SUPPLEMENTARY INFORMATION

Analyzing Mechanisms in Co(I) Redox Catalysis Using a Pattern Recognition Platform

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Contents

1. General Experimental

All air and water-sensitive reactions were carried out in dried glassware under a nitrogen atmosphere using standard Schlenk manifold techniques. Bulk solutions were evaporated under reduced pressure using a Büchi rotary evaporator. All solvents were commercially supplied or dried by a PureSolv system from InnovativeTechnology, Inc. All commercially available reagents and substrates were purchased from commercial suppliers and used without further purification, unless otherwise noted: benzyl bromide was distilled before use.

Flash column chromatography (FCC) was carried out using Silicycle SiliaFlash® F60 silica gel (40–63 μm). All reactions were followed by thin-layer chromatography (TLC) when practical, using Merck Kieselgel 60 F_{254} fluorescent treated silica which was visualised under UV light or by staining with aqueous basic potassium permanganate.

^{1}H, ^{2}H ^{13}C and ^{19}F NMR spectra were recorded using Oxford NMR 500 MHz, Bruker NMR 500 MHz and Oxford NMR 300 MHz spectrometers. Chemical shifts (δ) are given in parts per million (ppm), and coupling constants (J) are given in Hertz (Hz). The ^{1}H NMR spectra are reported as follows: ppm (multiplicity, coupling constants, number of protons).

High resolution mass spectra (**HRMS**) were recorded on a Waters LCP Premier XE TOF instrument by Electrospray Ionization (ESI). **IR spectra** were recorded on a Thermo Nicolet FT-IR as a thin film. Only selected absorption maxima (ν_{max}) are reported in wavenumbers (cm^{-1}). **Melting points** were recorded in degrees Celsius (°C), using a Thomas Hoover capillary melting point apparatus and are reported uncorrected. **Optical rotation** ($[\alpha]_D^T$) was measured (Na D line) on a Perkin Elmer Model 343 polarimeter fitted with a micro cell with a 1 dm path length and is quoted in (° ml)(g dm)$^{-1}$, concentrations are reported in g/100 mL.

Compound names are those generated by ChemBioDraw 18.2 software (PerkinElmer), following the IUPAC nomenclature.

All **electrochemical experiments** were conducted using a BioLogic SP-150 potentiostat.

2. Electrochemical Analysis

All electrochemical experiments were performed using a three-electrode configuration with a 3 mm (0.071 cm^2) boron-doped diamond working electrode, a platinum mesh counter electrode, and a fritted $Ag/AgNO_3$ reference electrode under an Ar environment containing 3.2% H_2. Each sample was then calibrated to a Fc/Fc^+ reference potential by square wave voltammetry (SWV) after the addition of 1.0 mM Fc. Tetrabutylammonium hexafluorophosphate was dried in a vacuum oven overnight at 90 °C to ensure anhydrous conditions. SWVs were performed with pulse height = 20 mV, pulse width = 20 ms (50 Hz), and a step height = 2 mV. Potential windows for cyclic voltammograms (CVs) were set to be 0.35 V ± $E_{1/2}$ for complex with ligand **3** and 0.25 V± $E_{1/2}$ for complex with ligand **2** to minimize the overlap between redox couples from bis-ligated and mono-ligated complexes. CVs and SWVs are plotted in polarographic notation with positive currents corresponding to reduction.

The activation of benzyl bromide rate constant of Co(I) ligated by ligand **3** was calculated as per a previous report.[1,2] Oxidative addition rate constants were measured by mixing 1.0 mM $CoBr_2$, 2.0 mM ligand, 1.0 mM substrate in a 100 mM Bu_4NPF_6 acetonitrile solution. By focusing on the Co(II)/Co(I) redox couple and varying the scan rate from 100 mV s^{-1} to 3 V s^{-1}, we measured variations in peak cathodic and anodic currents (i_{pc} and i_{pa} respectively) as an analogue for the amounts of Co(I) species generated by the electrode ($[Co(I)]_0$) and that of Co(I) remaining at the electrode surface ($[Co(I)]_t$) after the time required to reach the peak anodic current. In other words, for a CV potential window $E_i \rightarrow E_R$, then the reaction time (t) can be calculated as:

$$t = \frac{\left|E_R - E_{pc}\right| + \left|E_R - E_{pa}\right|}{\nu}$$

where ν is the scan rate, E_{pc} is the peak cathodic current, and E_{pa} is the peak anodic potential.

From the Randles-Sevcik equation at 25 °C (for a one-electron transfer), the peak current in the cathodic direction, i_{pc}, can be described by:

$$i_{pc} = 2.69 \times 10^5 A v^{\frac{1}{2}} [Co(II)]_{bulk} D_{Co(II)}^{\frac{1}{2}}$$

where A is the area of the electrode.

Similarly, given that the concentration of the Co(I) complex at the electrode at the peak cathodic potential is equal to (or, tends to) the bulk solution concentration of Co(II), the peak anodic current is dependent on the concentration of Co(I) remaining at the surface of the electrode after time, t:

$$i_{pa} = 2.69 \times 10^5 A v^{\frac{1}{2}} [Co(I)]_t D_{Co(I)}^{\frac{1}{2}}$$

From the division of the two above equations, it follows that:

$$\frac{i_{pa}}{i_{pc}} = \frac{[Co(I)]_t D_{Co(I)}^{\frac{1}{2}}}{[Co(II)]_{bulk} D_{Co(II)}^{\frac{1}{2}}}$$

which, with the assumption that the diffusion coefficients for the Co(II) and Co(I) species ($D_{Co(II)}$ and $D_{Co(I)}$) are approximately equivalent, then becomes:

$$\frac{i_{pa}}{i_{pc}} = \frac{[Co(I)]_t}{[Co(II)]_{bulk}}$$

According to the second order reaction between Co(I) and BnBr:

Co(I) + BnBr = Co(II) + Bn· + Br^-

A second-order kinetic equation can be derived as below (based on the approximation that the substrate and cobalt complex are in 1:1 equivalency, on account of their stoichiometry and negating the effect of diffusion to the electrode):

$$\frac{1}{[Co(I)]_t} - \frac{1}{[Co(II)]_{bulk}} = k_{obs}\, t$$

As a result, the second-order equation can be represented as:

$$\frac{1}{\frac{i_{pa}}{i_{pc}}[Co(II)]_{bulk}} - \frac{1}{[Co(II)]_{bulk}} = k_{obs}\, t$$

Since $[Co(II)]_{bulk}$ and k are constants while $\frac{i_{pa}}{i_{pc}}$ and t can be derived from CVs, plotting $\frac{1}{\frac{i_{pa}}{i_{pc}}[Co(II)]_{bulk}}$ against t across different scan rates resulted in a linear fit with a slope which is equal to the k_{obs}.

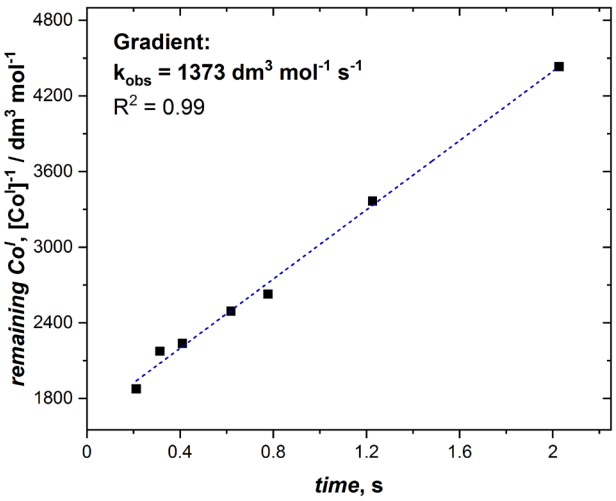


Figure S1. A second order kinetic plot describing the amount of electrochemically generated Co(I) species remaining in solution after a time, *t*. Experiments were performed using a solution of 1 mM $CoBr_2$ with 2 mM of ligand **3** and 1.0 mM benzyl bromide (**8**) in solution of acetonitrile containing 100 mM NBu_4PF_6 at 25 °C.

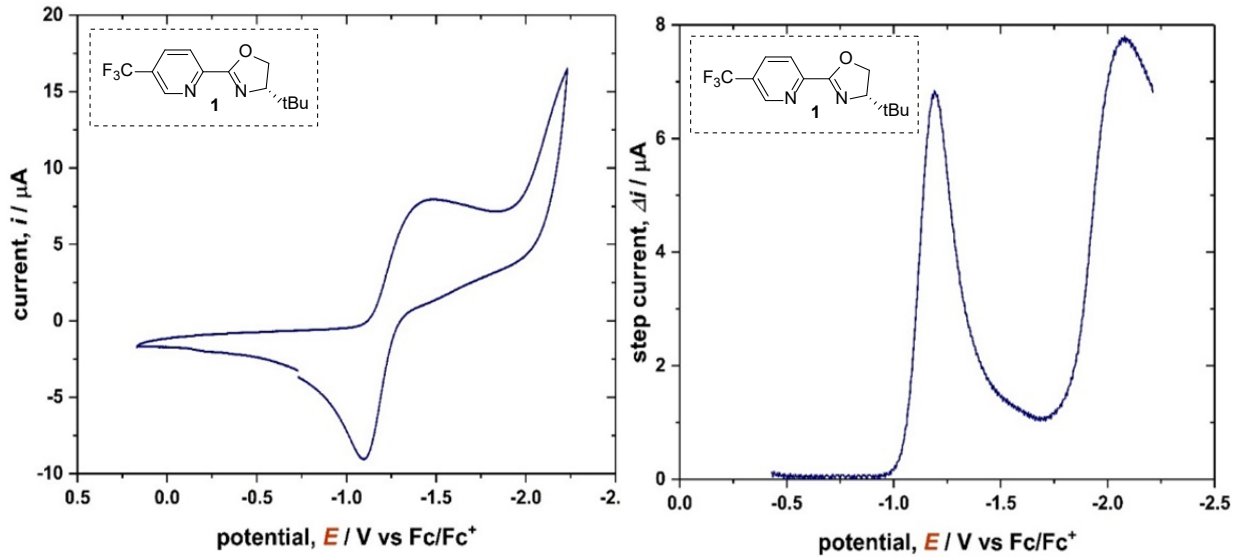
Discussion of some of the approximations in this methodology:

1. The diffusion coefficients of both complexes are assumed to be equal. Any deviation from this approximation is inconsequential when comparing the relative rates of different substrates with the same complex.
2. The substrate and cobalt complex are assumed to have equal concentrations, and the substrate is consumed by the reaction with Co(I) without being replenished through diffusion. This assumption may lead to an over-estimation of the absolute rate constants, but minimal impact on the relative rate constants of the varying substrates.
3. Once the Co(I) reacts with the substrate, it is "consumed" and does not undergo further electrochemistry (i.e., the ensuing Co(II) is not reduced again). This assumption was originally made according to the mechanism of an oxidative addition reaction which forms Co(III). In our previous work,[2] we found that, although the mechanism did proceed via a Co(II) intermediate, the observed rate constant was in agreement with CV simulations. In the outer-sphere electron transfer mechanism found with the BPP ligand in this study, the EC' nature of the mechanism suggests that this assumption may no longer hold entirely true. Nevertheless, trends in relative rate constants can be investigated through these results. A more rigorous method to obtain rate constants for these catalytic reactions (foot-of-the-wave analysis,[17] or using the plateau current of a CV within the "pure kinetics" domain[18]) may provide a more accurate value for absolute rate constants, but is not required in this work for comparing relative rate constants.

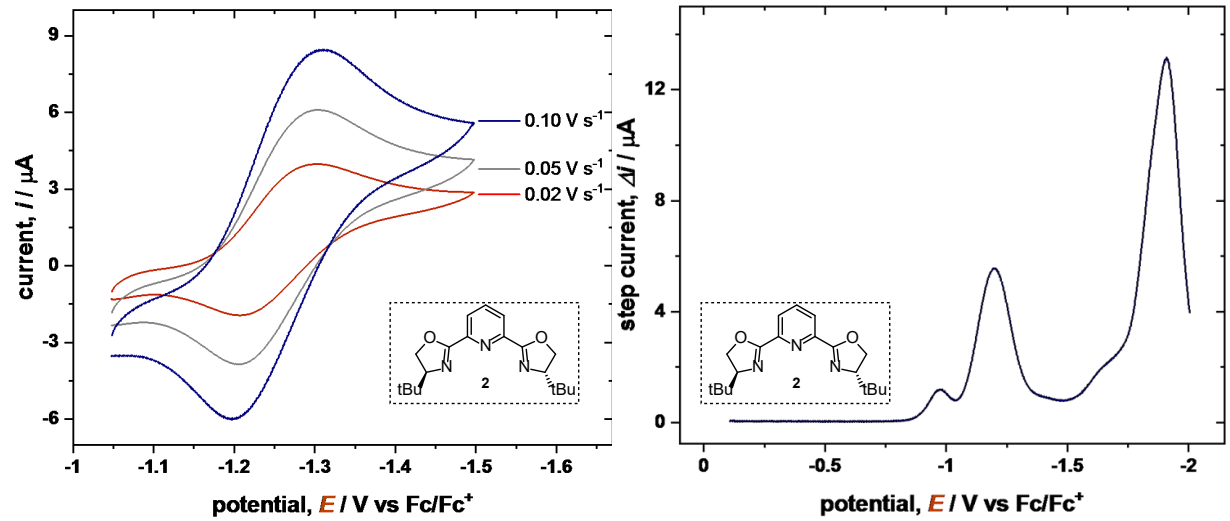
3. CVs and SWVs of Cobalt Complex

The below CVs were performed at a scan rate of 100, 50, 20, 10 mV s^{-1}, SWVs performed as noted above. Spectra for complexes ligated with ligand **2** and **3** are measured for this work while ligand **1** taken from the Supporting Information of a previous study.[2]

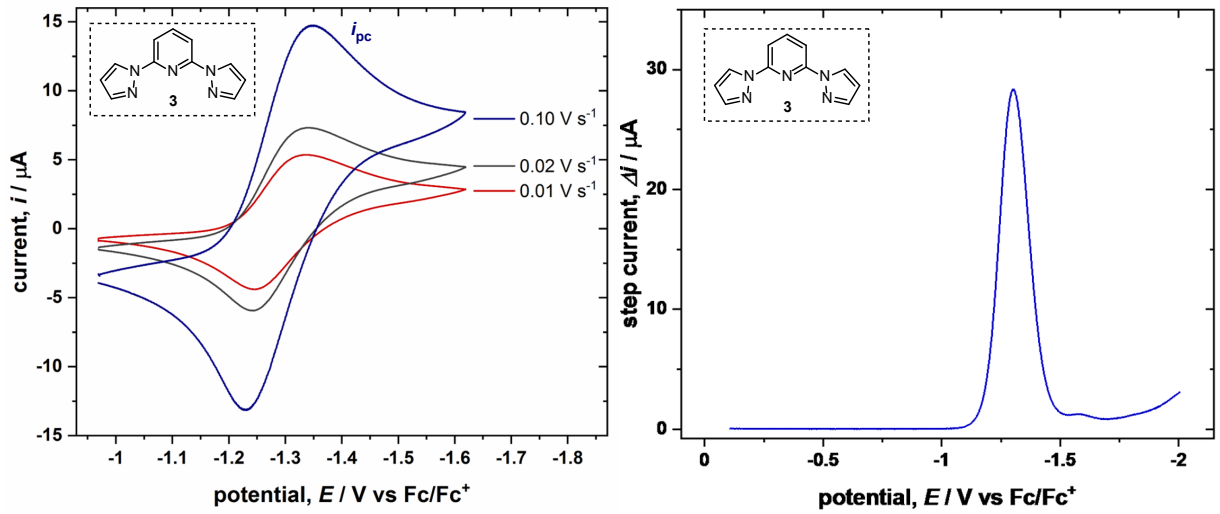
CV (100 mV s^{-1}) and SWV of $CoBr_2$ in the presence of 1.0 equiv **1**



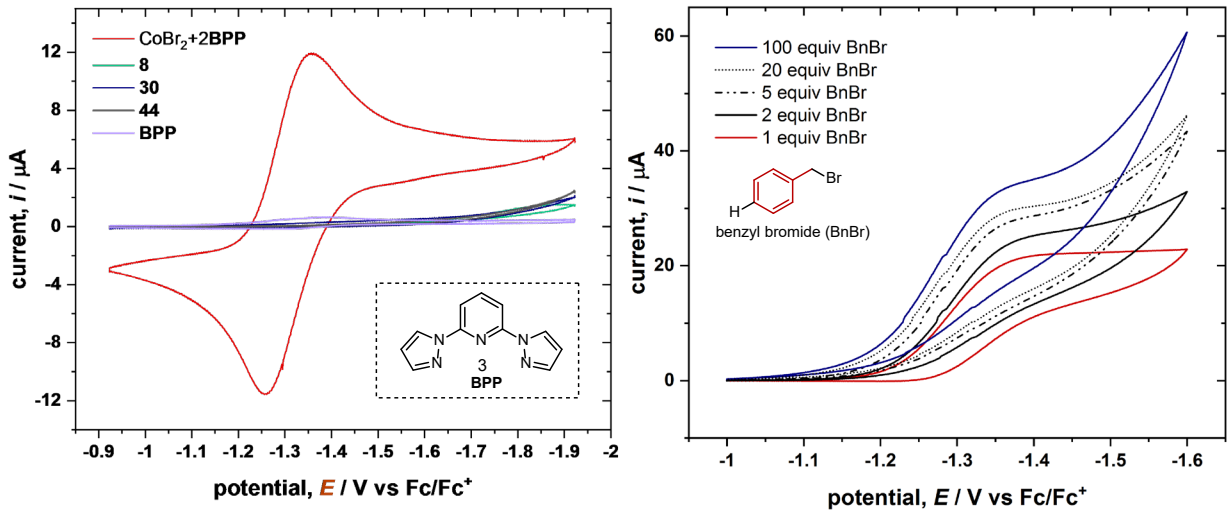
CV (100, 50, 20 mV s^{-1}) and SWV of $CoBr_2$ in the presence of 0.5 equiv **2**



CV (100, 20, 10 mV s^{-1}) and SWV of $CoBr_2$ in the presence of 2.0 equiv **3**



CV (20 mV s^{-1}, left figure below) of $CoBr_2$ in the presence of 2.0 equiv **3**, and CVs (20 mV s^{-1}, left figure below) of substrates **8**, **30**, **44** (for the numbering of substrates, please see section 5), and the pure ligand **3**. This CV (left figure below) demonstrates that the cobalt complex is the only redox active species in the potential window selected. CVs (100 mV s^{-1}, right figure below) of $CoBr_2$ and 2.0 equiv **3** in the presence of 1.0, 2.0, 5.0, 20, 100 equiv **5**. A plateau current was not observed at high substrate loadings and the increment in the catalytic current with additional substrate equivalents is reduced above 5 equiv. of substrate. This may be a consequence of catalyst degradation caused by the rebound of the benzyl radical to the ligand, or the slow heterogeneous electron-transfer kinetics of the cobalt complex.



4. Tabulated Experimental Properties for Cobalt Complexes Without Substrate

Ligand	$E_{1/2}$ / V *vs* Fc/Fc$^+$	$k_{disprop}$ / dm^3 mol^{-1} s^{-1}	[LCo(II)]$^{2+}$ or [L$_2$Co(II)]$^{2+}$ / mM
1	−1.21	13	0.75[1]
2	−1.25	48	~0.50[a]
3	−1.29	*n.d.*[b]	0.75[c]

[a]Estimated value, which influences the absolute value of the measured rate constants but not the relative value, which was in this work. [b]We were unable to determine the disproportionation rate constant for this complex due to excellent stability, even under low scan rates (10 mV s^{-1}), suggesting that any disproportionation is slower than the detection limit of our experimental assay. [c]Calculated from square-wave voltammograms shown in Figure S2.

Table S1. $E_{1/2}$ corresponds to the Co(II)/Co(I) redox couple; Effective concentration of mono-ligated complex in solution obtained from square-wave voltammetry by sequentially adding more ligand and monitoring change in peak heights.[1]

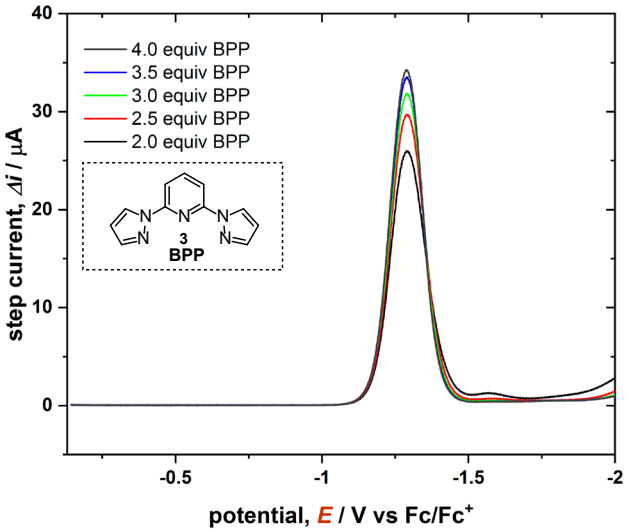
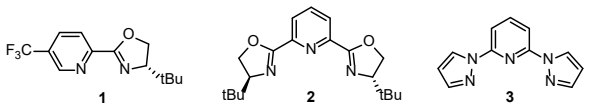


Figure S2. SWV of $CoBr_2$ (1 mM) in the presence of 2.0, 2.5, 3.0, 3.5, and 4.0 equiv **3**, conducted as noted above. The peak current kept increasing upon adding more ligands until adding 4.0 equiv **3**, from which we approximated the concentration of bis-ligated complex to be 0.75 mmol when 2.0 equiv ligand **3** was added.

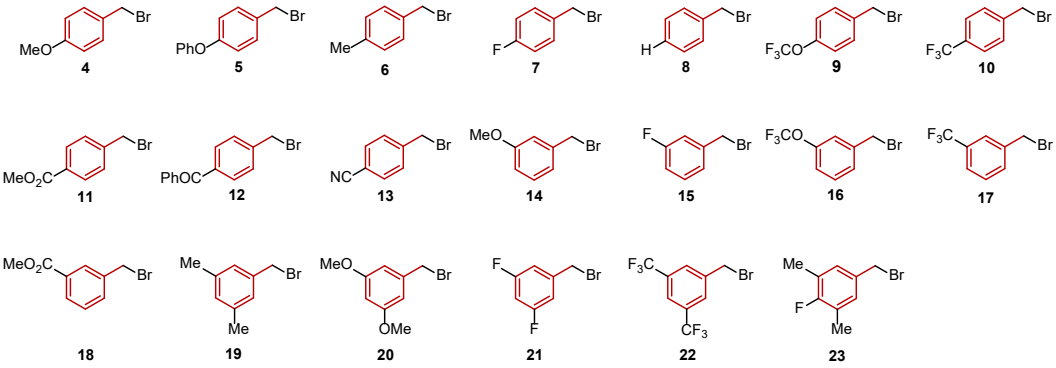
5. Numbering of Ligands and Substrates Studied

Ligands



1 **2** **3**

non-ortho primary substrates

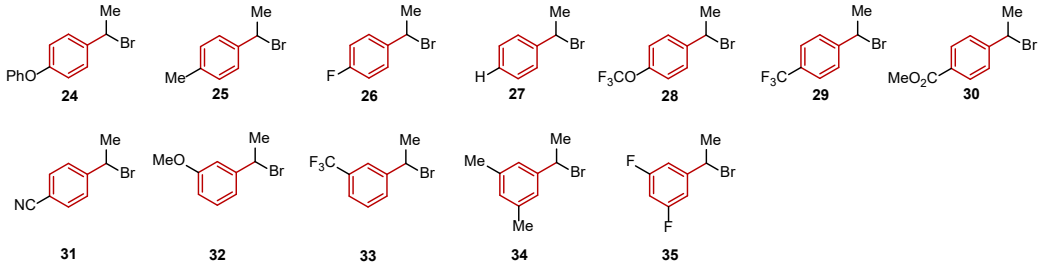


4 **5** **6** **7** **8** **9** **10**

11 **12** **13** **14** **15** **16** **17**

18 **19** **20** **21** **22** **23**

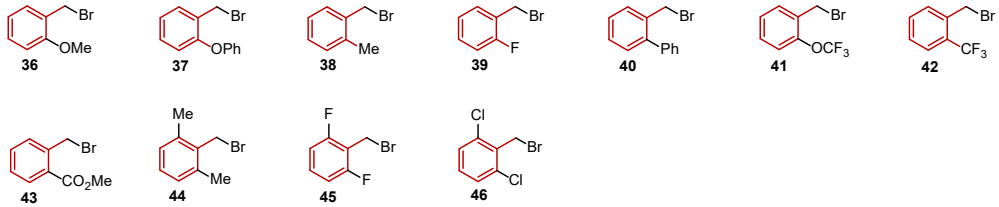
secondary substrates



24 **25** **26** **27** **28** **29** **30**

31 **32** **33** **34** **35**

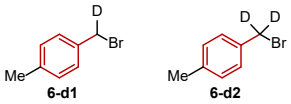
ortho-substituted substrates



36 **37** **38** **39** **40** **41** **42**

43 **44** **45** **46**

deuterated substrates



6-d1 **6-d2**

6. Complexation Studies for Cobalt with Ligand 2 and 3

6.1 Complexation Studies for Ligand 2

Upon electroreduction, we discovered two reversible responses in the cyclic voltammogram shown in the figure below, of which the first peak has $E_{1/2} = -0.95$ V (vs Fc/Fc^+), and the second peak has $E_{1/2} = -1.26$ V (vs Fc/Fc^+). In order to assign peaks to possible cobalt redox couples and cobalt complexes with different ligations, complexation studies were conducted.

It was proposed that the first peak (−0.95 V vs Fc/Fc^+) is from bis-ligated complex Co(II)/Co(I) couple, while the second peak (−1.26 V vs Fc/Fc^+) is from the mono-ligated complex Co(II)/Co(I) couple, which was supported by the CV and SWV studies shown below. As we added more ligand **2**, the first peak had a higher response in peak current, in both CV and SWV diagrams (Figure S3). We argued this was consistent with the proposal, according to which the more ligands added the higher concentration of bis-ligated complex, leading to higher response in peak current.

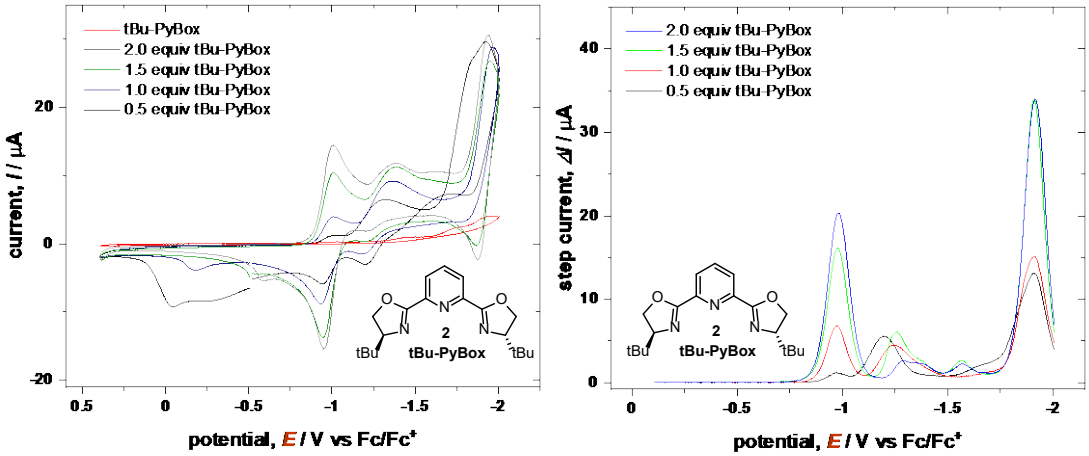


Figure S3. Cyclic voltammograms on the left were measured using a solution of 1 mM $CoBr_2$ with 0.5, 1.0, 1.5, 2.0 mM of ligand **2** in solution of acetonitrile containing 100 mM NBu_4PF_6 at 25 °C. Square wave voltammetry on the right was performed as noted above, with 1 mM $CoBr_2$ and 0.5, 1.0, 1.5, 2.0 mM of ligand **2** respectively.

Our hypothesis was further supported by ^{1}H NMR titration studies. To make comparison between the $[CoPyBox]^{2+}$ and $[Co(PyBox)_2]^{2+}$, we synthesized both of them according to previously reported methods,[3] of which the ^{1}H NMR spectrums in CD_3CN are presented on the bottom in Figure S4. With these two spectrums of the cobalt complexes as a reference, we were able to assign peaks in the spectra of complexes formed *in situ*. As is depicted in the figure, going from 1.0 equiv. to 2.0 equiv. ligand **2** (the signal in the spectrum with 0.5 equiv. ligand **2** was too low to be analysed), the concentration of bis-ligated complex increased referenced to the mono-ligated one. The trend in the ^{1}H NMR titration studies was then consistent with our CV and SWV studies, all leading to our proposed CV response assignment.

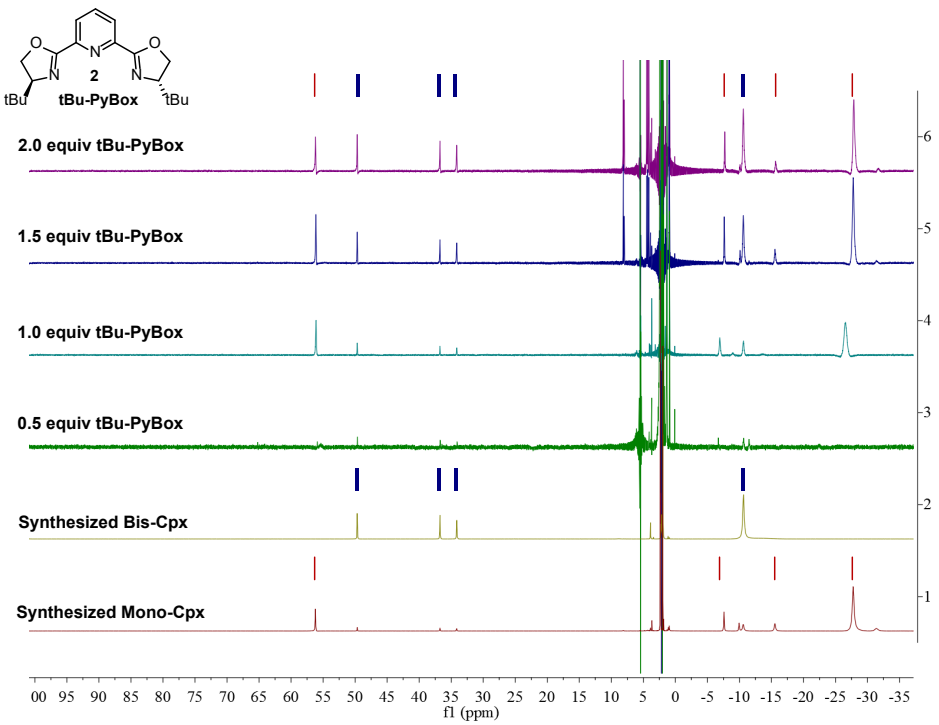


Figure S4. ^{1}H NMR spectrums of cobalt complexes (in CD_3CN): from the bottom to the top, synthesized $[CoPyBox]Br_2$, synthesized $[Co(PyBox)_2](BF_4)_2$, mixture of 2 mM $CoBr_2$ and 1 mM ligand **2**, mixture of 2 mM $CoBr_2$ and 2 mM ligand **2**, mixture of 2 mM $CoBr_2$ and 3 mM ligand **2**, mixture of 2 mM $CoBr_2$ and 4 mM ligand **2**.

6.1 Complexation Studies for Ligand 3

Distinct from ligand **2**, the cyclic voltammogram of ligand **3** with cobalt only afforded one reversible redox couple ($E_{1/2}$ = −1.29 V vs Fc/Fc^+), as well as in the square-wave voltammogram, depicted in Figure S5. According to previously reported studies of $[Co(BPP)_2]^{2+}$, the bis-ligation of cobalt was stable and could be maintained in acetonitrile solution.[4] Thus, we proposed that the CV response ($E_{1/2}$ = −1.29 V vs Fc/Fc^+) corresponded to a bis-ligated Co(II)/Co(I) redox couple. This hypothesis was supported by the fact that in both the CV and SWV the current response kept increasing after addition of ligands.

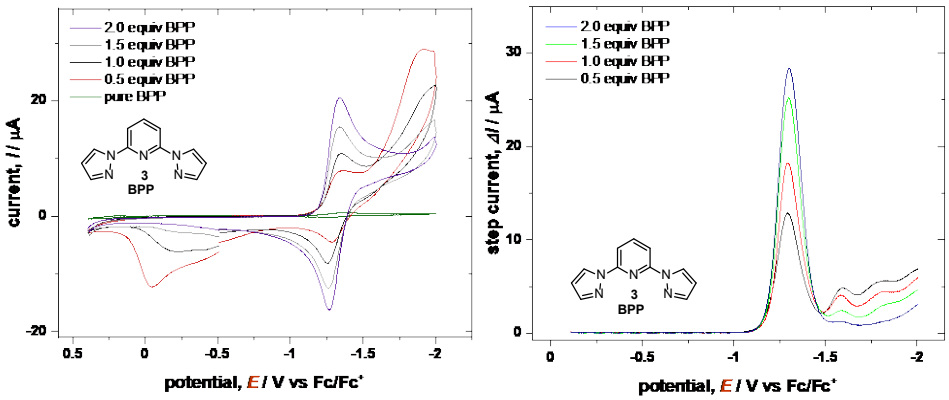


Figure S5. Cyclic voltammograms on the left were measured using a solution of 1 mM $CoBr_2$ with 0.5, 1.0, 1.5, 2.0 mM of ligand **3** in solution of acetonitrile containing 100 mM NBu_4PF_6 at 25 °C. Square wave voltammetry on the right was performed as noted above, with 1 mM $CoBr_2$ and 0.5, 1.0, 1.5, 2.0 mM of ligand **3** respectively.

Our ligand and bromide CV titration studies further supported to our proposal. To make comparison with a complex with a confirmed ligation state, we synthesized the $[Co(BPP)_2](BF_4)_2$ complex (Cpx-**1**) according to previously reported literature.[4] As is shown on the left in Figure S6, as more equivalents of ligand were added, the peak current for the redox couple increased, consistent with the bis-ligation of the complex. The synthesized bis-ligated complex Cpx-**1** possessed the same $E_{1/2}$ as the complex formed from *in situ*. We also conducted a bromide titration study (right side of Figure S6), wherein a decreasing peak current was observed upon the addition of more TBABr, suggesting a decreasing concentration of the complex. Such a trend can be interpreted by more bromide disfavouring bis-ligation and instead favouring another ligation state, possibly mono-ligation. As we added 10 equiv. bromide, we ended up with a redox couple with a different $E_{1/2}$, assigned to the mono-ligated cobalt complex. As a result, the combination of the observation from CVs supports the bis-ligation proposal.

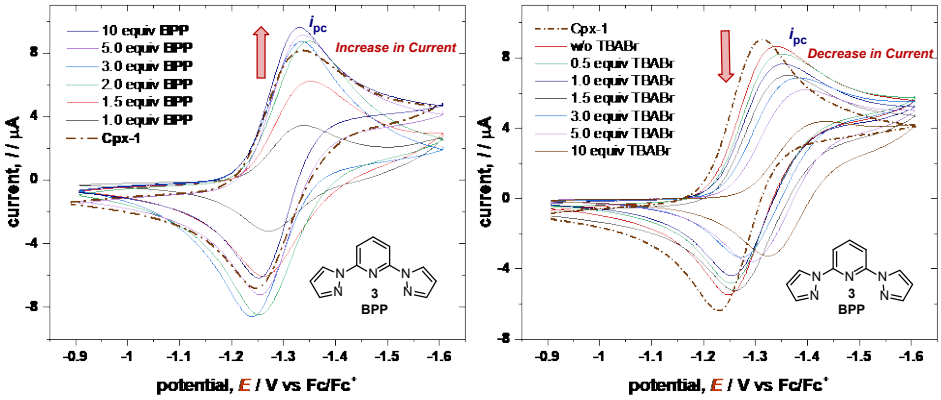


Figure S6. Cyclic voltammograms on the left were measured using a solution of 1 mM $CoBr_2$ with 1.0, 1.5, 2.0, 3.0, 5.0, 10 mM of ligand **3** in solution of acetonitrile containing 100 mM NBu_4PF_6 at 25 °C, compared to 1.0 mM Cpx-**1** ($[Co(BPP)_2](BF_4)_2$). Cyclic Voltammograms on the right were recorded using a solution of 1 mM $CoBr_2$ and 2.0 mM of ligand **3** with 0, 0.5, 1.0, 1.5, 3.0, 5.0, 10 mM TBABr in solution of acetonitrile containing 100 mM NBu_4PF_6 at 25 °C, compared to 1.0 mM Cpx-**1** ($[Co(BPP)_2](BF_4)_2$).

7. Hammett Studies

7.1 Tabulated Hammett Parameters for Substrates Studied

Substrate	σ	σ^+	σ^-
4	−0.27	−0.76	−0.26
5	−0.03	−0.50	0.10
6	−0.17	−0.37	−0.17
7	0.06	−0.07	−0.03
8	0.00	0.00	0.00
9	0.35		0.27
10	0.54	0.61	0.65
11	0.45	0.49	0.75
12	0.43	0.51	0.83
13	0.66	0.66	1.00

Table S2: Hammett Parameter Data collected from the following sources[5]

7.2 Tabulated Measured Rate Constants for Hammett Correlation

	Ligand 2		Ligand 3	
Substrate	k_{obs} (dm^3 mol^{-1} s^{-1})	$\log_{10}(k_X/k_H)$	k_{obs} (dm^3 mol^{-1} s^{-1})	$\log_{10}(k_X/k_H)$
4	2180	0.518	679	−0.306
5	1550	0.370	1170	−0.070
6	992	0.175	959	−0.156
7	729	0.041	1300	−0.024
8	663	0.000	1370	0.000
9	902	0.134	3370	0.390
10	1420	0.332	18200	1.12
11	3020	0.658	42800	1.49
12	21500	1.51	25900	1.28
13	4960	0.874	122000	1.95

Table S3: (1) Measurement for each ligand's Hammett data set was conducted on the same day to avoid deviations caused by equipment. Values are quoted to 3 significant figures (2) Kinetic data for ligand **1** was directly exported from the previous study.[2]

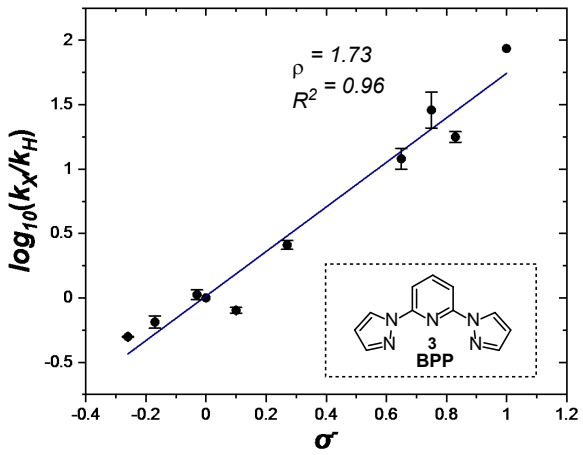
7.3 Hammett Correlation of Data for Ligand 3 with Standard Deviations.

Substrate	Ligand 3						
	k_{obs} (dm^3 mol^{-1} s^{-1})				Standard Deviation	$\log_{10}(k_X/k_H)$	Standard Error of the Mean (log units)
	Run 1	*Run 2*	*Run 3*	*Mean*			
4	679	699	732	703	22	−0.303	0.003
5	1170	1060	1170	1130	53	−0.097	0.022
6	959	776	1020	917	102	−0.188	0.048
7	1300	1470	1710	1500	169	0.025	0.038
8	1370	1410	1460	1410	35	0.000	0
9	3370	3360	4190	3640	386	0.411	0.035
10	18200	12800	19900	17000	3030	1.08	0.080
11	42800	24700	54400	40600	12200	1.46	0.139
12	25900	21700	27600	25100	2480	1.25	0.040
13	122000			122000	n.d.[a]	1.94	n.d.

[a]Multiple measurements weren't completed with substrate **13** since the large rate constants are at the maximum values capable for our assay.

Table S4: Three measurements for each substrate (except **13**) were conducted to ensure the reproducibility of the Hammett plot for ligand **3**. Values are quoted to 3 significant figures

Hammett plot for ligand **3** with averaged rate constants and error bars:



8. Kinetic Isotope Effect and Secondary Substrate Effect Studies

	Ligand 2			
Substrate	**Run**	k_{obs} **(dm^3 mol^{-1} s^{-1})**	**KIE**	**KIE *per* Deuterium**
6	1	713		
6	2	470		
6	3	607		
	Mean	660		
6-d_1	1	451	1.46	1.46
6-d_1	2	471	1.40	1.40
6-d_2	1	394	1.68	1.29
6-d_2	2	387	1.71	1.31
			Mean	1.37
			Standard Deviation	0.07

Table S5. Kinetic Isotope Effect results for the combination of substrate **6** with tBu-PyBox (**2**). Due to the change of measurement apparatus, the absolute values of rate constants shown in this table are different from Hammett measurements, but the relative values remain the same.

	Ligand 3			
Substrate	**Run**	k_{obs} **(dm^3 mol^{-1} s^{-1})**	**KIE**	**KIE *per* Deuterium**
6	1	505		
6	2	567		
	Mean	536		
6-d_1	1	500	1.07	1.07
6-d_1	2	468	1.15	1.15
6-d_2	1	445	1.20	1.10
6-d_2	2	399	1.34	1.16
			Mean	1.12
			Standard Deviation	0.04

Table S6. Kinetic Isotope Effect results for the combination of substrate **6** with BPP (**3**). Due to the change of measurement apparatus, the absolute values of rate constants shown in this table are different from Hammett measurements, but the relative values remain the same.

	Ligand 2		
Substrate	**Run**	k_{obs} **(dm^3 mol^{-1} s^{-1})**	**$k_{2°}/k_{1°}$**
8	**1**	663	
27	1	1680	2.54
27	2	1450	2.19
		Mean	2.36
		Error Bar	0.17

[a]Error bar determined by deviation to the mean

Table S7. Secondary substrate effect results for the combination of substrate **8** and **27** with tBu-PyBox (**2**). The data was measured on a single day so two secondary substrate rate constants can be averaged.

	Ligand 3		
Substrate	**Run**	k_{obs} **(dm^3 mol^{-1} s^{-1})**	**$k_{2°}/k_{1°}$**
8	1	1370	
27	1	983	0.72
8	2	1080	
27	2	778	0.72
		Mean	0.72
		Error Bar	0.01

[a]Error bar determined by deviation to the mean

Table S8. Secondary substrate effect results for the combination of substrate **8** and **27** with BPP (**3**). Due to the change of measurement apparatus, the absolute values of rate constants shown in this table are different, but the relative values remain the same.

9. Tabulated Experimental Rate Constants

	Ligand 3		
Substrate	k_{obs} (dm^3 mol^{-1} s^{-1})	$\log_{10}(k_X/k_H)$	referenced k_H[a]
4	679	−0.306	1370
5	1170	−0.070	
6	959	−0.156	
7	1300	−0.024	
8	1370	0.00	
9	3370	0.390	
10	18200	1.124	
11	42800	1.493	
12	25900	1.276	
13	122000	1.949	
14	2050	0.175	
15	6470	0.674	
16	6240	0.658	
17	5930	0.636	
18	4020	0.466	
19	781	−0.245	
20	2450	0.252	
21	17200	1.099	
22	23300	1.230	
23	964	−0.154	
24	456	−0.385	1110
25	535	−0.316	
26	1040	−0.028	
27	778	−0.142	
28	1430	0.111	
29	9560	0.936	
30	147000	2.122	
31	188000	2.230	
32	1380	0.094	
33	5170	0.669	
34	610	−0.262	
35	9160	0.918	
36	904	−0.088	
37	3270	0.470	
38	1760	0.201	
39	5740	0.726	
40	5470	0.694	
41	11800	1.027	

42	55800	1.714
43	28200	1.417
44	43500	1.594
45	43100	1.590
46	120000	2.035

[a] k_X referenced to the same k_H were measured on the same day to make sure all the relative rate constants can be cross-compared.

Table S9. Tabulated experimental substrate activation kinetics by cobalt with BPP (**3**). Values are quoted to 3 significant figures

10. Computational Details

All computations were carried out using Gaussian 16 RevC.01.[6] Multiple conformations were considered for each compound, with only the lowest-energy geometry considered in the parameterization. All computations in this section were performed at the M06-2X/def2-TZVP//M06-2X/6-31G(d,p) level with an ultrafine integration grid.[7-10] All optimized structures have been confirmed as ground states by the absence of negative eigenvalues in the frequency analysis at the same level of theory. Optimized structures are visualized using CYLview.[11]

The following parameters were considered in the modeling study:

E (TZ), G (TZ): Triple-zeta (triple-ζ) electronic energy and Gibbs free energy for each structure. The former is used in the calculation of the bond-dissociation energy (see below), and the latter used to determine the ground-state conformation; *included only for reference and not a parameter for the modeling*.

HOMO, ***LUMO energies***: Energies of the highest occupied and lowest virtual (Kohn−Sham) orbital ("HOMO" and "LUMO").

Dihedral Angle: The dihedral angles of the C−Br bond referenced to the phenyl ring plane, which can be obtained using GaussView 6.0.

BDE: Bond-dissociation energy; the energy required to homolytically cleave the C−Br bond to form two radicals in the gaseous phase. The bond-dissociation energies of the benzyl bromide substrates are given by

$$\boldsymbol{BDE = E\,(TZ)_{Rad} + E\,(TZ)_{Br\ atom} - E\,(TZ)_{Substrate}}$$

where $\mathbf{E\,(TZ)_{Rad}}$ is the triple-zeta (triple-ζ) electronic energy of the benzylic radical, $\mathbf{E\,(TZ)_{Br\ atom}}$ is the triple-zeta (triple-ζ) electronic energy of the bromine (or chlorine) atom, and $\mathbf{E\,(TZ)_{Substrate}}$ is the triple-zeta (triple-ζ) electronic energy of the starting material benzyl bromide.

11. Tabulated Selected Computational Parameters for the Substrates

	Benzyl Bromide Parameters					*Benzyl Radical Parameters*		
Substrate	**HOMO / Hartree**	**LUMO / Hartree**	**Dihedral Angle / Degree**	**E (TZ) / Hartree**	**G (TZ) / Hartree**	**E (TZ) / Hartree**	**G (TZ) / Hartree**	**BDE / kcal mol^{-1}**
4	−0.2799	0.0043	66.29	−2959.66	−2956.99	−385.41	−385.15	62.28
5	−0.2790	−0.0056	67.29	−3151.39	−3148.61	−577.14	−576.78	62.11
6	−0.2954	−0.0014	63.58	−2884.44	−2881.81	−310.19	−309.98	62.26
7	−0.3055	−0.0074	63.20	−2944.39	−2941.75	−370.14	−369.92	62.10
8	−0.3063	−0.0052	61.71	−2907.23	−2842.54	−270.88	−270.70	62.20
9	−0.3179	−0.0172	61.38	−3257.45	−3254.67	−621.55	−682.84	61.75
10	−0.3262	−0.0255	57.96	−3182.22	−3179.48	−546.74	−607.64	61.34
11	−0.3159	−0.0339	60.09	−3073.02	−3070.30	−438.00	−498.46	60.87
12	−0.3129	−0.0468	60.53	−3189.51	−3186.71	−554.45	−614.88	60.91
13	−0.3245	−0.0432	57.96	−2937.38	−2934.75	−302.84	−362.92	60.39
14	−0.2831	0.0003	60.20	−2959.66	−2956.99	−323.37	−385.15	62.14
15	−0.3085	−0.0115	60.37	−2944.39	−2941.75	−308.48	−369.92	61.75
16	−0.3109	−0.0148	60.06	−3257.45	−3254.67	−621.81	−682.84	61.49
17	−0.3250	−0.0234	57.66	−3182.22	−3179.48	−546.52	−607.64	61.55
18	−0.3149	−0.0309	61.00	−3073.02	−3070.30	−436.73	−498.46	62.14
19	−0.2956	−0.0010	62.69	−2923.75	−2921.09	−287.23	−349.25	62.37
20	−0.2761	0.0022	56.85	−3074.19	−3071.44	−438.21	−499.60	61.82
21	−0.3180	−0.0184	56.39	−3043.64	−3040.96	−408.06	−469.13	61.42
22	−0.3403	−0.0379	57.02	−3519.31	−3516.41	−884.14	−944.58	61.03
23	−0.2943	−0.0021	63.91	−3023.01	−3020.30	−386.58	−448.47	62.28
24	−0.2777	−0.0006	55.29	−2884.44	−3187.88	−249.10	−616.05	61.20
25	−0.2940	0.0041	54.29	−3190.70	−2921.08	−555.04	−349.25	61.51
26	−0.3038	−0.0026	53.83	−2923.75	−2981.02	−288.29	−409.19	61.32
27	−0.3047	0.0003	53.07	−2983.70	−2881.81	−348.14	−309.98	61.41
28	−0.3162	−0.0117	52.51	−3296.76	−3293.94	−661.82	−722.11	60.79
29	−0.3239	−0.0212	52.53	−3221.54	−3218.75	−587.05	−646.92	60.33
30	−0.3138	−0.0303	52.59	−3112.33	−3109.57	−478.27	−537.74	59.91
31	−0.3227	−0.0394	52.20	−2976.69	−2974.03	−343.20	−402.20	59.34
32	−0.2834	0.0003	51.55	−2998.97	−2996.26	−363.62	−424.43	61.20
33	−0.3232	−0.0185	52.07	−3221.54	−3218.75	−586.88	−646.92	60.51
34	−0.2943	0.0042	54.16	−2963.06	−2960.36	−327.29	−388.53	61.63
35	−0.3165	−0.0135	51.45	−3082.95	−3080.24	−448.41	−508.41	60.39
36	−0.2827	−0.0030	76.28	−2959.66	−2956.99	−323.12	−385.15	62.39
37	−0.2812	−0.0079	77.72	−3151.39	−3148.61	−514.59	−576.78	62.66
38	−0.2998	−0.0072	79.37	−2884.44	−2881.81	−247.50	−309.98	62.80
39	−0.3088	−0.0128	77.21	−2944.39	−2941.75	−308.39	−369.92	61.85

40	−0.2891	−0.0146	75.46	−3076.18	−3073.43	−439.03	−501.59	62.99
41	−0.3160	−0.0165	72.44	−3257.45	−3254.67	−621.75	−682.84	61.55
42	−0.3209	−0.0252	82.83	−3182.22	−3179.47	−546.82	−607.64	61.26
43	−0.3130	−0.0316	72.08	−3073.02	−3070.29	−436.97	−498.46	61.90
44	−0.2964	−0.0080	89.38	−2923.76	−2921.08	−286.81	−349.25	62.79
45	−0.3191	−0.0193	88.93	−3043.64	−3040.96	−408.12	−469.13	61.36
46	−0.3136	−0.0248	89.88	−3764.34	−3761.70	−1128.63	−1189.86	61.56

Table S10. Computational parameters for the substrates. The BDE was calculated using calculated Br^{-} E(TZ) = −2574.15 Hartree.

12. Multivariable Linear-Regression (MLR) Models

In order to investigate the relationship between substrate effects and electron transfer kinetics, multivariable parameter-based modeling was used to delve into possible molecular descriptors for the molecules in question. Model development was performed as described previously using normalized parameters (subtract mean, divide by standard deviation)[12] in MATLAB R2019a. In order to test our hypothesis on the electron transfer, it was necessary to discover a descriptor or combination of descriptors to describe the reduction and bond cleavage process.

While the results of the MLR modeling were presented in the manuscript, here we demonstrate the non-collinearity between the parameters we applied to modeling (Figure S7).

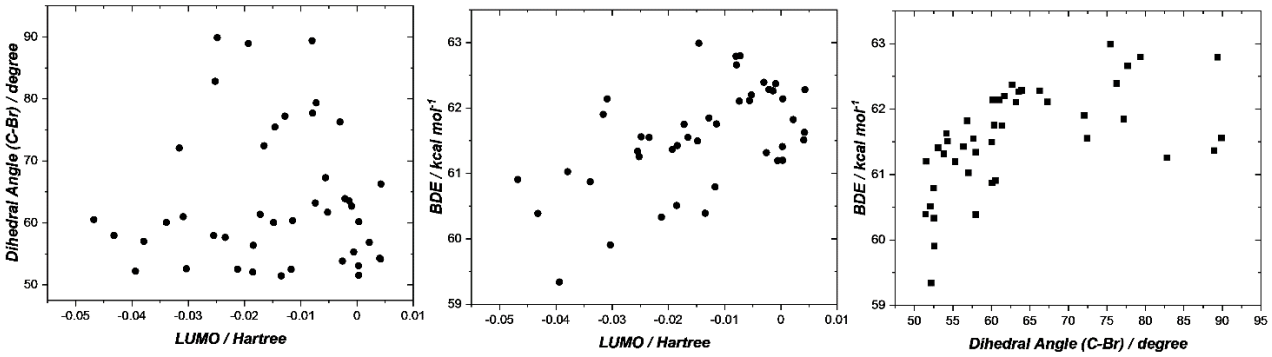


Figure S7. Intercorrelation between LUMO (Hartree), Dihedral Angle (C−Br) (degree), and BDE (kcal mol^{-1}), the scattering patterns presented in the diagrams demonstrate non-collinearity between these parameters.

Additionally, we demonstrate that taking one parameter out from the MLR modeling we presented in the manuscript would cause a statistically degradation of the modeling.

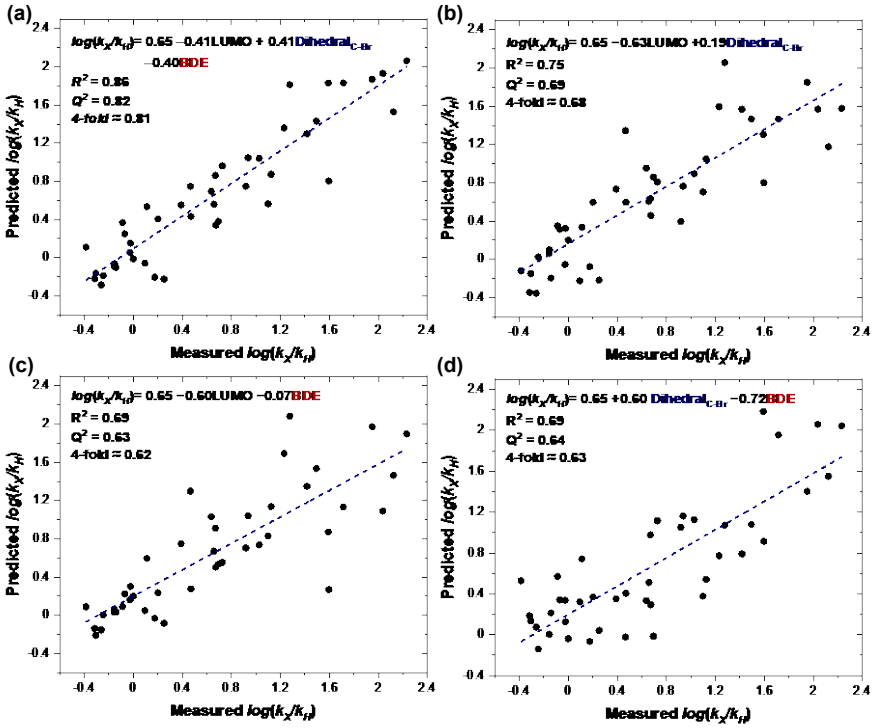


Figure S8. (a) Multivariable linear regression modeling of kinetic data with three parameters: LUMO energy of the substrates (**LUMO**), the C–Br bond dihedral angle (**Dihedral**$_{\text{C-Br}}$), and the C–Br bond-dissociation energy (**BDE**). This model has different statistics to that presented in the manuscript Figure 8.b, since in this case we have not partitioned the data into a separate training and validation set. (b) Model with **BDE** parameter taken out from (a). (c) Model with **Dihedral**$_{\text{C-Br}}$ parameter taken out from (a). (d) Model with **LUMO** parameter taken out from (a).

13. Synthesis of Ligands and Substrates

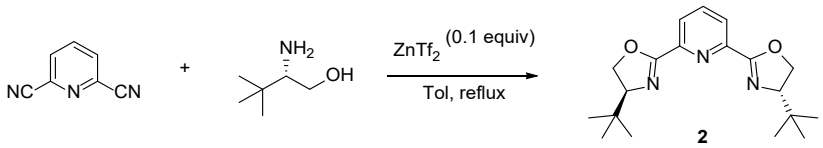
The following ligands and substrates were commercially available:

Ligand **1**, Substrate **4**-**23**, **27**, **30**, **38**-**45**.

*The deuterated substrates (**6-d**$_1$, **6-d**$_2$) were prepared according to our previous report.*[2]

The following ligands were prepared by an alternative procedure to that previously reported, yields are not optimized:

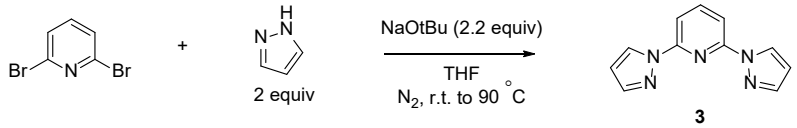
2,6-Bis((*S*)-4-(tert-butyl)-4,5-dihydrooxazol-2-yl)pyridine (2)



According to a literature procedure,[13] to a dried round bottom flask were added pyridine-2,6-dicarbonitrile (390 mg, 3.00 mmol, 1.00 equiv), L-*tert*-Leucinol (725 mg, 6.20 mmol, 2.10 equiv), and $ZnTf_2$ (109 mg, 0.300 mmol, 0.100 equiv) in toluene (30 mL). The reaction mixture was stirred at reflux (115 °C) for 17 h. Upon being cooled to room temperature, the mixture was diluted with ethyl acetate (20 ml), and washed with brine (3 x 10 ml) and sat. $NaHCO_3$ (2 x 10 ml), dried (Na_2SO_4), filtered and concentrated. The crude product was purified by trituration with hexane/ethyl acetate (9/1) to afford title compound **1** (732 mg, 74% yield) as a white powder solid.

[a]$_D^{20}$ = −174.1 (*c* 1.01, $CHCl_3$); **MP:** 239 – 241 °C (lit. 236 – 238 °C[13]); **^{1}H NMR** ($CDCl_3$, 500 MHz) δ 8.24 (d, J = 7.8 Hz, 2H), 7.85 (t, J = 7.9 Hz, 1H), 4.50 – 4.44 (m, 2H), 4.32 (t, J = 8.7 Hz, 2H), 4.11 (dd, J = 10.3, 8.5 Hz, 2H), 0.97 (s, 18H); **^{13}C NMR** ($CDCl_3$, 126 MHz) δ 162.20, 146.91, 137.10, 125.84, 76.40, 69.50, 34.00, 25.97; **IR** (neat) 2995, 1642, 1363, 1106, 971, 931, 906, 727 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H]^+$ ($C_{14}H_{19}N_2O_3^+$) requires *m/z* 330.2176, found *m/z* 330.2184. Data matches literature precedent.[13]

2,6-Di(1H-pyrazol-1-yl)pyridine (3)

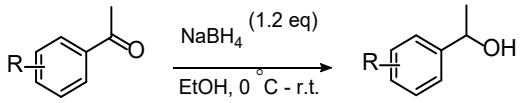


According to a literature procedure,[14] to a dried pressure vessel was added pyrazole (1.36 g, 20.0 mmol, 2.00 equiv) in 25 ml THF under nitrogen at room temperature. Then sodium *tert*-butoxide (2 M in THF, 11.0 ml, 22.0 mmol, 2.20 equiv) was added dropwise. The resulting mixture was stirred at room temperature for 5 min before 2,6-dibromopyridine (2.37 g, 10.0 mmol, 1.00 equiv) was added in one portion. The reactor was then heated at 90 °C, and the reaction was stirred for 36 h. Afterwards, the reaction was quenched by water and the resulting mixture was extracted

by ethyl acetate (3 x 40 ml). The collected organic phase was dried with Na_2SO_4, filtered, and concentrated under reduced pressure. The crude was further purified by recrystallization with DCM/MeOH. Ligand **3** was then afforded as a white solid (1.23 g, 58 % yield). **^{1}H NMR** ($CDCl_3$, 500 MHz) δ 8.58 (dd, J = 2.6, 0.8 Hz, 2H), 7.95 (dd, J = 8.7, 7.1 Hz, 1H), 7.88 – 7.84 (m, 2H), 7.77 (dd, J = 1.6, 0.7 Hz, 2H), 6.50 (dd, J = 2.6, 1.7 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 126 MHz) δ 150.05, 142.40, 141.44, 127.02, 109.39, 107.99; Data matches literature precedent.[14]

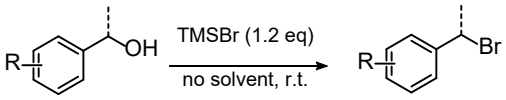
Synthesis of non-commercial substrates for the activation kinetic studies. Yields for these reactions were not optimized. Compounds are ordered according to the substrate numbering chart.

General Procedure A



To a 20 ml scintillation vial was added the methyl aryl ketone (3.00 mmol, 1.00 equiv), dissolved in ethanol (10 ml). After the reaction was cooled to 0 °C, $NaBH_4$ (137 mg, 3.60 mmol, 1.20 equiv) was added in one portion, and the resulting solution was stirred at room temperature overnight. The reaction progress was monitored by TLC, and upon complete consumption of the ketone starting material, the reaction was quenched by water and extracted by DCM (20 ml) three times. The collected organic phase was dried with Na_2SO_4, filtered, and concentrated under reduced pressure. The crude was then redissolved in DCM (2 ml), filtered through a pad of silica gel with hexane:ethyl acetate (5:1, 100 ml). By concentration under reduced pressure, the benzyl alcohol crude product was afforded for the following bromination reaction without further purification and characterization. The yield for this step was not recorded.

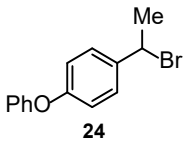
General Procedure B



According to the literature procedure, to the 1-dram scintillation vial was added the corresponding benzyl alcohol (0.50 mmol, 1.00 equiv), either from a commercial source or the crude product of general procedure A. Then trimethylsilyl bromide (80 µl, 0.60 mmol, 1.20 equiv) was injected in one portion via a syringe. The reaction was stirred overnight at room temperature. Then the reaction was concentrated under vacuum to remove excess trimethylsilyl bromide and side

products, affording the benzyl bromide product without the requirement of further purification if not specifically noted. The yield for this step was recorded for each substrate in the below.

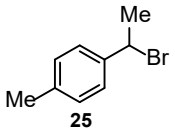
1-(1-Bromoethyl)-4-phenoxybenzene (**24**):



24

The general procedure A was followed using the corresponding methyl aryl ketone (636 mg, 3.00 mmol), affording the corresponding benzyl alcohol crude product. Then the general procedure B was followed using the corresponding benzyl alcohol (107 mg, 0.50 mmol). Product **24** was afforded as a pale yellow oil (142 mg, 99 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.45 – 7.40 (m, 2H), 7.37 (td, J = 8.3, 7.3, 1.9 Hz, 2H), 7.18 – 7.13 (m, 1H), 7.08 – 7.03 (m, 2H), 6.98 (dd, J = 8.8, 2.3 Hz, 2H), 5.26 (q, J = 7.1 Hz, 1H), 2.07 (d, J = 7.0 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.42, 156.71, 137.94, 129.88, 128.36, 123.72, 119.35, 118.56, 49.41, 26.97; **IR** (neat) 1588, 1506, 1487, 1167, 870, 837, 735, 691, 581, 548 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_{14}H_{13}O^+$) requires *m/z* 197.0960, found *m/z* 197.0968.

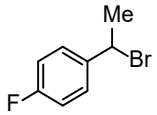
1-(1-Bromoethyl)-4-methylbenzene (**25**):



25

The general procedure B was followed using the corresponding benzyl alcohol (68 mg, 0.50 mmol). Product **25** was afforded as a pale yellow oil (93 mg, 94 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39 – 7.35 (m, 2H), 7.18 (dd, J = 8.2, 2.3 Hz, 2H), 5.25 (q, J = 7.1 Hz, 1H), 2.37 (s, 3H), 2.07 (d, J = 7.1 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 140.42, 138.29, 129.39, 126.75, 49.86, 26.87, 21.22; **IR** (neat) 1513, 1176, 1042, 816, 718, 586 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_9H_{11}^+$) requires *m/z* 119.0855, found *m/z* 119.0863.

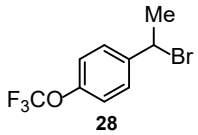
1-(1-Bromoethyl)-4-fluorobenzene (**26**):



26

The general procedure B was followed using the corresponding benzyl alcohol (70 mg, 0.50 mmol). Product **26** was afforded as a pale yellow oil (97 mg, 96 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.46 – 7.39 (m, 2H), 7.03 (t, J = 8.6 Hz, 2H), 5.21 (q, J = 6.9 Hz, 1H), 2.04 (d, J = 6.9 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.38 (d, J = 247.5 Hz), 139.21 (d, J = 3.3 Hz), 128.61 (d, J = 8.3 Hz), 115.58 (d, J = 21.8 Hz), 48.54, 26.97; **^{19}F NMR** ($CDCl_3$, 471 MHz) δ −113.23 (dd, J = 9.4, 5.0 Hz); **IR** (neat) 1604, 1509, 1222, 1179, 1159, 1042, 833, 720, 585 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_8H_8F^+$) requires *m/z* 123.0604, found *m/z* 123.0627.

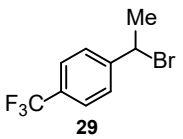
1-(1-Bromoethyl)-4-(trifluoromethoxy)benzene (**28**):



28

The general procedure A was followed using the corresponding methyl aryl ketone (612 mg, 3.00 mmol), affording the corresponding benzyl alcohol crude product. Then the general procedure B was followed using the corresponding benzyl alcohol (103 mg, 0.50 mmol). Product **28** was afforded as a pale yellow oil (124 mg, 92 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.53 – 7.42 (m, 2H), 7.23 – 7.13 (m, 2H), 5.20 (q, J = 6.9 Hz, 1H), 2.04 (d, J = 6.9 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.86, 141.93, 121.45, 120.43 (q, J = 258.3 Hz), 117.35, 47.85, 26.84; **^{19}F NMR** ($CDCl_3$, 471 MHz) δ −57.86 (s); **IR** (neat) 1509, 1265, 1213, 1154, 1112, 1043, 1018, 851, 815, 589 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_9H_8F_3O^+$) requires *m/z* 189.0521, found *m/z* 189.0524.

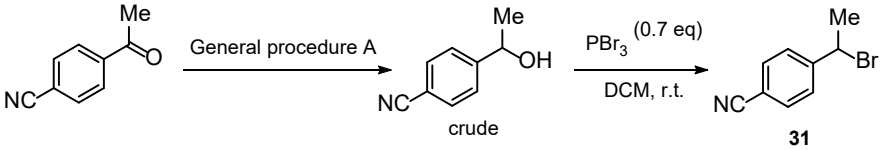
1-(1-Bromoethyl)-4-(trifluoromethyl)benzene (**29**):



29

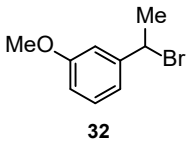
The general procedure B was followed using the corresponding benzyl alcohol (95 mg, 0.50 mmol). Product **29** was afforded as a pale yellow oil (125 mg, 98 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (d, J = 8.2 Hz, 2H), 7.56 (d, J = 8.2 Hz, 2H), 5.20 (q, J = 6.9 Hz, 1H), 2.05 (d, J = 7.0 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 145.12, 128.47 (q, J = 32.6 Hz), 125.32, 123.79 (q, J = 3.8 Hz), 121.98 (q, J = 272.1 Hz), 45.58, 24.68; **^{19}F NMR** ($CDCl_3$, 471 MHz) δ −62.70 (s); **IR** (neat) 1322, 1164, 1114, 1071, 1063, 1018, 840, 740, 613 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_9H_8F_3^+$) requires *m/z* 173.0572, found *m/z* 173.0578.

4-(1-Bromoethyl)benzonitrile (**31**):



The general procedure A was followed using the corresponding methyl aryl ketone (425 mg, 3.00 mmol), affording the corresponding benzyl alcohol crude product. Then to a 1-dram vial was added the corresponding benzyl alcohol (74 mg, 0.50 mmol), dissolved in DCM (1.5 ml). Phosphorous tribromide (33 µl, 0.35 mmol, 0.70 equiv) was added to the resulting solution, and the reaction was stirred under room temperature overnight. The solution was then concentrated under reduced pressure. The crude product was purified by prep-TLC with the developing solvent of hexane:ethyl acetate (15:1). Product **31** was afforded as a colorless oil (65 mg, 62 % yield), R_f = 0.35 (10% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.73 – 7.60 (m, 2H), 7.56 – 7.51 (m, 2H), 5.16 (q, J = 7.0 Hz, 1H), 2.02 (d, J = 6.9 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.17, 132.57, 127.67, 118.43, 112.06, 47.05, 26.38; **IR** (neat) 2229, 1067, 1042, 1020, 837, 799, 593, 560 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_9H_8N^+$) requires *m/z* 130.0651, found *m/z* 130.0662.

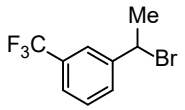
1-(1-Bromoethyl)-3-methoxybenzene (**32**):



The general procedure A was followed using the corresponding methyl aryl ketone (450 mg, 3.00 mmol), affording the corresponding benzyl alcohol crude product. Then the general procedure

B was followed using the corresponding benzyl alcohol (76 mg, 0.50 mmol). Product **32** was afforded as a pale brown oil (94 mg, 88 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.27 (t, J = 8.0 Hz, 1H), 7.03 (dd, J = 7.3, 1.7 Hz, 1H), 7.01 – 6.98 (m, 1H), 6.84 (ddd, J = 8.3, 2.6, 1.4 Hz, 1H), 5.19 (q, J = 7.0 Hz, 1H), 3.83 (s, 3H), 2.05 (d, J = 7.0 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.72, 144.75, 129.72, 119.13, 113.81, 112.62, 55.31, 49.42, 26.84; **IR** (neat) 1598, 1585, 1487, 1456, 1436, 1287, 1256, 1182, 1157, 1036, 778, 693, 547 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_9H_{11}O^+$) requires *m/z* 135.0804, found *m/z* 135.0810.

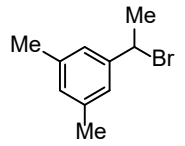
1-(1-Bromoethyl)-3-(trifluoromethyl)benzene (**33**):



33

The general procedure B was followed using the corresponding benzyl alcohol (95 mg, 0.50 mmol). Product **33** was afforded as a pale yellow oil (117 mg, 92 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.64 (d, J = 7.7 Hz, 1H), 7.56 (d, J = 7.8 Hz, 1H), 7.48 (t, J = 7.8 Hz, 1H), 5.22 (q, J = 7.0 Hz, 1H), 2.07 (d, J = 7.0 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 142.30, 129.16 (q, J = 32.5 Hz), 128.37, 127.35, 123.19 (q, J = 3.8 Hz), 121.97 (q, J = 273.4 Hz), 121.70 (q, J = 3.9 Hz), 45.72, 24.75; **^{19}F NMR** ($CDCl_3$, 471 MHz) δ −62.70 (s); **IR** (neat) 1324, 1165, 1123, 1074, 802, 741, 698, 656, 572 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_9H_8F_3^+$) requires *m/z* 173.0572, found *m/z* 173.0574.

1-(1-Bromoethyl)-3,5-dimethylbenzene (**34**):

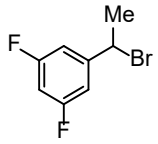


34

The general procedure A was followed using the corresponding methyl aryl ketone (444 mg, 3.00 mmol), affording the corresponding benzyl alcohol crude product. Then the general procedure B was followed using the corresponding benzyl alcohol (75 mg, 0.50 mmol). Product **34** was afforded as a pale yellow oil (107 mg, 99 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.10 – 6.99 (m, 2H), 6.94 – 6.89 (m,

1H), 5.16 (q, J = 6.9 Hz, 1H), 2.31 (s, 6H), 2.03 (d, J = 6.9 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 143.15, 138.28, 130.14, 124.61, 50.05, 26.86, 21.31; **IR** (neat) 1264, 1184, 1065, 849, 734, 699, 607 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_{10}H_{13}^+$) requires *m/z* 133.1011, found *m/z* 133.1021.

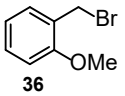
1-(1-Bromoethyl)-3,5-difluorobenzene (**35**):



35

The general procedure B was followed using the corresponding benzyl alcohol (79 mg, 0.50 mmol). Product **35** was afforded as a brown oil (90 mg, 81 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.99 – 6.93 (m, 2H), 6.73 (tt, J = 8.8, 2.3 Hz, 1H), 5.09 (q, J = 6.9 Hz, 1H), 2.00 (d, J = 6.9 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$)δ 162.91 (dd, J = 249.1, 12.9 Hz), 146.86 (t, J = 9.0 Hz), 109.96 (dd, J = 19.9, 6.2 Hz), 103.73 (t, J = 25.3 Hz), 46.76 (t, J = 2.3 Hz), 26.50; **^{19}F NMR** ($CDCl_3$, 471 MHz) δ −108.95 (t, J = 8.0 Hz); **IR** (neat) 1623, 1597, 1463, 1340, 1119, 981, 856, 735, 686, 616 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_8H_7F_2^+$) requires *m/z* 141.0510, found *m/z* 141.0508.

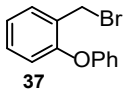
1-(Bromomethyl)-2-methoxybenzene (**36**):



36

The general procedure B was followed using the corresponding benzyl alcohol (69 mg, 0.50 mmol). Product **36** was afforded via bulb-to-bulb distillation as a colorless oil that slowly solidified in the freezer (52 mg, 52 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (dd, J = 7.5, 1.7 Hz, 1H), 7.32 – 7.28 (m, 1H), 6.94 (td, J = 7.5, 1.0 Hz, 1H), 6.89 (d, J = 8.3 Hz, 1H), 4.59 (s, 2H), 3.90 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.50, 130.93, 130.24, 126.14, 120.71, 111.00, 55.61, 29.07; **IR** (neat) 1492, 1464, 1437, 1292, 1250, 1220, 1047, 1026, 746, 604 cm^{-1}; Spectroscopic data matches literature precedent.[15] **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_8H_9O^+$) requires *m/z* 121.0647, found *m/z* 121.0659. Spectroscopic data matches literature precedent.[15]

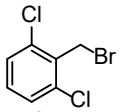
1-(Bromomethyl)-2-phenoxybenzene (**37**):



37

The general procedure B was followed using the corresponding benzyl alcohol (100 mg, 0.50 mmol). Product **37** was afforded as a purple oil (133 mg, 99 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.47 (dq, J = 7.8, 1.7 Hz, 1H), 7.41 – 7.33 (m, 2H), 7.29 – 7.24 (m, 1H), 7.17 – 7.13 (m, 1H), 7.12 – 7.08 (m, 1H), 7.07 – 7.04 (m, 2H), 6.88 – 6.84 (m, 1H), 4.61 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.02, 155.37, 131.35, 130.15, 129.86, 128.88, 123.64, 123.61, 119.02, 118.71, 28.16; **IR** (neat) 1581, 1492, 1453, 1243, 1201, 1160, 890, 810, 735, 719, 606 cm^{-1}; **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_{13}H_{11}O^+$) requires *m/z* 183.0804, found *m/z* 183.0811.

2-(Bromomethyl)-1,3-dichlorobenzene (**46**):



46

The general procedure B was followed using the corresponding benzyl alcohol (89 mg, 0.50 mmol). Product **46** was afforded as a white solid (118 mg, 99 % yield). ^{1}H NMR revealed a clean product with no further purification required; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.32 (dd, J = 8.1, 1.9 Hz, 2H), 7.18 (t, J = 8.1 Hz, 1H), 4.76 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 135.93, 133.66, 130.06, 128.58, 27.52; **IR** (neat) 1562, 1421, 1212, 1091, 906, 890, 778, 732, 705, 608 cm^{-1}; Spectroscopic data matches literature precedent.[16] **HRMS** (ESI) exact mass calculated for $[M+H-HBr]^+$ ($C_7H_5Cl_2^+$) requires *m/z* 158.9762, found *m/z* 158.9770.

14. References

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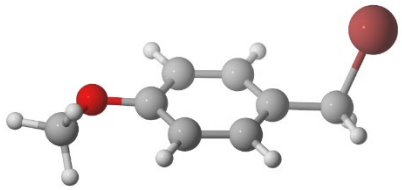
15. Cartesian Coordinates of Substrates

All computations herein are computed at the M06-2X/def2-TZVP//M06-2X/ 6-31G(d,p) level of theory

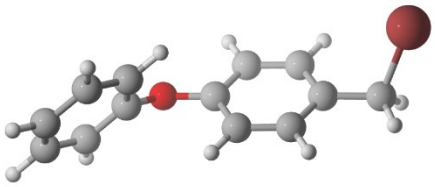
4



19

C	1.53269	1.30977	0.37462
C	0.21225	1.00872	0.64309
C	-0.24785	-0.31468	0.59371
C	0.65138	-1.31858	0.25644
C	1.98994	-1.03347	-0.01813
C	2.43237	0.28664	0.04233
C	-1.66865	-0.63738	0.92174
Br	-2.91891	0.12166	-0.39998
O	3.70659	0.68303	-0.20364
C	4.64243	-0.31308	-0.55355
H	1.90344	2.32816	0.40864
H	-0.48740	1.80576	0.88041
H	0.31081	-2.34921	0.20523
H	2.66434	-1.84029	-0.27671
H	-1.98926	-0.20717	1.86935
H	-1.85867	-1.70906	0.91822
H	5.58948	0.20131	-0.71172
H	4.75904	-1.05082	0.24927
H	4.34983	-0.82870	-1.47588

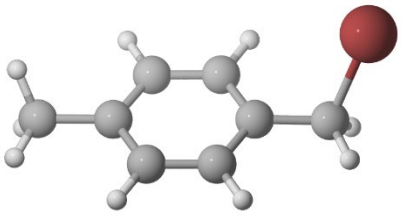
5



26

C	-1.47724	1.36678	-0.49140
C	-1.79129	0.57402	0.61714
C	-0.75326	-0.00836	1.34147
C	0.57667	0.19503	0.98451
C	0.86716	0.98569	-0.12446
C	-0.15953	1.57430	-0.86448
H	-2.28116	1.80530	-1.07641
H	-0.98188	-0.62691	2.20492
H	1.37952	-0.25475	1.55781
H	0.10133	2.18361	-1.72243
C	-3.21415	0.37572	1.02824
H	-3.29987	-0.18146	1.95918
H	-3.76235	1.31339	1.10539
O	2.14707	1.28281	-0.51713
C	3.15722	0.37307	-0.28933
C	3.01385	-0.97568	-0.61063
C	4.35852	0.86780	0.20580
C	4.09158	-1.83381	-0.42007
H	2.06922	-1.33779	-1.00306
C	5.43178	-0.00064	0.38266
H	4.43218	1.92422	0.43872
C	5.30181	-1.35228	0.07555
H	3.98526	-2.88466	-0.66897
H	6.37132	0.38282	0.76693
H	6.13863	-2.02719	0.21870
Br	-4.22136	-0.66882	-0.30439

6

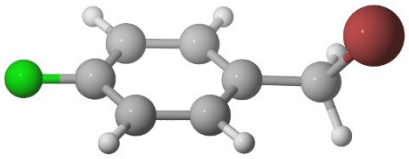


18

C	-1.97840	-1.14224	0.34914
C	-0.65254	-0.86057	0.63630
C	-0.15247	0.43599	0.47591
C	-1.00693	1.43287	0.01490
C	-2.34027	1.14492	-0.27243
C	-2.84602	-0.14257	-0.11018
C	1.26701	0.75271	0.82743
Br	2.53930	-0.23099	-0.30556
C	-4.28359	-0.46734	-0.42364
H	-2.35396	-2.15408	0.47829
H	0.01547	-1.64941	0.97224
H	-0.63162	2.44365	-0.12066
H	-2.99433	1.93481	-0.63112

H	1.52187	0.45265	1.84290
H	1.50021	1.80596	0.68298
H	-4.83183	0.42300	-0.73833
H	-4.35146	-1.20752	-1.22660
H	-4.79078	-0.88686	0.45025

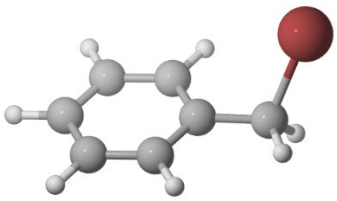
7



15

C	2.38624	1.13159	-0.28345
C	1.05765	1.41800	0.01981
C	0.19584	0.41911	0.47049
C	0.67818	-0.88670	0.60617
C	1.99832	-1.19113	0.30843
C	2.83182	-0.17042	-0.13167
C	-1.21801	0.74623	0.83701
Br	-2.50864	-0.21071	-0.29526
F	4.10812	-0.45859	-0.42126
H	3.07165	1.89374	-0.63502
H	0.69048	2.43357	-0.09627
H	0.00125	-1.67177	0.93148
H	2.39245	-2.19596	0.40547
H	-1.44004	1.80372	0.70717
H	-1.46660	0.43883	1.85173

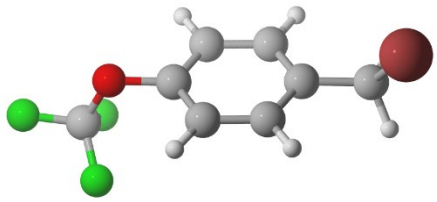
8



15

C	-2.827229	0.942809	-0.385067
C	-1.530826	1.298733	-0.017822
C	-0.627351	0.327642	0.409716
C	-1.031789	-1.009519	0.457412
C	-2.322865	-1.365267	0.091586
C	-3.225091	-0.388116	-0.329813
H	-3.522500	1.706952	-0.716890
H	-1.219870	2.338864	-0.063367
H	-0.317526	-1.768275	0.765789
H	-2.627983	-2.405850	0.131251
H	-4.233448	-0.667318	-0.617388
C	0.749415	0.720192	0.850700
H	0.967404	0.395265	1.867180
H	0.918028	1.791706	0.761163
Br	2.140866	-0.130006	-0.245372

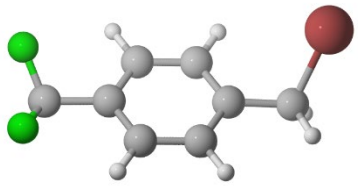
9



19

C	0.90971	1.32050	-0.46734
C	-0.40233	1.52358	-0.04757
C	-1.18663	0.45212	0.37681
C	-0.64762	-0.83824	0.36837
C	0.65781	-1.05575	-0.04702
C	1.41842	0.03203	-0.46048
C	-2.58221	0.68647	0.86953
Br	-3.90654	-0.27774	-0.21076
O	2.71524	-0.18698	-0.93153
C	3.68885	-0.14652	0.00585
F	4.84475	-0.36843	-0.59642
F	3.74457	1.03912	0.61995
F	3.51275	-1.07338	0.95258
H	1.53527	2.13965	-0.80268
H	-0.81682	2.52729	-0.05111
H	-1.26857	-1.67596	0.67236
H	1.09499	-2.04745	-0.06278
H	-2.86300	1.73654	0.81629
H	-2.72944	0.31574	1.88301

10

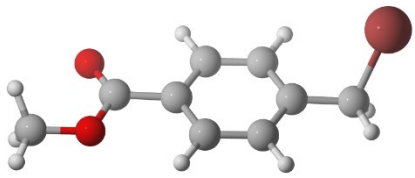


18

C	-1.00736	-0.95048	0.48018
C	0.34140	-0.70621	0.68242
C	0.87243	0.56685	0.44910
C	0.03515	1.58558	-0.00010
C	-1.32172	1.34713	-0.20438

C	-1.83709	0.08093	0.03857
C	2.32032	0.84873	0.71963
Br	3.49971	-0.33594	-0.30295
C	-3.30547	-0.18734	-0.12716
F	-3.94334	-0.17335	1.05380
F	-3.89751	0.72719	-0.90729
F	-3.52658	-1.39294	-0.67163
H	-1.42138	-1.93849	0.65229
H	1.00229	-1.50678	1.00147
H	0.44347	2.57305	-0.19380
H	-1.97358	2.13725	-0.55954
H	2.58340	0.67091	1.76169
H	2.59694	1.86281	0.43769

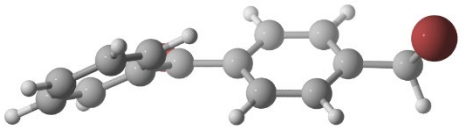
11



21

C	0.87197	1.12275	0.46704
C	-0.47425	0.85769	0.65607
C	-0.95609	-0.45200	0.55638
C	-0.07199	-1.48731	0.25492
C	1.28137	-1.22697	0.06280
C	1.75355	0.07941	0.17067
C	-2.40273	-0.74970	0.81199
Br	-3.57441	0.21925	-0.42683
C	3.19105	0.42237	-0.02392
O	3.94322	-0.65333	-0.30954
O	3.64245	1.53956	0.06346
C	5.32875	-0.37476	-0.50657
H	1.26682	2.13032	0.54066
H	-1.17039	1.66518	0.86431
H	-0.44375	-2.50433	0.17004
H	1.97096	-2.02927	-0.17261
H	-2.71908	-0.42599	1.80283
H	-2.63302	-1.80468	0.67662
H	5.79705	-1.33260	-0.72485
H	5.46188	0.31924	-1.33881
H	5.75852	0.06986	0.39322

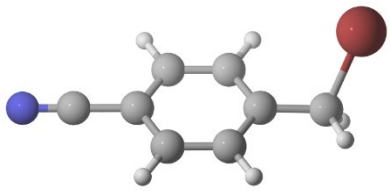
12



27

C	0.18406	0.03698	0.78389
C	-1.19137	-0.07806	0.92629
C	-2.04560	0.84311	0.31481
C	-1.50173	1.88976	-0.43107
C	-0.12434	2.01869	-0.55925
C	0.72791	1.08528	0.03225
C	-3.52935	0.73828	0.49670
Br	-4.22499	-0.96880	-0.17606
C	2.20557	1.30416	-0.10713
C	3.14374	0.13632	-0.06730
O	2.63847	2.43182	-0.25275
C	4.45652	0.37373	0.35125
C	5.38218	-0.66098	0.36908
C	5.00906	-1.93593	-0.05555
C	3.71080	-2.17250	-0.49885
C	2.77610	-1.14100	-0.50024
H	0.83950	-0.67607	1.27342
H	-1.61627	-0.89651	1.50057
H	-2.16080	2.60973	-0.90781
H	0.31315	2.83972	-1.11734
H	-4.06399	1.51311	-0.04924
H	-3.81723	0.75943	1.54703
H	4.72727	1.37941	0.65549
H	6.39640	-0.47587	0.70725
H	5.73383	-2.74379	-0.04714
H	3.42530	-3.15973	-0.84668
H	1.76854	-1.32286	-0.86070

13

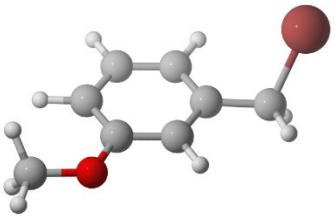


16

C	-1.72924	-1.05848	0.44020
C	-0.39135	-0.77160	0.65469
C	0.10389	0.51711	0.43083
C	-0.75940	1.51416	-0.02194
C	-2.10428	1.23930	-0.24166
C	-2.59035	-0.04864	-0.00857
C	1.54042	0.83971	0.71601

Br	2.75927	-0.30739	-0.30070
C	-3.98182	-0.34111	-0.23338
N	-5.10064	-0.57580	-0.41256
H	-2.11725	-2.05610	0.61267
H	0.28904	-1.55286	0.98026
H	-0.37931	2.51482	-0.20424
H	-2.77730	2.01263	-0.59447
H	1.79757	0.66553	1.76022
H	1.78993	1.86260	0.44082

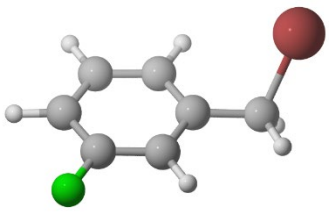
14



19

C	1.22957	1.95476	0.02638
C	-0.00339	1.42263	0.36167
C	-0.13052	0.04008	0.54976
C	0.97497	-0.78177	0.39215
C	2.22035	-0.23768	0.05308
C	2.35219	1.13688	-0.13037
C	-1.44267	-0.55315	0.96562
Br	-2.85929	-0.18629	-0.34331
O	3.23310	-1.13366	-0.07427
C	4.50350	-0.63189	-0.42694
H	1.33364	3.02481	-0.12161
H	-0.87701	2.05944	0.46016
H	0.90548	-1.85682	0.52596
H	3.30489	1.57854	-0.39493
H	-1.81179	-0.12311	1.89577
H	-1.39314	-1.63676	1.05188
H	5.16655	-1.49439	-0.48246
H	4.47767	-0.12951	-1.40119
H	4.88010	0.06819	0.32836

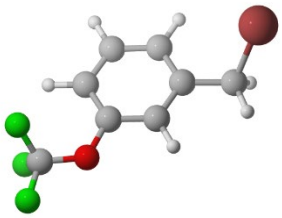
15



15

C	1.77010	1.79084	0.02188
C	0.51891	1.30758	0.38239
C	0.30183	-0.06894	0.49451
C	1.34475	-0.95506	0.23528
C	2.58489	-0.44525	-0.12325
C	2.82289	0.91373	-0.23499
C	-1.03073	-0.59743	0.93377
Br	-2.46852	-0.06081	-0.28756
F	3.58379	-1.30464	-0.37061
H	1.93276	2.85990	-0.06395
H	-0.30575	1.99115	0.56020
H	1.21329	-2.02969	0.30592
H	3.80867	1.26181	-0.52016
H	-1.32931	-0.20062	1.90313

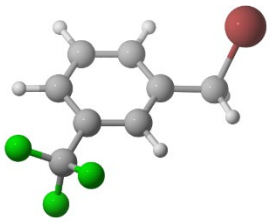
16



19

C	0.90971	1.32050	-0.46734
C	-0.40233	1.52358	-0.04757
C	-1.18663	0.45212	0.37681
C	-0.64762	-0.83824	0.36837
C	0.65781	-1.05575	-0.04702
C	1.41842	0.03203	-0.46048
C	-2.58221	0.68647	0.86953
Br	-3.90654	-0.27774	-0.21076
O	2.71524	-0.18698	-0.93153
C	3.68885	-0.14652	0.00585
F	4.84475	-0.36843	-0.59642
F	3.74457	1.03912	0.61995
F	3.51275	-1.07338	0.95258
H	1.53527	2.13965	-0.80268
H	-0.81682	2.52729	-0.05111
H	-1.26857	-1.67596	0.67236
H	1.09499	-2.04745	-0.06278
H	-2.86300	1.73654	0.81629
H	-2.72944	0.31574	1.88301

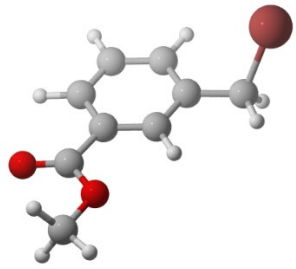
17



18

C	0.45130	2.29079	-0.01382
C	-0.69005	1.58187	0.33463
C	-0.63651	0.19776	0.52750
C	0.57469	-0.46554	0.35814
C	1.71822	0.25141	0.01101
C	1.66595	1.62675	-0.17617
C	-1.85646	-0.56380	0.95200
Br	-3.34100	-0.32965	-0.30623
C	3.02746	-0.47566	-0.10816
F	3.88529	0.16997	-0.90968
F	3.62698	-0.60761	1.08561
F	2.86235	-1.71298	-0.59847
H	0.39724	3.36317	-0.16653
H	-1.64340	2.09237	0.43860
H	0.63521	-1.54211	0.48795
H	2.56270	2.16786	-0.45682
H	-2.24528	-0.21453	1.90776
H	-1.67074	-1.63506	0.99940
H	-1.05144	-1.68516	0.95730

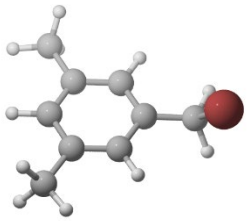
18



21

C	0.19924	2.48035	-0.00797
C	-0.87525	1.67315	0.34389
C	-0.69622	0.30235	0.55649
C	0.57053	-0.25217	0.40181
C	1.65016	0.55985	0.04751
C	1.46714	1.92551	-0.15634
C	-1.84710	-0.55713	0.98355
Br	-3.29261	-0.55211	-0.34417
C	3.02493	0.01027	-0.13042
O	3.08208	-1.31399	0.08769
C	4.37825	-1.88846	-0.07505
O	3.98844	0.67146	-0.43618
H	0.04858	3.54219	-0.17028
H	-1.87169	2.09623	0.44000
H	0.72962	-1.31463	0.55487
H	2.32487	2.52923	-0.43253
H	-2.31355	-0.19773	1.89984
H	-1.55540	-1.59893	1.10108
H	4.26138	-2.95057	0.13137
H	4.73841	-1.72983	-1.09339
H	5.08507	-1.43420	0.62213

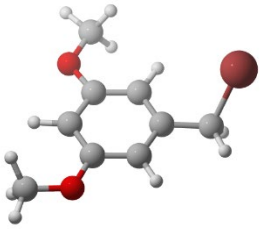
19



21

C	-1.76240	1.34987	0.05903
C	-2.67497	0.31675	-0.19505
C	-2.31053	-1.02104	-0.09897
C	-0.99386	-1.33003	0.26486
C	-0.07309	-0.32389	0.52732
C	-0.46385	1.01539	0.41908
C	1.31748	-0.67024	0.96208
Br	2.66734	-0.00798	-0.30475
C	-2.19338	2.78836	-0.06987
C	-3.29748	-2.12546	-0.37849
H	-3.69464	0.57046	-0.47856
H	-0.69105	-2.37225	0.34304
H	0.26916	1.79791	0.60205
H	1.47302	-1.74578	1.02078
H	1.58388	-0.20432	1.90981
H	-1.39147	3.46969	0.22127
H	-2.47522	3.02005	-1.10147
H	-3.06279	2.99595	0.56077
H	-2.94307	-2.77215	-1.18660
H	-3.44211	-2.75549	0.50433
H	-4.27002	-1.72304	-0.66913

20

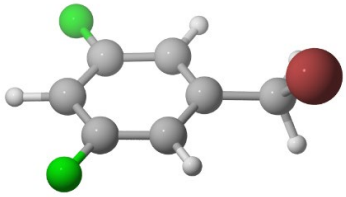


23

C	2.05166	-0.95270	0.04755
C	2.29004	0.40580	-0.09057
C	1.22777	1.30939	0.07440
C	-0.05053	0.86213	0.37798
C	-0.27078	-0.51672	0.51587
C	0.76225	-1.42047	0.35048
C	-1.62868	-1.01842	0.90777
Br	-3.02875	-0.41596	-0.32979
O	3.00048	-1.91176	-0.09505
O	1.56334	2.61468	-0.08750

C	4.30919	-1.48804	-0.41007
C	0.53176	3.56983	0.04057
H	3.26449	0.81121	-0.32942
H	-0.88644	1.54312	0.48211
H	0.60880	-2.48962	0.44845
H	-1.94169	-0.63690	1.87897
H	-1.67742	-2.10528	0.90281
H	4.91250	-2.39213	-0.48231
H	4.33488	-0.95438	-1.36734
H	4.71666	-0.83888	0.37385
H	0.99428	4.54098	-0.13152
H	-0.25814	3.40404	-0.70096
H	0.09185	3.54836	1.04453

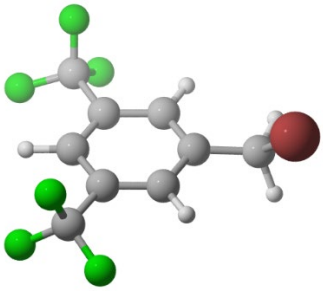
21



15

C	-1.75463	1.31492	0.06054
C	-2.73371	0.36524	-0.20147
C	-2.35331	-0.96302	-0.12283
C	-1.06081	-1.35453	0.20153
C	-0.10754	-0.37239	0.46137
C	-0.45320	0.97892	0.38858
C	1.27776	-0.77806	0.87200
Br	2.64809	0.02428	-0.27258
F	-2.09143	2.60742	-0.01004
F	-3.26685	-1.90788	-0.37245
H	-3.74477	0.65149	-0.46063
H	-0.82118	-2.41095	0.24470
H	0.28073	1.75860	0.55909
H	1.42085	-1.85443	0.80309
H	1.51847	-0.43695	1.87812

22



21

C	1.56037	-0.84290	-0.10403
C	1.67697	0.53313	0.00814
C	0.53764	1.31897	-0.16267
C	-0.69089	0.74185	-0.44306
C	-0.80170	-0.64683	-0.56546
C	0.32974	-1.43497	-0.38905
C	-2.11176	-1.27768	-0.93464
Br	-3.53132	-0.78845	0.31933
C	2.75383	-1.73004	0.11998
C	0.65002	2.80909	0.01139
F	-0.34603	3.45674	-0.60561
F	0.60986	3.15306	1.30557
F	1.80779	3.26999	-0.48180
F	2.78845	-2.73103	-0.77167
F	3.90344	-1.05259	0.02135
F	2.72100	-2.29238	1.33596
H	2.63749	0.99136	0.21564
H	-1.57163	1.36624	-0.55918
H	0.26575	-2.51531	-0.48261
H	-2.05555	-2.36432	-0.92035
H	-2.46575	-0.93998	-1.90796

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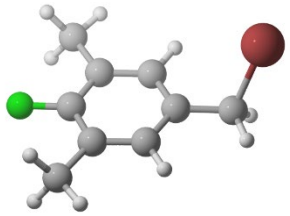

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C	1.52244	1.24643	0.15576
C	2.36031	0.15998	-0.08294
C	1.95832	-1.16636	-0.01531
C	0.62369	-1.40421	0.31737
C	-0.25654	-0.35483	0.57142
C	0.20145	0.96228	0.48399
C	-1.67171	-0.63675	0.96782
Br	-2.95618	0.06511	-0.34650
C	2.94444	-2.26531	-0.29924
F	3.64422	0.41504	-0.40433
C	2.06348	2.64480	0.04629
H	0.27209	-2.43134	0.37769
H	-0.49322	1.78087	0.65731
H	-1.94804	-0.14999	1.90194
H	-1.87393	-1.70410	1.03302
H	2.47245	-3.24376	-0.19583
H	3.34392	-2.17915	-1.31339
H	3.79439	-2.21559	0.38674
H	1.28408	3.37752	0.26105
H	2.88990	2.80026	0.74516
H	2.45151	2.83501	-0.95806

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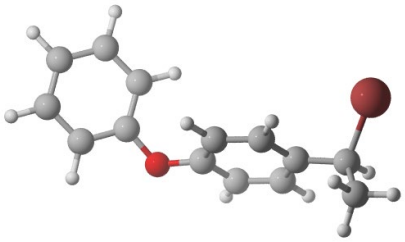

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C	-1.09255300	-1.15637400	-0.22021500
C	-0.26067500	-1.90486400	-1.04481000
C	1.11722500	-1.72709500	-0.97012100
C	1.67311300	-0.80654400	-0.08345600
C	0.82010800	-0.06132200	0.73561500
C	-0.55509700	-0.23145000	0.67820300
H	-0.70688900	-2.61320300	-1.73361600
H	1.76607100	-2.31163500	-1.61674000
H	1.24401700	0.67717900	1.41057600
H	-1.21350300	0.34877300	1.31545100
C	3.16748000	-0.68887300	0.03470500
C	3.70881700	-1.20736900	1.35821900
H	3.64956900	-1.18996600	-0.80531600
H	3.26302600	-0.66243000	2.19359800
H	3.44952800	-2.26586000	1.46013800
H	4.79345900	-1.09643900	1.40728000
Br	3.73016800	1.19821900	-0.16701500
O	-2.43780800	-1.41953800	-0.29336200
C	-3.34186000	-0.39510100	-0.11791900
C	-3.15268800	0.86444000	-0.68445500
C	-4.49948200	-0.69268800	0.59362800
C	-4.13696900	1.83372000	-0.52059400
H	-2.24656000	1.07482700	-1.24285700
C	-5.47939100	0.28392400	0.74142500
H	-4.61221700	-1.68549800	1.01471900
C	-5.30112700	1.55015200	0.19016600
H	-3.99311100	2.81566200	-0.95955300
H	-6.38362600	0.05304200	1.29509600
H	-6.06459900	2.31084000	0.31130800

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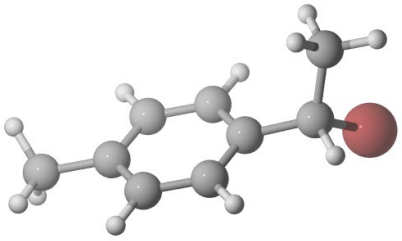

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C	-2.99508000	-0.20571400	0.00792500
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C	-0.72432300	-0.55947500	-0.77239700
C	-0.26174700	0.47959200	0.04135300
C	-1.17488500	1.16425200	0.83786400
C	-2.52696100	0.82529900	0.81879900
H	-2.41416700	-1.70661000	-1.42093500
H	-0.01299500	-1.12046000	-1.37271700
H	-0.83085100	1.97178700	1.47900800
H	-3.22542700	1.36966300	1.44834300
C	1.17567000	0.92161300	0.00492200
C	1.56621100	1.57509100	-1.31201500
H	1.38492900	1.58456000	0.84512300
H	0.93934200	2.45789800	-1.47252800
H	2.61537500	1.87570700	-1.30340800
H	1.40608800	0.88410900	-2.14293200
Br	2.38296800	-0.61489700	0.31487800
C	-4.45161500	-0.59140300	-0.01070500
H	-5.05142800	0.09568200	0.58976500
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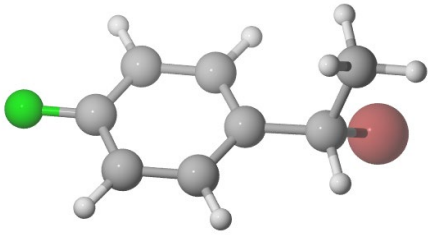
H	-4.59442900	-1.60027300	0.38851600

26



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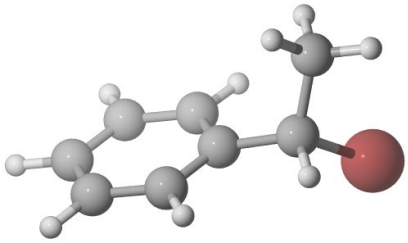
C	2.97658200	-0.24179200	-0.00633200
C	2.08342700	-0.94889700	0.78815700
C	0.74389300	-0.58746600	0.76655400

C	0.30033200	0.46691800	-0.03766700
C	1.22281200	1.15151300	-0.82774900
C	2.57132200	0.80376400	-0.81808100
H	2.44692100	-1.76747200	1.39845800
H	0.02185800	-1.14473500	1.35664200
H	0.88771800	1.96855900	-1.46060100
H	3.30214200	1.32228800	-1.42751600
C	-1.13252300	0.92577500	-0.00086600
C	-1.51631300	1.57994500	1.31782100
H	-1.33185400	1.59471000	-0.83870200
H	-2.56159800	1.89343800	1.30828000
H	-1.36681400	0.88436600	2.14694500
H	-0.87926700	2.45460100	1.48270900
Br	-2.35591700	-0.59431400	-0.31836300
F	4.27120000	-0.58925800	0.00949700

27



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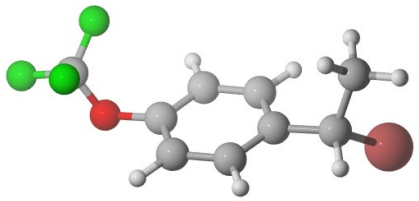
C	-3.34691500	-0.54568300	-0.00062200
C	-2.37676900	-1.17761700	-0.77818500
C	-1.06301300	-0.72772700	-0.75759200
C	-0.70262300	0.36093600	0.04085100
C	-1.67519300	0.98538600	0.82006300
C	-2.99381600	0.53526100	0.79928800
H	-4.37209700	-0.90092700	-0.01526900
H	-2.64548000	-2.02763400	-1.39697100
H	-0.29751200	-1.23430900	-1.33899900
H	-1.40049200	1.82962600	1.44706000
H	-3.74127000	1.02787500	1.41263900
C	0.69292700	0.92523100	0.00704900
C	1.02211800	1.61222600	-1.30984000
H	0.84300900	1.60357200	0.84760900
H	2.04054600	2.00449300	-1.30196700
H	0.92250700	0.91029000	-2.14103800
H	0.31956500	2.43639300	-1.46878400
Br	2.02831200	-0.49878500	0.31513300

28



22

C	1.62119000	-0.22617100	-0.52713600
C	0.81554100	-1.04081200	0.25948100
C	-0.51416800	-0.68998400	0.44445200
C	-1.03418000	0.46443200	-0.14822900
C	-0.20375600	1.26053200	-0.93625700
C	1.13273400	0.92152200	-1.12990600
H	1.23700800	-1.93484600	0.70451200
H	-1.16932000	-1.32794500	1.03036300
H	-0.60174100	2.15604100	-1.40484700
H	1.79242300	1.52595600	-1.74171400
C	-2.44863300	0.90817000	0.11836700
C	-2.65385700	1.39982700	1.54359200
H	-2.74193200	1.67195900	-0.60249900
H	-2.40989700	0.61057200	2.25852600
H	-1.99060800	2.25051600	1.72910100
H	-3.68804700	1.70952300	1.70297500
Br	-3.71358000	-0.56788100	-0.22238200
O	2.94620500	-0.60473500	-0.75936600
C	3.84886900	-0.12984900	0.12788500
F	3.58657000	-0.53203600	1.37514800
F	5.04195300	-0.58029300	-0.22173500
F	3.88206600	1.20632400	0.14307300

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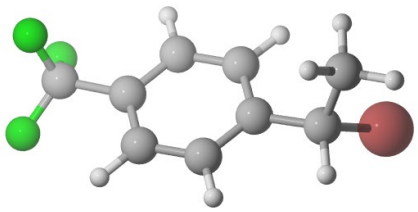

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C	2.01467900	0.04224700	-0.04663900
C	1.51033400	1.08241300	-0.81720300
C	0.14164300	1.33590400	-0.81429700
C	-0.72196900	0.55765700	-0.04520100
C	-0.20180700	-0.49062500	0.71989200
C	1.16060000	-0.74855100	0.72145300
H	2.18125900	1.68136300	-1.42299900
H	-0.25702000	2.14535800	-1.41913900
H	-0.87938700	-1.12049600	1.28878300
H	1.56570100	-1.56893900	1.30419000
C	-2.18499500	0.91265700	0.01106400
C	-2.59062500	1.52004400	1.34600700
H	-2.43847600	1.57997200	-0.81308200
H	-3.65456400	1.76256200	1.35459700
H	-2.38321000	0.82322500	2.16140600
H	-2.01190300	2.43326900	1.51633600
Br	-3.29669100	-0.68309400	-0.31648300
C	3.49437700	-0.20929100	0.00179500
F	3.76960500	-1.51485900	0.13524500
F	4.11099700	0.22657900	-1.10571500
F	4.06699300	0.41686400	1.04220200

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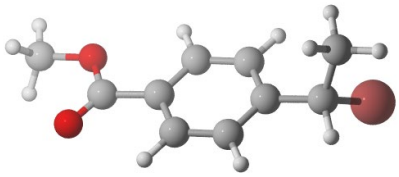
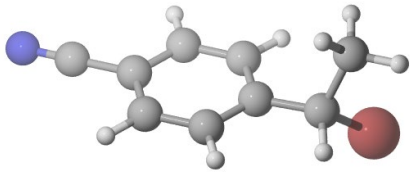


24

C	1.95440700	0.29025300	-0.05666200
C	1.16767500	-0.73251300	0.48041900
C	-0.20842200	-0.57663800	0.55496000
C	-0.81396000	0.59733500	0.09696800
C	-0.02172800	1.61171700	-0.44204300
C	1.35790900	1.46131500	-0.51870900
H	1.64035000	-1.64305300	0.82996600
H	-0.83100000	-1.37697000	0.94440600
H	-0.48784800	2.52397700	-0.80375200
H	1.98968500	2.23763100	-0.93685100
C	-2.29472000	0.82305500	0.25501300
C	-2.70613000	1.02706400	1.70577800
H	-2.61206900	1.66449600	-0.36147500
H	-3.78302600	1.18470600	1.78572600
H	-2.43320400	0.15591500	2.30580700
H	-2.18354000	1.90076800	2.10766900
Br	-3.30986300	-0.70308600	-0.47588100
C	3.43650800	0.17827200	-0.16622500
O	4.15335400	1.03737800	-0.62238600
O	3.90012000	-0.99233600	0.30172200
C	5.31574400	-1.14875000	0.21615400
H	5.81958200	-0.36998700	0.79209500
H	5.53195400	-2.13304600	0.62707600
H	5.64281900	-1.08343700	-0.82344500

31



19

C	2.74694300	-0.07992100	-0.01242200
C	1.85799300	-0.84240500	0.75586800
C	0.50498800	-0.54495500	0.73650600
C	0.02126000	0.51108800	-0.04216300
C	0.91348900	1.26123900	-0.80806300
C	2.27322300	0.97282100	-0.79785400
H	2.23628700	-1.66280400	1.35545500
H	-0.19488600	-1.14879300	1.30640600
H	0.54354100	2.07933300	-1.41921400
H	2.96738600	1.55347000	-1.39497700
C	-1.43169700	0.90728900	-0.00174500
C	-1.82818400	1.54488800	1.32208200
H	-1.66020800	1.57004200	-0.83679400
H	-2.88498400	1.81667100	1.31922100
H	-1.64610800	0.85421900	2.14868600
H	-1.22605600	2.44440400	1.48390300
Br	-2.58268200	-0.66160600	-0.31507900

C	4.15340400	-0.38609200	0.00381800
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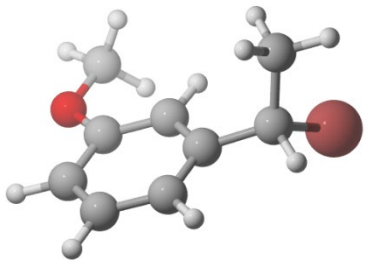
32



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C	2.82382600	1.04320300	-0.38639600
C	2.22886300	-0.17757700	-0.03889400
C	0.85861200	-0.24530400	0.19363200
C	0.07712200	0.90987500	0.07507900
C	0.66504300	2.11922700	-0.27533400
C	2.04262100	2.17841800	-0.50284300
H	3.89304500	1.06196500	-0.56532300
H	0.37018400	-1.18352500	0.43220100
H	0.05543300	3.01276000	-0.37004700
H	2.50424400	3.12079000	-0.77917800
C	-1.38829900	0.87883300	0.42280500
C	-1.63719000	0.72596900	1.91596800
H	-1.88174900	1.77046700	0.03530000
H	-2.70641200	0.70546900	2.13388000
H	-1.18516700	-0.19768900	2.28478800
H	-1.17768300	1.56851200	2.44218200
Br	-2.30410000	-0.60300000	-0.51148500
O	3.07092600	-1.23926800	0.04202600
C	2.50775900	-2.49269700	0.36427600
H	1.76701400	-2.80102600	-0.38269000
H	3.33321100	-3.20346100	0.37196200
H	2.03382100	-2.47480300	1.35294500

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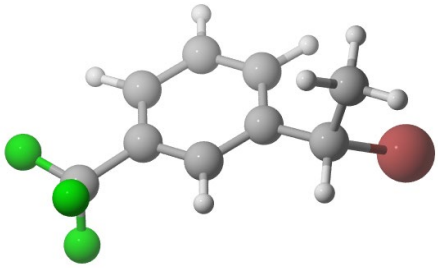
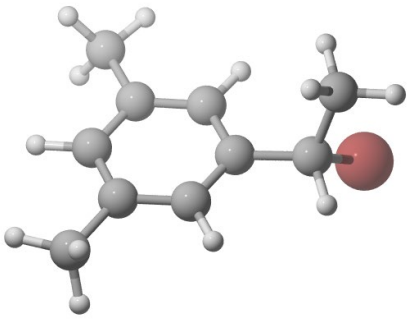


21

C	-1.83279200	1.65557200	0.07628400
C	-1.89355200	0.26908800	0.04360300
C	-0.73635700	-0.49928000	0.16418800
C	0.49866100	0.12092800	0.31968600
C	0.56045000	1.51815700	0.34872800
C	-0.59476200	2.27814200	0.22971400
H	-2.74191200	2.23858600	-0.01688300
H	-0.80806800	-1.58343100	0.14278800
H	1.52904500	2.00131700	0.44119000
H	-0.53435500	3.36083700	0.25205500
C	1.72629600	-0.72256100	0.54532400
C	2.22534400	-0.66150900	1.98142500
H	1.53139900	-1.75223500	0.24432800
H	3.11637900	-1.27831300	2.10942400
H	2.46832400	0.36724500	2.25760400
H	1.43851000	-1.02268800	2.65103600
Br	3.18643200	-0.15094400	-0.65085600
C	-3.20317000	-0.43501500	-0.16934000
F	-4.24936000	0.36942600	0.06019400
F	-3.31891000	-0.89070500	-1.42590300
F	-3.32341500	-1.49976500	0.63912300

34



24

C	-2.81840800	0.39753000	-0.13645400
C	-1.84228900	1.37172000	0.11154900
C	-0.52679400	0.96555200	0.29540500
C	-0.18090800	-0.38856100	0.23487800
C	-1.16557200	-1.33534900	-0.01815800
C	-2.49949200	-0.95344800	-0.20747000
H	-3.85093300	0.70864000	-0.28329500
H	0.25292100	1.70542500	0.46112000
H	-0.89975100	-2.38957100	-0.06897900
C	1.22317700	-0.84426100	0.53019100
C	1.61742600	-0.64828500	1.98624400
H	1.35016800	-1.88465400	0.22947200
H	2.64128200	-0.98284300	2.16257000
H	1.53927200	0.40535100	2.26388200
H	0.93571600	-1.22322700	2.62093400
Br	2.52295800	0.12697100	-0.60007500
C	-2.22478900	2.82866100	0.16575300
H	-1.36180200	3.45604700	0.39742500

H	-2.63667600	3.16060100	-0.79200400
H	-2.98886300	3.00545300	0.92857800
C	-3.55170600	-1.99367800	-0.49531000
H	-3.54288300	-2.78299600	0.26189000
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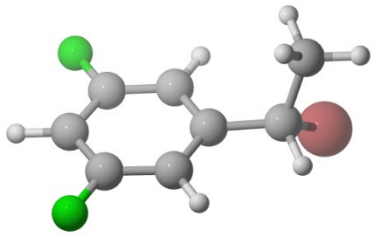
H	-3.37563500	-2.46941400	-1.46502200

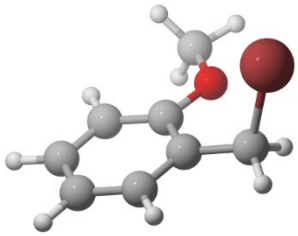
35



18

C	-2.87318100	0.41810900	-0.13576400
C	-2.50244300	-0.90924500	-0.26414400
C	-1.19095500	-1.33882500	-0.11072500
C	-0.20558900	-0.39890900	0.18553000
C	-0.54116500	0.94975100	0.32111900
C	-1.86319600	1.32480700	0.15773600
H	-3.89949600	0.73627400	-0.26518500
H	-0.96103400	-2.39234500	-0.22527400
H	0.21454200	1.70185600	0.51883900
C	1.19934100	-0.87766200	0.44923700
C	1.56670500	-0.82305300	1.92496000
H	1.32797900	-1.88492700	0.05263400
H	2.58649200	-1.17782700	2.08309300
H	1.48834700	0.19991200	2.30001000
H	0.87455500	-1.45368300	2.49162100
Br	2.50120200	0.19946600	-0.56330100
F	-2.18898000	2.61628000	0.28326800
F	-3.44552700	-1.81410400	-0.55081300

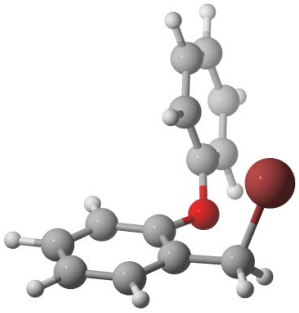
36



19

C	2.42095700	0.48365900	-0.33440300
C	1.12827100	0.54056400	0.18218800
C	0.44754200	-0.64227000	0.52444600
C	1.07947200	-1.86439200	0.32981300
C	2.37276000	-1.93242200	-0.18572000
C	3.03389400	-0.75680400	-0.51490200
H	2.95320500	1.38904700	-0.59894000
H	0.54563600	-2.77532800	0.58683500
H	2.85374600	-2.89324600	-0.32973000
H	4.04059000	-0.79303400	-0.91867400
C	-0.93207900	-0.55428600	1.07897800
H	-1.25294700	-1.49366000	1.52397300
H	-1.04410000	0.26773600	1.78208100
Br	-2.25050400	-0.17006300	-0.33578800
O	0.43637100	1.68683100	0.39926200
C	1.04956900	2.90427600	0.03333800
H	0.32764900	3.68727400	0.26099900
H	1.96812000	3.07572700	0.60682600
H	1.28246000	2.92309600	-1.03731400

37

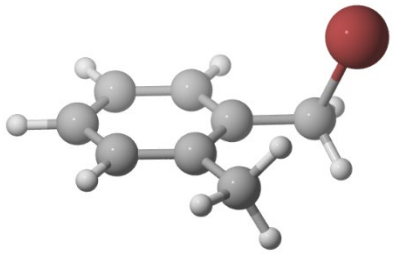


26

C	0.46655000	2.38269300	0.03037700
C	0.62982400	1.08960800	0.51530600
C	1.86458000	0.43804200	0.44472100
C	2.94522100	1.11707700	-0.11680800
C	2.79857400	2.41340000	-0.60039800
C	1.55704100	3.04103000	-0.52960000
H	-0.50801400	2.85520400	0.09603800
H	3.90668900	0.61535800	-0.18107600
H	3.64729500	2.92930000	-1.03561900
H	1.43503400	4.05098400	-0.90678300
C	1.97997500	-0.96319600	0.94255300
H	1.50014300	-1.10407900	1.90829400
H	3.01182600	-1.30681800	0.96606900
Br	1.02991200	-2.20282900	-0.25793000
O	-0.39455100	0.41390000	1.13315500
C	-1.61279900	0.33724100	0.48975300
C	-1.70279700	0.14287200	-0.88694400
C	-2.75206700	0.40942100	1.28315300
C	-2.96117100	0.02742300	-1.46789300
H	-0.79610400	0.05877800	-1.47668500
C	-4.00359300	0.28448600	0.68783100
H	-2.63782800	0.55741500	2.35126000
C	-4.11346600	0.09911400	-0.68775600

H	-3.03878800	-0.12846900	-2.53901100
H	-4.89553200	0.33863700	1.30350300
H	-5.09047900	0.00623600	-1.14943100

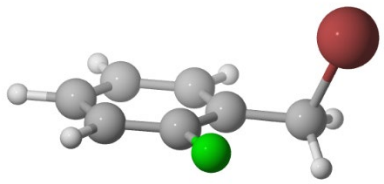
38



18

C	-2.47463000	0.93954300	-0.36734000
C	-1.17832900	0.95553200	0.14577400
C	-0.59283100	-0.26583300	0.52321600
C	-1.30386200	-1.45656500	0.37326800
C	-2.59692700	-1.45580300	-0.13869400
C	-3.18348000	-0.25069700	-0.50922900
H	-2.93460500	1.87875400	-0.66195100
H	-0.83314000	-2.39327500	0.66010300
H	-3.13955100	-2.38874100	-0.24840800
H	-4.19130900	-0.23439000	-0.91145300
C	0.78983200	-0.30718200	1.08763500
H	1.00858700	0.52846900	1.75022400
H	0.99861900	-1.24760200	1.59337200
Br	2.15854600	-0.18204400	-0.33103600
C	-0.42315700	2.25158700	0.28825600
H	-0.26114800	2.50347900	1.34252000
H	0.55971600	2.18640200	-0.18790100
H	-0.97595900	3.07494300	-0.16757600

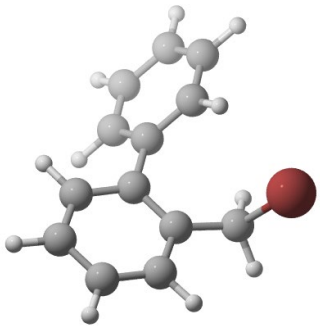
39



15

C	-2.41422700	1.03023500	-0.33673300
C	-1.13619900	0.91622100	0.18033700
C	-0.57100100	-0.30781900	0.53043600
C	-1.33662900	-1.45589900	0.33069000
C	-2.62519800	-1.37245400	-0.18932500
C	-3.16102400	-0.13090900	-0.52215200
H	-2.79967100	2.01195000	-0.58594700
H	-0.91132700	-2.42184800	0.58782200
H	-3.20872100	-2.27441600	-0.33614500
H	-4.16455100	-0.06156700	-0.92808200
C	0.81139700	-0.34845000	1.08614800
H	1.03394800	-1.30391800	1.55606800
H	1.00383200	0.47155900	1.77440300
Br	2.15017300	-0.13172600	-0.33839600
F	-0.40136400	2.02256500	0.36659100

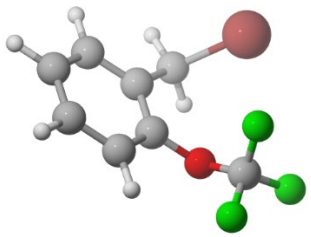
40



25

C	-0.50755500	2.50723000	-0.51417900
C	-0.36221500	1.20524700	-0.01575100
C	0.90014700	0.80626400	0.45865900
C	1.97449600	1.69862200	0.39331800
C	1.81763700	2.98011500	-0.11353000
C	0.56423200	3.38787900	-0.56553700
H	-1.48007200	2.81339000	-0.88794300
H	2.94709500	1.36757500	0.74870200
H	2.66438400	3.65701700	-0.15489400
H	0.42448500	4.38690200	-0.96538400
C	1.14042700	-0.53187200	1.08517600
H	0.22537500	-1.05046800	1.35957600
H	1.80488600	-0.45736700	1.94399900
Br	2.08571200	-1.74474800	-0.14986000
C	-1.55305400	0.31243700	-0.00720100
C	-1.50228600	-0.97767300	-0.54935200
C	-2.76796000	0.77806000	0.50883000
C	-2.63801100	-1.78156700	-0.56501600
H	-0.56877300	-1.34892300	-0.96311400
C	-3.90246500	-0.02649400	0.49193400
H	-2.81259400	1.77422400	0.93988000
C	-3.84047900	-1.30951900	-0.04540900
H	-2.58285900	-2.77796600	-0.99148900
H	-4.83456700	0.34773100	0.90307300
H	-4.72476500	-1.93832400	-0.05894400

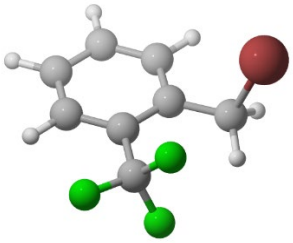
41



19

C	2.38676300	-0.42507500	-0.02105700
C	1.11814500	-0.09421700	0.43033700
C	0.68025500	1.22866600	0.51453200
C	1.55790300	2.23543800	0.11690200
C	2.83254800	1.92653400	-0.34969600
C	3.24294100	0.59915700	-0.41961400
H	2.69385600	-1.46313200	-0.05590200
H	1.23131200	3.26987700	0.17074600
H	3.50308800	2.72131200	-0.65721100
H	4.23630000	0.35288400	-0.77873300
C	-0.69188800	1.53123800	1.02060900
H	-0.82818800	2.59498700	1.20227200
H	-0.94173400	0.95418100	1.90816900
Br	-2.05943000	1.03166700	-0.29810500
O	0.22269600	-1.05947800	0.88388200
C	-0.10055100	-2.07014400	0.04097300
F	-1.18349600	-2.66109700	0.51410600
F	0.87647600	-2.98730700	-0.03051300
F	-0.33218500	-1.64628500	-1.19744200

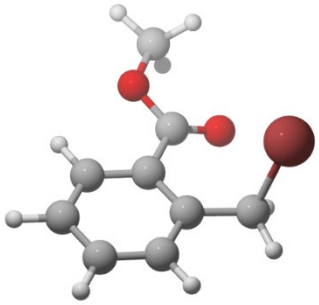
42



18

C	2.39993500	0.64979800	-0.46313500
C	1.26289000	0.01697200	0.02916600
C	0.18913100	0.76346000	0.53219400
C	0.28018200	2.15498800	0.51203700
C	1.41404100	2.79147500	0.02000900
C	2.47782300	2.03857200	-0.46732600
H	3.21829500	0.05022900	-0.84401900
H	-0.55816000	2.73963000	0.88056500
H	1.46552100	3.87513300	0.01596400
H	3.36542800	2.52865400	-0.85209600
C	-1.05822000	0.12549600	1.06649300
H	-1.48542500	0.71598400	1.87449600
H	-0.91872700	-0.90160300	1.39010000
Br	-2.44623500	0.06377000	-0.31761800
C	1.19634700	-1.48659800	0.03099800
F	1.16853200	-1.97792700	1.28505900
F	2.24806000	-2.03915200	-0.58397900
F	0.08991200	-1.93458500	-0.58007700

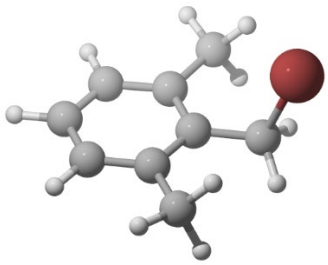
43



21

C	-2.33951100	0.66918500	-0.31541300
C	-1.11608200	0.20906500	0.17484000
C	-0.10304100	1.12719400	0.51083700
C	-0.35537400	2.48782000	0.33696600
C	-1.58028700	2.94232400	-0.14167200
C	-2.57721200	2.03043700	-0.46884300
H	-3.10415200	-0.05389700	-0.57292100
H	0.42765500	3.20091300	0.57797700
H	-1.75069900	4.00716000	-0.26229900
H	-3.53447100	2.37421600	-0.84554800
C	1.24542700	0.71390900	1.02029400
H	1.81390400	1.57800200	1.35786300
H	1.19442300	-0.05397800	1.78476700
Br	2.31758700	-0.08301200	-0.41949400
C	-0.90958700	-1.26104800	0.35315700
O	-0.06529200	-1.77261500	1.05082200
O	-1.79624000	-1.98296400	-0.35145600
C	-1.65971600	-3.39642900	-0.20689200
H	-2.43467600	-3.83443900	-0.83287700
H	-1.79396900	-3.68753600	0.83683300
H	-0.66899500	-3.71512700	-0.53609100

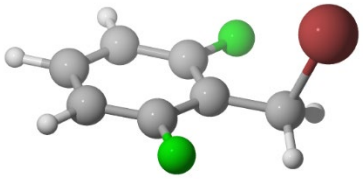
44



21

C	2.48446300	-1.20371600	-0.32487700
C	1.18935700	-1.22124700	0.19121700
C	0.55493400	-0.00000600	0.47258900
C	1.18932500	1.22125400	0.19122600
C	2.48443000	1.20376200	-0.32486800
C	3.13425300	0.00003300	-0.57274300
H	2.98100200	-2.14497600	-0.54248900
H	2.98094400	2.14503700	-0.54247500
H	4.14221600	0.00004800	-0.97523000
C	-0.82174400	-0.00002600	1.05195500
H	-1.03775200	0.88865800	1.63960900
H	-1.03774100	-0.88873300	1.63957700
Br	-2.19167900	-0.00000600	-0.37377400
C	0.47298700	2.52991300	0.41208200
H	-0.52096200	2.50914800	-0.04670300
H	0.34198600	2.74653800	1.47818100
H	1.03571300	3.35620000	-0.02584500
C	0.47305700	-2.52992700	0.41206700
H	0.34206400	-2.74656100	1.47816500
H	-0.52089300	-2.50918800	-0.04671700
H	1.03580600	-3.35619500	-0.02586500

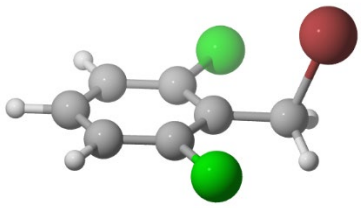
45



15

C	-2.45131000	-1.21184000	-0.34474200
C	-1.17511300	-1.18296800	0.19320700
C	-0.50409200	0.00001800	0.49264600
C	-1.17518000	1.18296200	0.19318800
C	-2.45137700	1.21175400	-0.34476300
C	-3.08225900	-0.00006300	-0.61359600
H	-2.92160700	-2.16582400	-0.54801800
H	-2.92172400	2.16570900	-0.54805800
H	-4.08034100	-0.00009500	-1.03760700
C	0.87153100	0.00005700	1.05764700
H	1.06825400	-0.89639300	1.63927700
H	1.06823300	0.89656400	1.63919600
Br	2.21361200	0.00000600	-0.37706300
F	-0.54908800	2.33621200	0.45836100
F	-0.54896000	-2.33617800	0.45840300

46



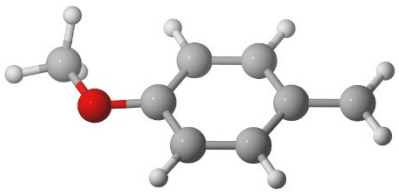
15

C	-2.43269300	-1.20572900	-0.41011300
C	-1.14752500	-1.19122700	0.11726600
C	-0.47379600	0.00000100	0.41634500
C	-1.14752800	1.19122600	0.11726400
C	-2.43269600	1.20572300	-0.41011500
C	-3.07407000	-0.00000400	-0.66672100
H	-2.91275900	-2.15420800	-0.61909000
H	-2.91276500	2.15420100	-0.61909200
H	-4.07725400	-0.00000500	-1.07854400
C	0.90014800	0.00000700	0.99758500
H	1.09311000	-0.89393500	1.58345500
H	1.09310600	0.89395700	1.58344400
Br	2.24610600	0.00000100	-0.42815900
Cl	-0.35436100	2.71924600	0.38724400
Cl	-0.35435600	-2.71924600	0.38724600

16. Cartesian Coordinates of Benzylic Radicals

All computations herein are computed at the M06-2X/def2-TZVP//M06-2X/ 6-31G(d,p) level of theory

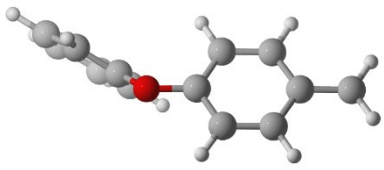
Benzylic Radical of Compound 4



18

C	-0.38248	-1.01820	-0.00012
C	0.99065	-1.20827	-0.00002
C	1.89902	-0.12200	-0.00002
C	1.33475	1.18489	0.00015
C	-0.02646	1.38068	0.00003
C	-0.90185	0.28126	-0.00012
H	-1.03879	-1.88022	-0.00008
H	1.38623	-2.21995	0.00003
H	2.00165	2.04233	0.00036
H	-0.45768	2.37596	0.00004
C	3.29161	-0.32249	-0.00000
H	3.97570	0.51674	0.00011
H	3.71116	-1.32068	-0.00002
O	-2.22542	0.58273	-0.00035
C	-3.13884	-0.49189	0.00029
H	-3.02003	-1.11619	0.89387
H	-4.13310	-0.04661	0.00009
H	-3.02017	-1.11712	-0.89271

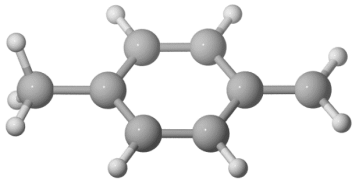
Benzylic Radical of Compound 5



25

C	1.80595	1.34848	0.61086
C	3.08507	0.82974	0.58165
C	3.37613	-0.38581	-0.09289
C	2.29545	-1.03780	-0.74451
C	1.01554	-0.51917	-0.72378
C	0.76712	0.67534	-0.03743
H	1.57972	2.27519	1.12676
H	3.89030	1.35414	1.08770
H	2.48878	-1.96378	-1.27821
H	0.20280	-1.02585	-1.23334
C	4.67770	-0.91997	-0.11691
H	4.89068	-1.84639	-0.63522
H	5.49637	-0.41540	0.38050
O	-0.46405	1.28154	-0.02676
C	-1.60403	0.51251	0.02666
C	-2.69903	0.96272	-0.70457
C	-1.69758	-0.62445	0.82808
C	-3.90054	0.26534	-0.63416
H	-2.58886	1.85390	-1.31232
C	-2.90334	-1.31629	0.88190
H	-0.83577	-0.95489	1.39815
C	-4.00721	-0.87768	0.15424
H	-4.75525	0.61628	-1.20328
H	-2.97966	-2.20156	1.50499
H	-4.94405	-1.42184	0.20357

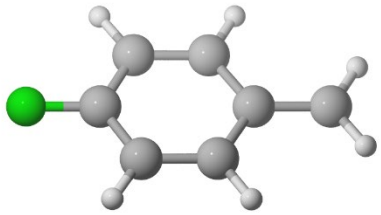
Benzylic Radical of Compound 6



17

C	-0.63155	-1.19833	-0.00003
C	0.74877	-1.20989	-0.00003
C	1.49313	-0.00060	-0.00000
C	0.75623	1.21002	0.00002
C	-0.62768	1.20530	0.00002
C	-1.35146	0.00711	-0.00001
H	-1.17633	-2.13938	-0.00005
H	1.28537	-2.15466	-0.00004
H	1.29645	2.15264	0.00004
H	-1.16677	2.14908	0.00003
C	2.90215	-0.00553	0.00001
H	3.46270	0.92092	-0.00055
H	3.45640	-0.93575	0.00056
C	-2.85658	-0.00219	0.00001
H	-3.24824	-0.52077	-0.88091
H	-3.24822	-0.52039	0.88117
H	-3.25941	1.01291	-0.00020
H	-3.02017	-1.11712	-0.89271

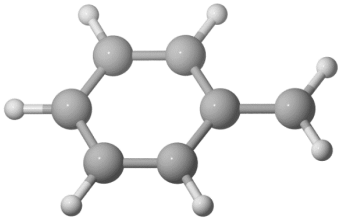
Benzylic Radical of Compound 7



14

C	-0.68751	-1.21708	0.00001
C	0.69485	-1.21331	0.00002
C	1.43296	0.00000	0.00004
C	0.69486	1.21331	0.00002
C	-0.68751	1.21708	0.00001
C	-1.36168	0.00000	0.00003
H	-1.25848	-2.13863	0.00000
H	1.23582	-2.15501	-0.00002
H	1.23582	2.15501	-0.00001
H	-1.25848	2.13863	-0.00000
C	2.84226	0.00000	-0.00001
H	3.40005	0.92795	-0.00015
H	3.40005	-0.92795	-0.00012
F	-2.70269	0.00000	-0.00004

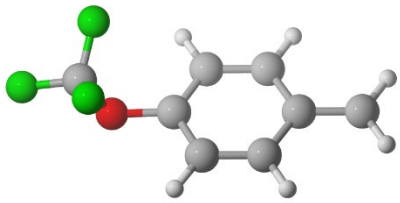
Benzylic Radical of Compound 8



14

C	-1.13130	-1.20788	-0.00002
C	0.25228	-1.21307	-0.00003
C	0.98756	-0.00000	-0.00001
C	0.25228	1.21307	0.00002
C	-1.13129	1.20788	0.00003
C	-1.83420	0.00000	0.00000
H	-1.67292	-2.14858	-0.00004
H	0.79550	-2.15390	-0.00005
H	0.79551	2.15389	0.00004
H	-1.67292	2.14858	0.00005
H	-2.91895	0.00000	0.00001
C	2.39843	-0.00000	-0.00001
H	2.95564	0.92840	-0.00057
H	2.95565	-0.92839	0.00065

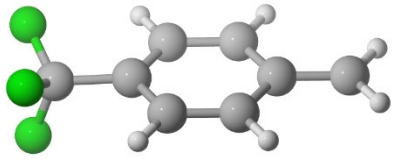
Benzylic Radical of Compound 9



18

C	0.72274	-1.21624	-0.38799
C	2.06848	-1.21457	-0.07212
C	2.78337	-0.00004	0.09623
C	2.06860	1.21458	-0.07203
C	0.72287	1.21639	-0.38790
C	0.06294	0.00011	-0.54390
H	0.16933	-2.13924	-0.51926
H	2.59530	-2.15584	0.05101
H	2.59552	2.15578	0.05117
H	0.16953	2.13945	-0.51910
C	4.15623	-0.00011	0.41800
H	4.69823	0.92835	0.54456
H	4.69805	-0.92863	0.54493
O	-1.28374	0.00022	-0.91615
C	-2.16992	-0.00001	0.10434
F	-3.38817	0.00021	-0.41193
F	-2.03642	-1.07566	0.88611
F	-2.03628	1.07519	0.88672

Benzylic Radical of Compound 10

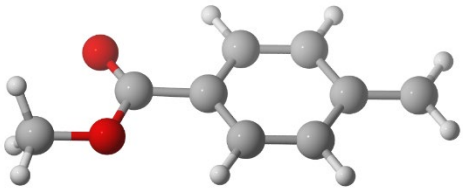


17

C	-0.35405	-1.21249	-0.02784
C	-1.73513	-1.21476	-0.00771
C	-2.46884	0.00000	0.00449
C	-1.73511	1.21475	-0.00771
C	-0.35403	1.21247	-0.02784
C	0.34081	-0.00002	-0.03776
H	0.19807	-2.14607	-0.04453
H	-2.27708	-2.15558	-0.00442
H	-2.27705	2.15559	-0.00442
H	0.19810	2.14604	-0.04453
C	-3.87823	0.00001	0.02372
H	-4.43496	0.92848	0.03158
H	-4.43498	-0.92844	0.03157
C	1.83904	-0.00000	0.00107
F	2.30638	0.00027	1.26094
F	2.35244	-1.08311	-0.60178

F	2.35242	1.08286	-0.60224

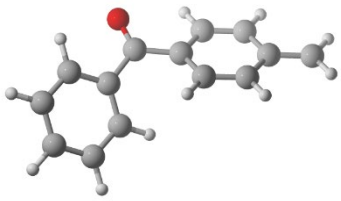
Benzylic Radical of Compound 11



20

C	-0.38437	-1.12489	-0.00002
C	-1.75656	-1.26754	-0.00001
C	-2.61277	-0.13287	0.00000
C	-2.00684	1.15347	0.00001
C	-0.63538	1.29036	0.00000
C	0.18846	0.15547	-0.00001
H	0.26152	-1.99544	-0.00003
H	-2.20139	-2.25828	-0.00002
H	-2.64434	2.03266	0.00002
H	-0.16466	2.26776	0.00001
C	-4.01066	-0.27767	0.00001
H	-4.66059	0.58845	0.00003
H	-4.46992	-1.25832	0.00001
C	1.65692	0.36649	-0.00001
O	2.19414	1.45054	-0.00002
O	2.34591	-0.79000	0.00001
C	3.76319	-0.63618	0.00002
H	4.17275	-1.64472	0.00036
H	4.08715	-0.08842	-0.88732

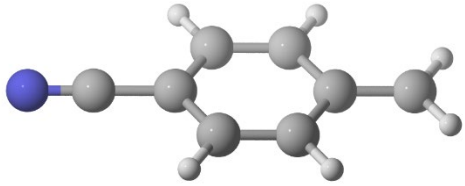
Benzylic Radical of Compound 12



26

C	-1.98353	1.28432	0.46647
C	-3.26170	0.77375	0.43988
C	-3.52152	-0.52219	-0.08744
C	-2.41677	-1.26236	-0.58719
C	-1.13544	-0.75031	-0.54007
C	-0.89665	0.52580	-0.00303
H	-1.78377	2.27983	0.84875
H	-4.09358	1.36065	0.81837
H	-2.59493	-2.24424	-1.01578
H	-0.31059	-1.32785	-0.94474
C	-4.82367	-1.04725	-0.12023
H	-5.01828	-2.03204	-0.52648
H	-5.66357	-0.47837	0.25864
C	0.45149	1.16427	0.01543
O	0.55213	2.37923	0.01822
C	1.68912	0.31610	0.02869
C	2.84609	0.84971	-0.54653
C	1.74376	-0.93053	0.65844
C	4.03409	0.13096	-0.52483
H	2.78942	1.83284	-1.00205
C	2.94004	-1.64147	0.69556
H	0.85818	-1.33268	1.14055
C	4.08161	-1.11681	0.09593
H	4.92619	0.54366	-0.98447
H	2.98103	-2.60330	1.19612
H	5.01139	-1.67631	0.11882

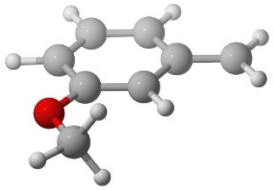
Benzylic Radical of Compound 13



15

C	-0.34599	-1.21762	0.00000
C	1.03210	-1.21695	-0.00000
C	1.76714	0.00000	-0.00001
C	1.03209	1.21695	-0.00001
C	-0.34599	1.21761	-0.00001
C	-1.04857	-0.00001	-0.00000
H	-0.89899	-2.15049	0.00001
H	1.57441	-2.15743	-0.00000
H	1.57440	2.15743	-0.00001
H	-0.89901	2.15048	-0.00001
C	3.17187	0.00001	-0.00001
H	3.72907	0.92834	0.00017
H	3.72908	-0.92832	-0.00000
C	-2.48275	-0.00001	0.00000
N	-3.64120	0.00001	0.00001

Benzylic Radical of Compound 14

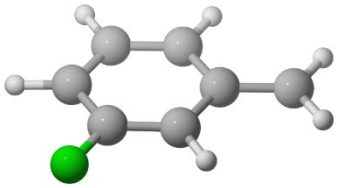


18

C	1.17614	1.75104	-0.00000

C	1.98403	0.62363	0.00002
C	1.40734	-0.66826	0.00002
C	-0.00992	-0.77770	0.00001
C	-0.79965	0.36060	-0.00000
C	-0.20891	1.63531	-0.00002
H	1.62729	2.73821	-0.00001
H	3.06520	0.71947	0.00003
H	-0.45072	-1.76796	0.00001
H	-0.85780	2.50356	-0.00003
C	2.21658	-1.82332	0.00003
H	1.77861	-2.81364	-0.00028
H	3.29629	-1.74418	-0.00010
O	-2.15997	0.35334	-0.00002
C	-2.80227	-0.90126	0.00002
H	-2.54332	-1.48304	-0.89291
H	-2.54337	-1.48296	0.89301
H	-3.87238	-0.69640	-0.00002

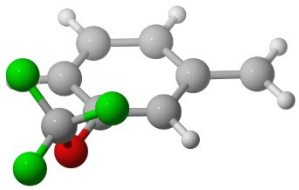
Benzylic Radical of Compound 15



14

C	0.04097	1.77053	0.00000
C	-1.17891	1.11731	0.00003
C	-1.24792	-0.30023	0.00004
C	-0.02899	-1.02378	-0.00000
C	1.16616	-0.33863	-0.00003
C	1.23808	1.05109	-0.00001
H	0.07185	2.85523	0.00001
H	-2.10379	1.68586	0.00001
H	-0.02301	-2.10854	-0.00002
H	2.20683	1.53601	-0.00002
C	-2.48977	-0.96947	0.00002
H	-2.54182	-2.05087	0.00011
H	-3.41949	-0.41469	-0.00040
F	2.31241	-1.03821	0.00000

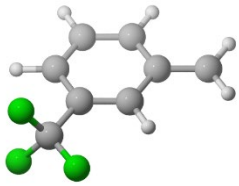
Benzylic Radical of Compound 16



18

C	-1.91347	1.78159	-0.11261
C	-2.78302	0.71217	-0.23618
C	-2.35094	-0.61731	0.00669
C	-0.99800	-0.81373	0.38030
C	-0.15772	0.27316	0.49603
C	-0.58203	1.57723	0.25539
H	-2.26646	2.78959	-0.30263
H	-3.81684	0.88102	-0.52157
H	-0.61522	-1.80882	0.58022
H	0.12022	2.39542	0.36090
C	-3.23535	-1.70956	-0.11814
H	-2.90042	-2.72191	0.06786
H	-4.26821	-1.55739	-0.40404
O	1.16037	0.06562	0.91915
C	2.05762	-0.16681	-0.06328
F	3.24651	-0.31956	0.49734
F	2.12234	0.84357	-0.93600
F	1.76909	-1.27103	-0.75946

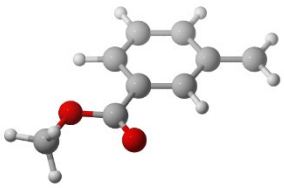
Benzylic Radical of Compound 17



17

C	1.46525	1.83675	0.00079
C	2.43566	0.84833	0.00413
C	2.08503	-0.52502	-0.00054
C	0.70442	-0.85123	-0.00766
C	-0.24961	0.14666	-0.01067
C	0.11343	1.49796	-0.00704
H	1.75870	2.88114	0.00303
H	3.48755	1.11855	0.00958
H	0.39910	-1.89226	-0.01268
H	-0.65422	2.26436	-0.01295
C	3.06938	-1.53501	0.00122
H	2.79311	-2.58165	-0.00266
H	4.12264	-1.28495	0.00674
C	-1.71310	-0.19113	-0.00028
F	-2.30105	0.21724	1.13533
F	-1.93409	-1.50750	-0.11421
F	-2.36149	0.41592	-1.00676

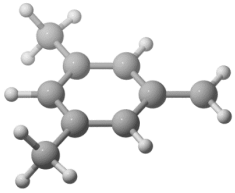
Benzylic Radical of Compound 18



20

C	-1.53864	1.85387	-0.00003
C	-2.56055	0.92008	-0.00000
C	-2.28466	-0.47189	0.00002
C	-0.92616	-0.86747	-0.00001
C	0.08990	0.07610	-0.00005
C	-0.20444	1.44518	-0.00005
H	-1.77674	2.91252	-0.00005
H	-3.59652	1.24707	0.00001
H	-0.65968	-1.92001	-0.00001
H	0.60203	2.16831	-0.00008
C	-3.32331	-1.42796	0.00009
H	-3.10220	-2.48755	0.00010
H	-4.36186	-1.12206	0.00014
C	1.49361	-0.42913	-0.00007
O	1.80017	-1.59787	-0.00013
O	2.39848	0.56444	0.00007
C	3.75720	0.13041	0.00011
H	4.35982	1.03672	0.00027
H	3.96408	-0.47148	0.88727
H	3.96418	-0.47123	-0.88720

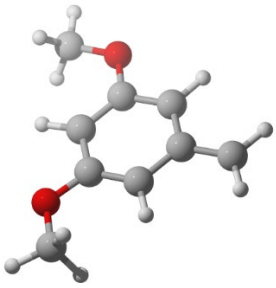
Benzylic Radical of Compound 19



20

C	1.22240	-0.63911	0.00001
C	1.21350	0.74697	-0.00000
C	0.00001	1.47941	-0.00001
C	-1.21350	0.74698	-0.00000
C	-1.22240	-0.63910	0.00000
C	-0.00000	-1.32349	0.00001
H	2.15435	1.29234	0.00000
H	-2.15434	1.29235	-0.00000
H	-0.00001	-2.41199	0.00001
C	0.00001	2.88930	-0.00001
H	-0.92847	3.44651	0.00036
H	0.92848	3.44652	-0.00029
C	-2.51785	-1.41097	-0.00001
C	2.51785	-1.41097	0.00001
H	-2.58991	-2.05517	0.88140
H	-3.37925	-0.73983	0.00014
H	-2.59004	-2.05492	-0.88159
H	2.58997	-2.05506	-0.88148
H	2.58997	-2.05505	0.88150
H	3.37925	-0.73983	0.00001

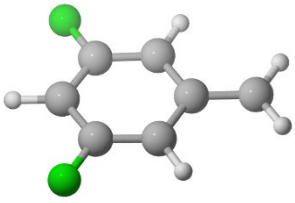
Benzylic Radical of Compound 20



22

C	-0.448278	-0.928077	-0.000222
C	-1.362445	0.121009	-0.000343
C	-0.923992	1.445395	-0.000192
C	0.451710	1.738050	0.000075
C	1.386934	0.666017	0.000266
C	0.928814	-0.638102	0.000117
C	0.901888	3.078156	0.000236
O	1.731993	-1.736250	0.000269
O	-2.710863	-0.052611	-0.000771
C	-3.195691	-1.376769	0.000669
C	3.124893	-1.518922	-0.000305
H	-0.744138	-1.968693	-0.000497
H	-1.663006	2.238963	-0.000301
H	2.445022	0.896711	0.000577
H	1.959181	3.311141	0.000486
H	0.197423	3.899976	0.000120
H	-4.282703	-1.302666	0.001393
H	-2.868937	-1.923214	-0.892055
H	-2.867595	-1.921671	0.893847
H	3.587552	-2.505395	-0.000778
H	3.442165	-0.967142	-0.893229
H	3.442999	-0.967649	0.892639

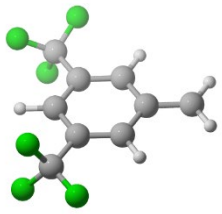
Benzylic Radical of Compound 21



14

C	0.67396	1.18440	0.00000
C	-0.70439	1.21779	-0.00000
C	-1.42891	-0.00001	-0.00001
C	-0.70437	-1.21780	-0.00000
C	0.67396	-1.18439	0.00000
C	1.40354	0.00001	0.00000
H	-1.21611	2.17324	-0.00000
H	-1.21609	-2.17325	-0.00000
H	2.48549	0.00001	0.00000
C	-2.84127	-0.00002	-0.00001
H	-3.39635	-0.92906	0.00007
H	-3.39636	0.92902	-0.00001
F	1.35025	-2.34089	-0.00000
F	1.35022	2.34091	0.00000

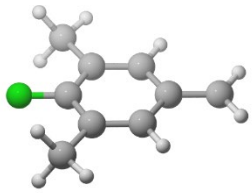
Benzylic Radical of Compound 22



20

C	1.19478	0.06682	-0.03282
C	1.21486	1.45050	-0.02839
C	0.00754	2.19059	-0.00096
C	-1.20990	1.46305	0.01972
C	-1.20435	0.08197	0.01237
C	-0.00765	-0.63784	-0.01350
H	2.16436	1.97546	-0.05181
H	-2.15330	1.99816	0.04143
H	-0.01363	-1.72242	-0.02344
C	0.01452	3.60053	0.00325
H	-0.91129	4.16068	0.02416
H	0.94592	4.15150	-0.01376
C	-2.49410	-0.69110	0.00128
C	2.48758	-0.70126	-0.00095
F	-3.55812	0.09913	0.19120
F	-2.50559	-1.62803	0.95994
F	3.50239	0.01114	-0.50845
F	2.39713	-1.84075	-0.70019
F	2.82627	-1.03599	1.25245
F	-2.66783	-1.32805	-1.16567

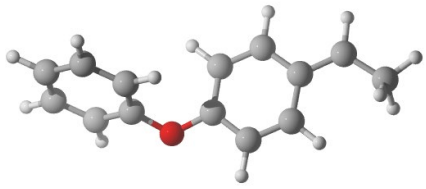
Benzylic Radical of Compound 23



20

C	-0.33926	1.23227	-0.00005
C	1.04600	1.21420	-0.00005
C	1.78003	-0.00001	-0.00003
C	1.04600	-1.21420	-0.00005
C	-0.33926	-1.23227	-0.00005
C	-0.99295	-0.00000	-0.00005
H	1.58818	2.15636	-0.00009
H	1.58817	-2.15637	-0.00007
C	3.18914	0.00001	0.00016
H	3.74644	-0.92822	0.00002
H	3.74642	0.92824	-0.00002
C	-1.14739	-2.50072	-0.00003
C	-1.14739	2.50071	-0.00003
H	-0.49335	-3.37423	0.00047
H	-1.79538	-2.55136	0.87926
H	-1.79474	-2.55182	-0.87974
H	-1.79494	2.55169	-0.87961
H	-1.79520	2.55146	0.87940
H	-0.49337	3.37424	0.00023
F	-2.34130	0.00001	0.00014

Benzylic Radical of Compound 24

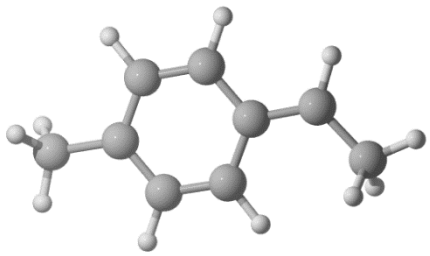


28

C	-0.29518000	0.70853000	-0.10748500
C	-1.32648500	1.35505700	0.57302000
C	-2.61524800	0.85496300	0.51208400
C	-2.91661600	-0.31609900	-0.22887000
C	-1.84147500	-0.94327900	-0.91110200
C	-0.55562300	-0.44354800	-0.85921200
H	-1.09182400	2.24904900	1.14054300
H	-3.40817100	1.36779500	1.04700500
H	-2.04462500	-1.83649700	-1.49530600

H	0.25366300	-0.93147400	-1.39240800
C	-4.22541900	-0.85069800	-0.29915800
C	-5.40211300	-0.24354200	0.38949700
H	-4.37238500	-1.74932900	-0.88960100
H	-5.58346200	0.78530600	0.05126200
H	-6.31031900	-0.81847100	0.20404500
H	-5.25461200	-0.19365700	1.47646500
O	0.94739300	1.29447700	-0.06707800
C	2.06803500	0.50338700	0.03048400
C	2.09653300	-0.66319500	0.79360200
C	3.21249600	0.95905300	-0.61799100
C	3.28640800	-1.37755300	0.89309700
H	1.19779600	-0.99930300	1.29953800
C	4.39629500	0.23831800	-0.50277800
H	3.15248300	1.87287100	-1.19859200
C	4.43846000	-0.93378100	0.24845900
H	3.31138400	-2.28556400	1.48702900
H	5.28853300	0.59391000	-1.00789400
H	5.36198600	-1.49612200	0.33265700

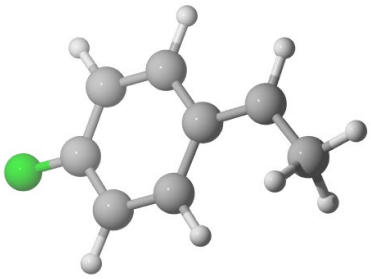
Benzylic Radical of Compound 25



20

C	1.83266700	-0.11597500	0.00001100
C	0.93835100	-1.19045700	0.00001500
C	-0.43350300	-0.99125500	0.00000900
C	-0.98081100	0.31425500	0.00000200
C	-0.06405000	1.39720300	0.00000300
C	1.29926800	1.18303700	0.00001000
H	1.33047300	-2.20435100	0.00002300
H	-1.09808900	-1.84977900	0.00001100
H	-0.45464400	2.41147100	0.00000300
H	1.97677900	2.03360400	0.00001500
C	-2.37795100	0.55131500	-0.00000400
C	-3.39911800	-0.53697100	-0.00001000
H	-2.71466400	1.58310400	-0.00001400
H	-3.29875400	-1.18626100	0.87979200
H	-4.41179300	-0.13149400	0.00000700
H	-3.29877400	-1.18623400	-0.87983600
C	3.32261600	-0.33116100	-0.00002000
H	3.78766300	0.12240800	-0.88121300
H	3.78775600	0.12275000	0.88094600
H	3.56922800	-1.39516900	0.00016900

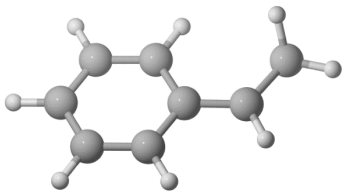
Benzylic Radical of Compound 26



17

C	-1.83446000	-0.13138500	-0.00001600
C	-0.97283400	-1.22114000	-0.00002900
C	0.39389400	-0.99629800	-0.00000800
C	0.92490600	0.31859700	0.00002400
C	0.00077000	1.39485900	0.00004700
C	-1.36441400	1.17834300	0.00002400
H	-1.38660200	-2.22321200	-0.00004800
H	1.06953600	-1.84545700	0.00000700
H	0.38251900	2.41180200	0.00007800
H	-2.07464500	1.99729600	0.00003600
C	2.32070800	0.56823600	0.00003700
C	3.35085500	-0.51121500	-0.00003700
H	2.64753900	1.60293500	0.00021000
H	4.35958700	-0.09636800	-0.00056600
H	3.25748200	-1.16080300	0.88037100
H	3.25676400	-1.16135600	-0.87994800
F	-3.15874800	-0.34720200	-0.00004400

Benzylic Radical of Compound 27

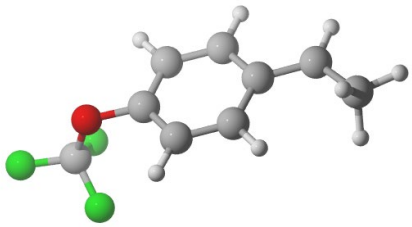


17

C	-2.28831400	0.35863200	0.00001200
C	-1.32059200	1.36453700	-0.00003300
C	0.02796400	1.04600400	-0.00004700
C	0.45677300	-0.30459900	0.00002900
C	-0.54418400	-1.30846400	0.00003800
C	-1.88794000	-0.98055300	0.00004100
H	-3.34257500	0.61401300	-0.00003200
H	-1.62497900	2.40664300	-0.00005200
H	0.76770000	1.84055600	-0.00012500
H	-0.23719900	-2.35093800	0.00007200

H	-2.63424000	-1.76887800	0.00008200
C	1.83062700	-0.65862900	-0.00009100
C	2.94027000	0.33904200	0.00009900
H	2.07885600	-1.71518100	-0.00067800
H	3.91481200	-0.15085100	0.00055400
H	2.89535600	0.99423800	-0.87982800
H	2.89464700	0.99457600	0.87971600

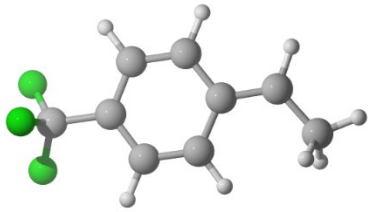
Benzylic Radical of Compound 28



21

C	0.38874100	0.12837100	-0.57599400
C	-0.37598100	-1.03253600	-0.53746100
C	-1.72992000	-0.94134000	-0.26340600
C	-2.34581300	0.31269500	-0.02049200
C	-1.52501300	1.46869500	-0.07002900
C	-0.17338500	1.38131200	-0.34330900
H	0.10277700	-1.98726400	-0.72463500
H	-2.32802400	-1.84602900	-0.23430700
H	-1.97603800	2.43964900	0.11226800
H	0.45861300	2.26139600	-0.38280700
C	-3.73046900	0.42759600	0.26210300
C	-4.65791300	-0.73879000	0.33169300
H	-4.12747600	1.42240800	0.43591900
H	-4.68949100	-1.28711200	-0.61893600
H	-4.34433700	-1.45892800	1.09867800
H	-5.67474700	-0.42313000	0.56748300
O	1.74501300	0.04165700	-0.90483500
C	2.58635700	-0.11994800	0.13950300
F	2.33746800	-1.24488300	0.81764200
F	3.82093700	-0.17604500	-0.33402400
F	2.50815000	0.89086300	1.01075600

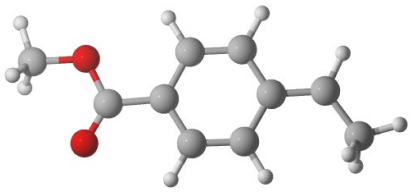
Benzylic Radical of Compound 29



20

C	0.78582600	0.04099800	0.03859900
C	0.21486200	1.31707600	0.02567400
C	-1.15863700	1.45550000	0.00854100
C	-2.01239100	0.32258600	0.00251400
C	-1.40480900	-0.95843900	0.01758700
C	-0.02833300	-1.09286100	0.03459200
H	0.85675500	2.19158300	0.03758100
H	-1.60359500	2.44627400	0.00304900
H	-2.02821600	-1.84646400	0.01940900
H	0.42653300	-2.07757700	0.05319200
C	-3.41991300	0.48600500	-0.01350200
C	-4.38416200	-0.65209300	-0.01897600
H	-3.80793800	1.49946900	-0.02223200
H	-5.41534700	-0.29810300	-0.03690000
H	-4.23652500	-1.30088000	-0.89194500
H	-4.26259600	-1.28718200	0.86804400
C	2.27583600	-0.10703400	-0.00295500
F	2.89411700	0.90689000	0.62256900
F	2.68037500	-1.24820300	0.57576600
F	2.74342600	-0.12508100	-1.26307400

Benzylic Radical of Compound 30

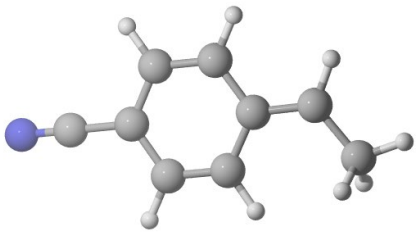


23

C	-0.65528200	0.10628900	-0.00000400
C	0.23670100	1.18671500	-0.00000600
C	1.59942400	0.96956200	-0.00000500

C	2.12628300	-0.34978400	0.00000500
C	1.20175200	-1.42833000	-0.00000400
C	-0.15940800	-1.20603200	-0.00000500
H	-0.17339400	2.19121700	-0.00001300
H	2.27852100	1.81602400	-0.00000900
H	1.58626000	-2.44437000	-0.00001000
H	-0.85521700	-2.03727600	-0.00000600
C	3.51660000	-0.60269300	0.00001300
C	4.55537300	0.46837800	0.00000300
H	3.83837000	-1.63940000	-0.00001400
H	5.56070400	0.04600800	0.00011700
H	4.46346200	1.11767000	-0.88001400
H	4.46332200	1.11781800	0.87989500
C	-2.10699200	0.40724400	0.00000000
O	-2.57798100	1.52198800	0.00000400
O	-2.86665400	-0.70492900	-0.00000100
C	-4.27118900	-0.46289700	0.00000400
H	-4.56062900	0.10447200	-0.88700300
H	-4.74326100	-1.44379000	-0.00000800
H	-4.56062600	0.10444700	0.88702900

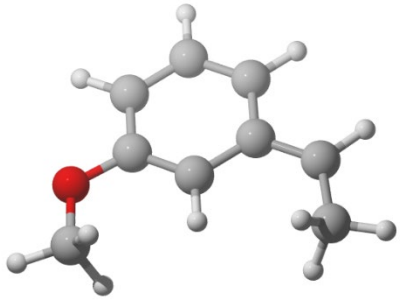
Benzylic Radical of Compound 31



18

C	1.53845200	-0.02833800	-0.00000600
C	0.69389700	-1.15038400	-0.00000700
C	-0.67614000	-0.98673700	-0.00000600
C	-1.25976500	0.30825700	-0.00001000
C	-0.38277400	1.42604800	-0.00000600
C	0.98541200	1.26434500	-0.00000800
H	1.13039000	-2.14329900	-0.00000500
H	-1.31697400	-1.86211800	0.00000400
H	-0.80866100	2.42502800	-0.00000200
H	1.64465000	2.12546400	-0.00000400
C	-2.65930500	0.49884300	0.00001000
C	-3.64881600	-0.61754600	0.00000400
H	-3.02638000	1.52024900	0.00006000
H	-4.67166300	-0.24022500	-0.00002400
H	-3.52802800	-1.26164100	-0.88028600
H	-3.52807100	-1.26162300	0.88031000
C	2.96216400	-0.20106900	0.00000500
N	4.11228400	-0.34033600	0.00001300

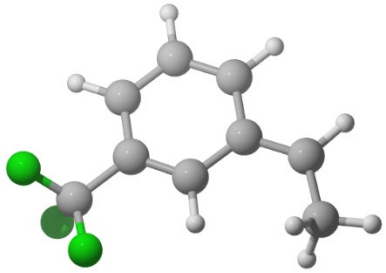
Benzylic Radical of Compound 32



21

C	1.30511100	1.57700700	0.00007200
C	1.21235600	0.17664500	0.00049600
C	-0.02595800	-0.44852200	0.00055700
C	-1.21728200	0.32431600	0.00012700
C	-1.10440700	1.73367600	-0.00033000
C	0.14278500	2.33954200	-0.00030800
H	2.29007200	2.02938300	-0.00001500
H	-0.10052700	-1.52896300	0.00118700
H	-2.00851300	2.33479700	-0.00074400
H	0.21664900	3.42246400	-0.00062000
C	-2.49521200	-0.28997800	-0.00017000
C	-2.70396500	-1.76731100	0.00011800
H	-3.36427000	0.35976300	-0.00063700
H	-3.76527700	-2.01892400	-0.00110700
H	-2.24703800	-2.24042800	-0.87930300
H	-2.24931400	-2.23980100	0.88108200
O	2.40300900	-0.48273100	0.00092800
C	2.36638600	-1.89126500	-0.00101200
H	1.85990400	-2.27737300	-0.89398700
H	3.40399900	-2.22379300	-0.00226400
H	1.86135100	-2.27993400	0.89168700

Benzylic Radical of Compound 33

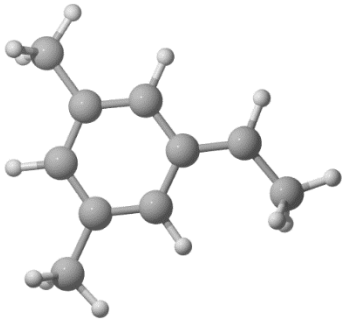


20

C	0.63172800	1.67800300	-0.01702200
C	0.60133100	0.28127100	-0.02327800
C	-0.59441800	-0.41377700	-0.01484400

C	-1.82785000	0.28328900	0.00091400
C	-1.77912900	1.69924300	0.00935500
C	-0.57343100	2.37936500	0.00021600
H	1.58251100	2.19967000	-0.03095800
H	-0.58038300	-1.49792700	-0.02482500
H	-2.71416700	2.25224900	0.02133900
H	-0.56568500	3.46425300	0.00379900
C	-3.07140000	-0.39825400	0.00625500
C	-3.19728000	-1.88455900	-0.00368600
H	-3.97402700	0.20390900	0.01866400
H	-4.24294600	-2.19369800	0.00157800
H	-2.72192500	-2.32383900	-0.89030900
H	-2.70937800	-2.33669900	0.86958200
C	1.90863400	-0.45825500	-0.00052800
F	2.50829100	-0.35938300	1.19678700
F	1.75984400	-1.76443200	-0.26218600
F	2.76929700	0.03871900	-0.90273100

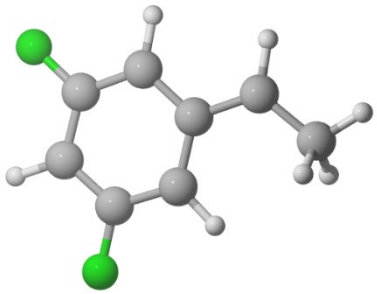
Benzylic Radical of Compound 34



23

C	-1.68510100	0.48992800	0.00063600
C	-0.60727600	1.38236000	-0.00052600
C	0.68610200	0.87799500	-0.00084800
C	0.93368500	-0.51604100	0.00039300
C	-0.18616900	-1.38329600	0.00180600
C	-1.48370400	-0.89643900	0.00150300
H	-2.70096100	0.88090900	0.00112700
H	1.52429300	1.56953100	-0.00156800
H	-0.01487500	-2.45754300	0.00311200
C	2.24924800	-1.04506000	0.00052700
C	3.47998700	-0.20099600	-0.00092800
H	2.35798000	-2.12496200	0.00172000
H	4.38219100	-0.81414600	-0.00117200
H	3.52005700	0.45421200	-0.88106600
H	3.52134100	0.45538000	0.87828900
C	-0.86148300	2.86899500	0.00026400
H	0.07435300	3.43172200	-0.01213500
H	-1.44772800	3.16686200	-0.87421300
H	-1.42559500	3.16944000	0.88840100
C	-2.66740700	-1.83072300	-0.00166800
H	-3.32038300	-1.63955000	0.85511200
H	-3.26900200	-1.69775000	-0.90603000
H	-2.34896900	-2.87444400	0.04146100

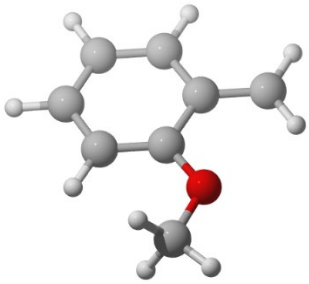
Benzylic Radical of Compound 35



17

C	-1.77329500	0.44571000	-0.00002600
C	-1.46225500	-0.91015000	-0.00003500
C	-0.16774500	-1.38368900	0.00001900
C	0.91143700	-0.46619100	0.00004900
C	0.61715400	0.91893600	0.00004400
C	-0.70034500	1.32937700	0.00001100
H	-2.79741400	0.79442200	-0.00005800
H	0.00874700	-2.45331300	0.00003400
H	1.40066200	1.66699100	0.00005000
C	2.24948400	-0.94034400	0.00007500
C	3.43975200	-0.04225300	-0.00006500
H	2.40124500	-2.01444600	-0.00002300
H	4.36808600	-0.61419400	-0.00016100
H	3.44876600	0.61363700	-0.88024900
H	3.44893300	0.61366800	0.88009200
F	-0.96628100	2.64318000	0.00000000
F	-2.47418000	-1.78930500	-0.00001300

Benzylic Radical of Compound 36

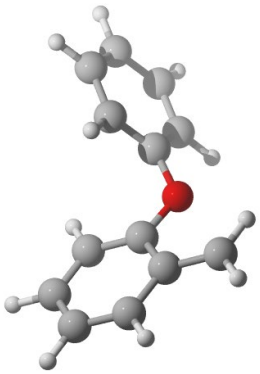


18

C	0.07147100	-1.35834900	0.00029100
C	0.46208200	-0.02708900	0.00024900
C	-0.50900500	1.02427000	0.00005000
C	-1.87300400	0.64118600	-0.00020300

C	-2.25845100	-0.68798600	-0.00019100
C	-1.28781900	-1.68916600	0.00007700
H	0.81051400	-2.15019100	0.00052800
H	-2.62142100	1.42846400	-0.00043100
H	-3.31125100	-0.94896400	-0.00039200
H	-1.57880700	-2.73412200	0.00011800
C	-0.11618500	2.37164100	0.00002000
H	-0.86439900	3.15423200	-0.00014700
H	0.92742700	2.65013600	0.00008100
O	1.75464100	0.38712600	0.00048400
C	2.76031400	-0.60123900	-0.00051100
H	3.71074800	-0.06877100	-0.00109200
H	2.69751600	-1.23392400	0.89268200
H	2.69612300	-1.23348100	-0.89391100

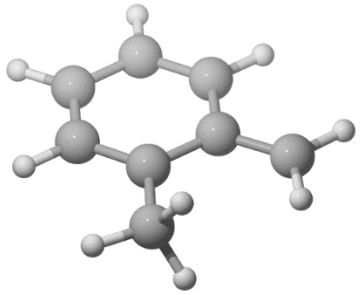
Benzylic Radical of Compound 37



25

C	1.06837300	-1.13666500	-0.58970500
C	1.04981600	0.20330400	-0.23409100
C	2.22472800	0.87669100	0.20392800
C	3.41543400	0.10643600	0.26232100
C	3.43341600	-1.23154800	-0.08243400
C	2.25898500	-1.85850300	-0.51016300
H	0.15336900	-1.61095700	-0.92818700
H	4.32501400	0.59919200	0.59333300
H	4.35891300	-1.79425200	-0.02301400
H	2.26796000	-2.90622600	-0.79024000
C	2.19723400	2.23566300	0.56345300
H	1.28050500	2.80547500	0.51919000
H	3.10308800	2.72811700	0.89323900
O	-0.07750500	0.97920000	-0.34466500
C	-1.31644200	0.42326100	-0.11678500
C	-1.56019100	-0.40862600	0.97515900
C	-2.34264600	0.78752600	-0.98180400
C	-2.85008200	-0.88239500	1.18884200
H	-0.74540200	-0.67503000	1.64012000
C	-3.63023600	0.31244500	-0.75078600
H	-2.11414500	1.43971300	-1.81737900
C	-3.88835700	-0.52574600	0.33049300
H	-3.04470900	-1.52954700	2.03797100
H	-4.43273300	0.59664500	-1.42365400
H	-4.89199900	-0.89778400	0.50536500

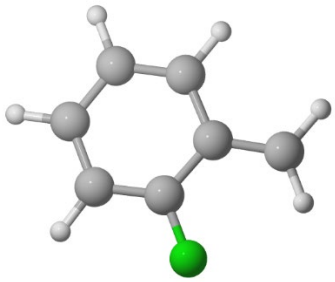
Benzylic Radical of Compound 38



17

C	0.53280700	-1.42483100	0.00004600
C	-0.59866300	-0.62163200	-0.00005600
C	-0.44214000	0.79906400	-0.00008200
C	0.87536900	1.32805500	-0.00012300
C	1.98509500	0.50426800	-0.00002200
C	1.81975400	-0.88231700	0.00009700
H	0.40813700	-2.50453600	0.00003800
H	0.99722700	2.40777200	-0.00026700
H	2.98101800	0.93540400	-0.00004200
H	2.68428000	-1.53767800	0.00027100
C	-1.54937100	1.66958400	0.00019300
H	-2.56799800	1.30633700	0.00010300
H	-1.40040400	2.74233100	0.00018200
C	-1.97268400	-1.23421600	-0.00007000
H	-2.54538600	-0.92702000	0.88161600
H	-2.54571000	-0.92624300	-0.88126000
H	-1.91217300	-2.32422100	-0.00054100

Benzylic Radical of Compound 39

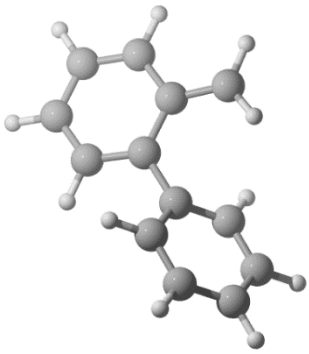


14

C	0.72253200	-1.36125000	0.00001100
C	-0.48966400	-0.70670700	0.00003500
C	-0.61341700	0.70292100	0.00008100
C	0.60418300	1.43105100	-0.00000200
C	1.83025100	0.78982000	-0.00001900
C	1.89759800	-0.60672500	0.00000100
H	0.73458000	-2.44517000	-0.00000800

H	0.55222800	2.51576100	-0.00006900
H	2.74376700	1.37469100	-0.00003300
H	2.85856800	-1.10887800	-0.00008100
C	-1.87822400	1.31950300	-0.00002500
H	-1.96080200	2.39842300	0.00003900
H	-2.78306600	0.72883500	-0.00012600
F	-1.62053600	-1.43059300	-0.00002400

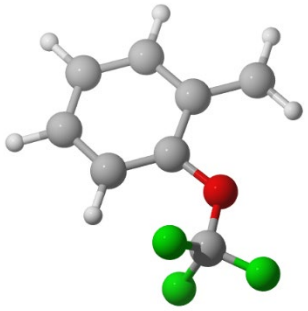
Benzylic Radical of Compound 40



24

C	-1.28586900	-1.40241200	-0.32488200
C	-0.66730900	-0.19024400	-0.02770200
C	-1.47521900	0.95782500	0.25129900
C	-2.88557100	0.80934700	0.16137000
C	-3.47247500	-0.40108500	-0.14972500
C	-2.67257800	-1.52240200	-0.38749300
H	-0.65945000	-2.26354000	-0.54006700
H	-3.50573900	1.67796900	0.36441700
H	-4.55340100	-0.48041500	-0.20519800
H	-3.12429300	-2.47754000	-0.63282500
C	-0.93648400	2.19702100	0.65498700
H	0.12097400	2.33350800	0.83130800
H	-1.59742200	3.03287900	0.84909300
C	0.81637800	-0.12884300	-0.01891700
C	1.50827100	0.83238500	-0.76724300
C	1.55565600	-1.07344700	0.70216600
C	2.89866000	0.85097800	-0.78703300
H	0.94426100	1.55680600	-1.34757600
C	2.94676600	-1.05415900	0.68391700
H	1.02764000	-1.81678500	1.29255900
C	3.62281500	-0.09098200	-0.05982600
H	3.41829100	1.59832700	-1.37826700
H	3.50313700	-1.79010900	1.25566800
H	4.70776000	-0.07499200	-0.07461400

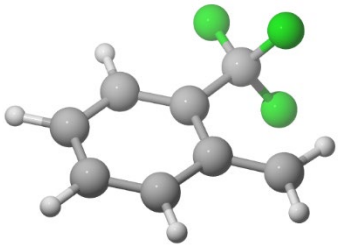
Benzylic Radical of Compound 41



18

C	0.62125700	-1.25935300	0.00977500
C	0.42678800	0.10993500	0.01006000
C	1.50998100	1.03034100	0.00264300
C	2.81301700	0.47211800	-0.00502800
C	3.01779400	-0.89491300	-0.00604600
C	1.92455600	-1.76233900	0.00116900
H	-0.21917200	-1.94079900	0.01640800
H	3.65789300	1.15413100	-0.01054100
H	4.02694400	-1.29219100	-0.01231300
H	2.07558500	-2.83592500	0.00061900
C	1.30054900	2.42184100	0.00281900
H	2.14949400	3.09305000	-0.00281200
H	0.30628700	2.84359600	0.00811600
O	-0.82145300	0.71982600	0.01971300
C	-1.94642200	-0.02485100	-0.00180300
F	-2.97493000	0.80692500	-0.00305400
F	-2.04866900	-0.82364200	1.06491300
F	-2.02423800	-0.79852100	-1.08838300

Benzylic Radical of Compound 42

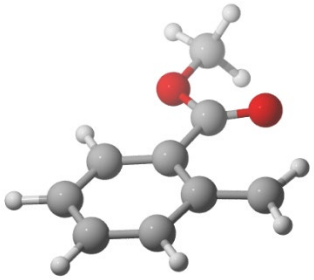


17

C	0.72990300	-1.43425000	-0.00002000
C	0.04723600	-0.22991500	0.00000000
C	0.74392800	1.01360500	-0.00003200
C	2.16085700	0.95156700	0.00001300
C	2.83431200	-0.25609600	0.00002400
C	2.12502900	-1.45878300	-0.00000500

H	0.16706000	-2.36046300	-0.00002400
H	2.71553600	1.88513700	0.00003300
H	3.91944200	-0.26641800	0.00004200
H	2.65008200	-2.40721200	-0.00001000
C	0.09394200	2.26541000	-0.00001300
H	0.68456700	3.17273500	-0.00011000
H	-0.98196700	2.35937000	0.00006000
C	-1.45434400	-0.23269600	-0.00001300
F	-1.95568100	0.39800500	1.07683400
F	-1.95972700	-1.47342100	-0.00003400
F	-1.95569200	0.39806000	-1.07676700

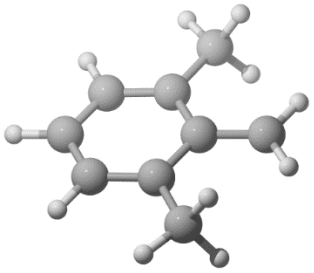
Benzylic Radical of Compound 43



20

C	0.54646500	-1.41387300	0.00014600
C	0.15713500	-0.07342600	0.00003700
C	1.15080800	0.95927500	-0.00015800
C	2.51168900	0.54126800	-0.00012900
C	2.87286900	-0.78888600	0.00001000
C	1.88634400	-1.78165500	0.00015400
H	-0.22242700	-2.17654500	0.00027700
H	3.27790900	1.31103700	-0.00026600
H	3.92286000	-1.06366900	0.00000700
H	2.16111900	-2.83057500	0.00030400
C	0.88554800	2.34274100	-0.00032500
H	1.72497700	3.02824100	-0.00039200
H	-0.11616400	2.73874800	-0.00020100
C	-1.29514500	0.25150500	0.00018600
O	-1.78172300	1.36080600	0.00076300
O	-2.06580700	-0.85559200	-0.00027900
C	-3.46802600	-0.60335200	-0.00034900
H	-3.94554000	-1.58161300	-0.00279900
H	-3.75390600	-0.03236200	-0.88609900
H	-3.75471000	-0.03655700	0.88787000

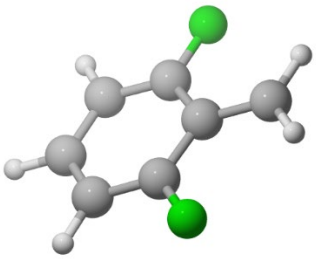
Benzylic Radical of Compound 44



20

C	1.20623800	1.39728200	-0.00000900
C	1.23189200	0.01138100	-0.00000300
C	0.00000000	-0.71863400	0.00001600
C	-1.23189200	0.01138100	0.00000200
C	-1.20623800	1.39728200	-0.00000600
C	0.00000000	2.09820300	-0.00001400
H	2.14627600	1.94217900	0.00000900
H	-2.14627600	1.94217900	0.00001200
H	0.00000000	3.18311700	-0.00006300
C	0.00000000	-2.12433300	-0.00004600
H	-0.92155200	-2.68994700	-0.00017100
H	0.92155200	-2.68994700	0.00002800
C	-2.54706700	-0.72008400	0.00003200
H	-2.64661100	-1.36265900	-0.88137600
H	-2.64664500	-1.36256100	0.88151100
H	-3.38103100	-0.01575100	-0.00002600
C	2.54706700	-0.72008400	0.00002600
H	2.64664100	-1.36256800	0.88150100
H	2.64661400	-1.36265200	-0.88138600
H	3.38103100	-0.01575100	-0.00002300

Benzylic Radical of Compound 45

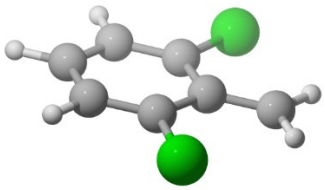


14

C	-1.21275700	1.36730200	-0.00002300
C	-1.19010700	-0.01066600	0.00006200
C	0.00000000	-0.77636200	0.00001500
C	1.19010700	-0.01066600	0.00006100

C	1.21275600	1.36730300	-0.00002400
C	0.00000000	2.06055300	-0.00003600
H	-2.16742300	1.87923700	-0.00002100
H	2.16742300	1.87923800	-0.00002200
H	-0.00000100	3.14427100	-0.00014300
C	0.00000000	-2.18039000	-0.00009900
H	-0.93301200	-2.72452600	-0.00012800
H	0.93301400	-2.72452600	-0.00009300
F	2.34734700	-0.68645200	0.00003700
F	-2.34734700	-0.68645200	0.00003700

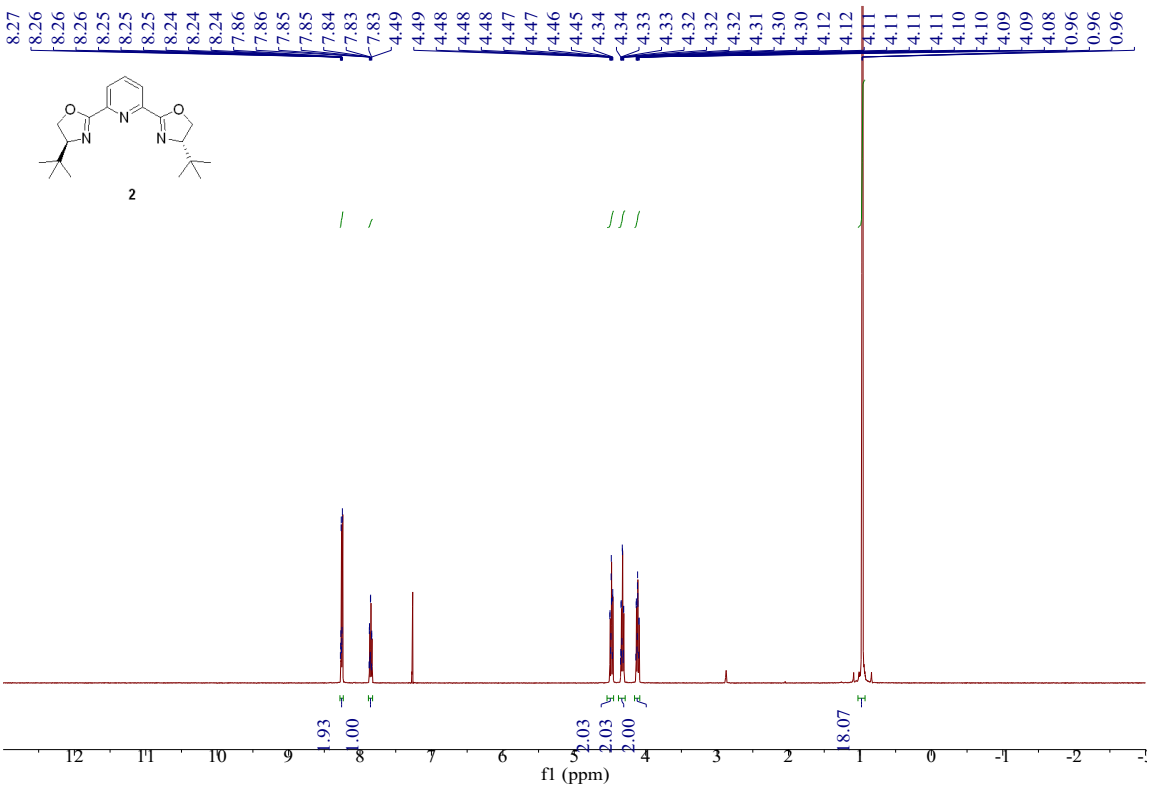
Benzylic Radical of Compound 46

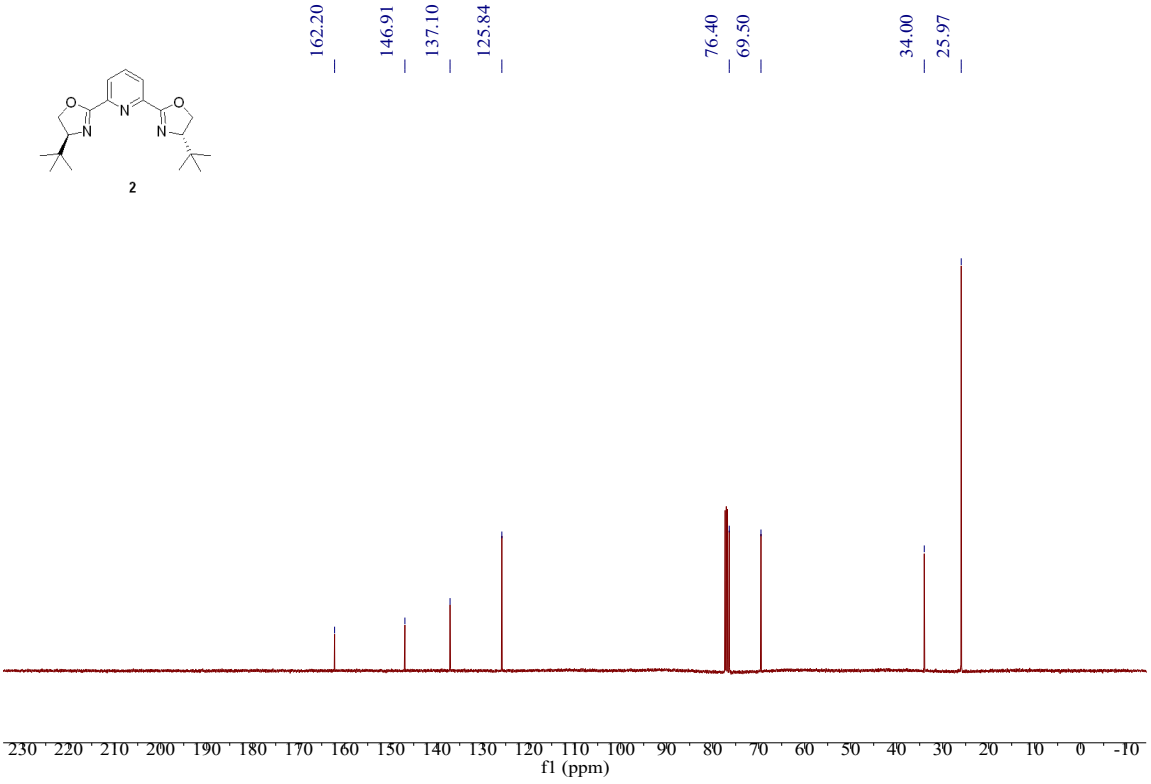


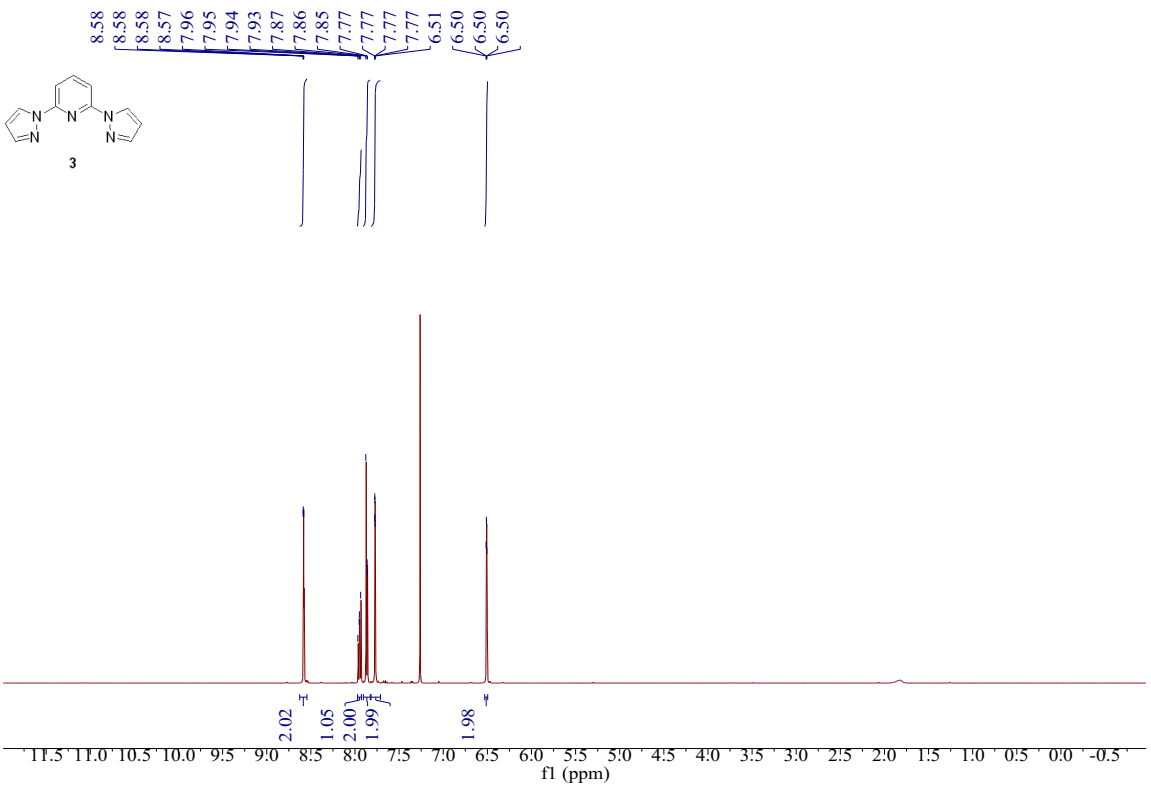
14

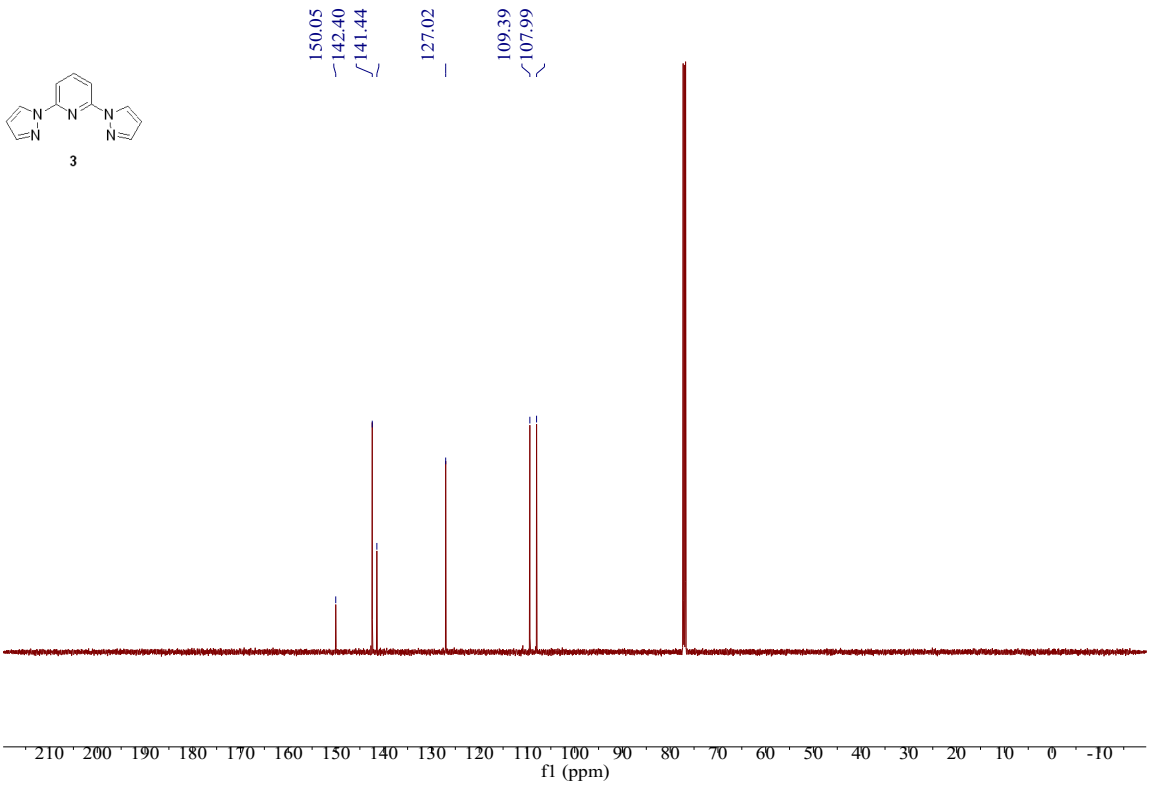
C	-1.20727000	1.56653900	0.00002800
C	-1.20061500	0.18474700	0.00004600
C	0.00000000	-0.58646100	0.00004000
C	1.20061500	0.18474700	0.00004300
C	1.20726900	1.56653900	0.00002500
C	0.00000000	2.26337300	0.00005000
H	-2.15482600	2.09223100	-0.00004900
H	2.15482600	2.09223100	-0.00005200
H	0.00000000	3.34724400	-0.00001700
C	0.00000000	-1.99024400	0.00004100
H	-0.92916200	-2.54002800	0.00024400
H	0.92916200	-2.54002800	0.00046000
Cl	2.73881600	-0.63491400	-0.00006700
Cl	-2.73881600	-0.63491400	-0.00006400

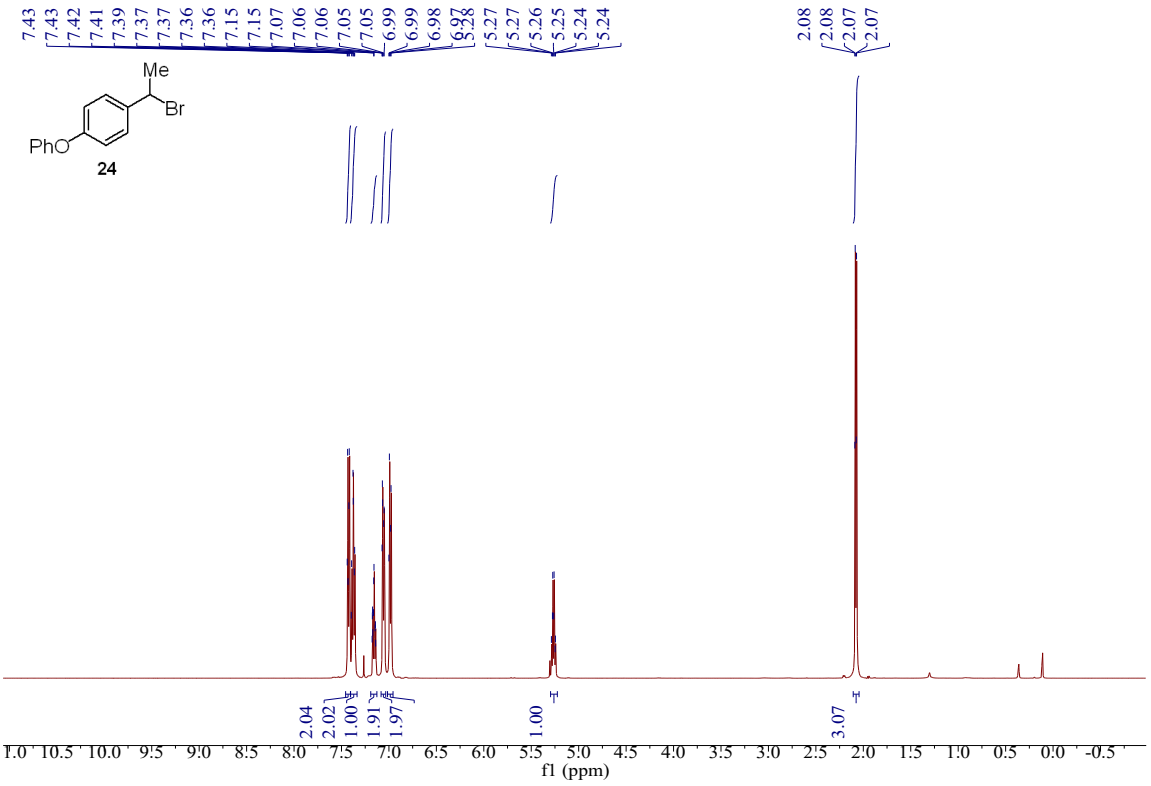
17. NMR Spectra *(Synthesized ligand and benzyl bromides)*

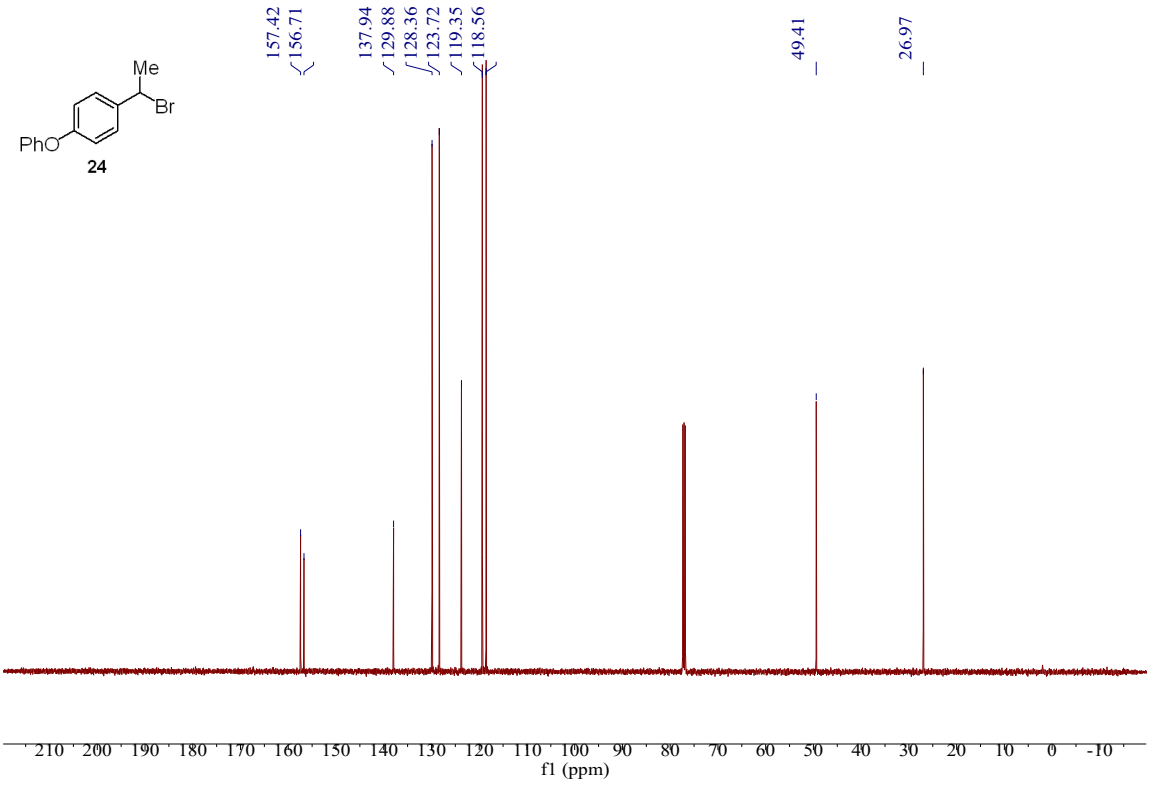


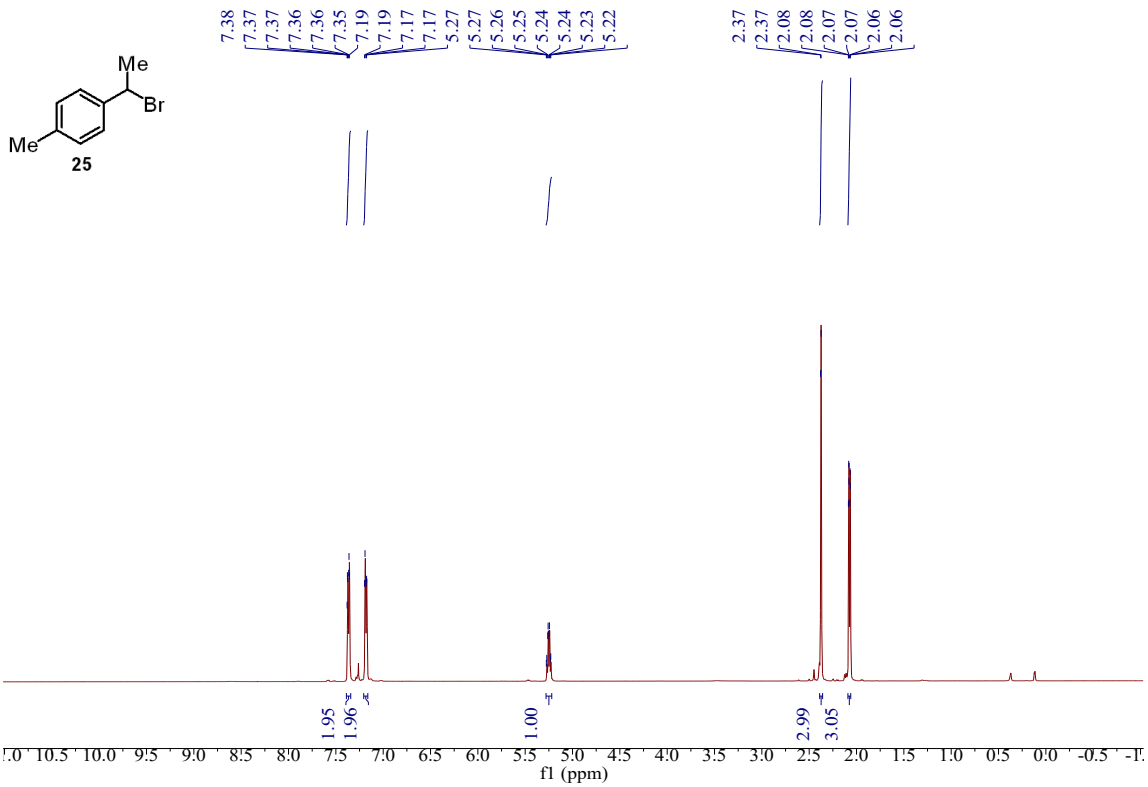


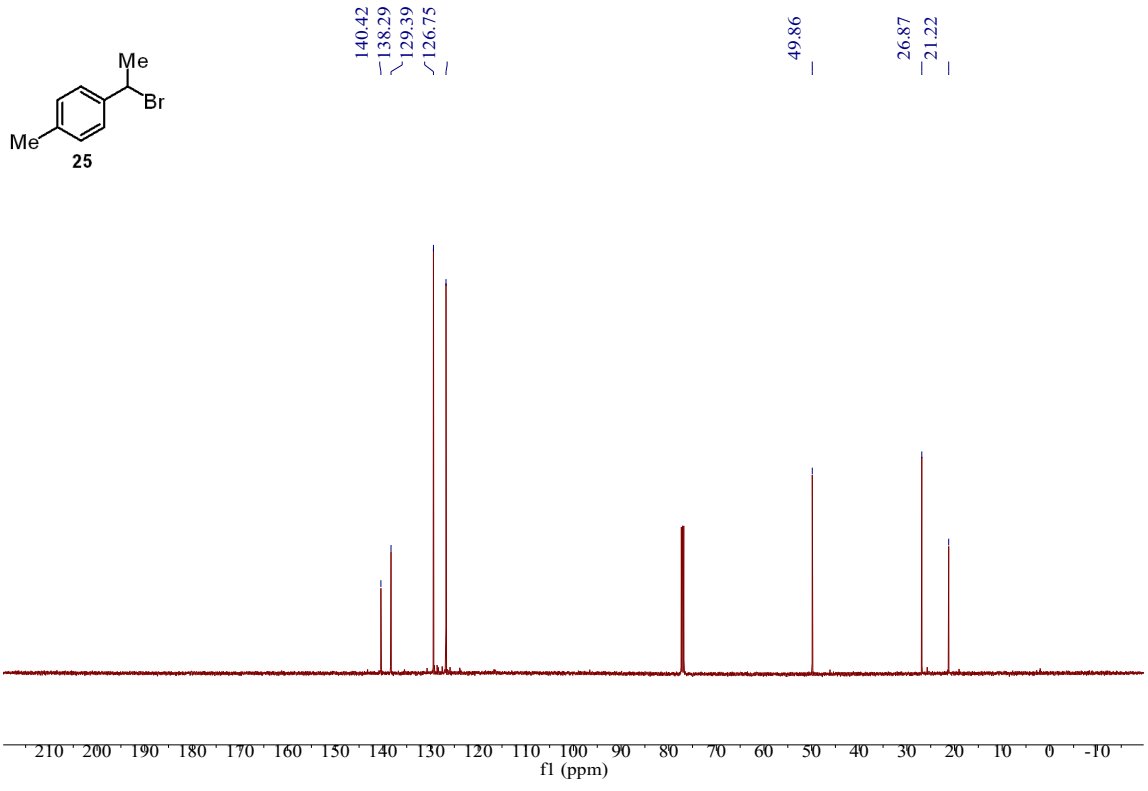

8.58
8.58
8.58
8.57
7.96
7.95
7.94
7.93
7.87
7.86
7.85
7.77
7.77
7.77
7.77
6.51
6.50
6.50
6.50
3
2.02
1.05
2.00
1.99
1.98
f1 (ppm)

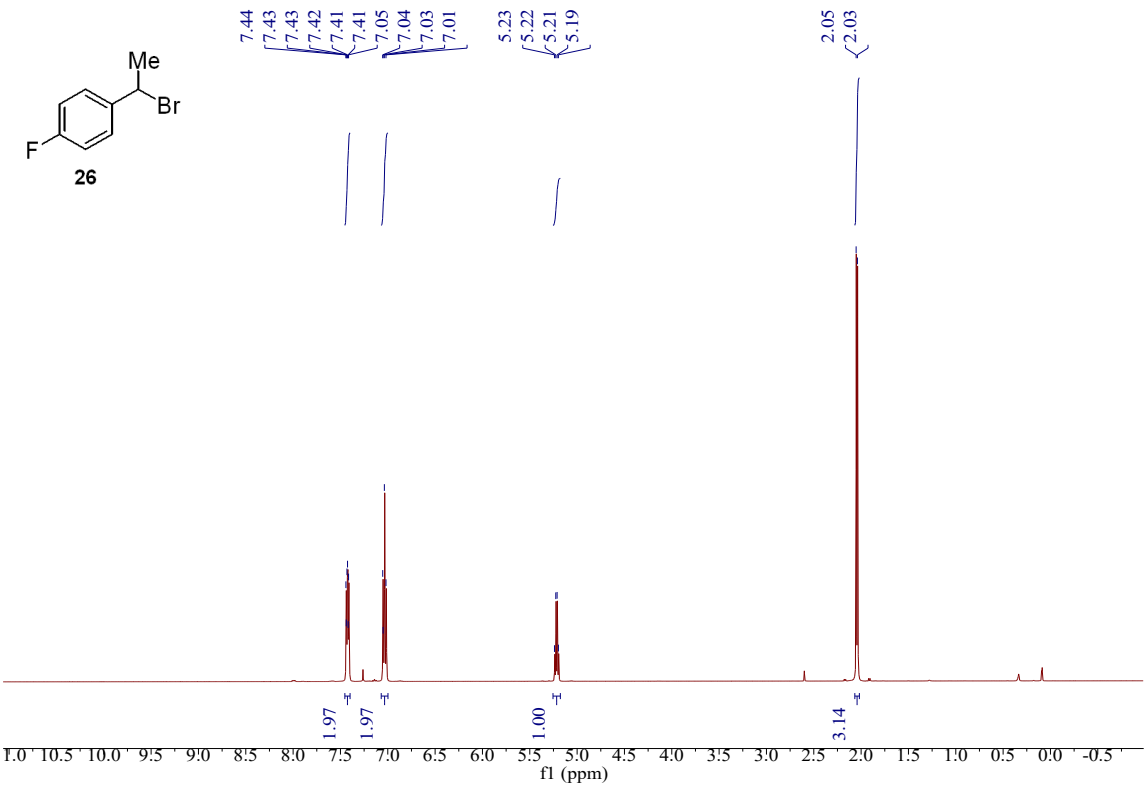

150.05
142.40
141.44
127.02
109.39
107.99
3
f1 (ppm)

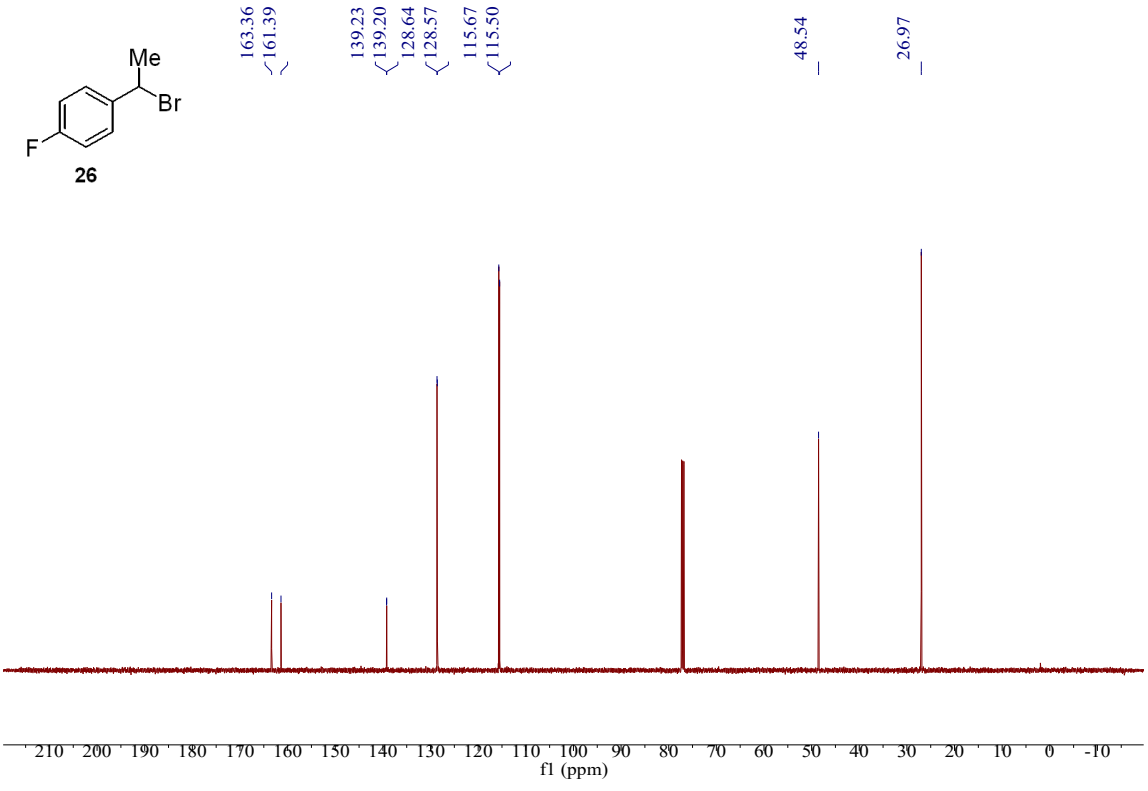

7.43
7.43
7.42
7.41
7.39
7.37
7.37
7.36
7.36
7.15
7.15
7.07
7.06
7.06
7.05
7.05
6.99
6.99
6.98
6.97
5.28
5.27
5.27
5.26
5.25
5.24
5.24
2.08
2.08
2.07
2.07
Me
Br
PhO
24
2.04
2.02
1.00
1.91
1.97
1.00
3.07
f1 (ppm)

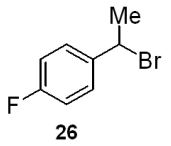

157.42
156.71
137.94
129.88
128.36
123.72
119.35
118.56
49.41
26.97
Me
Br
PhO
24
f1 (ppm)


Me
Br
Me
25
7.38
7.37
7.37
7.36
7.36
7.35
7.19
7.19
7.17
7.17
5.27
5.27
5.26
5.25
5.24
5.24
5.23
5.22
2.37
2.37
2.08
2.08
2.07
2.07
2.06
2.06
1.95
1.96
1.00
2.99
3.05
fl (ppm)


Me
Br
Me
25
140.42
138.29
129.39
126.75
49.86
26.87
21.22
fl (ppm)

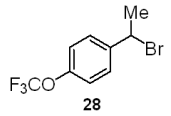

Me
Br
F
26
7.44
7.43
7.43
7.42
7.41
7.41
7.05
7.04
7.03
7.01
5.23
5.22
5.21
5.19
2.05
2.03
1.97
1.97
1.00
3.14
fl (ppm)


Me
Br
F
26
163.36
161.39
139.23
139.20
128.64
128.57
115.67
115.50
48.54
26.97
fl (ppm)


Me
Br
F

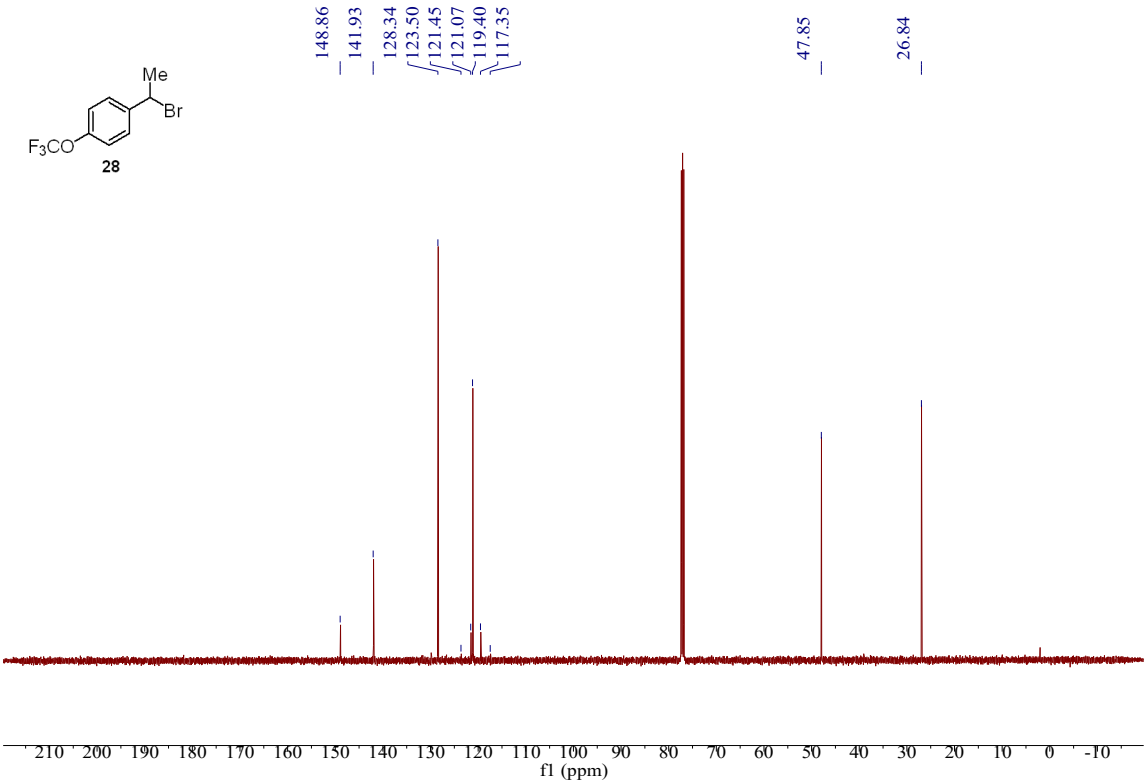
26

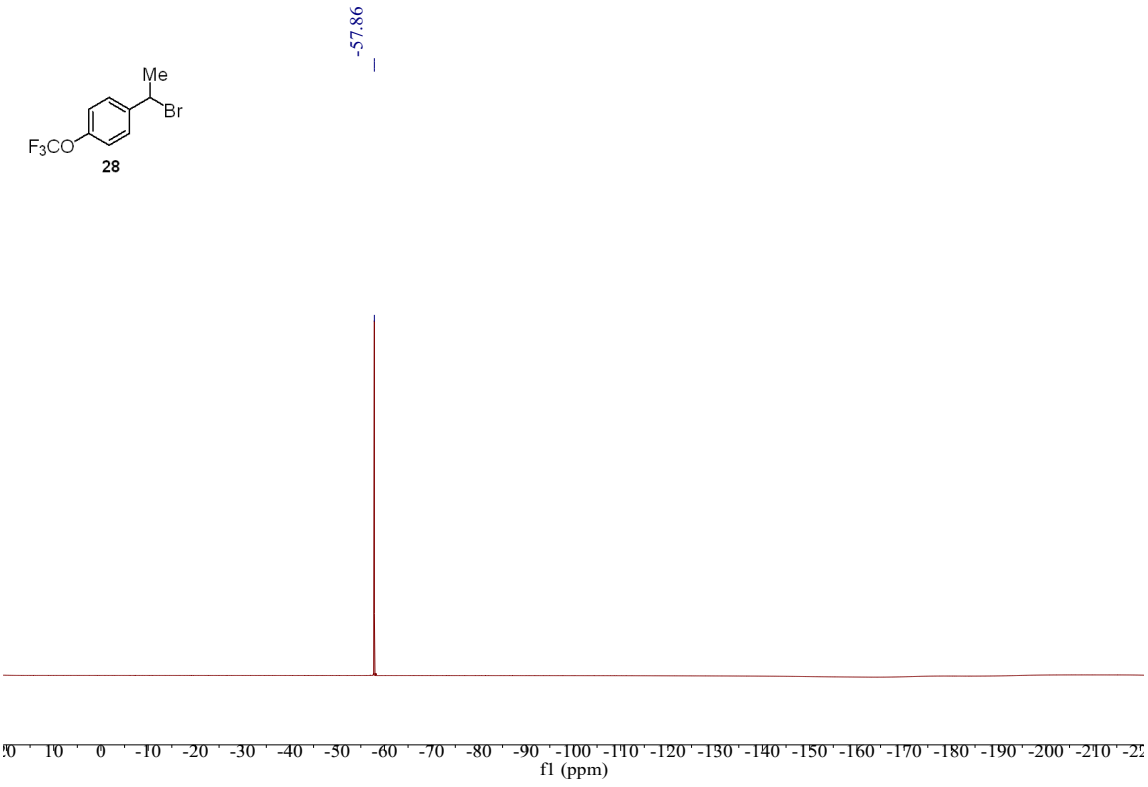
-113.22
-113.23
-113.24
-113.25
-113.26
f1 (ppm)

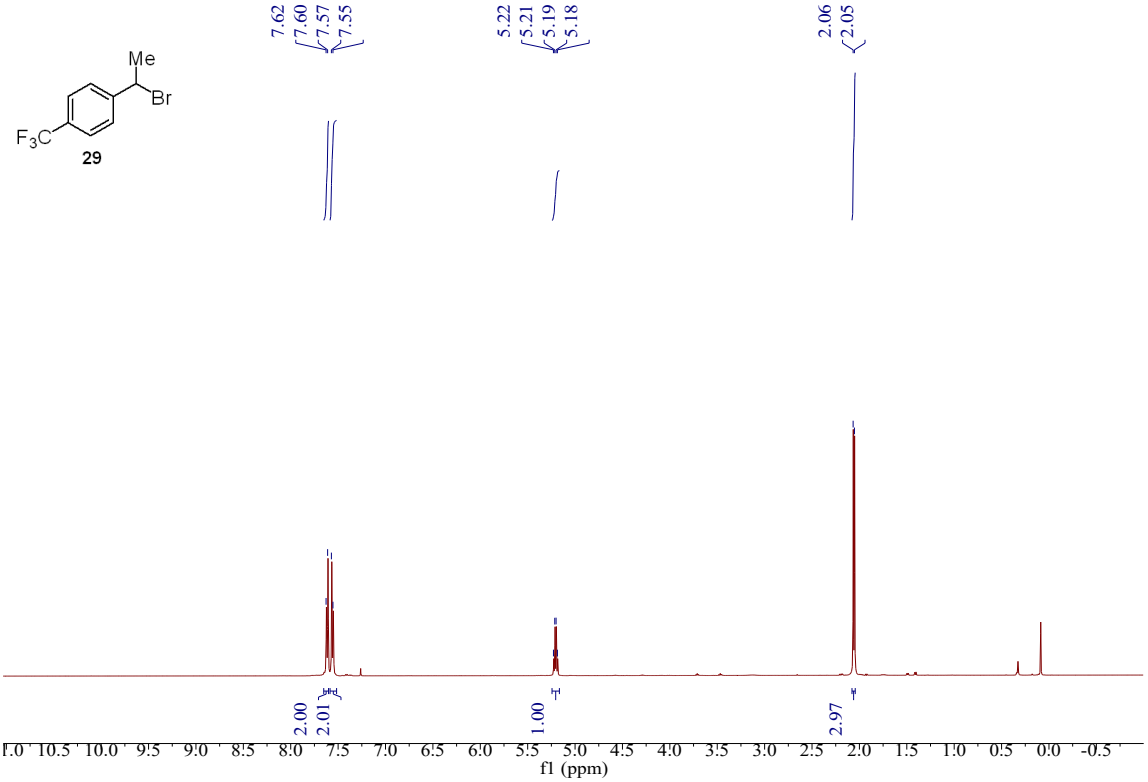

Me
Br
F3CO

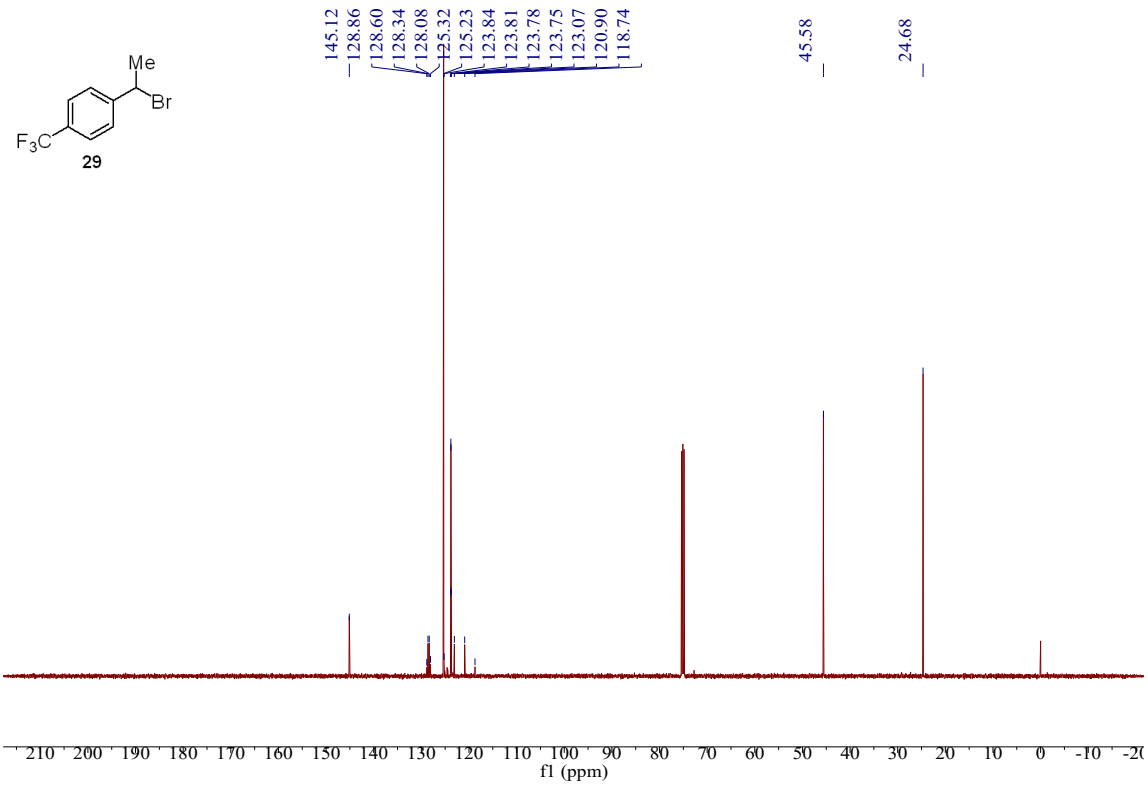
28

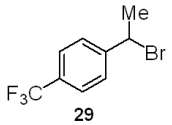
7.48
7.48
7.47
7.46
7.46
7.45
7.20
7.20
7.18
5.22
5.20
5.19
5.18
2.05
2.03
2.02
2.09
1.00
3.05
f1 (ppm)


148.86
141.93
128.34
123.50
121.45
121.07
119.40
117.35
47.85
26.84
Me
Br
F3CO
28
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-57.86
Me
Br
F3CO
28
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

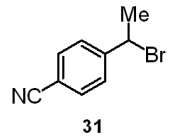

Me
Br
F3C
29
7.62
7.60
7.57
7.55
5.22
5.21
5.19
5.18
2.06
2.05
2.00
2.01
1.00
2.97
f1 (ppm)


Me
Br
F3C
29
145.12
128.86
128.60
128.34
128.08
125.32
125.23
123.84
123.81
123.78
123.75
123.07
120.90
118.74
45.58
24.68
f1 (ppm)


Me
Br
F3C

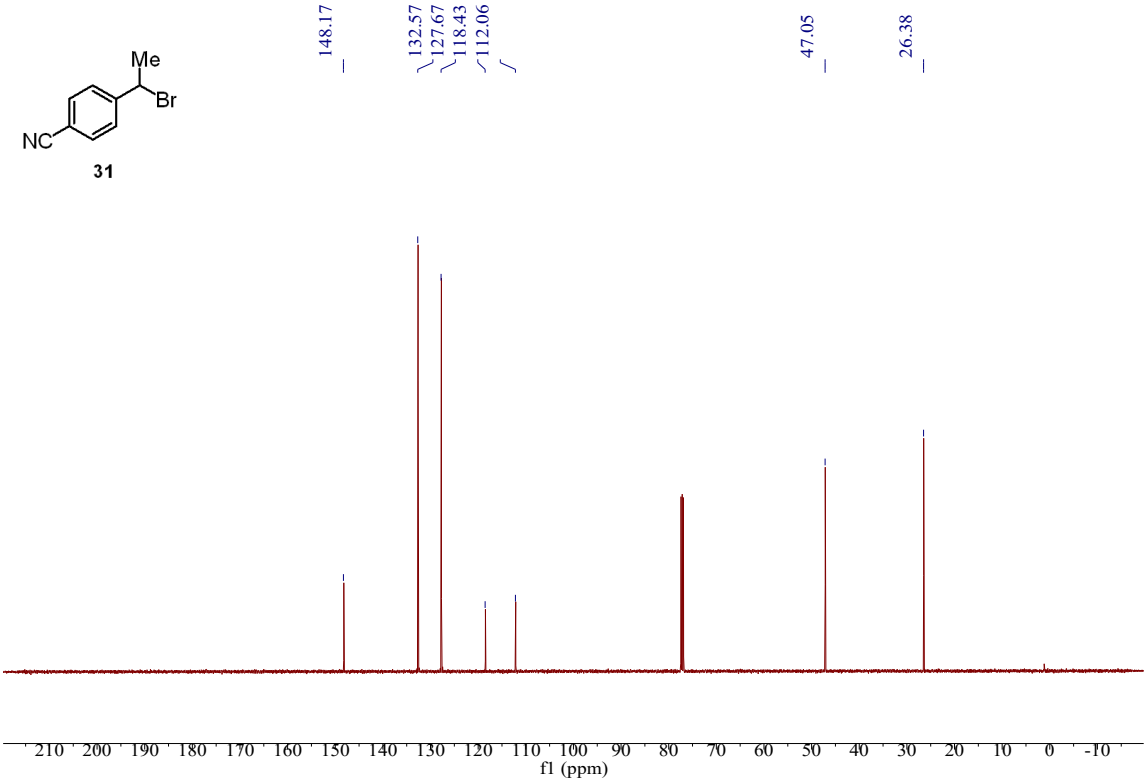
29

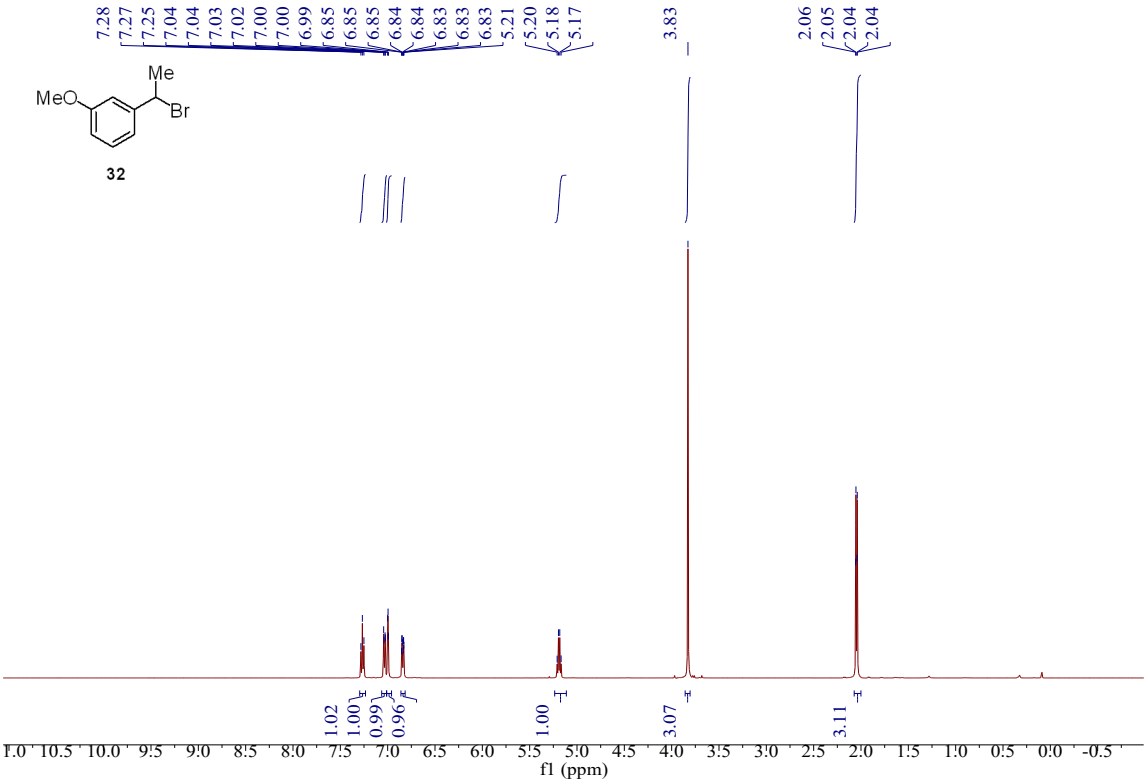
-62.70
f1 (ppm)

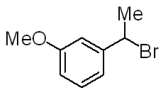

Me
Br
NC

31

7.64
7.63
7.62
7.62
7.54
7.54
7.53
7.52
5.18
5.16
5.15
5.14
2.03
2.02
1.95
2.00
1.00
3.10
f1 (ppm)

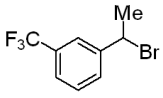

Me
Br
NC
31
148.17
132.57
127.67
118.43
112.06
47.05
26.38
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.28
7.27
7.25
7.04
7.04
7.03
7.02
7.00
7.00
6.99
6.85
6.85
6.85
6.84
6.84
6.83
6.83
6.83
5.21
5.20
5.18
5.17
3.83
2.06
2.05
2.04
2.04
Me
MeO
Br
32
1.02
1.00
0.99
0.96
1.00
3.07
3.11
f1 (ppm)


Me
MeO
Br

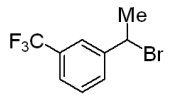
32

159.72
144.75
129.72
119.13
113.81
112.62
55.31
49.42
26.84
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Me
F3C
Br

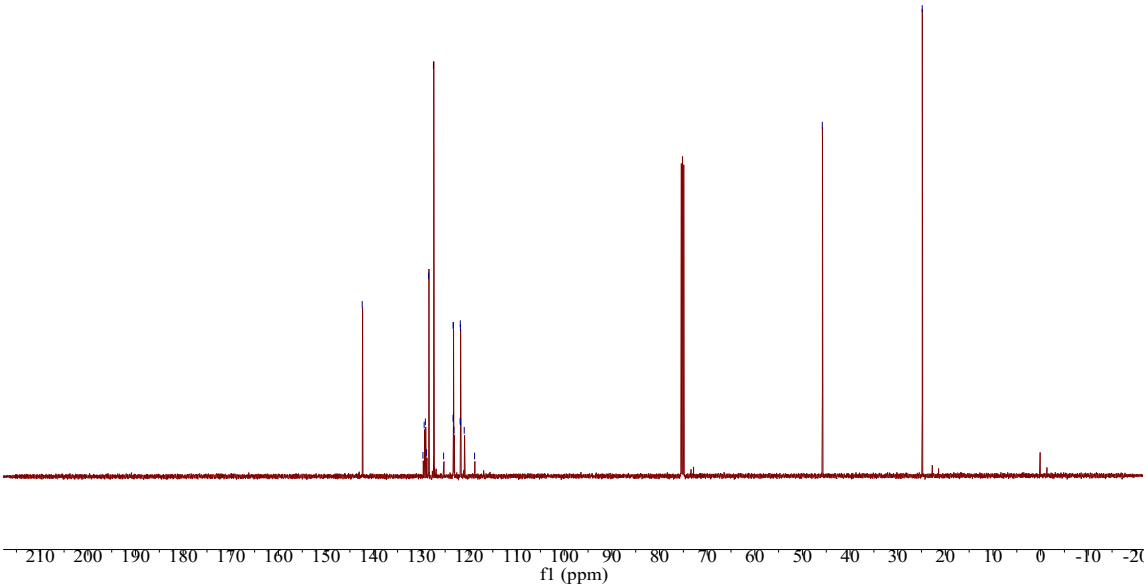
33

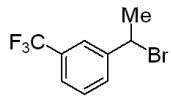
7.70
7.65
7.63
7.57
7.55
7.49
7.48
7.46
5.24
5.23
5.21
5.20
2.07
2.06
0.99
1.04
1.03
1.06
1.00
3.17
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Me
F3C
Br

33

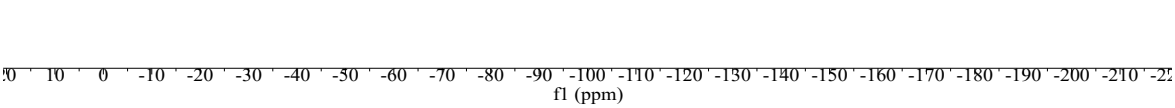

142.30
129.55
129.29
129.04
128.78
128.37
127.35
125.21
123.23
123.20
123.17
123.14
123.05
121.74
121.71
121.68
121.65
120.88
118.72
45.72
24.75

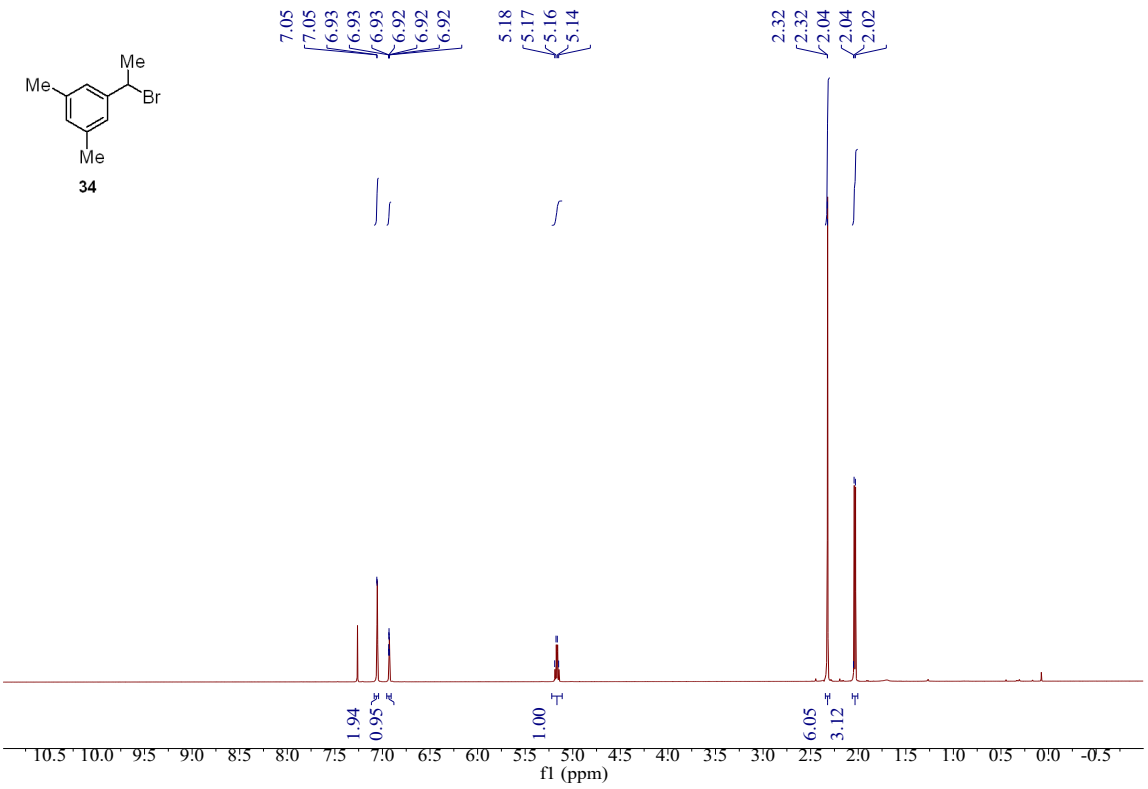

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

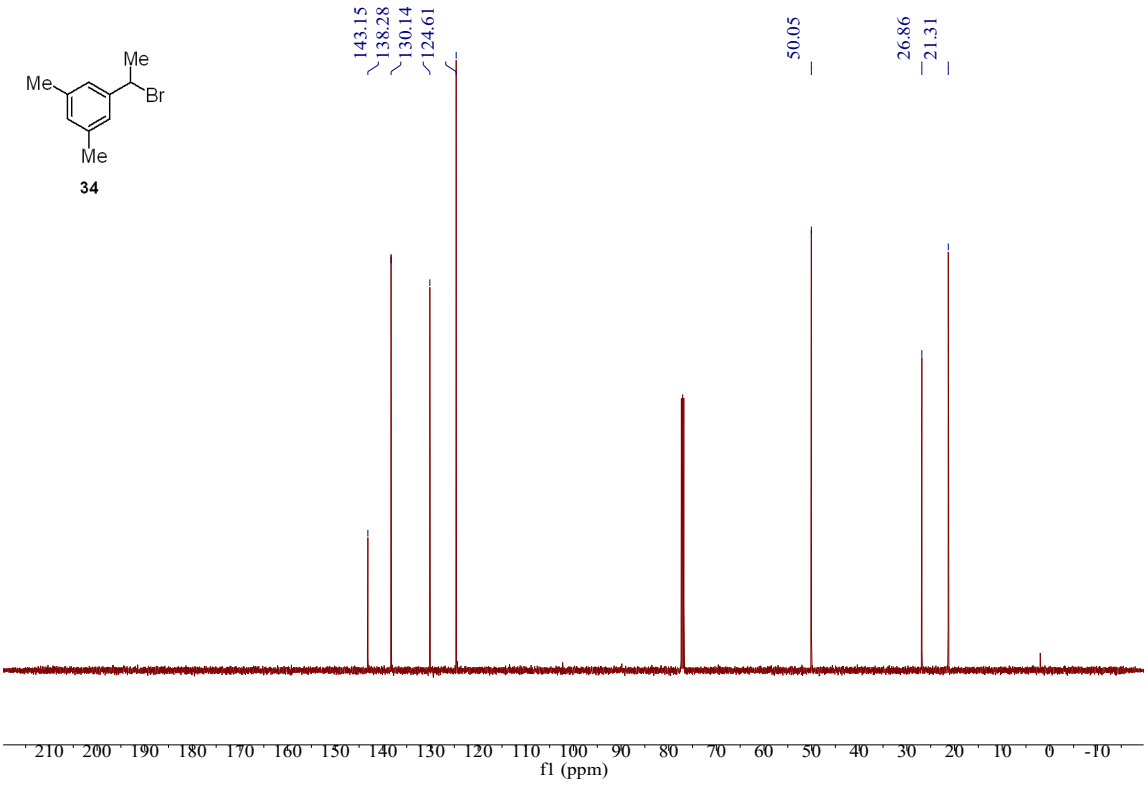

Me
F3C
Br

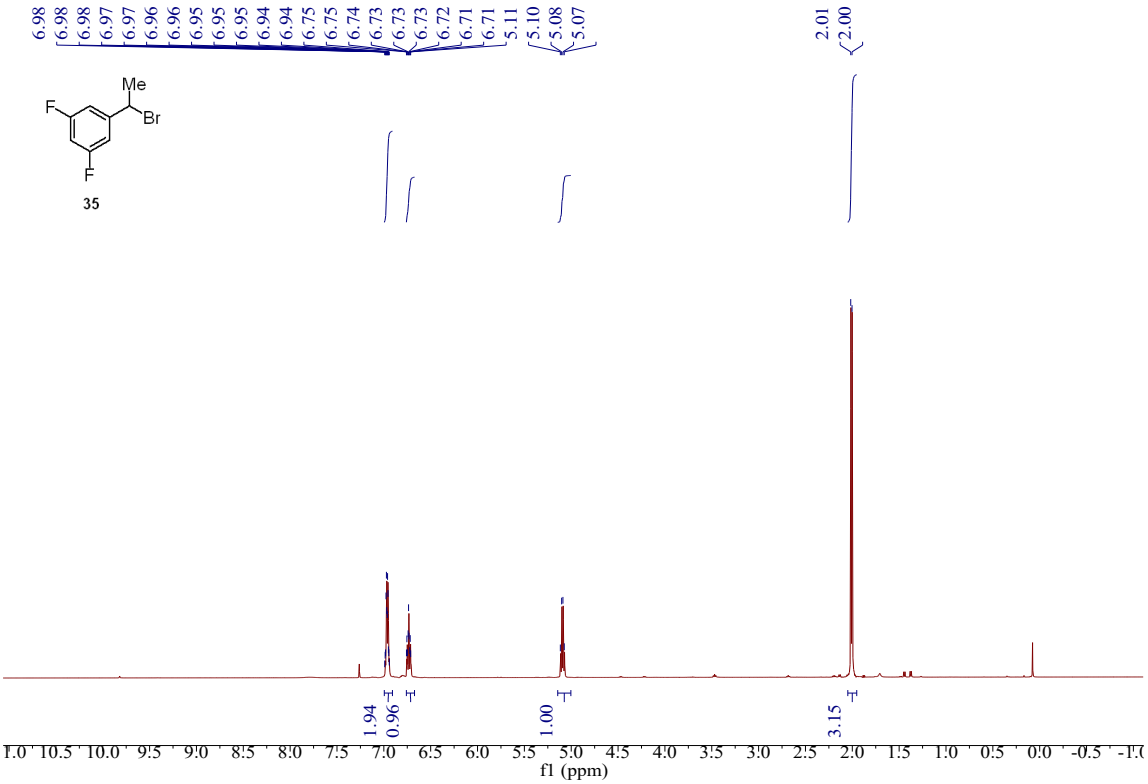
33

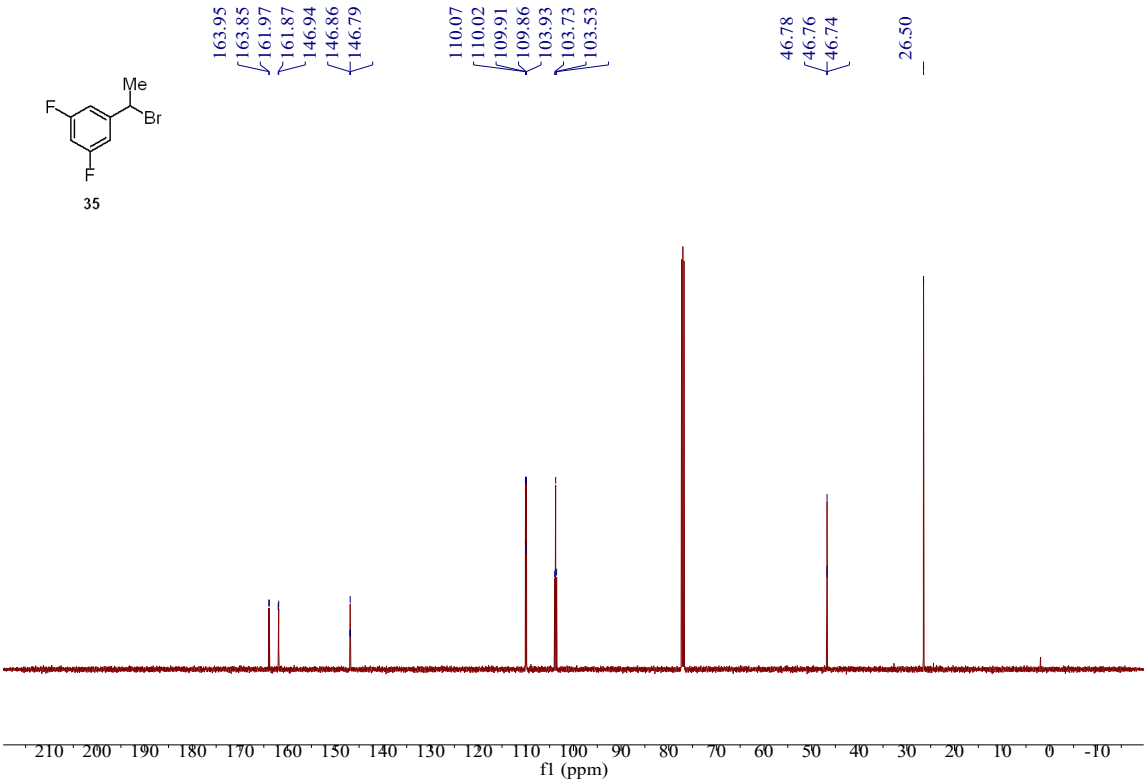
-62.70

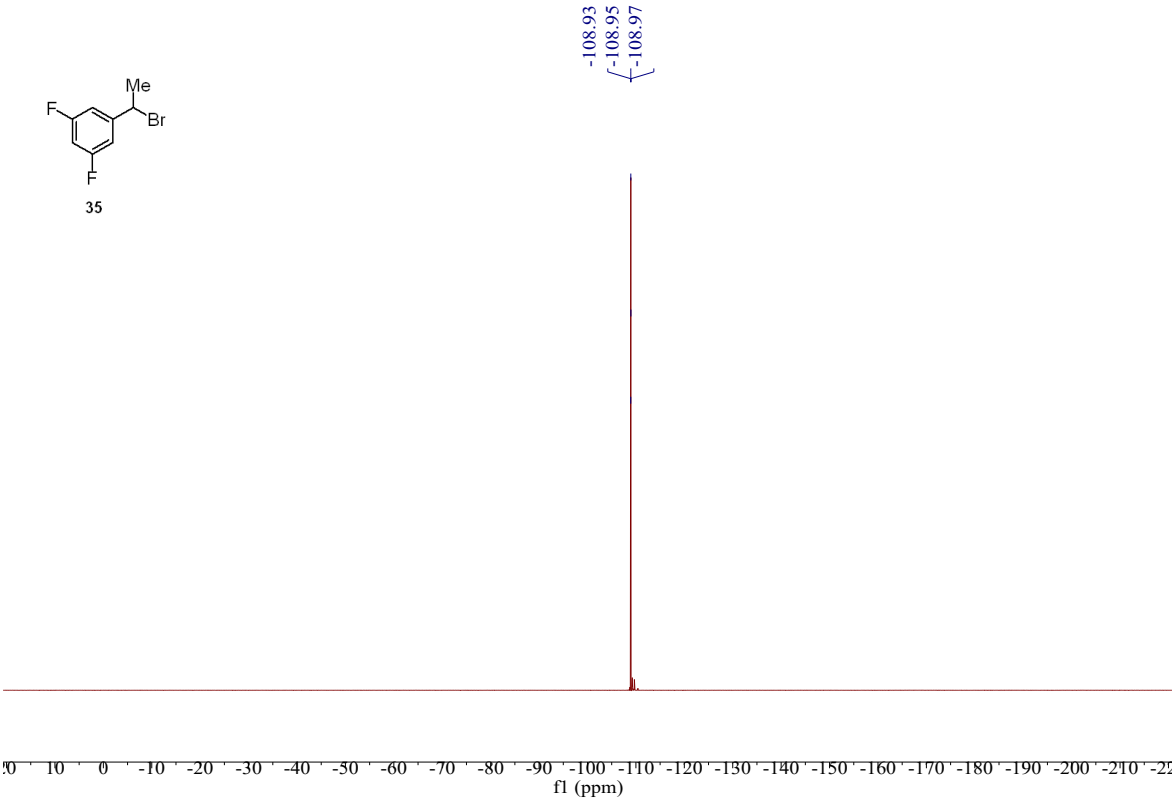

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

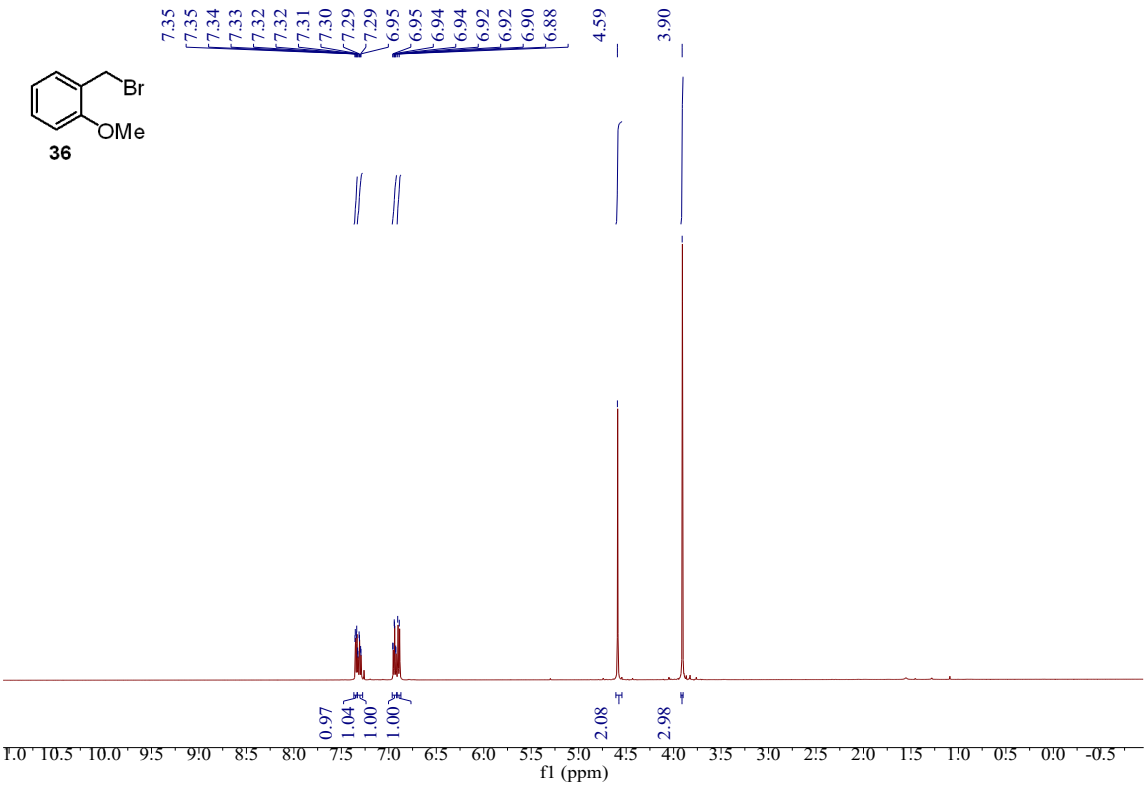

Me
Me
Br
Me
34
7.05
7.05
6.93
6.93
6.93
6.92
6.92
6.92
5.18
5.17
5.16
5.14
2.32
2.32
2.04
2.04
2.02
1.94
0.95
1.00
6.05
3.12
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

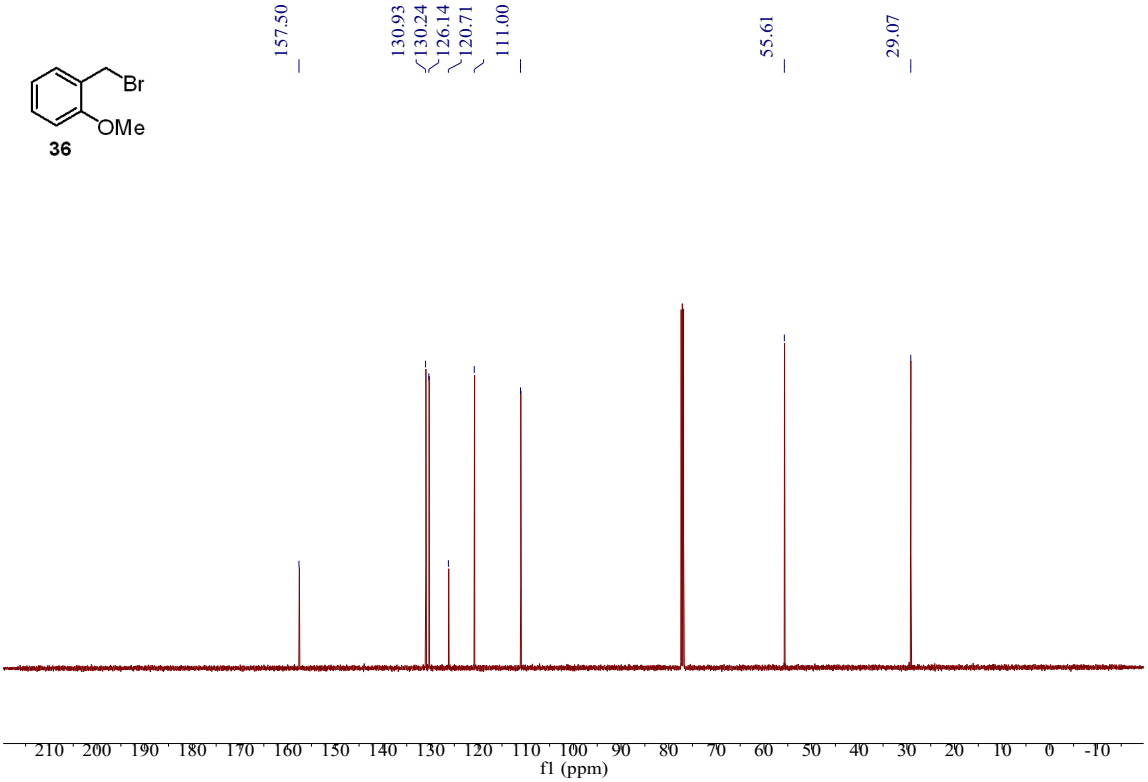

Me
Me
Br
Me
34
143.15
138.28
130.14
124.61
50.05
26.86
21.31
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

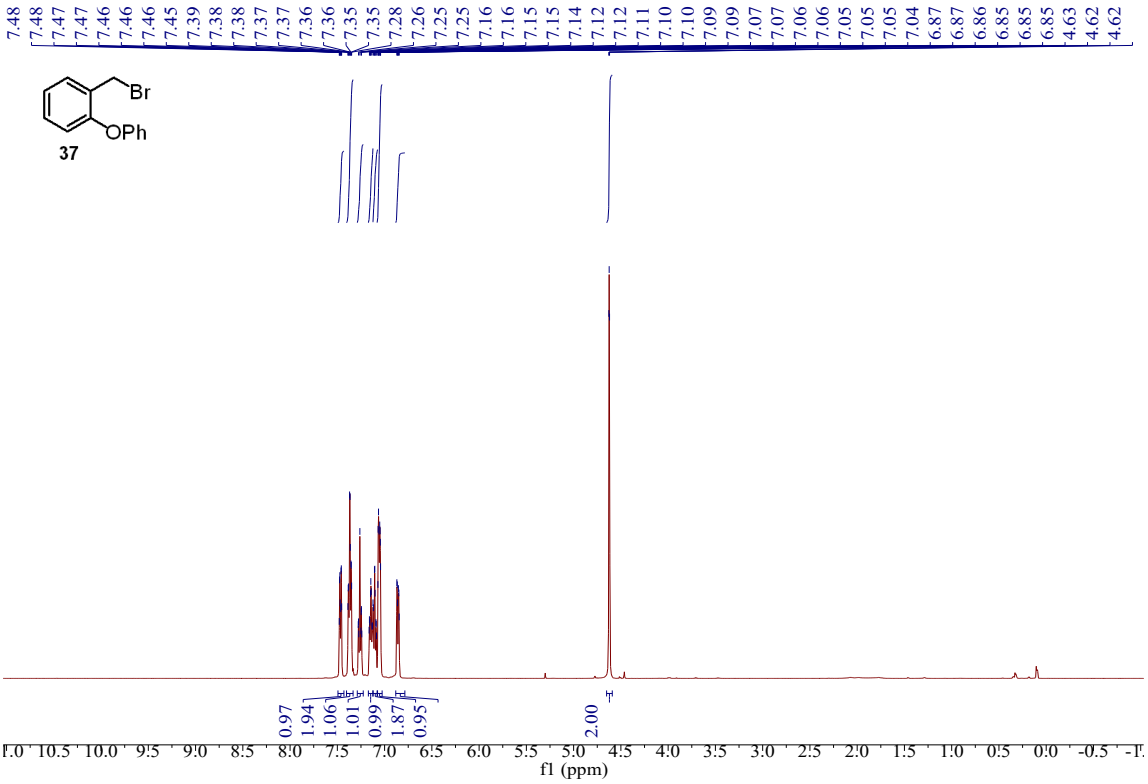

6.98
6.98
6.98
6.97
6.97
6.96
6.96
6.95
6.95
6.95
6.94
6.94
6.75
6.75
6.74
6.73
6.73
6.73
6.72
6.71
6.71
5.11
5.10
5.08
5.07
2.01
2.00
Me
F
Br
F
35
1.94
0.96
1.00
3.15
fl (ppm)

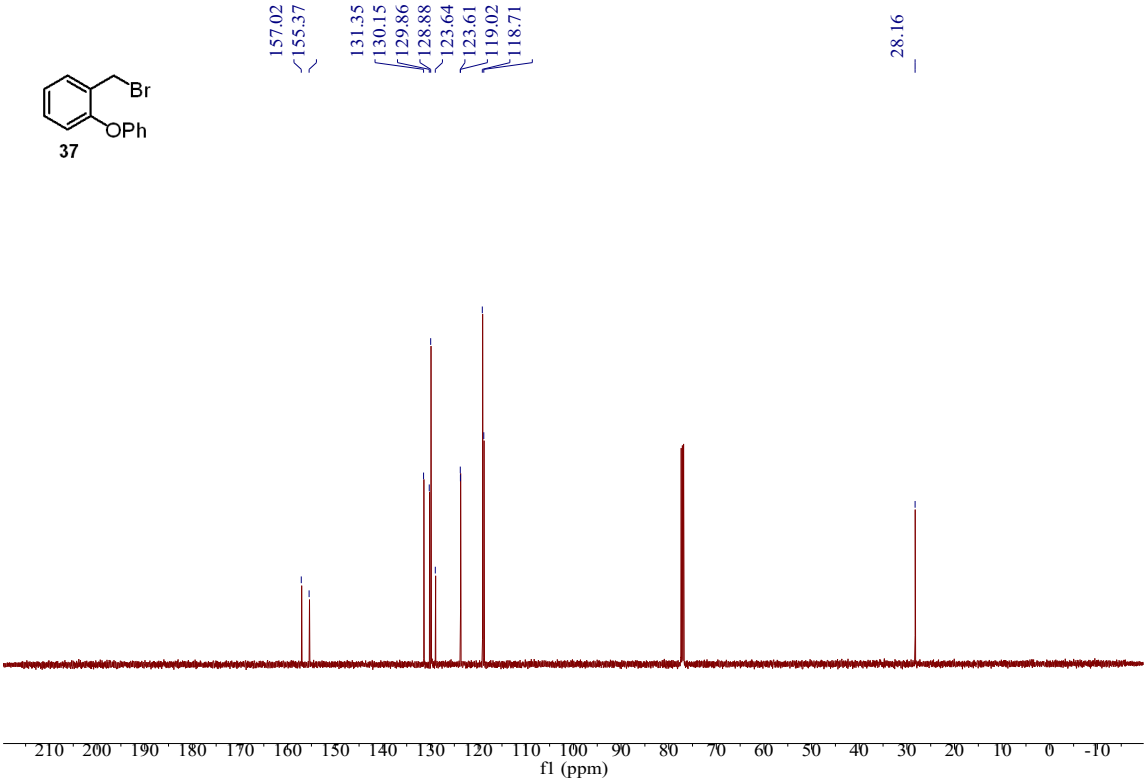

163.95
163.85
161.97
161.87
146.94
146.86
146.79
110.07
110.02
109.91
109.86
103.93
103.73
103.53
46.78
46.76
46.74
26.50
Me
F
Br
F
35
fl (ppm)

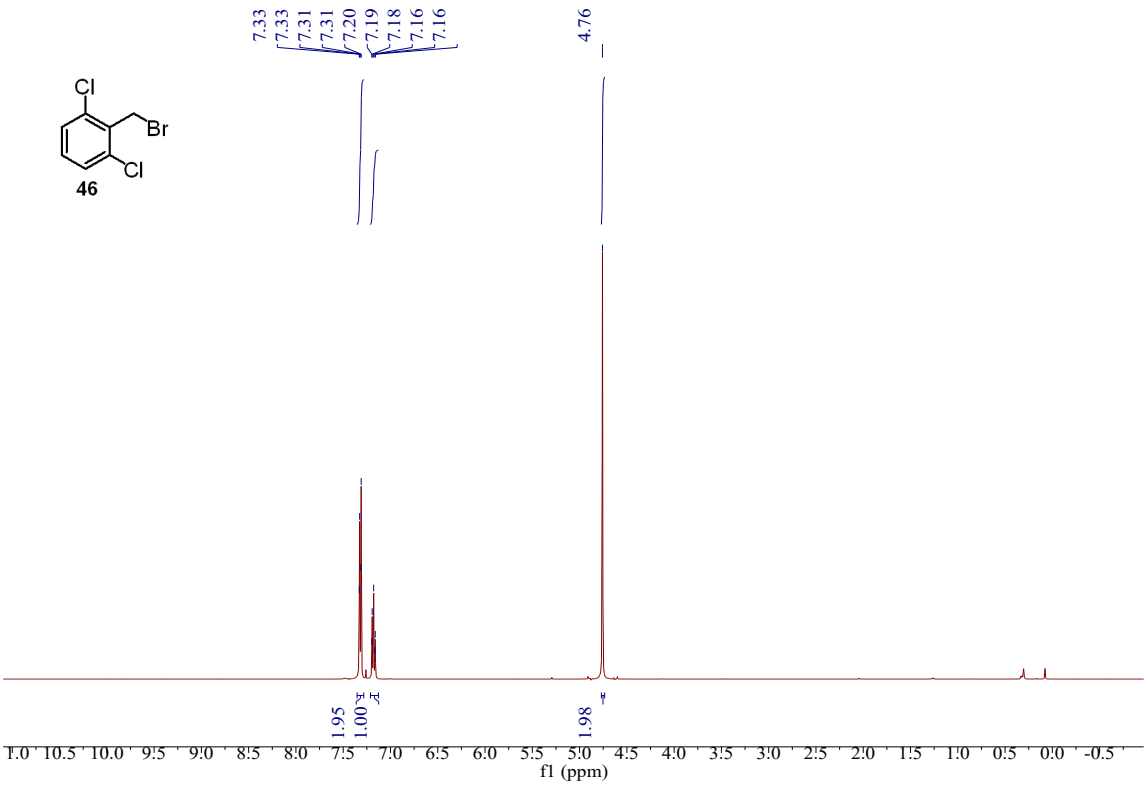

Me
F
Br
F
35
-108.93
-108.95
-108.97
f1 (ppm)

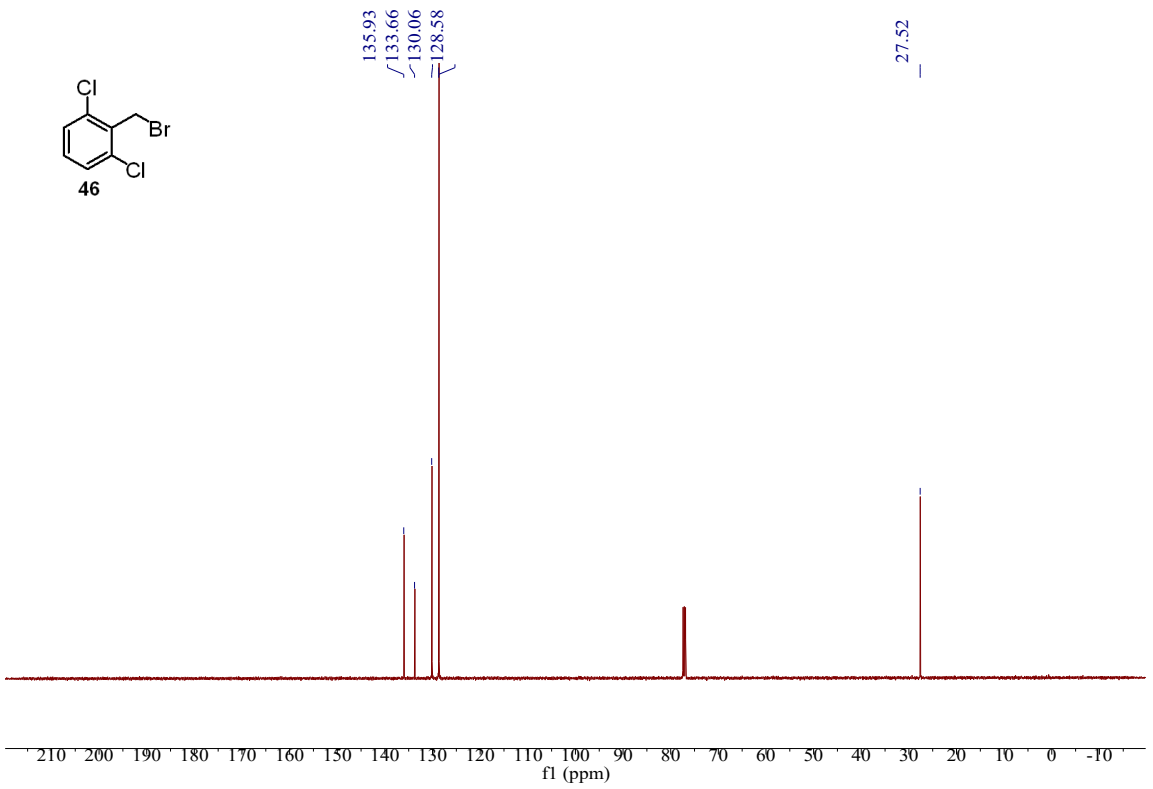

Br
OMe
36
7.35
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.29
7.29
6.95
6.95
6.94
6.94
6.92
6.92
6.90
6.88
4.59
3.90
0.97
1.04
1.00
1.00
2.08
2.98
f1 (ppm)


Br
OMe
36
157.50
130.93
130.24
126.14
120.71
111.00
55.61
29.07
fl (ppm)


Br
OPh
37
0.97
1.94
1.06
1.01
0.99
1.87
0.95
2.00
fl (ppm)


157.02
155.37
131.35
130.15
129.86
128.88
123.64
123.61
119.02
118.71
28.16
Br
OPh
37
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.33
7.33
7.31
7.31
7.20
7.19
7.18
7.16
7.16
4.76
Cl
Br
Cl
46
1.95
1.00
1.98
1.0 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
f1 (ppm)


Cl
Br
Cl
46
135.93
133.66
130.06
128.58
27.52
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)