{12}$O$_3$Na$^+$, [M+Na]$^+$, 203.0679, found: 203.0677.

3,4-diphenyl-butyric acid (1z), white solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.32 – 7.17 (m, 8H), 7.09 – 7.07 (m, 2H), 3.47 – 3.39 (m, 1H), 2.99 – 2.90 (m, 2H), 2.76 – 2.64 (m, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 178.4, 143.1, 139.3, 129.2, 128.5, 128.3, 127.5, 126.7, 126.3, 43.6, 43.0, 39.8. HRMS (ESI) calcd for C$_{16}$H$_{15}$O$_2$, [M-H]$^-$, 239.1078, found: 239.1078.

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NMR Spectra of Products and Substrates

3aa

3ba

S34
3ad
3bf
3qa

Chemical shifts and other spectral data for the compounds are shown in the diagram.
3ya

O

O

11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

O

O

2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

S77
1c

\[
\begin{align*}
\text{OH} & \quad \text{H} \quad \text{O} \\
\text{Ar} & \quad \text{Ar} \\
\end{align*}
\]

S86
S101
1t
General Computational Calculation Details

Thermal correction to Gibbs Free Energy = 0.164101
Sum of electronic and thermal Free Energies = -1459.988004

\begin{align*}
\text{C} & : 0.07663800 \quad 0.97883300 \quad 0.17407700 \\
\text{H} & : 0.32595600 \quad 1.86034300 \quad -0.43586400 \\
\text{C} & : 1.09855400 \quad -0.09083200 \quad -0.19648100 \\
\text{C} & : 0.73999500 \quad -1.38195100 \quad -0.59571300 \\
\text{C} & : 2.46988900 \quad 0.19721800 \quad -0.16397800 \\
\text{C} & : 1.69550000 \quad -2.34200000 \quad -0.91940800 \\
\text{H} & : -0.31124200 \quad -1.64226500 \quad -0.66415300 \\
\text{C} & : 3.44048100 \quad -0.74616500 \quad -0.48301600 \\
\text{C} & : 3.04911700 \quad -2.02798900 \quad -0.85746300 \\
\text{H} & : 1.37672200 \quad -3.33429000 \quad -1.22246500 \\
\text{H} & : 4.48996900 \quad -0.47381200 \quad -0.44394800 \\
\text{H} & : 3.80229700 \quad -2.76848100 \quad -1.10693400 \\
\text{C} & : -1.35480000 \quad 0.62982800 \quad -0.22562600 \\
\text{C} & : -2.18512900 \quad -0.24926800 \quad 0.48014500 \\
\text{C} & : -1.89942000 \quad 1.23120200 \quad -1.36619200 \\
\text{C} & : -3.49075300 \quad -0.51816200 \quad 0.07865000 \\
\text{C} & : -3.20153200 \quad 0.97742500 \quad -1.78458400 \\
\text{H} & : -1.27735500 \quad 1.91944300 \quad -1.93237500 \\
\text{C} & : -4.00168900 \quad 0.10051600 \quad -1.05791000 \\
\text{H} & : -4.09810300 \quad -1.20795500 \quad 0.65537100 \\
\text{H} & : -3.58859800 \quad 1.46583400 \quad -2.67322000 \\
\text{H} & : -5.02085300 \quad -0.10635800 \quad -1.36849900
\end{align*}
C                  0.18937000    1.39265600    1.61184900
H                 -0.35840200    2.26316700    1.95369400
H                  0.77985200    0.82917700    2.32178700
Cl                 -1.60715200   -1.08758900    1.90972800
Cl                  3.02611900    1.81037300    0.25206600

Thermal correction to Gibbs Free Energy=         0.159911
Sum of electronic and thermal Free Energies=      -1459.935281

C                  -0.04200500   -0.74946400   -0.22796300
H                  -0.37990900   -1.64391900   -1.04798900
C                 -1.15059900    0.18186600    0.06089400
C                 -0.84974600    1.45352700    0.58975600
C                 -2.51748500   -0.08855300   -0.14548100
C                 -1.83599100    2.37583400    0.91095500
H                  0.19134600    1.70856000    0.76302800
C                 -3.51569200    0.82415000    0.17807400
C                 -3.17931900    2.06210500    0.71510500
H                 -1.55188200    3.33924000    1.32268600
H                 -4.55275500    0.56416400   -0.00713800
H                 -3.96050000    2.77214500    0.96565400
C                  1.30144100   -0.17286400   -0.50617700
C                  2.35404500   -0.21729400    0.41835500
C                  1.55430400    0.45749600   -1.73292700
C                  3.61317400    0.30056400    0.12915900
C                  2.80258000    0.98748700   -2.03628200

S114
H  0.74555700  0.51328400 -2.45685400
C  3.83783700  0.89944500 -1.10663200
H  4.40289900  0.24558500  0.87136700
H  2.96963800  1.46222500 -2.99792600
H  4.81939400  1.30255000 -1.33491200
C -0.10011500 -2.18195300  0.15730000
H  0.79475700 -2.77521900  0.01945900
H -0.94367400 -2.58027000  0.70547900
Cl 2.08873600 -0.87470900  2.02067200
Cl -3.03988000 -1.57837400 -0.91641700

Thermal correction to Gibbs Free Energy= 0.164769
Sum of electronic and thermal Free Energies= -1460.010337

C  -0.03483800  0.0.65128900 -0.25860700
H  -0.43832600 -2.39674800 -1.46765800
C  -1.15057300  0.19865400  0.07815900
C  -0.88504600  1.45369800  0.69323000
C  -2.52578000 -0.09872300 -0.10645200
C  -1.88585800  2.31327200  1.10811300
H   0.15016500  1.72738300  0.86869100
C  -3.53631000  0.75904300  0.31146700
C  -3.22567600  1.96747300  0.92626100
H  -1.62150400  3.25202500  1.58464700
H  -4.57045800  0.48093000  0.13650100
H  -4.02213100  2.62961900  1.24920600

S115
C   1.29124300  -0.02055300  -0.44934800
C   2.39618200  -0.30039500   0.36638000
C   1.49163600   0.88555800  -1.50294500
C   3.64894800   0.25933300   0.13798200
C   2.73652900   1.45336600  -1.74782800
H   0.64612500   1.12828400  -2.14088200
C   3.81945200   1.13437900  -0.93049600
H   4.79577600   1.57179100  -1.11331200
C  -0.10150300  -2.13801500  -0.45564100
H   0.89302400  -2.57449100  -0.33293500
H  -0.78077200  -2.62119100   0.25247900
Cl   2.19829100  -1.32912100   1.77298300
Cl  -3.05828800  -1.53298100  -0.96591500

Thermal correction to Gibbs Free Energy=  0.164838
Sum of electronic and thermal Free Energies=  -1459.966972

C   0.03617700  -0.60022500  -0.08804000
H  -0.08275400  -1.32198300  -0.89792200
C  -1.25084400   0.12712900   0.20632600
C  -1.26866300   1.38107800   0.90203200
C  -2.51605700  -0.30980700  -0.30028700
C  -2.44171800   2.06678100   1.13378500
H  -0.32716600   1.77718200   1.27015300

S116
| Atoms | x     | y     | z     |
|-------|-------|-------|-------|
| C     | -3.68915500 | 0.38220800 | -0.06292600 |
| C     | -3.66747600 | 1.57509500 | 0.66260700 |
| H     | -2.40795100 | 3.00434200 | 1.68058000 |
| H     | -4.62341200 | -0.00536900 | -0.45712100 |
| H     | -4.59027400 | 2.11529900 | 0.84304900 |
| C     | 1.30619100  | 0.18938700 | -0.26005100 |
| C     | 2.55172500  | -0.33093600 | 0.10626600 |
| C     | 1.29624700  | 1.44832000 | -0.87106600 |
| C     | 3.73488300  | 0.37744400 | -0.08275100 |
| C     | 2.46791600  | 2.16971100 | -1.07415300 |
| H     | 0.34478900  | 1.86535400 | -1.18830400 |
| C     | 3.68985300  | 1.63765800 | -0.6696500  |
| H     | 4.67940800  | -0.06168800 | 0.2208300  |
| H     | 2.42495700  | 3.14504400 | -1.54812200 |
| H     | 4.61042500  | 2.19323700 | -0.81759400 |
| C     | -0.31420000 | -1.16327300 | 1.23236900 |
| H     | -0.83738100 | -2.10957800 | 1.30200400 |
| H     | 0.05330800  | -0.69422500 | 2.13735600 |
| Cl    | 2.67575600  | -1.94531800 | 0.78064400 |
| Cl    | -2.60829800 | -1.79650700 | -1.22478700 |

Thermal correction to Gibbs Free Energy = 0.165942
Sum of electronic and thermal Free Energies = -1459.979258

| Atoms | x     | y     | z     |
|-------|-------|-------|-------|
| C     | 0.03111100 | -0.66199700 | -0.23456500 |
| H     | -0.19812900 | -1.24329900 | -1.12571000 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -1.23756400 | -0.06900300 | 0.43991900 |
| C       | -1.12947100 | 1.22880600 | 1.13211400 |
| C       | -2.54837800 | -0.28427700 | -0.20127000 |
| C       | -2.13985000 | 2.14598300 | 1.12649300 |
| H       | -0.20351200 | 1.42950200 | 1.66307300 |
| C       | -3.54190500 | 0.65548300 | -0.19923000 |
| C       | -3.35786400 | 1.89079300 | 0.45354600 |
| H       | -2.00810400 | 3.08549600 | 1.65535700 |
| H       | -4.48084000 | 0.43987000 | -0.70000900 |
| H       | -4.15274800 | 2.62744400 | 0.44687100 |
| C       | 1.28482700  | 0.14215200 | -0.33420200 |
| C       | 2.53329200  | -0.36980000 | 0.03408800 |
| C       | 1.25673200  | 1.44000100 | -0.86060400 |
| C       | 3.70397000  | 0.37441000 | -0.08566600 |
| C       | 2.41470900  | 2.19847900 | -0.99150100 |
| H       | 0.29886900  | 1.85245200 | -1.16547300 |
| C       | 3.64068400  | 1.66643000 | -0.59687400 |
| H       | 4.65207200  | -0.06028100 | 0.21318100 |
| H       | 2.36007000  | 3.20259600 | -1.39973500 |
| H       | 4.55122900  | 2.24954300 | -0.69135900 |
| C       | -0.45352800 | -1.23981000 | 1.04188400 |
| H       | -0.91876700 | -2.22033700 | 1.02156600 |
| H       | 0.09151500  | -0.99972800 | 1.95032200 |
| Cl      | 2.67149900  | -2.01252900 | 0.63156100 |
| Cl      | -2.83222000 | -1.81506900 | -0.99702400 |
Thermal correction to Gibbs Free Energy = 0.164640

Sum of electronic and thermal Free Energies = -1459.975367

|   |     C   |     H   |     C   |     C   |     C   |     C   |     C   |     H   |     C   |     H   |     C   |     H   |     H   |     H   |     C   |     C   |     C   |     C   |     C   |     C   |     C   |     C   |     C   |
|---|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| C | 0.02777300 | -0.82631900 | -0.52944700 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| H | -0.44266600 | -1.01075000 | -1.49071300 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | -1.28302200 | -0.27840400 | 0.56277600 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | -0.90899100 | 0.84249500 | 1.39129800 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | -2.56371500 | -0.15583000 | -0.08644100 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | -1.66561200 | 1.98834300 | 1.44380700 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| H | 0.01280900 | 0.76295900 | 1.96134400 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | -3.31281800 | 1.00020700 | -0.03322200 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | -2.86663900 | 2.09353700 | 0.71918100 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| H | -1.33660100 | 2.81592000 | 2.06525600 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| H | -4.25695100 | 1.04869500 | -0.56664700 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| H | -3.45914300 | 3.00081600 | 0.75629100 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | 1.24648000 | -0.00355800 | -0.54264600 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | 2.47656700 | -0.37928200 | 0.01651500 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | 1.18736900 | 1.26719700 | -1.14310300 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | 3.58287300 | 0.46628100 | 0.00663300 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | 2.28339400 | 2.11803500 | -1.17183100 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| H | 0.24208600 | 1.58036100 | -1.57954700 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | 3.48467500 | 1.72103800 | -0.58470700 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| H | 4.51616000 | 0.13213400 | 0.44750000 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| H | 2.19903800 | 3.09276600 | -1.64170500 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| H | 4.34773000 | 2.37898500 | -0.59257800 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| C | -0.50380300 | -1.56097300 | 0.63734400 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |

S119
H        -1.05481900  -2.47697300  0.43694700
H        0.13565200  -1.62392000  1.51393900
Cl       2.70379000  -1.98419200  0.68731300
Cl       -3.17499500  -1.51331400  -1.00655000

Thermal correction to Gibbs Free Energy=         0.165036
Sum of electronic and thermal Free Energies=      -1460.005274

C        0.60057600  0.73467300  -1.54077900
H        0.69974000  1.70835700  -2.00849700
C        -1.59102200  -0.24322000  -0.66253900
C        -2.09001100  -1.54077900  -0.40337300
C        -2.02766300  0.78176900  0.18320800
C        -2.95512200  -1.77825100  0.65614800
H        -1.78560200  -2.33863700  -1.05399000
C        -2.88616500  0.55167200  1.25447600
C        -3.34737500  -0.73850500  1.49507900
H        -3.31894500  -2.78672200  0.82592500
H        -3.19287500  1.37904600  1.88579100
H        -4.01581300  -0.92272300  2.33010100
C        1.62083000  0.44544400  -0.58312500
C        1.92917500  -0.80051600  0.01757400
C        2.43703200  1.53565000  -0.16960400
C        2.91637700  -0.93611100  0.98552200
C        3.42466700  1.40909100  0.78880300
H        2.24517400  2.50535300  -0.62109600

S120
C    3.66257100    0.16829900    1.38630100
H    3.10891900   -1.91525600    1.41188600
H    4.00966500    2.27680000    1.07721600
H    4.43080400    0.05362900    2.14378300
C    -0.67108200   -0.00415500   -1.84952200
H    -1.21664000   -0.97187500   -2.59039900
H    -0.47431500   -0.97372700   -2.32007700
Cl    1.14372000   -2.27584500   -0.50646100
Cl   -1.53353400    2.44150100   -0.10696500

Thermal correction to Gibbs Free Energy=              0.170706
Sum of electronic and thermal Free Energies=          -1459.814049

C    0.01643000   -0.65513600    0.61366100
H    0.29783000   -1.00292100    1.61418800
C   -1.36841400   -0.05887000    0.66928500
C   -1.86854900    0.81377200    1.63180500
C   -2.20899900   -0.36582900   -0.38589100
C   -3.16071100    1.31929400    1.49445400
H   -1.24672600    1.09212700    2.47696100
C   -3.49023800    0.10106500   -0.58015000
C   -3.96056100    0.97080000    0.40587000
H   -3.55064300    1.99407700    2.24899700
H   -4.09591000   -0.18685400   -1.43159700
H   -4.96514800    1.36997900    0.31695800
C    1.07119100    0.30698000    0.08963900

S121
\[
\begin{array}{c}
\text{C} & 2.43199300 & 0.01668200 & 0.24852600 \\
\text{C} & 0.73716500 & 1.48224800 & -0.58730000 \\
\text{C} & 3.42751400 & 0.85588200 & -0.23528000 \\
\text{C} & 1.72195000 & 2.33245600 & -1.08363900 \\
\text{H} & -0.30792500 & 1.74385000 & -0.72402100 \\
\text{C} & 3.06588300 & 2.02115000 & -0.90641700 \\
\text{H} & 4.47088200 & 0.59831500 & -0.08746400 \\
\text{H} & 1.43395000 & 3.23824100 & -1.60692100 \\
\text{C} & -0.08689900 & -1.91679300 & -0.24420800 \\
\text{H} & 0.78515100 & -2.17542800 & -0.84374700 \\
\text{H} & -0.52326900 & -2.77322500 & 0.26843300 \\
\text{Cl} & -1.39791300 & -1.48725600 & -1.53243100 \\
\text{H} & 3.83918300 & 2.68021500 & -1.28749500 \\
\text{Cl} & 2.92121300 & -1.44924900 & 1.07793600 \\
\end{array}
\]

\[
\begin{array}{c}
\text{Thermal correction to Gibbs Free Energy=} & 0.166125 \\
\text{Sum of electronic and thermal Free Energies=} & -1459.795432 \\
\end{array}
\]
C        -3.82055100  0.96480500  0.99101900
H        -3.07157500  1.50686900  2.9363600
H        -4.29358900  0.30841100  -1.01313400
H        -4.79540800  1.41448300  1.14878600
C        1.14147600  0.19845100  -0.04540300
C        2.49458200  -0.06191400  0.20257700
C        0.80570400  1.41318600  -0.65041300
C        3.48414700  0.84933000  -0.14525000
C        1.78831500  2.32700700  -1.01395800
H        -0.23799300  1.64456800  -0.83930000
C        3.12723600  2.04518300  -0.76068700
H        4.52284100  0.62142800  0.06790900
H        1.50317500  3.25909600  -1.48976600
C        0.03226500  -2.05305500  -0.30312100
H        0.89583600  -2.44340300  -0.84136900
H        -0.78124200  -2.73955600  -0.07712200
Cl       -1.93471000  -0.99260600  -1.95583200
H        3.90071600  2.75494900  -1.03483400
Cl       2.99768600  -1.54100300  0.99555100

Thermal correction to Gibbs Free Energy=           0.167593
Sum of electronic and thermal Free Energies=      -1459.836067

C        0.02292800  -0.58780500  0.20607500
H        0.41553900  -2.14763500  1.52109900
C        -1.26179100  0.08898900  0.34492600

S123
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | -1.33260900 | 1.18562500 | 1.22795200 |
| C       | -2.45067600 | -0.34813800 | -0.27625700 |
| C       | -2.55305100 | 1.77272100 | 1.53115900 |
| H       | -0.42503100 | 1.52872400 | 1.71395400 |
| C       | -3.66219700 | 0.26465300 | -0.00536200 |
| C       | -3.71342800 | 1.31065700 | 0.91742300 |
| H       | -2.59374200 | 2.59344300 | 2.23870100 |
| H       | -4.55854200 | -0.06117000 | -0.52196000 |
| H       | -4.66947600 | 1.77464900 | 1.13702700 |
| C       | 1.17048900  | 0.19618000 | -0.10941400 |
| C       | 2.53641600  | -0.16634700 | 0.11953800 |
| C       | 0.93806200  | 1.42419500 | -0.79995800 |
| C       | 3.56601100  | 0.65458400 | -0.30003100 |
| C       | 1.97228000  | 2.22589200 | -1.23705100 |
| H       | -0.08183200 | 1.69814000 | -1.04181300 |
| C       | 3.28680700  | 1.84059900 | -0.98198200 |
| H       | 4.59240300  | 0.37373200 | -0.09329200 |
| H       | 1.75942800  | 3.13809600 | -1.78219000 |
| C       | 0.04952400  | -2.04021700 | 0.48735100 |
| H       | 0.73139400  | -2.59190700 | -0.16321900 |
| H       | -0.94971900 | -2.47134200 | 0.46908400 |
| Cl      | -2.40258500 | -1.55507300 | -1.53262400 |
| H       | 4.11301300  | 2.45968800 | -1.31711900 |
| Cl      | 3.00576100  | -1.57574700 | 1.00871300 |

![Chemical Structure](image)
Thermal correction to Gibbs Free Energy= 0.169303

Sum of electronic and thermal Free Energies= -1459.804684

|     | -0.04225600 | -0.51209900 | -0.23768100 |
|-----|-------------|-------------|-------------|
| C   | -0.11104100 | -1.16543900 | -1.09911600 |
| H   | -1.24842600 | 0.23137700  | 0.11216900  |
| C   | -1.20439800 | 1.37877500  | 0.92496500  |
| C   | -2.50507900 | -0.23333600 | -0.32229400 |
| C   | -2.36355600 | 2.06805500  | 1.24344100  |
| H   | -0.24274600 | 1.72690700  | 1.29148800  |
| C   | -3.66815700 | 0.45561600  | -0.00756000 |
| C   | -3.59254300 | 1.60626000  | 0.77362000  |
| H   | -2.31050300 | 2.95923000  | 1.85876500  |
| H   | -4.62452900 | 0.09210500  | -0.36698400 |
| H   | -4.50549700 | 2.13887000  | 1.01965400  |
| C   | 1.32970700  | 0.25227500  | -0.36135400 |
| C   | 2.46802900  | -0.37718000 | 0.14110800  |
| C   | 1.48601700  | 1.47802100  | -1.00077900 |
| C   | 3.74108800  | 0.15564800  | 0.03564400  |
| C   | 2.75402000  | 2.04280600  | -1.11913100 |
| H   | 0.61201300  | 1.98612200  | -1.39869800 |
| C   | 3.87130700  | 1.38728600  | -0.60556000 |
| H   | 4.60269000  | -0.36312800 | 0.44085200  |
| H   | 2.86925300  | 3.00040300  | -1.61570900 |
| H   | 4.85607700  | 1.83301800  | -0.69806200 |
| C   | -0.03083500 | -1.24191400 | 1.02548500  |
| H   | -0.58009400 | -2.17944300 | 1.09787400  |
| H   | 0.18242300  | -0.71430300 | 1.95219900  |
| Cl  | 2.21492800  | -1.94188100 | 0.93266400  |
| Cl  | -2.63990600 | -1.67364300 | -1.29117700 |

S125
Thermal correction to Gibbs Free Energy= 0.168727

Sum of electronic and thermal Free Energies= -1459.828575

\[
\begin{array}{cccc}
\text{C} & -0.04889100 & -0.70719500 & 0.24929000 \\
\text{H} & 0.25110300 & -1.18927200 & 1.17806900 \\
\text{C} & 1.27475400 & -0.05162300 & -0.42828600 \\
\text{C} & 1.10740600 & 1.16082200 & -1.16342000 \\
\text{C} & 2.53397800 & -0.28167300 & 0.21753200 \\
\text{C} & 2.12358600 & 2.08284700 & -1.24626100 \\
\text{H} & 0.15694900 & 1.33345300 & -1.66054700 \\
\text{C} & 3.54510100 & 0.65301000 & 0.14330900 \\
\text{C} & 3.33177500 & 1.82612600 & -0.58630200 \\
\text{H} & 1.99213600 & 2.99732300 & -1.81217300 \\
\text{H} & 4.49253700 & 0.47754600 & 0.64000500 \\
\text{H} & 4.13484100 & 2.55520100 & -0.63881200 \\
\text{C} & -1.27840700 & 0.13539400 & 0.34677300 \\
\text{C} & -2.52307600 & -0.35537600 & -0.05902600 \\
\text{C} & -1.22928800 & 1.40613500 & 0.92992100 \\
\text{C} & -3.68295100 & 0.40183700 & 0.08511500 \\
\text{C} & -2.37763600 & 2.17252500 & 1.07661100 \\
\text{H} & -0.26911200 & 1.79323300 & 1.26080300 \\
\text{C} & -3.60566800 & 1.66991700 & 0.64874300 \\
\text{H} & -4.63406600 & -0.00581700 & -0.24006100 \\
\text{H} & -2.31439400 & 3.15872600 & 1.52402500 \\
\text{H} & -4.50917300 & 2.26089200 & 0.75805100
\end{array}
\]
Thermal correction to Gibbs Free Energy = 0.168485

Sum of electronic and thermal Free Energies = -1459.826295
|   |  X    |  Y    |  Z    |
|---|-------|-------|-------|
| H | 0.58729500 | 1.39395000 | -2.12505000 |
| C | 3.59528300 | 1.64693700 | -0.59727900 |
| H | 4.41503900 | 0.20756000 | 0.78490800 |
| H | 2.57056400 | 2.87648500 | -2.04406500 |
| H | 4.47299900 | 2.28349600 | -0.54923600 |
| C | -0.56055200 | -1.64328000 | 0.11732900 |
| H | -1.17876800 | -2.39953700 | -0.36414200 |
| H | 0.00039700 | -2.02328500 | 0.96323600 |
| Cl | 2.55252700 | -1.83416200 | 1.01912900 |
| Cl | -3.15729100 | -0.99656700 | -1.48741500 |

Thermal correction to Gibbs Free Energy = 0.167648

Sum of electronic and thermal Free Energies = -1459.828883

|   |  X    |  Y    |  Z    |
|---|-------|-------|-------|
| C | 0.33875700 | -0.82559200 | 0.54497500 |
| H | -0.14211200 | -1.75455300 | 0.23764600 |
| C | -1.60654000 | 0.44002200 | 0.29859300 |
| C | -1.39369000 | 1.58108800 | -0.48231000 |
| C | -2.76448000 | -0.31081200 | 0.06771300 |
| C | -2.32493500 | 1.98231300 | -1.43262500 |
| H | -0.48922500 | 2.16238100 | -0.32454700 |
| C | -3.70607900 | 0.08010200 | -0.87782200 |
| C | -3.48155000 | 1.23061700 | -1.62840800 |
| H | -2.14677400 | 2.87796200 | -2.01831100 |
| H | -4.60286600 | -0.51254700 | -1.02385200 |
| H | -4.21486700 | 1.53474000 | -2.36823800 |
C   1.63324400  -0.67507000   0.04524800
C   2.56791000   0.38991500   0.28454100
C   2.06262700  -1.74660900  -0.80409800
C   3.81770000   0.36226400  -0.29539600
C   3.31119800  -1.76419400  -1.38257300
H   1.36480200  -2.55782000  -0.98709200
C   4.18352800  -0.70531800  -1.12463200
H   4.51873100   1.16697600  -0.10595600
H   3.61209000  -2.58398700  -2.02385200
H   5.17436500  -0.69985500  -1.56824100
C  -0.55365600   0.04399200  1.33261100
H  -1.00965300  -0.55685700   2.12690200
H  -0.09097500   0.92441500  1.76360200
Cl   2.21939200   1.73693900  1.30739500
Cl  -3.07102200  -1.76618400   0.98772500