Supporting Information

Branched-Selective Cross-Electrophile Coupling of 2-Alkyl Aziridines and (Hetero)aryl Iodides Using Ti/Ni Catalysis

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1. General Information

General Considerations: Manipulations of air-sensitive compounds were carried out under an atmosphere of nitrogen using standard Schlenk techniques or in a nitrogen-filled glovebox. All Ti/Ni-catalyzed cross-coupling reactions were set up in a nitrogen filled glovebox, using oven dried glass vials (140 °C) that were allowed to cool under vacuum prior to use in the glovebox. Branched/linear connectivity is confirmed for all cross-coupled products by HMBC. Unless otherwise noted yields are reported as a mixture of branched:linear (B:L) isomers and are reported as % yield (B:L).

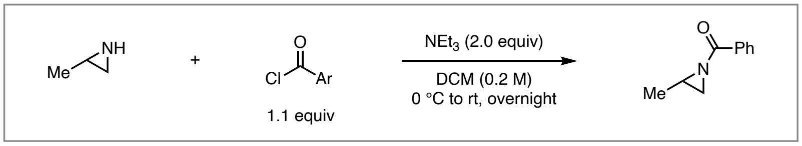
Materials: Tetrahydrofuran (THF) was distilled over Na/benzophenone, degassed by sparging with nitrogen, and stored over 4 Å sieves in a nitrogen-filled glovebox. All liquid reagents used in the glovebox were degassed by sparging with nitrogen for at least 30 minutes and were stored inside the glovebox.

Unless otherwise noted, commercial reagents were used as received. $NiBr_2$•diglyme, 4,4'-di-*tert*-butylbipyridine (dtbbpy), zinc (dust, <10 µm, ≥98%), and manganese (powder, ~325 mesh, ≥99% trace metal basis) were purchased from Sigma-Aldrich. Cp^*TiCl_3 (Cp^* = pentamethylcyclopentadienyl) was purchased from Strem. NEt_3•HBr was purchased from Acros Organics and was dried under vacuum overnight at 50 °C. Pyridine•HBr was purchased from Sigma-Aldrich and was dried under vacuum overnight at 50 °C. 2-methyl aziridine was purchased from Oakwood and used as received.

Instrumentation: Proton nuclear magnetic resonance (^1H NMR) spectra were recorded on Bruker spectrometers (at 400, 500, and 600 MHz). Carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker spectrometers (at 126 and 151 MHz). Fluorine nuclear magnetic resonance (^{19}F NMR) spectra were recorded on Bruker spectrometers (376, 471, and 565 MHz). Proton chemical shifts are reported in parts per million downfield from tetramethylsilane and referenced to residual protium in the NMR solvent ($CDCl_3$ = δ 7.26 ppm, Methanol-d_4 = 3.31 ppm). Carbon chemical shifts are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to the carbon resonance of the solvent ($CDCl_3$ = 77.16 ppm). NMR data are represented as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, h = sextet, hept = heptet, m = multiplet, br = broad), coupling constant in Hertz (Hz), integration. Gas chromatography with flame ionization detection (GC-FID) was performed using an Agilent 7890A GC. Low-resolution gas chromatography-mass spectrometry (GC-MS) was performed using an Agilent 8890 GC System/Agilent 5977B GC/MSD. High resolution mass spectra were obtained using a Thermo Scientific Thermo Exactive Plus MSD (DART-MS) equipped with an ID-CUBE ion source and a Vapur Interface (ION Sense Inc.) (atmospheric-pressure chemical ionization, APCI) or on an Agilent 6530 LC-QTOF by electrospray ionization (ESI) paired with a time of flight (TOF) mass spectrometer. FTIR spectra were obtained with an Agilent Cary 630 FTIR Spectrometer. Optical rotations were measured with a Rudolf Autopol III Automatic Polarimeter. Chiral SFC data was collected using an Agilent 1260 Infinity II LC system.

2. General Procedures

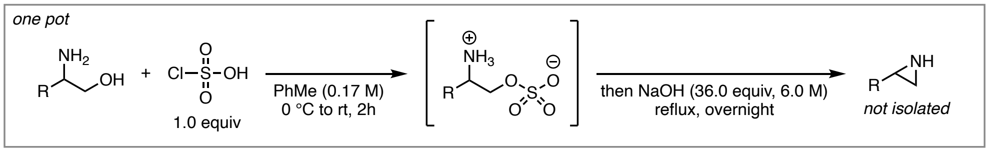
General Procedure A: Benzoyl protection of aziridines



A flame dried flask was charged with 2-methylaziridine (1.0 equiv), DCM (0.2 M), and triethylamine (2.0 equiv). The reaction was cooled to 0 °C and the acid chloride (1.1 equiv) was added dropwise. The reaction was stirred at room temperature overnight. The reaction mixture was then quenched with saturated $NaHCO_3$. The aqueous layer was extracted with DCM (2x). The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered, and concentrated. The aziridine was purified by flash chromatography and distilled where indicated.

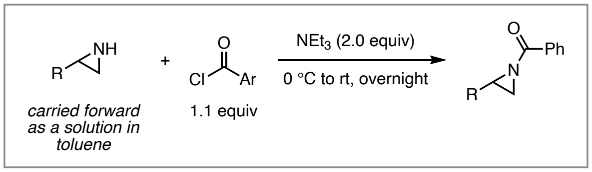
General Procedure B: Synthesis of benzoyl protected aziridines from amino alcohols

Note: Due to the commercial availability of enantioenriched amino alcohols, many of the aziridines (where specified) were prepared from enantioenriched amino alcohols resulting in enantioenriched aziridines.[1] We include the optical rotation for *N*-benzoyl-2-*n*-butyl aziridine (**3a**) and *N*-benzoyl-2-isopropyl aziridine (**6a**) to demonstrate that the resulting aziridines are also enantioenriched. However, subjection of enantioenriched aziridines to cross-coupling results in a racemic product (see **3b**). As the cross-coupling is stereoablative, we do not include additional characterization data for all enantioenriched aziridines or for the resulting cross-coupled products.



Unprotected aziridines were prepared according to a modified literature prep.[1] A flame dried flask was charged with amino alcohol (1.0 equiv) and toluene (0.17 M). The reaction mixture was cooled to 0 °C followed by the dropwise addition of chlorosulfonic acid (1.0 equiv). The reaction was stirred at room temperature for 2 hours to yield the hydrogen sulfate.

NaOH (36.0 equiv, 6.0 M) was added to this reaction mixture and the biphasic solution was heated under reflux overnight. The reaction was then allowed to cool to room temperature and the phases were separated. The aqueous phase was extracted with diethyl ether (3x) and the combined organic layers were washed with brine and dried over $MgSO_4$. The diethyl ether was gently removed under reduced pressure. Many 2-alkyl aziridines have low boiling points so the aziridine was carried forward as a solution of toluene.



To a solution of the aziridine in toluene was added triethylamine (2.0 equiv). The reaction was cooled to 0 °C and benzoyl chloride (1.1 equiv) was added dropwise. The reaction was stirred at room temperature overnight. The reaction mixture was then quenched with saturated $NaHCO_3$.

The aqueous layer was extracted with DCM or EtOAc (2x). The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered, and concentrated. The aziridine was purified by flash chromatography and distilled where indicated.

General Procedure C: Synthesis of cross-coupled products

All reaction preparation was done inside a nitrogen-filled glovebox in oven-dried vials.

The following stock solutions were prepared in 1-dram vials:

Stock Solution 1: Cp^*TiCl_3 (23.16 mg, 0.080 mmol, 20 mol%) and 889 μL of THF.

Stock Solution 2: $NiBr_2$•diglyme (7.05 mg, 0.020 mmol, 5 mol%), dtbbpy (8.05 mg, 0.030 mmol, 7.5 mol%), and 889 μL of THF. This vial was equipped with a Teflon stir bar, capped with a septum cap, and allowed to stir for 15 minutes forming a green suspension.

Stock Solution 3: Zn (78.46 mg, 1.20 mmol, 3.0 equiv) and 889 μL of THF. A suspension of Zn in THF was generated by pipetting up and down a few times before transferring to the reaction.

To a 2-dram vial equipped with a Teflon stir bar was added aziridine (0.40 mmol, 1.0 equiv) and ArI (0.40 mmol, 1.0 equiv). 889 μL of stock solution 1 was added. The reaction was allowed to stir for 15 minutes at which point NEt_3•HBr (145.69 mg, 0.800 mmol, 2.0 equiv), stock solution 2 (889 μL), and stock solution 3 (889 μL) were sequentially added. The reaction vial was capped with a septum cap, wrapped with electrical tape, and brought outside the glovebox. The reactions were set to stir (1200 rpm) at room temperature for 16 hours. After 16 hours the reactions were opened to air. EtOAc (~2 mL) was added to the vial and then the solution was passed through a celite plug with EtOAc to remove any solids. The eluate was concentrated and further purified by flash chromatography to yield the desired cross-coupled product.

3. Additive Screening

The following stock solutions were prepared:

Stock Solution 1: **1a** (12.09 mg, 0.075 mmol, 11.3 μL, 1.0 equiv), PhI (15.30 mg, 0.075 mmol, 8.4 μL, 1.0 equiv), dodecane (12.78 mg, 0.075 mmol, 17.0 μL, 1.0 equiv), and 113 μL of THF (assuming volumes are additive the total volume is 150 μL).

Stock Solution 2: Cp*TiCl3 (4.34 mg, 15.0 μmol, 20 mol%) in 100 μL of THF.

Stock Solution 3: $NiBr_2$•diglyme (1.32 mg, 3.8 μmol, 5 mol%) and dtbbpy (1.51 mg, 5.6 μmol, 7.5 mol%) in 125 μL of THF. This vial was equipped with a Teflon stir bar, capped with a septum cap, and allowed to stir for 15 minutes before use.

Stock Solution 4: Zn (14.71 mg, 0.225 mmol, 3.0 equiv) in 125 μL of THF.

Additive Stock Solution: Additive stock solutions were prepared such that we could keep 40 μL for GC-FID analysis to get absolute ratio of aziridine (based on response factors) to dodecane and a relative ratio of the additive to dodecane. A volume of 150 μL of the solution would be transferred to the reaction (such that 0.075 mmol of the aziridine, PhI, and additive is transferred to solution).

The following additive stock solutions were prepared by weighing out the specified amounts of additives (Mass in 190 μL (mg)) into separate vials. 190 μL of Stock Solution 1 was added to each vial to generate a stock solution with 0.075 mmol/150 μL of **1a**, PhI, dodecane, and additive. Styrene and tertbutyl acrylate were distilled before use.

Each additive was screened in a separate reaction.

Table S1. Additive stock solution amounts

Additive	Mass in 150 μL (mg)	Mass in 190 μL (mg)
1-decene	10.52	13.33
styrene	7.81	9.89
tert-butyl acrylate	9.61	12.18
2-ocatanone	9.62	12.18
4-ethylbenzonitrile	9.84	12.46
3-chloropropylbenzene	11.60	14.69
cyclohexyl chloride	8.90	11.27
1-bromoheptane	13.43	17.01
4-chlorobiphenyl	14.15	17.92
p-tolyl trifluoromethanesulfonate	18.02	22.82
phenylboronic acid pinacol ester	15.31	19.39
aniline	6.99	8.85
2-phenyl-1,3-dioxolane	11.26	14.27
N-methyl-*p*-toluenesulfonamide	13.89	17.60
N-(*tert*-butoxycarbonyl)methylamine	9.84	12.46
acetophenone	9.01	11.41
4-bromobiphenyl	17.48	22.14
benzyloxytrimethylsilane	13.52	17.13
1-nonyne	9.32	11.80
4-fluorobenzaldehyde	9.31	11.79
4-ethylbenzoic acid	11.26	14.26
4-ethylnitrobenzene	11.34	14.36
4-bromoheptane	13.43	17.01
1-iodooctane	18.01	22.81
iodocyclohexane	15.75	19.95
1-decylamine	11.80	14.95
cyclohexylmethanol	8.56	10.85
4-phenylphenol	12.77	16.18

To an oven dried 1-dram vial with a Teflon stir bar was added NEt_3•HBr (27.32 mg, 0.15 mmol, 2 equiv), Stock Solution 2 (100 μL), and the corresponding Additive Stock Solution (150 μL). The reactions were allowed to stir for 15 min at which point Stock Solution 3 (125 μL) and Stock Solution 4 (125 μL) were added. The reaction vial was capped with a septum cap, wrapped with electrical tape, and brought outside the glovebox. The reaction was set to stir (700 rpm) at room temperature for 16 hours. Yields and additive recovery were determined by GC-FID.

Table S2. GC-FID peak areas and ratios relative to dodecane of starting materials and additives.

	Peak Area			**Ratio (relative to dodecane)**	
Additive	Dodecane	**1a**	Additive	**1a** (corrected)	Additive
1-decene	607.1	412.1	450.3	0.97	0.74
styrene	668.8	454.9	350.8	0.98	0.52
tert-butyl acrylate	682.2	466.0	263.0	0.98	0.39
2-ocatanone	691.2	471.3	359.2	0.98	0.52
4-ethylbenzonitrile	677.8	461.9	484.3	0.98	0.71
3-chloropropylbenzene	670.7	457.0	477.5	0.98	0.71
cyclohexyl chloride	677.8	461.4	279.8	0.98	0.41
1-bromoheptane	612.1	417.1	336.1	0.98	0.55
4-chlorobiphenyl	621.7	425.8	641.2	0.98	1.03
p-tolyl trifluoromethanesulfonate	916.0	657.4	527.2	1.01	0.58
phenylboronic acid pinacol ester	1153.3	835.6	1204.0	1.01	1.04
aniline	686.0	468.7	301.9	0.98	0.44
2-phenyl-1,3-dioxolane	918.8	558	601.9	1.01	0.66
N-methyl-*p*-toluenesulfonamide	480.8	346.4	365.8	1.00	0.76
N-(*tert*-butoxycarbonyl)methylamine	1055.4	760.7	439.7	1.00	0.42
acetophenone	640.8	437.0	351.3	0.98	0.55
4-bromobiphenyl	603.2	415.0	655.6	0.99	1.09
benzyloxytrimethylsilane	918.4	660.9	688.9	1.00	0.75
1-nonyne	641.2	435.9	389.5	0.98	0.61
4-fluorobenzaldehyde	623.3	425.2	304.5	0.97	1.21
4-ethylbenzoic acid	636.5	428.2	N/D	0.97	2.43
4-ethylnitrobenzene	652.7	446.0	435.4	0.98	0.67
4-bromoheptane	596.3	404.8	310.7	0.97	0.52
1-iodooctane	599.3	406.0	369.2	0.97	0.62
iodocyclohexane	642.9	436.1	302.9	0.97	0.47
1-decylamine	634.1	433.1	216.7	0.98	0.34
cyclohexylmethanol	693.5	472.3	273.2	0.98	0.39
4-phenylphenol	629.0	437.5	504.9	1.00	0.80

[a] Reactions containing *p*-tolyl trifluoromethanesulfonate, phenylboronic acid pinacol ester, 2-pheny-1,3-dioxolane, *N*-methyl-*p*-toluenesulfonamide, *N*-(*tert*-butoxycarbonyl)methylamine, and benzyloxytrimethylsilane were performed following GC-FID maintenance and ratios were calculated using updated response factors.

Table S3. GC-FID peak areas and ratios relative to dodecane of products and additives.

	Peak Area				**Ratio (Relative to Dodecane)**[a]		
Additive	Dodecane	Branched	Linear	Additive	Branched (corrected)	Linear (corrected)	Additive
1-decene	557.9	399.6	36.3	351.9	0.58	0.04	0.63
styrene	535.7	366.1	35.4	198.5	0.55	0.05	0.37
tert-butyl acrylate	541.2	395.8	50.5	133.1	0.59	0.06	0.25
2-ocatanone	460.4	459.5	56.8	162.3	0.80	0.09	0.35
4-ethylbenzonitrile	454.5	398.8	35.1	231.5	0.71	0.05	0.51
3-chloropropylbenzene	472.6	426.8	45.3	337.9	0.73	0.07	0.71
cyclohexyl chloride	486.6	483.7	52.0	176.9	0.80	0.07	0.36
1-bromoheptane	536.5	473.1	42.4	202.6	0.71	0.05	0.38
4-chlorobiphenyl	435.5	391.8	40.0	428.1	0.72	0.06	0.98
p-tolyl trifluoromethanesulfonate	430.6	356.8	32.3	248.6	0.59	0.05	0.57
phenylboronic acid pinacol ester	423.2	448.6	46.6	456.9	0.72	0.07	1.06
aniline	623.5	576.5	64.4	253.5	0.74	0.07	0.41

N-methyl-*p*-toluenesulfonamide	520.6	429.4	87.0	394.3	0.58	0.12	0.76
N-(*tert*-butoxycarbonyl)methylamine	403.4	430.7	57.6	160.6	0.75	0.10	0.40
acetophenone	527.4	412.9	126.6	171.7	0.63	0.17	0.33
4-bromobiphenyl	511.6	453.6	50.1	292.2	0.71	0.07	0.57
benzyloxytrimethylsilane	410.2	299.5	46.3	308.4	0.51	0.08	0.75
1-nonyne	515.4	142.3	8.0	3.1	0.22	0.01	0.01
4-fluorobenzaldehyde	572.4	20.8	14.5	55.3	0.03	0.02	0.10
4-ethylbenzoic acid	551.1	2.7	0.0	N/D	0.00	0.00	N/D
4-ethylnitrobenzene	501.4	0.0	0.0	178	0.00	0.00	0.36
4-bromoheptane	599.2	374.7	31.8	25.1	0.50	0.04	0.04
1-iodooctane	560.2	447.3	38.1	0.0	0.64	0.05	0.00
iodocyclohexane	452.3	437	34.4	2.9	0.78	0.05	0.01
1-decylamine	436.2	261.1	57.6	0.0	0.48	0.09	0.00
cyclohexylmethanol	577.4	11.4	10.9	227.5	0.02	0.01	0.39
4-phenylphenol	507.5	60.6	36.0	367.2	0.10	0.05	0.72

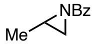
[a]Reactions containing *p*-tolyl trifluoromethanesulfonate, phenylboronic acid pinacol ester, 2-pheny-1,3-dioxolane, *N*-methyl-*p*-toluenesulfonamide, *N*-(*tert*-butoxycarbonyl)methylamine, and benzyloxytrimethylsilane were performed following GC-FID maintenance and ratios were calculated using updated response factors.

Table S4: Yields and additive recovery.

Additive	**Yield**	**B:L**	**Additive Remaining**
1-decene	64%	12.8	85%
styrene	61%	12.1	71%
tert-butyl acrylate	67%	9.1	64%
2-ocatanone	91%	9.4	68%
4-ethylbenzonitrile	78%	13.6	71%
3-chloropropylbenzene	81%	11.0	100%
cyclohexyl chloride	89%	10.8	88%
1-bromoheptane	78%	13.0	69%
4-chlorobiphenyl	80%	11.4	95%
p-tolyl trifluoromethanesulfonate	63%	11.2	100%
phenylboronic acid pinacol ester	79%	9.7	101%
aniline	83%	10.4	92%
2-phenyl-1,3-dioxolane	76%	9.9	81%
N-methyl-*p*-toluenesulfonamide	69%	5.0	100%
N-(*tert*-butoxycarbonyl)methylamine	84%	7.6	96%
acetophenone	81%	3.8	59%
4-bromobiphenyl	79%	10.6	53%
benzyloxytrimethylsilane	59%	6.5	100%
1-nonyne	24%	20.7	1%
4-fluorobenzaldehyde	5%	1.7	8%
4-ethylbenzoic acid	0%	N/D	0%
4-ethylnitrobenzene	0%	N/D	53%
4-bromoheptane	55%	13.7	8%
1-iodooctane	71%	13.7	0%
iodocyclohexane	85%	14.8	1%
1-decylamine	58%	5.3	0%
cyclohexylmethanol	3%	1.2	100%
4-phenylphenol	15%	2.0	90%

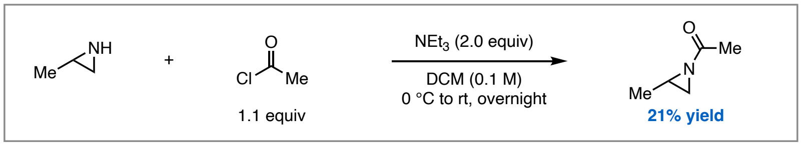
Functional groups we considered to be tolerated in the reaction had yield and additive recovery >60%. If the yield or the additive recovery was <15% we considered this functional group to be incompatible with the method. Potentially problematic functionalities fall in the range of 15-60% yield or additive recovery.

4. Aziridine Synthesis and Characterization



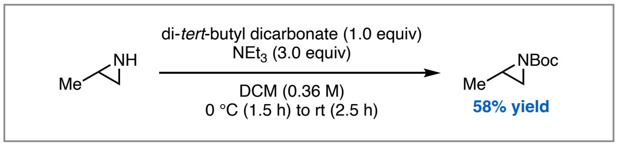
***N*-benzoyl-2-methyl aziridine (1a)** was prepared according to General Procedure A from 2-methyl aziridine (70.0 mmol) and benzoyl chloride. The resulting oil was purified by flash chromatography (8% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 80 °C, full vacuum) to give the product as a clear oil (83% yield). Spectral data are in agreement with reported literature values.[2]

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.06 – 7.99 (m, 2H), 7.59 – 7.51 (m, 1H), 7.49 – 7.41 (m, 2H), 2.58 (pd, *J* = 5.4, 3.5 Hz, 1H), 2.54 (d, *J* = 5.8 Hz, 1H), 2.14 (d, *J* = 3.6 Hz, 1H), 1.40 (d, *J* = 5.3 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 179.4, 133.7, 132.8, 129.2, 128.5, 34.7, 32.3, 17.9.
HRMS (APCI): calculated for $C_{10}H_{12}NO^+$ ($[M+H]^+$): 162.0913, found 162.0912.
FTIR (ATR, cm^{-1}): 3064, 2995, 2966, 2930, 1672, 1405, 1316, 1297, 703.



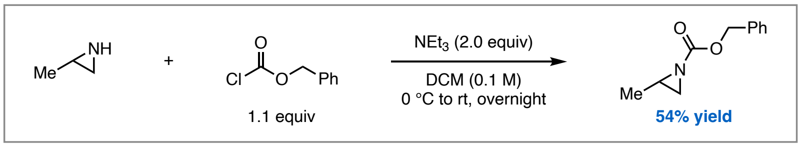
***N*-acetyl-2-methyl aziridine (S1):** A flame-dried flask was charged with 2-methylaziridine (500.0 mg, 0.62 mL, 8.8 mmol, 1.0 equiv), DCM (0.1 M, 87 mL), and triethylamine (1.77 g, 2.44 mL, 17.5 mmol, 2.0 equiv). The solution was cooled to 0 °C and acetyl chloride (756.1 mg, 0.68 mL, 9.6 mmol, 1.1 equiv) was added dropwise. The reaction was stirred at room temperature overnight. The reaction mixture was then quenched with saturated $NaHCO_3$. The aqueous layer was extracted with DCM (2x). The organic layers were combined and washed with brine, dried over $MgSO_4$, filtered, and concentrated. The resulting oil was purified by flash chromatography (25% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected yellow oil was further purified by distillation (hot plate temperature = 65 °C, 25 Torr) to give the product as a clear oil (21% yield). *Note:* the product is volatile under full vacuum. Spectral data are in agreement with reported literature values.[3]

^{1}H NMR (500 MHz, $CDCl_3$): δ 2.50 (pd, *J* = 5.6, 3.4 Hz, 1H), 2.32 (d, *J* = 5.8 Hz, 1H), 2.13 (s, 3H), 1.94 (d, *J* = 3.4 Hz, 1H), 1.32 (d, *J* = 5.5 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 183.3, 33.0, 31.7, 23.9, 17.8.
HRMS (APCI): calculated for $C_5H_{10}NO^+$ ($[M+H]^+$): 100.0757, found 100.0754.



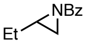
***N*-Boc-2-methyl aziridine (S2)** was prepared according to a modified literature procedure.[4] A flame-dried flask was charged with 2-methylaziridine (500.0 mg, 0.62 mL, 8.8 mmol, 1.0 equiv), DCM (0.36 M, 24 mL), and triethylamine (2.66 g, 3.66 mL, 26.3 mmol, 3.0 equiv). The solution was cooled to 0 °C and di-*tert*-butyl dicarbonate (1.91 g, 8.8 mmol, 1.0 equiv) was added. The reaction was stirred for 1.5 hours at 0 °C and then was warmed to room temperature and stirred for an additional 2 hours. The reaction mixture was then quenched with saturated $NaHCO_3$. The aqueous layer was extracted with DCM (2x). The organic layers were combined and washed with brine, dried over $MgSO_4$, filtered, and concentrated. The resulting oil was purified by flash chromatography (10% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, $KMnO_4$ stain) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 70 °C, 8 Torr) to give the product as a clear oil (58% yield). *Note:* the product is volatile under full vacuum. Spectral data are in agreement with reported values.[5]

^{1}H NMR (500 MHz, $CDCl_3$): δ 2.43 (pd, *J* = 5.6, 3.7 Hz, 1H), 2.23 (d, *J* = 5.9 Hz, 1H), 1.87 (d, *J* = 3.8 Hz, 1H), 1.45 (s, 9H), 1.26 (d, *J* = 5.6 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 162.6, 81.1, 33.7, 32.6, 28.1, 17.5.
HRMS (APCI): calculated for $C_8H_{16}NO_2^+$ ($[M+H]^+$): 158.1176, found 158.1176.
FTIR (ATR, cm^{-1}): 3001, 2976, 2932, 1712, 1474, 1457, 1367, 1304, 1222, 1148, 749.



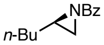
***N*-Cbz-2-methyl aziridine (S3):** A flame-dried flask was charged with 2-methylaziridine (500.0 mg, 0.62 mL, 8.8 mmol, 1.0 equiv), DCM (0.1 M, 87 mL), and triethylamine (1.77 g, 2.44 mL, 17.5 mmol, 2.0 equiv). The solution was cooled to 0 °C and benzyl chloroformate (1.64 g, 1.38 mL, 9.6 mmol, 1.1 equiv) was added dropwise. The reaction was stirred at room temperature overnight. The reaction mixture was then quenched with saturated $NaHCO_3$. The aqueous layer was extracted with DCM (2x). The organic layers were combined and washed with brine, dried over $MgSO_4$, filtered, and concentrated. The resulting oil was purified by flash chromatography (10% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 85 °C, full vacuum) to give the product as a clear oil (54% yield). Spectral data are in agreement with reported values.[6]

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.41 – 7.28 (m, 5H), 5.16 – 5.11 (m, 2H), 2.52 (pd, *J* = 5.6, 3.8 Hz, 1H), 2.33 (d, *J* = 5.9 Hz, 1H), 1.96 (d, *J* = 3.8 Hz, 1H), 1.28 (d, *J* = 5.6 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 163.5, 136.0, 128.7, 128.4, 128.3, 68.2, 34.0, 32.8, 17.6.
HRMS (APCI): calculated for $C_{11}H_{14}NO_2^+$ ($[M+H]^+$): 192.1019, found 192.1019.
FTIR (ATR, cm^{-1}): 3066, 3033, 3002, 2967, 2932, 1713, 1455, 1408, 1379, 1290, 1203, 1151, 1060, 1027, 695.



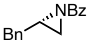
***N*-benzoyl-2-ethyl aziridine (2a)** was prepared according to General Procedure B from 2-aminobutan-1-ol (15.0 mmol). The product was isolated by flash chromatography (10% Et_2O/hexanes). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 80 °C, full vacuum) to give the product as a clear oil (31% yield).

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.03 (dd, *J* = 8.1, 1.3 Hz, 2H), 7.58 – 7.50 (m, 1H), 7.47 – 7.42 (m, 2H), 2.56 – 2.51 (m, 1H), 2.50 (d, *J* = 5.9 Hz, 1H), 2.19 (d, *J* = 3.6 Hz, 1H), 1.89 (dqd, *J* = 14.7, 7.4, 4.5 Hz, 1H), 1.51 (dp, *J* = 14.5, 7.4 Hz, 1H), 1.03 (t, *J* = 7.5 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 179.5, 133.6, 132.7, 129.2, 128.5, 39.9, 31.1, 25.3, 10.4.
HRMS (APCI): calculated for $C_{11}H_{14}NO^+$ ($[M+H]^+$): 176.1070, found 176.1076.
FTIR (ATR, cm^{-1}): 3060, 2966, 2931, 2878, 1670, 1315, 1294, 707.



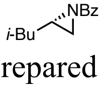
***N*-benzoyl-2-*n*-butyl aziridine (3a)** was prepared according to General Procedure B from (R)-2-aminohexan-1-ol hydrochloride (5.0 mmol). The product was isolated by flash chromatography (5% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 90 °C, full vacuum) to give the product as a clear oil (41% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 (dd, J = 8.3, 1.4 Hz, 2H), 7.65 – 7.49 (m, 1H), 7.49 – 7.38 (m, 2H), 2.58 – 2.52 (m, 1H), 2.50 (d, J = 5.9 Hz, 1H), 2.19 (d, J = 3.7 Hz, 1H), 1.94 – 1.80 (m, 1H), 1.51 – 1.33 (m, 5H), 0.91 (t, J = 7.2 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 179.5, 133.6, 132.7, 129.2, 128.5, 38.7, 32.0, 31.8, 28.8, 22.5, 14.1.
HRMS (APCI): calculated for $C_{13}H_{18}NO^+$ ($[M+H]^+$): 204.1383, found 204.1383.
FTIR (ATR, cm^{-1}): 3058, 2992, 2957, 2859, 1672, 1449, 1315, 1297, 723, 707.
Optical Rotation: $[\alpha]_D^{23}$ (*c* 1.0 g/100 mL, $CHCl_3$) = -68.4.



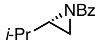
***N*-benzoyl-2-benzyl aziridine (4a)** was prepared according to General Procedure B from L-phenylalaninol (5.0 mmol). The product was isolated by flash chromatography (10% EtOAc/hexanes). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 125 °C, full vacuum) to give the product as a clear oil (29% yield). Spectral data are in agreement with reported values.[7]

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.05 – 7.96 (m, 2H), 7.54 (tt, *J* = 7.3, 1.9 Hz, 1H), 7.47 – 7.37 (m, 2H), 7.36 – 7.29 (m, 2H), 7.29 – 7.22 (m, 3H)[a], 3.22 – 3.15 (m, 1H), 2.86 – 2.75 (m, 2H), 2.58 – 2.53 (m, 1H), 2.30 – 2.26 (m, 1H).
[a]Overlaps with solvent residual peak.
^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 179.3, 137.5, 133.3, 132.8, 129.3, 129.0, 128.8, 128.5, 126.9, 38.8, 38.6, 31.7.
HRMS (APCI): calculated for $C_{16}H_{16}NO^+$ ($[M+H]^+$): 238.1226, found 238.1228.
FTIR (ATR, cm^{-1}): 3084, 3060, 3028, 2994, 2916, 1670, 1316, 1294, 723, 699.



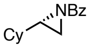
***N*-benzoyl-2-isobutyl aziridine (5a)** was prepared according to General Procedure B from L-leucinol (5.0 mmol). The product was isolated by flash chromatography (3% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 70 °C, full vacuum) to give the product as a clear oil (27% yield).

^{1}H NMR (600 MHz, CDCl$_3$): δ 8.05 – 8.02 (m, 2H), 7.57 – 7.52 (m, 1H), 7.48 – 7.42 (m, 2H), 2.61 – 2.56 (m, 1H), 2.53 – 2.50 (m, 1H), 2.20 (d, *J* = 3.7 Hz, 1H), 1.86 – 1.75 (m, 2H), 1.33 – 1.19 (m, 1H), 1.00 – 0.96 (m, 6H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 179.5, 133.6, 132.7, 129.2, 128.5, 41.4, 37.5, 32.5, 27.1, 22.9, 22.6.
HRMS (APCI): calculated for $C_{13}H_{18}NO^+$ ($[M+H]^+$): 204.1383, found 204.1389.
FTIR (ATR, cm^{-1}): 3060, 2991, 2956, 2926, 2870, 1671, 1316, 1300, 707.



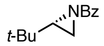
***N*-benzoyl-2-isopropyl aziridine (6a)** was prepared according to General Procedure B from L-valinol (10.0 mmol). The product was isolated by flash chromatography (10% Et$_2$O/hexanes). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 90 °C, full vacuum) to give the product as a clear oil (37% yield).

^{1}H NMR (500 MHz, CDCl$_3$): δ 8.05 – 8.01 (m, 2H), 7.57 – 7.51 (m, 1H), 7.47 – 7.41 (m, 2H), 2.44 (td, *J* = 6.1, 3.7 Hz, 1H), 2.40 (dd, *J* = 6.1, 0.6 Hz, 1H), 2.27 (dd, *J* = 3.5, 0.6 Hz, 1H), 1.87 – 1.74 (m, 1H), 1.08 (d, *J* = 6.7 Hz, 3H), 0.99 (d, *J* = 6.9 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 179.7, 133.5, 132.7, 129.3, 128.5, 43.8, 30.3, 30.0, 20.1, 18.4.
HRMS (APCI): calculated for $C_{12}H_{16}NO^+$ ($[M+H]^+$): 190.1226, found 190.1233.
IR (ATM cm^{-1}): 3061, 2960, 2928, 2874, 1670, 1316, 1290, 706.
Optical Rotation: $[\alpha]_D^{23}$ (*c* 1.0 g/100 mL, CHCl$_3$) = +109.2.



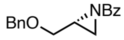
***N*-benzoyl-2-cyclohexyl aziridine (7a)** was prepared according to General Procedure B from (S)-2-amino-2-cyclohexylethanol (5.0 mmol). The product was isolated by flash chromatography (10% EtOAc/hexanes). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 100 °C, full vacuum) to give the product as a clear oil (28% yield).

^{1}H NMR (600 MHz, CDCl$_3$): δ 8.05 – 8.02 (m, 2H), 7.56 – 7.51 (m, 1H), 7.44 (t, J = 7.7 Hz, 2H), 2.46 – 2.42 (m, 1H), 2.39 (d, *J* = 6.2 Hz, 1H), 2.29 (d, *J* = 3.7 Hz, 1H), 1.91 – 1.84 (m, 1H), 1.81 – 1.74 (m, 3H), 1.72 – 1.65 (m, 1H), 1.48 – 1.37 (m, 1H), 1.33 – 1.14 (m, 4H), 1.14 – 1.04 (m, 1H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 179.8, 133.5, 132.7, 129.2, 128.5, 42.8, 39.7, 30.9, 30.8, 29.3, 26.4, 26.0, 25.9.
HRMS (APCI): calculated for $C_{15}H_{20}NO^+$ ($[M+H]^+$): 230.1539, found 230.1540.
IR (ATM cm^{-1}): 3064, 2986, 2922, 2850, 1672, 1317, 1305, 708.



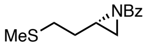
***N*-benzoyl-2-*tert*-butyl aziridine (8a)** was prepared according to General Procedure B from L-*tert*-leucinol (10.0 mmol). The product was isolated by flash chromatography (10% Et_2O/hexanes). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 115 °C, full vacuum) to give the product as a clear oil (51% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.09 – 8.01 (m, 2H), 7.59 – 7.50 (m, 1H), 7.48 – 7.39 (m, 2H), 2.47 (dd, J = 6.3, 3.9 Hz, 1H), 2.35 (dd, J = 3.8, 0.7 Hz, 1H), 2.29 (dd, J = 6.3, 0.7 Hz, 1H), 1.01 (s, 9H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 179.9, 133.5, 132.7, 129.3, 128.4, 46.5, 30.8, 29.7, 26.7.
HRMS (ESI-TOF): calculated for $C_{13}H_{18}NO^+$ ($[M+H]^+$): 204.1383, found 204.1389.
IR (ATM cm^{-1}): 3060, 3031, 2955, 2904, 2869, 1672, 1318, 1306, 1274, 714, 705.

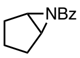


(R)-(2-((benzyloxy)methyl)aziridin-1-yl)(phenyl)methanone (9a) was prepared according to General Procedure B from H-Serinol(Bzl) (2.5 mmol). The product was isolated by flash chromatography (5% to 25% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated to give the product as a yellow oil (26% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.16 – 8.07 (m, 2H), 7.58 – 7.50 (m, 1H), 7.45 – 7.38 (m, 2H), 7.38 – 7.27 (m, 5H), 4.61 – 4.52 (m, 2H), 3.75 – 3.65 (m, 2H), 2.87 (tdd, J = 5.8, 4.4, 3.6 Hz, 1H), 2.57 (d, J = 6.1 Hz, 1H), 2.35 (d, J = 3.6 Hz, 1H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 178.8, 137.9, 133.1, 132.9, 129.5, 128.6, 128.5, 128.0, 127.9, 73.4, 70.6, 37.3, 29.1.
HRMS (APCI): calculated for $C_{17}H_{18}NO_2^+$ ($[M+H]^+$): 268.1332, found 268.1332.
IR (ATM cm^{-1}): 3062, 3029, 2997, 1670, 1449, 1342, 1315, 1297, 1224, 1094, 1073, 1026, 725, 698.

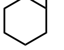


(S)-(2-(2-(methylthio)ethyl)aziridin-1-yl)(phenyl)methanone (10a) was prepared according to General Procedure B from (S)-2-amino-4-(methylthio)butan-1-ol (2.5 mmol). The product was isolated by flash chromatography (5% to 25% EtOAc/hexanes + 5% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated to give the product as a yellow oil (12% yield).
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.08 – 7.98 (m, 2H), 7.61 – 7.52 (m, 1H), 7.49 – 7.41 (m, 2H), 2.72 – 2.66 (m, 1H), 2.67 – 2.62 (m, 2H), 2.53 (d, J = 5.9 Hz, 1H), 2.28 (d, J = 3.6 Hz, 1H), 2.16 – 2.06 (m, 4H), 1.87 – 1.70 (m, 1H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 179.3, 133.4, 132.9, 129.2, 128.6, 37.4, 32.1, 32.0, 31.3, 15.9.
HRMS (APCI): calculated for $C_{12}H_{16}NOS^+$ ($[M+H]^+$): 222.0947, found 222.0947.
IR (ATM cm^{-1}): 3058, 2988, 2914, 2851, 2259, 1670, 1449, 1405, 1315, 1296, 708.



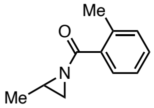
(6-azabicyclo[3.1.0]hexan-6-yl)(phenyl)methanone (11a) was prepared according to General Procedure A from 6-azabicyclo[3.1.0]hexane (3.0 mmol) and benzoyl chloride. The resulting oil was purified by flash chromatography (5% to 10% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 90 °C, full vacuum) to give the product as a clear oil (86% yield). Spectral data are in agreement with reported literature values.[8]

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 – 7.94 (m, 2H), 7.57 – 7.49 (m, 1H), 7.46 – 7.41 (m, 2H), 3.19 (s, 2H), 2.19 – 2.10 (m, 2H), 1.83 – 1.61 (m, 3H), 1.48 – 1.30 (m, 1H).
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ 178.3, 133.8, 132.5, 128.9, 128.5, 43.8, 27.1, 19.7.
HRMS (ESI-TOF): calculated for $C_{12}H_{14}NO^+$ ($[M+H]^+$): 188.1070, found 188.1070.
FTIR (ATR, cm^{-1}): 3058, 3027, 2956, 2859, 1664, 1381, 1318, 1282, 703.



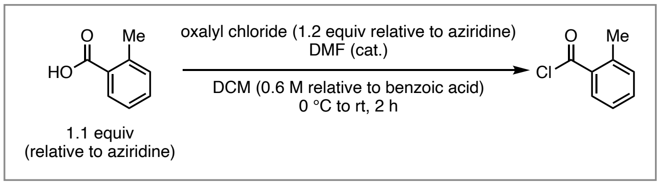
(7-azabicyclo[4.1.0]heptan-7-yl)(phenyl)methanone (12a) was prepared according to General Procedure B from trans-2-aminocyclohexan-1-ol (5.0 mmol). The product was isolated by flash chromatography (5% NEt_3/hexanes). Fractions containing product (determined by TLC, UV light) were collected and concentrated to give the product as a white solid (31% yield). Spectral data are in agreement with reported values.[8]

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.05 – 7.96 (m, 2H), 7.59 – 7.49 (m, 1H), 7.49 – 7.40 (m, 2H), 2.76 (m, 2H), 2.13 – 2.03 (m, 2H), 1.97 – 1.85 (m, 2H), 1.66 – 1.49 (m, 2H), 1.43 – 1.30 (m, 2H).
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ 180.4, 133.8, 132.6, 129.2, 128.5, 37.2, 24.1, 20.2.
HRMS (ESI-TOF): calculated for $C_{13}H_{16}NO^+$ ($[M+H]^+$): 202.1226, found 202.1225.
FTIR (ATR, cm^{-1}): 3060, 3030, 3005, 2933, 2858, 1670, 1312, 1288, 704.

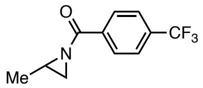


(2-methylaziridin-1-yl)(*o*-tolyl)methanone (13a) was prepared according to General Procedure A from 2-methyl aziridine (8.8 mmol) and synthesized 2-methylbenzoyl chloride (see below). The product was purified by flash chromatography (2% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 75 °C, full vacuum) to give the product as a clear oil (65% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.89 (dd, J = 7.8, 1.5 Hz, 1H), 7.37 (td, J = 7.5, 1.5 Hz, 1H), 7.29 – 7.19 (m, 2H), 2.53 (s, 3H), 2.52 – 2.48 (m, 1H), 2.46 (d, J = 5.7 Hz, 1H), 2.08 (d, J = 3.5 Hz, 1H), 1.30 (d, J = 5.4 Hz, 3H).
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ 181.1, 139.1, 134.0, 131.7, 131.3, 130.3, 125.8, 34.4, 32.3, 21.3, 17.8.
HRMS (APCI): calculated for $C_{11}H_{14}NO^+$ ($[M+H]^+$): 176.1070, found 176.1075.
IR (ATM cm^{-1}): 3062, 2990, 2966, 2928, 1673, 1404, 1306, 1286, 743.

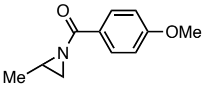


2-methylbenzoyl chloride: A flame-dried flask was charged with 2-methylbenzoic acid (1.311 g, 9.6 mmol, 1.1 equiv relative to aziridine). The flask was evacuated and backfilled with N_2 (3x). DCM (0.6 M relative to benzoic acid, 16 mL) and a few drops of DMF were added. The reaction was cooled to 0 °C and oxalyl chloride (1.334 g, 0.92 mL, 10.5 mmol, 1.2 equiv relative to aziridine) was added dropwise. The reaction was stirred at room temperature until the carboxylic acid had fully dissolved and bubbling had stopped (~2 hours). The reaction was concentrated under reduced pressure to yield 2-methylbenzoyl chloride that was used without further purification.



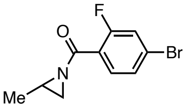
(2-methylaziridin-1-yl)(4-(trifluoromethyl)phenyl)methanone (14a) was prepared according to General Procedure A from 2-methyl aziridine (4.4 mmol) and 4-(trifluoromethylbenzoyl) chloride. The product was purified by flash chromatography (5% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 75 °C, full vacuum) to give the product as a clear oil (71% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, *J* = 8.1 Hz, 2H), 7.72 (d, *J* = 8.1 Hz, 2H), 2.62 (pd, *J* = 5.4, 3.6 Hz, 1H), 2.57 (d, *J* = 5.8 Hz, 1H), 2.19 (d, *J* = 3.6 Hz, 1H), 1.40 (d, *J* = 5.4 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 178.0, 136.8, 134.2 (q, *J* = 32.6 Hz), 129.5, 125.6 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 272.6 Hz), 35.0, 32.5, 17.8.
^{19}F NMR (376 MHz, $CDCl_3$): δ -63.0 (s).
HRMS (APCI): calculated for $C_{11}H_{11}F_3NO^+$ ($[M+H]^+$): 230.0787, found 230.0791.
IR (ATM cm^{-1}): 2998, 2970, 2932, 1675, 1411, 1312, 1164, 1126, 1107, 1065, 778, 717.



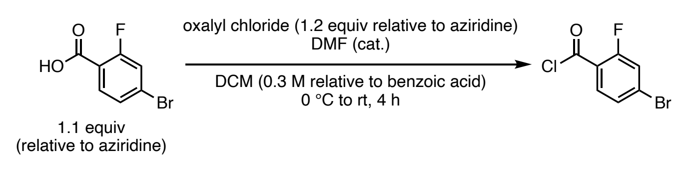
(4-methoxyphenyl)(2-methylaziridin-1-yl)methanone (15a) was prepared according to General Procedure A from 2-methyl aziridine (4.4 mmol) and 4-methoxybenzoyl chloride. The product was purified by flash chromatography (10% EtOAc/hexanes + 1% NEt_3). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 130 °C, full vacuum) to give the product as a clear oil (74% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 – 7.96 (m, 2H), 6.98 – 6.89 (m, 2H), 3.87 (s, 3H), 2.58 – 2.53 (m, 1H), 2.52 (d, *J* = 5.8 Hz, 1H), 2.11 (d, *J* = 3.6 Hz, 1H), 1.38 (d, *J* = 5.3 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 179.0, 163.3, 131.2, 126.3, 113.7, 55.6, 34.7, 32.2, 17.9.
HRMS (APCI): calculated for $C_{11}H_{14}NO^+$ ($[M+H]^+$): 192.1019, found 192.1025.
IR (ATM cm^{-1}): 3065, 2995, 2965, 2932, 2840, 1664, 1603, 1301, 1254, 1167, 776.



(4-bromo-2-fluorophenyl)(2-methylaziridin-1-yl)methanone (16a) was prepared according to a modified General Procedure A from 2-methyl aziridine (4.4 mmol) and synthesized 4-bromo-2-fluorobenzoyl chloride (see below). NEt_3 was added to a solution of 4-bromo-2-fluorobenzoyl chloride in DCM followed by addition of 2-methyl aziridine at 0 °C. The product was purified by flash chromatography (10% EtOAc/hexanes). Fractions containing product (determined by TLC, UV light) were collected and concentrated. The collected oil was further purified by distillation (hot plate temperature = 90 °C, full vacuum) to give the product as a clear oil (65% yield).

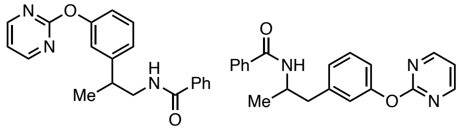
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.89 – 7.77 (m, 1H), 7.43 – 7.31 (m, 2H), 2.71 – 2.64 (m, 1H), 2.53 (dd, *J* = 5.8, 0.8 Hz, 1H), 2.17 (dd, *J* = 3.7, 1.0 Hz, 1H), 1.34 (d, *J* = 5.5 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 175.0 (d, *J* = 4.1 Hz), 161.1 (d, *J* = 262.1 Hz), 133.0 (d, *J* = 2.6 Hz), 127.8 (d, *J* = 3.8 Hz), 127.5 (d, *J* = 9.7 Hz), 121.3 (d, *J* = 11.5 Hz), 120.6 (d, *J* = 26.3 Hz), 35.3 (d, *J* = 1.9 Hz), 32.8 (d, *J* = 1.9 Hz), 17.7 (d, *J* = 1.4 Hz).
^{19}F NMR (565 MHz, $CDCl_3$): δ -106.9 (t, *J* = 9.0 Hz).
HRMS (ESI-TOF): calculated for $C_{10}H_{10}{}^{79}BrFNO^{+}$ ($[M+H]^{+}$): 257.9924, found 257.9924.
IR (ATM cm^{-1}): 3069, 2995, 2969, 2932, 1663, 1597, 1405, 1311, 1214, 772.



4-bromo-2-fluorobenzoyl chloride: A flame-dried flask was charged with 4-bromo-2-fluorobenzoic acid (1.055 g, 4.8 mmol, 1.1 equiv relative to aziridine). The flask was evacuated and backfilled with N_2 (3x). DCM (0.6 M relative to benzoic acid, 8 mL) and a few drops of DMF were added. The reaction was cooled to 0 °C and oxalyl chloride (666.8 mg, 0.46 mL, 5.3 mmol, 1.2 equiv relative to aziridine) was added dropwise. The reaction was stirred at room temperature for 4 hours (DCM (8 mL) added at 1.5 hours). The reaction was concentrated under reduced pressure to yield 4-bromo-2-fluorobenzoyl chloride that was used without further purification. At the time this manuscript was prepared, 4-bromo-2-fluorobenzoyl chloride was commercially available.

5. Characterization of Cross-Coupled Products

5.1. Cross-Coupling of 1a with Aryl Iodides



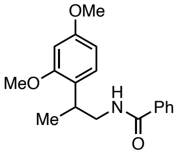
major (branched) *minor (linear)*

***N*-(2-(4-(pyrimidin-2-yloxy)phenyl)propyl)benzamide (A-1)** was prepared according to General Procedure C from **1a** and 2-(4-iodophenoxy)pyrimidine. The product was isolated by flash chromatography (35% acetone/hexanes + 1% NEt$_3$) to produce **A-1** as a yellow oil (45% yield (14:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 53% yield (12.5:1)
Run 2: 37% yield (15.4:1)

Branched Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 8.48 (d, J = 4.9 Hz, 2H), 7.66 – 7.61 (m, 2H), 7.48 – 7.32 (m, 4H), 7.15 (dt, J = 7.7, 1.4 Hz, 1H), 7.11 – 7.06 (m, 2H), 7.01 (t, J = 4.8 Hz, 1H), 6.20 (br s, 1H), 3.90 – 3.81 (m, 1H), 3.38 (ddd, J = 13.5, 8.8, 5.0 Hz, 1H), 3.18 – 3.07 (m, 1H), 1.35 (d, J = 7.0 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 167.7, 165.4, 159.8, 153.3, 146.3, 134.8, 131.5, 130.1, 128.6, 127.0, 124.5, 120.7, 120.0, 116.3, 46.7, 39.7, 19.1.

Linear Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 8.56 (d, J = 4.7 Hz, 2H), 7.70 – 7.67 (m, 2H), 7.54 – 7.31 (m, 4H), 7.21 – 6.96 (m, 4H), 6.04 (d, J = 8.3 Hz, 1H), 4.55 – 4.42 (m, 1H), 2.98 (dd, J = 13.5, 5.4 Hz, 1H), 2.90 (dd, J = 13.6, 6.9 Hz, 1H), 1.24 (d, J = 6.7 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$)[a,b]: δ 166.98, 165.47, 159.90, 153.01, 139.81, 129.75, 128.65, 126.94, 126.91, 124.46, 123.03, 120.63, 119.85, 116.27, 46.40, 42.12, 19.99.
[a] Two decimal places shown to distinguish between peaks at δ 126.94 and 126.91.
[b] Due to a trace impurity in the sample, ^{13}C{^{1}H} assignments for the linear isomer are less certain.

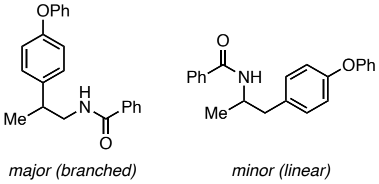
Mixture of Isomers:
HRMS (APCI): calculated for $C_{20}H_{20}N_3O_2^+$ ([M+H]$^+$): 334.1550, found 334.1549.
IR (ATM cm^{-1}): 3313 (br), 3071, 3062, 2967, 2928, 2915, 1641, 1571, 1540, 1488, 1405, 1305, 698.



***N*-(2-(2,4-dimethoxyphenyl)propyl)benzamide (B-1)** was prepared according to General Procedure C from **1a** and 1-iodo-2,4-dimethoxybenzene. The product was isolated by flash chromatography (20% acetone/hexanes) to produce **B-1** as a white solid (22% yield (>20:1)). The product was isolated with high selectivity for the branched isomer (>20:1); as such, only branched isomer characterization data is provided.

Run 1: 21% yield (>20:1)
Run 2: 22% yield (>20:1)

^{1}H NMR (500 MHz, CDCl$_3$): δ 7.63 (d, *J* = 7.4 Hz, 2H), 7.48 – 7.41 (m, 1H), 7.42 – 7.34 (m, 2H), 7.14 (d, *J* = 8.4 Hz, 1H), 6.50 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.47 (d, *J* = 2.4 Hz, 1H), 6.28 (br s, 1H), 3.83 – 3.76 (m, 6H), 3.74 – 3.65 (m, 1H), 3.52 – 3.40 (m, 2H), 1.30 (d, *J* = 6.4 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$)^a: δ 167.52, 159.53, 158.13, 135.10, 131.27, 128.56, 127.75, 126.86, 124.56, 104.65, 98.83, 55.53, 55.47, 46.46, 31.93, 18.28.
^{a}Two decimal places shown to distinguish between peaks at δ 55.53 and 55.47.
HRMS (APCI): calculated for $C_{18}H_{22}NO_3^+$ ([M+H]$^+$): 300.1594, found 300.1594.
IR (ATM cm^{-1}): 3320 (br), 3067, 3004, 2995, 2958, 2934, 2876, 2837, 1639, 1612, 1582, 1540, 1506, 1489, 1457, 1292, 1261, 1208, 1158, 1034, 933, 711, 695.

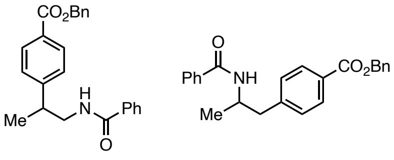


***N*-(2-(4-phenoxyphenyl)propyl)benzamide (C-1)** was prepared according to General Procedure C from **1a** and benzyl 1-iodo-4-phenoxybenzene. The product was isolated by flash chromatography (15% acetone/hexanes) to produce **C-1** as a white solid (71% yield (11:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 74% yield (10.0:1)
Run 2: 68% yield (11.1:1)
Partial isolation of branched and linear isomers was done via preparative thin layer chromatography (20% EtOAc/hexanes) to aid in characterization.

Branched Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 7.66 – 7.61 (m, 2H), 7.51 – 7.44 (m, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.37 – 7.29 (m, 2H), 7.25 – 7.20 (m, 2H), 7.13 – 7.07 (m, 1H), 7.05 – 6.97 (m, 4H), 6.01 (br s, 1H), 3.82 (dt, *J* = 13.5, 6.4 Hz, 1H), 3.41 (ddd, *J* = 13.6, 8.8, 5.0 Hz, 1H), 3.13 – 3.04 (m, 1H), 1.34 (d, *J* = 7.0 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 167.6, 157.4, 156.1, 139.0, 134.8, 131.5, 129.9, 128.7, 128.6, 126.9, 123.4, 119.3, 118.9, 46.8, 39.3, 19.5.

Linear Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 7.70 (d, *J* = 6.9 Hz, 2H), 7.51 – 7.31 (m, 5H), 7.23 – 7.17 (m, 2H), 7.12 – 7.09 (m, 1H), 7.02 – 6.94 (m, 4H), 5.93 (br s, 1H), 4.52 – 4.40 (m, 1H), 2.92 (dd, *J* = 13.6, 5.7 Hz, 1H), 2.84 (dd, *J* = 13.6, 7.0 Hz, 1H), 1.24 (d, *J* = 6.7 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 166.9, 157.5, 156.0, 135.0, 132.9, 131.5, 130.9, 129.9, 128.7, 127.0, 123.3, 119.1, 118.9, 46.7, 41.8, 20.2.

Mixture of Isomers:
HRMS (APCI): calculated for $C_{22}H_{22}NO_2^+$ ([M+H]$^+$): 332.1645, found 332.1644.
IR (ATM cm^{-1}): 3319 (br), 3060, 3038. 2967, 2930, 2873, 1636, 1540, 1507, 1489, 1237, 870, 848, 692.



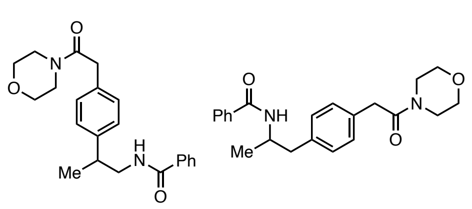
major (branched) *minor (linear)*

Benzyl 4-(1-benzamidopropan-2-yl)benzoate (D-1) was prepared according to General Procedure C from **1a** and benzyl 4-iodobenzoate. The product was isolated by flash chromatography (20% acetone/hexanes) to produce **D-1** as a white solid (87% yield (8:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 89% yield (8.3:1)
Run 2: 85% yield (6.9:1)
Partial isolation of branched and linear products was done via preparative thin layer chromatography (20% EtOAc/hexanes) to aid in characterization.

Branched Isomer
^{1}H NMR (500 MHz, CDCl$_3$): δ 8.05 (d, J = 8.1 Hz, 2H), 7.61 (d, J = 7.2 Hz, 2H), 7.50 – 7.28 (m, 10H), 6.00 (br s, 1H), 5.36 (s, 2H), 3.83 (dt, J = 12.8, 6.4 Hz, 1H), 3.44 (ddd, J = 13.7, 8.7, 5.2 Hz, 1H), 3.23 – 3.11 (m, 1H), 1.35 (d, J = 7.0 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$)[a]: δ 167.63, 166.39, 149.85, 136.18, 134.60, 131.62, 130.37, 128.91, 128.74, 128.73, 128.40, 128.31, 127.47, 126.87, 66.80, 46.51, 40.08, 19.20.
[a]Two decimal places shown to distinguish between peaks at δ 128.74 and 128.73.

Linear Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 8.01 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 7.3 Hz, 2H), 7.50 – 7.28 (m, 10H), 5.93 (br s, 1H), 5.35 (s, 2H), 4.49 (hept, J = 6.8 Hz, 1H), 3.02 (dd, J = 13.5, 5.7 Hz, 1H), 2.91 (dd, J = 13.5, 7.1 Hz, 1H), 1.22 (d, J = 6.7 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 166.94, 166.47, 143.69, 136.20, 134.76, 131.63, 130.01, 129.72, 128.76[b], 128.73[c], 128.64, 128.37, 128.34[d], 126.88, 66.78, 42.54, 30.75, 20.08.
[a]Two decimal places shown to distinguish between peaks at δ 128.76 and 128.73.
[b–d]Peak overlaps with branched isomer, appears to be linear isomer based on sample with higher concentration of linear sample.

Mixture of Isomers:
HRMS (APCI): calculated for $C_{24}H_{24}NO_3^+$ ([M+H]$^+$): 374.1751, found 374.1747.
IR (ATM cm^{-1}): 3326 (br), 3069, 2963, 2932, 1716, 1639, 1540, 1272, 1102, 707, 696.



major (branched) *minor (linear)*

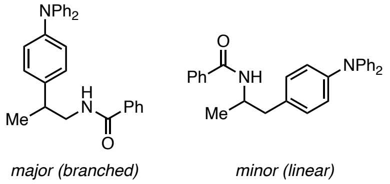
***N*-(2-(4-(2-morpholino-2-oxoethyl)phenyl)propyl)benzamide (E-1)** was prepared according to General Procedure C from **1a** and 2-(4-iodophenyl)-1-morpholinoethan-1-one. The product was isolated by flash chromatography (40% acetone/hexanes) to produce a **E-1** as a slightly yellow oil (62% yield (12:1)). The product was isolated and characterized as a mixture of isomers.

Run 1: 59% yield (12.5:1)
Run 2: 66% yield (11.1:1)

Branched Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 7.64 – 7.60 (m, 2H), 7.51 – 7.43 (m, 1H), 7.41 – 7.35 (m, 2H), 7.24 – 7.19 (m, 4H), 5.99 (br s, 1H), 3.81 (dt, *J* = 13.0, 6.4 Hz, 1H), 3.71 (s, 2H), 3.65 – 3.63 (m, 4H), 3.51 – 3.38 (m, 5H), 3.12 – 3.02 (m, 1H), 1.33 (d, *J* = 7.0 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 169.8, 167.6, 142.9, 134.8, 133.4, 131.5, 129.2, 128.7, 127.8, 126.9, 66.9[a], 66.6[a], 46.7[b], 46.6[b], 42.3, 40.4, 39.6, 19.4.
[a,b]Rotamer

Linear Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 7.68 (d, *J* = 7.5 Hz, 2H), 7.52 – 7.32 (m, 3H), 7.25 – 7.15 (m, 4H), 5.91 (d, *J* = 8.2 Hz, 1H), 4.52 – 4.40 (m, 1H), 3.70 (s, 2H), 3.63 – 3.62 (m, 4H), 3.52 – 3.38 (m, 4H), 2.92 (dd, *J* = 13.6, 5.8 Hz, 1H), 2.84 (dd, *J* = 13.6, 7.0 Hz, 1H), 1.22 (d, *J* = 6.6 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 169.8, 166.9, 142.9, 136.7, 134.9, 133.1, 131.6, 130.1, 128.8, 126.9, 66.6[a], 46.6[b,c], 42.2, 40.6, 20.2.
[a,b]Only single signal for rotameric carbon is reported due to overlap with branched isomer.
[c]Two carbons, see HMBC.

Mixture of Isomers:
HRMS (APCI): calculated for $C_{22}H_{27}N_2O_3^+$ ([M+H]$^+$): 367.2016, found 367.2015.
IR (ATM cm^{-1}): 3324 (br), 2972, 2898, 2867,1636, 1538, 1458, 1431, 1299, 115, 717, 697.



***N*-(2-(4-(diphenylamino)phenyl)propyl)benzamide (F-1)** was prepared according to General Procedure C from **1a** and 4-iodo-*N*,*N*-diphenylaniline. The product was isolated by flash chromatography (15% acetone/hexanes) to produce **F-1** as an off-white solid (63% yield (11:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 63% yield (10.0:1)
Run 2: 62% yield (11.3:1)

Branched Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 7.64 (d, *J* = 7.5 Hz, 2H), 7.51 – 7.45 (m, 1H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.27 – 7.21 (m, 4H), 7.13 (d, *J* = 8.4 Hz, 2H), 7.10 – 7.04 (m, 6H), 7.01 (t, *J* = 7.3 Hz, 2H), 6.00 (br s, 1H), 3.81 (dt, *J* = 13.1, 6.4 Hz, 1H), 3.41 (ddd, *J* = 12.0, 8.0, 4.2 Hz, 1H), 3.09 – 2.99 (m, 1H), 1.34 (d, *J* = 7.0 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 167.5, 147.9, 146.7, 138.3, 135.0, 131.5, 129.4, 128.7, 128.1, 126.9, 124.5, 124.2, 122.8, 46.8, 39.3, 19.4.

Linear Isomer:

^{1}H NMR (500 MHz, CDCl$_3$): δ 7.69 (d, *J* = 7.4 Hz, 2H), 7.51 – 7.17 (m, 7H), 7.17 – 6.97 (m, 10H), 5.92 (d, *J* = 8.1 Hz, 1H), 4.45 (hept, *J* = 6.8 H, 1H), 2.88 (dd, *J* = 13.6, 6.0 Hz, 1H), 2.82 (dd, *J* = 13.6, 6.9 Hz, 1H), 1.26 (d, *J* = 6.4 Hz, 3H).

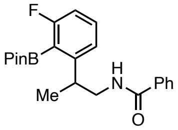
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$)[a]: δ 166.87, 147.97, 146.50, 135.10, 132.33, 131.49, 131.46, 130.44, 129.33, 126.95, 124.35, 124.17, 122.75, 46.71, 42.01, 20.34.

[a] Two decimal places shown to distinguish between peaks at δ 131.49 and 131.46.

Mixture of Isomers:

HRMS (APCI): calculated for $C_{28}H_{27}N_2O^+$ ([M+H]$^+$): 407.2118, found 407.2118.

IR (ATM cm^{-1}): 3322 (br), 3056, 3028, 2965, 2930, 1636, 1588, 1540, 1508, 1491, 1313, 1278, 754, 712, 695.



***N*-(2-(3-fluoro-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propyl)benzamide (G-1)** was prepared according to General Procedure C from **1a** and 2-(2-fluoro-6-iodophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane. Yields were determined by ^{19}F NMR versus 1-fluoronaphthalene as an external standard (25% yield (>20:1)). The product was isolated for characterization by preparative thin layer chromatography (60% Et$_2$O/hexanes). The product was isolated with high selectivity for the branched isomer (>20:1); as such, only branched characterization data is provided.
Run 1: 27% yield (>20:1)
Run 2: 22% yield (>20:1)

^{1}H NMR (500 MHz, CDCl$_3$): δ 7.71 (d, *J* = 7.3 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.41 – 7.32 (m, 3H), 7.13 (d, *J* = 7.8 Hz, 1H), 6.89 (5, *J* = 8.5 Hz, 1H), 6.73 (br s, 1H), 3.70 (dt, *J* = 13.3, 4.3 Hz, 1H), 3.57 (ddd, *J* = 13.2, 10.8, 5.3 Hz, 1H), 3.20 – 3.09 (m, 1H), 1.40 – 1.33 (m, 15H).

^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 167.5, 165.7 (d, *J* = 243.8 Hz), 150.9 (d, *J* = 7.6 Hz), 134.6, 132.4 (d, *J* = 9.0 Hz), 131.3, 128.4, 127.2, 121.3 (d, *J* = 2.8 Hz), 117.5[a], 113.2 (d, *J* = 23.7 Hz), 85.0, 48.0, 38.9, 25.1[b], 24.8[b], 20.3.

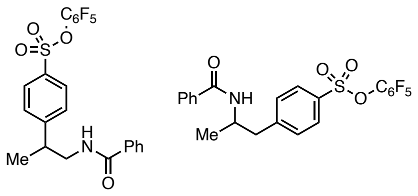
[a] Carbon directly connected to boron not observed in ^{13}C{^{1}H} NMR but observed in HMBC.

[b] Rotameric carbons on the methyl substituents of the BPin.

^{19}F NMR (376 MHz, CDCl$_3$): δ -104.3 (ddd, *J* = 9.2, 6.5, 3.7 Hz).

HRMS (APCI): calculated for $C_{22}H_{28}BFNO_3^+$ ([M+H]$^+$): 384.2141, found 384.2138.

IR (ATM cm^{-1}): 3354 (br), 3059, 2976, 2932, 2874, 1644, 1613, 1534, 1489, 1452, 1381, 1366, 1317, 1224, 1142, 855, 738, 712, 693.



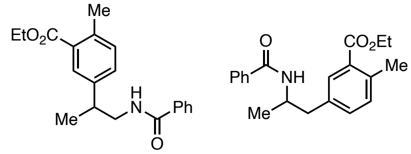
major (branched) *minor (linear)*

Perfluorophenyl 4-(1-benzamidopropan-2-yl)benzenesulfonate (H-1) was prepared according to General Procedure C from **1a** and perfluorophenyl 4-iodobenzenesulfonate. The product was isolated by flash chromatography (20% acetone/hexanes) to produce a **H-1** as a white solid (90% yield (7:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 94% yield (7.3:1)
Run 2: 85% yield (7.4:1)

Branched Isomer:
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.95 (d, *J* = 8.5 Hz, 2H), 7.66 – 7.61 (m, 2H), 7.54 – 7.47 (m, 3H), 7.43 – 7.38 (m, 2H), 6.03 (br s, 1H), 3.82 (dt, *J* = 13.3, 6.4 Hz, 1H), 3.53 (ddd, *J* = 13.9, 8.5, 5.7 Hz, 1H), 3.40 – 3.24 (m, 1H), 1.40 (d, *J* = 7.0 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 167.76, 153.04, 143.32 – 141.31 (m), 141.37 – 139.32 (m), 139.03 – 136.73 (m), 134.29, 132.89, 131.69, 128.96, 128.65, 128.63, 126.85, 124.28 – 123.95 (m), 46.37, 40.10, 18.96.
^{19}F NMR (565 MHz, $CDCl_3$): δ -150.80 (d, *J* = 19.9 Hz, 2F), -155.25 (t, *J* = 22.0 Hz, 1F), -161.03 (t, *J* = 21.1 Hz, 2F).

Linear Isomer:
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.91 (d, *J* = 8.2 Hz, 2H), 7.72 – 7.68 (m, 2H), 7.53 – 7.38 (m, 5H), 5.90 (d, *J* = 7.8 Hz, 1H), 4.52 (hept, *J* = 6.9 Hz, 1H), 3.15 (dd, *J* = 13.4, 5.6 Hz, 1H), 2.98 (dd, *J* = 13.4, 7.3 Hz, 1H), 1.25 (d, *J* = 6.6 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$)[a]: δ 167.1, 147.1, 134.4, 132.9, 132.7, 131.7, 130.6, 128.7, 126.9, 46.6, 42.5, 19.9.
[a]Due to overlap with the branched isomer in both ^{13}C{^{1}H} and ^{13}C{^{19}F} NMR, perfluoroarene peaks were not observed.
^{19}F NMR (565 MHz, $CDCl_3$): δ -150.73 (d, *J* = 19.9 Hz, 2F), -155.23 – -155.35 (m, 1F)[a], -161.01 – -161.14 (m, 2F)[b].
[a,b]Could not observe all peaks due to overlap with branched isomer.

Mixture of Isomers:
HRMS (APCI): calculated for $C_{22}H_{17}F_5NO_4S^+$ ($[M+H]^+$): 486.0793, found 486.0786.
IR (ATR cm^{-1}): 3325 (br), 3082, 3031, 2972, 2933, 1642, 1519, 1392, 1198, 1183, 997, 716.



major (branched) *minor (linear)*

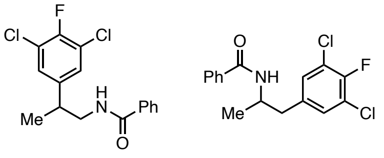
Ethyl 5-(1-benzamidopropan-2-yl)-2-methylbenzoate (I-1) was prepared according to General Procedure C from **1a** and ethyl 5-iodo-2-methylbenzoate. The product was isolated by flash

chromatography (17% acetone/hexanes) to produce **I-1** as a yellow oil (84% yield (10:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 84% yield (10.0:1)
Run 2: 85% yield (10.8:1)

Branched Isomer:
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.78 (d, *J* = 2.0 Hz, 1H), 7.63 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.38 (dd, *J* = 8.3, 7.0 Hz, 2H), 7.29 (dd, *J* = 7.8, 2.1 Hz, 1H), 7.22 (d, *J* = 7.8 Hz, 1H), 5.99 (br s, 1H), 4.35 (q, *J* = 7.2 Hz, 2H), 3.83 (dt, *J* = 13.2, 6.5 Hz, 1H), 3.41 (ddd, *J* = 13.5, 8.7, 5.0 Hz, 1H), 3.16 – 3.07 (m, 1H), 2.57 (s, 3H), 1.41 – 1.31 (m, 6H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 167.8, 167.7, 141.7, 138.5, 134.8, 132.3, 131.5, 130.7, 130.5, 129.4, 128.7, 126.9, 61.0, 46.6, 39.4, 21.5, 19.3, 14.5.

Linear Isomer:
^{1}H NMR (500 MHz, CDCl3): δ 7.75 (d, *J* = 1.9 Hz, 1H), 7.70 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.51 – 7.35 (m, 4H), 7.18 (d, *J* = 7.8 Hz, 1H), 5.91 (d, *J* = 8.1 Hz, 1H), 4.53 – 4.43 (m, 1H), 4.39 – 4.30 (m, 2H), 2.94 (dd, *J* = 13.6, 5.6 Hz, 1H), 2.87 (dd, *J* = 13.6, 6.9 Hz, 1H), 2.56 (s, 3H), 1.41 – 1.31 (m, 3H), 1.22 (d, *J* = 6.7 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 167.8, 166.9, 141.7^a, 138.4, 135.4, 134.9, 133.1, 132.0, 131.6, 130.1, 128.7, 126.9, 60.9, 46.5, 41.7, 23.0, 20.0, 14.5.
^{a}Not fully resolved in HMBC, some uncertainty.

Mixture of Isomers:
HRMS (APCI): calculated for $C_{20}H_{24}NO_3^+$ ($[M+H]^+$): 326.1751, found 326.1753.
IR (ATR cm^{-1}): 3314 (br), 3071, 3064, 3027, 2967, 2931, 2875, 1718, 1639, 1540, 1294, 1262, 1196, 1077, 711, 694.



major (branched) *minor (linear)*

***N*-(2-(3,5-dichloro-4-fluorophenyl)propyl)benzamide (J-1)** was prepared according to General Procedure C from **1a** and 1,3-dichloro-2-fluoro-5-iodobenzene. The product was isolated by flash chromatography (17% acetone/hexanes) to produce **J-1** as an off-white solid (76% yield (8:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 78% yield (7.7:1)
Run 2: 73% yield (8.2:1)

Branched Isomer:
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.51 – 7.43 (m, 1H), 7.42 – 7.34 (m, 2H), 7.15 (d, *J* = 6.2 Hz, 2H), 6.48 (br s, 1H), 3.64 (dt, *J* = 13.3, 6.5 Hz, 1H), 3.37 (ddd, *J* = 13.7, 8.1, 5.7 Hz, 1H), 3.04 (h, *J* = 7.1 Hz, 1H), 1.27 (d, *J* = 7.0 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 167.9, 152.9 (d, *J* = 249.2 Hz), 141.7 (d, *J* = 4.8 Hz), 134.4, 131.7, 128.7, 127.8, 126.9, 122.4 (d, *J* = 17.6 Hz), 46.6, 39.1, 19.0.
^{19}F NMR (565 MHz, Chloroform-*d*): δ -118.5 (t, *J* = 6.1 Hz).

Linear Isomer:

^{1}H NMR (500 MHz, CDCl$_3$): δ 7.70 (d, *J* = 7.9 Hz, 2H), 7.51 – 7.43 (m, 1H), 7.42 – 7.34 (m, 2H), 7.15 (d, *J* = 6.2 Hz, 2H), 6.28 (d, *J* = 8.0 Hz, 1H), 4.34 (hept, *J* = 6.8 Hz, 1H), 2.90 (dd, *J* = 13.6, 5.7 Hz, 1H), 2.70 (dd, *J* = 13.6, 7.3 Hz, 1H), 1.21 (d, *J* = 6.7 Hz, 3H).

^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$)^{a}: δ 167.22, 152.99 (d, *J* = 249.0 Hz), 135.64 (d, *J* = 5.1 Hz), 134.58, 131.66, 129.78, 126.90, 126.87, 122.11 (d, *J* = 17.6 Hz), 46.71, 41.42, 19.84.

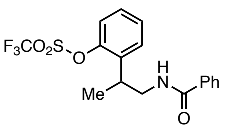
^{a}Two decimal places shown to distinguish between peaks at δ 126.90 and 126.87.

^{19}F NMR (565 MHz, Chloroform-*d*): δ -119.0 (t, *J* = 6.2 Hz).

Mixture of Isomers:

HRMS (APCI): calculated for $C_{16}H_{15}{}^{35}Cl_2NO^+$ ($[M+H]^+$): 326.0509, found 326.0509.

IR (ATR cm^{-1}): 3295 (br), 3081, 3071, 3059, 2970, 2934, 1636, 1578, 1540, 1483, 1412, 1270, 812, 705, 695.



2-(1-benzamidopropan-2-yl)phenyl trifluoromethanesulfonate (K-1) was prepared according to General Procedure C from **1a** and 2-iodophenyl trifluoromethanesulfonate. Yields were determined by ^{19}F NMR versus 1-fluoronaphthalene as an external standard (5% yield ((>20:1). Product for characterization was isolated via preparative thin layer chromatography (1% MeOH in DCM, ran in a fridge kept at 4 °C to prevent decomposition). The product was isolated with high selectivity for the branched isomer (>20:1); as such, only branched characterization data is provided.

Run 1: 6% yield (>20:1)

Run 2: 5% yield (>20:1)

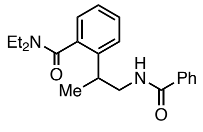
^{1}H NMR (500 MHz, CDCl$_3$): δ 7.65 – 7.61 (m, 2H), 7.49 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.43 – 7.36 (m, 3H), 7.32 (ddd, *J* = 8.2, 7.2, 1.7 Hz, 1H), 7.29 – 7.24 (m, 1H), 6.09 (br s, 1H), 3.80 – 3.72 (m, 2H), 3.48 (dp, *J* = 8.5, 6.9 Hz, 1H), 1.35 (d, *J* = 6.9 Hz, 3H).

^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$)^{a}: δ 167.68, 147.63, 137.10, 134.48, 131.57, 129.30, 128.67, 128.66, 128.56, 126.94, 121.77, 118.70 (q, *J* = 320.1 Hz), 45.29, 33.26, 19.59.

^{a}Two decimal places shown to distinguish between peaks at δ 128.67 and 128.66.

^{19}F NMR (565 MHz, CDCl$_3$): δ -73.50 (s).

HRMS (APCI): calculated for $C_{17}H_{17}F_3NO_4S^+$ ($[M+H]^+$): 388.0825, found 388.0818.



(mixture of rotamers)

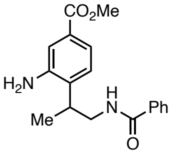
2-(1-benzamidopropan-2-yl)-*N*,*N*-diethylbenzamide (O-1) was prepared according to General Procedure C from **1a** and *N*,*N*-diethyl-2-iodobenzamide. The product was isolated by flash chromatography (20% acetone/hexanes) to produce **O-1** as a white solid (55% yield (>20:1)). The product was isolated with high selectivity for the branched isomer (>20:1); as such, only branched characterization data is provided.

Run 1: 51% yield (>20:1)

Run 2: 58% yield (>20:1)

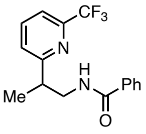
Compound **O-1** was produced as a mixture of atropisomers (~6:1).[9] Characterization for the major atropisomer in $CDCl_3$ is provided; however, exchange in $CDCl_3$ was not observed. In CD_3OD the two rotamers can equilibrate (reaching a ratio of ~2:1). In addition, exchange is observed in the NOESY as confirmation that the two isomers arise from conformational isomerism, not from the presence of two regioisomers. Specifically, the exchange cross-peak from the two methyl peaks at 1.1 and 0.9 serves an indicator of conformational isomerism. These peaks have sufficient resolution and distinct enough integrations (2:1) to assign them as terminal methyl groups on different atropisomers. While exchange cross-peaks are observed in the δ 3.9 – 2.8 range (4 sets with sufficient resolution from the diagonal), this region of the ^{1}H NMR does not have sufficient resolution to obtain good integration values to determine if these cross-peaks are from exchange between the two atropisomers or rotation amongst the C–N tertiary amide bond within the same isomer. However, the number of exchange peaks observed is greater than what would be observed with rotation about the amide bond with two regioisomers (1 exchange set x 2 isomers = 2 exchange sets).

^{1}H NMR (500 MHz, Chloroform-*d*): δ 8.27 (br s, 1H), 7.87 (d, *J* = 6.7 Hz, 2H), 7.83 (d, *J* = 7.7 Hz)[a], 7.46 – 7.40 (m, 1H), 7.40 – 7.30 (m, 4H), 7.25 – 7.19 (m, 1H), 7.19 – 7.13 (m, 1H), 3.72 – 3.47 (m, 4H), 3.37 – 3.25 (m, 1H), 3.25 – 3.12 (m, 1H), 3.12 – 3.01 (m, 1H), 1.38 (d, *J* = 7.0 Hz, 3H), 1.30 (t, *J* = 7.1 Hz, 3H), 1.09 (t, *J* = 7.0 Hz, 3H).
[a]Resolved minor atropisomer peak used for quantification.
^{1}H NMR (500 MHz, Methanol-*d*$_4$)[a]: δ 7.82 – 7.76 (m, 2H), 7.75 – 7.70 (m)[b], 7.58 – 7.06 (m, 7H), 4.01 – 2.80 (m, 7H)[c], 1.43 – 1.19 (m, 6H), 1.10 (t, *J* = 7.1 Hz, 3H)[d], 0.95 (t, *J* = 7.1 Hz)[d].
[a]Amide proton not observed.
[b]Resolved minor atropisomer peak.
[c]Overlaps with solvent residual peak.
[d]Resolved peaks for the two atropisomers for which exchange is observed and used for quantification.
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ 171.8, 167.6, 141.5, 136.5, 134.5, 130.9, 129.8, 128.3, 127.5, 126.6, 126.5, 125.1, 49.1, 43.3, 39.3, 34.7, 19.8, 14.3, 13.1.
HRMS (APCI): calculated for $C_{21}H_{27}N_2O_2^+$ ($[M+H]^+$): 339.2067, found 339.2068.
IR (ATR cm^{-1}): 3291 (br), 3066, 2970, 2935, 2875, 1655, 1636, 1612, 1598, 1540, 1491, 1433, 1292, 1077, 713, 695.

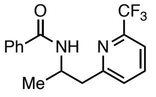


Methyl 3-amino-4-(1-benzamidopropan-2-yl)benzoate (P-1) was prepared according to General Procedure C from **1a** and methyl 3-amino-4-iodobenzoate. The product was isolated by flash chromatography (30% acetone/hexanes) to produce a **P-1** as a yellow solid (28% yield (>20:1)). The product was isolated with high selectivity for the branched isomer (>20:1); as such, only branched characterization data is provided.
Run 1: 28% yield (>20:1)
Run 2: 27% yield (>20:1)

^{1}H NMR (500 MHz, CDCl$_3$): δ 7.74 (d, J = 8.4 Hz, 2H), 7.53 – 7.49 (m, 1H), 7.46 – 7.40 (m, 3H), 7.25 – 7.19 (m, 1H), 7.19 – 7.13 (m, 1H), 6.65 (br s, 1H), 4.55 (br s, 2H), 3.88 (s, 3H), 3.75 (dt, J = 14.1, 5.4 Hz, 1H), 3.35 – 3.24 (m, 1H), 3.17 – 3.08 (m, 1H), 1.39 (d, J = 5.8 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 168.6, 167.4, 145.3, 134.3, 132.5, 131.9, 129.3, 128.8, 127.0, 126.0, 119.5, 116.6, 52.1, 47.1, 33.2, 17.2.
HRMS (APCI): calculated for $C_{18}H_{21}N_2O_3^+$ ([M+H]$^+$): 313.1547, found 313.1545.
IR (ATR cm^{-1}): 3357 (br), 3267 (br), 3074, 3048, 2980, 2961, 2900, 2887, 2875, 1714, 1638, 1578, 1534, 1438, 1298, 1243, 1118, 998, 714, 693.



major (branched)



minor (linear)

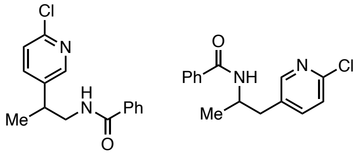
***N*-(2-(6-(trifluoromethyl)pyridin-2-yl)propyl)benzamide (het-1)** was prepared according to General Procedure C from **1a** and 2-iodo-6-(trifluoromethyl)pyridine. The product was isolated by flash chromatography (25% acetone/hexanes) to produce **het-1** as a yellow oil (83% yield (11:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 84% yield (10.0:1)
Run 2: 81% yield (11.1:1)

Branched Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 7.86 – 7.78 (m, 1H), 7.80 – 7.73 (m, 2H), 7.59 (br s, 1H)[a], 7.54 (d, J = 7.8 Hz, 1H), 7.49 – 7.32 (m, 4H), 3.87 – 3.73 (m, 2H), 3.34 (pd, J = 7.1, 4.2 Hz, 1H), 1.37 (d, J = 7.1 Hz, 3H).
[a] In samples of lower concentration, the amide proton is not observed, likely due to intramolecular hydrogen bonding.
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 167.4, 165.4, 147.3 (q, J = 34.3 Hz), 138.3, 134.5, 131.4, 128.5, 126.9, 125.4, 121.6 (q, J = 274.1 Hz), 118.4 (q, J = 2.9 Hz), 44.3, 40.3, 18.4.
^{19}F NMR (565 MHz, CDCl$_3$): δ -68.0 (s).

Linear Isomer:
^{1}H NMR (500 MHz, CDCl$_3$)[a]: δ 7.87 – 7.73 (m, 3H), 7.57 – 7.52 (m, 1H), 7.49 – 7.32 (m, 4H), 4.66 – 4.56 (m, 1H), 3.22 (dd, J = 14.3, 4.8 Hz, 1H)[b], 3.04 (dd, J = 14.3, 6.2 Hz, 1H), 1.24 (d, J = 6.7 Hz, 3H).
[a] Amide proton not directly observed, likely due to overlap with amide proton of branched isomer or intramolecular hydrogen bonding.
[b] In repeated samples, this peak exhibits significant broadening; therefore, integration values are higher than expected in ^{1}H NMR.
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 166.5, 160.1, 147.5 (q, J = 34.4 Hz), 138.2, 134.6, 131.4, 128.5, 127.3, 127.0, 121.6 (q, J = 274.2 Hz), 118.7 – 118.6 (m), 45.4, 42.7, 20.1.
^{19}F NMR (565 MHz, CDCl$_3$): δ -67.9 (s).

Mixture of Isomers:
HRMS (ESI-TOF): calculated for $C_{16}H_{16}F_3N_2O^+$ ([M+H]$^+$): 309.1209, found 309.1194.

IR (ATR cm^{-1}): 3326 (br), 3069, 2970, 2936, 2895, 2872, 1641, 1601, 1579, 1534, 1489, 1467, 1339, 1309, 1186, 1161, 1139, 1096, 993, 819, 750, 711, 695.



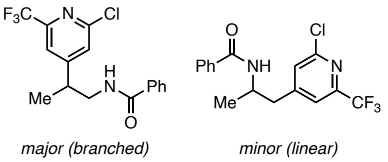
major (branched) *minor (linear)*

***N*-(2-(6-chloropyridin-3-yl)propyl)benzamide (het-2)** was prepared according to General Procedure C from **1a** and 2-chloro-5-iodopyridine. The product was isolated by flash chromatography (25% acetone/hexanes) to produce **het-2** as a yellow solid (72% yield (10:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 73% yield (10.0:1)
Run 2: 71% yield (9.1:1)

Branched Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 8.10 (s, 1H), 7.66 – 7.62 (m, 2H), 7.53 – 7.46 (m, 1H), 7.46 – 7.41 (m, 1H), 7.37 – 7.30 (m, 2H), 7.25 – 7.19 (m, 1H), 6.68 (br s, 1H), 3.75 – 3.58 (m, 1H), 3.49 – 3.36 (m, 1H), 3.10 (h, *J* = 7.1 Hz, 1H), 1.28 (d, *J* = 7.2 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$): δ 167.9, 149.7, 148.9, 138.6, 137.6, 134.4, 131.6, 128.6, 126.9, 124.4, 46.4, 36.9, 18.9.

Linear Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 8.12 (s, 1H), 7.69 – 7.66 (m, 2H), 7.54 – 7.48 (m, 1H), 7.47 – 7.40 (m, 1H), 7.40 – 7.30 (m, 2H), 7.25 – 7.19 (m, 1H), 6.32 (br s, 1H), 4.38 (hept, *J* = 7.0, 6.5 Hz, 1H), 2.89 (dd, *J* = 13.8, 6.0 Hz, 1H), 2.80 (dd, *J* = 14.0, 6.8 Hz, 1H), 1.20 (d, *J* = 6.7 Hz, 3H).
^{13}C{1H} NMR (126 MHz, CDCl$_3$): δ 167.2, 150.2, 149.7, 139.8, 134.5, 132.7, 131.6, 128.7, 126.9, 124.1, 46.3, 38.7, 19.9.

Mixture of Isomers:
HRMS (APCI): calculated for $C_{15}H_{16}{}^{35}ClN_2O^+$ ([M+H]$^+$): 275.0946, found 275.0945.
IR (ATR cm^{-1}): 3306 (br), 3089, 3080, 3056, 2971, 2822, 2872, 1636, 1603, 1540, 1458, 1308, 1143, 1108, 742, 711, 695.



major (branched) *minor (linear)*

***N*-(2-(2-chloro-6-(trifluoromethyl)pyridin-4-yl)propyl)benzamide (het-3)** was prepared according to General Procedure C from **1a** and 2-chloro-4-iodo-6-(trifluoromethyl)pyridine. The product was isolated by flash chromatography (25% acetone/hexanes) to produce **het-3** as a white solid (69% yield (8:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 60% yield (7.1:1)
Run 2: 77% yield (8.3:1)

Branched Isomer:

^{1}H NMR (600 MHz, CDCl$_3$): δ 7.68 – 7.64 (m, 2H), 7.55 – 7.47 (m, 2H), 7.47 – 7.39 (m, 3H), 6.19 (br s, 1H), 3.71 (dt, *J* = 13.4, 6.5 Hz, 1H), 3.53 (ddd, *J* = 13.9, 8.0, 6.1 Hz, 1H), 3.29 (h, *J* = 7.1 Hz, 1H), 1.38 (d, *J* = 7.0 Hz, 3H).

^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 168.0, 158.8, 152.6, 148.7 (q, *J* = 35.8 Hz), 134.1, 132.0, 128.9, 126.9, 126.4, 120.8 (q, *J* = 274.5 Hz), 118.5 (q, *J* = 2.9 Hz), 46.1, 39.6, 18.3.

^{19}F NMR (565 MHz, CDCl$_3$): δ -67.9 (s).

Linear Isomer:

^{1}H NMR (600 MHz, CDCl$_3$): δ 7.71 – 7.69 (m, 2H), 7.55 – 7.47 (m, 2H), 7.47 – 7.39 (m, 3H), 5.96 (br s, 1H), 4.46 (hept, *J* = 6.9 Hz, 1H), 3.12 (dd, *J* = 13.5, 5.5 Hz, 1H), 2.91 (dd, *J* = 13.5, 7.4 Hz, 1H), 1.27 (d, *J* = 6.8 Hz, 3H).

^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$)[a,b]: δ 167.31, 152.65, 152.31, 149.23 – 148.16 (m), 134.25, 131.99, 128.22, 126.93, 126.87, 120.45 (q, *J* = 2.2 Hz), 46.24, 41.77, 19.95.

[a] Two decimal places shown to distinguish between peaks at δ 126.93 and 126.87.

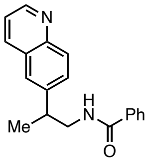
[b] Trifluoromethyl carbon not observed.

^{19}F NMR (565 MHz, CDCl$_3$): δ -68.0 (s).

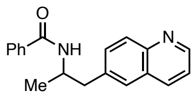
Mixture of Isomers:

HRMS (ESI-TOF): calculated for $C_{16}H_{15}{}^{35}ClF_3N_2O^+$ ([M+H]$^+$): 343.0820, found 343.0817.

IR (ATR cm^{-1}): 3288 (br), 3096, 3066, 2973, 2932, 1636, 1603, 1540, 1429, 1325, 1193, 1142, 910, 837, 708, 694.



major (branched)



minor (linear)

***N*-(2-(quinolin-6-yl)propyl)benzamide (het-4)** was prepared according to General Procedure C from **1a** and 6-iodoquinoline. The product was isolated by flash chromatography (35% EtOAc/hexanes + 10% NEt$_3$) to produce **het-4** as a pink oil (48% yield (10:1)). The product was isolated and characterized as a mixture of isomers.

Run 1: 43% yield (10.0:1)
Run 2: 53% yield (10.0:1)

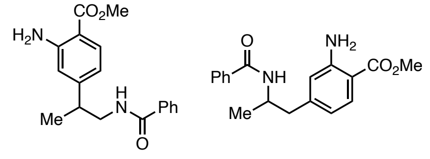
Branched Isomer:

^{1}H NMR (600 MHz, CDCl$_3$): δ 8.89 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.13 – 8.10 (m, 1H), 8.09 (d, *J* = 8.5 Hz, 1H), 7.73 – 7.57 (m, 4H), 7.46 – 7.42 (m, 1H), 7.41 – 7.38 (m, 1H), 7.37 – 7.33 (m, 2H), 6.08 (br s, 1H), 3.92 (ddd, *J* = 13.3, 6.8, 6.0 Hz, 1H), 3.54 (ddd, *J* = 13.7, 8.7, 5.1 Hz, 1H), 3.32 (dp, *J* = 8.9, 6.9 Hz, 1H), 1.44 (d, *J* = 7.0 Hz, 3H).

^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 167.7, 150.3, 147.7, 142.6, 135.9, 134.7, 131.6, 130.1, 129.3, 128.7, 128.5, 126.9, 125.7, 121.5, 46.7, 40.0, 19.5.

Linear Isomer:
^{1}H NMR (600 MHz, CDCl$_3$): δ 8.90 – 8.86 (m, 1H), 8.05 (d, *J* = 8.6 Hz, 1H), 7.73 – 7.57 (m, 3H), 7.50 – 7.46 (m, 2H), 7.46 – 7.32 (m, 4H), 5.99 (d, *J* = 7.9 Hz, 1H), 4.64 – 4.53 (m, 1H), 3.18 (dd, *J* = 13.6, 5.5 Hz, 1H), 3.03 (dd, *J* = 13.6, 7.3 Hz, 1H), 1.27 (d, *J* = 6.7 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 167.0, 150.2, 147.5, 136.6, 135.8, 134.8, 131.8, 129.6, 128.7, 128.6, 128.4, 127.8, 126.9, 121.4, 46.8, 42.5, 20.1.

Mixture of Isomers:
HRMS (ESI-TOF): calculated for $C_{19}H_{19}N_2O^+$ ([M+H]$^+$): 291.1492, found 291.1497.
IR (ATR cm^{-1}): 3476 (br shoulder), 3299 (br), 3058, 3029, 2963, 2926, 2873, 1636, 1577, 1540, 1500, 1490, 1453, 1307, 1292, 1121, 1074, 1029, 837, 800, 696.



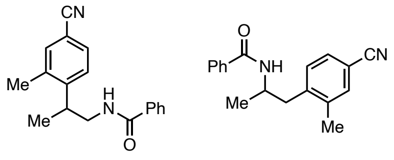
major (branched) *minor (linear)*

Methyl 2-amino-4-(1-benzamidopropan-2-yl)benzoate (I-2) was prepared according to General Procedure C from **1a** and methyl 2-amino-4-iodobenzoate. The product was isolated by flash chromatography (25% acetone/hexanes) to produce a **I-2** as a yellow oil (71% yield (6:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 72% yield (6.7:1)
Run 2: 71% yield (6.3:1)

Branched Isomer:
^{1}H NMR (600 MHz, CDCl$_3$)^a: δ 7.82 (d, *J* = 8.2 Hz, 1H), 7.66 – 7.62 (m, 2H), 7.46 – 7.42 (m, 1H), 7.39 – 7.34 (m, 2H), 6.61 – 6.53 (m, 2H), 6.18 (br s, 1H), 3.85 (s, 3H), 3.79 (ddd, *J* = 13.2, 7.0, 6.0 Hz, 1H), 3.37 (ddd, *J* = 13.6, 8.8, 5.0 Hz, 1H), 2.99 (dp, *J* = 9.0, 6.9 Hz, 1H), 1.28 (d, *J* = 7.0 Hz, 3H).
[a]Aniline protons not observed possibly due to intramolecular hydrogen bonding.
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 168.4, 167.6, 151.0, 150.0, 134.6, 131.9, 131.5, 128.7, 126.9, 116.1, 115.8, 110.1, 51.7, 46.2, 39.9, 19.0.

Linear Isomer:
^{1}H NMR (600 MHz, CDCl$_3$)^a: δ 7.78 (d, *J* = 8.1 Hz, 1H), 7.72 – 7.69 (m, 2H), 7.49 – 7.42 (m, 1H), 7.41 – 7.33 (m, 2H), 6.61 – 6.53 (m, 2H), 6.10 (d, *J* = 8.1 Hz, 1H), 4.48 – 4.40 (m, 1H), 3.84 (s, 3H), 2.88 (dd, *J* = 13.4, 5.7 Hz, 1H), 2.72 (dd, *J* = 13.4, 7.3 Hz, 1H), 1.21 (d, *J* = 6.7 Hz, 3H).
[a]Aniline protons not observed possibly due to intramolecular hydrogen bonding.
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 168.5, 167.0, 149.8, 144.9, 134.8, 131.5, 128.7, 128.6, 127.0, 118.5, 117.8, 109.9, 51.6, 46.4, 42.5, 20.1.

Mixture of Isomers:
HRMS (APCI): calculated for $C_{18}H_{21}N_2O_3^+$ ([M+H]$^+$): 313.1547, found 313.1547.
IR (ATR cm^{-1}): 3458 (br), 3363 (br), 3060, 3028, 2951, 2928, 2876, 1685, 1653, 1636, 1618, 1602, 1591, 1577, 1539, 1523, 1487, 1437, 1298, 1248, 1189, 1103, 906, 726.



major (branched) *minor (linear)*

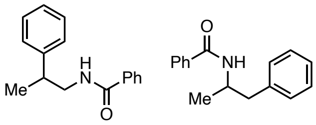
***N*-(2-(4-cyano-2-methylphenyl)propyl)benzamide (L-2)** was prepared according to General Procedure C from **1a** and 4-iodo-3-methylbenzonitrile. The product was isolated by flash chromatography (25% to 50% EtOAc/hexanes) to produce a **L-2** as a light brown solid (42% yield (9:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 41% yield (9.3:1)
Run 2: 42% yield (7.7:1)

Branched Isomer:
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.66 – 7.62 (m, 2H), 7.50 – 7.45 (m, 2H), 7.44 – 7.36 (m, 3H), 7.34 (d, *J* = 8.0 Hz, 1H), 6.21 (br s, 1H), 3.68 (dt, *J* = 13.0, 6.5 Hz, 1H), 3.56 – 3.45 (m, 2H), 2.38 (s, 3H), 1.30 (d, *J* = 6.7 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 167.8, 148.3, 137.9, 134.4, 134.0, 131.7, 130.3, 128.8, 126.9, 126.4, 119.1, 110.2, 45.9, 35.1, 19.5, 18.7.

Linear Isomer:
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.72 – 7.69 (m, 2H), 7.53 – 7.22 (m, 6H), 6.10 (d, *J* = 8.0 Hz, 1H), 4.49 – 4.39 (m, 1H), 3.11 (dd, *J* = 13.7, 6.1 Hz, 1H), 2.78 (dd, *J* = 13.5, 7.7 Hz, 1H), 2.44 (s, 3H), 1.25 (d, *J* = 6.7 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 167.0, 142.5, 138.4, 134.6, 133.9, 131.7, 130.9, 129.6, 128.8, 126.9, 119.2, 110.5, 45.9, 40.6, 20.3, 19.6.

Mixture of Isomers:
HRMS (APCI): calculated for $C_{18}H_{19}N_2O^+$ ($[M+H]^+$): 279.1492, found 279.1493.
IR (ATR cm^{-1}): 3325, 3062, 2970, 2929, 2231, 1636, 1604, 1578, 1539, 1490, 1311, 1293, 712, 696.

5.2. Aziridine Substrate Scope



major (branched) *minor (linear)*

***N*-(2-phenylpropyl)benzamide (1b)** was prepared according to General Procedure C from **1a** and phenyl iodide. The product was isolated by flash chromatography (15% acetone/hexanes) to produce a white solid (81% yield (11:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 82% yield (11.1:1)
Run 2: 80% yield (10.0:1)
Partial isolation of branched and linear products was done via preparative thin layer chromatography (20% EtOAc/hexanes) to aid in characterization. Spectral data are in agreement with reported literature values.[10,11]

Branched Isomer:

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.64 – 7.58 (m, 2H), 7.49 – 7.44 (m, 1H), 7.41 – 7.33 (m, 4H), 7.28 – 7.24 (m, 3H), 5.95 (br s, 1H), 3.86 (ddd, *J* = 13.1, 7.1, 5.9 Hz, 1H), 3.41 (ddd, *J* = 13.5, 8.9, 4.8 Hz, 1H), 3.08 (dp, *J* = 9.0, 6.9 Hz, 1H), 1.35 (d, *J* = 7.0 Hz, 3H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 167.6, 144.2, 134.8, 131.5, 129.0, 128.7, 127.4, 127.0, 126.9, 46.7, 40.0, 19.4.

Linear Isomer:

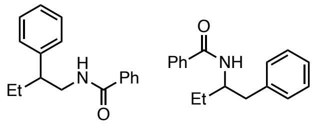
^{1}H NMR (500 MHz, CDCl3): δ 7.69 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.51 – 7.20 (m, 8H), 5.88 (br s, 1H), 4.55 – 4.40 (m, 1H), 2.95 (dd, *J* = 13.5, 5.6 Hz, 1H), 2.87 (dd, *J* = 13.5, 7.0 Hz, 1H), 1.23 (d, *J* = 6.7 Hz, 3H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 166.9, 137.9, 135.0, 131.5, 129.7, 128.7, 128.6, 126.9, 126.7, 46.6, 42.5, 20.1.

Mixture of Isomers:

HRMS (APCI): calculated for $C_{16}H_{18}NO^+$ ($[M+H]^+$): 240.1383, found 240.1384.

IR (ATM cm^{-1}): 3321 (br), 3060, 3028, 2964, 2927, 1636, 1542, 1535, 1491, 698.



major (branched) *minor (linear)*

***N*-(2-phenylbutyl)benzamide (2b)** was prepared according to General Procedure C from **2a** and phenyl iodide. The product was isolated by flash chromatography (12 to 20% EtOAc/hexanes) to produce a white solid (67% yield (>20:1)).

Run 1: 63% yield (>20:1)

Run 2: 70% yield (>20:1)

As the branched isomer could be cleanly isolated, we obtained ^{1}H NMR yield and selectivity versus ethylene carbonate as an external standard (82% yield (9:1)). Linear isomer yield based on literature characterization data.[12]

^{1}H NMR run 1: 84% yield (9.1:1)

^{1}H NMR run 2: 80% yield (9.5:1)

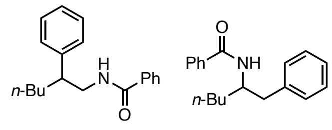
Branched Isomer:

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 – 7.54 (m, 2H), 7.50 – 7.40 (m, 1H), 7.40 – 7.31 (m, 4H), 7.31 – 7.18 (m, 3H), 5.89 (br s, 1H), 3.97 (ddd, *J* = 13.3, 7.2, 5.4 Hz, 1H), 3.37 (ddd, *J* = 13.7, 9.6, 4.5 Hz, 1H), 2.86 – 2.75 (m, 1H), 1.88 – 1.74 (m, 1H), 1.73 – 1.60 (m, 1H), 0.86 (t, *J* = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 167.5, 142.7, 134.9, 131.4, 128.9, 128.6, 128.0, 127.0, 126.9, 47.7, 45.4, 26.9, 12.1.

HRMS (ESI-TOF): calculated for $C_{17}H_{20}NO^+$ ($[M+H]^+$): 254.1539, found 254.1538.

IR (ATM cm^{-1}): 3305 (br), 3080, 3061, 3028, 2962, 2928, 2873, 1636, 1578, 1540, 1491, 1307, 699.

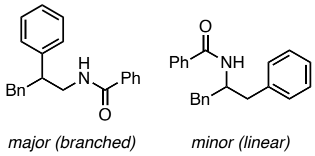


major (branched) *minor (linear)*

***N*-(2-phenylhexyl)benzamide (3b)** was prepared according to General Procedure C from **3a** and phenyl iodide. The product was isolated by flash chromatography (10 to 40% EtOAc/hexanes) to produce a white solid (74% yield (>20:1)).
Run 1: 77% yield (>20:1)
Run 2: 72% yield (>20:1)
As the branched isomer could be cleanly isolated, we obtained ^{1}H NMR yield and selectivity versus ethylene carbonate as an external standard (91% yield (9:1)).
^{1}H NMR run 1: 92% yield (9.1:1)
^{1}H NMR run 2: 89% yield (9.2:1)

Branched Isomer:
^{1}H NMR (600 MHz, CDCl$_3$): δ 7.58 – 7.54 (m, 2H), 7.47 – 7.42 (m, 1H), 7.40 – 7.32 (m, 4H), 7.29 – 7.23 (m, 1H), 7.24 – 7.19 (m, 2H), 5.87 (br s, 1H), 3.97 (ddd, *J* = 13.4, 7.3, 5.3 Hz, 1H), 3.34 (ddd, *J* = 13.4, 9.7, 4.5 Hz, 1H), 2.88 (tt, *J* = 9.5, 5.4 Hz, 1H), 1.74 (ddt, *J* = 13.4, 10.4, 5.4 Hz, 1H), 1.65 (dtd, *J* = 13.5, 9.6, 5.3 Hz, 1H), 1.36 – 1.12 (m, 4H), 0.84 (t, *J* = 7.2 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 167.5, 143.0, 134.9, 131.4, 129.0, 128.7, 128.0, 127.0, 126.9, 46.0, 45.7, 33.6, 29.6, 22.8, 14.1.
HRMS (ESI-TOF): calculated for $C_{19}H_{24}NO^+$ ($[M+H]^+$): 282.1852, found 282.1853.
IR (ATM cm^{-1}): 3300 (br), 3060, 3028, 2956, 2928, 2858, 1636, 1603, 1579, 1540, 1491, 1453, 1307, 1292, 699.

Linear Isomer:
^{1}H NMR (600 MHz, CDCl$_3$): δ 7.73 – 7.68 (m, 2H), 7.54 – 7.48 (m, 1H), 7.46 – 7.41 (m, 2H), 7.34 – 7.30 (m, 2H), 7.26 – 7.22 (m, 3H), 5.82 (d, *J* = 8.7 Hz, 1H), 4.42 (tq, *J* = 8.6, 6.0 Hz, 1H), 2.96 (dd, *J* = 13.7, 6.5 Hz, 1H), 2.92 (dd, *J* = 13.7, 5.9 Hz, 1H), 1.68 – 1.26 (m, 6H)[a], 0.90 (t, *J* = 7.2 Hz, 3H).
[a]Overlap with H_2O and with branched isomer
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 167.1, 138.0, 135.1, 131.5, 129.8, 128.7, 128.6, 126.9, 126.6, 50.6, 40.9, 33.9, 28.4, 22.7, 14.2.
HRMS (ESI-TOF): calculated for $C_{19}H_{24}NO^+$ ($[M+H]^+$): 282.1852, found 282.1854.
IR (ATM cm^{-1}): 3314 (br), 3070, 3027, 2950, 2926, 2854, 1634, 1535, 1311, 694.



major (branched) *minor (linear)*

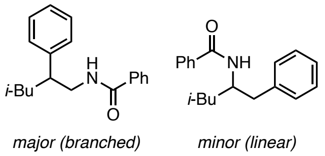
***N*-(2,3-diphenylpropyl)benzamide (4b)** was prepared according to General Procedure C from **4a** and phenyl iodide. The product was isolated by flash chromatography (20% acetone/hexanes) to produce a yellow solid (87% yield (6:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 87% yield (5.9:1)
Run 2: 86% yield (5.3:1)

Partial isolation of branched and linear products was done via preparative thin layer chromatography (20% EtOAc/hexanes) to aid in characterization.

Branched Isomer:
^{1}H NMR (600 MHz, CDCl$_3$): δ 7.53 – 7.48 (m, 2H), 7.46 – 7.40 (m, 1H), 7.37 – 7.29 (m, 4H), 7.27 – 7.19 (m, 5H), 7.19 – 7.14 (m, 1H), 7.13 – 7.09 (m, 2H), 5.84 (br s, 1H), 3.94 (ddd, *J* = 13.5, 6.7, 5.7 Hz, 1H), 3.55 (ddd, *J* = 13.5, 9.1, 5.0 Hz, 1H), 3.24 (dtd, *J* = 9.1, 7.5, 5.6 Hz, 1H), 3.07 – 2.97 (m, 2H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 167.4, 142.2, 139.6, 134.7, 131.5, 129.2, 128.9, 128.6, 128.5, 128.0, 127.2, 126.8, 126.3, 47.6, 45.0, 41.0.

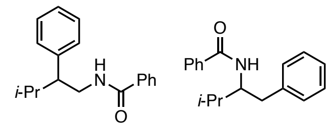
Linear Isomer:
^{1}H NMR (600 MHz, CDCl$_3$): δ 7.57 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.49 – 7.43 (m, 1H), 7.38 (dd, *J* = 8.3, 7.0 Hz, 2H), 7.34 – 7.28 (m, 4H), 7.27 – 7.20 (m, 6H), 5.85 (d, *J* = 8.2 Hz, 1H), 4.68 (dp, *J* = 8.2, 6.6 Hz, 1H), 2.97 (dd, *J* = 14.0, 6.3 Hz, 2H), 2.90 (dd, *J* = 14.0, 6.9 Hz, 2H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 166.5, 138.0, 134.5, 131.5, 129.6, 128.7[a], 126.8, 126.8, 51.7, 39.8.
[a] Two carbons, see HSQC

Mixture of Isomers:
HRMS (APCI): calculated for $C_{22}H_{22}NO^+$ ($[M+H]^+$): 316.1696, found 316.1696.
IR (ATM cm^{-1}): 3315 (br), 3060, 3026, 2923, 1636, 1579, 1540, 1490, 1453, 1307, 1291, 697.



***N*-(4-methyl-2-phenylpentyl)benzamide (5b)** was prepared according to General Procedure C from **5a** and phenyl iodide. The product was isolated by flash chromatography (13% acetone/hexanes) to produce a white solid (83% yield (>20:1)). The product was isolated and characterized as a mixture of isomers. While minor amounts of linear isomer are observed by ^{1}H NMR, due to the high selectivity of the reaction, only branched isomer characterization data is provided.
Run 1: 83% yield (20.6:1)
Run 2: 83% yield (20.0:1)

^{1}H NMR (600 MHz, CDCl$_3$): δ 7.59 (d, *J* = 7.3 Hz, 2H), 7.43 (t, *J* = 7.4 Hz, 1H), 7.39 – 7.31 (m, 4H), 7.28 – 7.20 (m, 3H), 6.09 (br s, 1H), 3.91 (dt, *J* = 12.1, 5.8 Hz, 1H), 3.31 (ddd, *J* = 13.6, 9.5, 4.6 Hz, 1H), 3.01 (tt, *J* = 10.0, 5.3 Hz, 1H), 1.64 (ddd, *J* = 13.3, 9.9, 5.0 Hz, 1H), 1.55 – 1.41 (m, 2H), 0.88 (d, *J* = 3.7 Hz, 3H), 0.87 (d, *J* = 3.8 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 167.4, 142.9, 134.8, 131.3, 128.8, 128.5, 127.9, 126.9, 126.8, 46.0, 43.6, 42.9, 25.4, 23.5, 21.9.
HRMS (APCI): calculated for $C_{19}H_{24}NO^+$ ($[M+H]^+$): 282.1852, found 282.1852.
IR (ATM cm^{-1}): 3320 (br), 3028, 2955, 2927, 1636, 1540, 1490, 1307, 1293, 699.

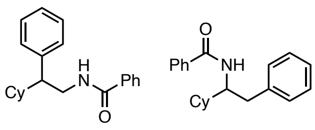


major (branched) *minor (linear)*

N-(3-methyl-2-phenylbutyl)benzamide (6b) was prepared according to General Procedure C from **6a** and phenyl iodide. Yields were determined by ^{1}H NMR versus ethylene carbonate as an external standard (86% yield (2:1)).
^{1}H NMR run 1: 86% yield (2.2:1)
^{1}H NMR run 2: 86% yield (2.0:1)
Partial isolation of branched and linear products was done via preparative thin layer chromatography (20% EtOAc/hexanes) to aid in characterization.

Branched Isomer:
^{1}H NMR (600 MHz, CDCl$_3$): δ 7.50 – 7.48 (m, 2H), 7.45 – 7.40 (m, 1H), 7.38 – 7.31 (m, 4H), 7.28 – 7.24 (m, 1H), 7.22 – 7.19 (m, 2H), 5.74 (br s, 1H), 4.18 (ddd, J = 13.4, 7.3, 4.8 Hz, 1H), 3.39 (ddd, J = 13.4, 10.9, 4.0 Hz, 1H), 2.61 (ddd, J = 10.8, 8.4, 4.8 Hz, 1H), 1.96 (dhept, J = 8.4, 6.7 Hz, 1H), 1.09 (d, J = 6.6 Hz, 3H), 0.78 (d, J = 6.7 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$)[a]: δ 167.43, 141.97, 134.90, 131.38, 128.84, 128.6[b], 127.02, 126.81, 52.98, 43.07, 31.87, 21.04, 21.02.
[a] Two decimal places shown to distinguish between peaks at δ 21.04 and 21.02.
[b] Likely two carbons
HRMS (APCI): calculated for $C_{18}H_{22}NO^+$ ($[M+H]^+$): 268.1696, found 268.1697.
IR (ATM cm^{-1}): 3314 (br), 3083, 3062, 3028, 2959, 2928, 2872, 1636, 1542, 1307, 1293, 700.

Linear Isomer:
^{1}H NMR (600 MHz, CDCl$_3$): δ 7.67 – 7.59 (m, 2H), 7.49 – 7.45 (m, 1H), 7.42 – 7.38 (m, 2H), 7.30 – 7.26 (m, 2H), 7.25 – 7.22 (m, 2H), 7.22 – 7.17 (m, 1H), 5.83 (d, J = 9.3 Hz, 1H), 4.32 (ddt, J = 9.3, 7.7, 5.9 Hz, 1H), 2.96 (dd, J = 14.1, 6.1 Hz, 1H), 2.84 (dd, J = 14.1, 7.8 Hz, 1H), 1.95 – 1.88 (m, 1H), 1.05 (d, J = 6.8 Hz, 3H), 1.00 (d, J = 6.8 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 167.3, 138.4, 135.3, 131.4, 129.4, 128.7, 128.6, 126.8, 126.6, 55.6, 38.1, 30.8, 19.9, 17.9.
HRMS (APCI): calculated for $C_{18}H_{22}NO^+$ ($[M+H]^+$): 268.1696, found 268.1696.
IR (ATM cm^{-1}): 3301 (br), 3084, 3076, 3058, 3023, 3010, 2955, 2925, 1636, 1534, 1336, 1288, 1196, 698.



major (branched) *minor (linear)*

N-(2-cyclohexyl-2-phenylethyl)benzamide (7b) was prepared according to General Procedure C from **7a** and phenyl iodide. Yields were determined by ^{1}H NMR versus ethylene carbonate as an external standard (87% yield (4:1)).
Run 1: 85% yield (3.9:1)
Run 2: 89% yield (4.0:1)
Partial isolation of branched and linear products was done via preparative thin layer chromatography (15% EtOAc/hexanes) to aid in characterization.

Branched Isomer:

^{1}H NMR (600 MHz, CDCl$_3$): δ 7.50 – 7.47 (m, 2H), 7.44 – 7.39 (m, 1H), 7.36 – 7.31 (m, 4H), 7.29 – 7.23 (m, 1H), 7.21 – 7.18 (m, 2H), 5.73 (s, 1H), 4.20 (ddd, *J* = 13.3, 7.3, 4.8 Hz, 1H), 3.37 (ddd, *J* = 13.3, 10.9, 3.9 Hz, 1H), 2.66 (ddd, *J* = 10.9, 8.4, 4.8 Hz, 1H), 2.04 – 1.99 (m, 1H), 1.81 – 1.75 (m, 1H), 1.64 – 1.59 (m, 3H), 1.48 – 1.41 (m, 1H), 1.33 – 1.03 (m, 4H)[a], 0.90 – 0.79 (m, 1H)[a].

[a] Cyclohexyl peaks exhibit overlap with the linear isomer in a sample with a B:L ratio of 10:1.

^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$)[a]: δ 167.27, 141.87, 134.80, 131.22, 128.70, 128.53, 128.47, 126.83, 126.68, 51.82, 42.59, 41.39, 31.18, 31.13, 26.43, 26.35, 26.32.

[a] Two decimal places shown to distinguish between peaks at δ 26.35 and 26.32.

HRMS (APCI): calculated for $C_{21}H_{26}NO^+$ ($[M+H]^+$): 308.2009, found 308.2010.

IR (ATM cm^{-1}): 3310 (br), 3082, 3060, 3027, 2922, 2850, 1635, 1540, 1489, 1305, 1293, 700.

Linear Isomer:

^{1}H NMR (600 MHz, CDCl$_3$): δ 7.67 – 7.62 (m, 2H), 7.51 – 7.46 (m, 1H), 7.46 – 7.39 (m, 2H), 7.32 – 7.29 (m, 2H), 7.26 – 7.20 (m, 3H), 5.84 (d, *J* = 9.4 Hz, 1H), 4.34 (ddt, *J* = 9.4, 7.8, 6.0 Hz, 1H), 3.02 (dd, *J* = 14.1, 5.8 Hz, 1H), 2.86 (dd, *J* = 14.1, 7.8 Hz, 1H), 1.96 – 1.83 (m, 2H), 1.83 – 1.75 (m, 2H), 1.70 (d, *J* = 11.9 Hz, 1H), 1.37 – 1.02 (m, 6H)[a].

[a] Cyclohexyl peaks exhibit overlap with the branched isomer in a sample with a B:L ratio of 1:15.

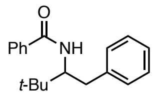
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$)[a]: δ 167.08, 138.35, 135.13, 131.23, 129.29, 128.54, 128.48, 126.71, 126.41, 54.85, 40.77, 37.70, 30.22, 28.50, 26.41, 26.15[b].

[a] Two decimal places shown to distinguish between peaks at δ 128.54 and 128.48.

[b] Likely two carbons.

HRMS (APCI): calculated for $C_{21}H_{26}NO^+$ ($[M+H]^+$): 308.2009, found 308.2008.

IR (ATM cm^{-1}): 3291 (br), 3062, 3028, 2915, 1849, 1634, 1543, 699.



***N*-(3,3-dimethyl-1-phenylbutan-2-yl)benzamide (8b)** was prepared according to General Procedure C from **8a** and phenyl iodide. Yields were determined by ^{1}H NMR versus ethylene carbonate as an external standard (12% yield (<1:20)).

^{1}H NMR run 1: 15% yield (<1:20)

^{1}H NMR run 2: 9% yield (<1:20)

Isolation was done via preparative thin layer chromatography (100% DCM) to aid in characterization. The product was isolated with high selectivity for the linear isomer (<1:20); as such, only linear characterization data is provided.

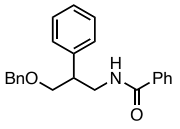
^{1}H NMR (500 MHz, CDCl$_3$): δ 7.48 (d, *J* = 8.0 Hz, 2H), 7.45 – 7.39 (m, 1H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.24 – 7.20 (m, 4H), 7.17 – 7.10 (m, 1H), 5.68 (d, *J* = 9.9 Hz, 1H), 4.36 (td, *J* = 10.8, 3.5 Hz, 1H), 3.18 (dd, *J* = 14.3, 3.6 Hz, 1H), 2.50 (dd, *J* = 14.4, 11.4 Hz, 1H), 1.06 (s, 9H).

^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$)[a]: δ 167.64, 139.06, 135.62, 131.17, 128.99, 128.61, 128.55, 126.71, 126.42, 58.41, 36.80, 35.48, 26.75.

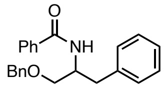
[a] Two decimal places shown to distinguish between peaks at δ 128.61 and 128.55.

HRMS (ESI-TOF): calculated for $C_{19}H_{24}NO^+$ ($[M+H]^+$): 282.1852, found 282.1852.

IR (ATM cm^{-1}): 3306 (br), 3060, 3032, 2966, 2865, 1634, 1578, 1492, 1368, 1107, 741, 694.



major (branched)



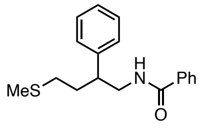
minor (linear)

***N*-(3-(benzyloxy)-2-phenylpropyl)benzamide (9b)** was prepared according to General Procedure C from **9a** and phenyl iodide. The product was isolated by flash chromatography (15% acetone/hexanes) to produce a yellow oil (78% yield (2:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 76% yield (2.0:1)
Run 2: 80% yield (2.1:1)

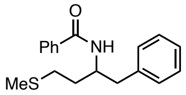
Branched Isomer:
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.59 – 7.54 (m, 2H), 7.51 – 7.21 (m, 13H), 7.07 (br s, 1H), 4.72 – 4.41 (m, 2H), 3.92 (dt, *J* = 13.4, 6.1 Hz, 1H), 3.87 – 3.83 (m, 2H), 3.79 (ddd, *J* = 13.3, 8.5, 4.4 Hz, 1H), 3.30 (tt, *J* = 7.9, 5.7 Hz, 1H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 167.1, 140.0, 137.8, 134.5, 131.2, 128.8, 128.6, 128.4, 128.0, 127.9, 127.8, 127.2, 126.8, 74.9, 73.7, 45.2, 44.3.

Linear Isomer:
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.76 – 7.72 (m, 2H), 7.51 – 7.21 (m, 13H), 6.70 – 6.57 (br s, 1H), 4.61 – 4.51 (m, 3H), 3.52 (d, *J* = 3.7 Hz, 2H), 3.07 (dd, *J* = 13.4, 6.1 Hz, 1H), 3.01 (dd, *J* = 13.4, 8.4 Hz, 1H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$)[a]: δ 166.94, 138.03, 137.98, 134.66, 131.42, 129.46, 128.54, 128.51, 128.51, 127.91, 127.88, 126.95, 126.49, 73.29, 69.65, 50.79, 37.49.
[a] Two decimal places shown to distinguish between peaks at δ 138.03 and 137.98.

Mixture of Isomers:
HRMS (APCI): calculated for $C_{23}H_{24}NO_2^+$ ($[M+H]^+$): 346.1802, found 346.1802.
IR (ATM cm^{-1}): 3314 (br), 3062, 3028, 2923, 2857, 1636, 1577, 1528, 1487, 1453, 1289, 1088, 1073, 1027, 908, 730, 6943.



major (branched)



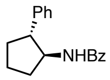
minor (linear)

***N*-(4-(methylthio)-2-phenylbutyl)benzamide (10b)** was prepared according to General Procedure C from **10a** and phenyl iodide. The product was isolated by flash chromatography (15% acetone/hexanes) to produce a yellow oil (54% yield (11:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 54% yield (10.0:1)
Run 2: 54% yield (12.5:1)

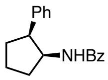
Branched Isomer:
^{1}H NMR (500 MHz, CDCl$_3$): δ 7.61 – 7.55 (m, 2H), 7.46 – 7.41 (m, 1H), 7.37 – 7.31 (m, 4H), 7.28 – 7.19 (m, 3H), 6.14 (br s, 1H), 3.94 – 3.84 (m, 1H), 3.41 (ddd, *J* = 13.5, 9.0, 4.8 Hz, 1H), 3.06 (tt, *J* = 9.8, 5.4 Hz, 1H), 2.43 – 2.29 (m, 2H), 2.11 – 1.97 (m, 4H), 1.98 – 1.79 (m, 1H).
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) δ 167.5, 141.7, 134.6, 131.5, 129.0, 128.6, 127.9, 127.2, 126.8, 45.3, 44.8, 33.0, 31.9, 15.5.

Linear Isomer:
Due to trace impurity, we did not obtain full characterization of the linear isomer. Below are listed the diagnostic peaks observed used to determine B:L ratio.
^{1}H NMR (500 MHz, CDCl$_3$): δ 2.96 (dd, *J* = 13.6, 6.1 Hz, 1H), 2.90 (dd, *J* = 13.2, 6.5 Hz, 1H).

Mixture of Isomers:
HRMS (APCI): calculated for $C_{18}H_{22}NOS^+$ ([M+H]$^+$): 300.1417, found 300.1421.
IR (ATM cm^{-1}): 3314 (br), 3062, 3028, 2923, 2857, 1636, 1577, 1528, 1487, 1453, 1289, 1088, 1073, 1027, 908, 730, 6943.

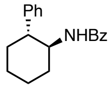


(+-)
major (trans)

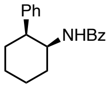


(+-)
minor (cis)

***N*-2-phenylcyclopentyl)benzamide (11b)** was prepared according to General Procedure C from **11a** and phenyl iodide. Yields were determined by ^{1}H NMR versus trimethoxy benzene as an external standard (60% yield (7:1)).
^{1}H NMR run 1: 57% yield (7.1:1)
^{1}H NMR run 2: 63% yield (5.9:1)
Isolation of the trans isomer was achieved by flash chromatography (15% EtOAc/hexanes) followed by recrystallization from hot EtOAc/hexanes. Spectral data for the trans isomer are in agreement with literature values.[13] Cis isomer yield based on literature characterization data from the same paper.
Trans Isomer:
^{1}H NMR (600 MHz, CDCl$_3$): δ 7.69 – 7.64 (m, 2H), 7.48 – 7.43 (m, 1H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.32 – 7.28 (m, 4H), 7.23 – 7.18 (m, 1H), 6.06 (br s, 1H), 4.50 (dq, *J* = 9.6, 7.8 Hz, 1H), 2.99 (td, *J* = 9.9, 8.0 Hz, 1H), 2.45 (dtd, *J* = 13.3, 7.9, 5.4 Hz, 1H), 2.27 – 2.17 (m, 1H), 1.93 – 1.86 (m, 2H), 1.83 – 1.76 (m, 1H), 1.70 – 1.54 (m, 1H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 167.5, 142.4, 134.9, 131.4, 128.8, 128.6, 127.4, 127.0, 126.8, 57.6, 52.3, 33.2, 32.9, 22.5.
HRMS (ESI-TOF): calculated for $C_{18}H_{20}NO^+$ ([M+H]$^+$): 266.1539, found 266.1538.
IR (ATM cm^{-1}): 3282 (br), 3062, 3028, 2958, 2872, 1632, 1578, 1540, 1491, 1317, 697.



(+-)
major (trans)



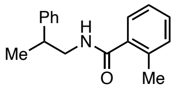
(+-)
minor (cis)

***N*-(2-phenylcyclohexyl)benzamide (12b)** was prepared according to General Procedure C from **12a** and phenyl iodide. Yields were determined by 1H NMR versus trimethoxy benzene as an external standard (29% yield (5:1)).

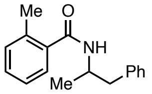
^{1}H NMR run 1: 26% yield (4.6:1)
^{1}H NMR run 2: 32% yield (5.2:1)
Isolation of the trans isomer was achieved by flash chromatography (10% EtOAc, 10% NEt_3, 80% hexanes). Under these column conditions the cis isomer coeluted with a side product of the reaction and the trans isomer could be collected cleanly. Partial isolation of the cis product was done via preparative thin layer chromatography (40% Et_2O/hexanes) to aid in characterization (collecting the top portion of the band to obtain cis isomer cleanly).

Trans Isomer:
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.44 – 7.35 (m, 3H), 7.33 – 7.22 (m, 6H), 7.20 – 7.13 (m, 1H), 5.70 (d, *J* = 8.3 Hz, 1H), 4.23 (tdd, *J* = 11.4, 8.1, 3.9 Hz, 1H), 2.54 (td, *J* = 11.6, 3.6 Hz, 1H), 2.41 – 2.34 (m, 1H), 2.02 – 1.95 (m, 1H), 1.91 – 1.80 (m, 2H), 1.69 – 1.20 (m, 4H)[a].
[a]Overlaps with H_2O.
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$): δ 167.1, 143.6, 135.3, 131.2, 128.8, 128.5, 127.5, 126.8, 126.8, 53.1, 51.1, 35.6, 34.2, 26.4, 25.5.
HRMS (ESI-TOF): calculated for $C_{19}H_{22}NO^+$ ($[M+H]^+$): 280.1696, found 280.1695.
IR (ATM cm^{-1}): 3295 (br), 3090, 3080, 3062, 3030, 2928, 2853, 1632, 1603, 1578, 1543, 1492, 1447, 1340, 1329, 755, 697, 669.

Cis Isomer:
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.55 – 7.49 (m, 2H), 7.47 – 7.40 (m, 1H), 7.39 – 7.32 (m, 2H), 7.32 – 7.24 (m, 4H), 7.24 – 7.15 (m, 1H), 6.05 (d, *J* = 7.9 Hz, 1H), 4.57 (dq, *J* = 7.7, 3.8 Hz, 1H), 3.08 (dt, *J* = 12.3, 3.9 Hz, 1H), 2.22 – 2.15 (m, 1H), 2.03 – 1.89 (m, 2H), 1.86 – 1.23 (m, 5H)[a].
[a]Overlaps with H_2O and grease
$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 167.00, 142.82, 135.32, 131.13, 128.49, 128.48, 127.31, 126.66, 126.60, 50.23, 44.74, 30.80, 26.00, 25.50, 20.96.
[a]Two decimal places shown to distinguish between peaks at δ 128.49 and 128.48.
HRMS (ESI-TOF): calculated for $C_{19}H_{22}NO^+$ ($[M+H]^+$): 280.1696, found 280.1696.



major (branched)



minor (linear)

2-methyl-*N*-(2-phenylpropyl)benzamide (13b) was prepared according to General Procedure C from **13a** and phenyl iodide. The product was isolated by flash chromatography (15% EtOAc/hexanes) to produce a yellow solid (58% yield (8:1)). The product was isolated and characterized as a mixture of isomers.
Run 1: 57% yield (9.1:1)
Run 2: 58% yield (7.7:1)

Branched Isomer:
^{1}H NMR (600 MHz, CDCl3): δ 7.36 – 7.32 (m, 2H), 7.29 – 7.19 (m, 4H), 7.18 – 7.15 (m, 2H), 7.14 – 7.10 (m, 1H), 5.74 (br s, 1H), 3.78 (dt, *J* = 13.5, 6.4 Hz, 1H), 3.45 (ddd, *J* = 13.4, 9.0, 5.3 Hz, 1H), 3.08 (dp, *J* = 9.2, 6.9 Hz, 1H), 2.33 (s, 3H), 1.34 (d, *J* = 7.0 Hz, 3H).
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$): δ 170.1, 144.1, 136.7, 136.0, 131.0, 129.8, 128.8, 127.3, 126.9, 126.7, 125.7, 46.4, 40.0, 19.7, 19.7.

Linear Isomer:

^{1}H NMR (600 MHz, CDCl3): δ 7.38 – 7.10 (m, 9H), 5.74 (br s, 1H), 4.52 – 4.42 (m, 1H), 2.90 (dd, J = 13.6, 6.6 Hz, 1H), 2.85 (dd, J = 13.7, 6.9 Hz, 1H), 2.33 (s, 3H), 1.24 (d, J = 6.8 Hz, 3H).

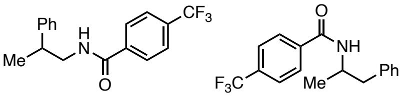
^{13}C{^{1}H} NMR (151 MHz, CDCl3): δ 169.48, 138.06, 136.86, 135.96, 130.93, 129.71, 129.50, 128.50, 127.31, 126.59, 126.58, 46.46, 42.63, 20.41, 19.63.

[a]Two decimal places shown to distinguish between peaks at δ 126.59 and 126.58.

Mixture of Isomers:

HRMS (APCI): calculated for $C_{17}H_{20}NO^+$ ([M+H]$^+$): 254.1539, found 254.1538.

IR (ATM cm^{-1}): 3268 (br), 3027, 2965, 2926, 2872, 1636, 1535, 1453, 1306, 760, 741, 699.



major (branched) *minor (linear)*

***N*-(2-phenylpropyl)-4-(trifluoromethyl)benzamide (14b)** was prepared according to General Procedure C from **14a** and phenyl iodide. The product was isolated by flash chromatography (15% EtOAc/hexanes) to produce a white solid (48% yield (20:1)). The product was isolated and characterized as a mixture of isomers. While minor amounts of linear isomer are observed by ^{1}H NMR, due to the high selectivity of the reaction, only branched isomer characterization data is provided.

Run 1: 52% yield (20:1)

Run 2: 44% yield (20:1)

Branched Isomer:

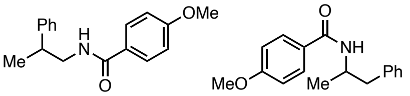
^{1}H NMR (600 MHz, CDCl3): δ 7.70 (d, J = 8.1 Hz, 2H), 7.62 (d, J = 8.1 Hz, 2H), 7.38 – 7.32 (m, 2H), 7.28 – 7.23 (m, 3H), 6.17 (br s, 1H), 3.83 (dt, J = 13.4, 6.3 Hz, 1H), 3.42 (ddd, J = 13.6, 8.9, 5.0 Hz, 1H), 3.09 (dp, J = 9.1, 6.9 Hz, 1H), 1.35 (d, J = 7.0 Hz, 3H).

^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 166.3, 143.9, 138.1, 133.2 (q, J = 32.7 Hz), 129.0, 127.4, 127.3, 127.1, 125.7 (q, J = 3.8 Hz), 123.8 (q, J = 272.6 Hz), 46.8, 39.8, 19.4.

^{19}F NMR (565 MHz, CDCl$_3$): δ -62.97 (s).

HRMS (APCI): calculated for $C_{17}H_{17}F_3NO^+$ ([M+H]$^+$): 308.1257, found 308.1257.

IR (ATM cm^{-1}): 3322 (br), 3028, 2965, 2932, 1642, 1546, 1327, 1165, 1126, 1069, 700.



major (branched) *minor (linear)*

4-methoxy-N-(2-phenylpropyl)benzamide (15b) was prepared according to General Procedure C from **15a** and phenyl iodide. The product was isolated by flash chromatography (10% to 15% acetone/hexanes) to produce a white solid (78% yield (10:1)). The product was isolated and characterized as a mixture of isomers.

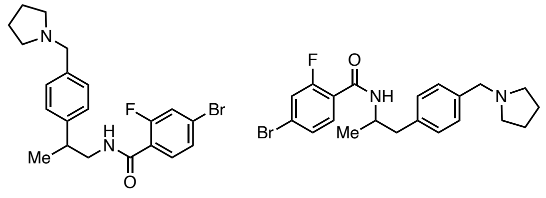
Run 1: 74% yield (9:1)

Run 2: 81% yield (10:1)

Branched Isomer:
^{1}H NMR (600 MHz, CDCl$_3$): δ 7.61 (d, *J* = 8.7 Hz, 2H), 7.36 – 7.29 (m, 2H), 7.25 – 7.19 (m, 3H), 6.84 (d, *J* = 8.8 Hz, 2H), 6.23 (br s, 1H), 3.83 – 3.73 (m, 4H), 3.39 (ddd, *J* = 13.4, 8.5, 5.0 Hz, 1H), 3.11 – 3.01 (m, 1H), 1.31 (d, *J* = 7.0 Hz, 3H).
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 167.0, 162.1, 144.3, 128.7, 128.6, 127.3, 127.0, 126.8, 113.7, 55.4, 46.6, 39.8, 19.3.

Linear Isomer:
^{1}H NMR (600 MHz, CDCl$_3$): δ 7.69 (d, *J* = 8.8 Hz, 2H), 7.37 – 7.18 (m, 5H), 6.84 (d, *J* = 8.8 Hz, 2H), 6.23 (br s, 1H), 4.48 – 4.41 (m, 1H), 3.83 – 3.73 (m, 3H)[a], 2.95 (dd, *J* = 13.5, 5.6 Hz, 1H), 2.81 (dd, *J* = 13.4, 7.2 Hz, 1H), 1.20 (d, *J* = 6.6 Hz, 3H).
[a]Not resolved from branched isomer.
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 166.4, 162.0, 138.1, 129.6, 128.7, 128.4, 127.2, 126.5, 113.6, 55.4, 46.5, 42.5, 20.0.

Mixture of Isomers:
HRMS (APCI): calculated for $C_{17}H_{20}NO^+$ ($[M+H]^+$): 270.1489, found 270.1489.
IR (ATM cm^{-1}): 3313 (br), 3059, 3028, 3001, 2961, 2928, 2871, 2838, 1631, 1606, 1545, 1504, 1253, 1178, 1032, 844, 763, 701.



major (branched) *minor (linear)*

16b was prepared according to a modified General Procedure C from **16a** and 1-(4-iodobenzyl)pyrrolidine (synthesized according to reference 14 and distilled at 100 °C under full vacuum before use; at the time this manuscript was prepared, 1-(4-iodobenzyl)pyrrolidine was commercially available).

The following stock solutions were prepared in 1-dram vials:
Stock Solution 1: Cp*TiCl$_3$ (23.16 mg, 0.080 mmol, 20 mol%) and 889 μL of THF.
Stock Solution 2: NiBr$_2$•diglyme (7.05 mg, 0.020 mmol, 5 mol%), dtbbpy (8.05 mg, 0.030 mmol, 7.5 mol%), and 889 μL of THF. This vial was equipped with a Teflon stir bar, capped with a septum cap, and allowed to stir for 15 minutes forming a green suspension.
Stock Solution 3: Zn (78.46 mg, 1.20 mmol, 3.0 equiv) and 889 μL of THF. A suspension of Zn in THF was generated by pipetting up and down a few times before transferring to the reaction.

To a 2-dram vial equipped with a Teflon stir bar was added pyridine•HBr (64.00 mg, 0.40 mmol, 1.0 equiv), aziridine (103.24 mg, 0.40 mmol, 1.0 equiv), and ArI (114.86 mg, 0.40 mmol, 1.0 equiv). 889 μL of stock solution 1 was added. The reaction was allowed to stir for 15 minutes at which point stock solution 2 (889 μL), and stock solution 3 (889 μL) were sequentially added. The reaction vial was capped with a septum cap, wrapped with electrical tape, and brought outside the glovebox. The reactions were set to stir (1200 rpm) at room temperature for 3 hours. After 3 hours the reactions were opened to air. EtOAc (~2 mL) was added to the vial and then the solution was passed through a celite plug with EtOAc to remove any solids. The eluate was concentrated and purified by flash chromatography (5% EtOAc/hexanes + 15% NEt$_3$) to produce a slightly pink solid (46% yield (10:1)). The product was isolated and characterized as a mixture of isomers. Spectral data are in agreement with literature values.[15]

Run 1: 47% yield (9.1:1)
Run 2: 45% yield (10.0:1)

Branched Isomer:

^{1}H NMR (600 MHz, CDCl$_3$): δ 7.96 – 7.85 (m, 1H), 7.37 – 7.34 (m, 1H), 7.30 – 7.27 (m, 2H), 7.23 – 7.19 (m, 1H), 7.19 – 7.16 (m, 2H), 6.57 – 6.47 (m, 1H), 3.78 (dtd, *J* = 12.8, 6.4, 1.7 Hz, 1H), 3.58 (s, 2H), 3.45 (dddd, *J* = 13.3, 8.5, 4.8, 1.2 Hz, 1H), 3.04 (dp, *J* = 8.6, 6.9 Hz, 1H), 2.57 – 2.40 (m, 4H), 1.86 – 1.68 (m, 4H), 1.32 (d, *J* = 7.0 Hz, 3H).

^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): = δ 162.4 (d, *J* = 3.3 Hz), 160.1 (d, *J* = 251.7 Hz), 142.4, 138.0, 133.2 (d, *J* = 2.9 Hz), 129.4, 128.3 (d, *J* = 3.3 Hz), 127.1, 126.2 (d, *J* = 10.3 Hz), 120.3 (d, *J* = 11.8 Hz), 119.6 (d, *J* = 28.2 Hz), 60.4, 54.2, 47.0, 39.3, 23.5, 19.3.

^{19}F NMR (565 MHz, CDCl$_3$): δ -111.6 (q, *J* = 10.9 Hz).

Linear Isomer:

^{1}H NMR (600 MHz, CDCl$_3$): δ 7.93 – 7.88 (m, 1H), 7.38 – 7.33 (m, 1H), 7.30 – 7.19 (m, 3H), 7.16 – 7.13 (m, 2H), 6.55 – 6.48 (m, 1H), 4.49 – 4.38 (m, 1H), 3.57 (s, 2H), 2.91 (dd, *J* = 13.5, 5.9 Hz, 1H), 2.79 (dd, *J* = 13.6, 7.1 Hz, 1H), 2.57 – 2.40 (m, 4H), 1.86 – 1.68 (m, 4H), 1.21 (d, *J* = 6.7 Hz, 3H).

^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$): δ 161.6 (d, *J* = 3.4 Hz), 160.1 (d, *J* = 251.4 Hz), 137.7, 136.3, 133.3 – 133.2 (m)[a], 129.4, 129.1, 128.4 – 128.3 (m)[b], 126.2 (d, *J* = 10.3 Hz), 120.5 (d, *J* = 11.9 Hz), 119.6 (d, *J* = 28.2 Hz), 60.5, 54.2[c], 47.1, 42.1, 23.5, 20.0.

[a,b] Overlap with branched isomer precluded full resolution of multiplet.

[c] Not observed in ^{13}C{^{1}H} NMR, assumed overlap with branched isomer.

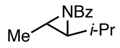
^{19}F NMR (565 MHz, CDCl$_3$): δ -111.3 (q, *J* = 10.9 Hz).

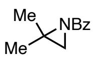
Mixture of Isomers:

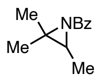
HRMS (ESI-TOF): calculated for $C_{21}H_{25}{}^{79}BrFN_2O^+$ ([M+H]$^+$): 419.1129, found 419.1126.

IR (ATM cm^{-1}): 3449 (br shoulder), 3385 (br), 2964, 2930, 2872, 2787, 1654, 1603, 1535, 1477, 1401, 1299, 1205, 1154, 1128, 1113, 877, 766.

Unsuccessful Aziridines:





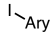


6. Construction of Aryl Iodide Chemical Space

6.1. Commercial Aryl Iodide Search

The search was performed on Reaxys® on Aug 24, 2022.

Initial Search:
The search was initiated under "Query builder" in Reaxys® on the following structure (where Ary=Aryl using the prebuilt functionality under "Reaxys Group Generics").



The following filters were also applied on this page:

- Molecular Weight <= 500 (*Identification→Molecular Weight*)
- Number of Fragments = 1 (*Identification→Number of Fragments*)

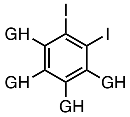
The search was performed in the "Commercial Substances" database (Search in Substances >> Change database from Reaxys® to Commercial Substances) to give 392,214 aryl iodides.

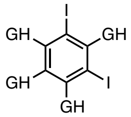
Subsequent Filters:
From the initial set of aryl iodides the following filters were applied:

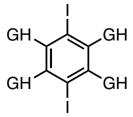
- Availability: Limit to "PubChem"
- Availability: Limit to "Reaxys"
- Price: Filter by Value <= 500
- Stock Availability: Limit to "In Stock"

This narrowed our initial search space to 4,284 aryl iodides.

Functional Group Filters:
We limited our search space to mono-substituted aryl iodides. This was done by using the "By Structure" filter in the lefthand column and excluding following structures: (GH=Any group or H)







This gave us a final aryl iodide search space of 4,116 aryl iodides.

6.2. Descriptor Generation

In order to compare aryl iodides in chemical space we first needed to generate descriptors for each aryl iodide. While many types of descriptors exist, we wanted descriptors that would distinguish aryl iodides based on their chemical reactivity. Thus, we turned to density functional theory (DFT) descriptors to capture electronic and local steric features as these features would most likely distinguish aryl iodide reactivity.

Global and common core atomic DFT descriptors were generated for the minimum energy conformer for the 4,116 aryl iodides using Auto-QChem. Calculations were performed using the APFD^{16} functional with the 6-31G** basis set$^{17–21}$ for light atoms and LanL2DZ basis set$^{22–24}$ for heavy atoms. All calculations for these descriptors were performed using the PCM solvation model^{25} for acetonitrile. From the initial list of descriptors, we hand selected the following features based on chemical intuition.

Global descriptors

homo_energy	lumo_energy

Atomic descriptors

Common Core
- I
- C_{ipso}
- C_{ortho_avg}
- C_{meta_avg}
- C_{para}

APT_charge	ES_root_Mulliken_charge	ES_root_NPA_Rydberg	ES_root_NPA_charge
ES_root_NPA_core	ES_root_NPA_total	ES_root_NPA_valence	Mulliken_charge
NMR_anisotropy	NMR_shift	NPA_Rydberg	NPA_charge
NPA_core	NPA_total	NPA_valence	VBur

Before we could use the descriptors in clustering, we standardized the descriptors using sklearn.preprocessing.scale (StandardScaler). We then removed any zero-variance features (descriptors that do not change across the data set) and highly correlated (>95%) features (this avoids “double counting” or “overweighting” of a single feature).

Table S5. Aryl iodide features used in clustering. Features highlighted in light grey do not vary across the dataset. Features highlighted in dark grey correlate with at least one non-highlighted feature above 95%. Features that are not highlighted are ones used for dimensionality reduction and clustering.

Global

homo_energy	lumo_energy

I

APT_charge	ES_root_Mulliken_charge	ES_root_NPA_Rydberg	ES_root_NPA_charge
ES_root_NPA_core	ES_root_NPA_total	ES_root_NPA_valence	Mulliken_charge
NMR_anisotropy	NMR_shift	NPA_Rydberg	NPA_charge
NPA_core	NPA_total	NPA_valence	VBur

C_ipso

APT_charge	ES_root_Mulliken_charge	ES_root_NPA_Rydberg	ES_root_NPA_charge
ES_root_NPA_core	ES_root_NPA_total	ES_root_NPA_valence	Mulliken_charge
NMR_anisotropy	NMR_shift	NPA_Rydberg	NPA_charge
NPA_core	NPA_total	NPA_valence	VBur

C_ortho_avg

APT_charge	ES_root_Mulliken_charge	ES_root_NPA_Rydberg	ES_root_NPA_charge
ES_root_NPA_core	ES_root_NPA_total	ES_root_NPA_valence	Mulliken_charge
NMR_anisotropy	NMR_shift	NPA_Rydberg	NPA_charge
NPA_core	NPA_total	NPA_valence	VBur

C_meta_avg

APT_charge	ES_root_Mulliken_charge	ES_root_NPA_Rydberg	ES_root_NPA_charge
ES_root_NPA_core	ES_root_NPA_total	ES_root_NPA_valence	Mulliken_charge
NMR_anisotropy	NMR_shift	NPA_Rydberg	NPA_charge
NPA_core	NPA_total	NPA_valence	VBur

C_para_avg

APT_charge	ES_root_Mulliken_charge	ES_root_NPA_Rydberg	ES_root_NPA_charge
ES_root_NPA_core	ES_root_NPA_total	ES_root_NPA_valence	Mulliken_charge
NMR_anisotropy	NMR_shift	NPA_Rydberg	NPA_charge
NPA_core	NPA_total	NPA_valence	VBur

6.3. Dimensionality Reduction

The next step of the workflow involves applying a dimensionality reduction technique. Principal Components Analysis (PCA) and Uniform Manifold Approximation and Projection (UMAP). For both algorithms, we tested several benchmark levels of compression from the original 45 dimensions to 20, 10, 5, 3, and 2 dimensions.

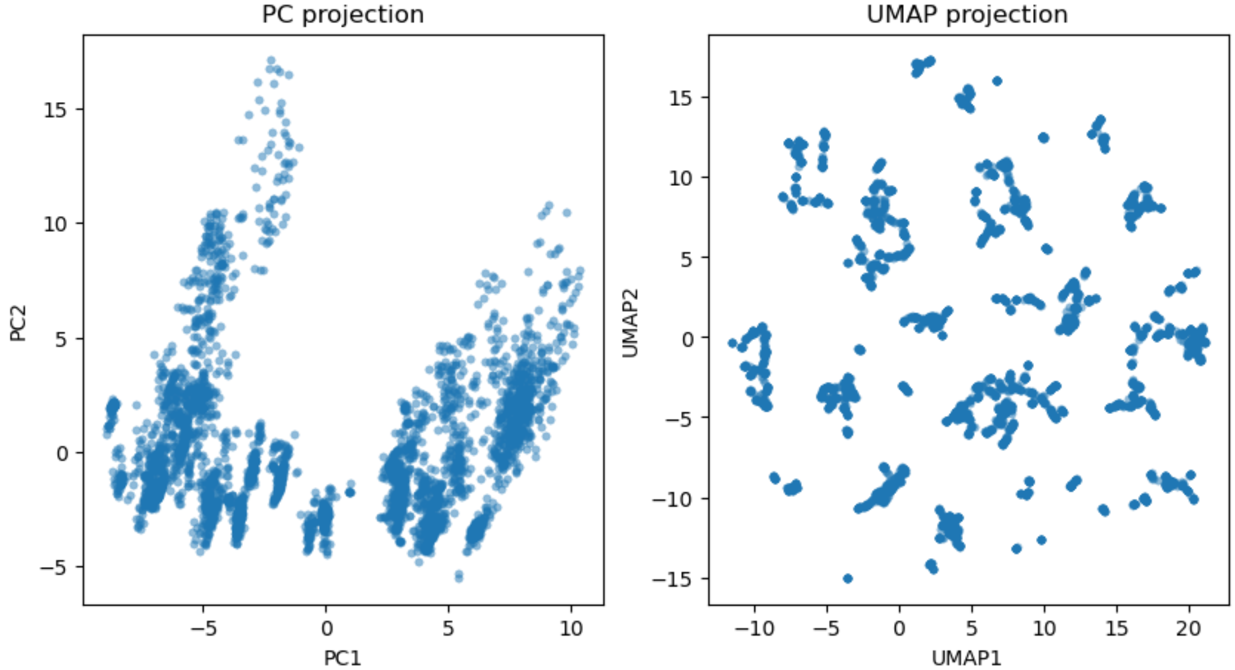


Figure S1. Two-dimensional imbedding of PCA and UMAP clustering methods

The quality of clustering was then tested by the silhouette value, a common clustering metric. For each sample (aryl iodide) $i \epsilon C_i$(data point i in cluster C_i) we compute two values:

Average distance of an aryl iodide to the other aryl iodides within its same cluster:

$$a(i) = \frac{1}{|C_i|-1} \sum_{j \epsilon C_i, i \neq j} d(i,j)$$ **SEq.1**

Average distance of an aryl iodide to other clusters:

$$b(i) = \min_{k \neq i} \frac{1}{|C_k|} \sum_{j \epsilon C_k} d(i,j)$$ **SEq.2**

The silhouette value is then defined by:

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$ **SEq.3**

This value can hypothetically span the range of $-1 \leq s(i) \leq 1$. Larger values mean that aryl iodides within the same cluster match the other aryl iodides within the same cluster while differing from those in other clusters. We computed silhouette scores for 5-45 clusters (aiming to have a high silhouette score).

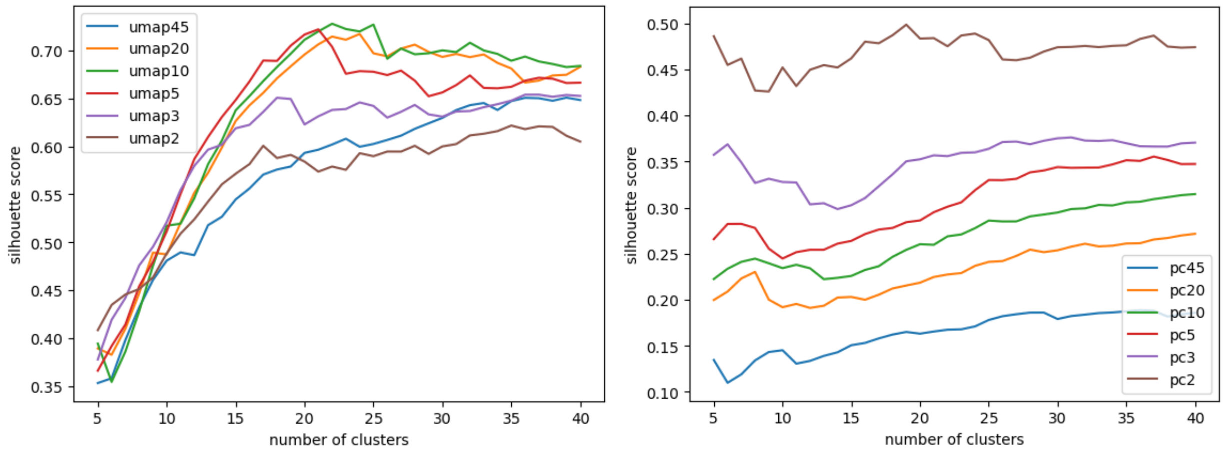


Figure S2. Average silhouette score as a function of number of clusters (5-45) for both UMAP (top) and PCA (bottom) clustering methods.

We found that overall UMAP provided higher silhouette scores, beginning low but then quickly rising until they begin to taper off around 15-20 clusters. For our substrate scope selection, we chose to proceed with UMAP clustering, at 10 dimensions and 16 clusters. A full list of aryl iodides sorted by cluster is included in section 12.

UMAP, like other non-linear dimensionality reduction techniques, involves the transformation of high-dimensional data into a lower-dimensional Euclidean space. This transformation requires warping the high-dimensional shape, which means that distances in the lower-dimensional space may not carry the same intuitive physical meaning as in linear reduction techniques, such as PCA.

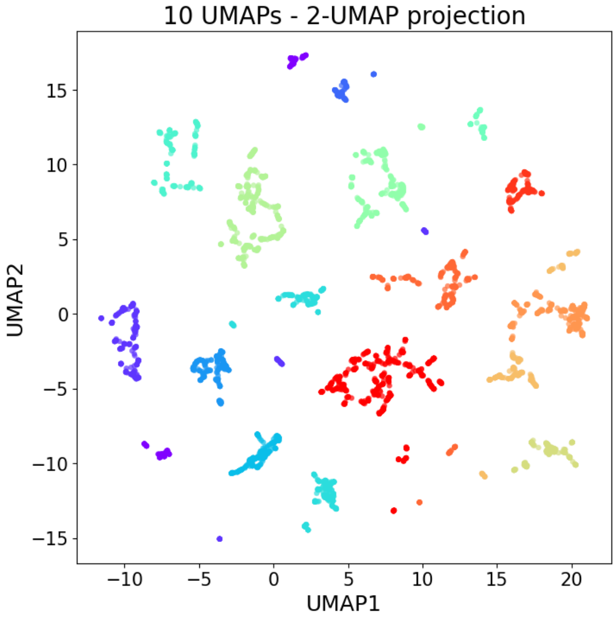


Figure S3. Clusters generated in 10-dimensions plotted on 2-dimension UMAP space.

6.4. Functional Group Filter

With initial clusters in hand, we next removed functional groups we envisioned would be incompatible with the method. These functional groups include those that gave either <15% yield or <15% additive recovery in the robustness screen. In addition, we also removed acid halides, sulfonyl halides, tertiary alkyl bromides, and anything with more than one iodide. We found that even without these aryl iodides we still had a good representation of ArI chemical space.

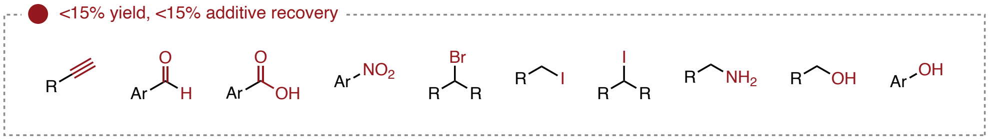


Figure S4. Functional groups that are not tolerated in the reaction as determined by Glorius additive screen.

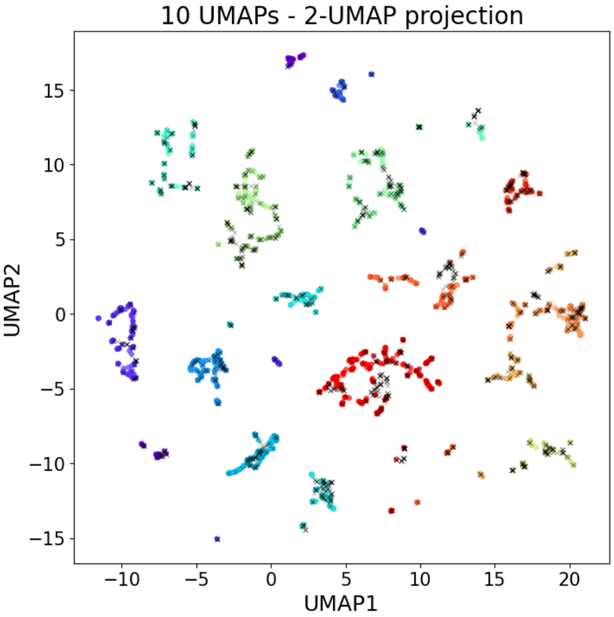


Figure S5. Chemical space with aryl iodides containing unsuitable functional groups marked with an “x”.

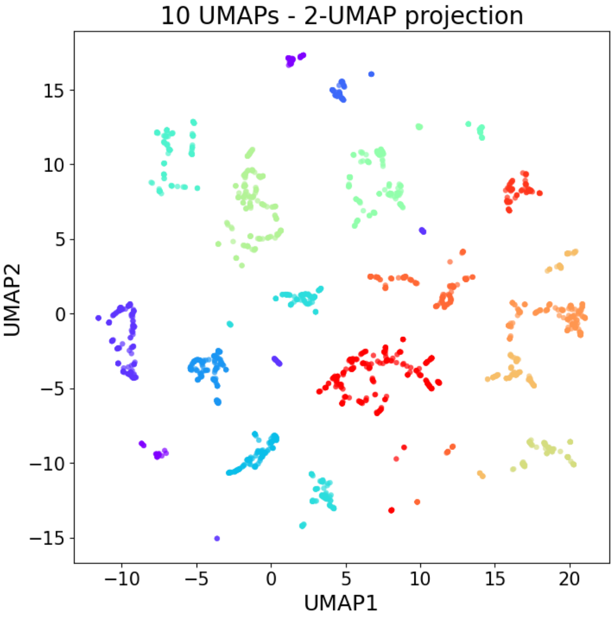


Figure S6. Chemical space following functional group filter.

6.5. Aryl Iodide Scope Selection

One aryl iodide from each cluster was hand selected for analysis in the substrate scope (Figure 4B). In selecting aryl iodides, we considered similarity to other aryl iodides in the cluster, distance to the centroid of the cluster (see section 6.6), vendor availability, and cost. Figure S7 shows an overlay of the observed reaction yields on the plot and Figure S8 shows an overlay of the predicted reaction yields on the plot. While cluster identity appears to be correlated with reactivity, we would recommend that a user apply the prediction model to assess the performance of an untested substrate rather than using the cluster identity of the unseen substrate.

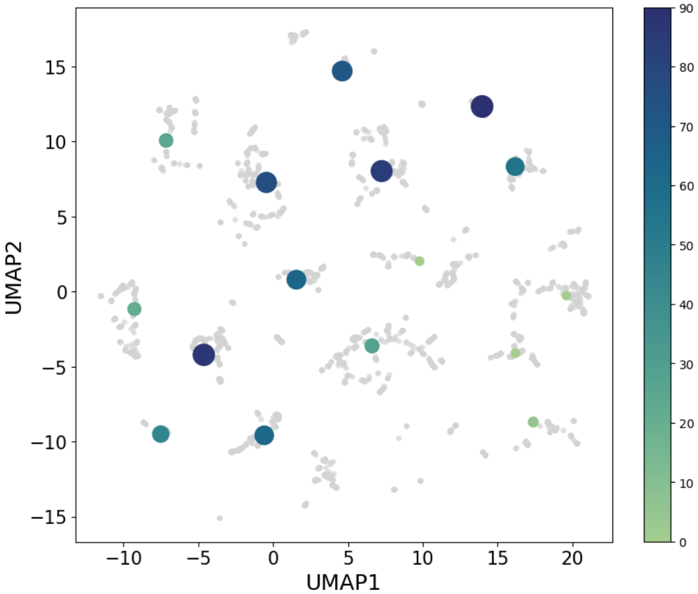


Figure S7. Heat map plot of observed yields across aryl iodide scope.

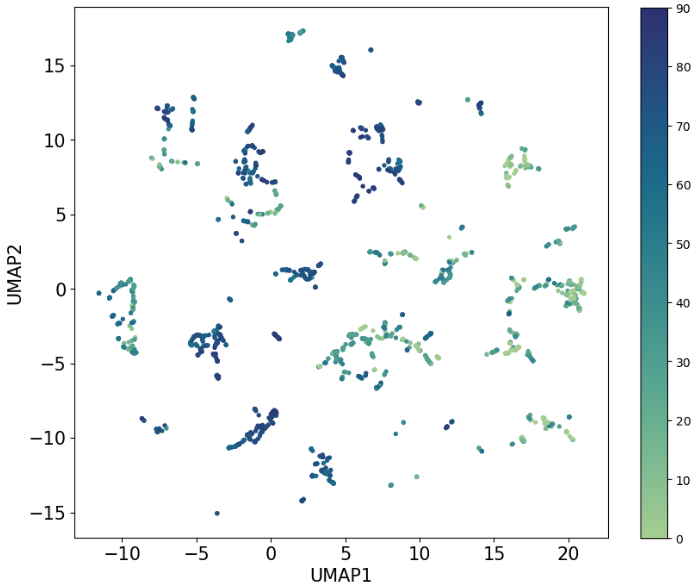
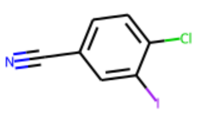


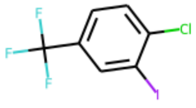
Figure S8. Heat map plot of predicted yields across all aryl iodides. Yields that are predicted to be less than 0% yield are set to 0% yield.

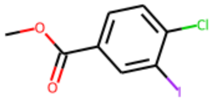
6.6. Center 50 Aryl Iodides in Each Cluster

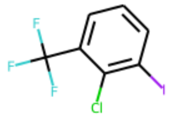
For each cluster we computed the centroid position based on 10 UMAP features from the full aryl iodide space. We then applied the functional group filter and sorted the remaining aryl iodides in order of distance to the centroid. Below the center 50 from each cluster are displayed. In cases where a cluster has fewer than fifty aryl iodides, all aryl iodides are displayed.

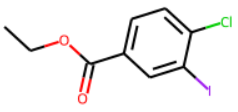
Cluster A:

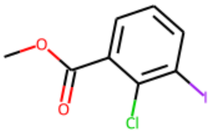


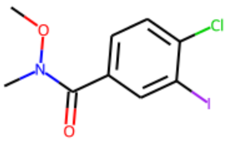


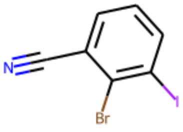


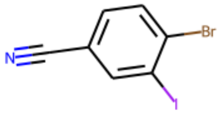


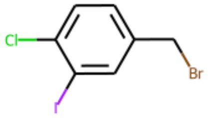


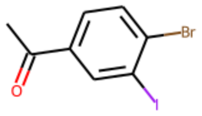


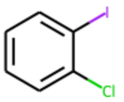


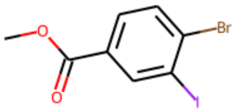


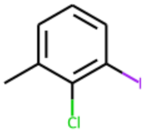


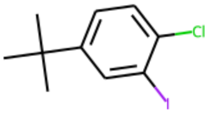


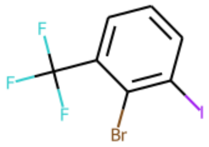


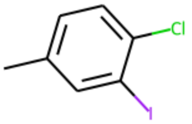


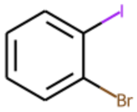


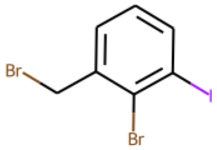


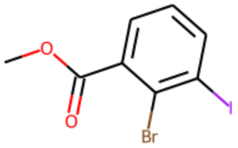


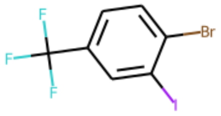


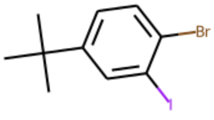


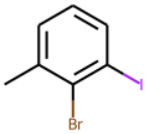


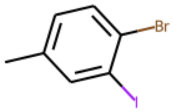


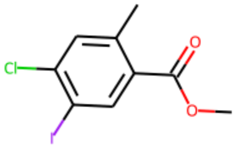


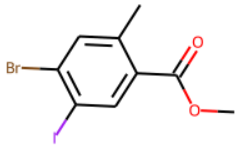


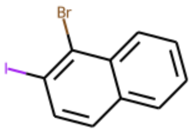


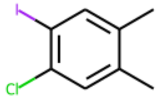


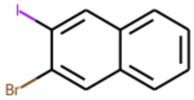


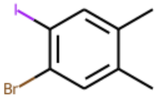


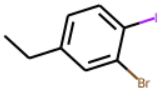


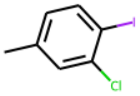


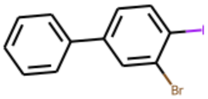


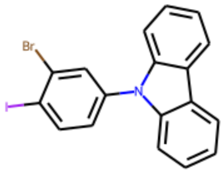


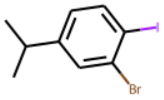


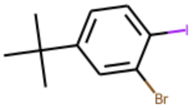


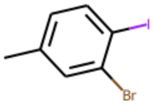


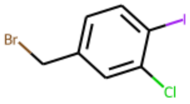


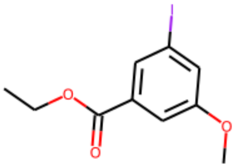


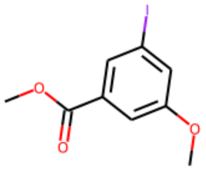


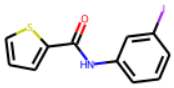


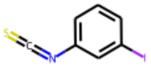


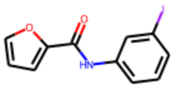


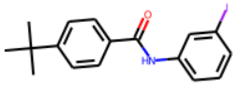


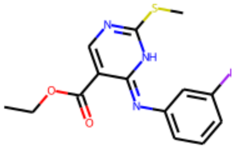


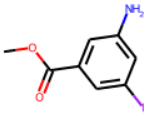


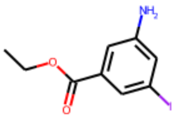


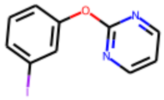


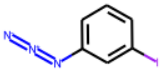






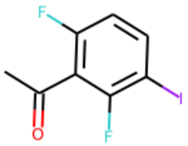


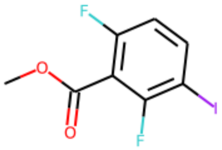


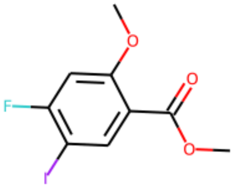


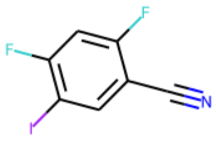
In this cluster we opted to select an aryl iodide that represented the substrates without a single *ortho* substituent as overall our substrate scope had several substrates with *ortho* substitution.

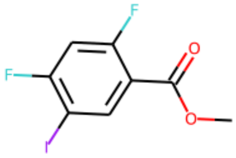
Cluster B:

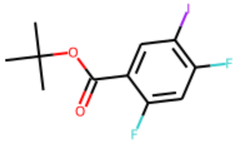
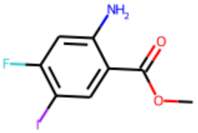
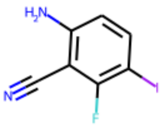
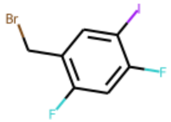
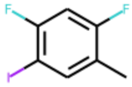
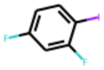
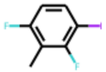
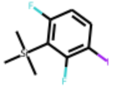
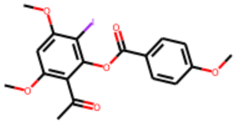
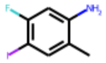
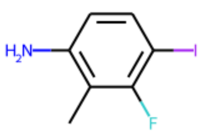
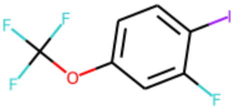
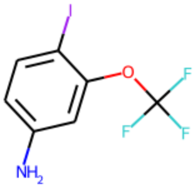
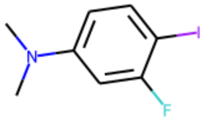
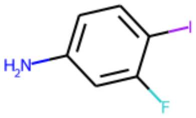
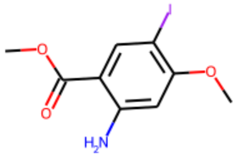
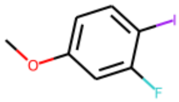
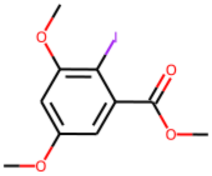
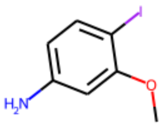
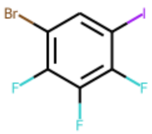
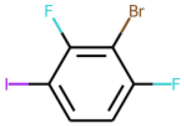
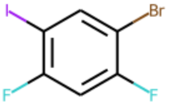
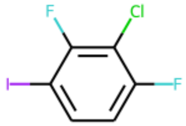
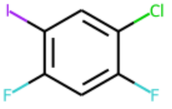


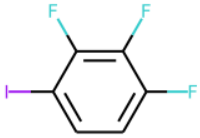
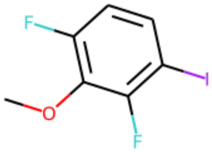
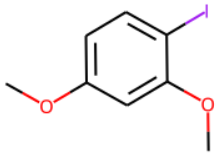
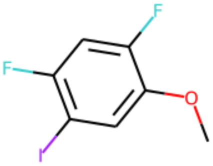
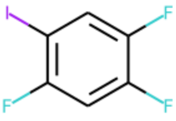


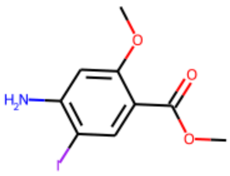
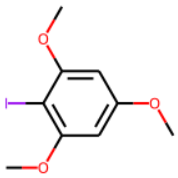
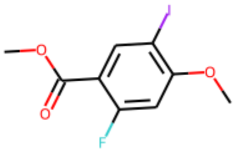
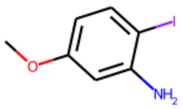
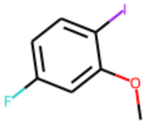
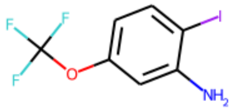
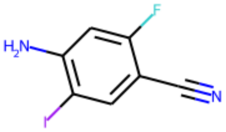
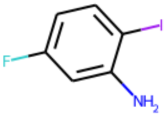
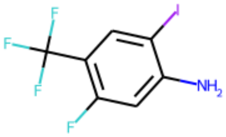
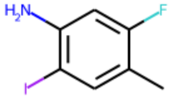
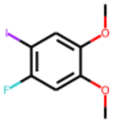
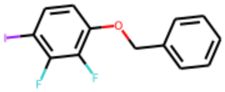
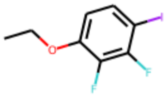
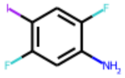
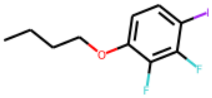






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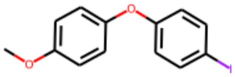
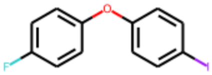
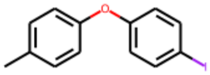
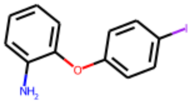
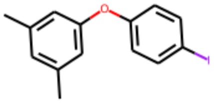
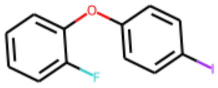
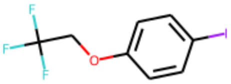
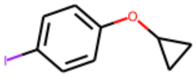
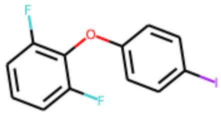
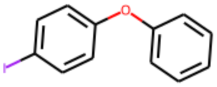
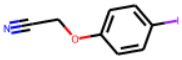
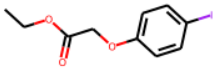
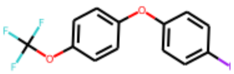
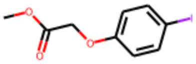
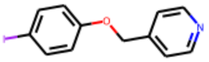

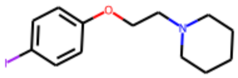
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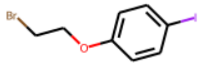
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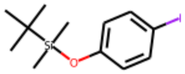
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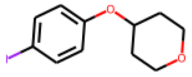
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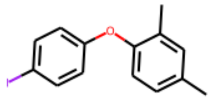
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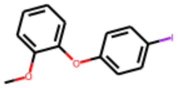
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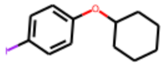
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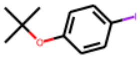
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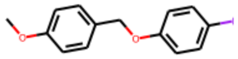
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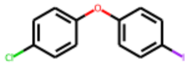
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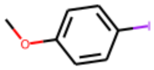
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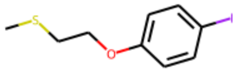
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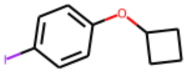
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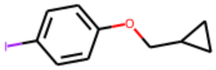
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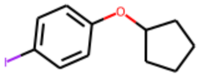
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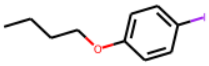
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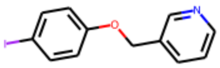
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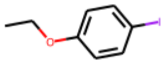
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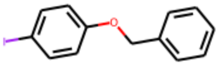
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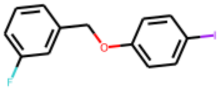
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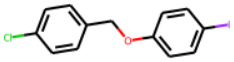
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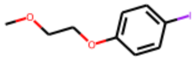
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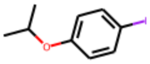
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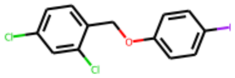
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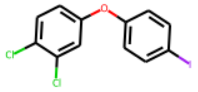
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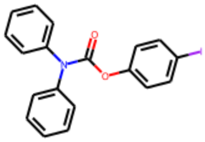
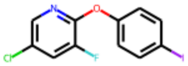
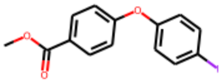
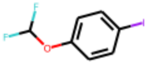
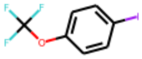
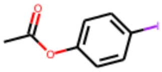
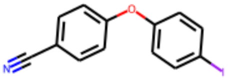
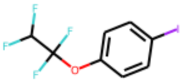
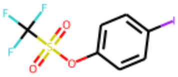
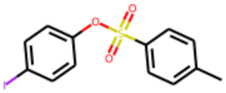

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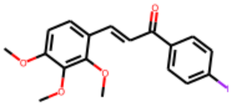
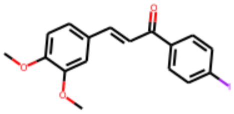
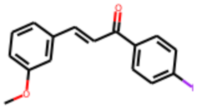
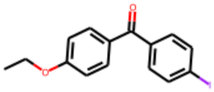
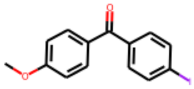
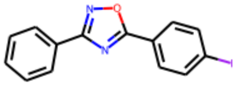
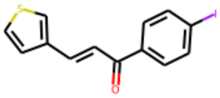
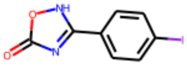
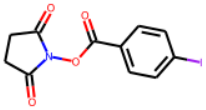
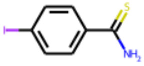
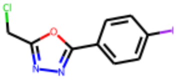
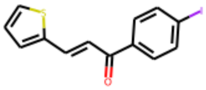
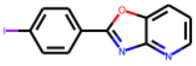
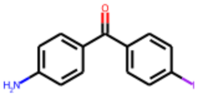
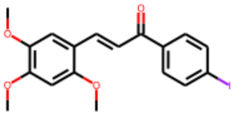
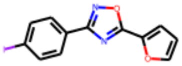
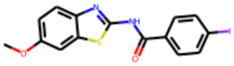
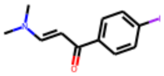
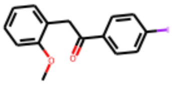
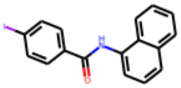

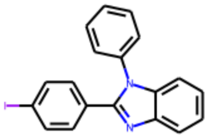
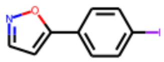
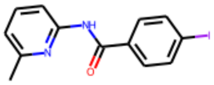
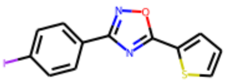
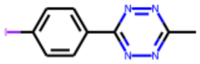
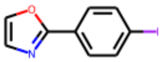
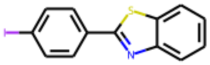
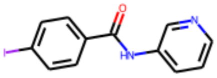
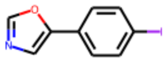
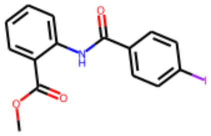
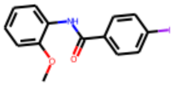
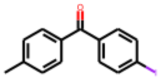
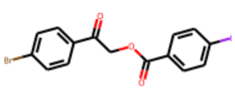
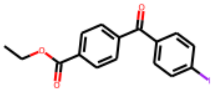
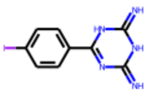
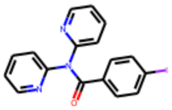
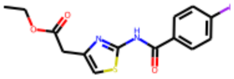
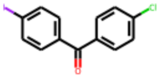
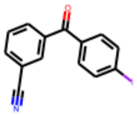
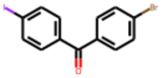
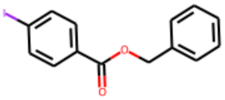
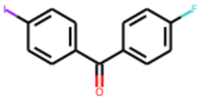
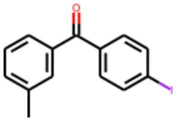
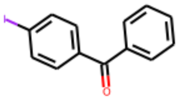
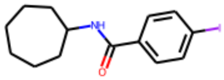
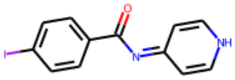
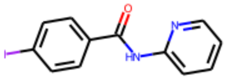
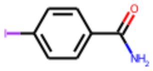
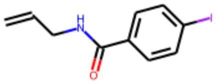
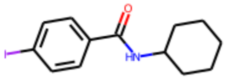

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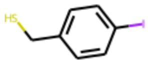
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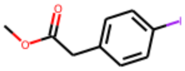
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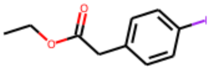
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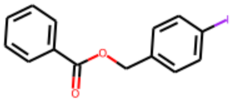
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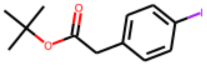
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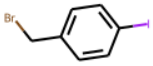
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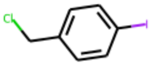
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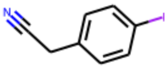
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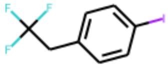
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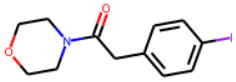
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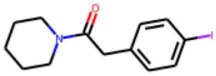
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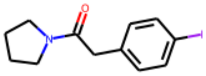
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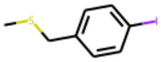
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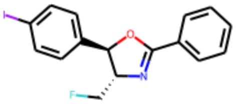
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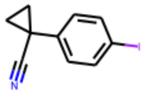
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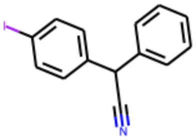
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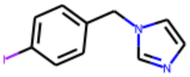
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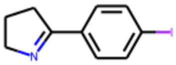
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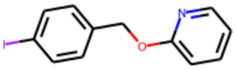
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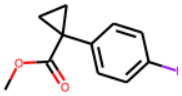
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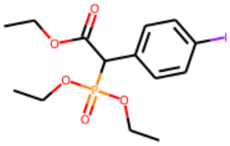
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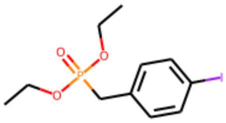
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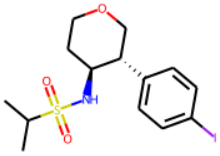
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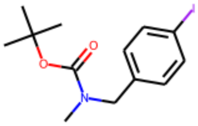
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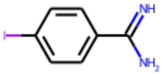
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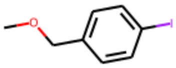
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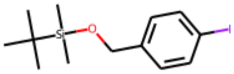
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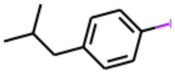
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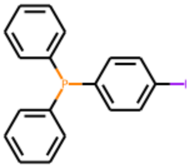
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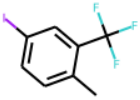
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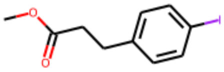
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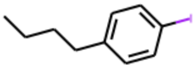
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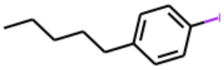
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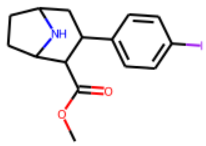
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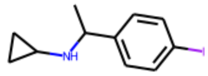
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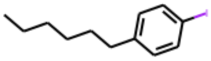
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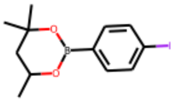
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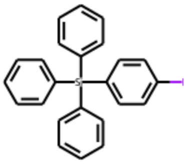
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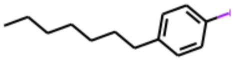
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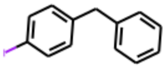
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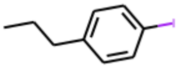
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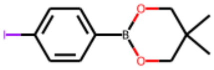
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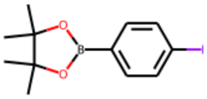
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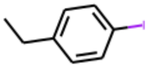
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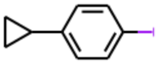
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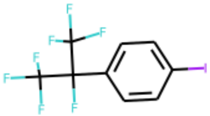
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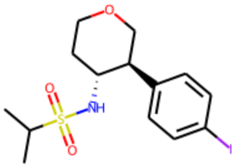
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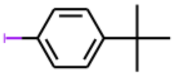
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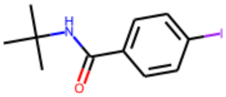
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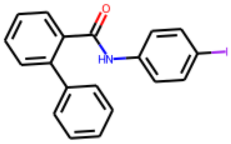
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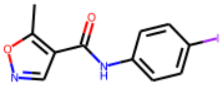
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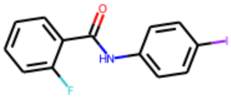
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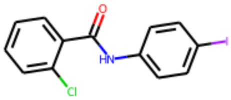
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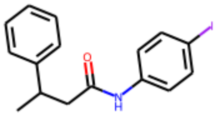
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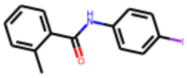
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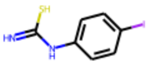
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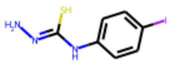
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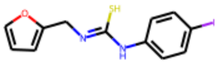
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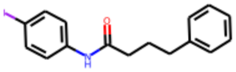
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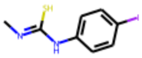
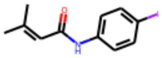
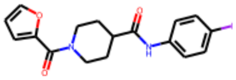
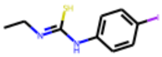
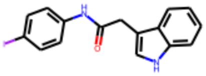
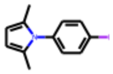
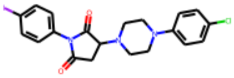
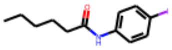
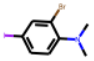
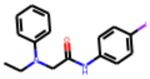
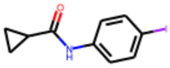
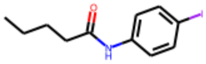
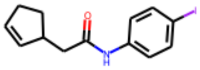
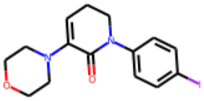
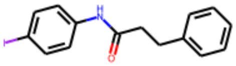
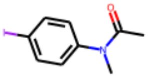
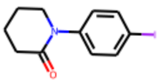
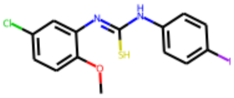
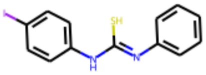
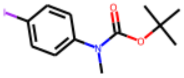
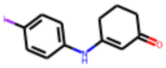
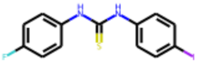
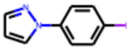
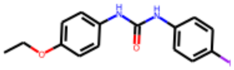
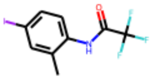
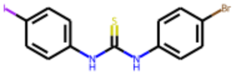
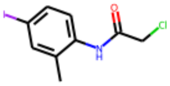
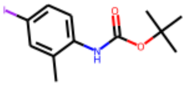
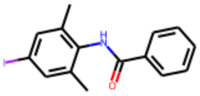
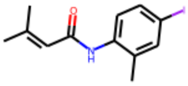
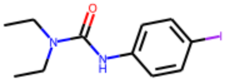
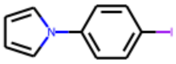
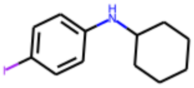
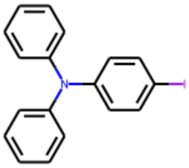
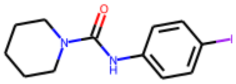































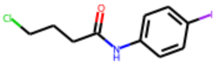


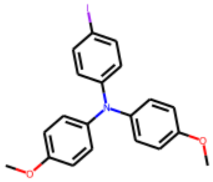


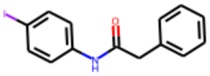


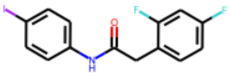


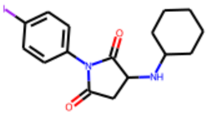






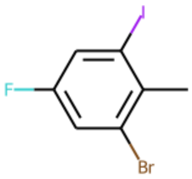


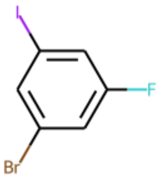


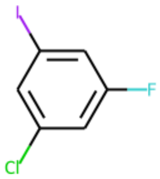


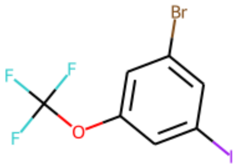
Many of the amides we tested were not soluble under reaction conditions. Thus, the selected aryl iodide does not contain the amide functionality.

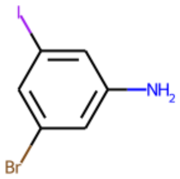
Cluster G:

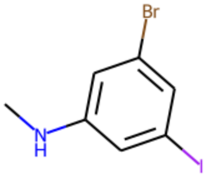


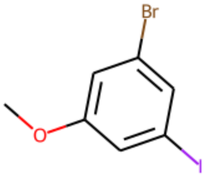


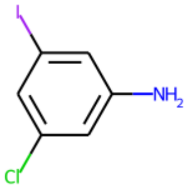


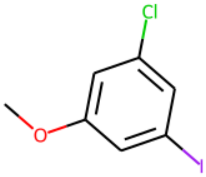


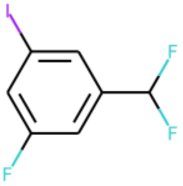


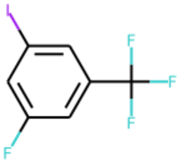


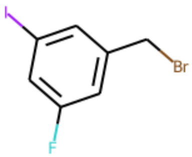


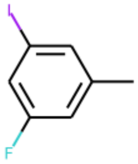


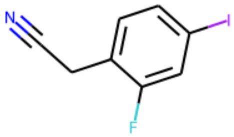


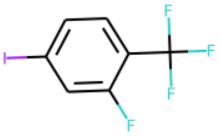


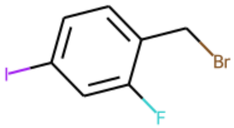


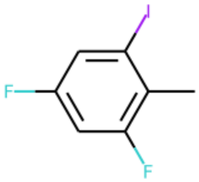


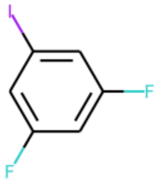


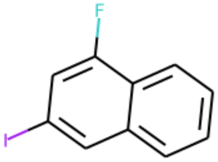


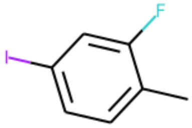


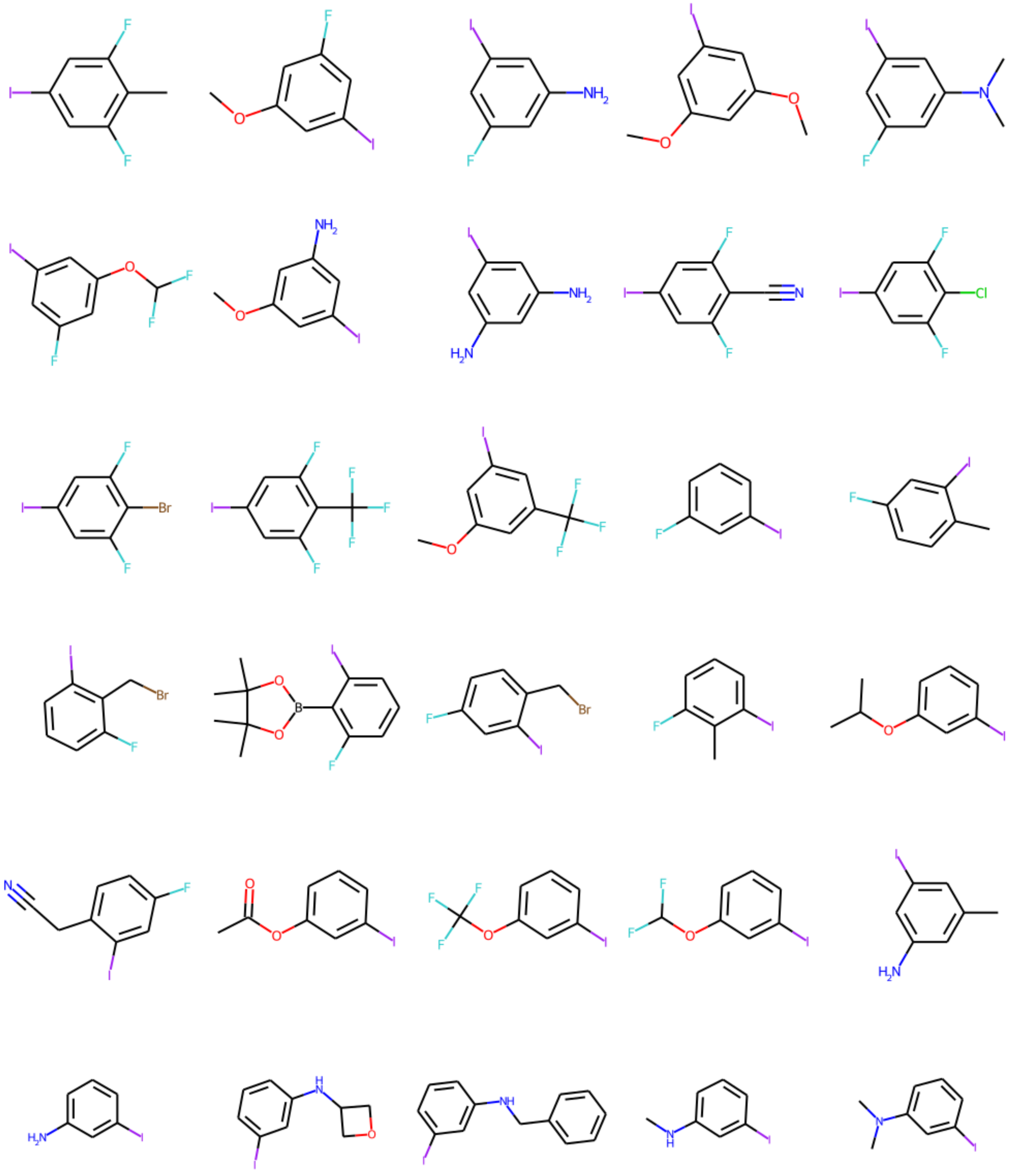






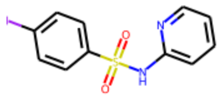
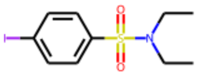
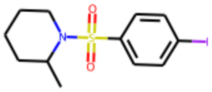
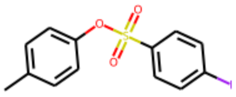
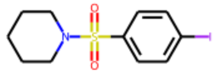
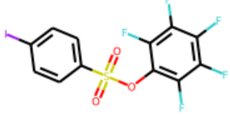
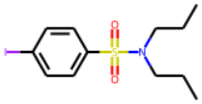
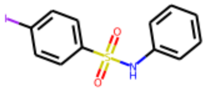
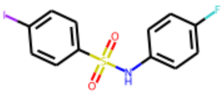
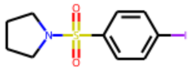
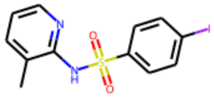
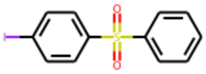
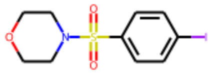
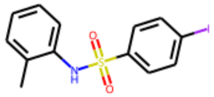
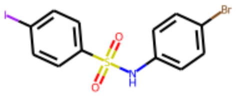
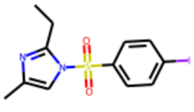
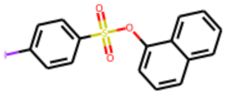
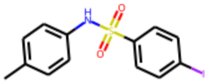
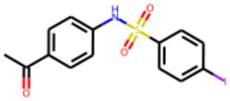
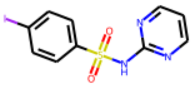
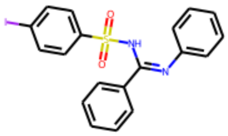
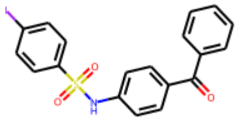
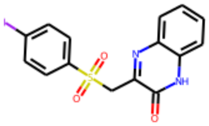
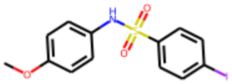


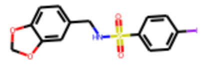
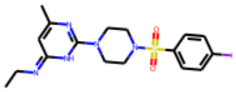
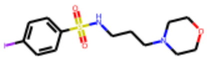
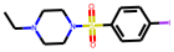
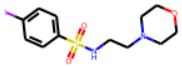


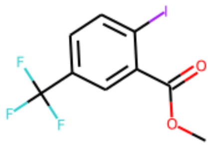


While this cluster has a spread of aryl iodides with and without a single *ortho* substituent, we found the *ortho* boronic acid pinacol ester substituent a particularly interesting stretch of our method as it contains a bulky *ortho* substituent that could be used for further diversification.

Cluster H: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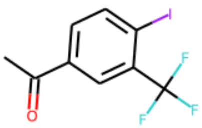
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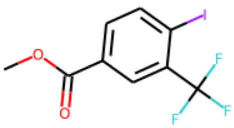
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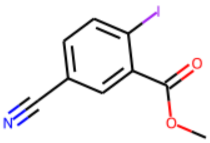
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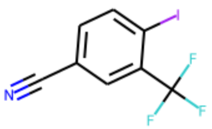
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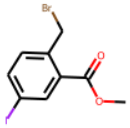
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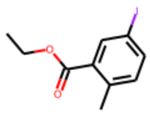
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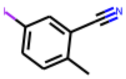
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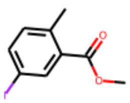
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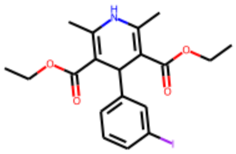
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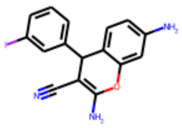
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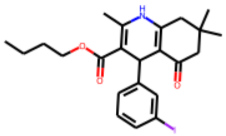
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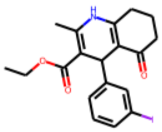
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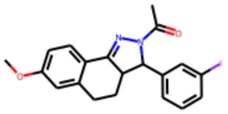
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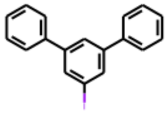
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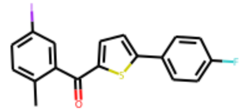
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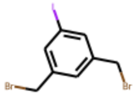
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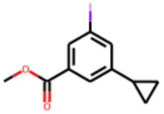
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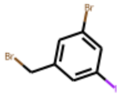
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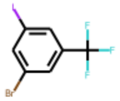
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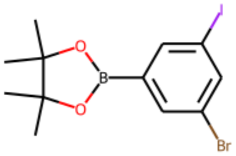
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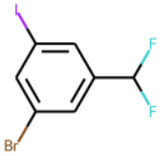
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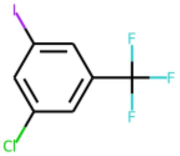
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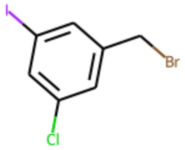
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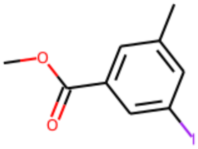
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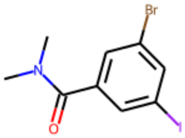
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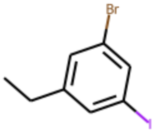
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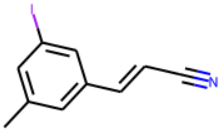
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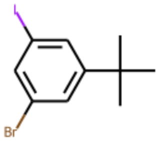
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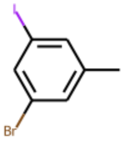
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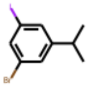
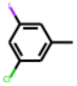
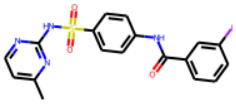
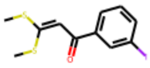
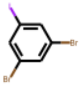
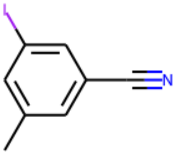
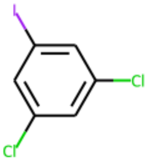
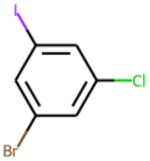
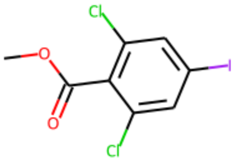
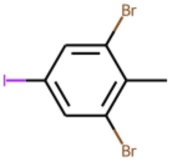
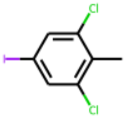
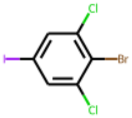
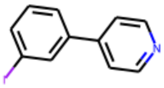
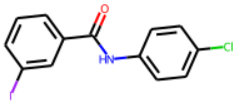
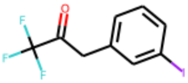
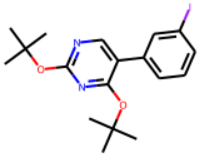
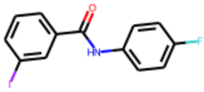
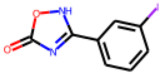
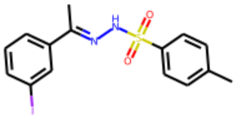
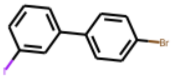
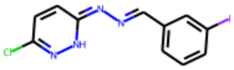
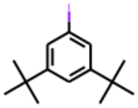
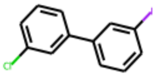
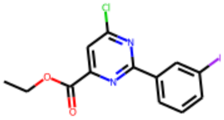
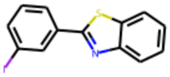

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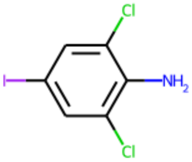
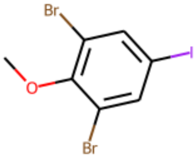
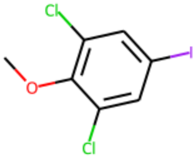
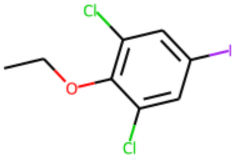
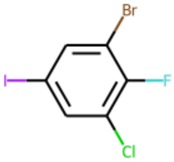

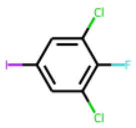
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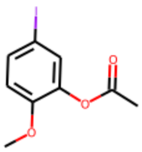
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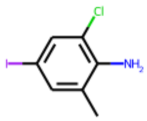
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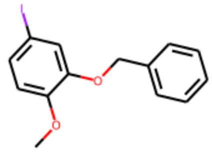
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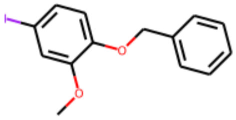
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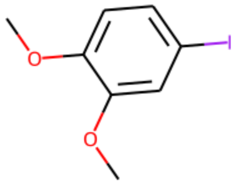
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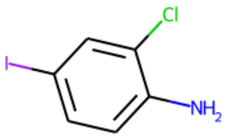
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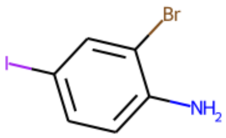
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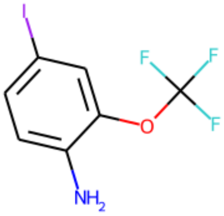
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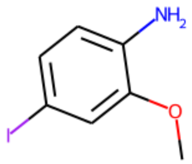
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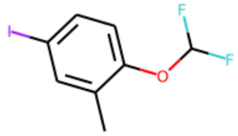
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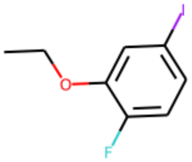
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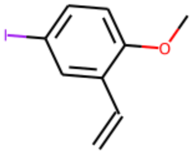
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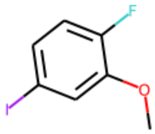
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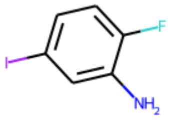
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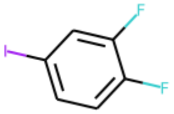
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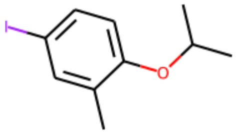
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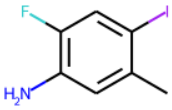
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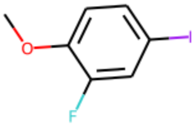
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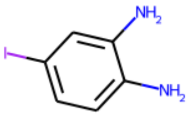
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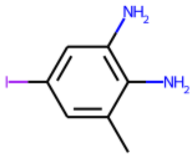
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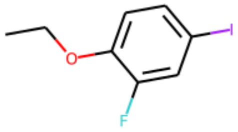
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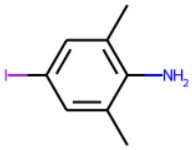
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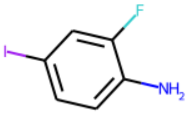
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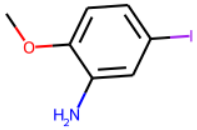
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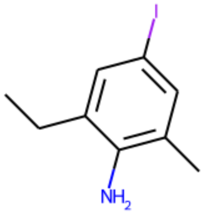
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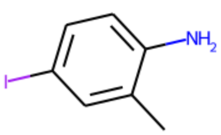
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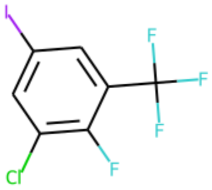
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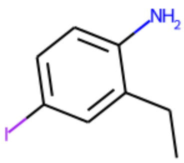
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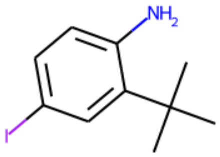
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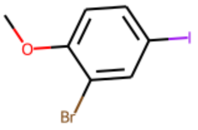

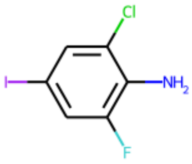
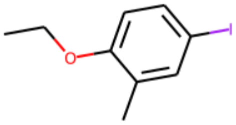
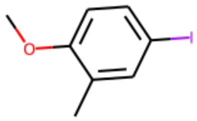

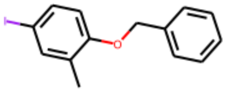
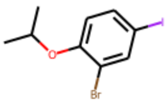
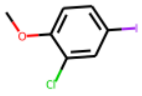

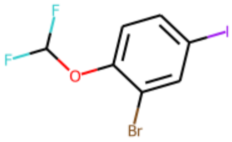
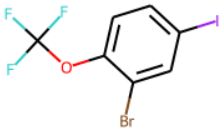
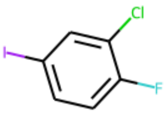
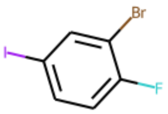
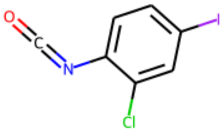

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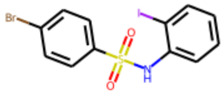
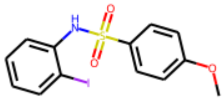
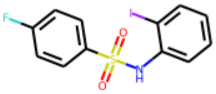
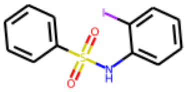
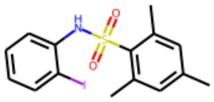
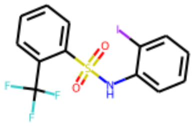
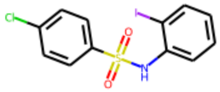
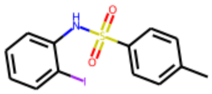
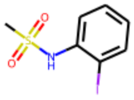
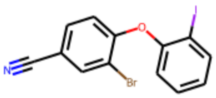
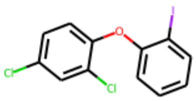
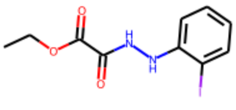
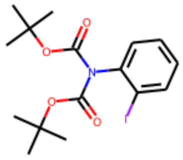

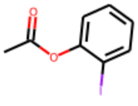

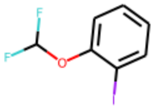
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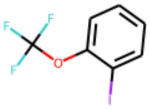
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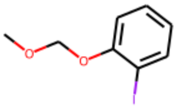
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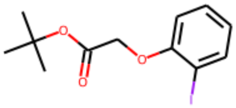
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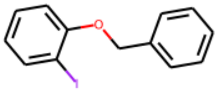
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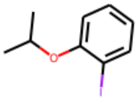
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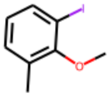
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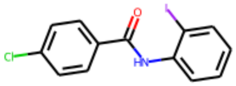
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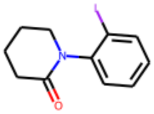
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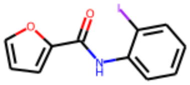
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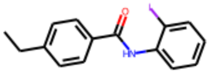
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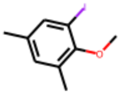
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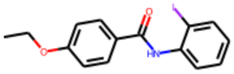
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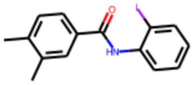
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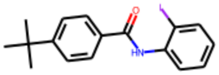
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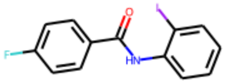
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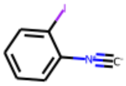
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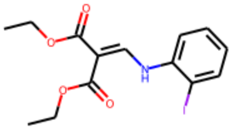
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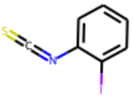
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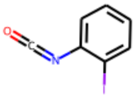
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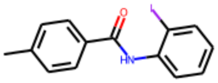
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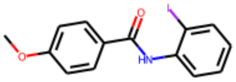
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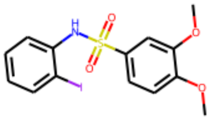
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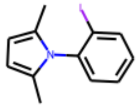
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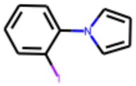
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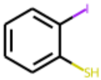
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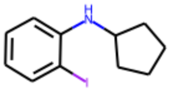
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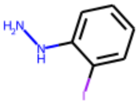
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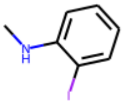
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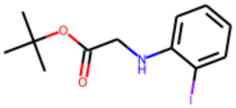
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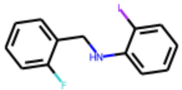
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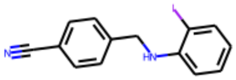
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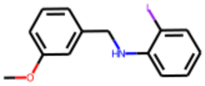
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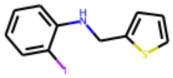
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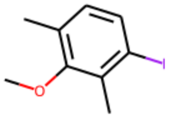
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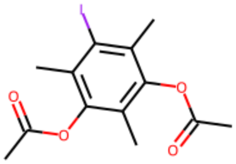
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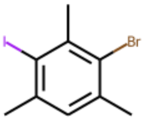
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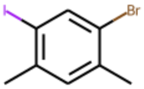
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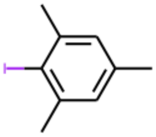
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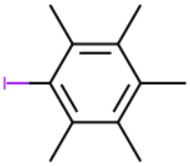
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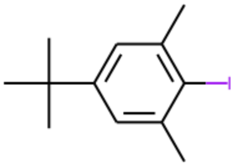
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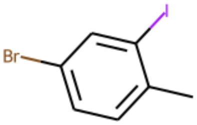
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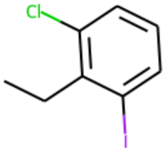
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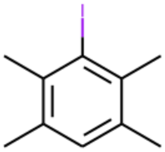
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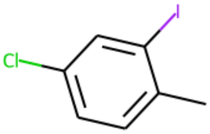
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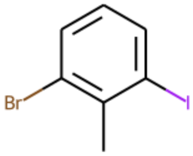
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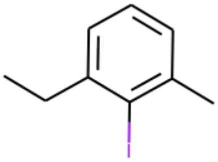
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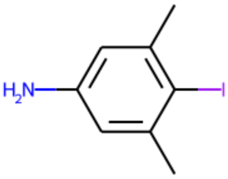
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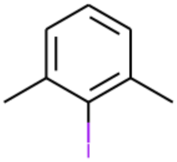
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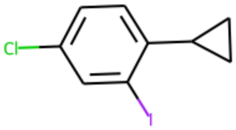
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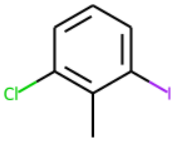
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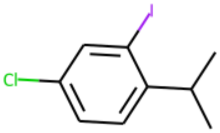
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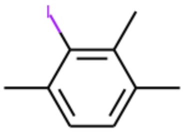
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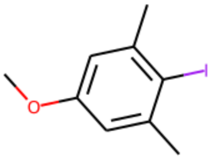
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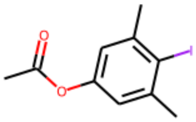
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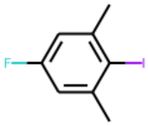
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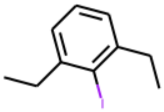
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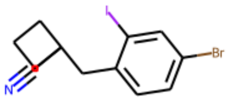
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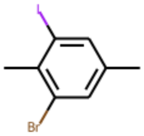
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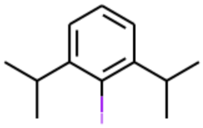
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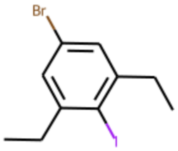
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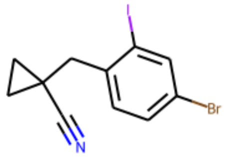
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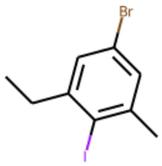
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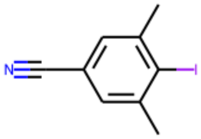
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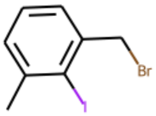
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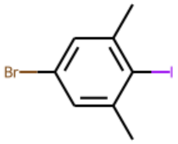
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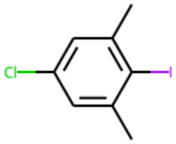
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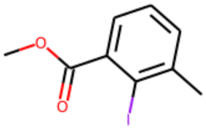
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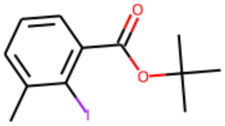
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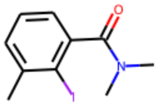
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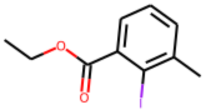
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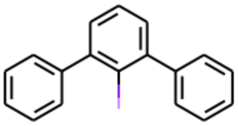
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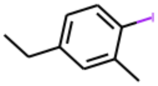
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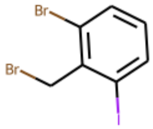
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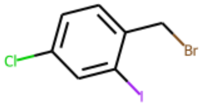
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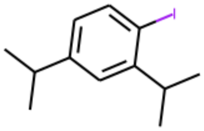
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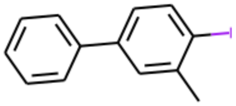
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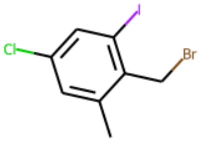
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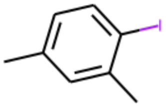
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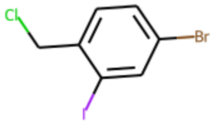
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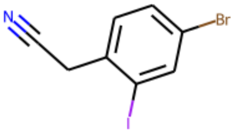
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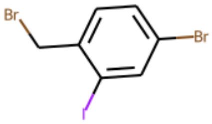
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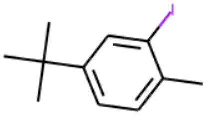
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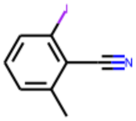
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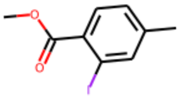
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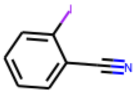
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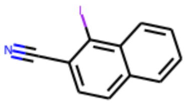
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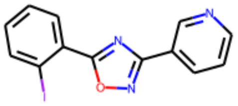
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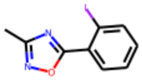
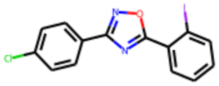
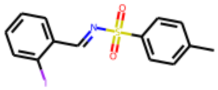
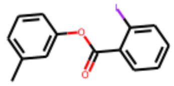
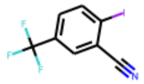
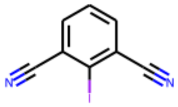
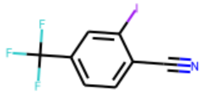
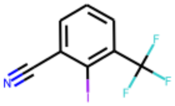
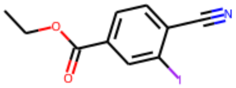
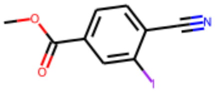
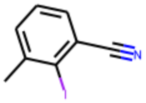
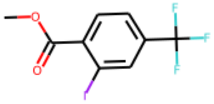
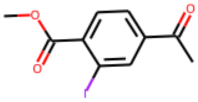
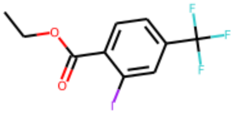
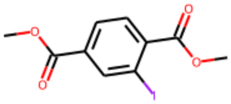
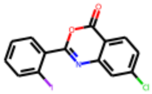

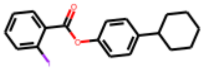
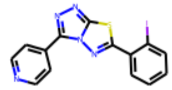
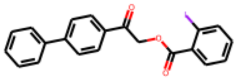
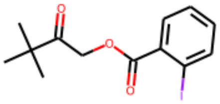
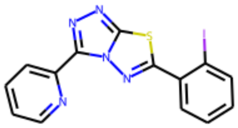
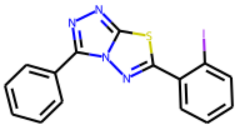
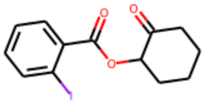
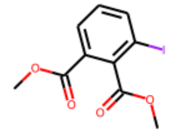

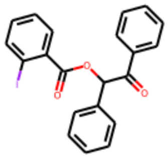
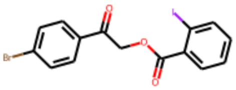
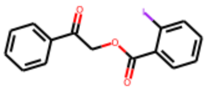
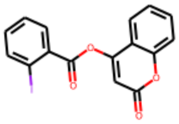

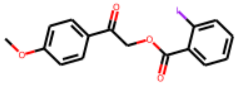
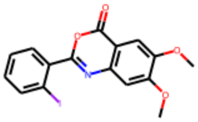
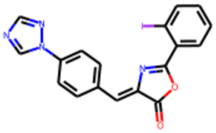
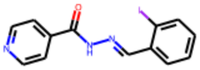
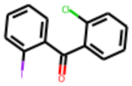
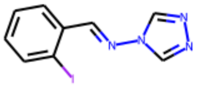
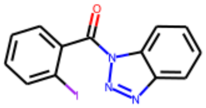
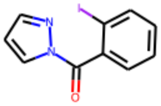
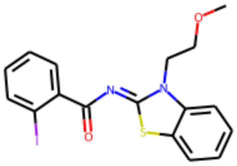
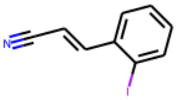
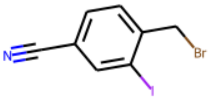
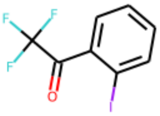
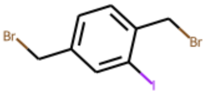
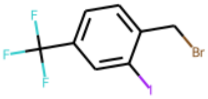
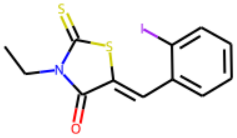

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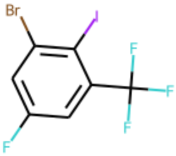
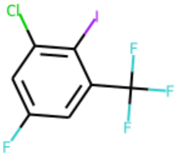
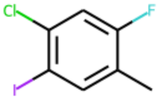
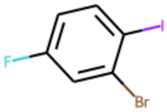
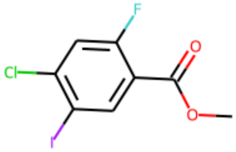
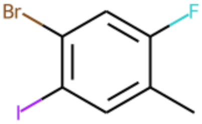
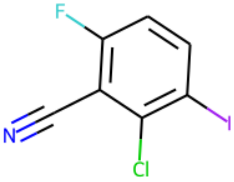
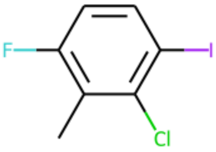
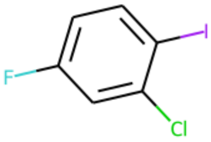
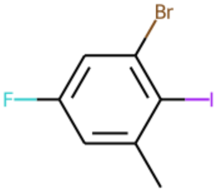
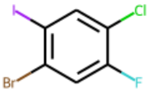
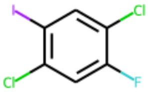
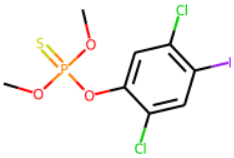
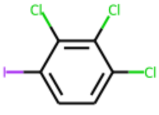
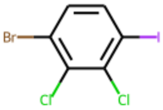

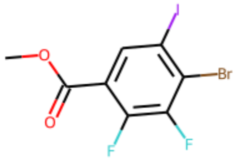
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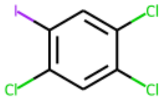
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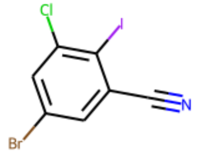
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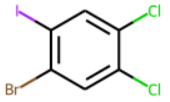
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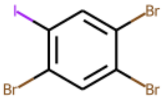
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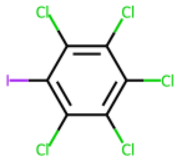
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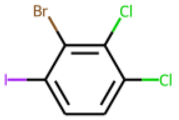
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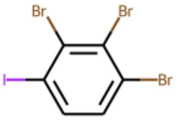
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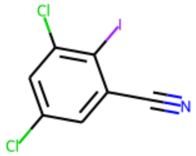
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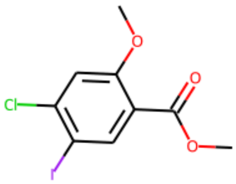
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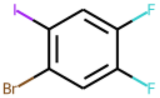
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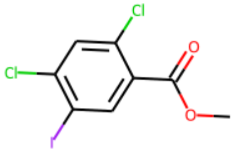
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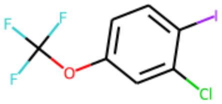
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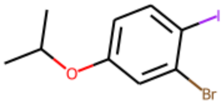
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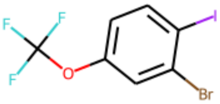
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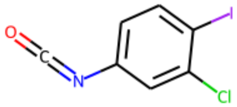
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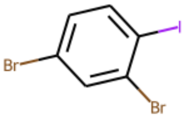
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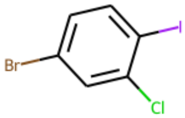
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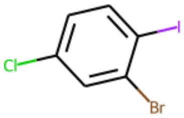
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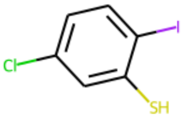
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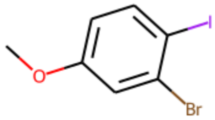
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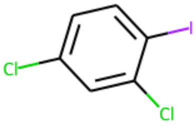
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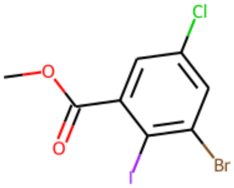
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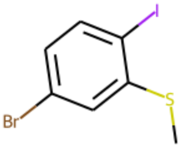
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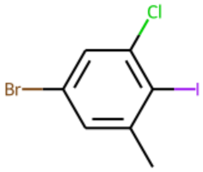
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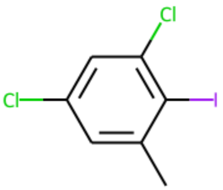
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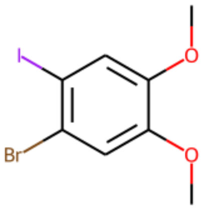
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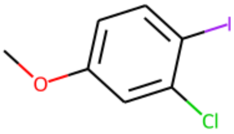
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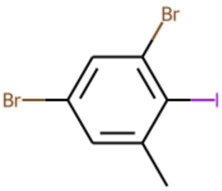
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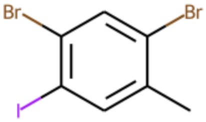
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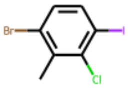
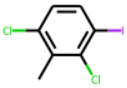
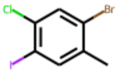
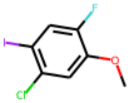
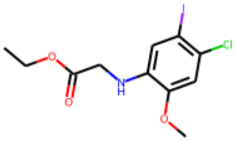




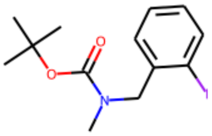
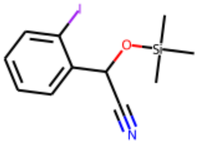
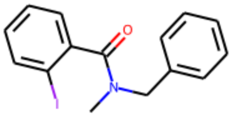
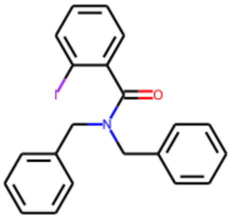
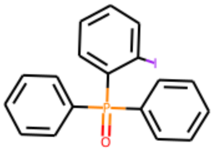
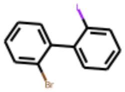
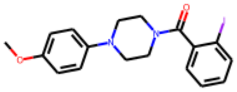
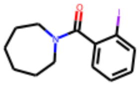
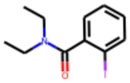
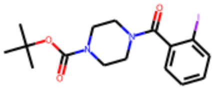
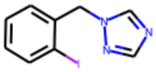
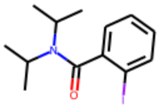
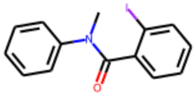
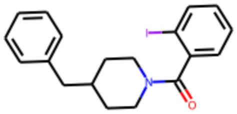
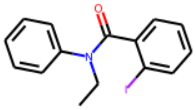
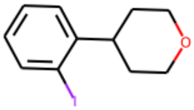
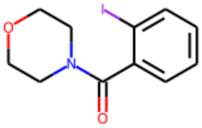
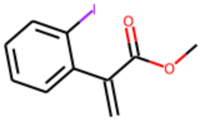
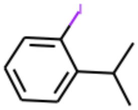
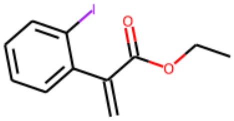


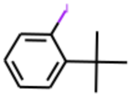
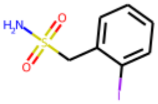
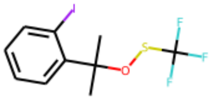


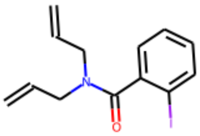
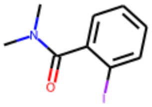
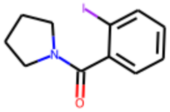
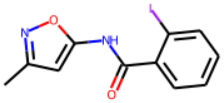
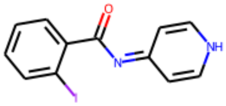


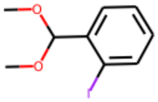
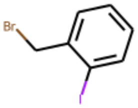
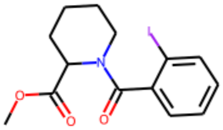
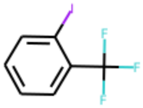
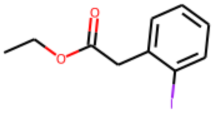
Although not featured prominently in the central region, this cluster comprised several aryl iodides characterized by 2,6-dihalide substitution reaction. While selecting our scope we sought to explore how the electronic properties at this location would influence reactivity. However, we ultimately found that di-*ortho* substituted aryl iodides were unreactive.

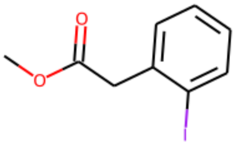
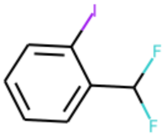
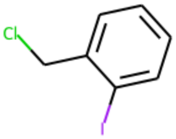
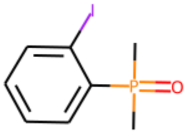
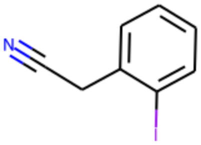
Cluster O:

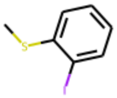
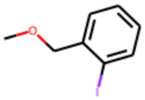
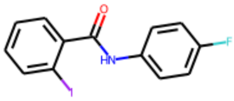
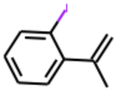
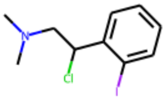





















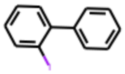
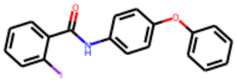
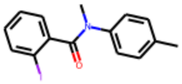
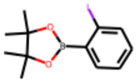
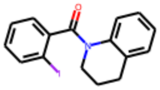




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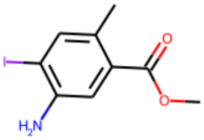
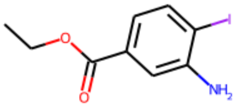
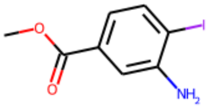
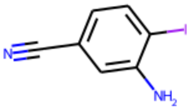
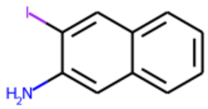
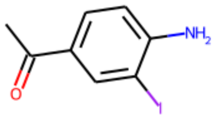
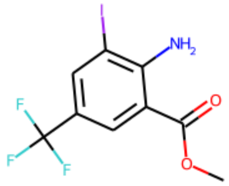
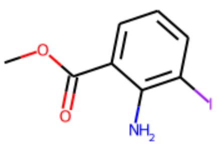
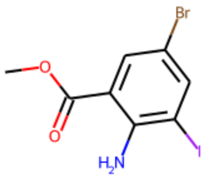
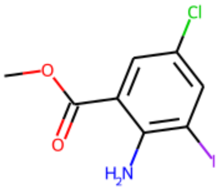
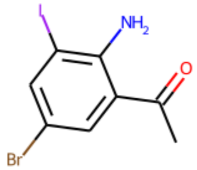
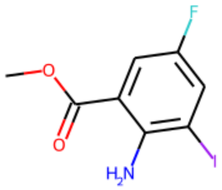
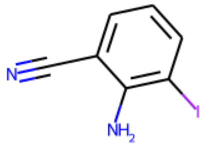
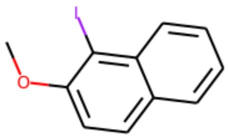
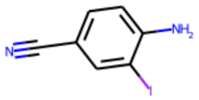
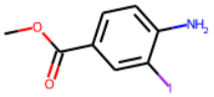
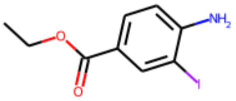
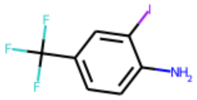
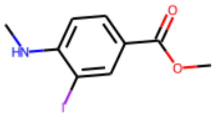
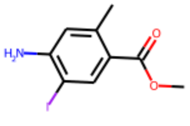
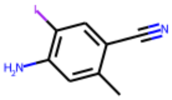
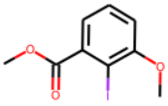
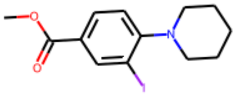
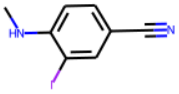
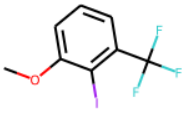
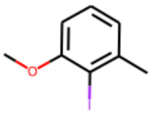
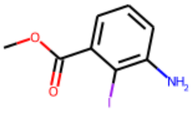
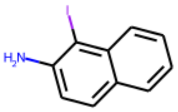
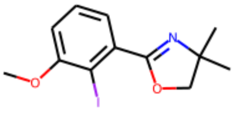
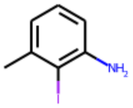
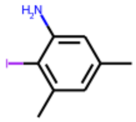
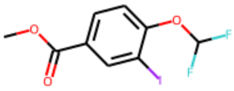
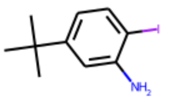
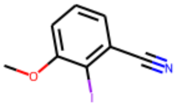
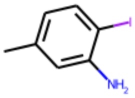
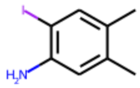
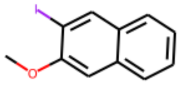
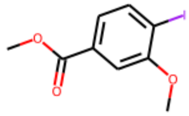





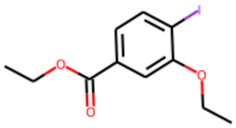































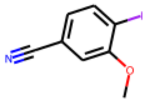


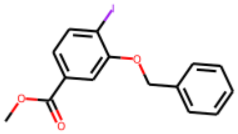


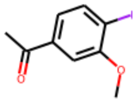


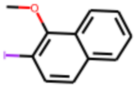


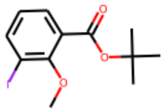


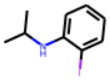


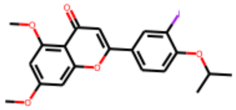


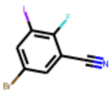


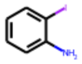


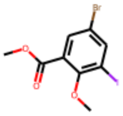












6.7. 2D-Feature Plots

In a retrospective analysis, we sought to explore how well our substrate scope covered steric and electronic feature space (Figure S9). This analysis revealed that we had excluded electron-deficient and -neutral aryl iodides with a single small *ortho* substituent from our scope. Initially, we overlooked this gap in the chemical space due to the presence of multiple mono-*ortho* substituted electron-deficient aryl iodides (**O**, **G**, **K**). However, the size of these *ortho* substituents prevented them from being included in this particular region of chemical space.

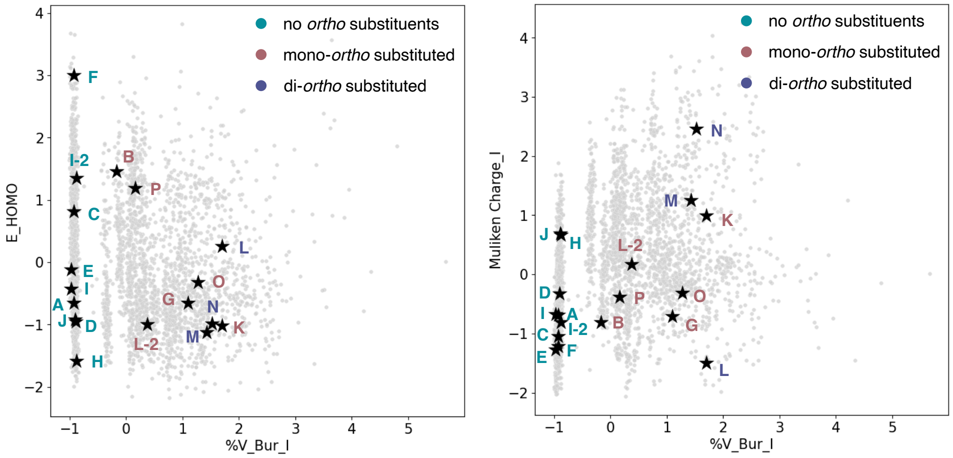


Figure S9. Selected aryl iodides plotted onto a bivariate steric (%V_{Bur_I}) and electronic (E_{HOMO} or Muliken Charge_I) feature space.

Therefore, when assessing the performance of our reactivity model (Figure 4B, 5) on unknown aryl iodides, we chose **L-2** to ensure coverage of this specific chemical space region. Gratifyingly, even though our reactivity model was not trained on this region of chemical space, it could still predict the performance of aryl iodides from this region.

7. Reaction Modeling

7.1. Aziridine B:L Selectivity Model

The aziridine B:L selectivity model was built using features from Auto-QChem. Specifically, the Boltzmann average $\%V_{Bur\_C}$ at 3.5 Å from DFT optimized geometries was used.

Table S6. Values used in aziridine reaction modeling.

Aziridine	$\%V_{Bur\_C}$	B:L
1a	60	11
2a	64	9
3a	65	6
4a	66	2
6a	68	0
7a	68	9
8a	72	20
5a	67	4

7.2. ArI Yield Model

The ArI model was built using features from Auto-QChem. The model was based on the minimum energy conformer of the respective aryl iodide. These features were preprocessed as part of the construction of chemical space (see above). $\%V_{Bur\_I}$ is calculated at 3.5 Å.

With only 14 points used to construct the model, we assessed its robustness using leave-one-out cross-validation (LOOCV), a k-fold cross-validation technique in which a single data point is excluded from the dataset, and the model is trained on the remaining points. Subsequently, we evaluated the model's performance by mean absolute error (MAE) values for both the training set and the excluded data point. This process was iterated over the entire dataset, the MAE values presented in Figure 4D represent the average of these values.

Table S7. Values used in ArI reaction modeling.

ArI	$\%V_{Bur\_I}$	E_{HOMO}	Observed % Yield	Predicted % Yield
B	-0.17	1.45	22	40
C	-0.93	0.81	71	68
D	-0.91	-0.93	87	80
E	-0.98	-0.13	62	76
F	-0.93	3.00	63	52
G	1.10	-0.67	25	16
H	-0.88	-1.59	90	84
I	-0.97	-0.44	84	78
J	-0.89	-0.97	76	80
K	1.71	-1.03	5	0
L	1.71	0.25	0	-9
M	1.43	-1.14	0	10

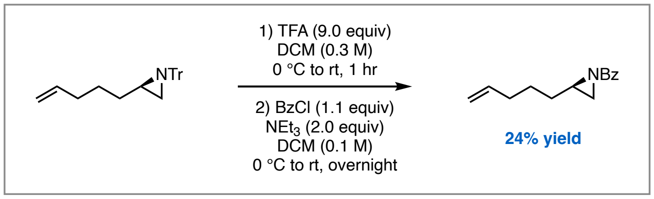
N	1.53	-1.00	0	6
P	0.16	1.18	28	32
A	-0.93	-0.66	45	79
O	1.28	-0.33	55	8

While not included in the model, we also evaluated two additional aryl iodides (Table S8) to assess the utility of the model in predicting substrates with multiple substitutions with competing effects on reactivity.

Table S8. Values used to compute yields of validation substrates.

Product	$\%V_{Bur\_I}$	E_{HOMO}	Observed % Yield	Predicted % Yield
I-2	-0.89	1.35	71	63
L-2	0.37	-1.00	42	34

8. Mechanistic Experiments

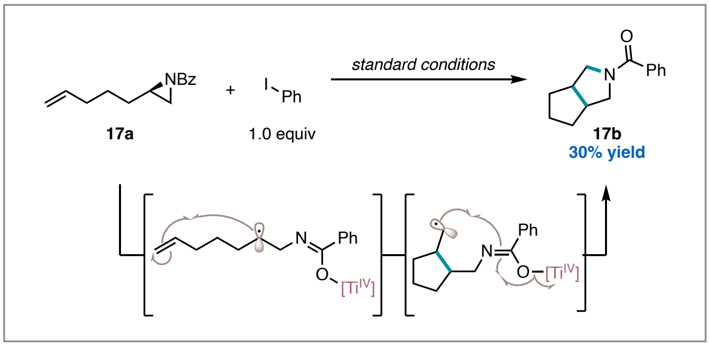


(2-(pent-4-en-1-yl)aziridin-1-yl)(phenyl)methanone (17a): To a round bottom flask was added 2-(pent-4-en-1-yl)tritylaziridine (1.9131 g, 4.8 mmol, 1.0 equiv)[26] and DCM (0.3 M, 16 mL). The reaction was cooled to 0 °C and trifluoroacetic acid (4.9425 g, 3.34 mL, 43.4 mmol, 9.0 equiv) was added dropwise. The reaction turned bright yellow and was stirred at room temperature for 1 hour. H_2O (16 mL) was added and the reaction was stirred until the bright yellow color of the trityl cation disappeared. $NaHCO_3$ was slowly added until bubbling ceased. The aqueous layer was extracted with DCM (16 mL, 2x). The organic layers were combined and washed with saturated $NaHCO_3$, washed with brine, dried over $MgSO_4$, and filtered.

The unprotected aziridine was taken forward as a mixture in DCM. NEt_3 (974.5 mg, 1.34 mL, 9.6 mmol, 2.0 equiv) was added to the reaction and the reaction was cooled to 0 °C. Benzoyl chloride (744.8 mg, 0.62 mL, 5.3 mmol, 1.1 equiv) was added dropwise. The reaction was stirred at room temperature overnight. The reaction mixture was then quenched with saturated $NaHCO_3$. The aqueous layer was extracted with DCM (2x). The organic layers were combined and washed with brine, dried over $MgSO_4$, filtered, and concentrated. The resulting oil was purified by flash chromatography (10% NEt_3/hexanes). Fractions containing product (determined by TLC, UV light) were collected and concentrated to yield **17a** as a slightly yellow oil (24% yield).

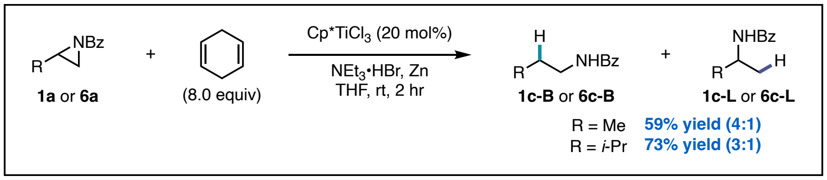
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.09 – 7.97 (m, 2H), 7.55 (tt, *J* = 6.8, 1.4 Hz, 1H), 7.45 (dd, *J* = 8.3, 7.0 Hz, 2H), 5.80 (ddt, *J* = 16.9, 10.1, 6.6 Hz, 1H), 5.02 (dq, *J* = 17.1, 1.7 Hz, 1H), 4.97 (ddt,

J = 10.2, 2.2, 1.3 Hz, 1H), 2.60 – 2.52 (m, 1H), 2.50 (d, J = 5.9 Hz, 1H), 2.20 (d, J = 3.6 Hz, 1H), 2.17 – 2.07 (m, 2H), 1.91 – 1.81 (m, 1H), 1.62 – 1.52 (m, 2H), 1.52 – 1.42 (m, 1H).
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ 179.5, 138.4, 133.5, 132.8, 129.2, 128.5, 115.1, 38.4, 33.4, 31.8, 31.7, 25.9.
HRMS (ESI-TOF): calculated for $C_{14}H_{18}NO^+$ ($[M+H]^+$): 216.1383, found 216.1382.
IR (ATR cm^{-1}): 3066, 2992, 2976, 2932, 2857, 1675, 1641, 1580, 1466, 1450, 1406, 1317, 1300, 1228, 1071, 1025, 993, 912, 723, 708, 689.



(Hexahydrocyclopenta[*c*]pyrrol-2(1*H*)-yl)(phenyl)methanone (17b) was observed in the cross-coupling of **17a** and phenyl iodide according to General Procedure C. **17b** likely arises from radical ring opening and sequential cyclizations. Yield was determined by GC-FID versus dodecane as an external standard. Authentic product for characterization and GC-FID response factors was purified by preparative thin layer chromatography (15% EtOAc/hexanes). Spectral data are in agreement with reported literature values.[27]

^1H NMR (500 MHz, $CDCl_3$): δ 7.51 – 7.44 (m, 2H), 7.42 – 7.36 (m, 3H), 3.86 (dd, J = 12.7, 8.6 Hz, 1H), 3.64 – 3.57 (m, 1H), 3.50 (dd, J = 13.0, 4.6 Hz, 1H), 3.19 (dd, J = 11.8, 4.5 Hz, 1H), 2.82 – 2.55 (m, 2H), 1.92 – 1.81 (m, 1H), 1.81 – 1.69 (m, 2H), 1.67 – 1.50 (m, 2H)[a], 1.39 – 1.33 (m, 1H).
[a]Overlaps with H_2O.
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ 169.6, 137.3, 129.8, 128.4, 127.2, 55.4, 51.9, 43.9, 42.1, 32.5, 31.9, 25.8.
HRMS (ESI-TOF): calculated for $C_{14}H_{18}NO^+$ ($[M+H]^+$): 216.1383, found 216.1384.
IR (ATR cm^{-1}): 3058, 2946, 2865, 1629, 1577, 1446, 1420, 1245, 791, 721, 700, 663.

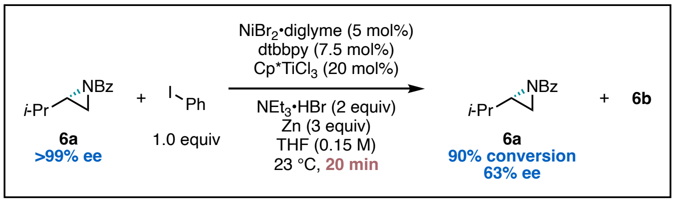


The following manipulations were performed in a nitrogen filled glovebox.
In a 1-dram vial the following stock solution was prepared:
Stock Solution 1: Cp^*TiCl_3 (2.89 mg, 0.01 mmol, 20 mol%), Zn (9.81 mg, 0.15 mmol, 3.0 equiv) and 333 μL of THF. This vial was equipped with a Teflon stir bar, capped with a septum cap, and allowed to stir for 10 min. The solution turned from red to blue.
In a separate 1-dram vial equipped with a Teflon stir bar was added aziridine (**1a** or **6a**) (0.05 mmol, 1.0 equiv), 1,4-cyclohexadiene (32.1 mg, 37.8 μL, 0.40 mmol, 8.0 equiv), and NEt_3•HBr

(18.2 mg, 0.10 mmol, 2.0 equiv). Stock solution 1 (333 µL) was then added and the solution rapidly turned back to red. The reaction vial was capped with a septum cap, wrapped with electrical tape, and brought outside the glovebox. The reaction vial was set to stir (700 rpm) for 2 hours. Yields were determined by GC with dodecane as an external standard.

1c-B and **1c-L**: Authentic product was obtained by flash chromatography (15 to 40% EtOAc/hexanes). Spectral data are in agreement with literature reports.[28]

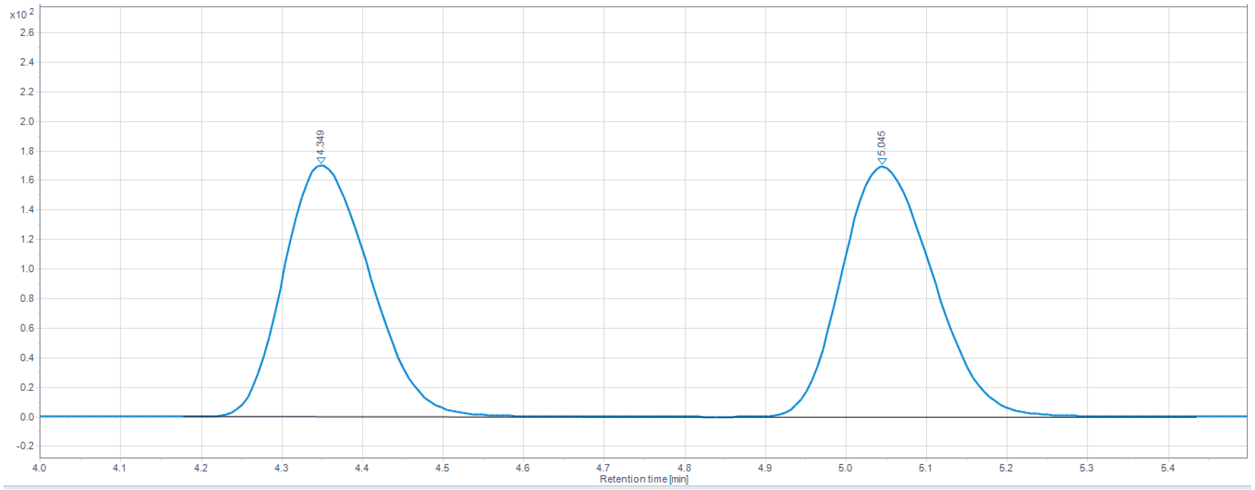
6c-B and **6c-L**: Authentic product was obtained by flash chromatography (15 to 20% EtOAc/hexanes). Spectral data are in agreement with literature reports.[29,30]

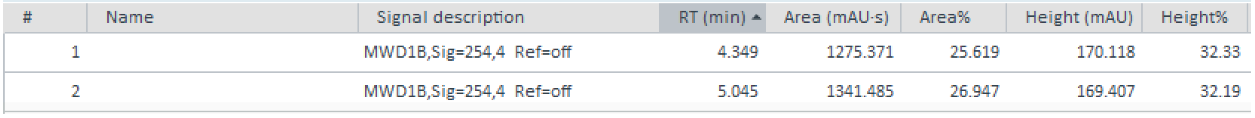


6a was subjected to General Procedure C with phenyl iodide (reaction was run on 0.1 mmol scale). The reaction was tracked by TLC and quenched after 20 minutes by passing through a plug of silica gel with EtOAc. The reaction had gone to 90% conversion (determined by ^{1}H NMR versus ethylene carbonate as an external standard). Starting material was recovered by flash chromatography (5% EtOAc/hexanes). % ee was determined by chiral SFC.

Chiral SFC traces (CHIRALPAK IC-10 SFC, 1.5 mL/min, 20% IPA in CO_2, 30 °C, 130.00 bar):

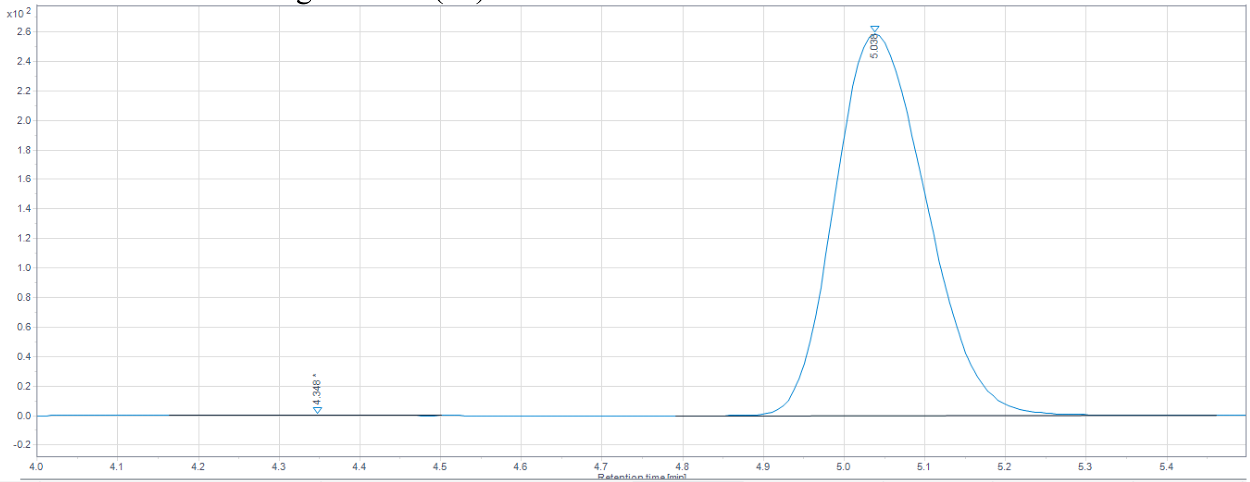
Mixture of isomers:





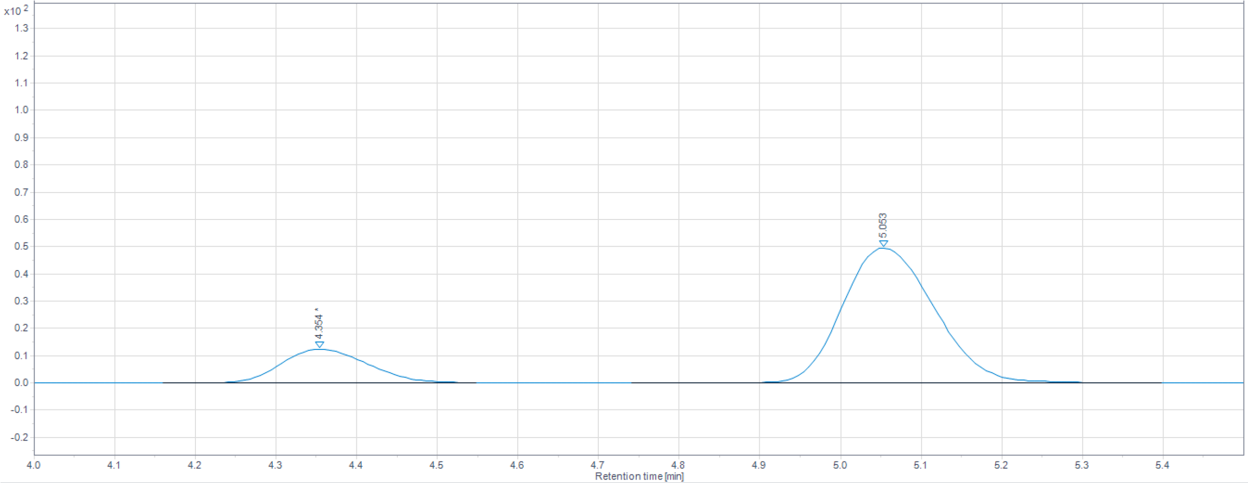
#	Name	Signal description	RT (min)	Area (mAU·s)	Area%	Height (mAU)	Height%
1		MWD1B,Sig=254,4 Ref=off	4.349	1275.371	25.619	170.118	32.33
2		MWD1B,Sig=254,4 Ref=off	5.045	1341.485	26.947	169.407	32.19

Enantioenriched starting material (**6a**):



	Name	Signal description	RT (min) ▲	Area (mAU·s)	Area%	Height (mAU)	Height%
1		MWD1B,Sig=254,4 Ref=off	4.348	4.192	0.096	0.566	0.13
2		MWD1B,Sig=254,4 Ref=off	5.038	2045.038	46.969	258.942	60.89

Recovered Starting Material:



	Name	Signal description	RT (min) ▲	Area (mAU·s)	Area%	Height (mAU)	Height%
1		MWD1B,Sig=254,4 Ref=off	4.354	90.551	2.990	12.314	5.68
2		MWD1B,Sig=254,4 Ref=off	5.053	392.948	12.977	49.606	22.90

9. DFT Calculations

DFT calculations were performed using the Gaussian16 software package. All geometries were optimized using the UM06 functional[31] and the 6-31g(d,p) basis set[17–21] for C, H, O, N, and Cl and the LanL2DZ pseudopotential/basis set[22–24] for Ti. Vibrational frequencies were computed at the same level of theory to confirm stationary points (zero negative frequencies) and transition states (one negative frequency). Corrections to vibrational frequencies were performed using the GoodVibes.py program.[32] Vibrational frequencies were corrected using Truhlar's quasiharmonic oscillator approximation,[33] setting all vibrational frequencies below 50 cm^{-1} to 50 cm^{-1}. Single-point energy calculations were performed using the UM06 functional with the Def2TZVP basis set[34,35] for all atoms. All calculations were preformed using the SMD solvation model[36] for tetrahydrofuran.

Full Gaussian16 Reference: Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

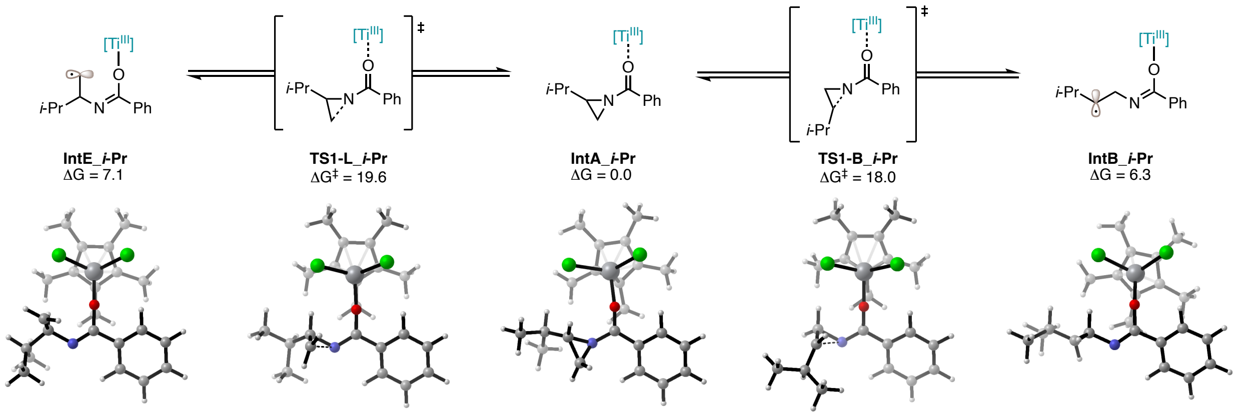


Figure S10. Ti^{III} induced radical ring-opening.

Table S9. Electronic (E) and free energies (G) for computed structures and single point energy calculations (SPC) reported in Hartree.

Structure	Imaginary Frequency	E_SPC	E	G(T)_SPC	qh-G(T)_SPC
IntA_*i*-Pr		-2756.06062	-1964.299925	-2755.656179	-2755.654431
TS1-B_*i*-Pr	-586.00	-2756.03003	-1964.268108	-2755.628258	-2755.625816
IntB_*i*-Pr		-2756.04957	-1964.284247	-2755.645801	-2755.644458
TS1-L_*i*-Pr	-677.32	-2756.02826	-1964.265741	-2755.624648	-2755.623168
IntE_*i*-Pr		-2756.04603	-1964.280985	-2755.645612	-2755.643162

XYZ Coordinates:

IntA_*i*-Pr:

C	3.32346400	1.93644800	-0.59639700
C	1.91078400	2.38896300	-0.72662600
H	3.79620100	1.47025600	-1.46042400
H	3.99825500	2.43906100	0.09533200
N	2.23761200	1.19702500	0.03044700
C	1.80838100	-0.04953400	-0.32426000
O	0.61889900	-0.20197000	-0.70499900
C	2.68933100	-1.20360000	-0.15657300
C	3.91213000	-1.09596000	0.52029500
C	2.27830700	-2.44909700	-0.65533100
C	4.71076200	-2.21841000	0.68944600
H	4.22430500	-0.13908900	0.93175900
C	3.08450000	-3.56512100	-0.48430800
H	1.32997900	-2.52345400	-1.18525800
C	4.30105300	-3.45198600	0.18697500
H	5.65546700	-2.13297200	1.22089900
H	2.76543200	-4.52715900	-0.87785800
H	4.93075500	-4.32857700	0.32052700
C	-1.95574900	0.55318100	1.53430200
C	-1.16171300	-0.62101000	1.67038400
C	-1.88640800	-1.70264200	1.08874600
C	-3.13323700	-1.19643700	0.61101900
C	-3.17452700	0.19410100	0.88547800
Ti	-1.33507600	-0.19955600	-0.56591600
C	-1.41144700	-3.11671200	1.03310800
H	-1.49776200	-3.59313600	2.01921700
H	-1.99196100	-3.71237300	0.32222900
H	-0.35664700	-3.18380400	0.73444400
C	-4.23325600	-1.97278600	-0.02729800
H	-5.01573700	-2.20975700	0.70672500
H	-4.70658200	-1.40589200	-0.83790700
H	-3.87637400	-2.91626100	-0.45129300
C	-4.31995000	1.09471800	0.57348900
H	-5.11807500	0.97744500	1.31943000
H	-4.02108100	2.14744400	0.56856700
H	-4.75446700	0.86977800	-0.40795700
C	-1.56424700	1.90486600	2.02866100
H	-0.49026600	2.08897500	1.88851400

H	-2.10786600	2.70398400	1.51414200
H	-1.76866700	1.99876300	3.10421900
C	0.15101000	-0.71588600	2.37307400
H	0.00278300	-0.79865100	3.45857500
H	0.71923700	-1.59782700	2.05507800
H	0.78017300	0.16779600	2.20257100
Cl	-1.62474400	-1.80525500	-2.23181200
Cl	-1.71683600	1.89005600	-1.49895200
C	1.33695600	3.58703900	-0.00636100
H	1.43884300	2.18528800	-1.69224600
C	1.45349600	4.80394300	-0.91418500
H	1.01073600	5.68890300	-0.44249900
H	2.50827000	5.02921900	-1.12660500
H	0.94265300	4.64160700	-1.87190400
H	0.26635800	3.36388100	0.13606500
C	1.96658000	3.84690300	1.35233000
H	3.00381200	4.19543300	1.25355000
H	1.41079800	4.63007200	1.88116600
H	1.96814500	2.95034700	1.98514100

TS1-B_*i*-Pr

C	-2.78235800	-2.09529300	-0.21615500
C	-1.86053400	-1.93178300	0.91538500
H	-2.39428100	-1.88107100	-1.21506400
N	-2.30495700	-0.55325800	0.89964600
C	-1.57295300	0.35143400	0.27385000
O	-0.40723800	0.07009200	-0.28004600
C	-2.06401300	1.72557900	0.13607600
C	-3.25852500	2.11707200	0.76084000
C	-1.34272400	2.67451300	-0.60414200
C	-3.71442400	3.42232200	0.64770000
H	-3.81497100	1.38340700	1.33903700
C	-1.80445200	3.98112500	-0.71049400
H	-0.42580200	2.37870200	-1.11110000
C	-2.98947400	4.36146900	-0.08565600
H	-4.64116200	3.71232000	1.13833900
H	-1.23697200	4.70499600	-1.29152200
H	-3.34906600	5.38446800	-0.17093400
C	2.19321300	-0.98017000	1.52224700
C	1.70091000	0.34817600	1.66169800
C	2.50393600	1.19981900	0.84851400
C	3.51008500	0.39882200	0.22951400
C	3.31311500	-0.94434200	0.63933200
Ti	1.37124200	-0.26637500	-0.53689500
C	2.32793300	2.67506400	0.72025300
H	2.68880200	3.18225900	1.62512800
H	2.88198100	3.07747100	-0.13300100
H	1.27357300	2.95362700	0.59436400
C	4.61674800	0.86309500	-0.65164500
H	5.55471000	0.91159700	-0.08192900
H	4.77947500	0.17745600	-1.49134400
H	4.42455300	1.85749100	-1.06462300
C	4.18214400	-2.09399800	0.26676800
H	5.09184300	-2.09353000	0.88281600
H	3.67640900	-3.05226500	0.41926500
H	4.49659900	-2.04265800	-0.78196100

C	1.68491400	-2.18951800	2.23000200
H	0.67230600	-2.03831500	2.61919500
H	1.67107500	-3.07119700	1.57938500
H	2.33153200	-2.42518800	3.08609100
C	0.59392200	0.79552900	2.55168600
H	0.98625100	1.03586900	3.54884600
H	0.10353900	1.69809400	2.16954000
H	-0.17526600	0.02550700	2.68130600
Cl	1.78035700	1.03287300	-2.37261400
Cl	1.30045700	-2.39170900	-1.37883500
H	-0.80056500	-2.10934500	0.70263800
H	-2.17057500	-2.43956900	1.83545400
C	-4.21704600	-2.44995500	-0.05535400
C	-4.40349200	-3.93573800	-0.38140700
H	-5.45196400	-4.23048300	-0.24647800
H	-4.12822700	-4.13959700	-1.42473200
H	-3.78394500	-4.57135200	0.26263100
H	-4.48423600	-2.28961600	1.00113400
C	-5.10539800	-1.58314300	-0.93777100
H	-4.98000100	-0.51924500	-0.70163900
H	-4.84982900	-1.72461800	-1.99702400
H	-6.16349400	-1.84315200	-0.81208000

IntB_*i*-Pr

C	-3.10430400	1.90079200	0.09762700
C	-2.15765600	1.87334800	-1.05090800
H	-3.01762600	2.73721500	0.79756300
H	-2.02225700	0.83355500	-1.39984200
N	-0.91447200	2.54362600	-0.72021300
C	0.17824400	1.89324400	-0.70128800
O	0.28641900	0.58133200	-0.99462700
C	1.46273300	2.54837800	-0.35856400
C	1.46394000	3.68690200	0.45305000
C	2.67480600	2.03173900	-0.82413500
C	2.66404400	4.28952400	0.80746700
H	0.51388400	4.07961900	0.80918500
C	3.87348800	2.64886400	-0.48220300
H	2.67607700	1.14603100	-1.45713900
C	3.87104500	3.77210800	0.33995400
H	2.65933900	5.16591800	1.45173100
H	4.81279700	2.24662100	-0.85506900
H	4.80999700	4.24657400	0.61674900
C	-0.78182800	-1.78435800	1.26723100
C	0.06928300	-0.69205100	1.60168200
C	1.41727600	-1.12180900	1.45157700
C	1.39659900	-2.49035600	1.05045200
C	0.04100500	-2.89809200	0.92877400
Ti	0.39753000	-1.19574400	-0.64600400
C	2.64706900	-0.32576900	1.72524300
H	3.42701400	-0.50738200	0.97628300
H	2.44673600	0.75107300	1.74654500
H	3.06448800	-0.60686200	2.70173300
C	2.58064900	-3.37782400	0.90300800
H	2.77099700	-3.89361400	1.85432700
H	2.42464700	-4.14519200	0.13746500
H	3.48394900	-2.81742500	0.64323800

C	-0.40093400	-4.26608500	0.53898900
H	-0.20143400	-4.97335600	1.35505200
H	-1.47117200	-4.30224400	0.31704300
H	0.13868400	-4.62909300	-0.34445000
C	-2.26823900	-1.73624900	1.33558300
H	-2.65180200	-0.79153900	0.92888300
H	-2.73579700	-2.55697800	0.78436400
H	-2.59823900	-1.79766800	2.38202000
C	-0.40582000	0.61801600	2.12404000
H	-0.64481400	0.51851500	3.19188500
H	0.34916200	1.40579500	2.03017000
H	-1.32194800	0.95777200	1.62039500
Cl	2.20991800	-1.79178800	-1.86597200
Cl	-1.31997700	-2.01583900	-1.87975600
H	-2.59632400	2.41745100	-1.91058000
C	-4.40467500	1.16875500	0.03567800
C	-5.40127500	1.90263600	-0.86914100
H	-6.35645500	1.36383100	-0.92077200
H	-5.60258200	2.90928800	-0.47728300
H	-5.01983700	2.00936800	-1.89173800
H	-4.22062300	0.17374800	-0.41003900
C	-4.99069700	0.98897300	1.43072100
H	-5.20904300	1.96820500	1.87976700
H	-5.92784200	0.41961800	1.40209300
H	-4.29321200	0.46702800	2.09938300

TS1-L_*i*-Pr

C	2.44091200	2.07168600	-1.72052500
C	1.80480100	2.19155500	-0.40071700
H	1.92181600	1.54704800	-2.51888400
H	3.46656600	2.38911200	-1.88272100
N	2.46299700	0.92609200	-0.15708100
C	1.79345700	-0.20445200	-0.31475500
O	0.51245700	-0.23388600	-0.64955500
C	2.47376600	-1.49261100	-0.17128400
C	3.81690000	-1.54271800	0.23393100
C	1.79407000	-2.69535900	-0.41842400
C	4.45634400	-2.76298500	0.39335700
H	4.34443100	-0.61120800	0.42291000
C	2.44100900	-3.91435200	-0.25465400
H	0.75903100	-2.66943000	-0.75435000
C	3.77198200	-3.95452800	0.15312400
H	5.49700300	-2.78728100	0.70949600
H	1.90282700	-4.83865300	-0.45364500
H	4.27626000	-4.90978900	0.28072800
C	-1.90042700	1.00667200	1.34656800
C	-1.10745000	-0.11630000	1.71796000
C	-1.82458600	-1.29526600	1.36361200
C	-3.07467600	-0.89775700	0.80205800
C	-3.11809900	0.51970100	0.78371600
Ti	-1.30706000	-0.14765400	-0.58091500
C	-1.36437200	-2.69488100	1.58973900
H	-1.63164200	-3.02551000	2.60247300
H	-1.82275100	-3.39315700	0.88179600
H	-0.27595200	-2.78852900	1.49425600
C	-4.18646800	-1.79017000	0.37567100

H	-4.93891200	-1.85267900	1.17375600
H	-4.69027300	-1.41165900	-0.52068500
H	-3.84112300	-2.80621700	0.16353400
C	-4.27283700	1.32973700	0.30629700
H	-5.08613700	1.29824600	1.04401900
H	-4.00151900	2.37824100	0.15299300
H	-4.67442700	0.94473600	-0.63863600
C	-1.54061700	2.43424400	1.57586800
H	-0.45570500	2.59106100	1.53973100
H	-2.00189700	3.09726700	0.83671100
H	-1.88078800	2.75543400	2.56971100
C	0.20276200	-0.06869500	2.42386500
H	0.04109600	0.00720900	3.50740400
H	0.79861000	-0.97075800	2.24583300
H	0.80769000	0.79576700	2.12559600
Cl	-1.87757500	-1.88219500	-1.94582200
Cl	-1.71813400	1.69847800	-1.86075100
C	2.22580200	3.32778800	0.52086800
H	0.70894600	2.13411700	-0.44595300
C	1.58279800	4.61672300	0.02694200
H	0.49016700	4.52840700	-0.04396300
H	1.81301600	5.45619300	0.69350800
H	1.95914300	4.87225600	-0.97385700
H	1.81174300	3.08350500	1.51487700
C	3.73149300	3.48685900	0.66093600
H	3.96391100	4.24059000	1.42268800
H	4.21523800	2.54809100	0.95261200
H	4.18599300	3.82826600	-0.27898200

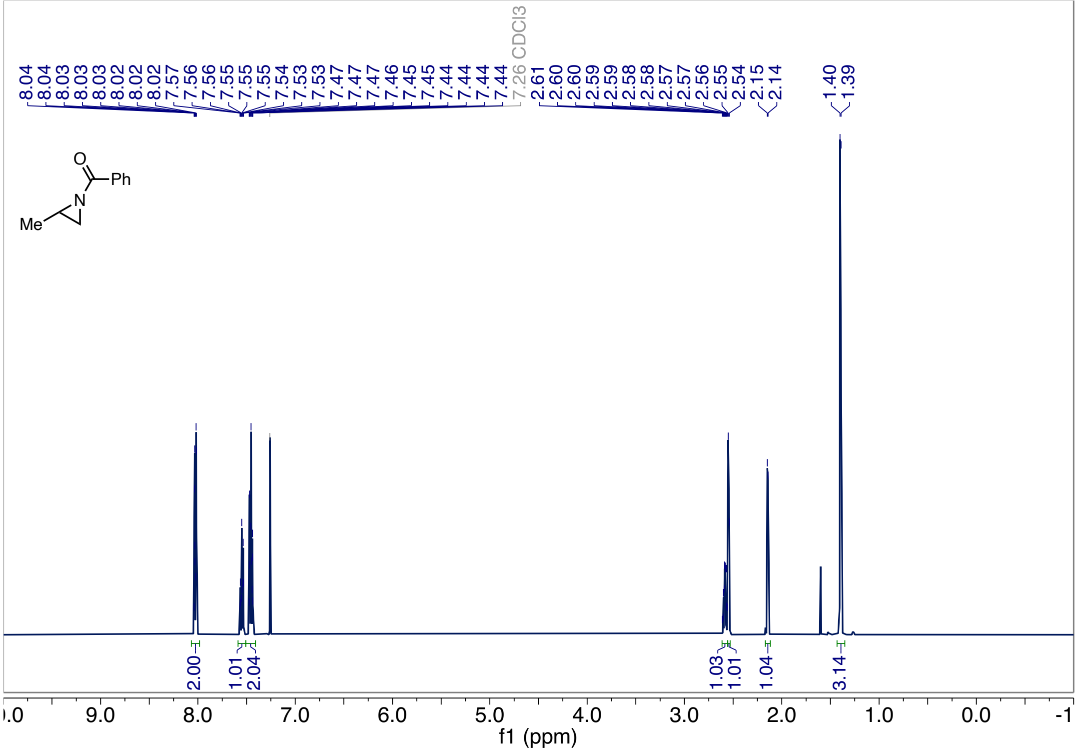
IntE_*i*-Pr

C	-1.71815300	-2.40233300	-1.89027300
C	-1.99625200	-2.10750100	-0.45854000
H	-1.90615200	-1.66820900	-2.66925900
H	-1.37238600	-3.39393600	-2.17586400
N	-2.52790200	-0.76325900	-0.28669800
C	-1.74859400	0.23497500	-0.41652400
O	-0.44540500	0.12325400	-0.73133400
C	-2.23451900	1.62473100	-0.24621400
C	-3.45621800	1.85142700	0.39614500
C	-1.48932200	2.71263700	-0.70969600
C	-3.92158400	3.14677200	0.57590600
H	-4.02735300	0.99805200	0.75482100
C	-1.96197300	4.00954400	-0.53236700
H	-0.54227800	2.54243900	-1.21897700
C	-3.17550000	4.22929400	0.11222300
H	-4.86916800	3.31489600	1.08279900
H	-1.37904000	4.85022400	-0.90198100
H	-3.54140800	5.24386800	0.25377000
C	1.72734500	-1.07933700	1.49147400
C	1.05574700	0.15562300	1.71225500
C	1.91211100	1.20667200	1.27364600
C	3.12621700	0.61828500	0.80772600
C	3.00837800	-0.79029700	0.93631500
Ti	1.35018600	-0.07151000	-0.58003700
C	1.60140000	2.66219800	1.34500600
H	1.77178400	3.03628300	2.36341600

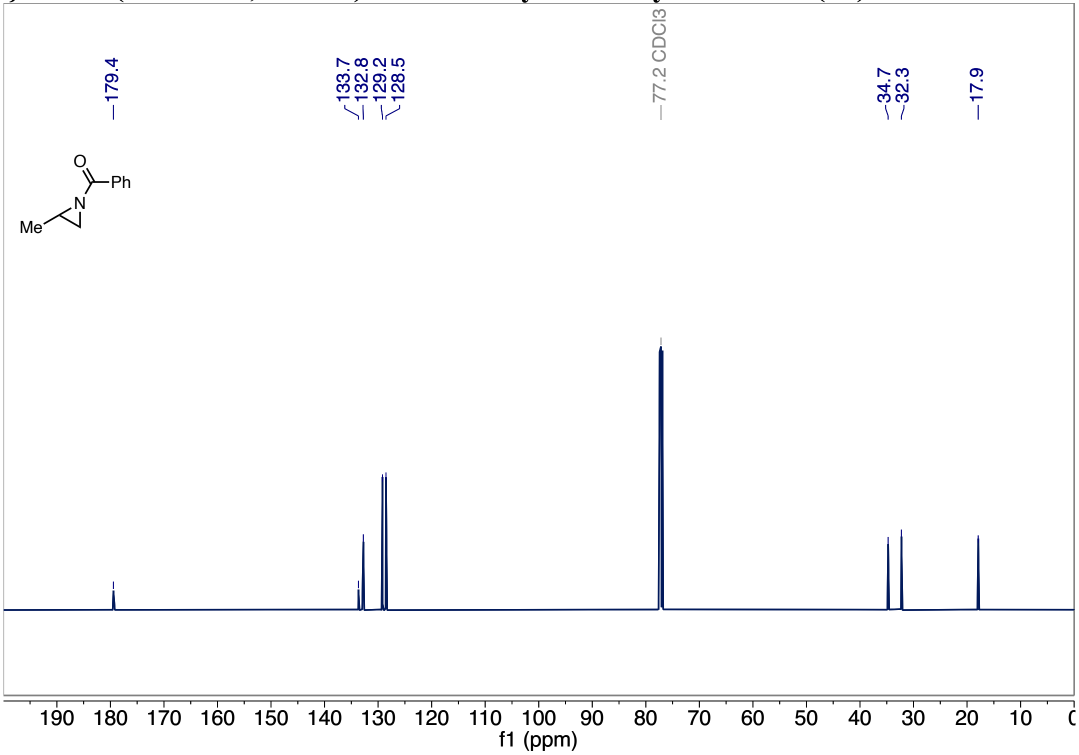
H	2.23044800	3.24604800	0.66626000
H	0.55438000	2.87144800	1.09398700
C	4.34755100	1.32595100	0.33602900
H	5.09121700	1.35892000	1.14385900
H	4.81044200	0.81152900	-0.51368000
H	4.13829500	2.35552500	0.03244000
C	4.07998300	-1.77558200	0.62677800
H	4.82440700	-1.78093900	1.43469800
H	3.68379400	-2.79084100	0.53096300
H	4.60681500	-1.52880800	-0.30205700
C	1.22124000	-2.43336400	1.85198900
H	0.14394600	-2.42066900	2.05141300
H	1.41363900	-3.17050700	1.06422700
H	1.72052600	-2.79012000	2.76297000
C	-0.26943700	0.32561100	2.36958200
H	-0.15298300	0.26266200	3.45964900
H	-0.71486700	1.30056000	2.14457300
H	-0.98743400	-0.44980200	2.07657800
Cl	2.07829000	1.50687800	-2.03644800
Cl	1.74380300	-1.99023600	-1.70716500
C	-2.97138800	-3.13290200	0.15624400
H	-2.50765600	-4.11995900	-0.00631300
H	-1.04347400	-2.20378300	0.10838600
C	-4.32102400	-3.11293000	-0.54525100
H	-4.99093200	-3.87812600	-0.13409400
H	-4.80697100	-2.13684000	-0.42033900
H	-4.21475000	-3.29760200	-1.62259900
C	-3.12452800	-2.91226300	1.65286200
H	-3.78556400	-3.66539400	2.09942300
H	-2.15764500	-2.96888500	2.17244900
H	-3.55964800	-1.92419700	1.85638900

10. NMR Spectra

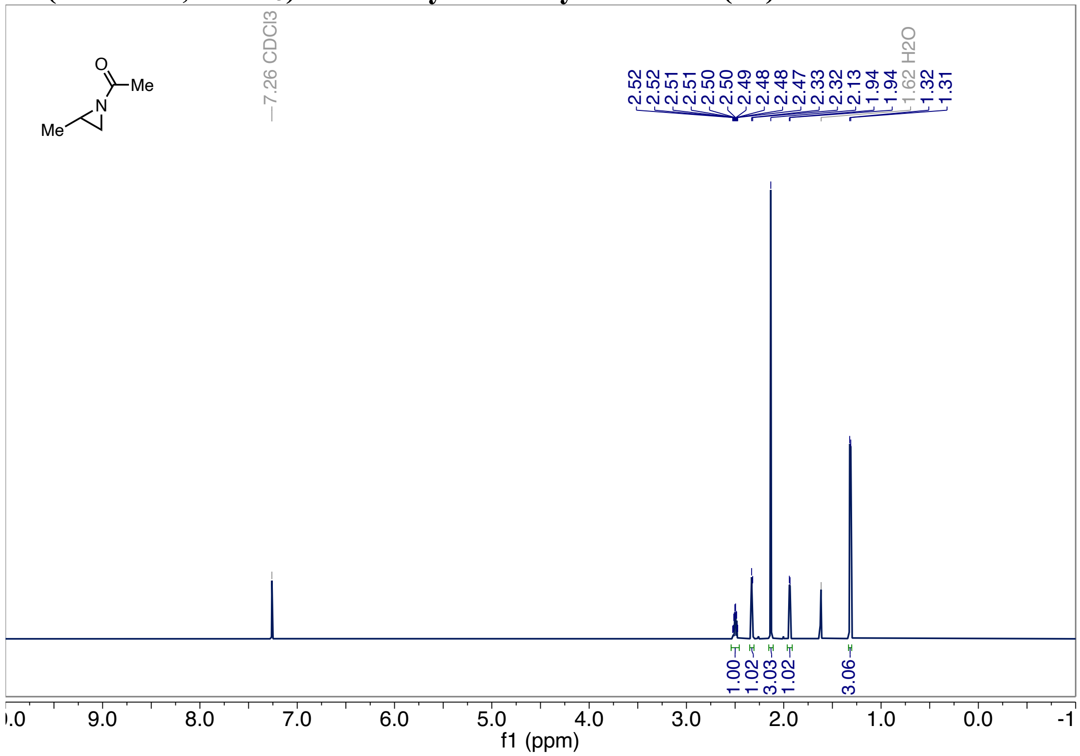
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-benzoyl-2-methyl aziridine (1a):



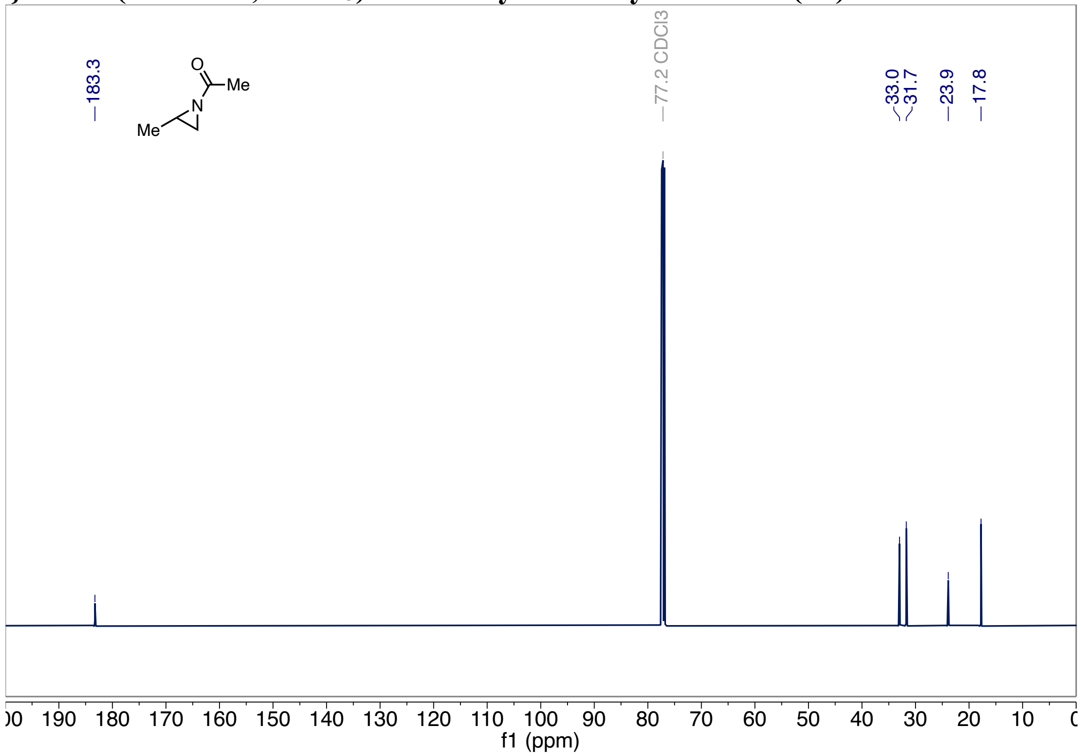
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-benzoyl-2-methyl aziridine (1a):



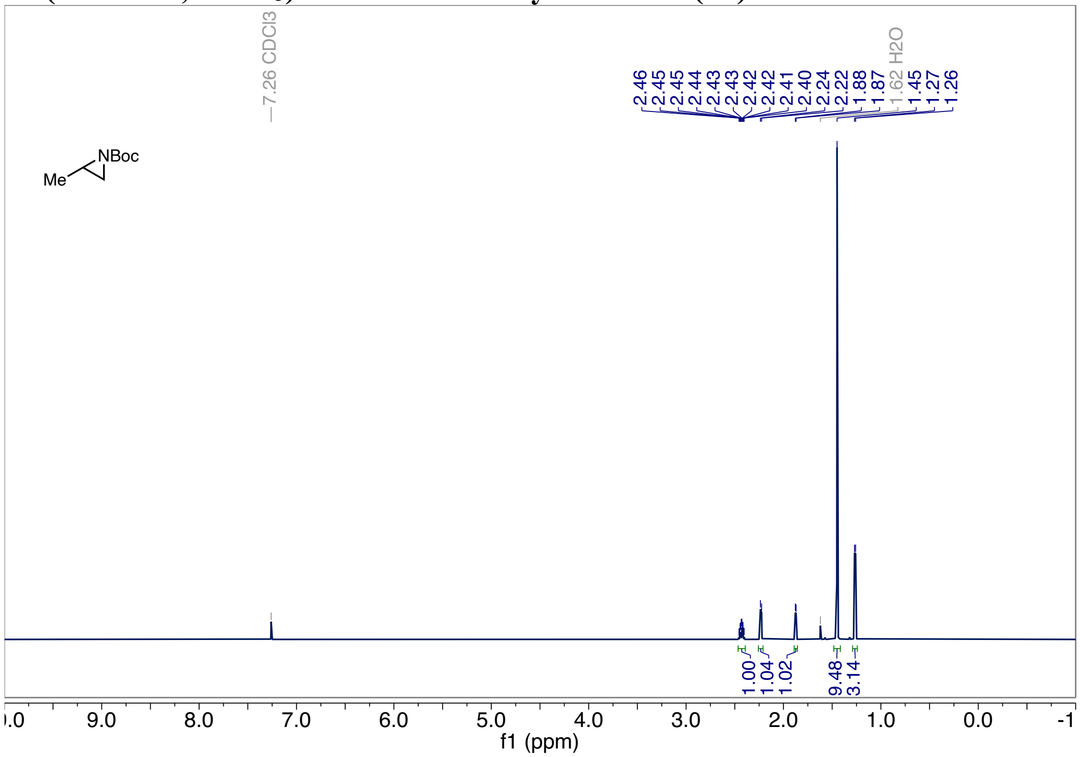
^{1}H NMR (500 MHz, $CDCl_3$) of *N*-acetyl-2-methyl aziridine (S1):



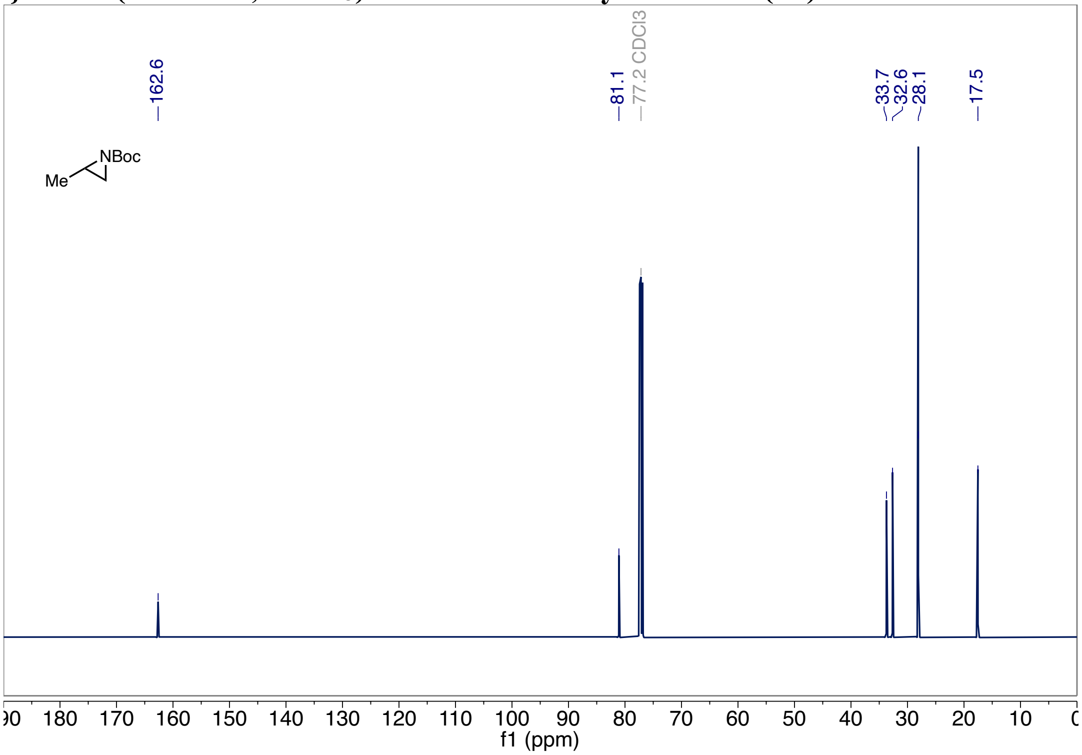
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) of *N*-acetyl-2-methyl aziridine (S1):



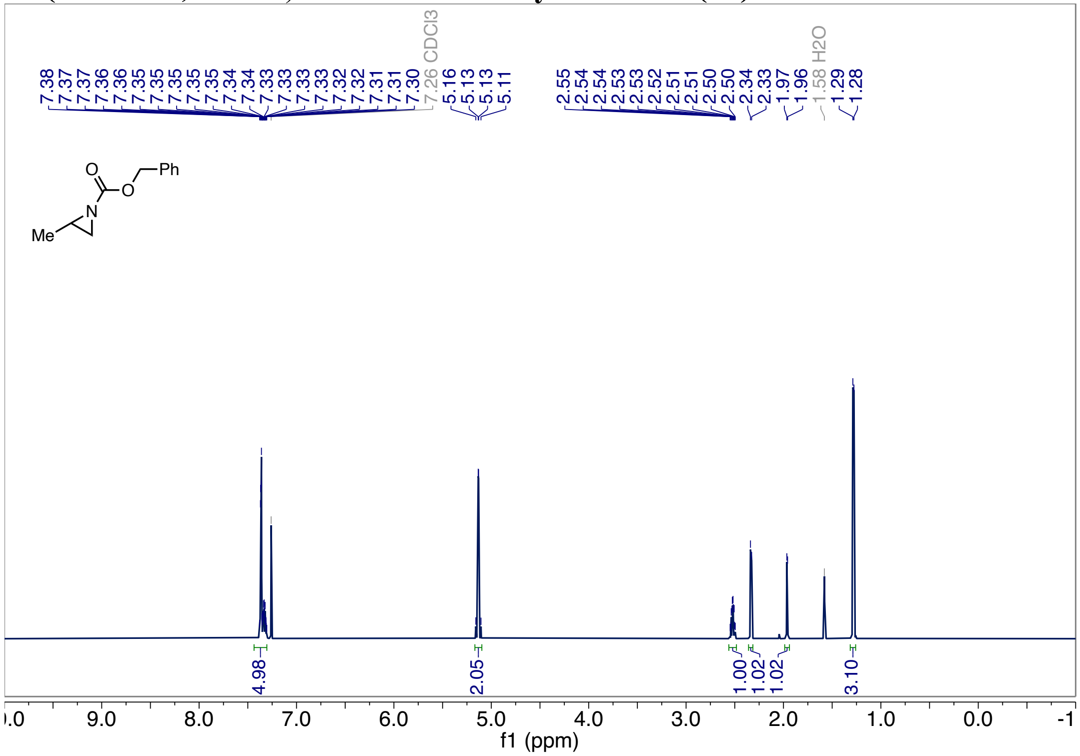
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-Boc-2-methyl aziridine (S2):



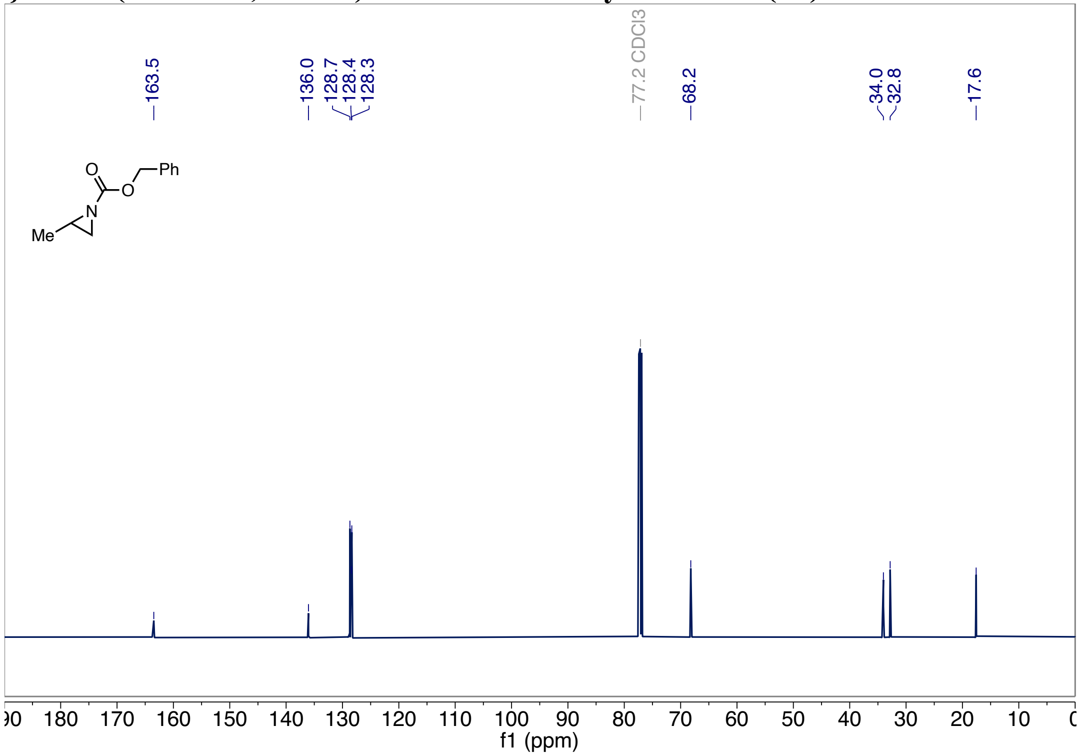
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-Boc-2-methyl aziridine (S2):



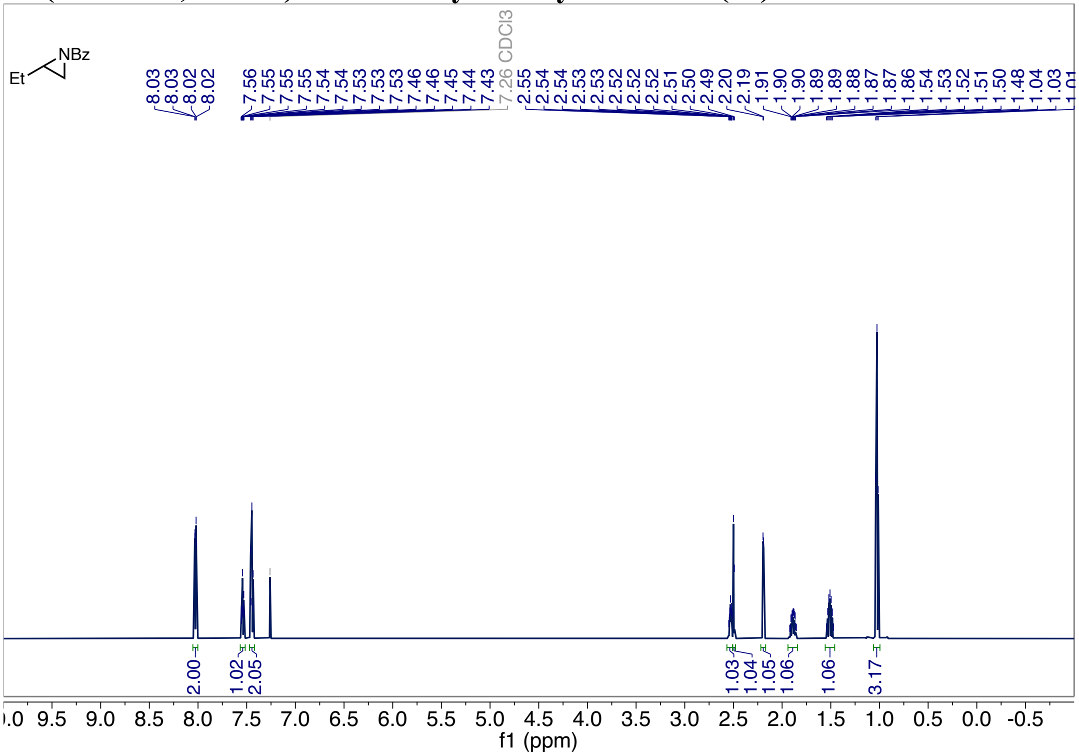
^1H NMR (500 MHz, $CDCl_3$) of *N*-Cbz-2-methyl aziridine (S3):



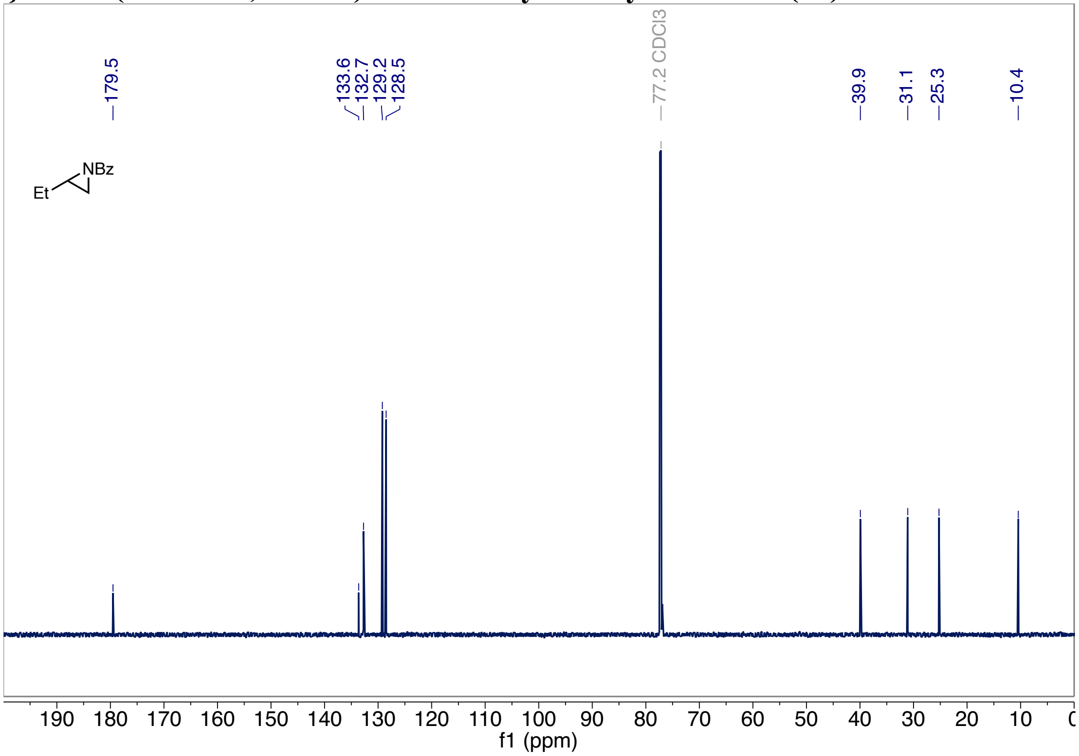
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) of *N*-Cbz-2-methyl aziridine (S3):



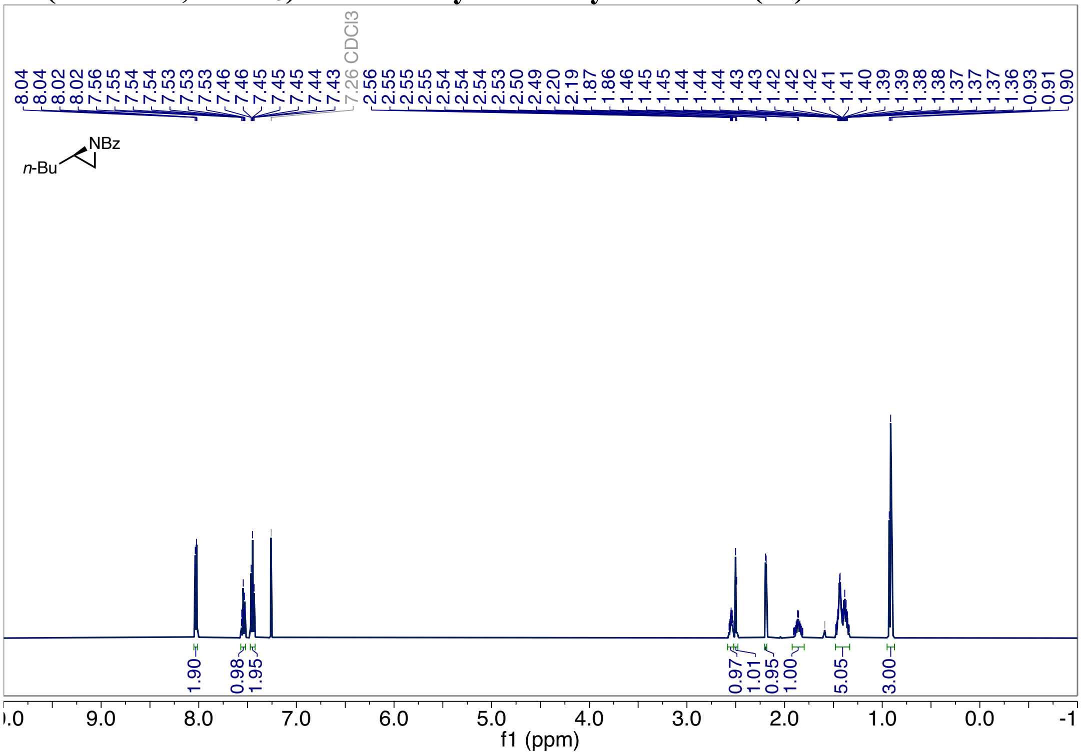
^{1}H NMR (600 MHz, CDCl$_3$) of *N*-benzoyl-2-ethyl aziridine (2a):



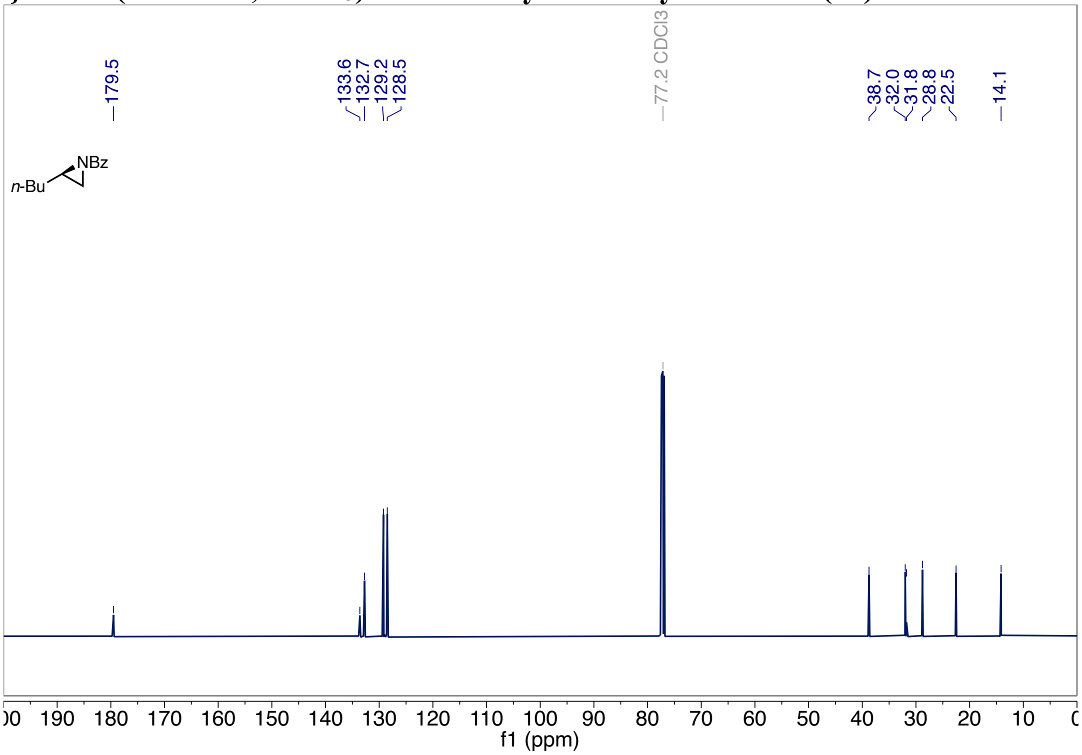
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of *N*-benzoyl-2-ethyl aziridine (2a):



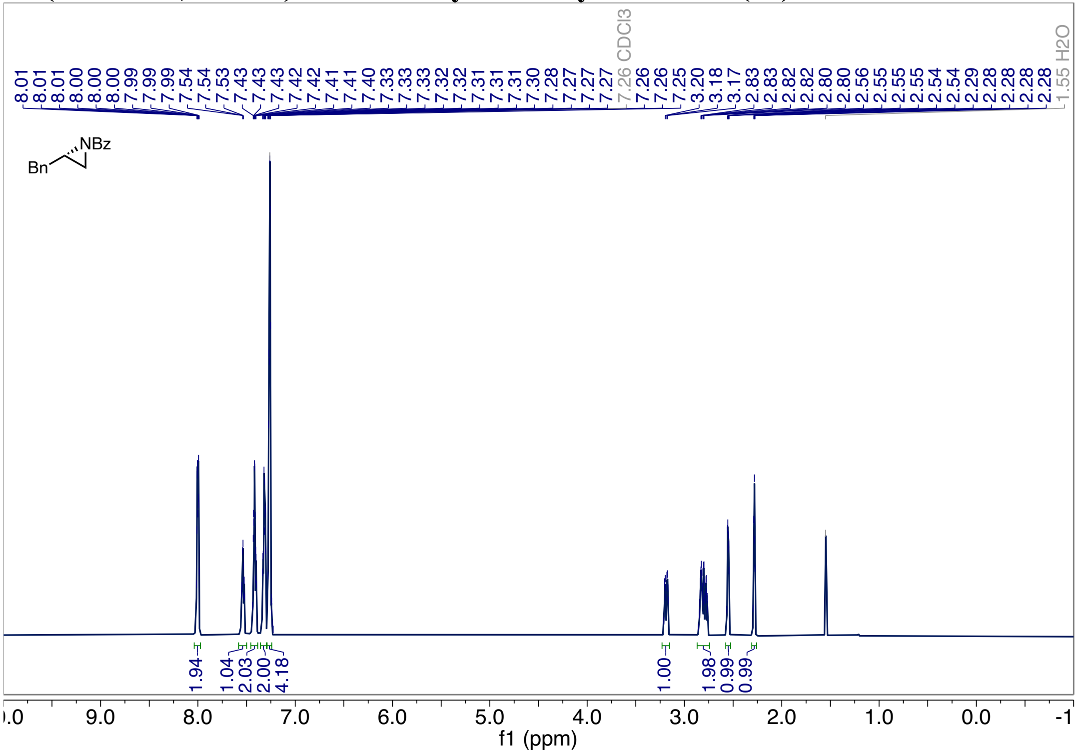
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-benzoyl-2-*n*-butyl aziridine (3a):



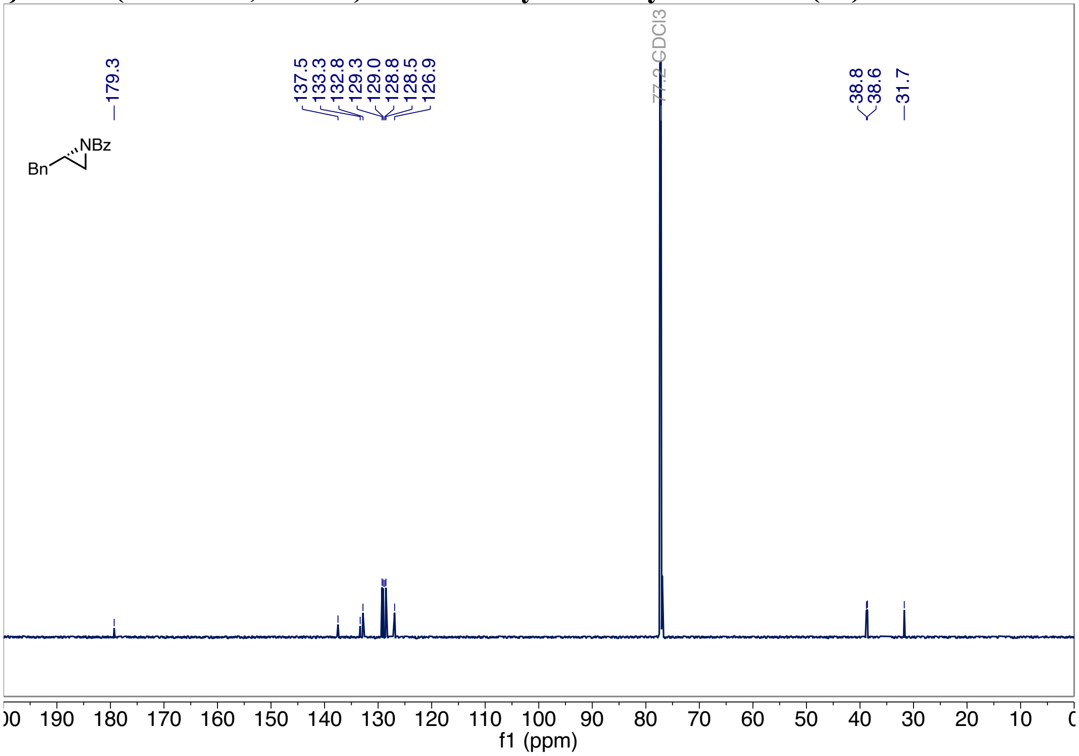
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-benzoyl-2-*n*-butyl aziridine (3a):



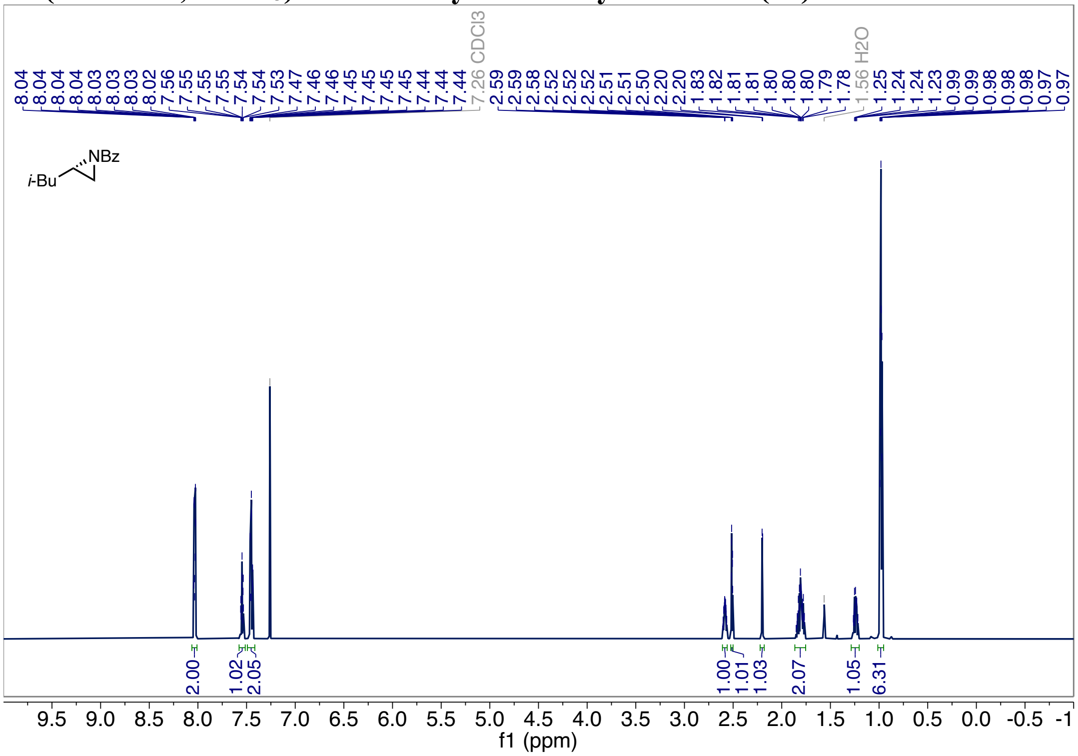
^{1}H NMR (600 MHz, $CDCl_3$) of *N*-benzoyl-2-benzyl aziridine (4a):



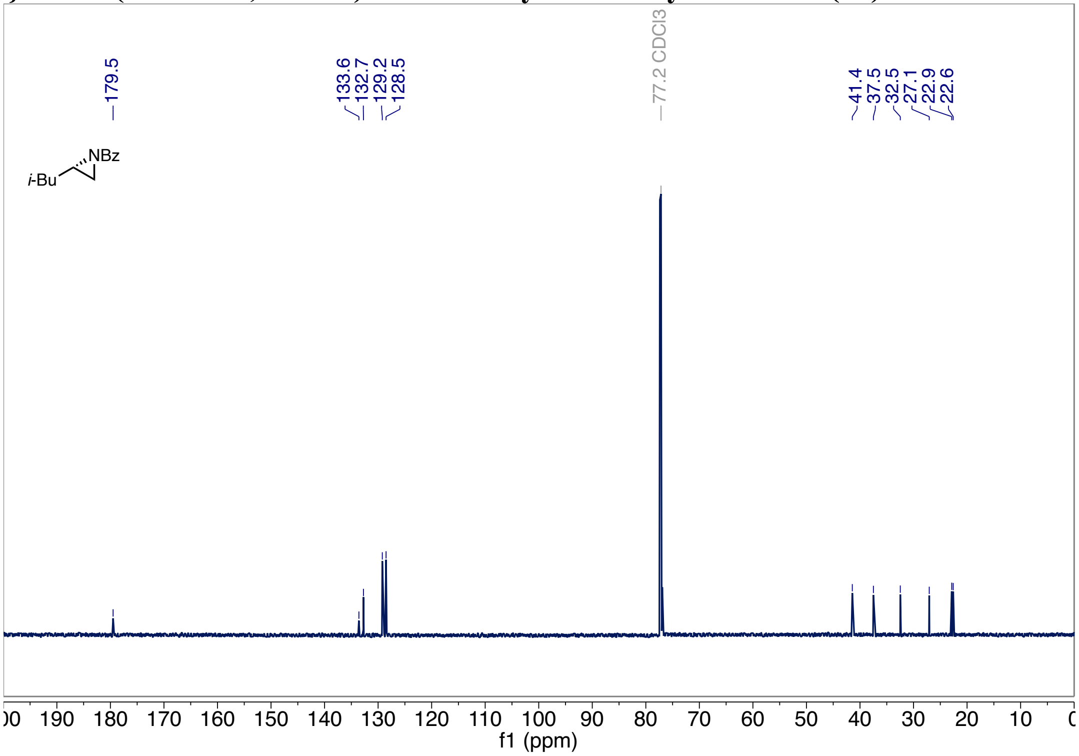
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) of *N*-benzoyl-2-benzyl aziridine (4a):



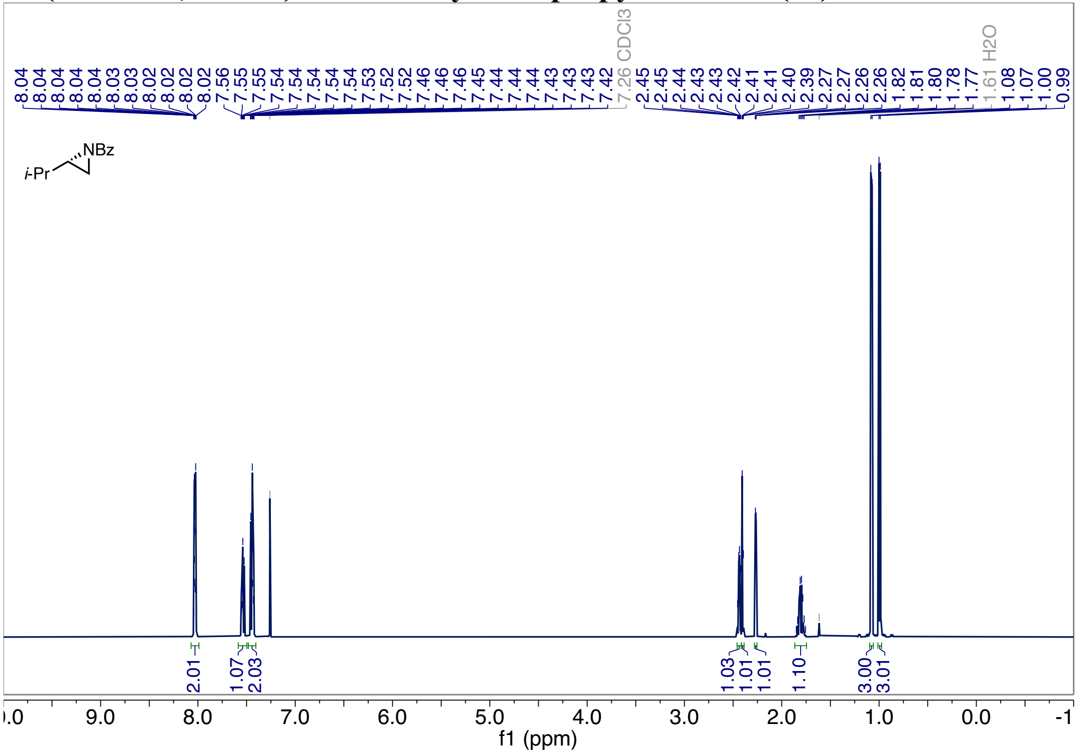
^{1}H NMR (600 MHz, $CDCl_3$) of *N*-benzoyl-2-isobutyl aziridine (5a):



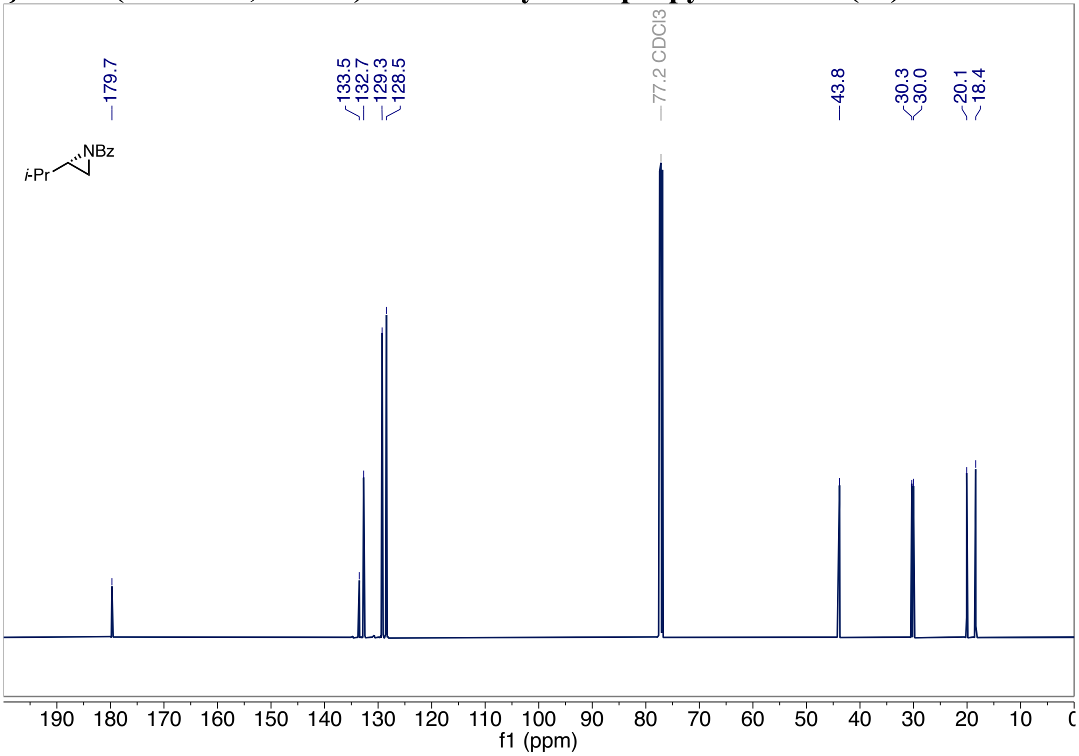
^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) of *N*-benzoyl-2-isobutyl aziridine (5a):



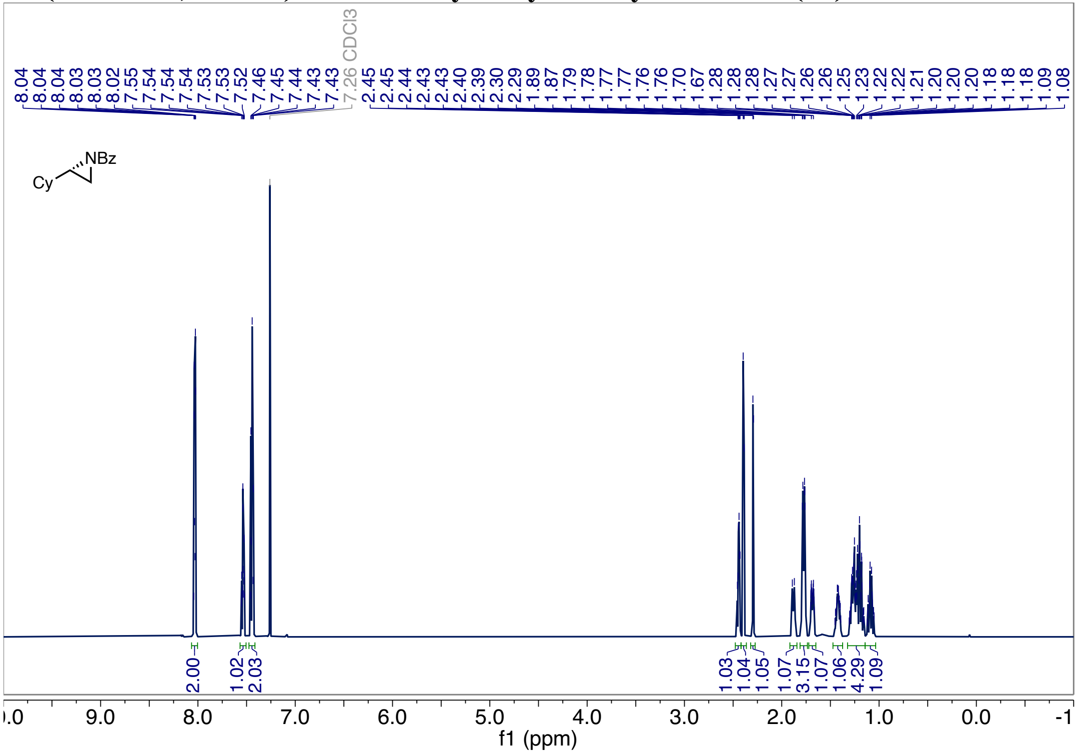
^{1}H NMR (500 MHz, $CDCl_3$) of *N*-benzoyl-2-isopropyl aziridine (6a):



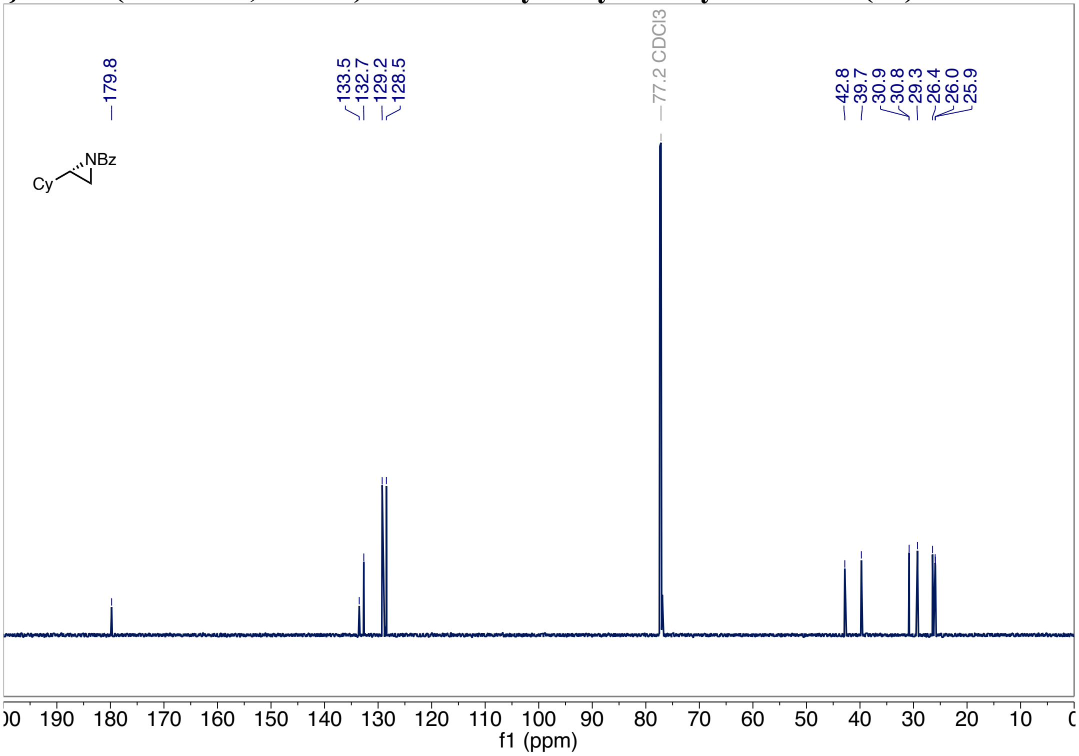
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) of *N*-benzoyl-2-isopropyl aziridine (6a):



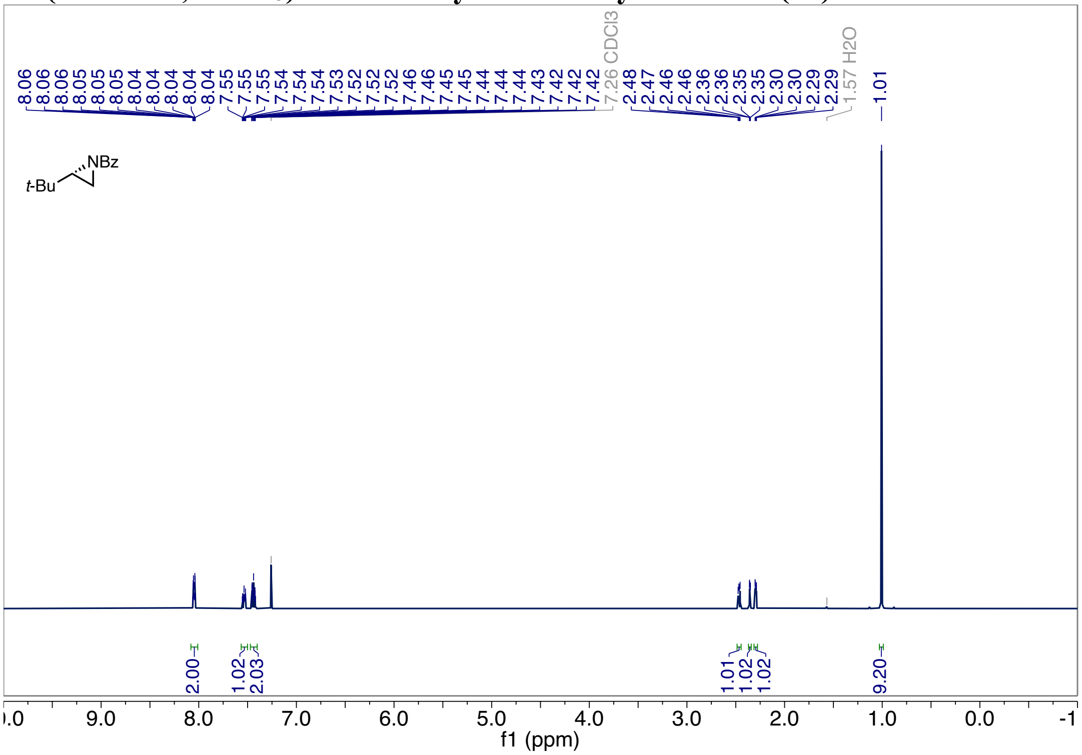
^{1}H NMR (600 MHz, CDCl$_3$) of *N*-benzoyl-2-cyclohexyl aziridine (7a):



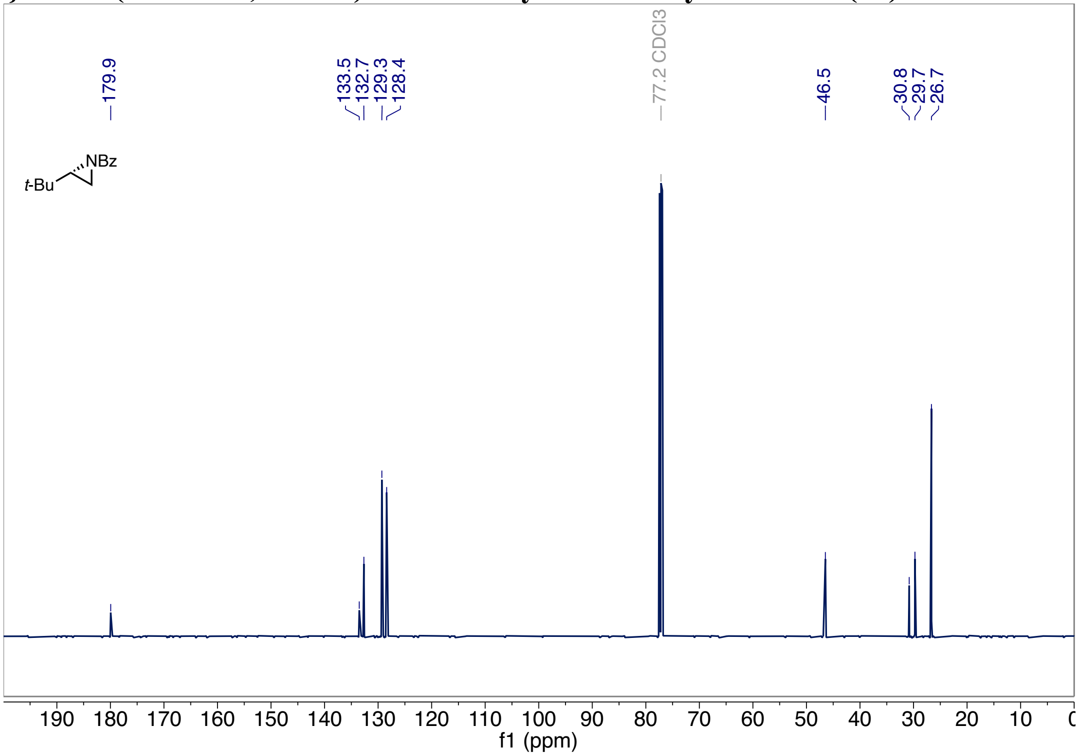
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of *N*-benzoyl-2-cyclohexyl aziridine (7a):



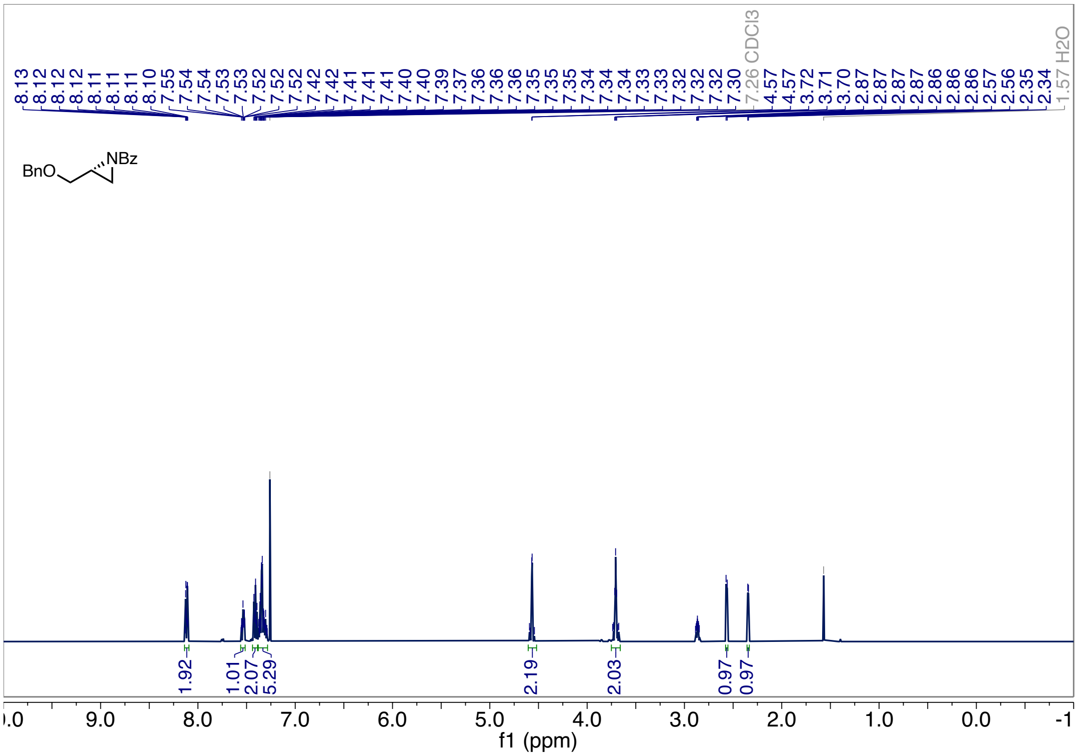
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-benzoyl-2-*tert*-butyl aziridine (8a):



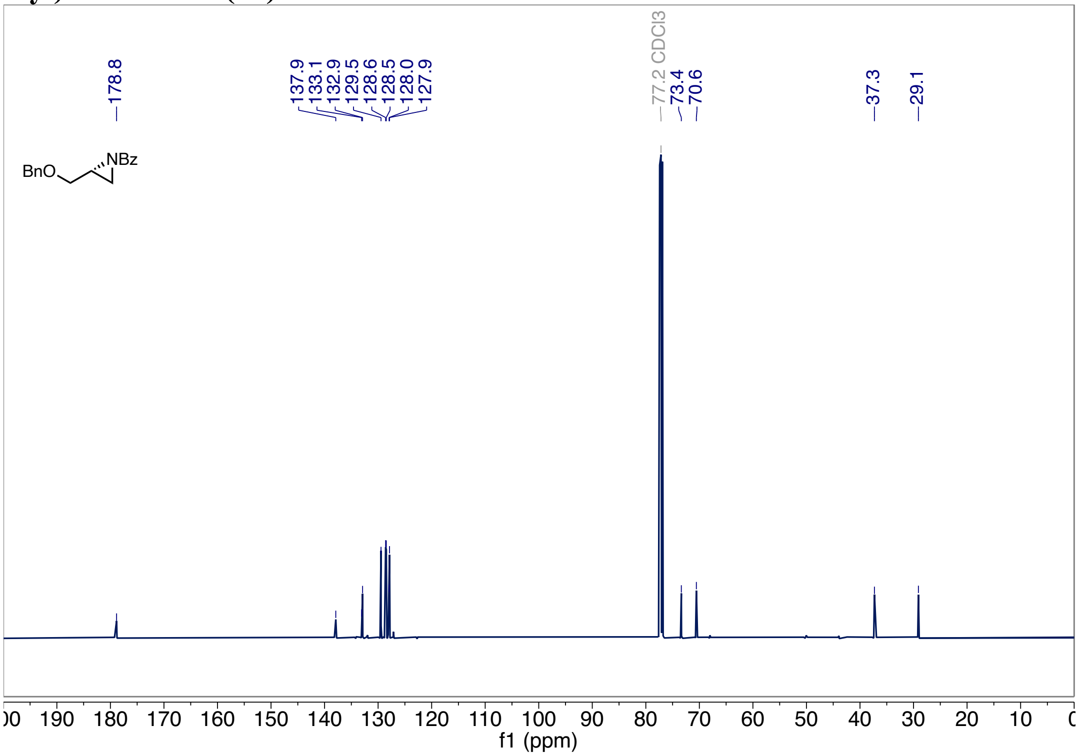
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-benzoyl-2-*tert*-butyl aziridine (8a):



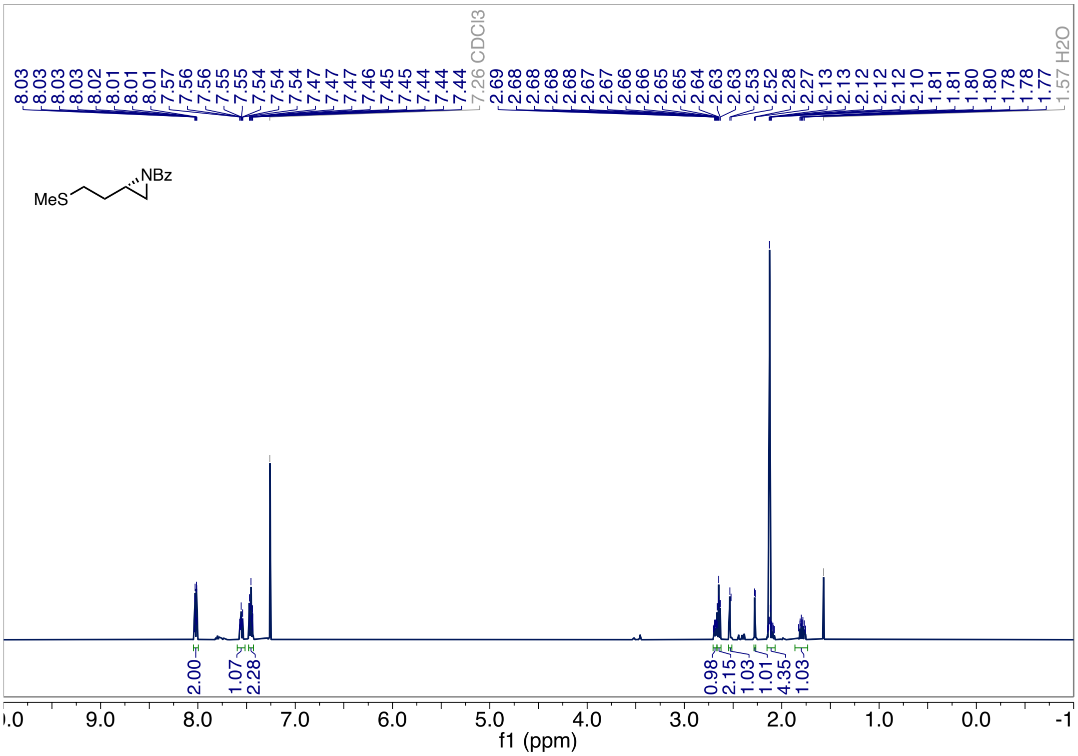
^{1}H NMR (500 MHz, CDCl$_3$) of (R)-(2-((benzyloxy)methyl)aziridin-1-yl)(phenyl)methanone (9a):



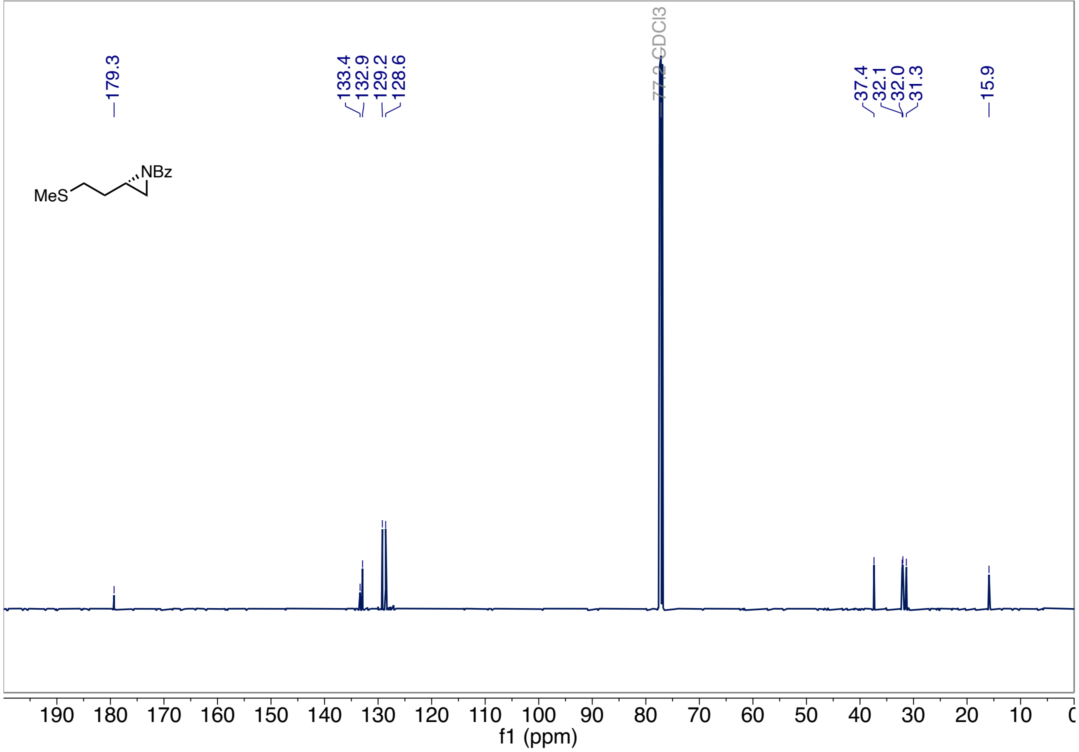
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of (R)-(2-((benzyloxy)methyl)aziridin-1-yl)(phenyl)methanone (9a):



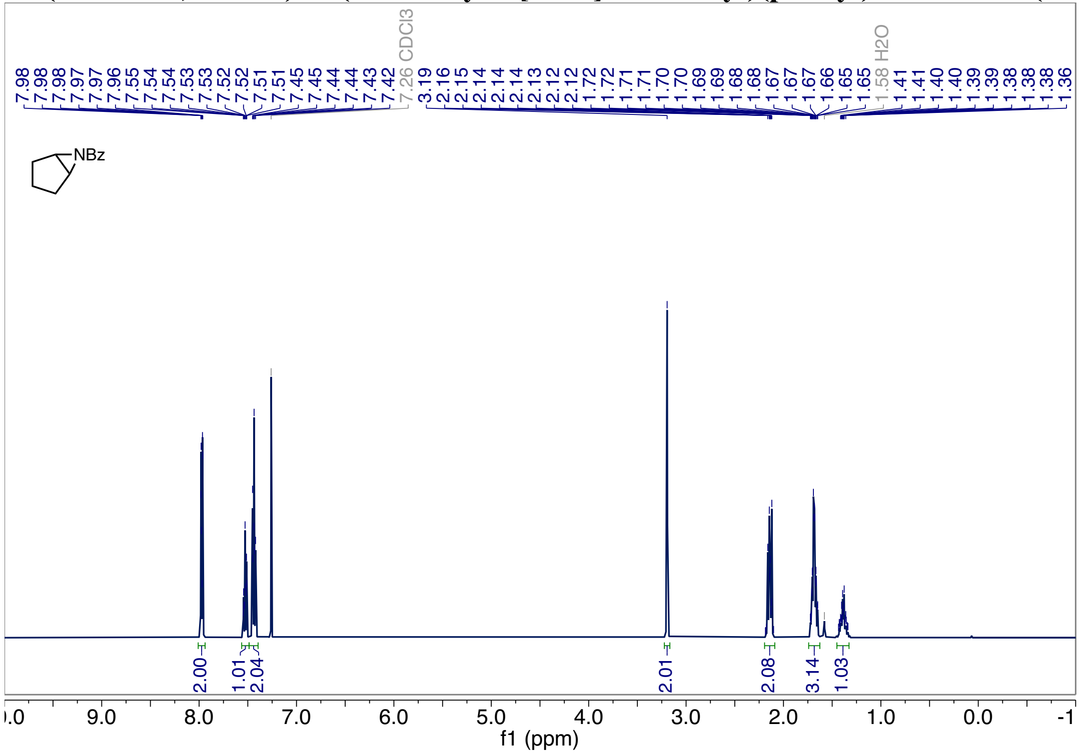
^{1}H NMR (500 MHz, CDCl$_3$) of (S)-(2-(2-(methylthio)ethyl)aziridin-1-yl)(phenyl)methanone (10a):



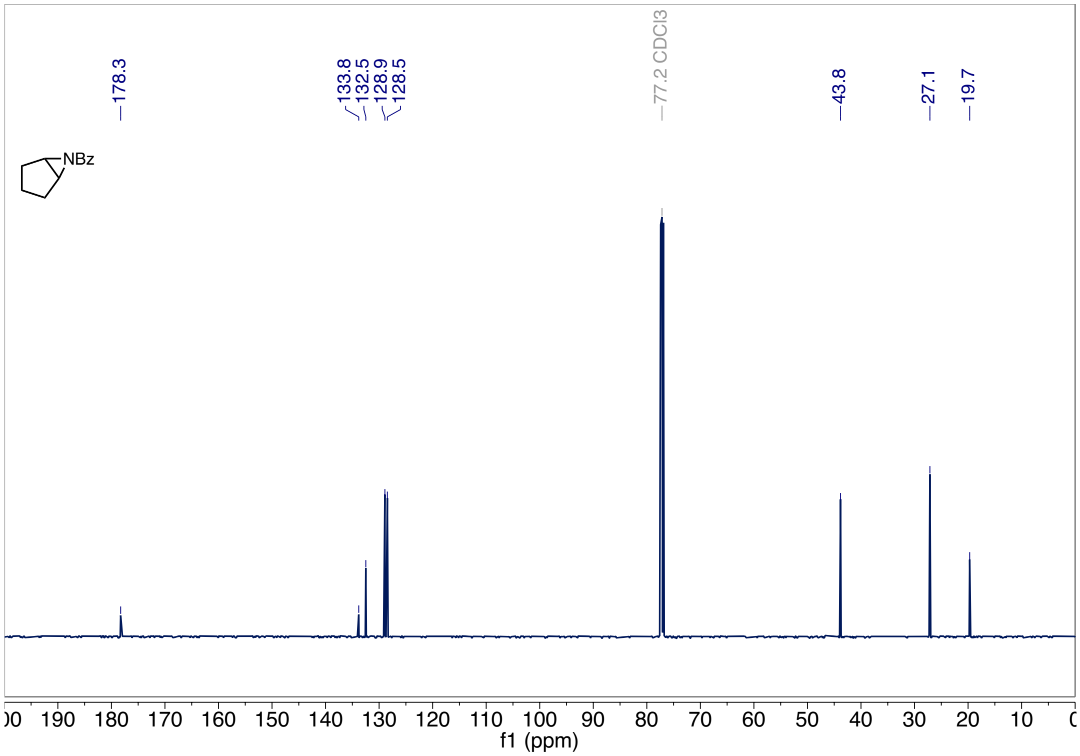
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of (S)-(2-(2-(methylthio)ethyl)aziridin-1-yl)(phenyl) methanone (10a):



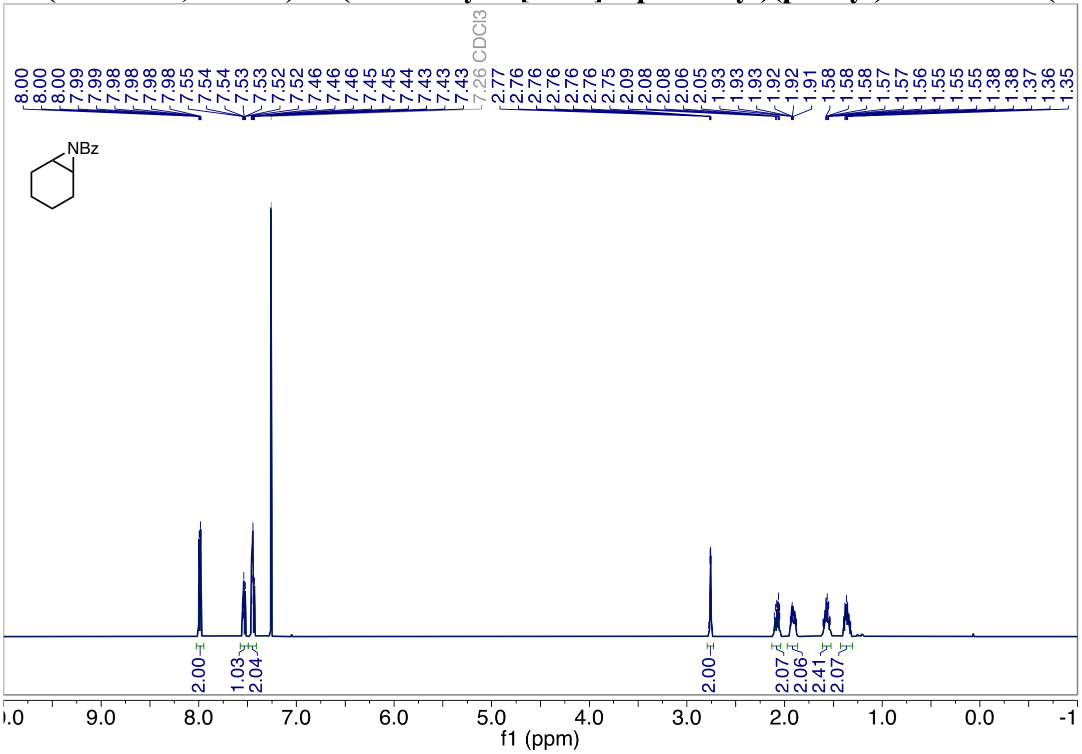
^{1}H NMR (500 MHz, $CDCl_3$) of (6-azabicyclo[3.1.0]hexan-6-yl)(phenyl)methanone (11a):



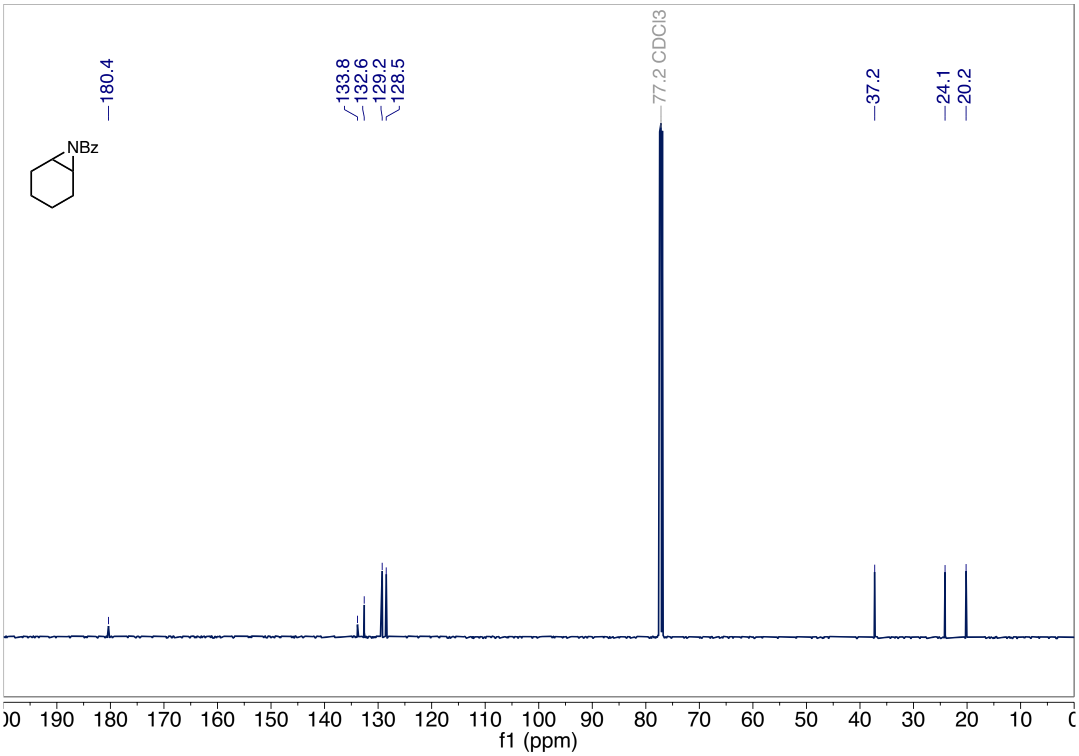
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) of (6-azabicyclo[3.1.0]hexan-6-yl)(phenyl)methanone (11a):



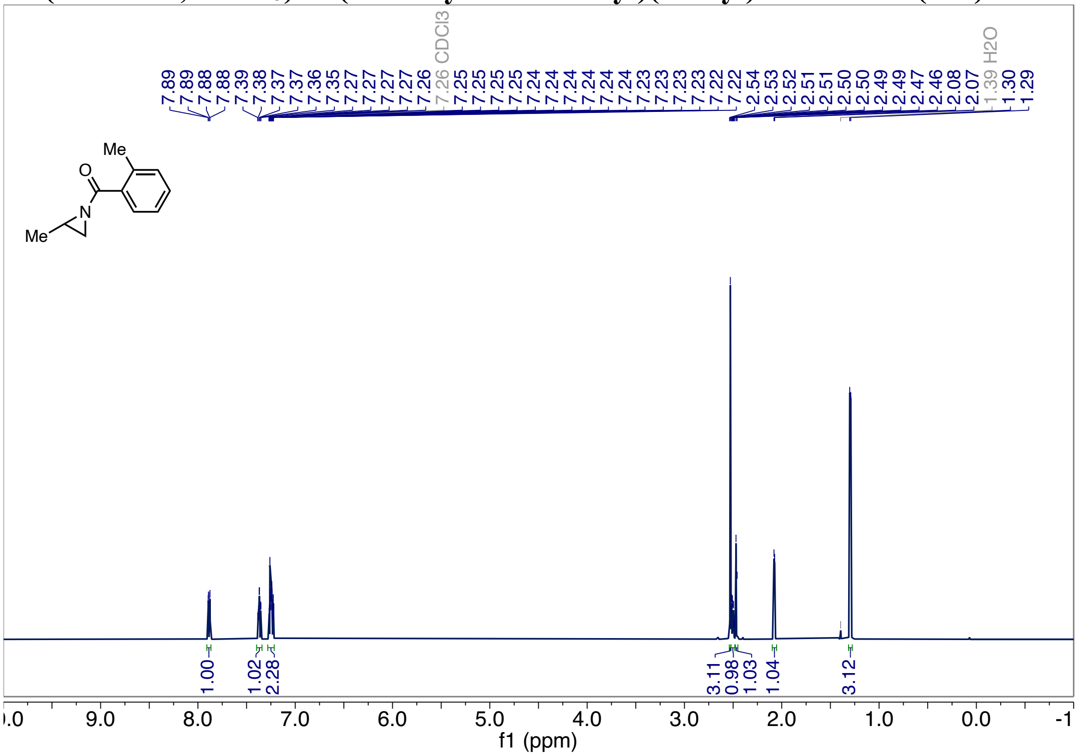
^1H NMR (500 MHz, $CDCl_3$) of (7-azabicyclo[4.1.0]heptan-7-yl)(phenyl)methanone (12a):



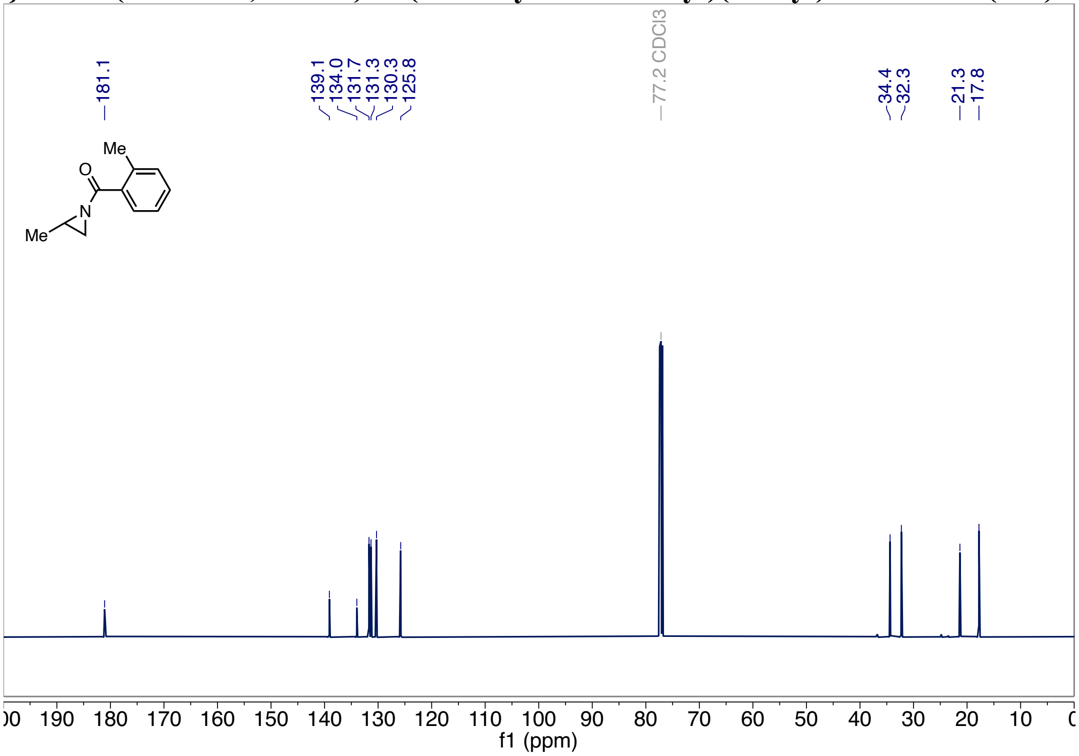
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) of (7-azabicyclo[4.1.0]heptan-7-yl)(phenyl)methanone (12a):



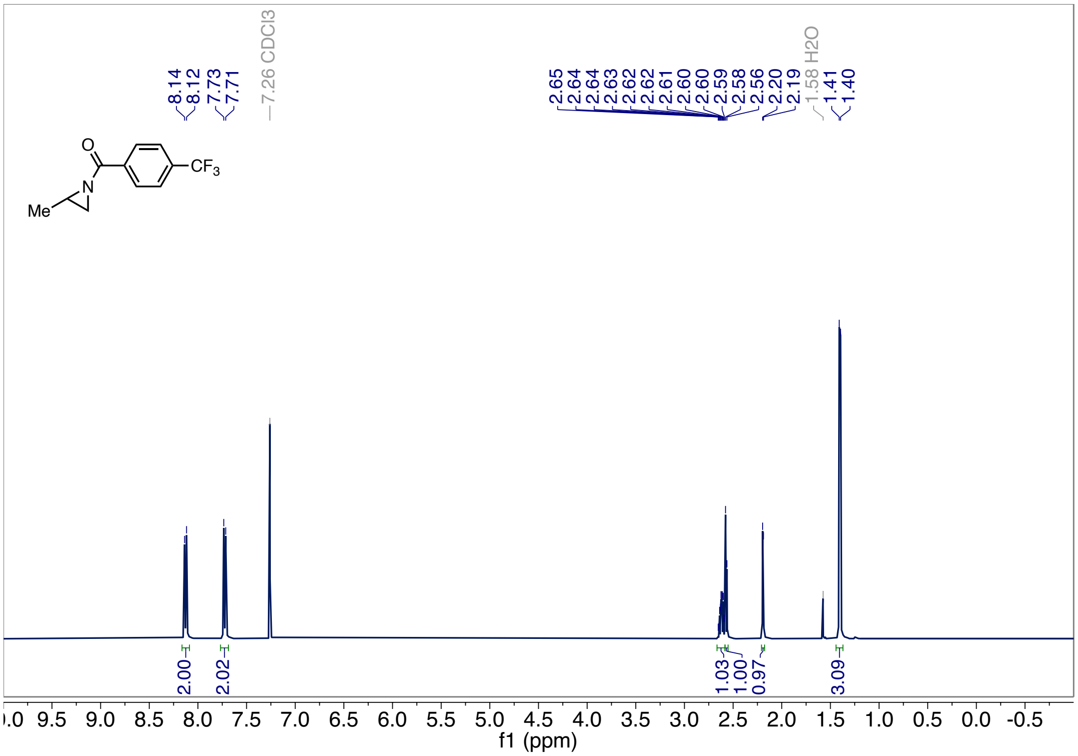
^{1}H NMR (500 MHz, $CDCl_3$) of (2-methylaziridin-1-yl)(*o*-tolyl)methanone (13a):



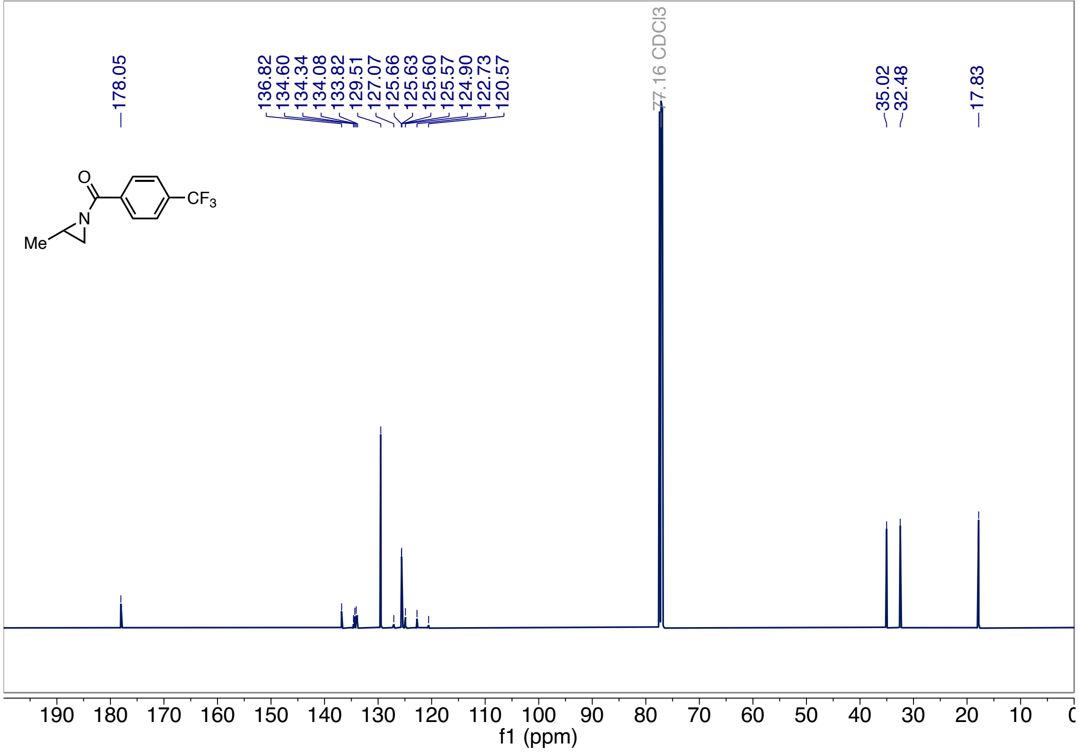
$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) of (2-methylaziridin-1-yl)(*o*-tolyl)methanone (13a):



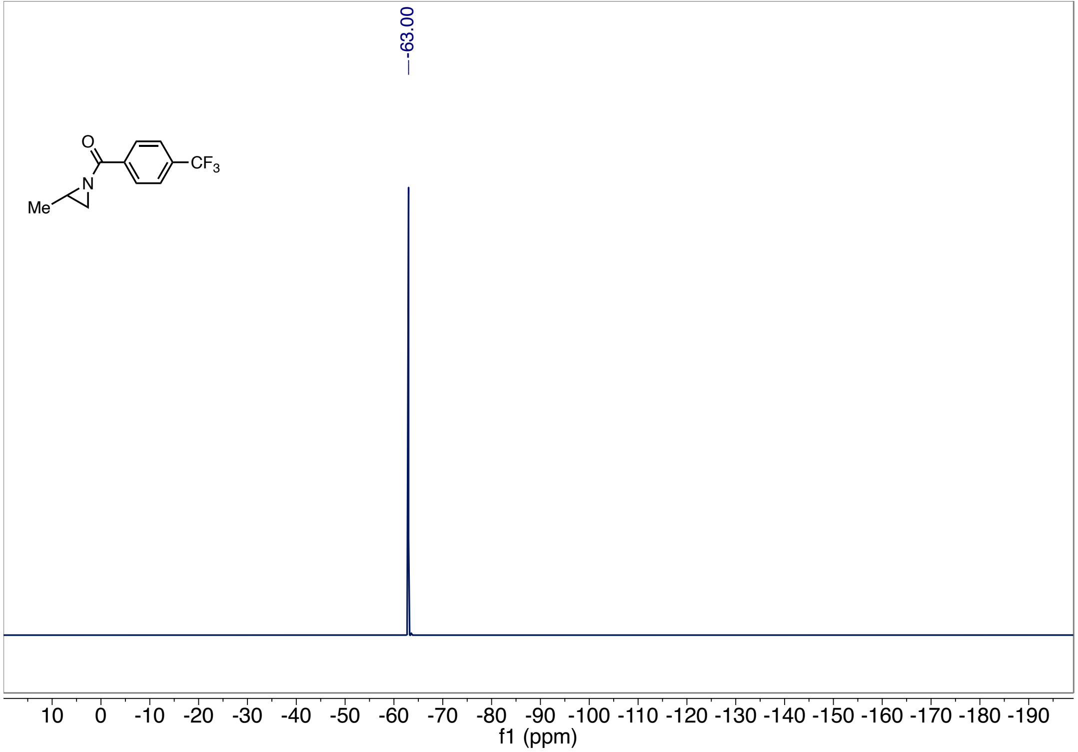
^{1}H NMR (400 MHz, CDCl$_3$) of (2-methylaziridin-1-yl)(4-(trifluoromethyl)phenyl)methanone (14a):



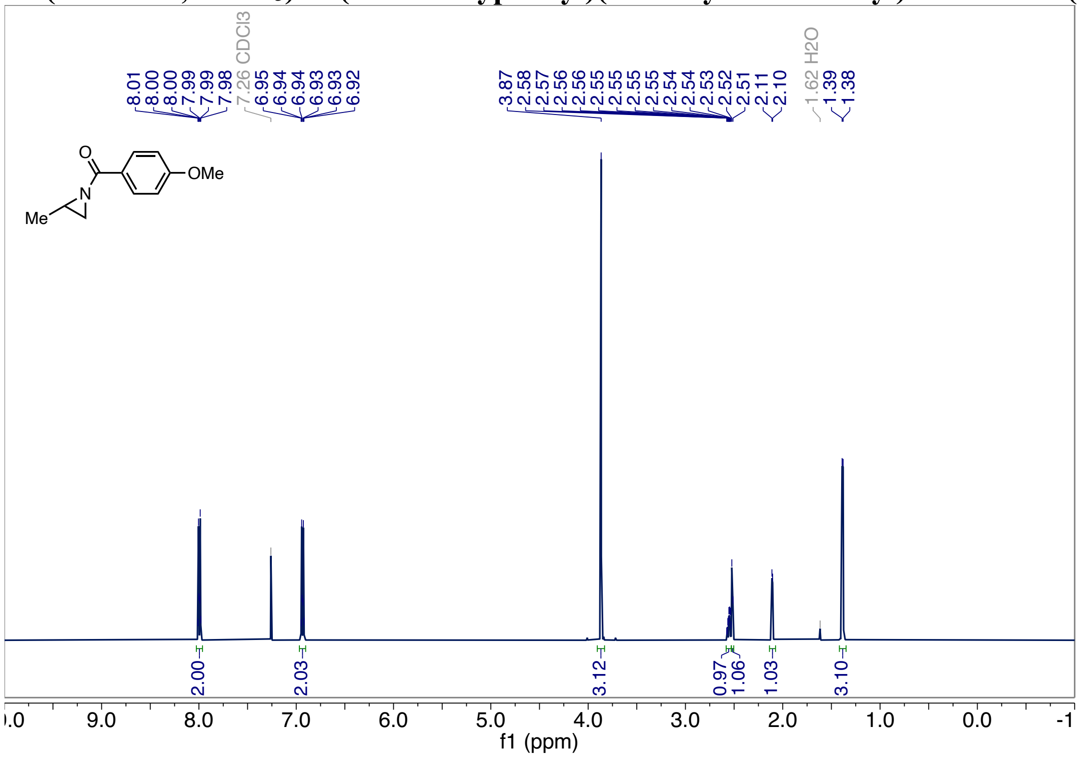
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of (2-methylaziridin-1-yl)(4-(trifluoromethyl)phenyl) methanone (14a):



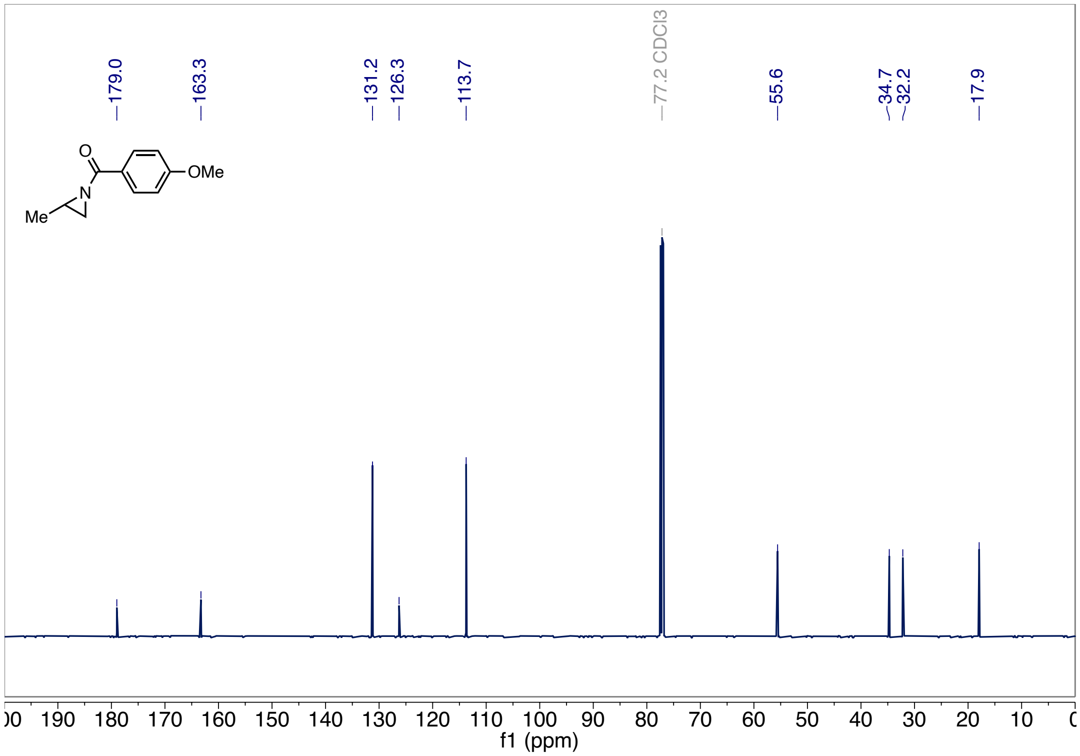
^{19}F NMR (376 MHz, $CDCl_3$) of (2-methylaziridin-1-yl)(4-(trifluoromethyl)phenyl) methanone (14a):



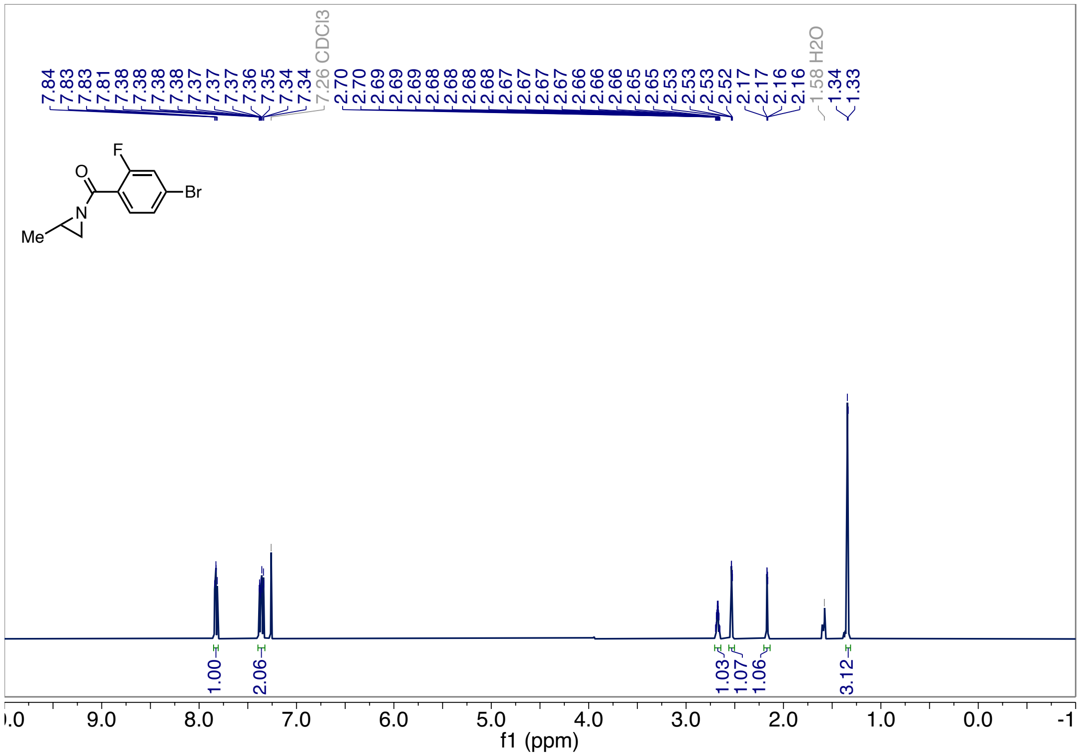
^{1}H NMR (500 MHz, CDCl$_3$) of (4-methoxyphenyl)(2-methylaziridin-1-yl)methanone (15a):



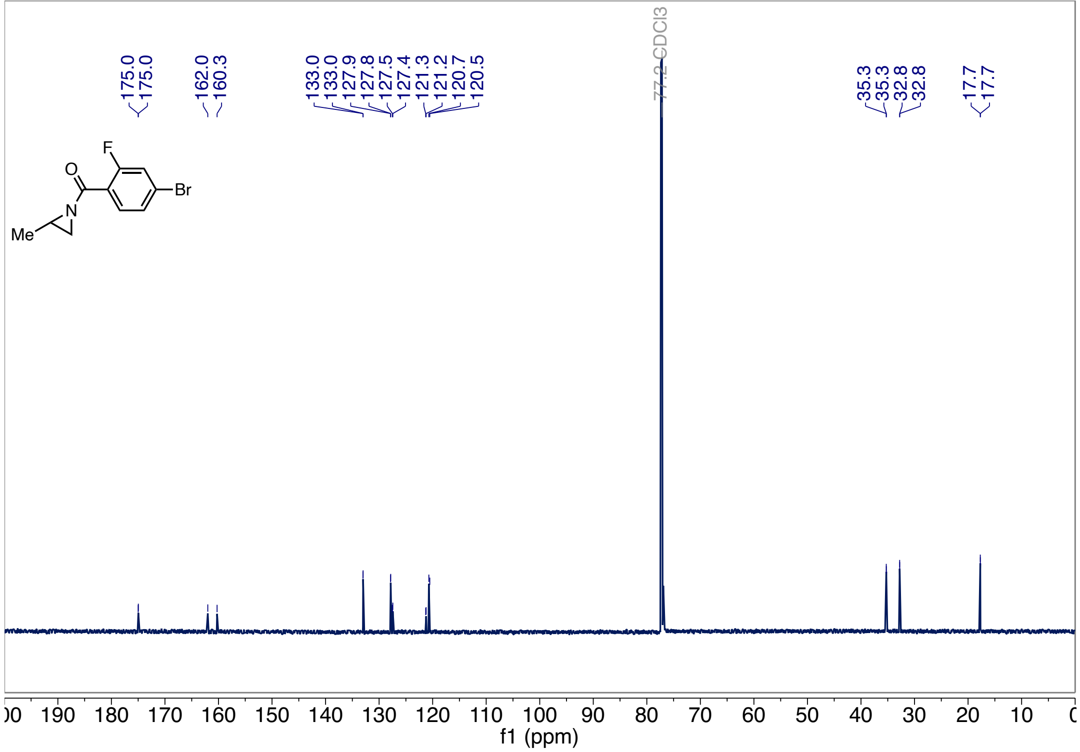
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of (4-methoxyphenyl)(2-methylaziridin-1-yl)methanone (15a):



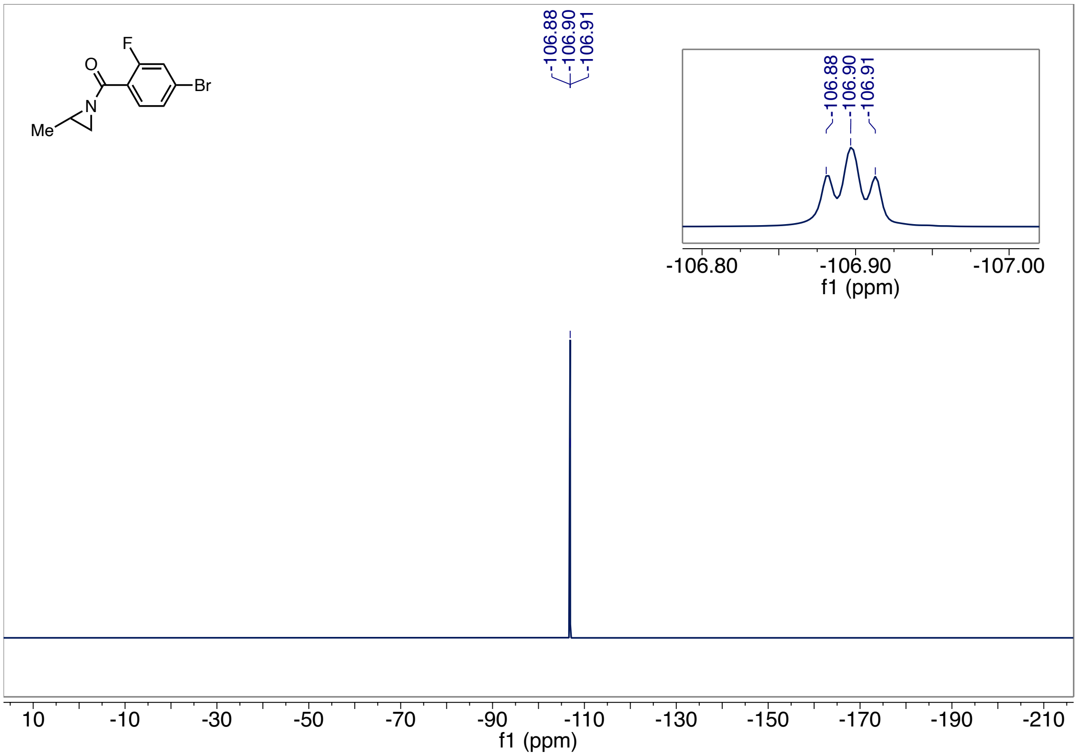
^{1}H NMR (600 MHz, CDCl$_3$) of (4-bromo-2-fluorophenyl)(2-methylaziridin-1-yl)methanone (16a):



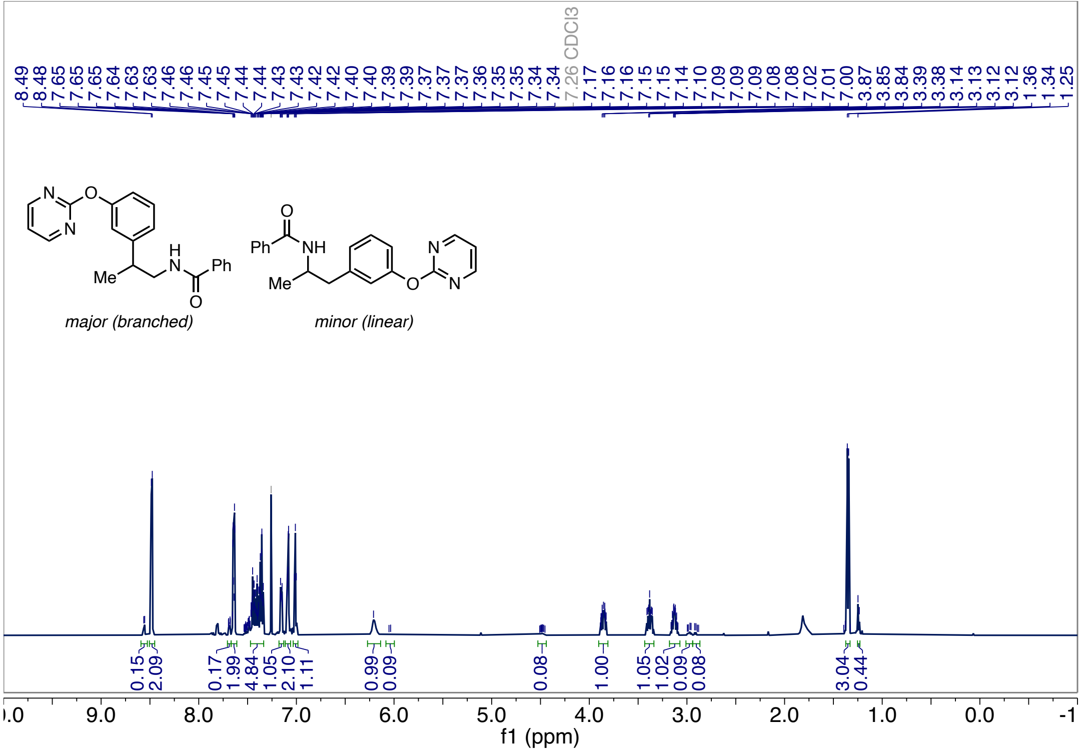
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of (4-bromo-2-fluorophenyl)(2-methylaziridin-1-yl) methanone (16a):



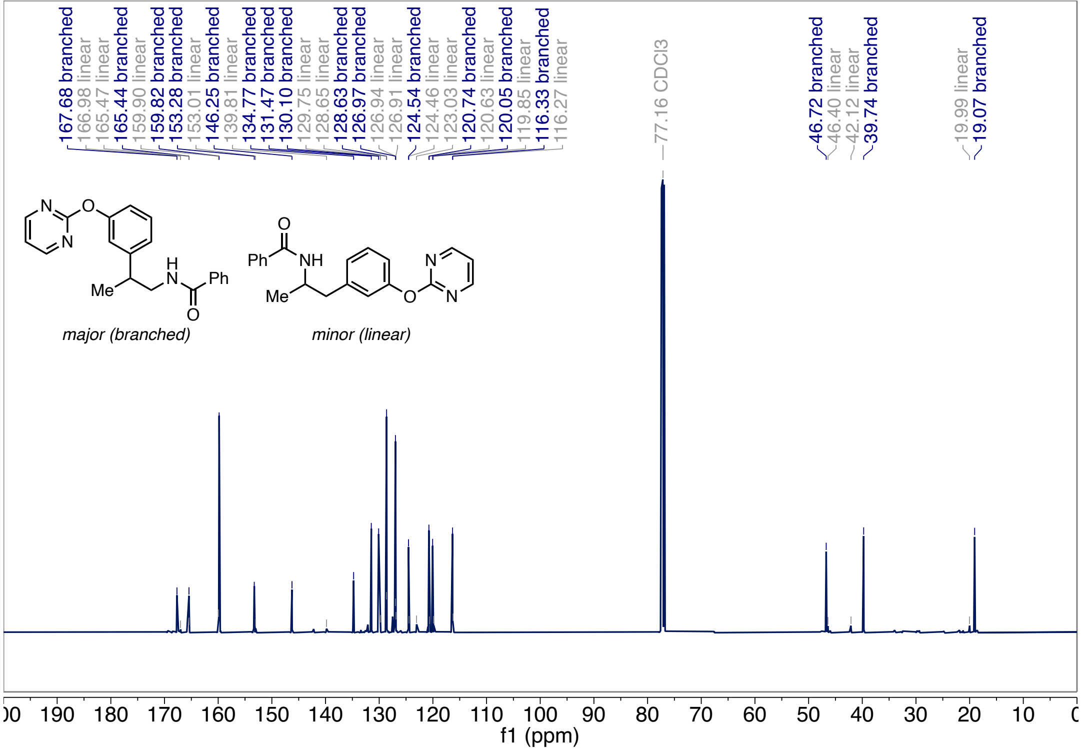
^{19}F NMR (565 MHz, CDCl$_3$) of (4-bromo-2-fluorophenyl)(2-methylaziridin-1-yl)methanone (16a):



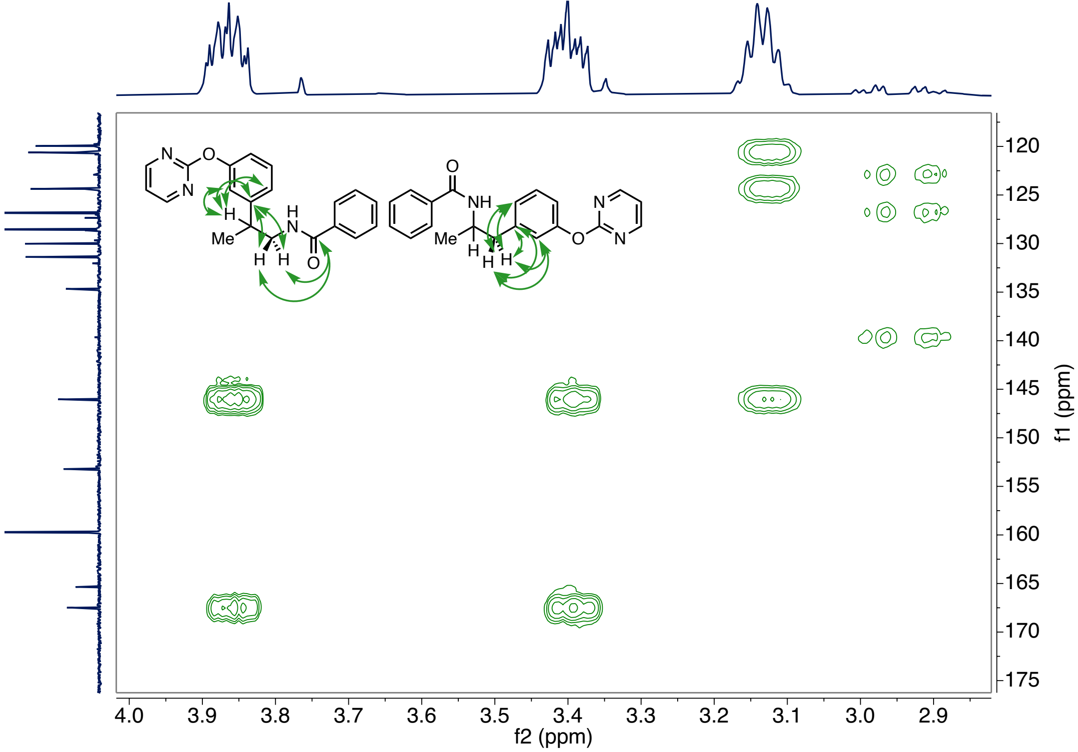
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-(4-(pyrimidin-2-yloxy)phenyl)propyl)benzamide (A-1), mixture of isomers (13:1):



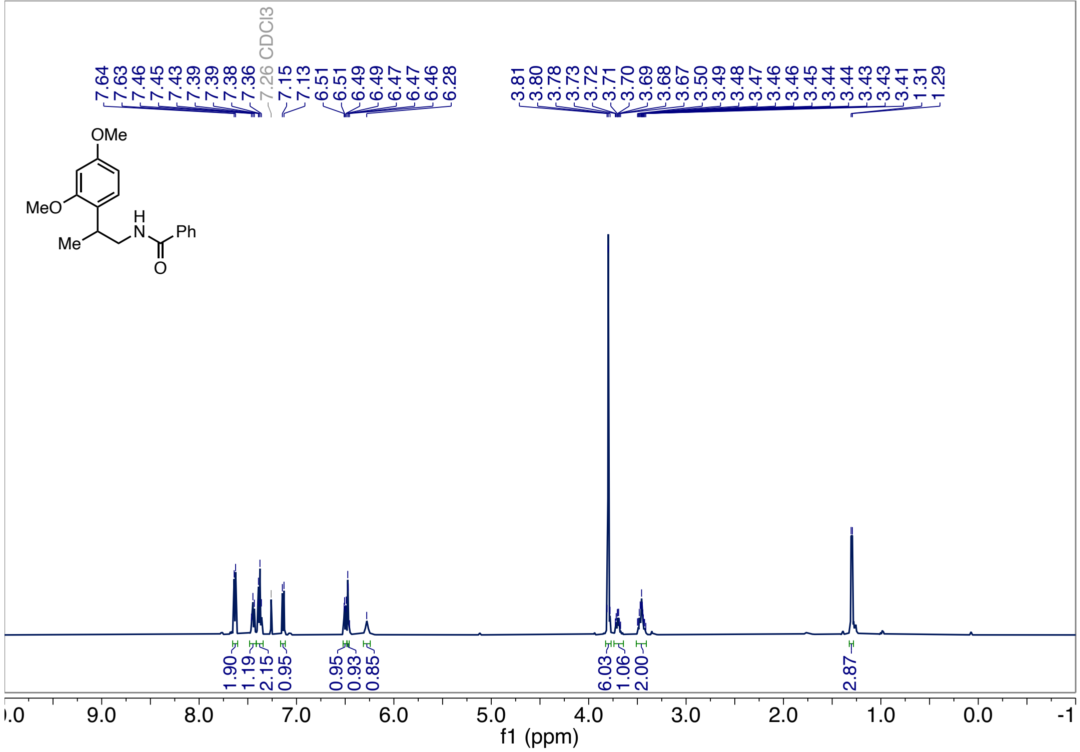
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-(4-(pyrimidin-2-yloxy)phenyl)propyl)benzamide (A-1), mixture of isomers (13:1):



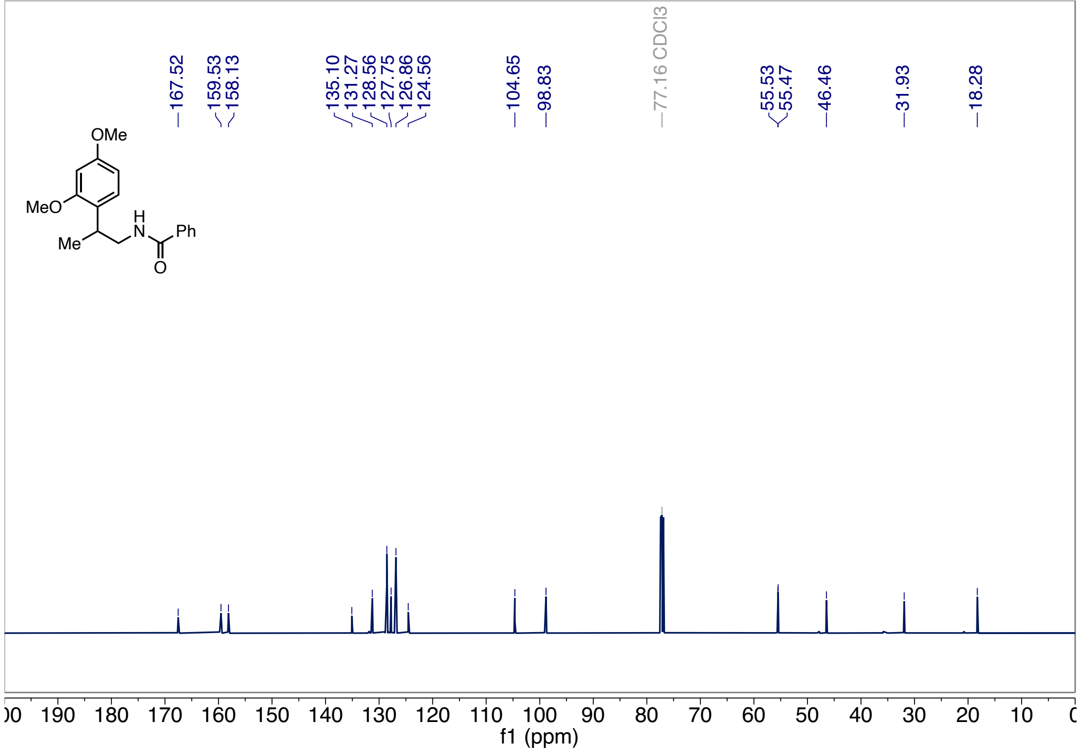
HMBC (500 MHz, CDCl₃) of *N*-(2-(4-(pyrimidin-2-yloxy)phenyl)propyl)benzamide (A-1), mixture of isomers (13:1):



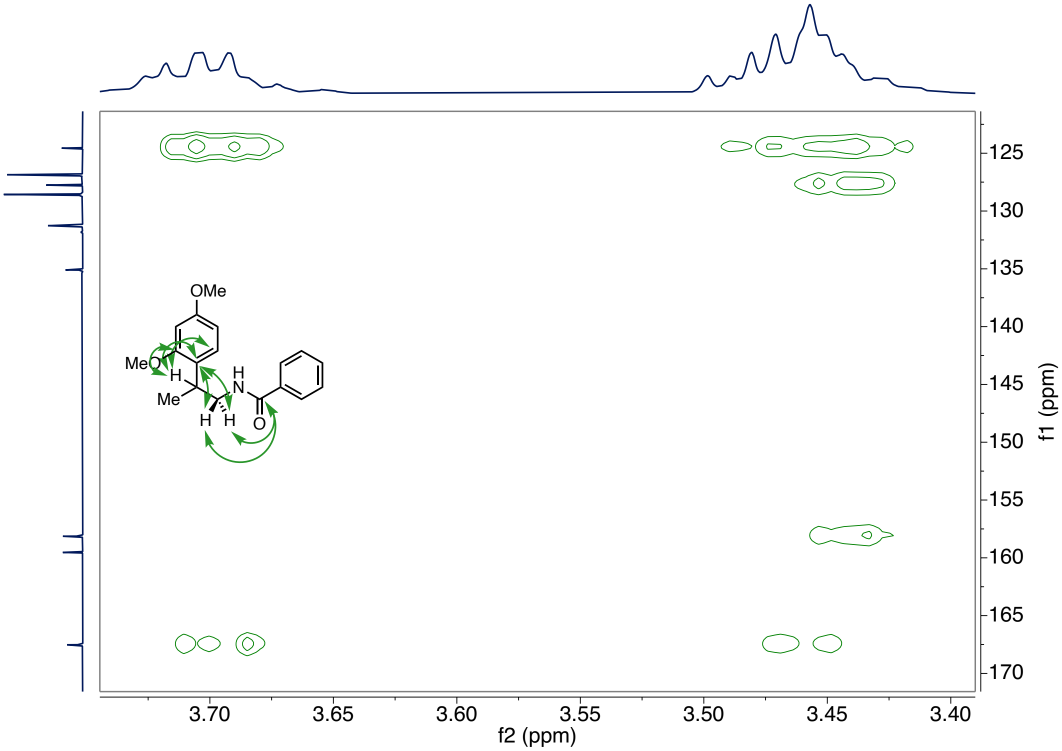
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-(2,4-dimethoxyphenyl)propyl)benzamide (B-1):



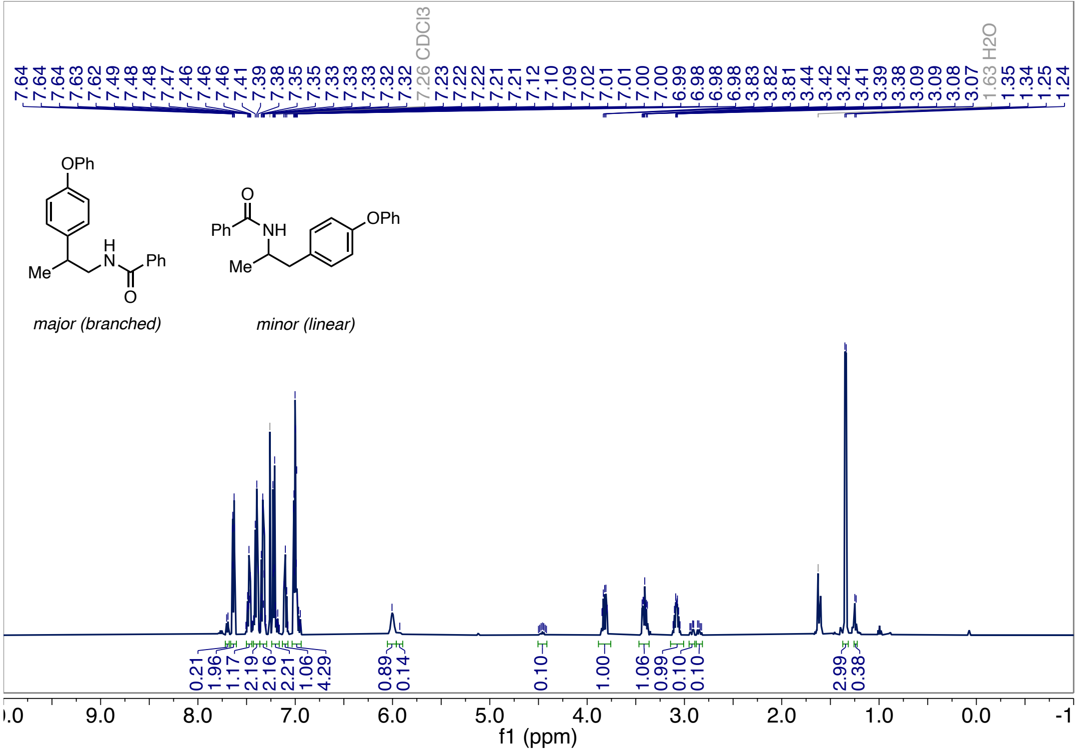
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-(2,4-dimethoxyphenyl)propyl)benzamide (B-1):



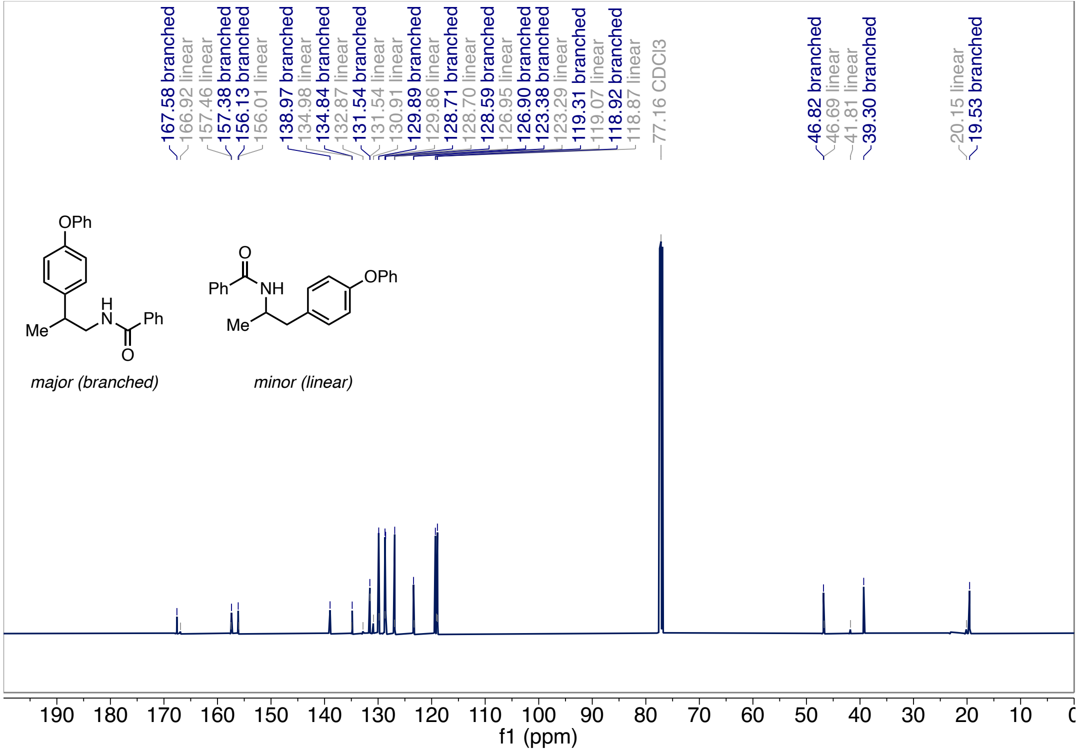
HMBC (500 MHz, CDCl$_3$) of *N*-(2-(2,4-dimethoxyphenyl)propyl)benzamide (B-1):



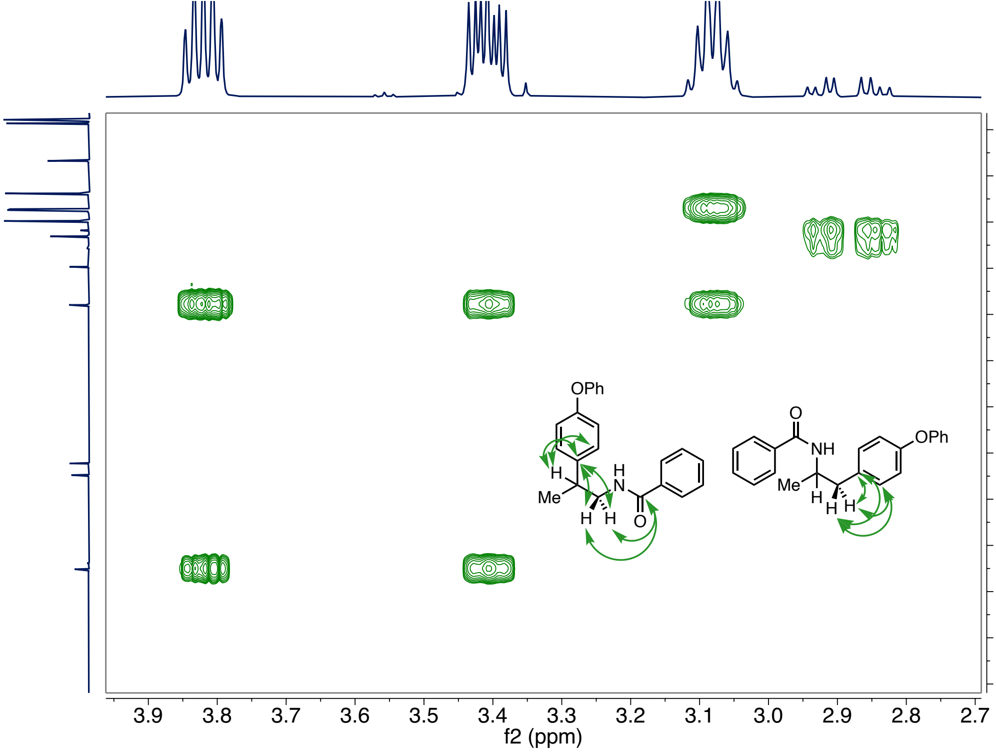
^{1}H NMR (500 MHz, CDCl3) of *N*-(2-(4-phenoxyphenyl)propyl)benzamide (C-1), mixture of isomers (10:1):



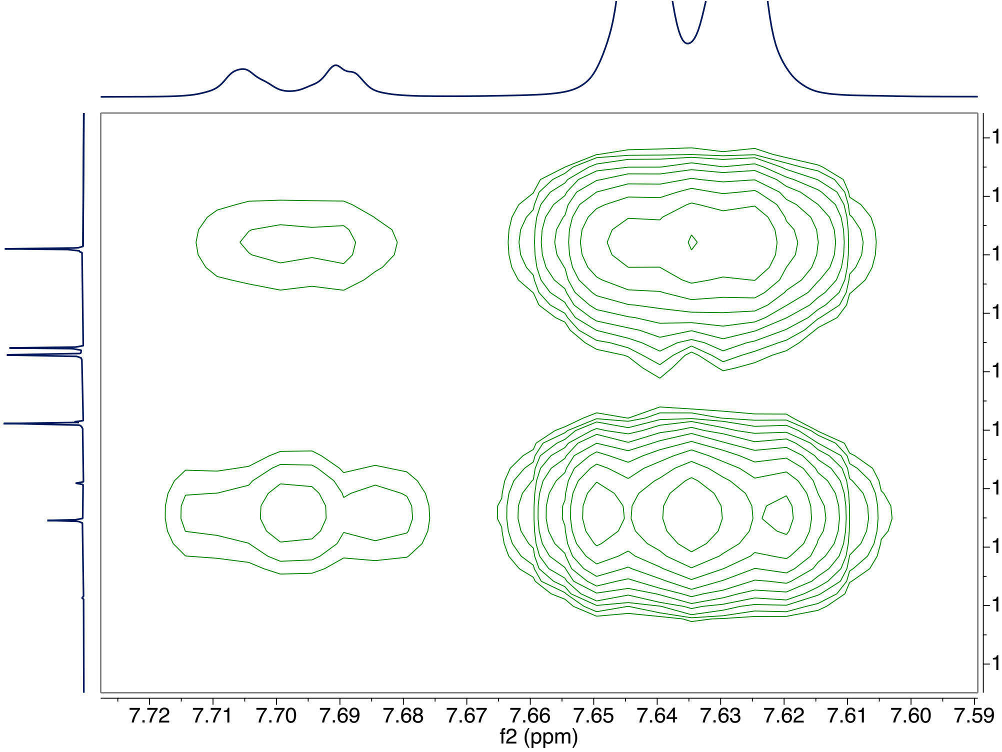
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-(4-phenoxyphenyl)propyl)benzamide (C-1), mixture of isomers (10:1):



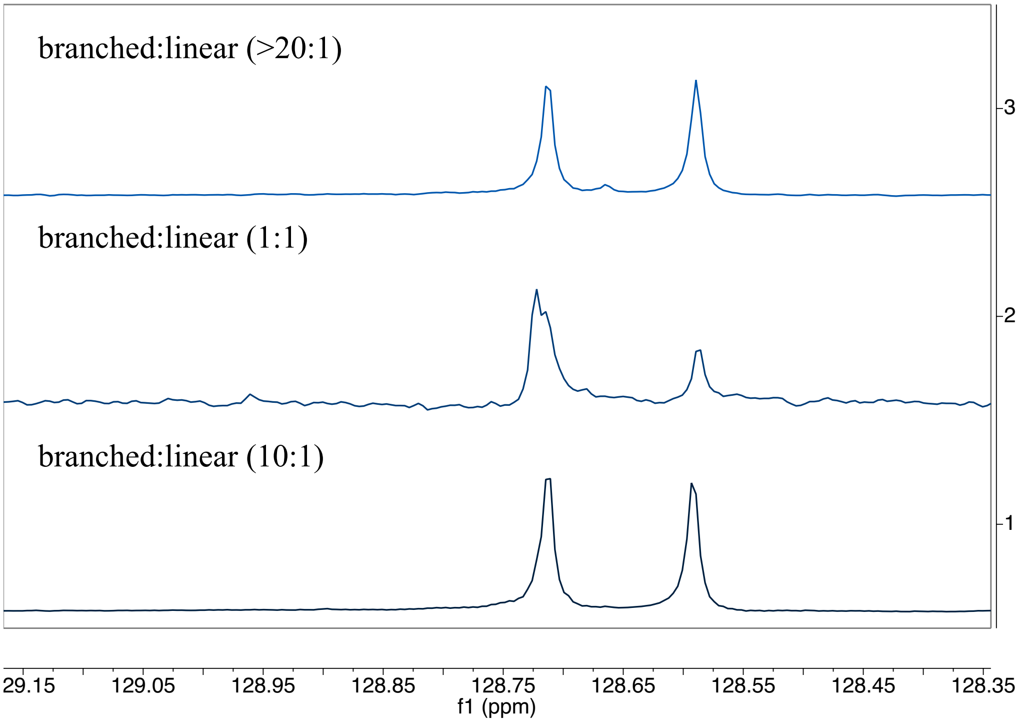
HMBC (500 MHz, CDCl3) of *N*-(2-(4-phenoxyphenyl)propyl)benzamide (C-1), mixture of isomers (10:1):



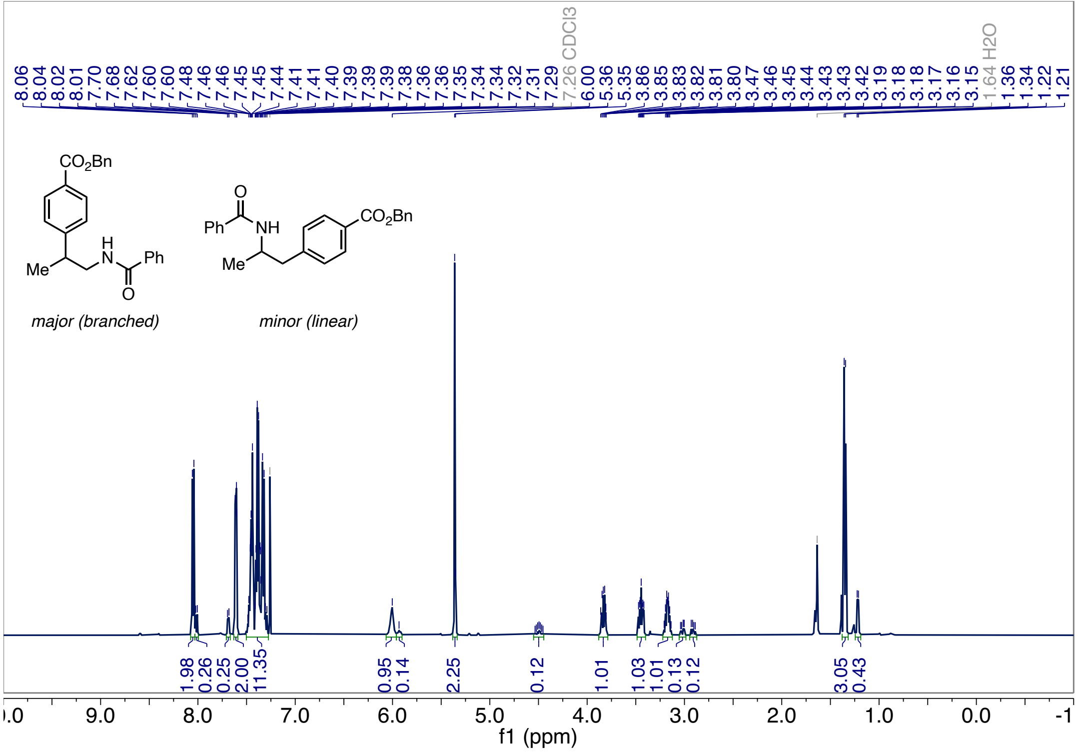
HMBC (500 MHz, CDCl$_3$) of *N*-(2-(4-phenoxyphenyl)propyl)benzamide (C-1) to demonstrate two carbons contributing to the signals at δ 131.5 and 126.9 in $^{13}C\{^{1}H\}$ NMR, mixture of isomers (10:1):



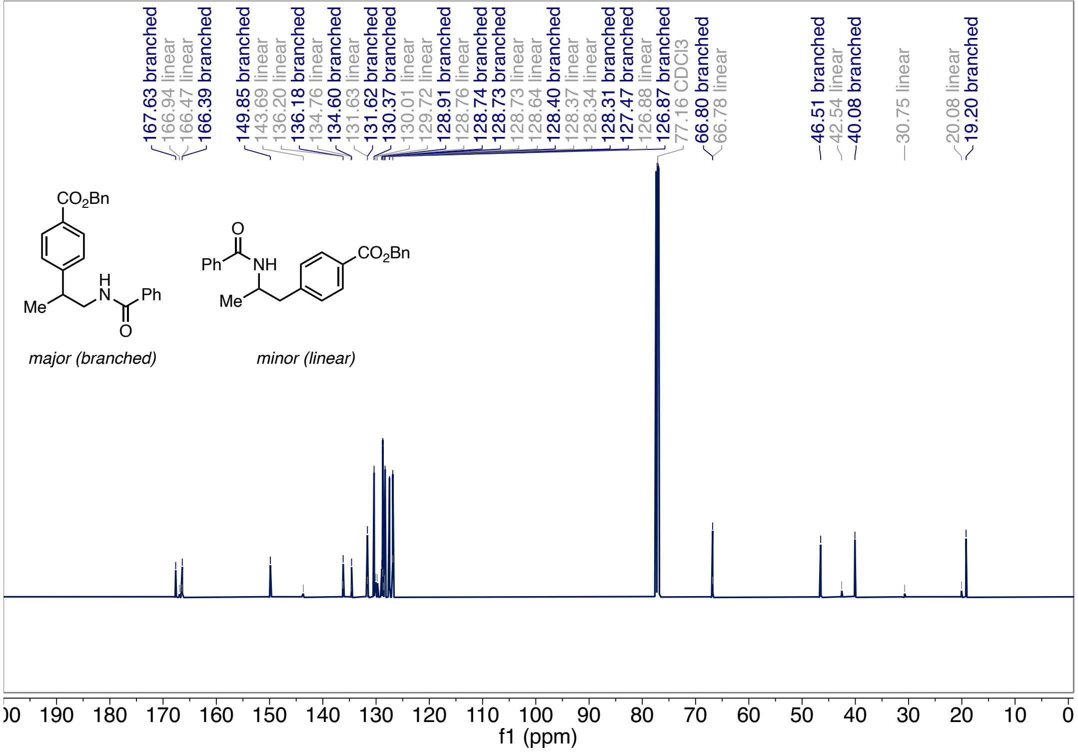
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) of *N*-(2-(4-phenoxyphenyl)propyl)benzamide (C-1) identifying overlapping peaks at δ 128.7:



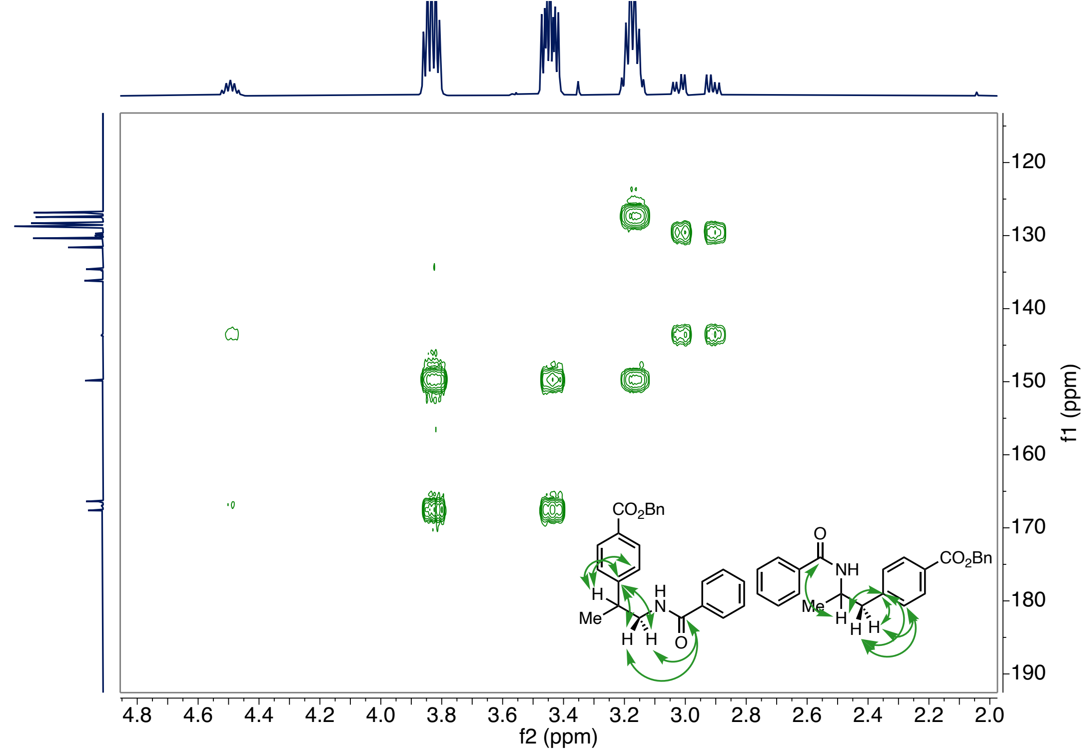
^{1}H NMR (500 MHz, $CDCl_3$) of Benzyl 4-(1-benzamidopropan-2-yl)benzoate (D-1), mixture of isomers (8:1):



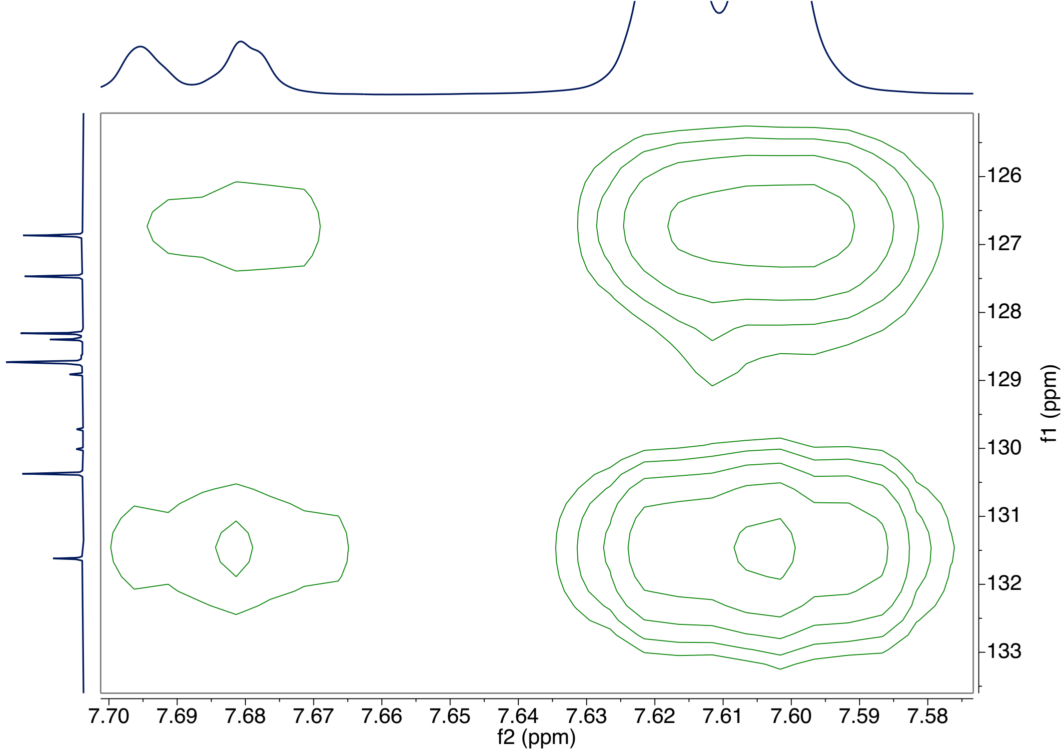
$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) of Benzyl 4-(1-benzamidopropan-2-yl)benzoate (D-1), mixture of isomers (8:1):



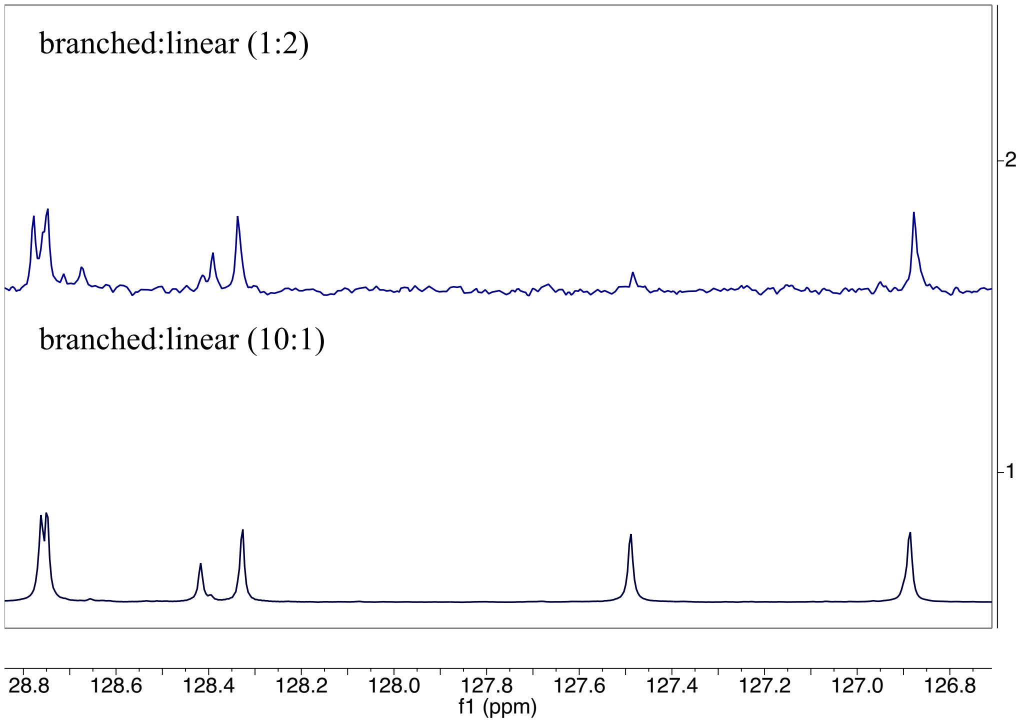
HMBC (500 MHz, CDCl₃) of Benzyl 4-(1-benzamidopropan-2-yl)benzoate (D-1), mixture of isomers (8:1):



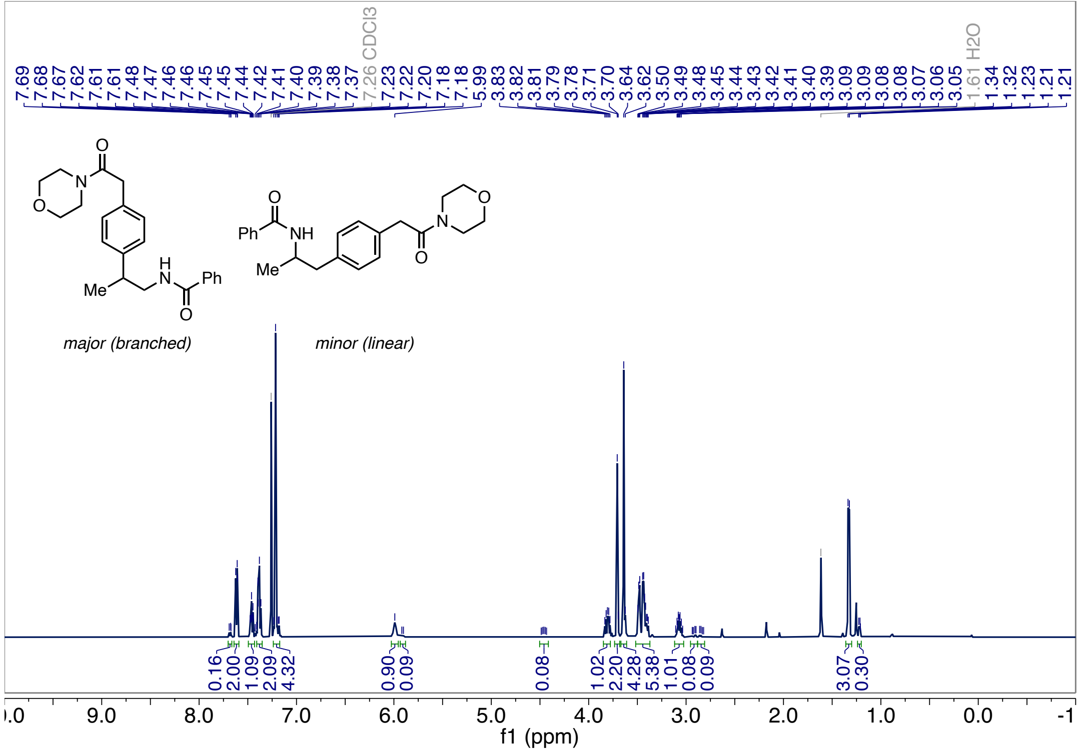
HMBC (500 MHz, CDCl₃) of Benzyl 4-(1-benzamidopropan-2-yl)benzoate (D-1) to demonstrate two carbons contributing to the signals at δ 131.62 and 126.87 in $^{13}C\{^{1}H\}$ NMR, mixture of isomers (8:1):



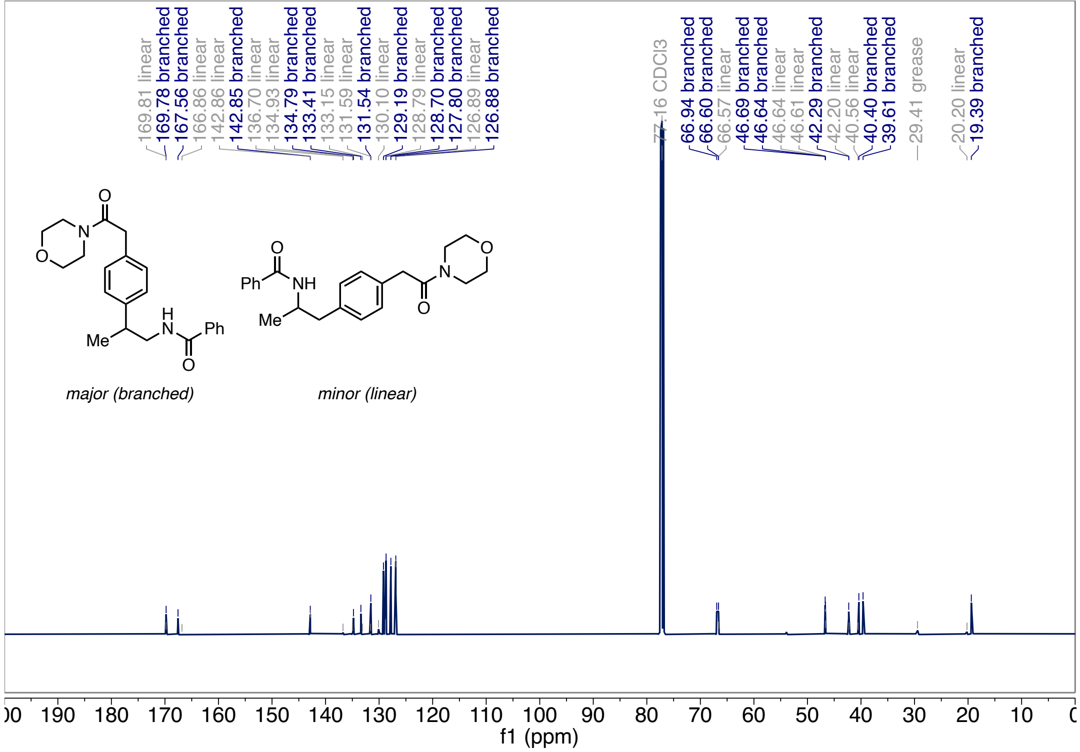
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) of Benzyl 4-(1-benzamidopropan-2-yl)benzoate (D-1) identifying overlapping peaks at δ 128.76, 128.73, and 128.34:



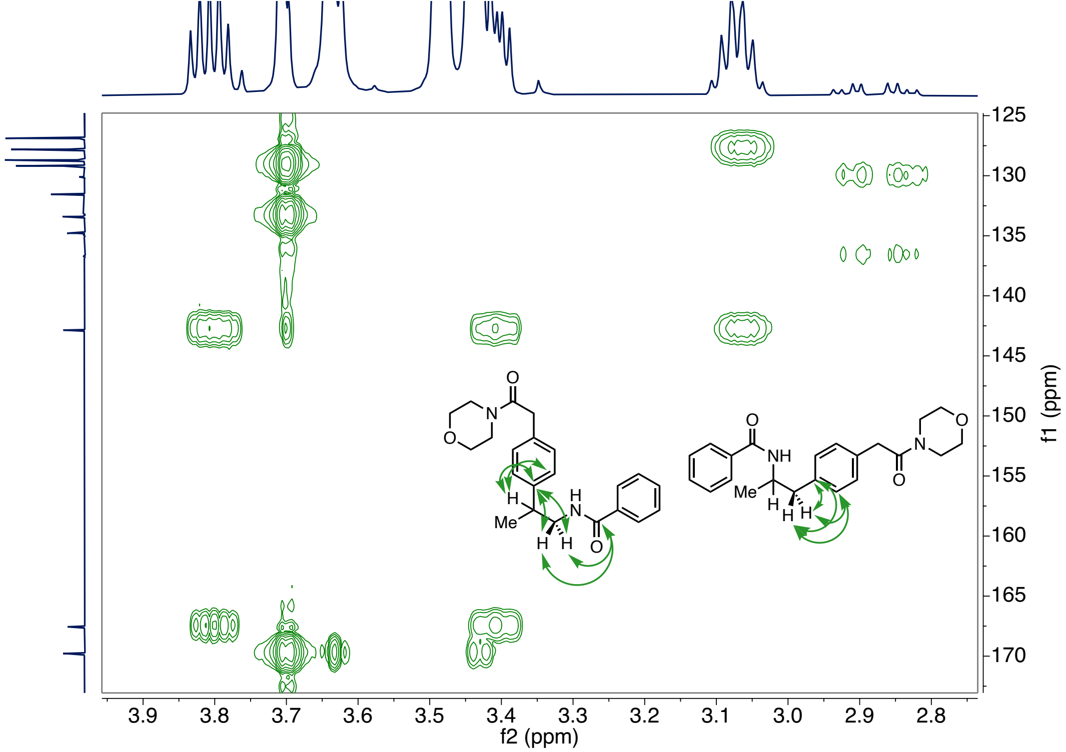
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-(4-(2-morpholino-2-oxoethyl)phenyl)propyl)benzamide (E-1), mixture of isomers (13:1):



^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-(4-(2-morpholino-2-oxoethyl)phenyl)propyl) benzamide (E-1), mixture of isomers (13:1):

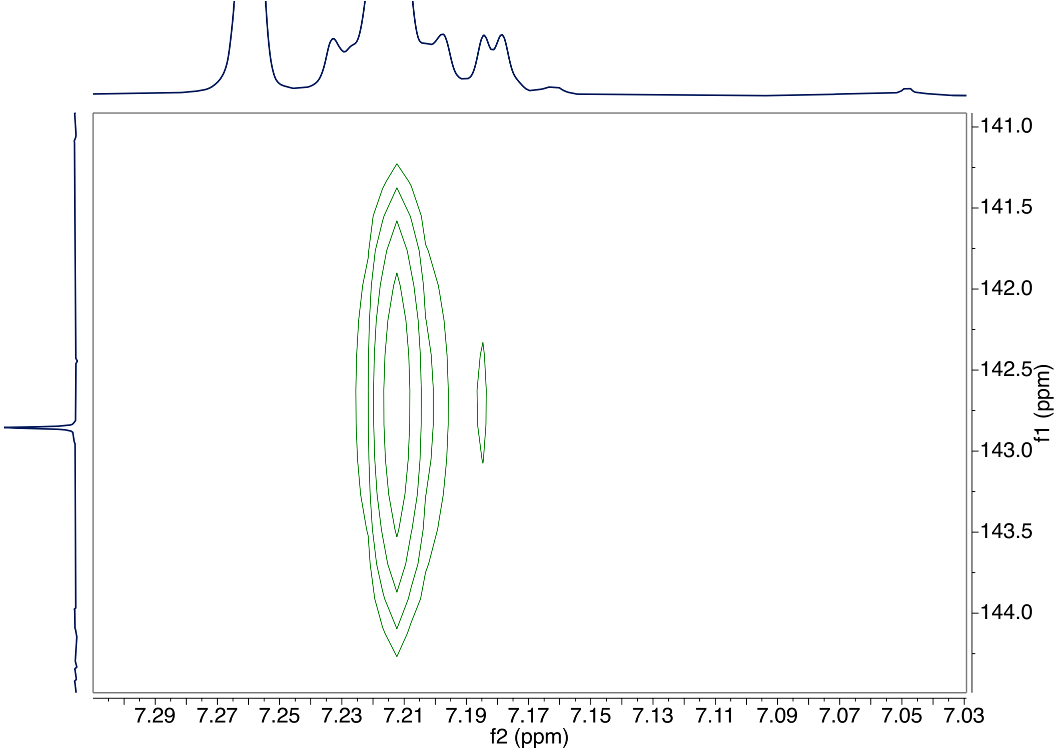


HMBC (500 MHz, CDCl$_3$) of *N*-(2-(4-(2-morpholino-2-oxoethyl)phenyl)propyl)benzamide (E-1), mixture of isomers (13:1):

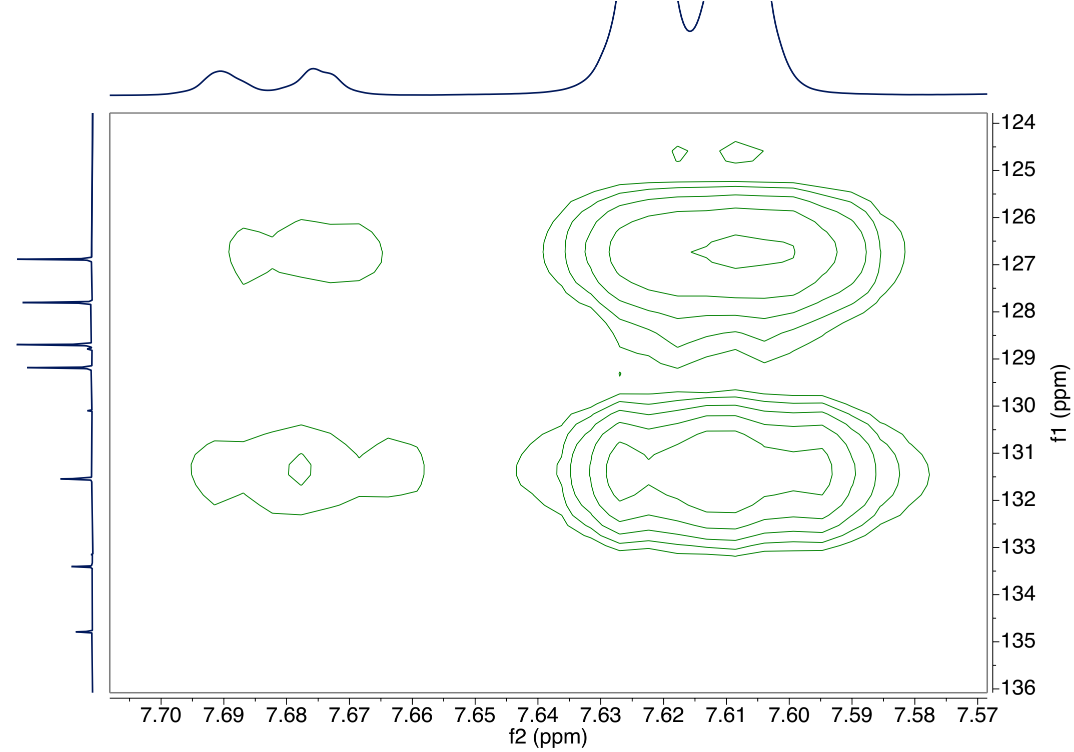


Only correlations necessary to establish branched/linear connectivity are identified.

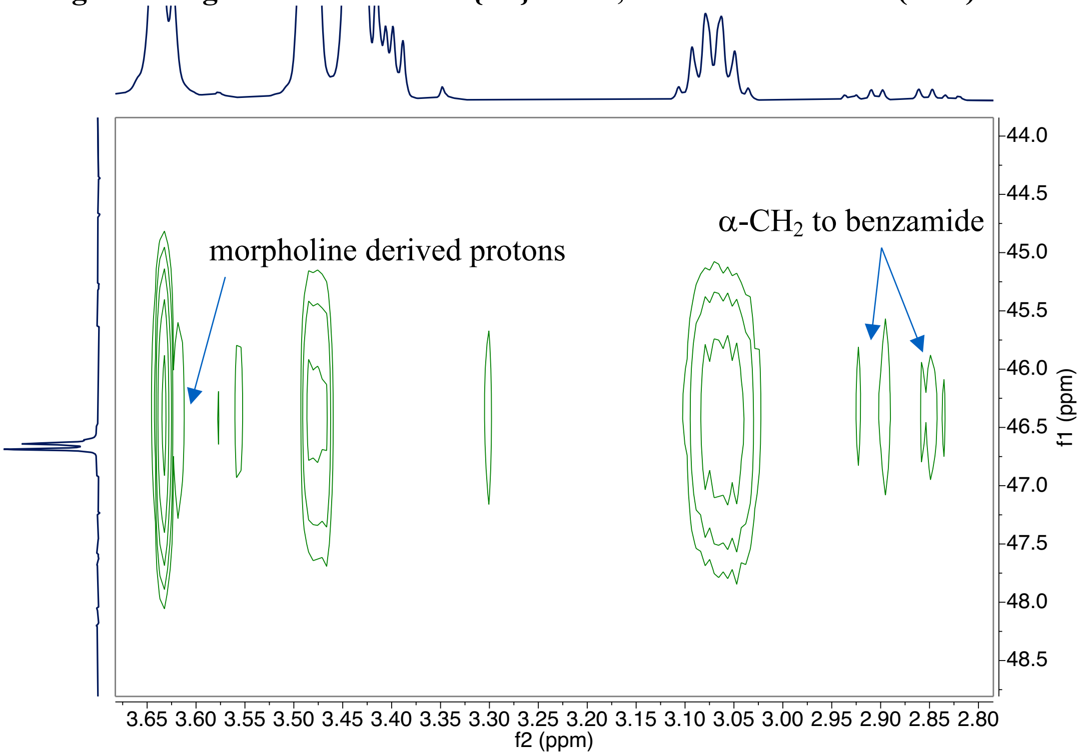
HMBC (500 MHz, CDCl$_3$) of E-1 to demonstrate two carbons contributing to the signal at δ 142.9 in ^{13}C{^{1}H} NMR, mixture of isomers (13:1):



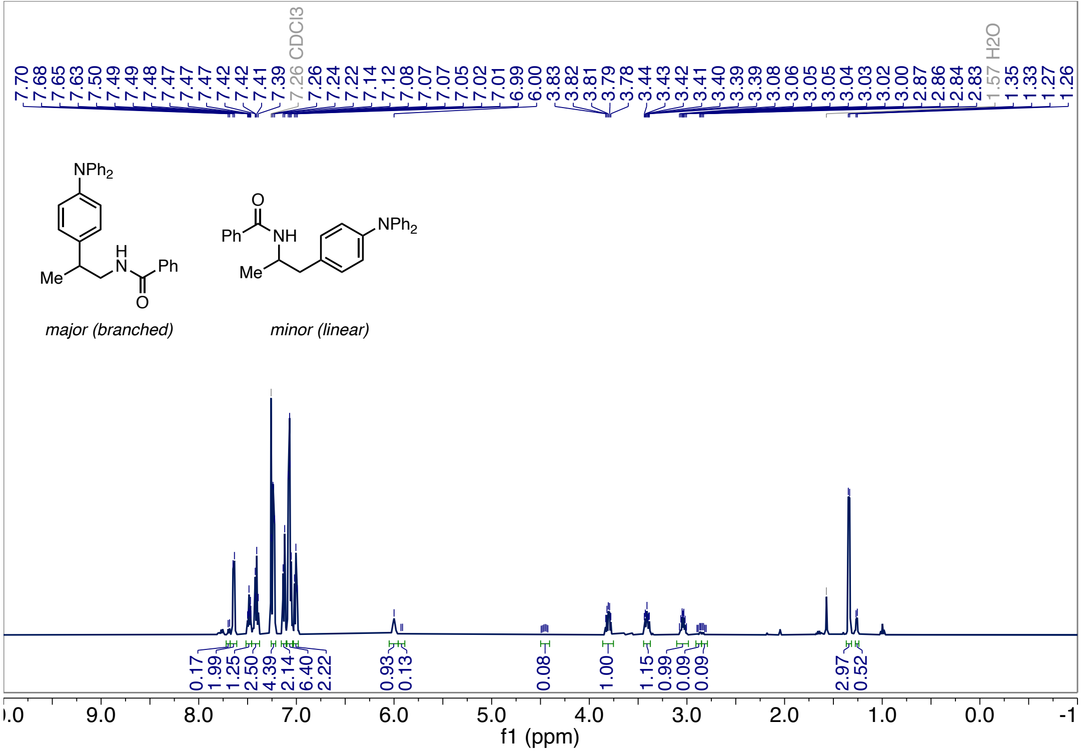
HMBC (500 MHz, $CDCl_3$) of E-1 to demonstrate two carbons contributing to the signals at δ 131.5 and 126.9 in $^{13}C\{^1H\}$ NMR, mixture of isomers (13:1):



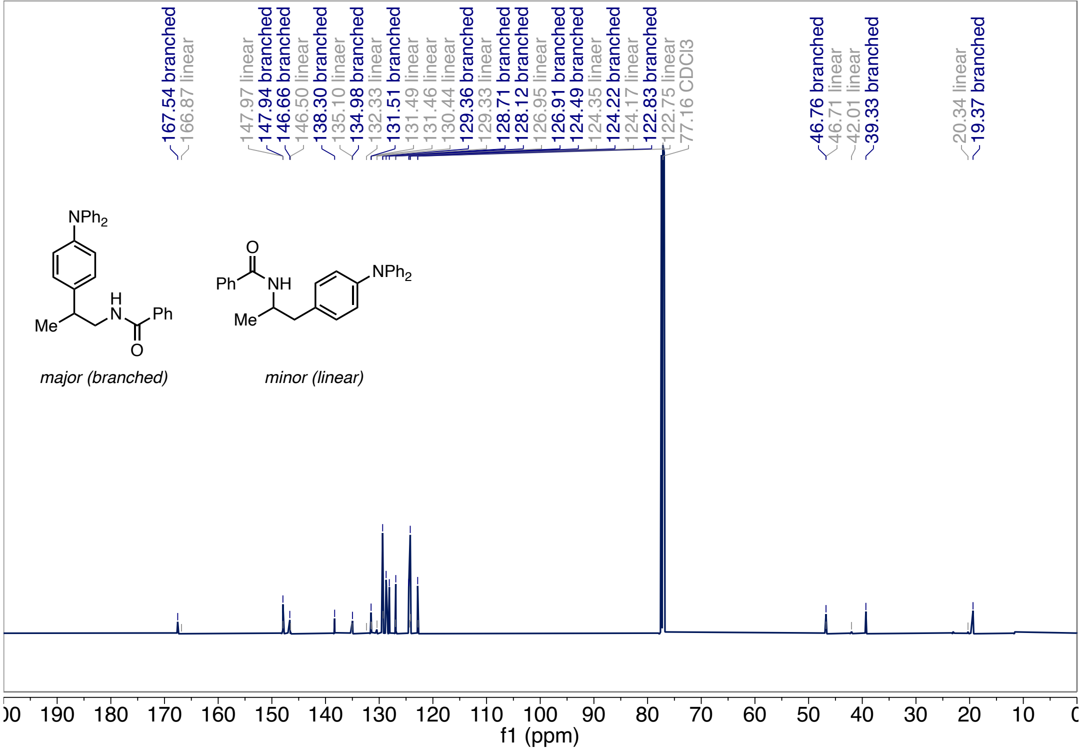
HMBC (500 MHz, $CDCl_3$) of E-1 to demonstrate two carbons from the linear isomer contributing to the signal at δ 46.6 in $^{13}C\{^1H\}$ NMR, mixture of isomers (13:1):



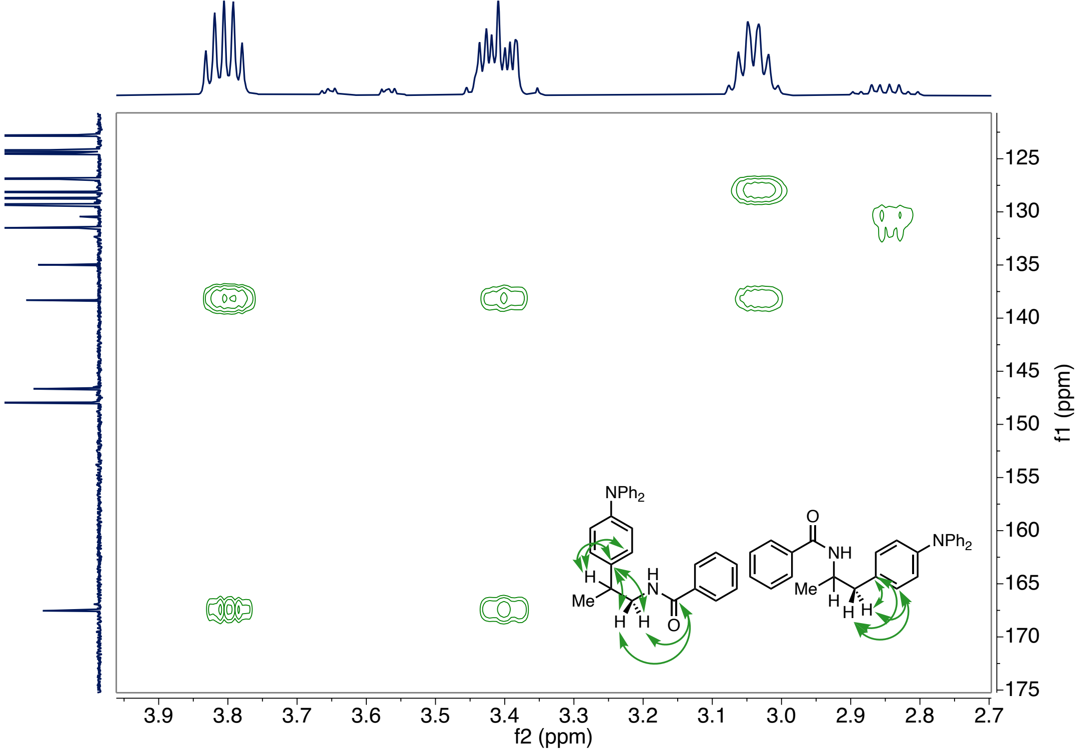
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-(4-(diphenylamino)phenyl)propyl)benzamide (F-1), mixture of isomers (11:1):



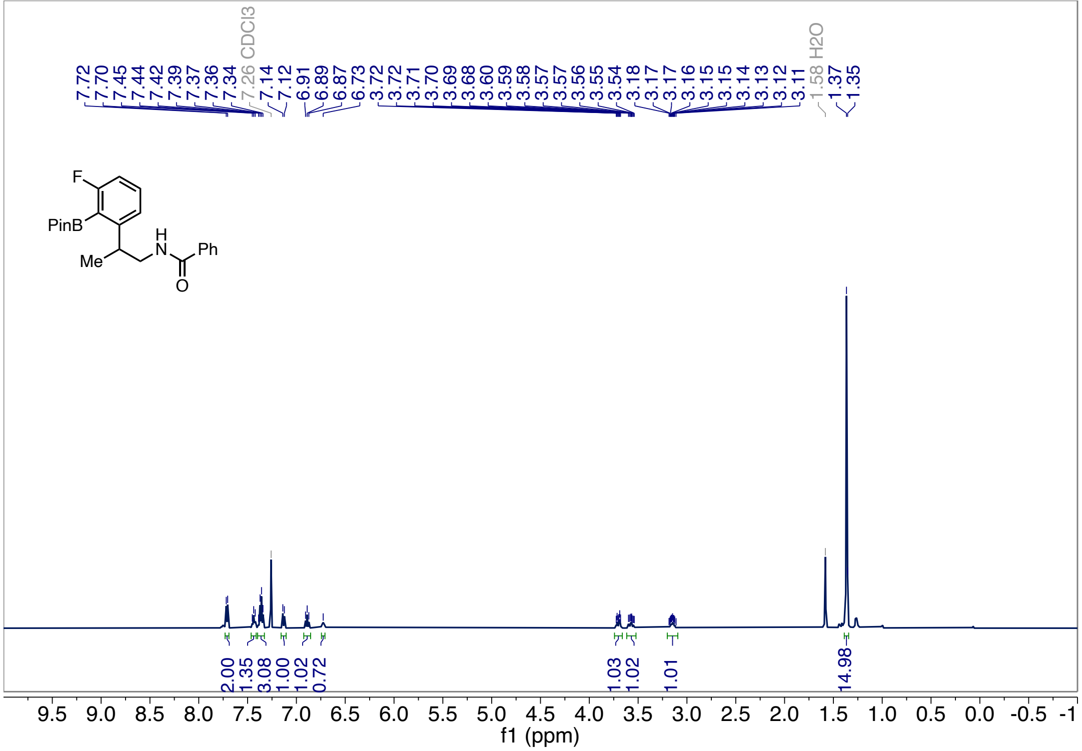
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-(4-(diphenylamino)phenyl)propyl)benzamide (F-1), mixture of isomers (11:1):



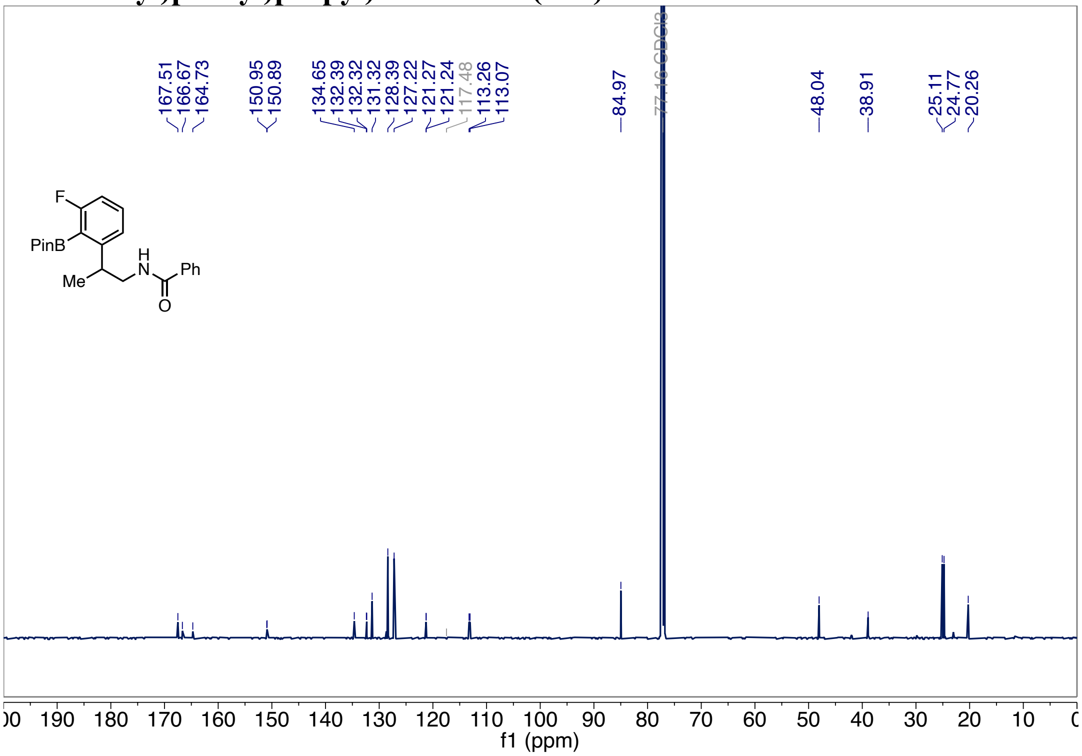
HMBC (500 MHz, CDCl₃) of *N*-(2-(4-(diphenylamino)phenyl)propyl)benzamide (F-1), mixture of isomers (11:1):



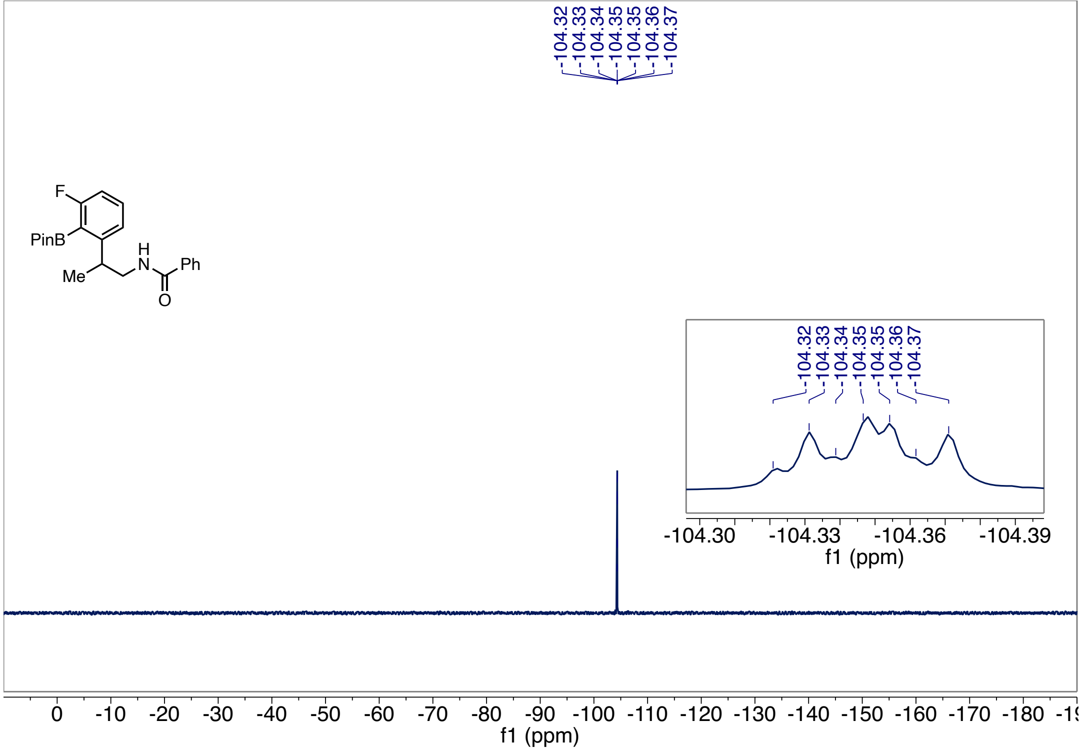
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-(3-fluoro-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propyl)benzamide (G-1):



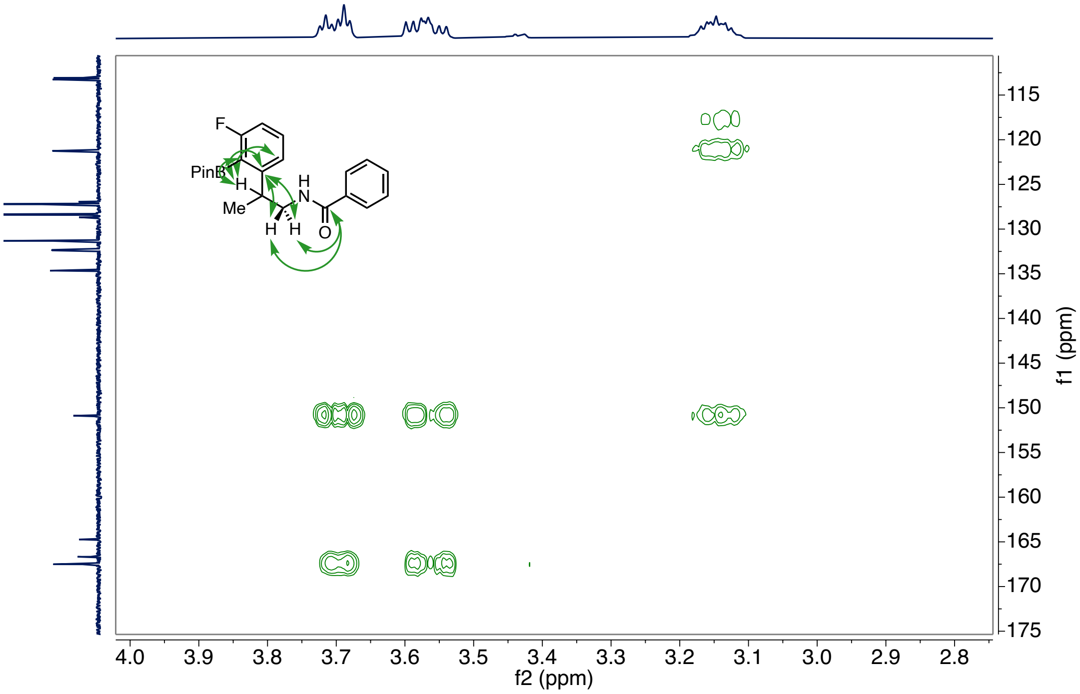
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-(3-fluoro-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propyl)benzamide (G-1):



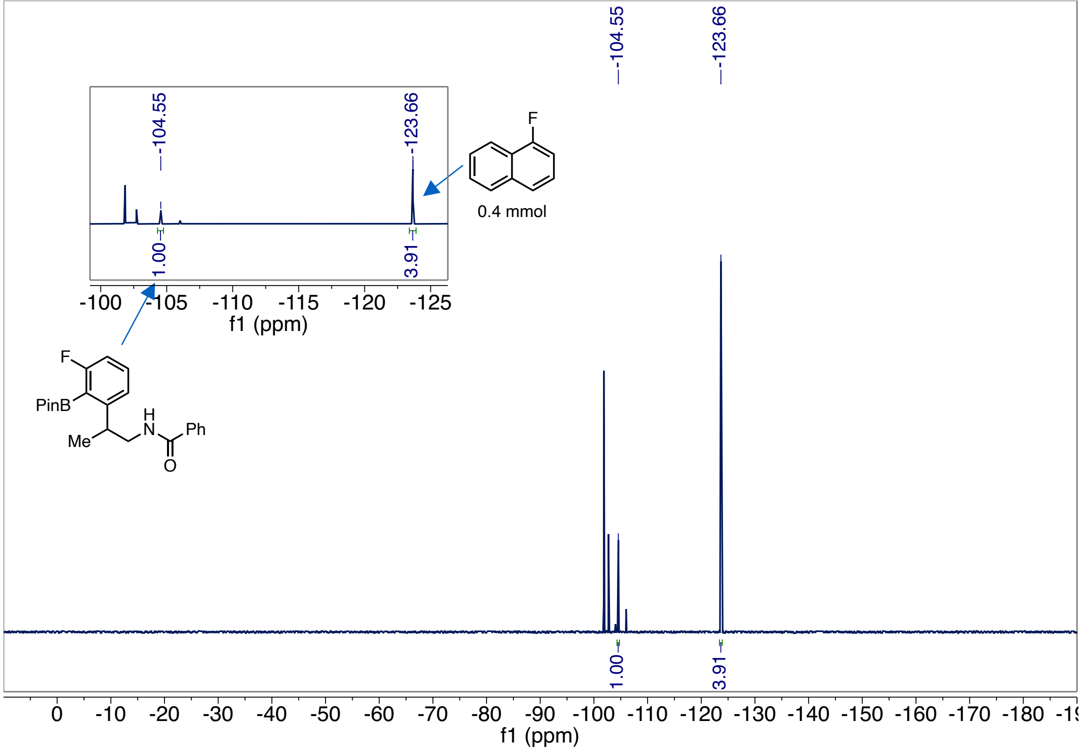
^{19}F NMR (376 MHz, CDCl$_3$) of *N*-(2-(3-fluoro-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propyl)benzamide (G-1):



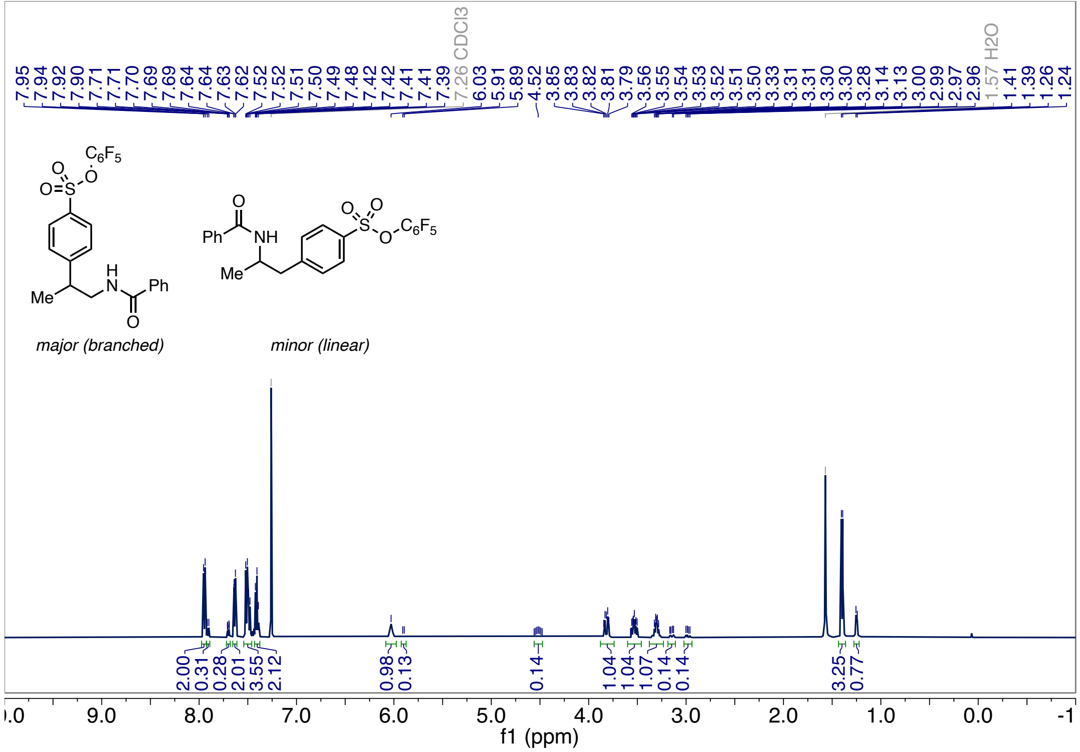
HMBC (500 MHz, CDCl$_3$) of *N*-(2-(3-fluoro-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propyl)benzamide (G-1):



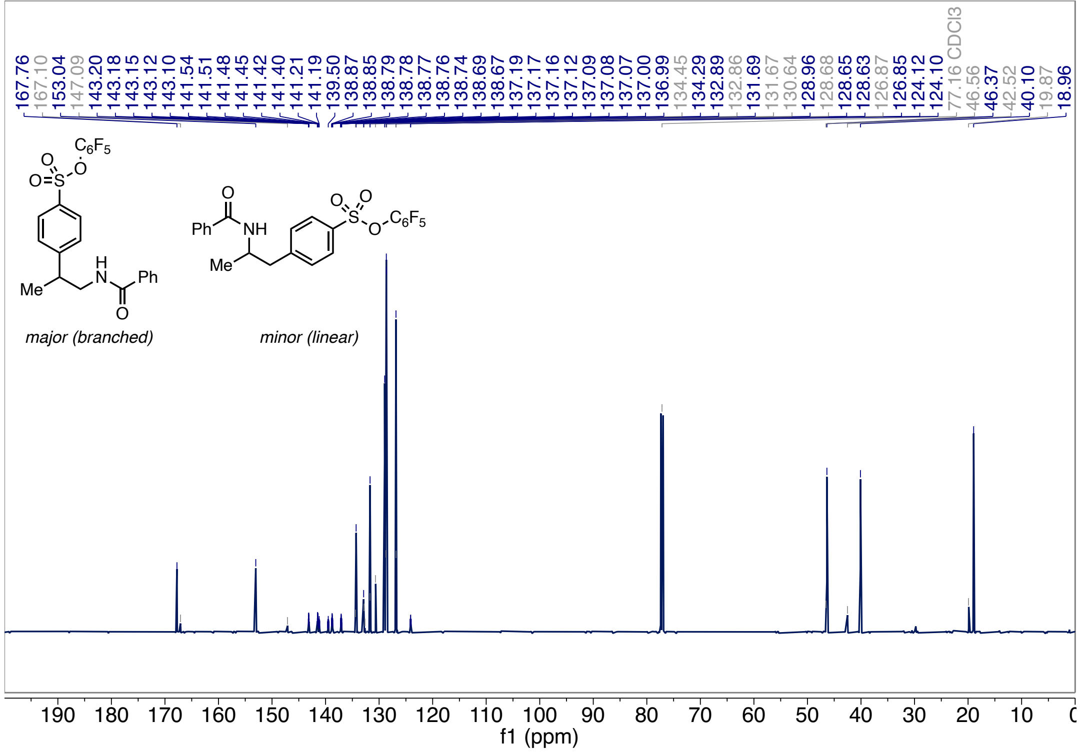
$^{19}F\{^1H\}$ NMR (376 MHz, $CDCl_3$) yield of *N*-(2-(3-fluoro-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propyl)benzamide (G-1) versus 1-fluoronaphthalene:



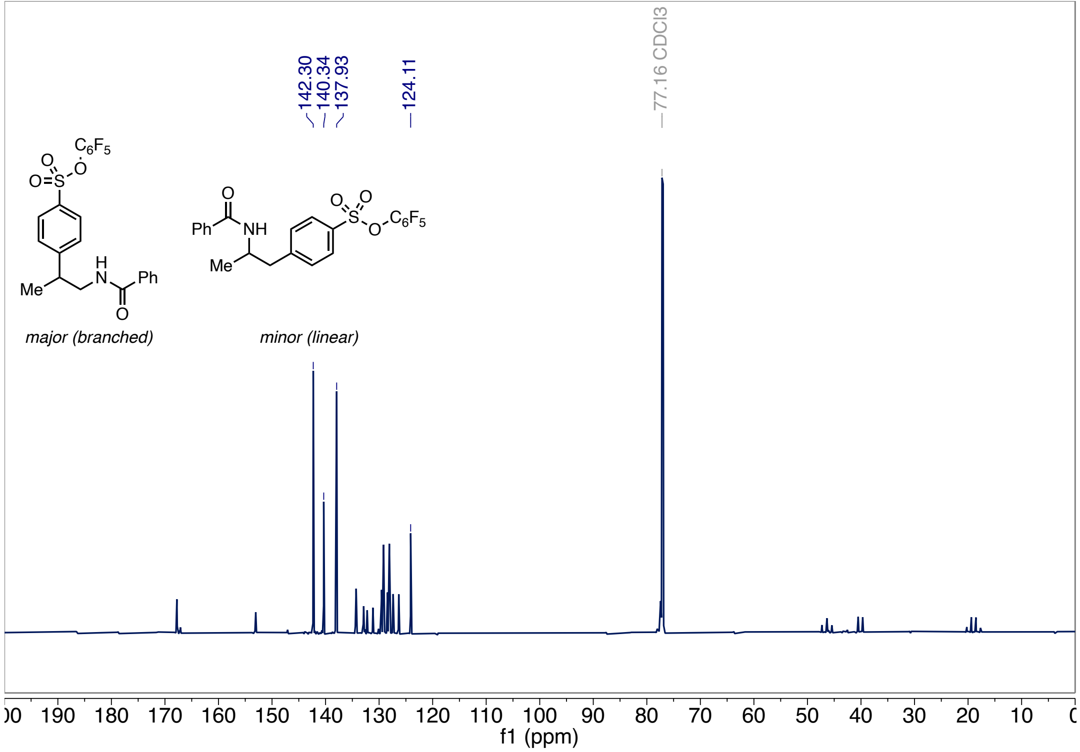
^{1}H NMR (500 MHz, CDCl$_3$) of perfluorophenyl 4-(1-benzamidopropan-2-yl) benzenesulfonate (H-1), mixture of isomers (7:1):



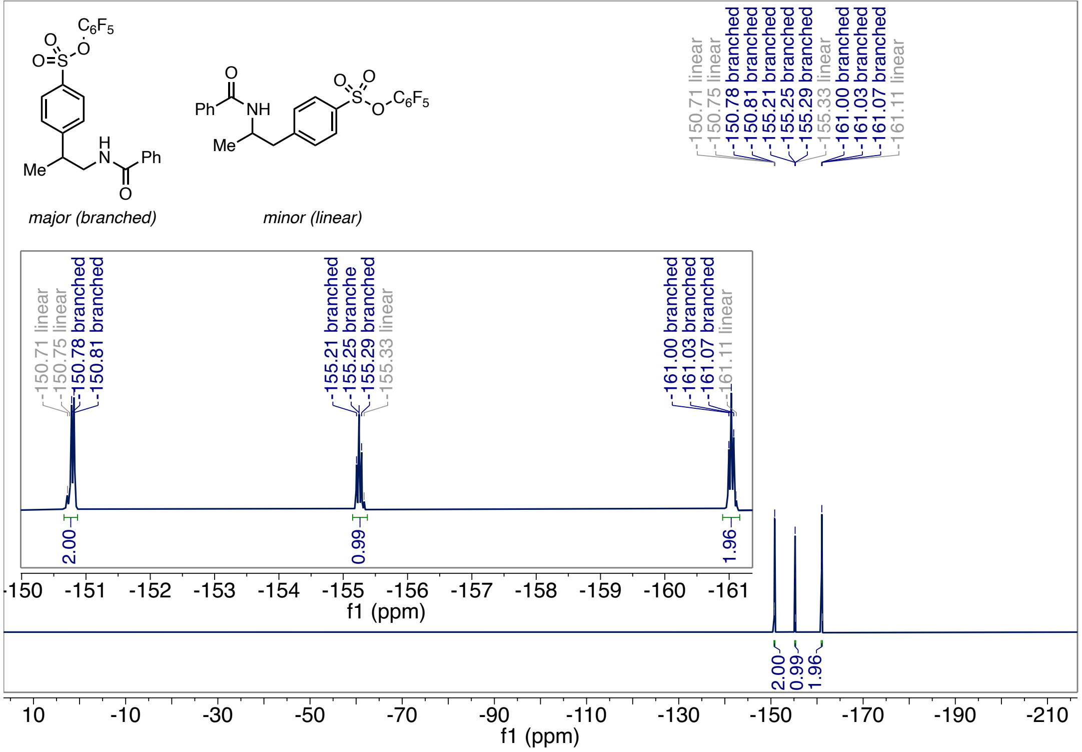
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of perfluorophenyl 4-(1-benzamidopropan-2-yl) benzenesulfonate (H-1), mixture of isomers (7:1):



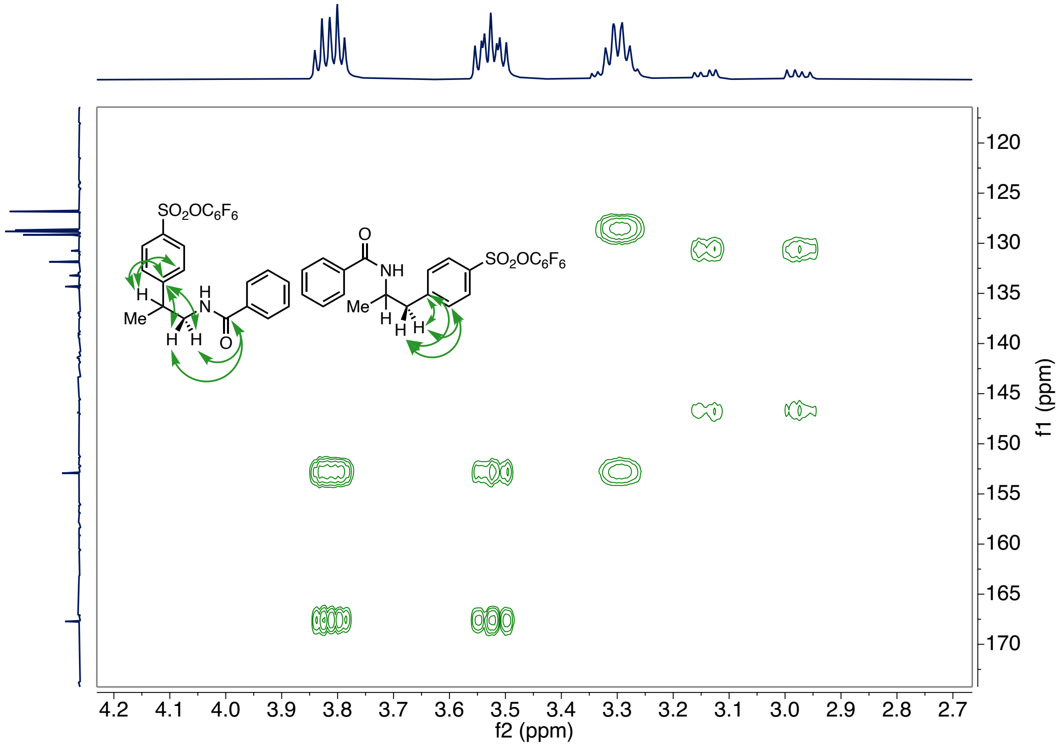
^{13}C{^{19}F} NMR (151 MHz, CDCl$_3$) of perfluorophenyl 4-(1-benzamidopropan-2-yl) benzenesulfonate (H-1), mixture of isomers (7:1):



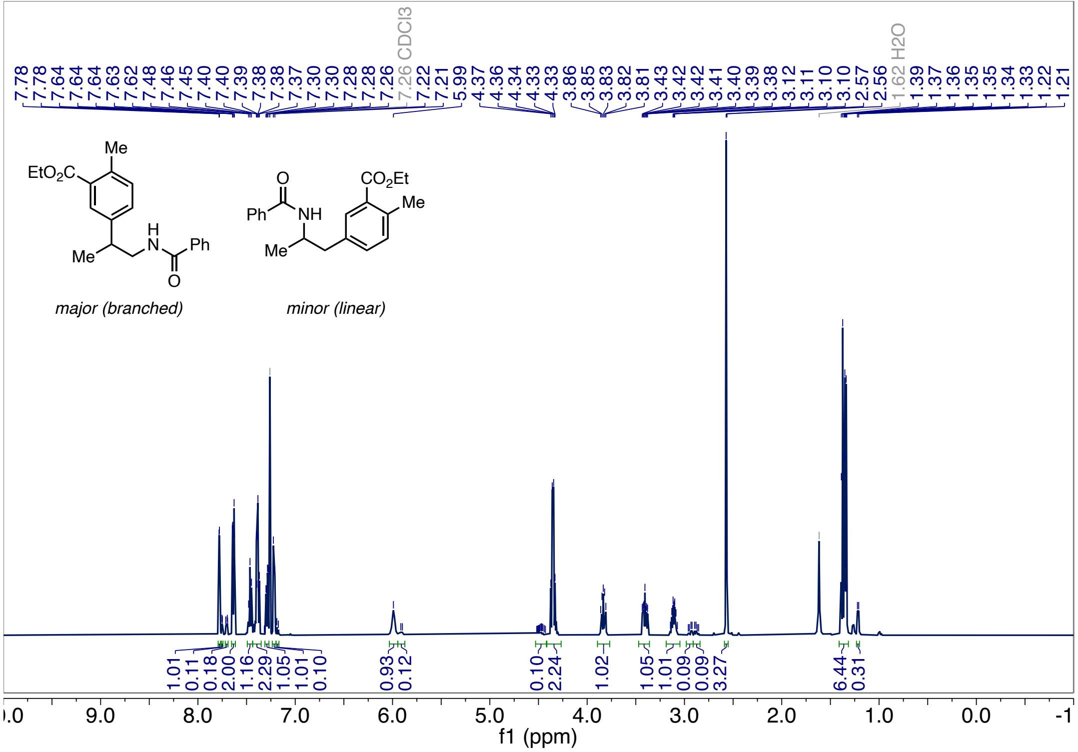
^{19}F NMR (565 MHz, CDCl$_3$) of perfluorophenyl 4-(1-benzamidopropan-2-yl) benzenesulfonate (H-1), mixture of isomers (7:1):



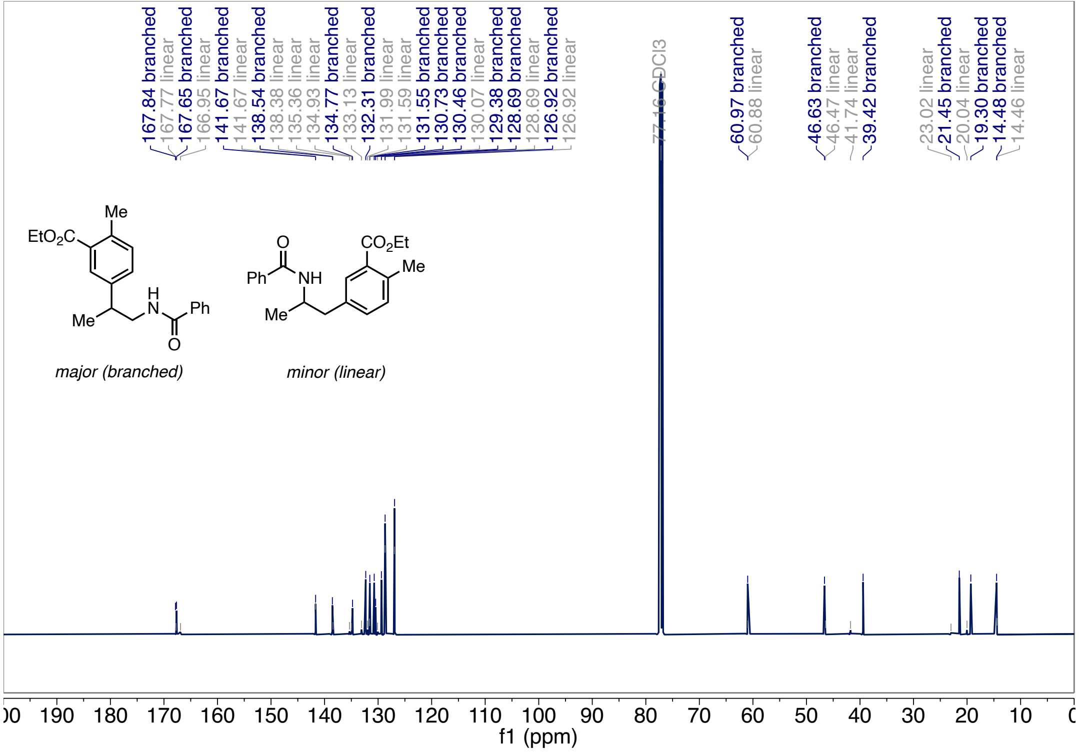
HMBC (500 MHz, CDCl₃) of perfluorophenyl 4-(1-benzamidopropan-2-yl)benzenesulfonate (H-1), mixture of isomers (7:1):



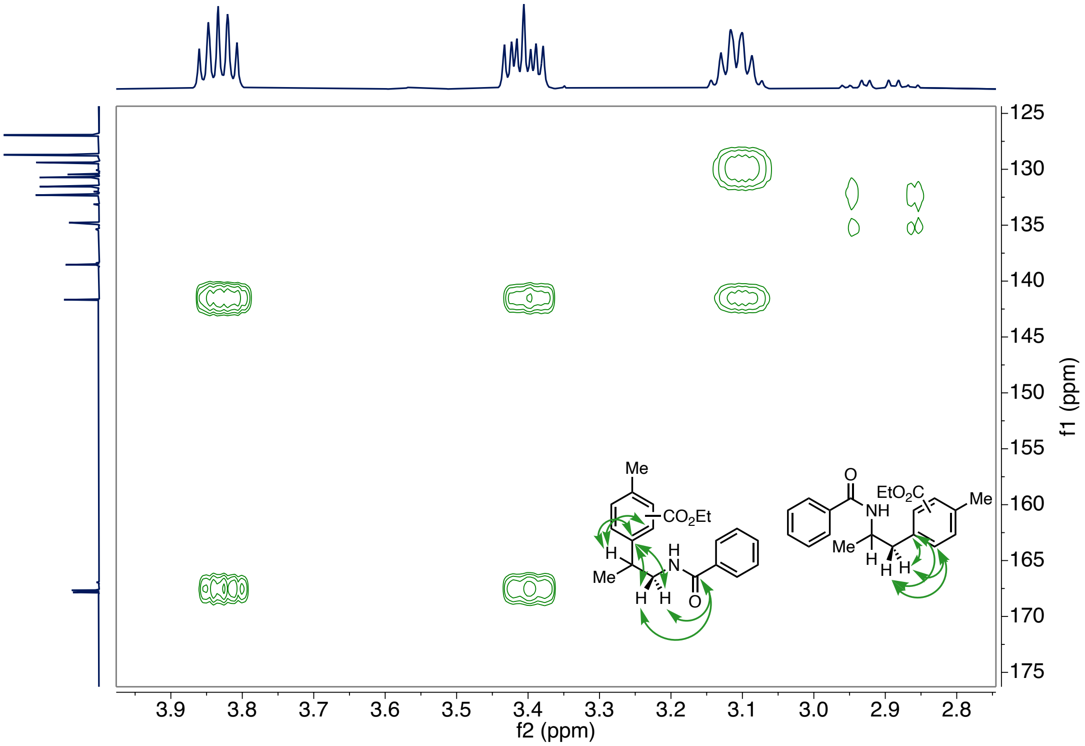
^{1}H NMR (500 MHz, CDCl$_3$) of ethyl 5-(1-benzamidopropan-2-yl)-2-methylbenzoate (I-1), mixture of isomers (10:1):



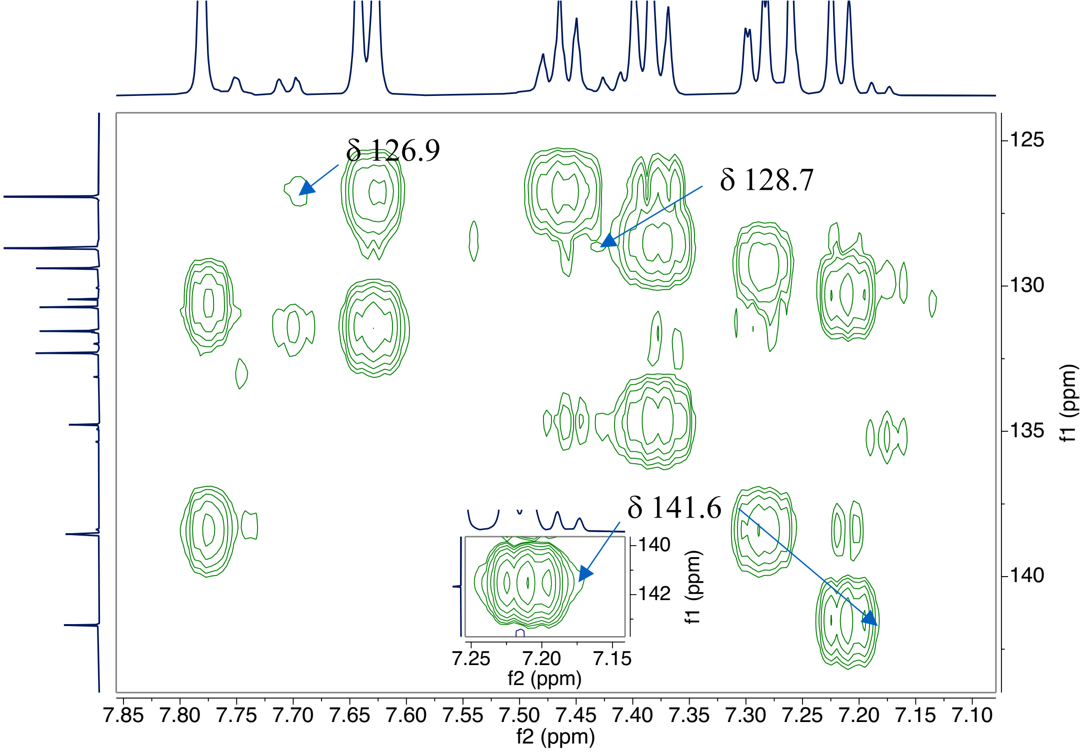
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of ethyl 5-(1-benzamidopropan-2-yl)-2-methylbenzoate (I-1), mixture of isomers (10:1):



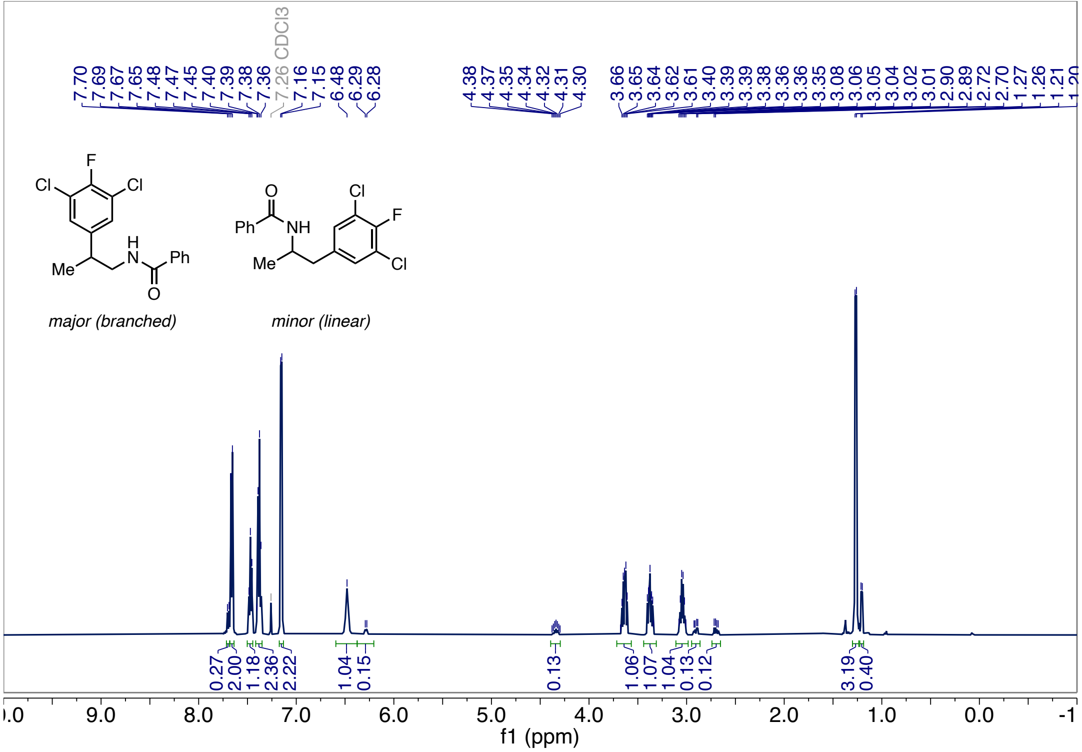
^{1}H NMR (500 MHz, CDCl$_3$) of ethyl 5-(1-benzamidopropan-2-yl)-2-methylbenzoate (I-1), mixture of isomers (10:1):



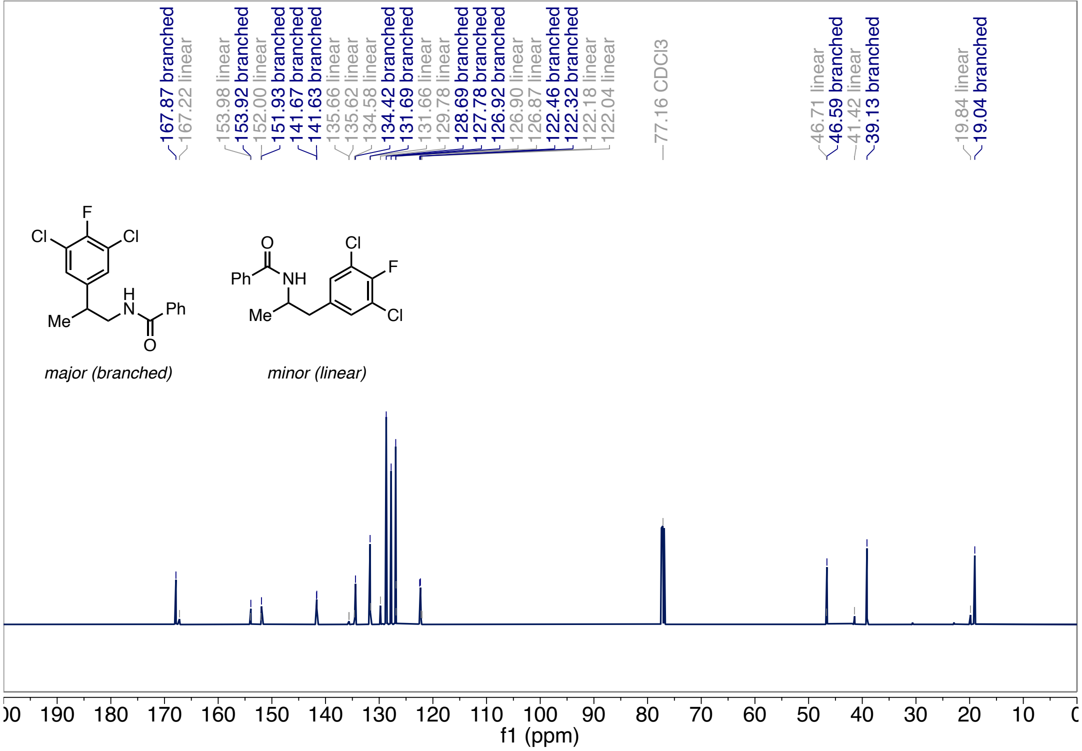
HMBC (500 MHz, CDCl$_3$) of I-1 to demonstrate overlap of carbons from the linear isomer at δ 141.6, 128.7, and 126.9 in ^{13}C{^{1}H} NMR, mixture of isomers (10:1):



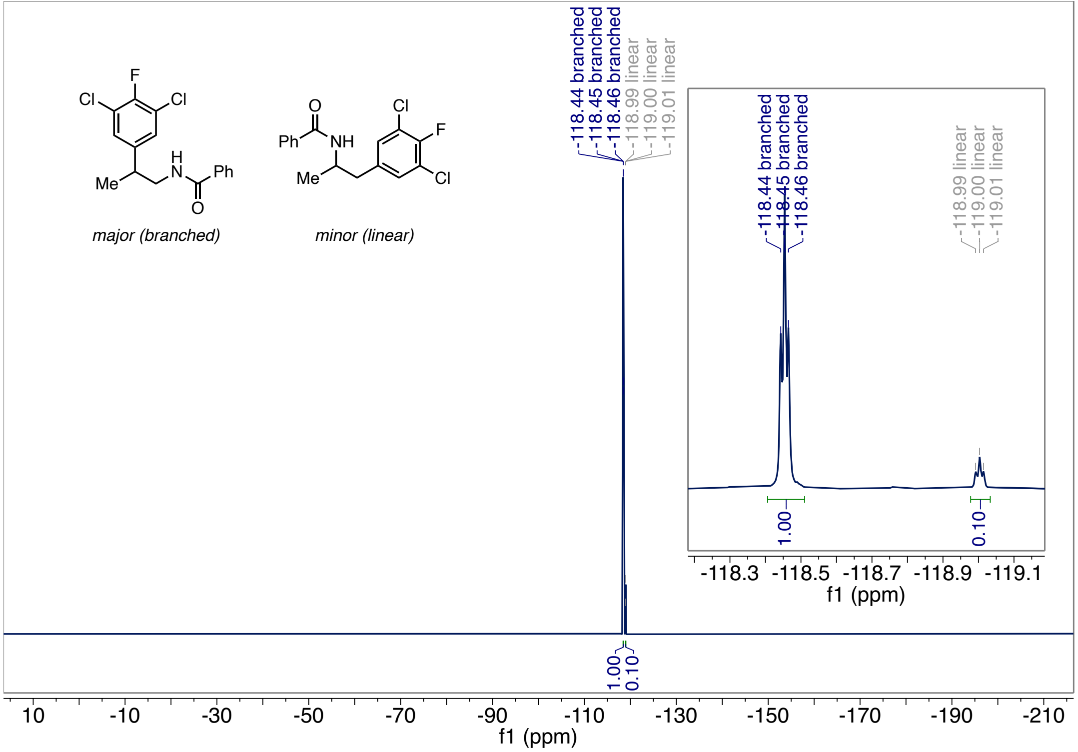
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-(3,5-dichloro-4-fluorophenyl)propyl)benzamide (J-1), mixture of isomers (8:1):



^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-(3,5-dichloro-4-fluorophenyl)propyl)benzamide (J-1) , mixture of isomers (8:1):

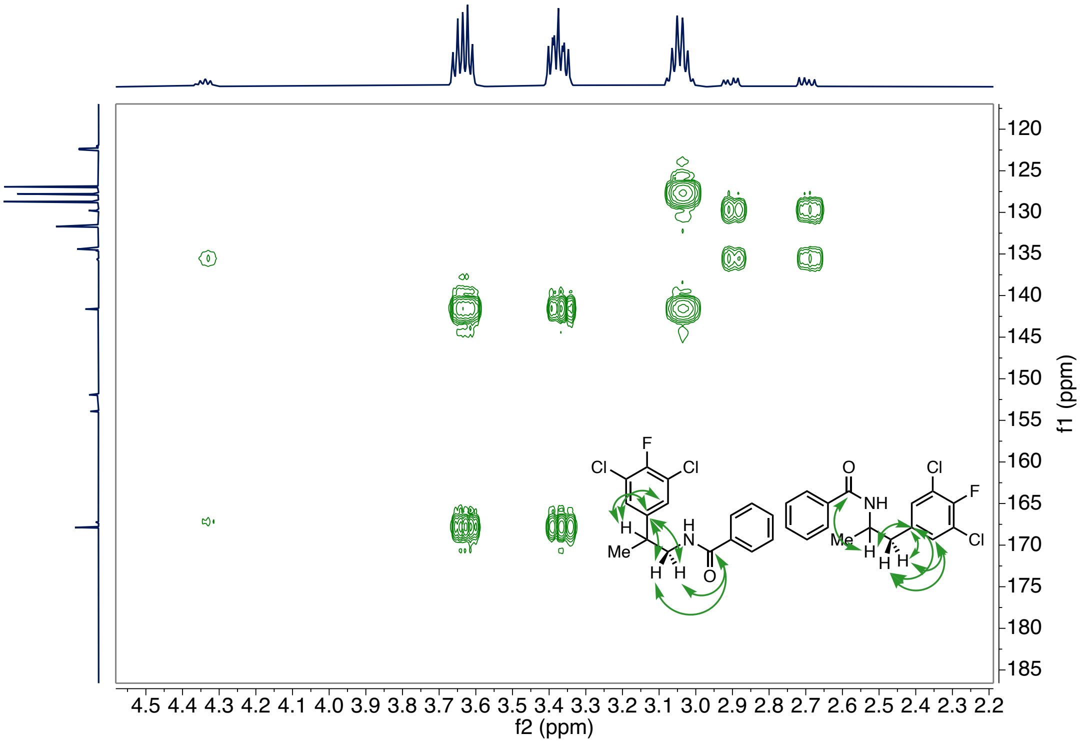


^{19}F NMR (565 MHz, CDCl$_3$) of *N*-(2-(3,5-dichloro-4-fluorophenyl)propyl)benzamide (J-1), mixture of isomers (8:1)[a]:

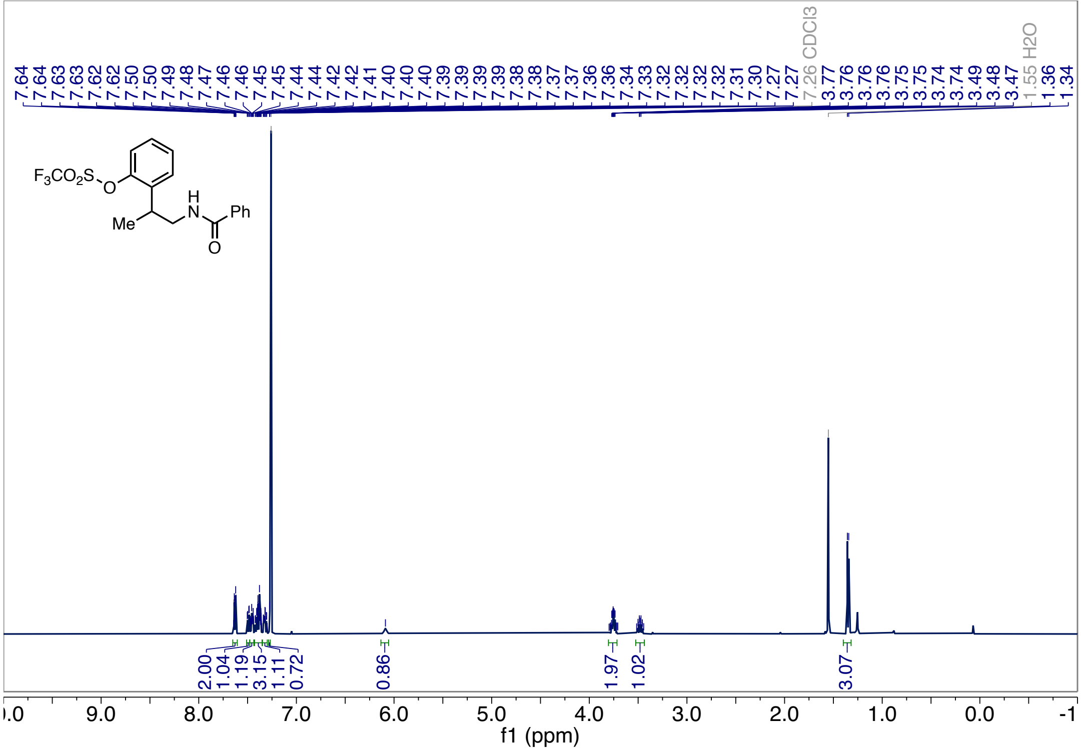


[a]Determined by ^{1}H NMR of same sample.

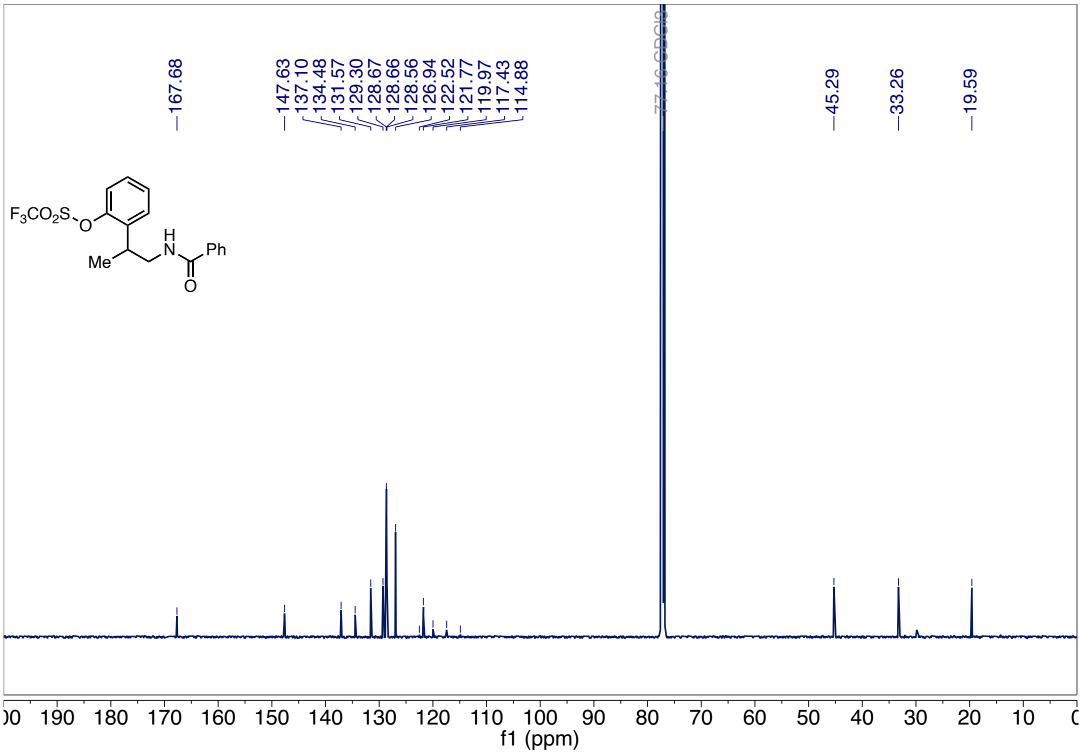
HMBC (500 MHz, CDCl$_3$) of *N*-(2-(3,5-dichloro-4-fluorophenyl)propyl)benzamide (J-1), mixture of isomers (8:1):



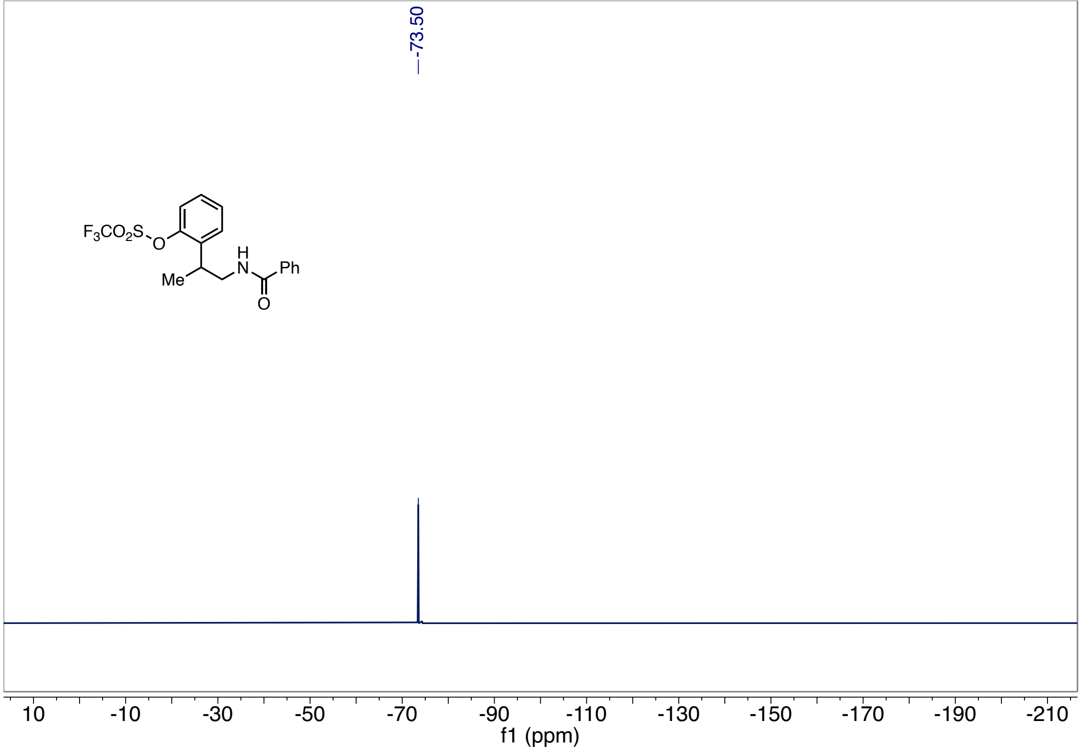
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-(3,5-dichloro-4-fluorophenyl)propyl) benzamide (K-1):



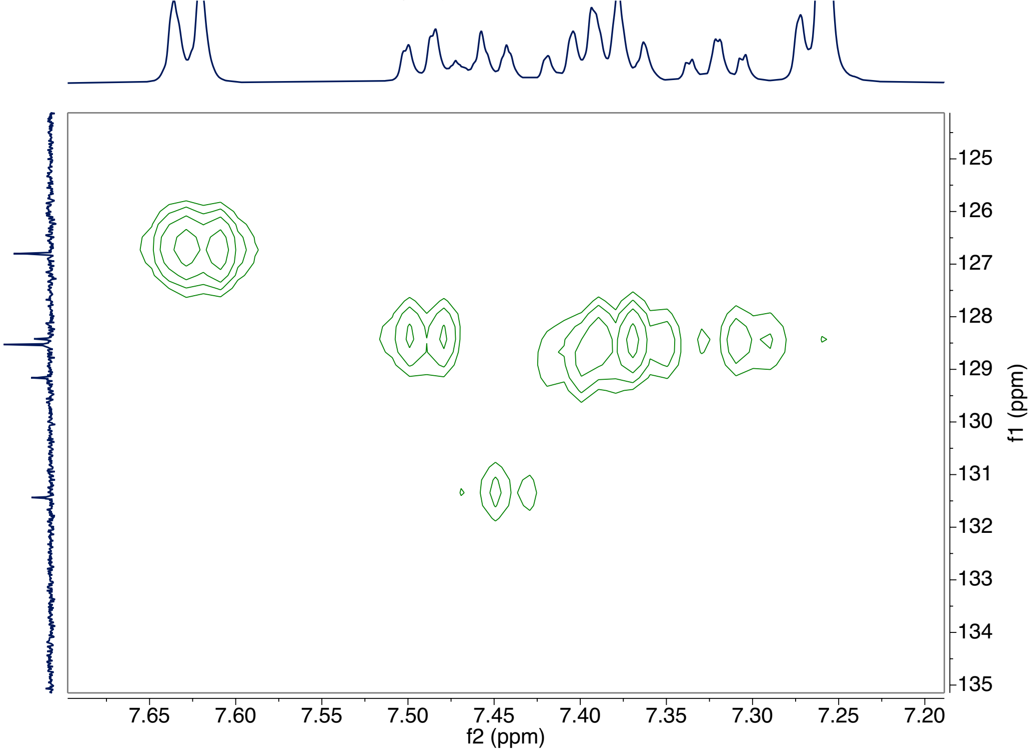
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-(3,5-dichloro-4-fluorophenyl)propyl) benzamide (K-1):



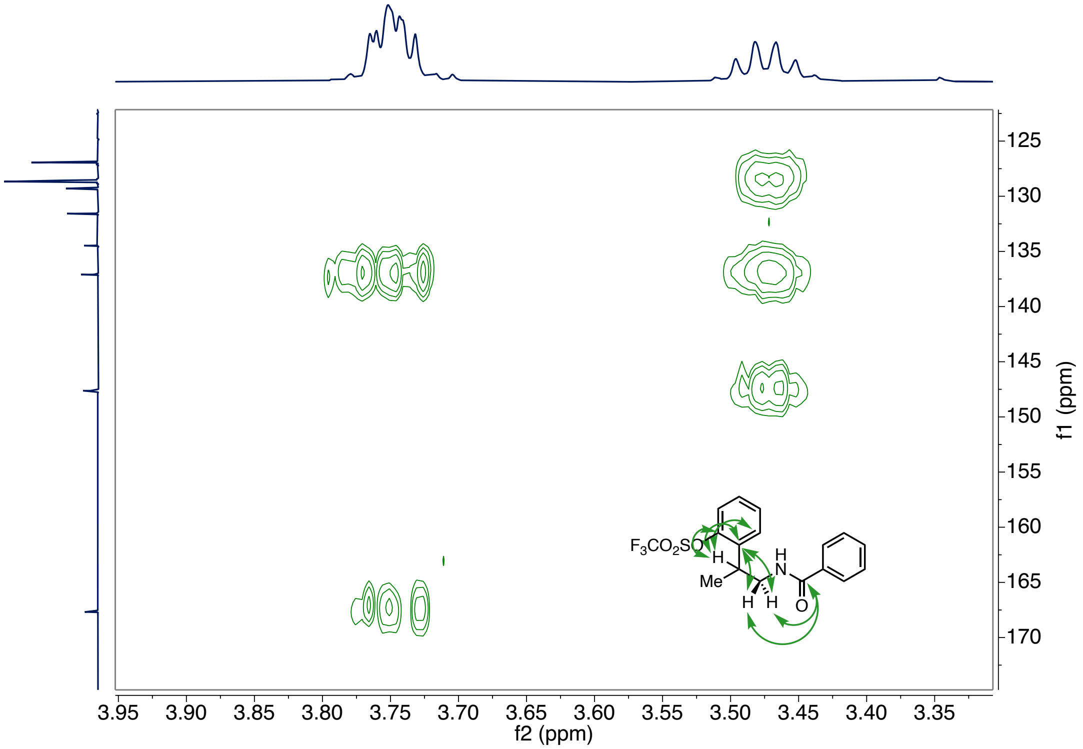
^{19}F NMR (565 MHz, CDCl$_3$) of *N*-(2-(3,5-dichloro-4-fluorophenyl)propyl) benzamide (K-1):



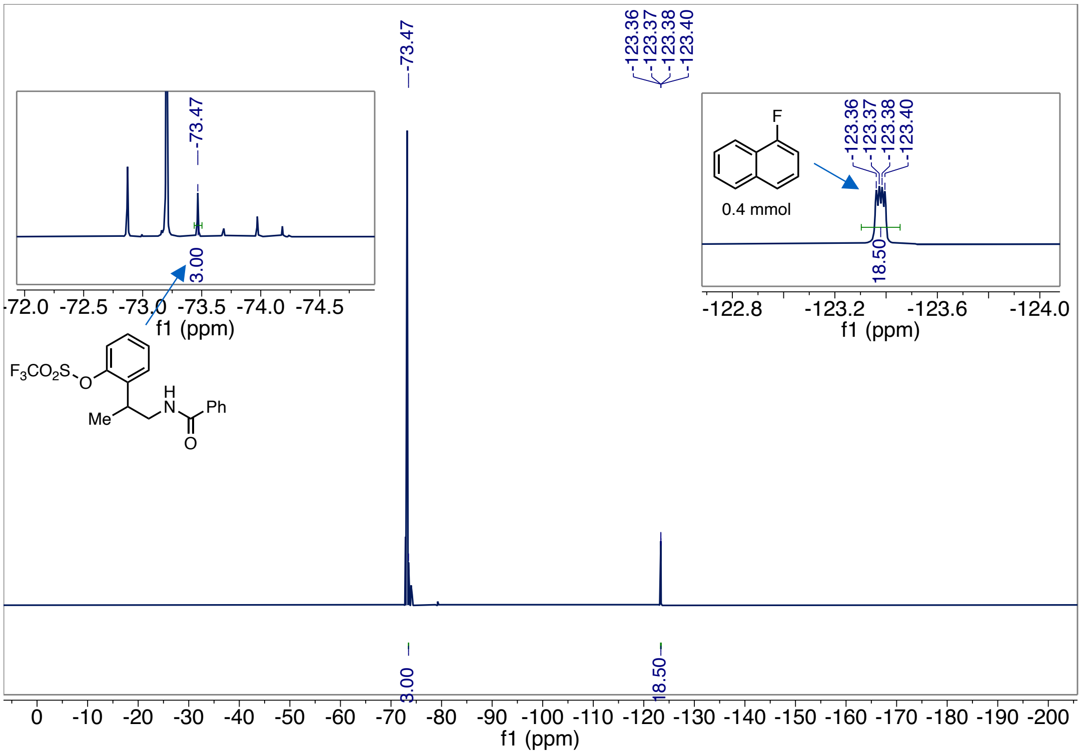
HSQC of *N*-(2-(3,5-dichloro-4-fluorophenyl)propyl) benzamide (K-1) to demonstrate three carbons between δ 128.7 – 128.5 in ^{13}C{^{1}H} NMR:



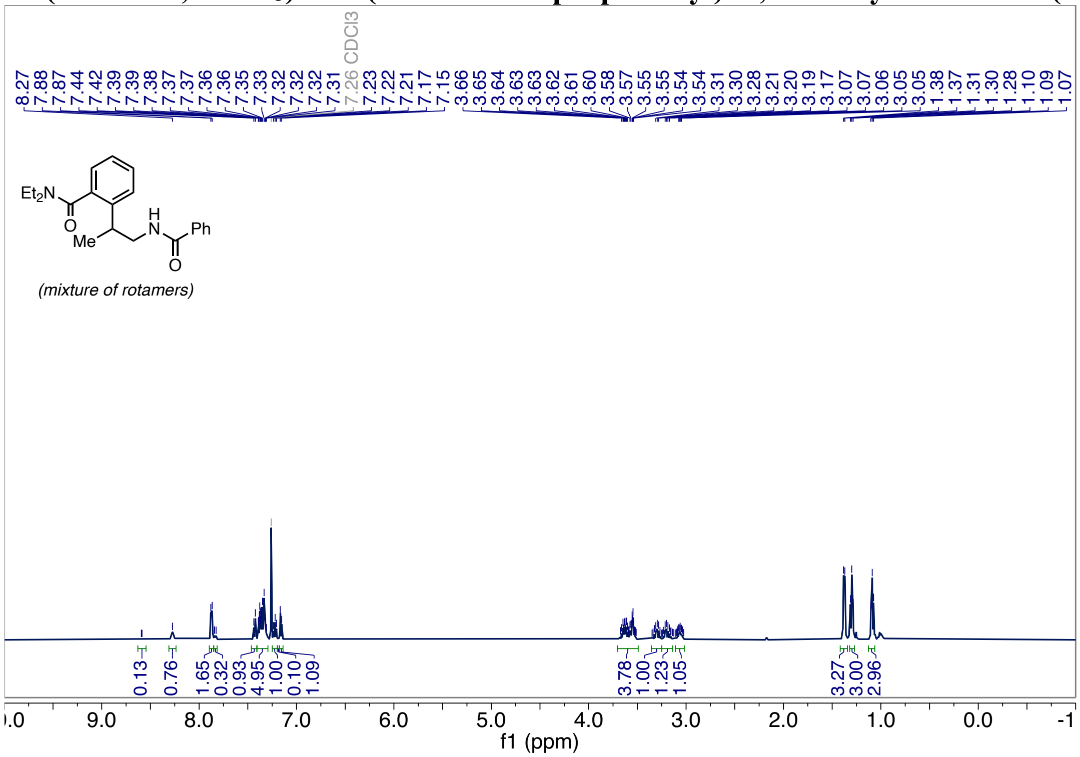
HMBC (500 MHz, CDCl₃) of *N*-(2-(3,5-dichloro-4-fluorophenyl)propyl) benzamide (K-1):



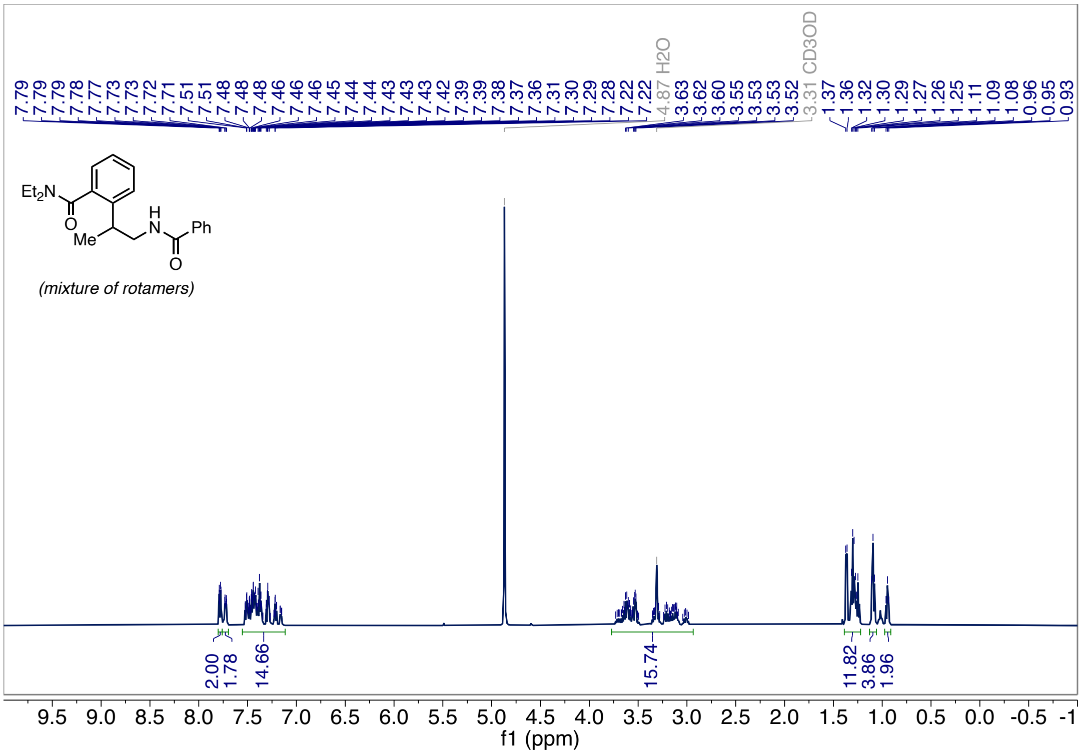
^{19}F NMR (471 MHz, CDCl₃) yield of *N*-(2-(3,5-dichloro-4-fluorophenyl)propyl) benzamide (K-1):



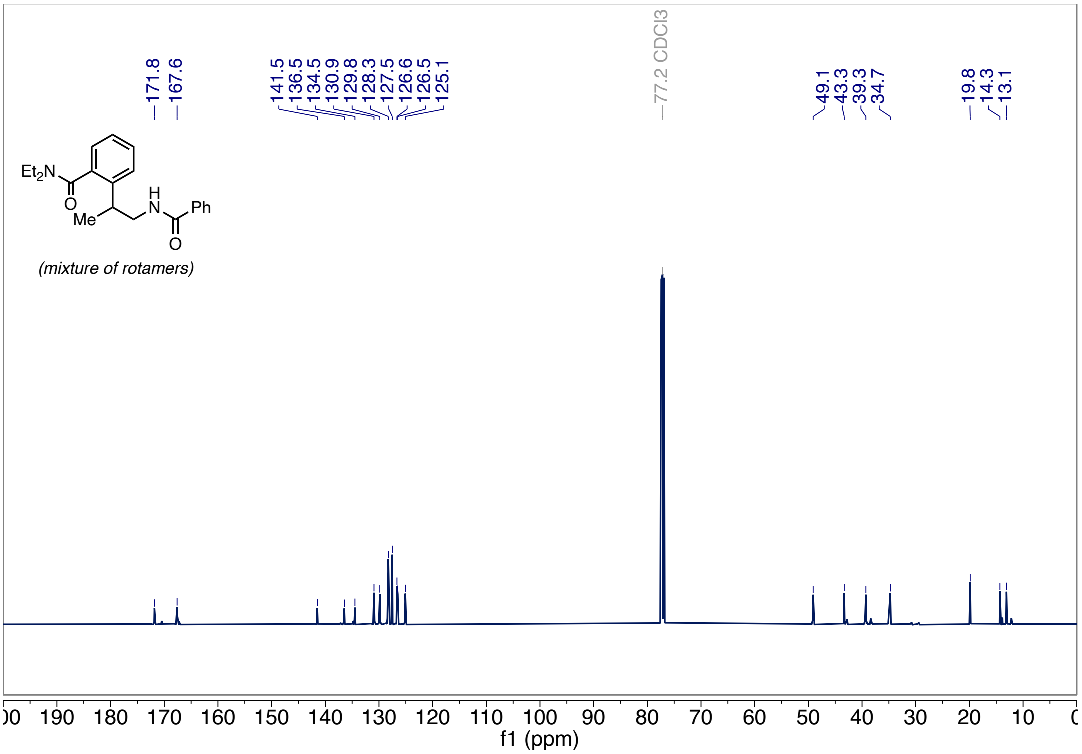
^{1}H NMR (500 MHz, CDCl$_3$) of 2-(1-benzamidopropan-2-yl)-*N*,*N*-diethylbenzamide (O-1):



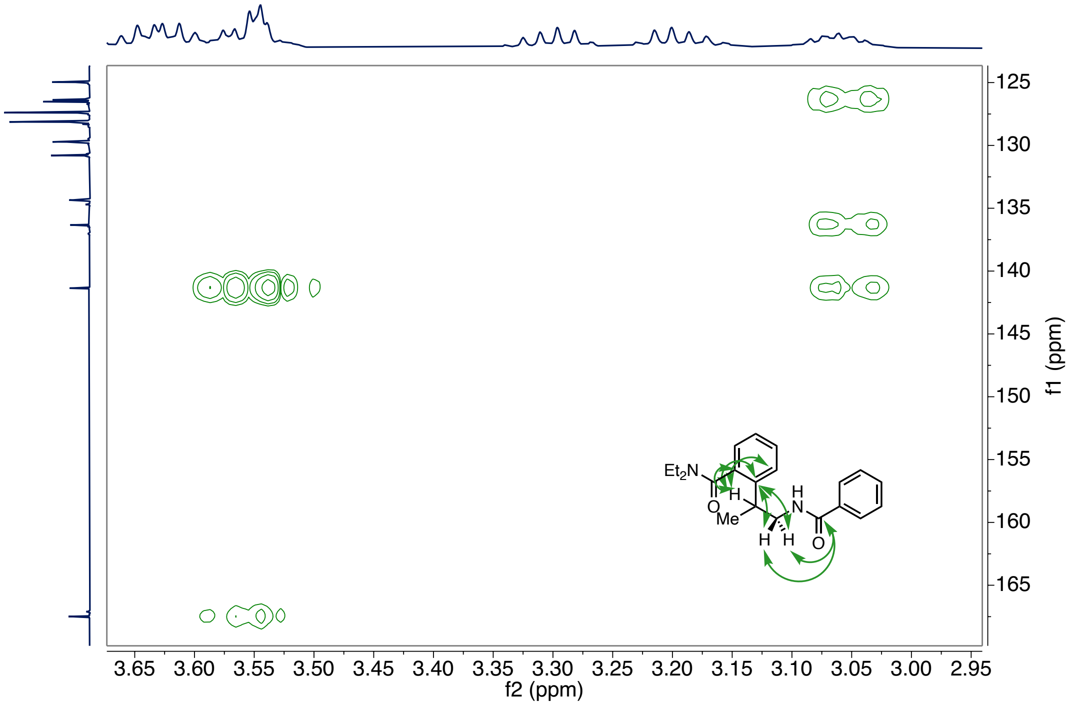
^{1}H NMR (500 MHz, Methanol-*d*$_4$) of 2-(1-benzamidopropan-2-yl)-*N*,*N*-diethylbenzamide (O-1):



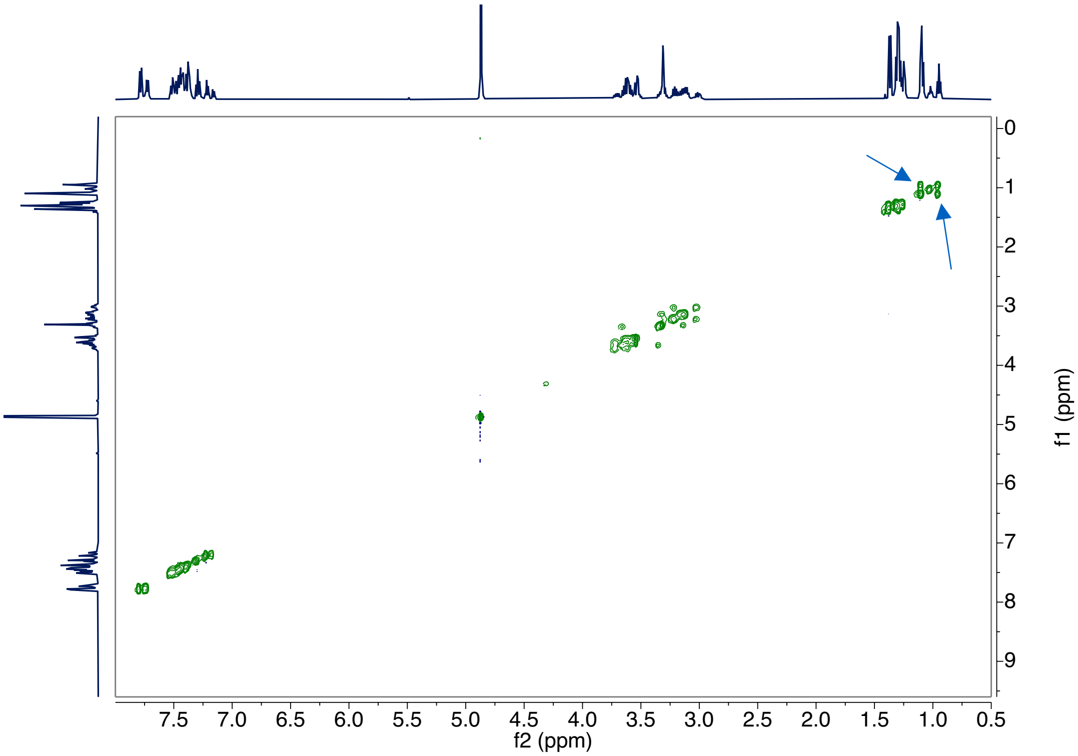
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) of 2-(1-benzamidopropan-2-yl)-*N*,*N*-diethylbenzamide (O-1):



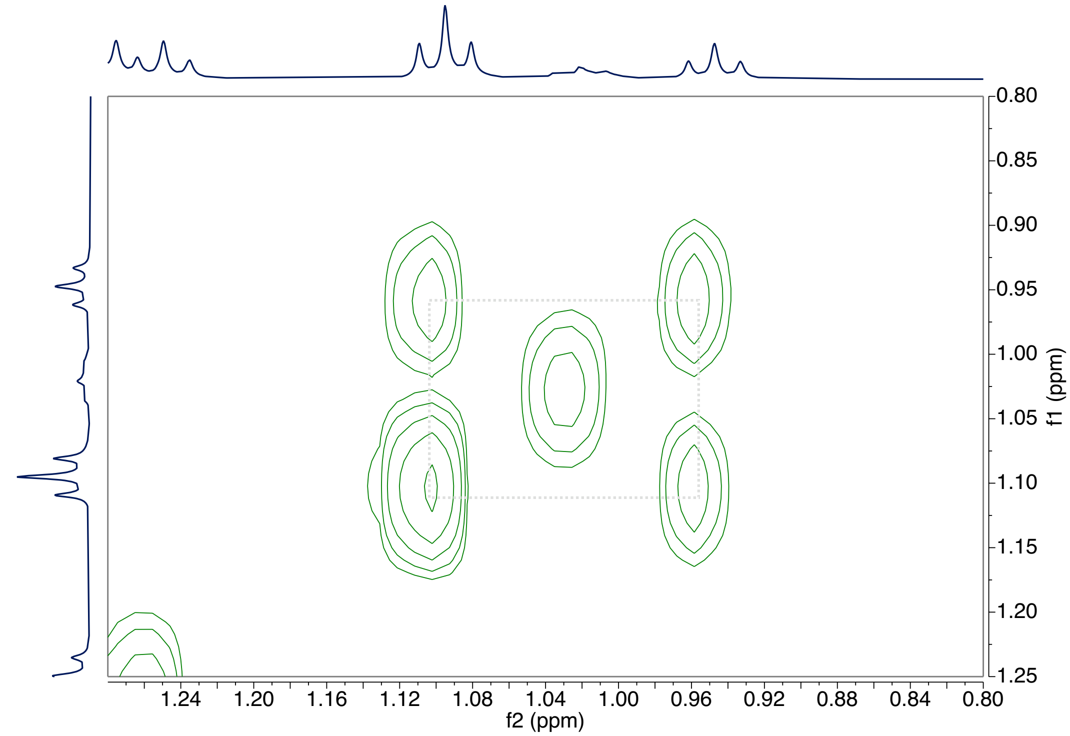
HMBC(500 MHz, $CDCl_3$) of 2-(1-benzamidopropan-2-yl)-*N*,*N*-diethylbenzamide (O-1):



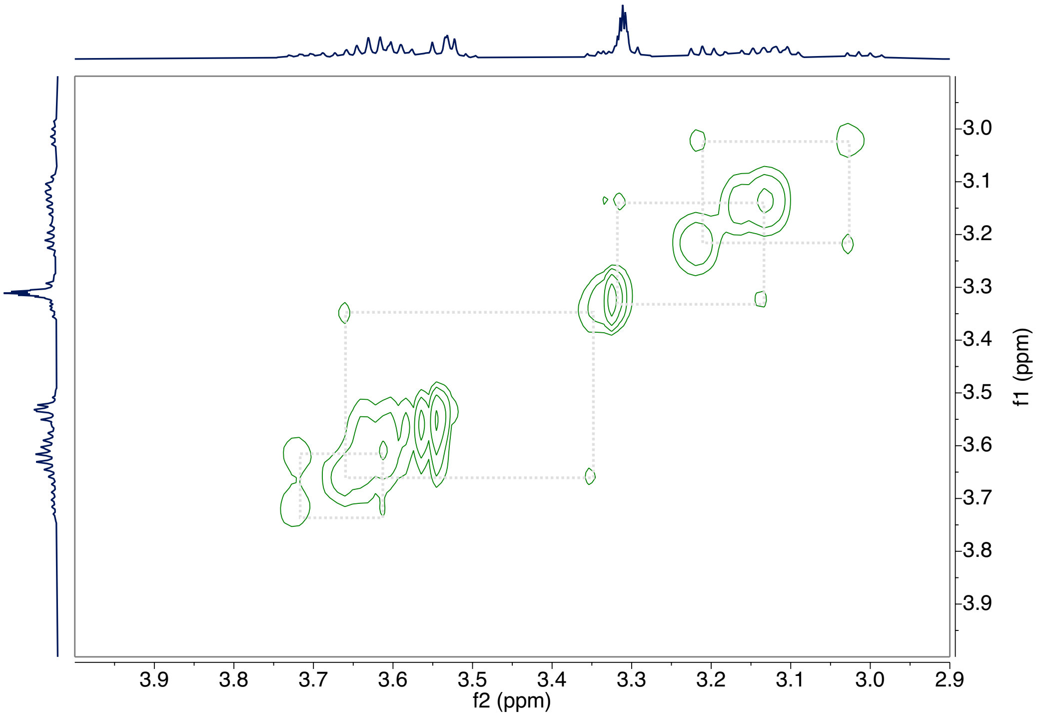
NOESY (500 MHz, Methanol-d_4) of 2-(1-benzamidopropan-2-yl)-*N*,*N*-diethylbenzamide (O-1):



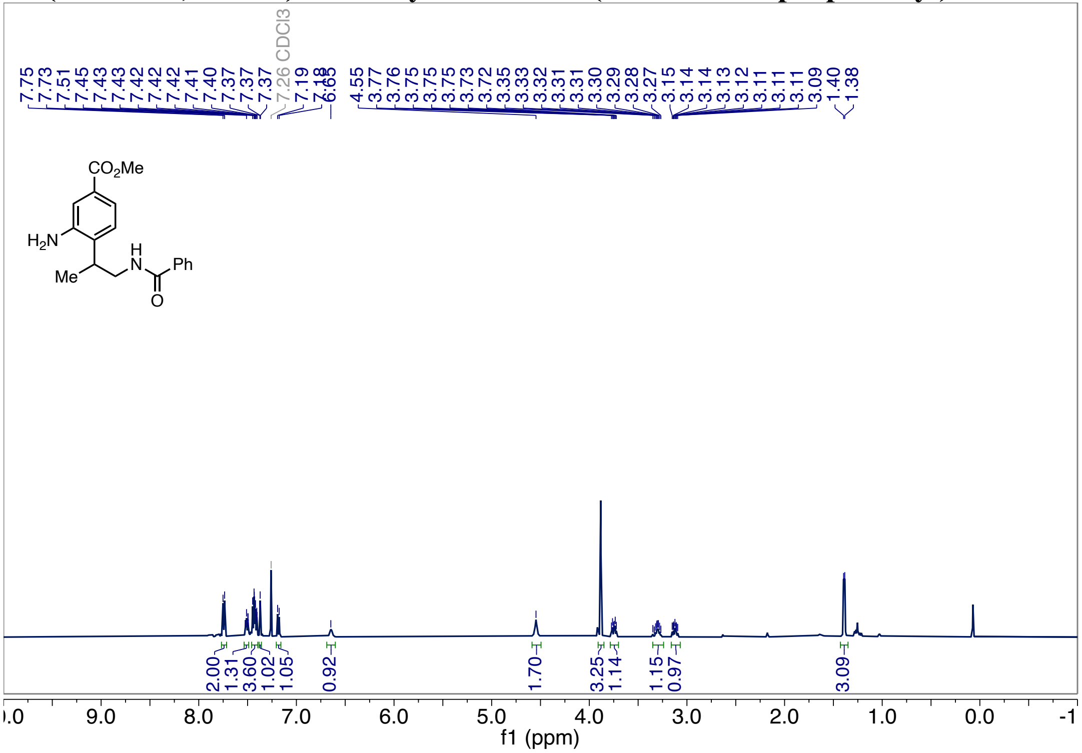
NOESY (500 MHz, Methanol-d_4) of 2-(1-benzamidopropan-2-yl)-*N*,*N*-diethylbenzamide (O-1):



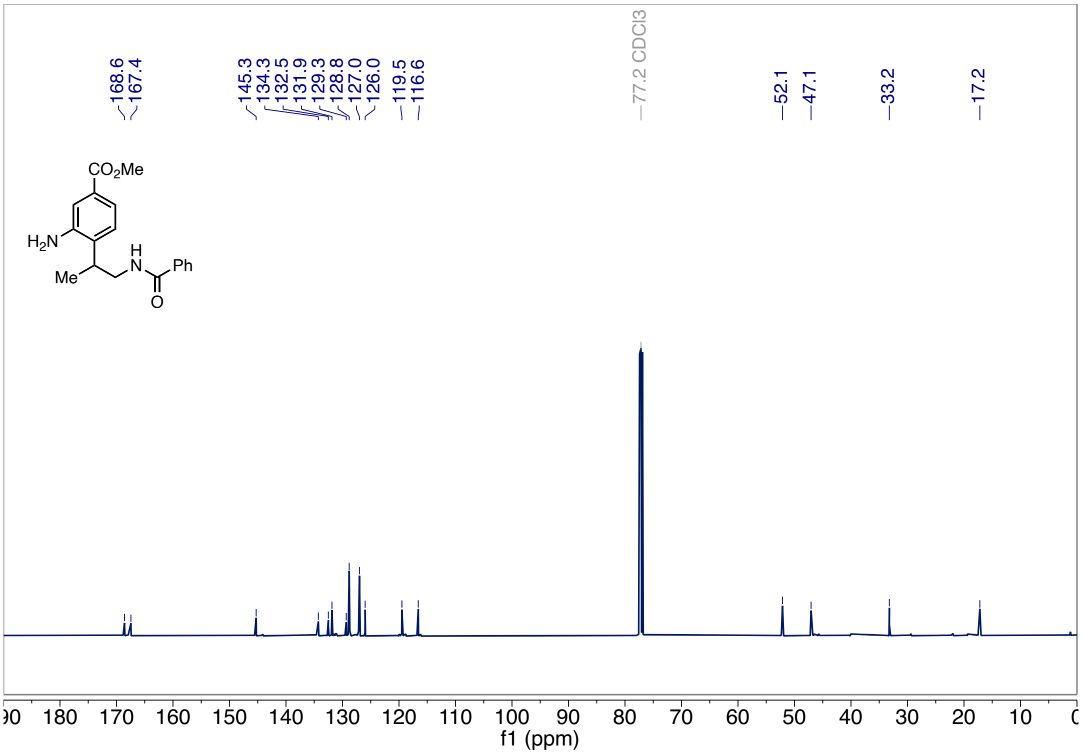
NOESY (500 MHz, Methanol-d_4) of 2-(1-benzamidopropan-2-yl)-*N*,*N*-diethylbenzamide (O-1):



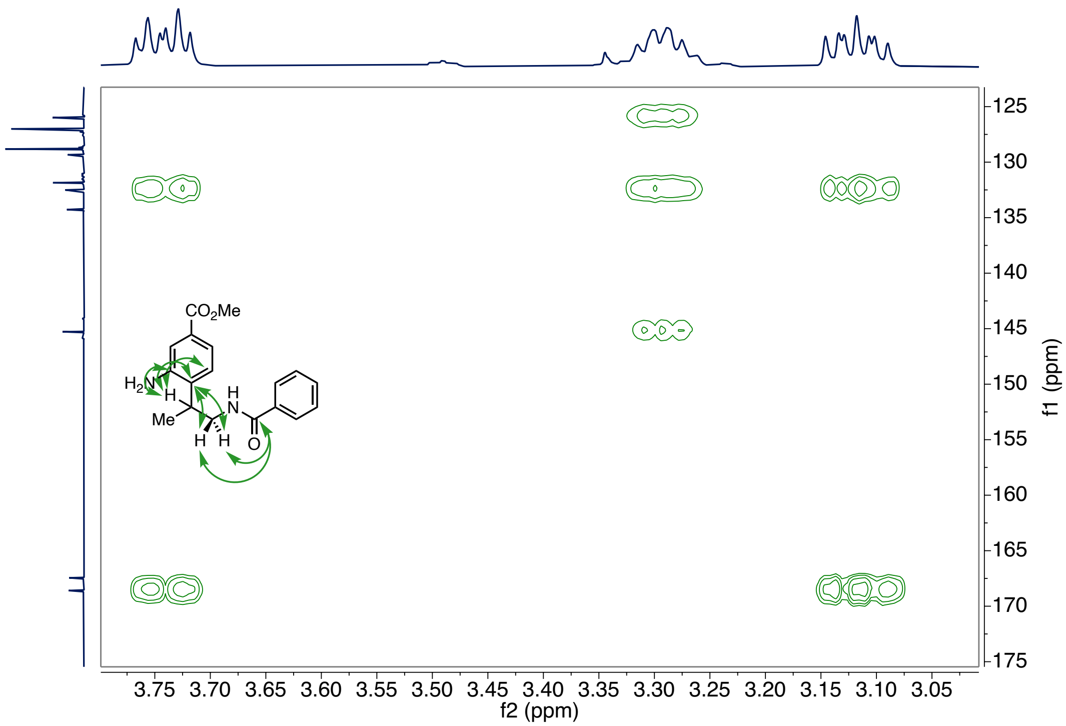
^{1}H NMR (500 MHz, CDCl$_3$) of methyl 3-amino-4-(1-benzamidopropan-2-yl)benzoate (P-1):



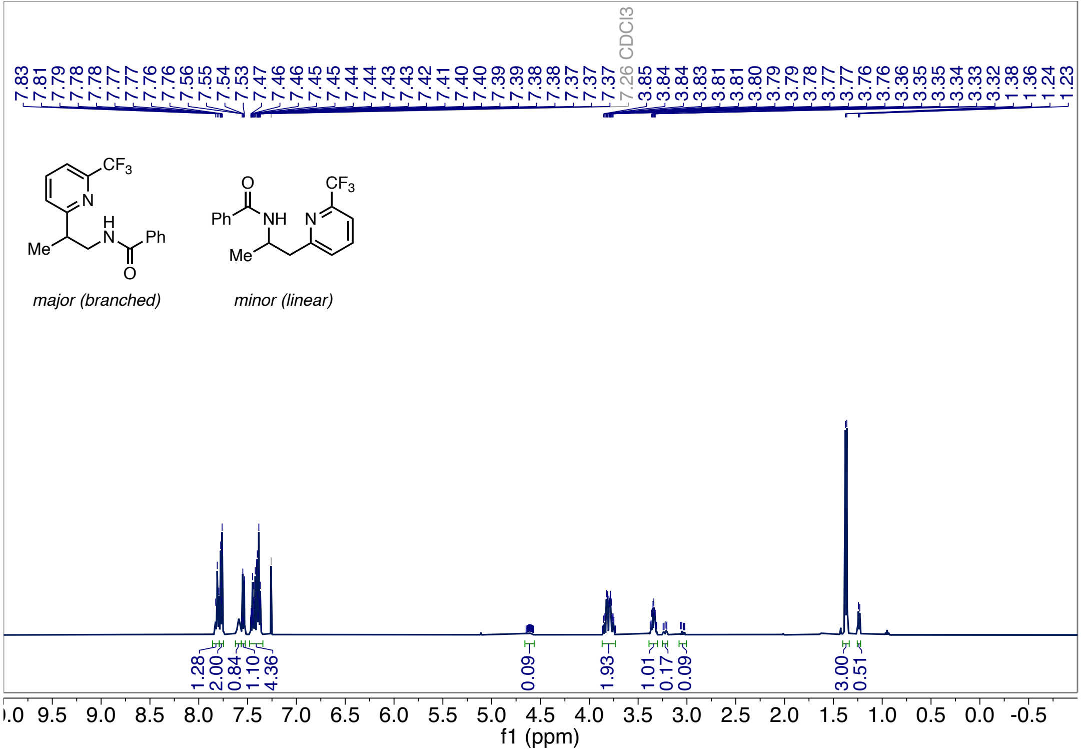
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of methyl 3-amino-4-(1-benzamidopropan-2-yl)benzoate (P-1):



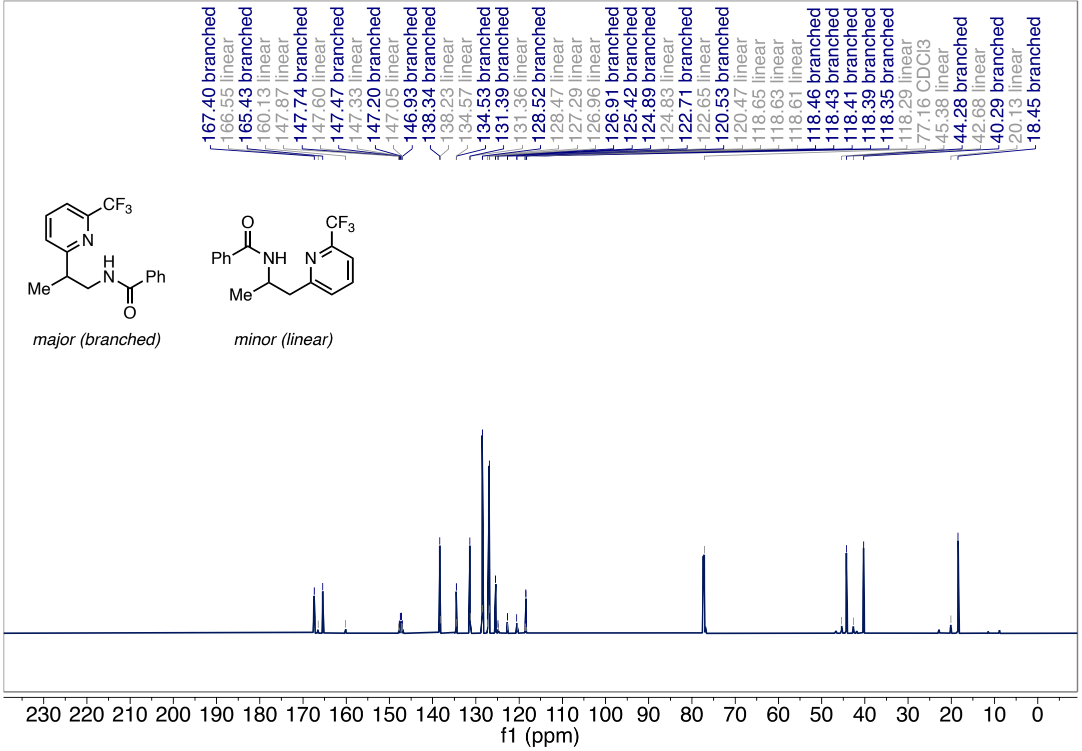
HMBC (500 MHz, CDCl$_3$) of methyl 3-amino-4-(1-benzamidopropan-2-yl)benzoate (P-1):



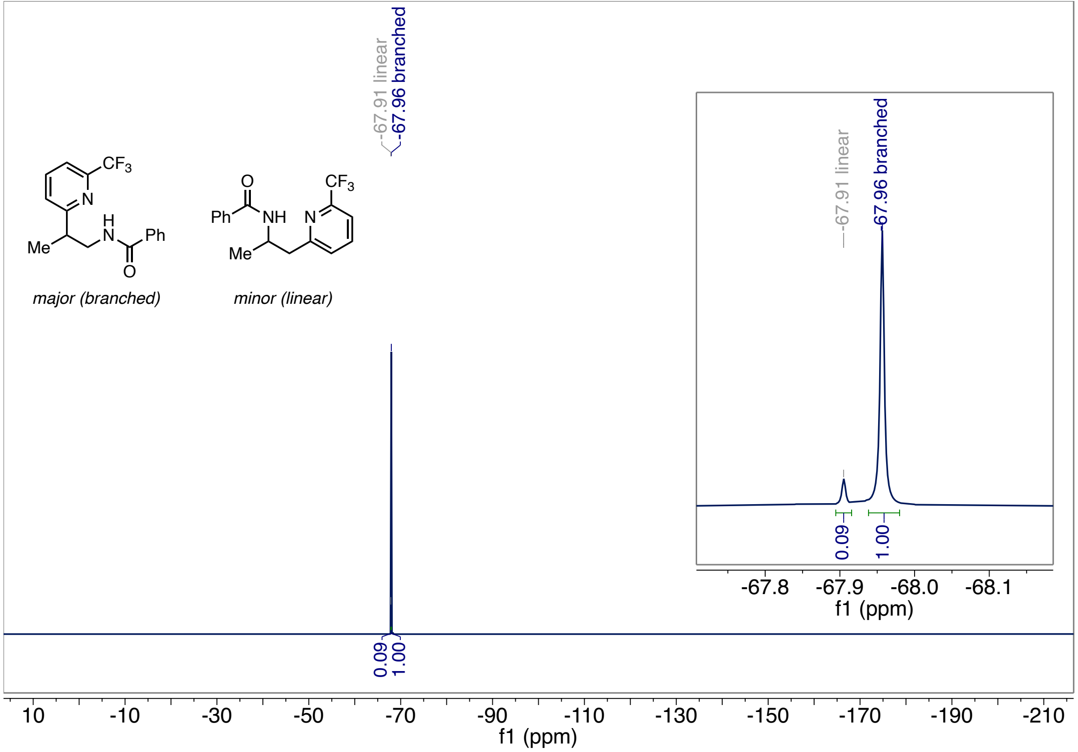
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-(6-(trifluoromethyl)pyridin-2-yl)propyl)benzamide (het-1), mixture of isomers (11:1):



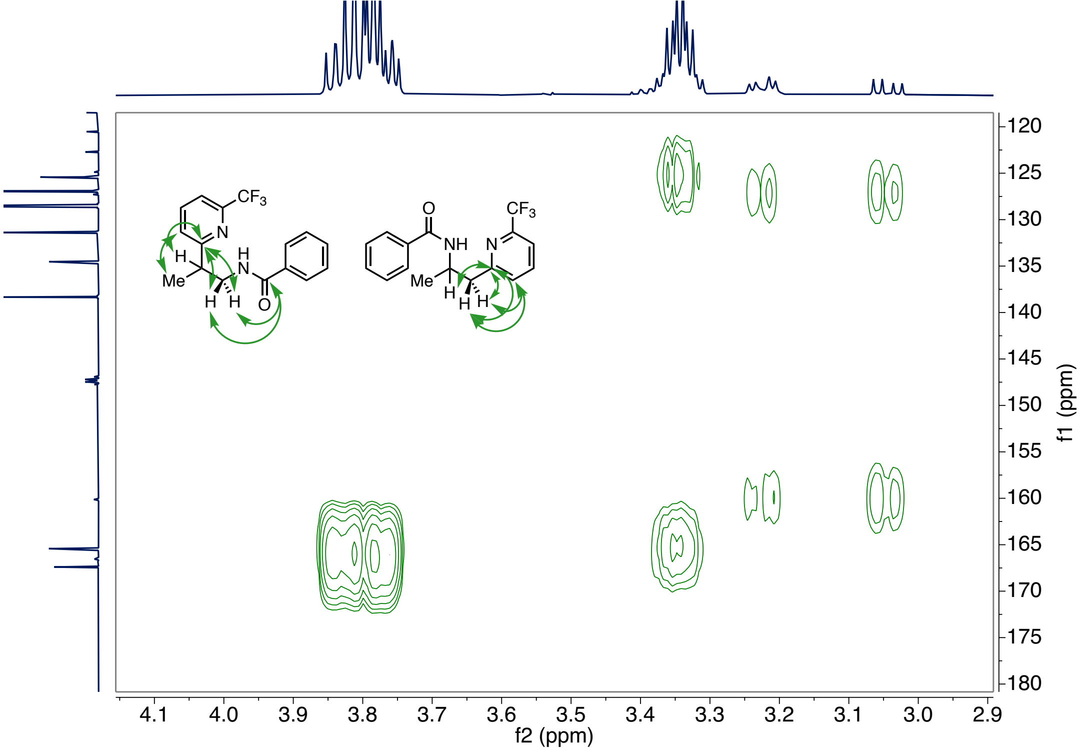
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-(6-(trifluoromethyl)pyridin-2-yl)propyl)benzamide (het-1), mixture of isomers (11:1):



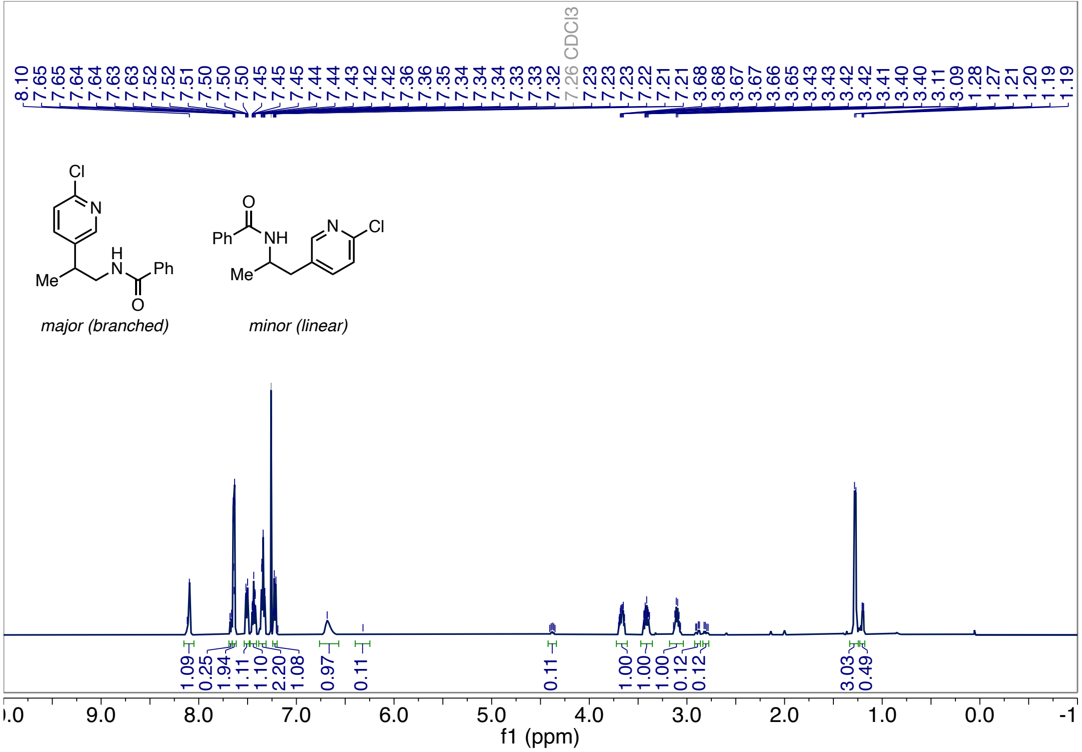
^{19}F NMR (565 MHz, $CDCl_3$) of *N*-(2-(6-(trifluoromethyl)pyridin-2-yl)propyl)benzamide (het-1), mixture of isomers (11:1):



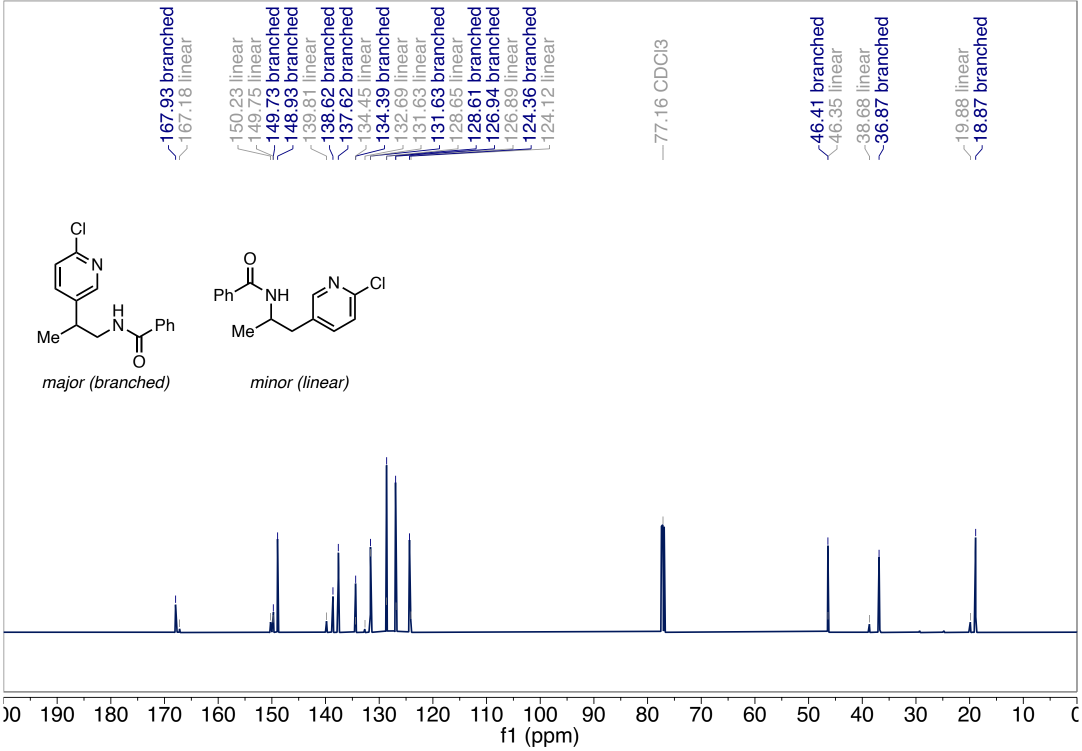
HMBC (500 MHz, $CDCl_3$) of *N*-(2-(6-(trifluoromethyl)pyridin-2-yl)propyl)benzamide (het-1), mixture of isomers (11:1):



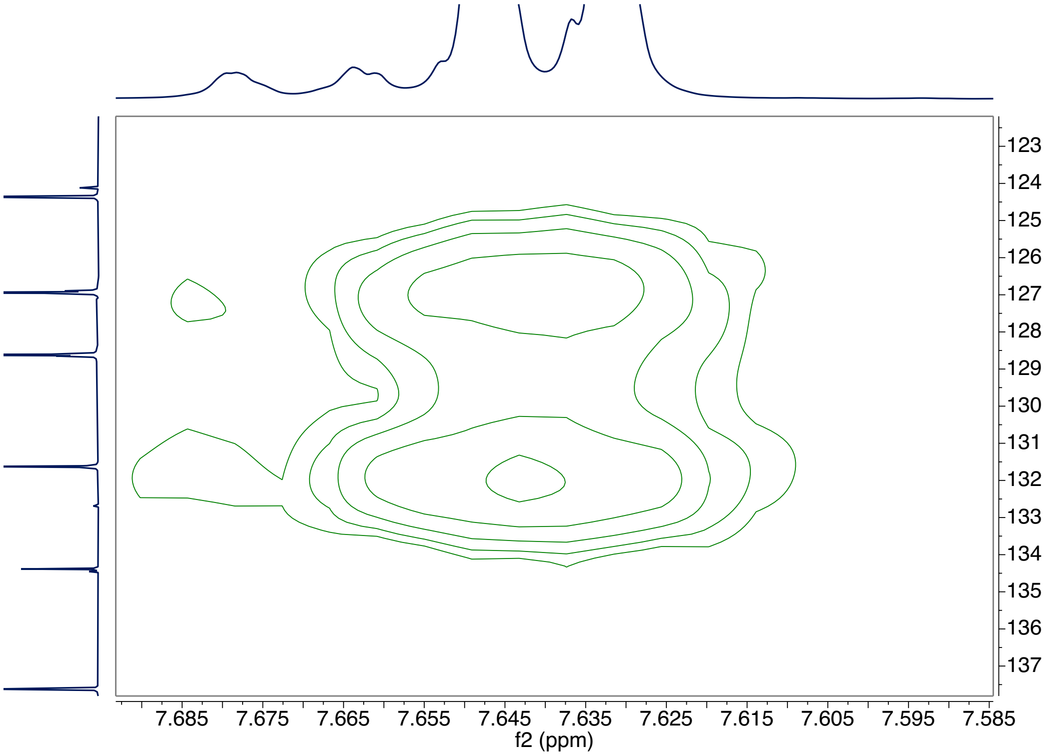
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-(6-chloropyridin-3-yl)propyl)benzamide (het-2), mixture of isomers (9:1):



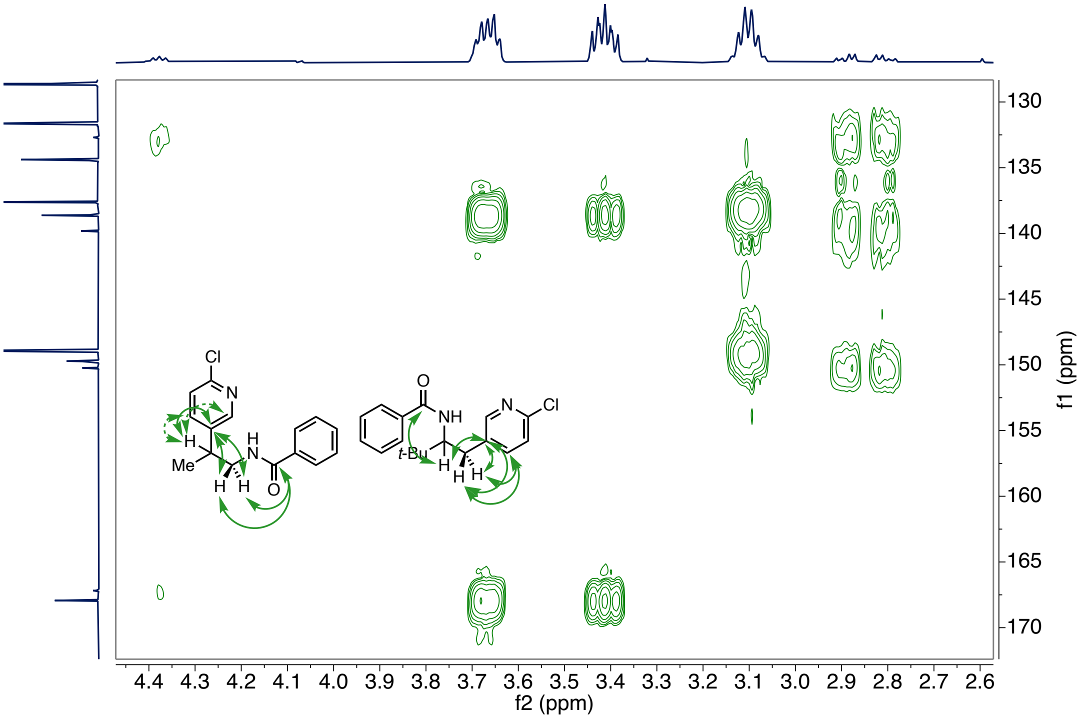
^{13}C{1H} NMR (126 MHz, CDCl$_3$) of *N*-(2-(6-chloropyridin-3-yl)propyl)benzamide (het-2), mixture of isomers (9:1):



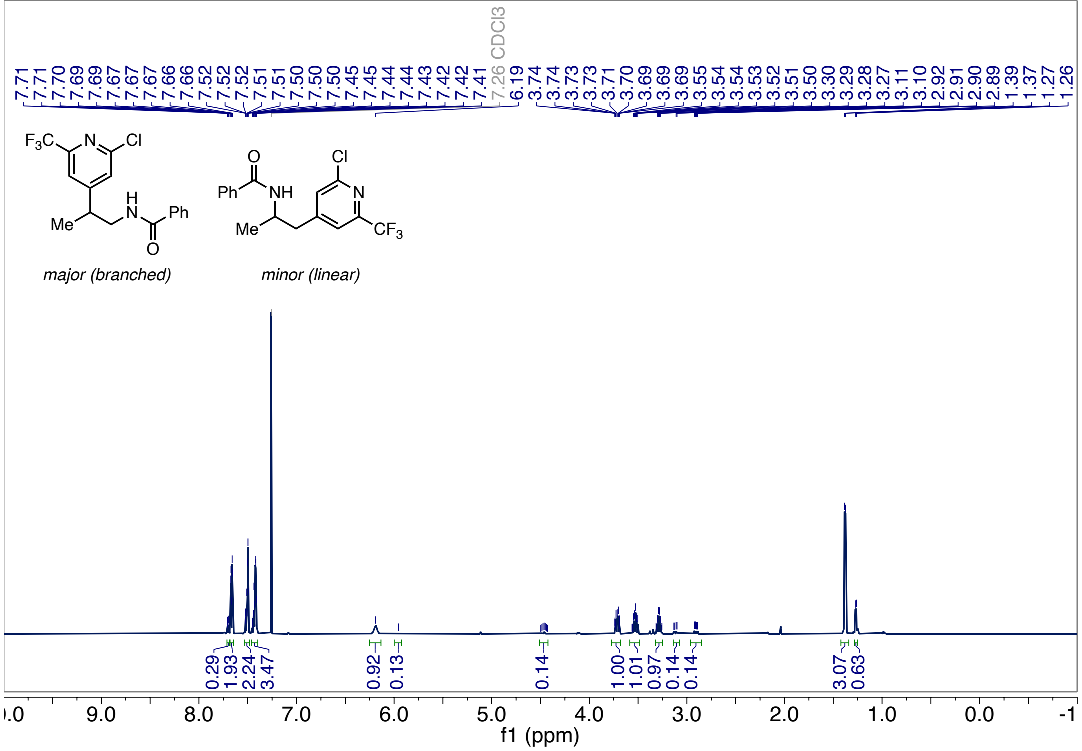
HMBC (500 MHz, CDCl₃) of het-2 to demonstrate overlap of carbon from the linear isomer at δ 131.6 in $^{13}C\{^{1}H\}$ NMR, mixture of isomers (9:1):



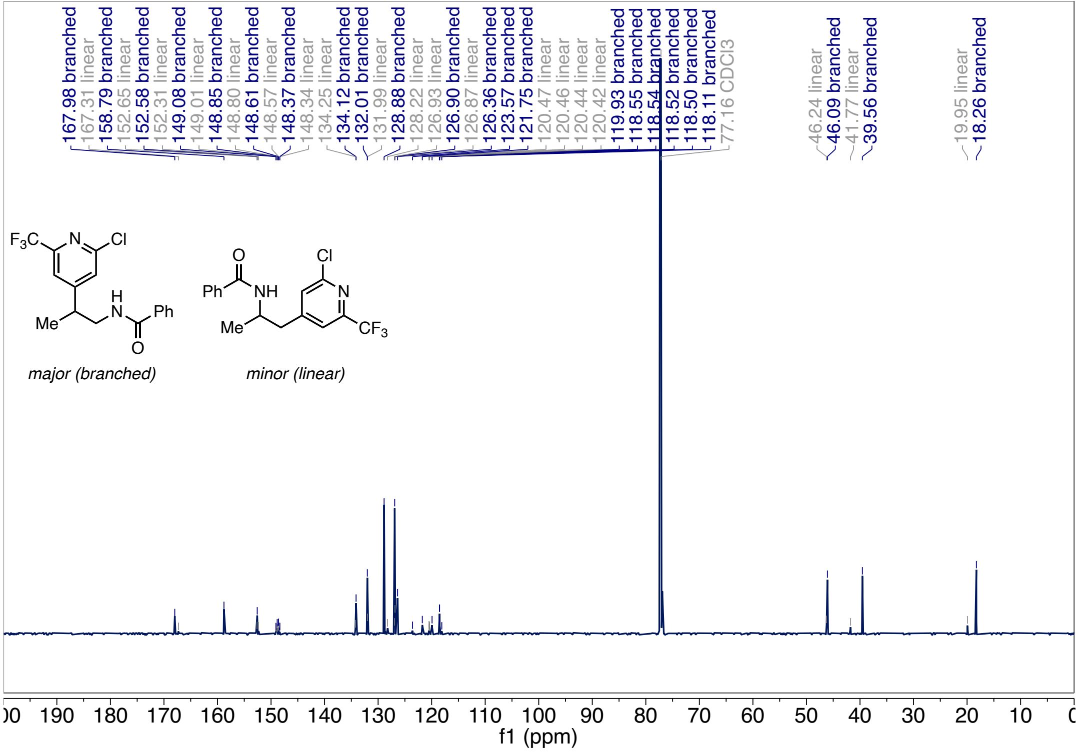
HMBC (500 MHz, CDCl₃) of *N*-(2-(6-chloropyridin-3-yl)propyl)benzamide (het-2), mixture of isomers (9:1):



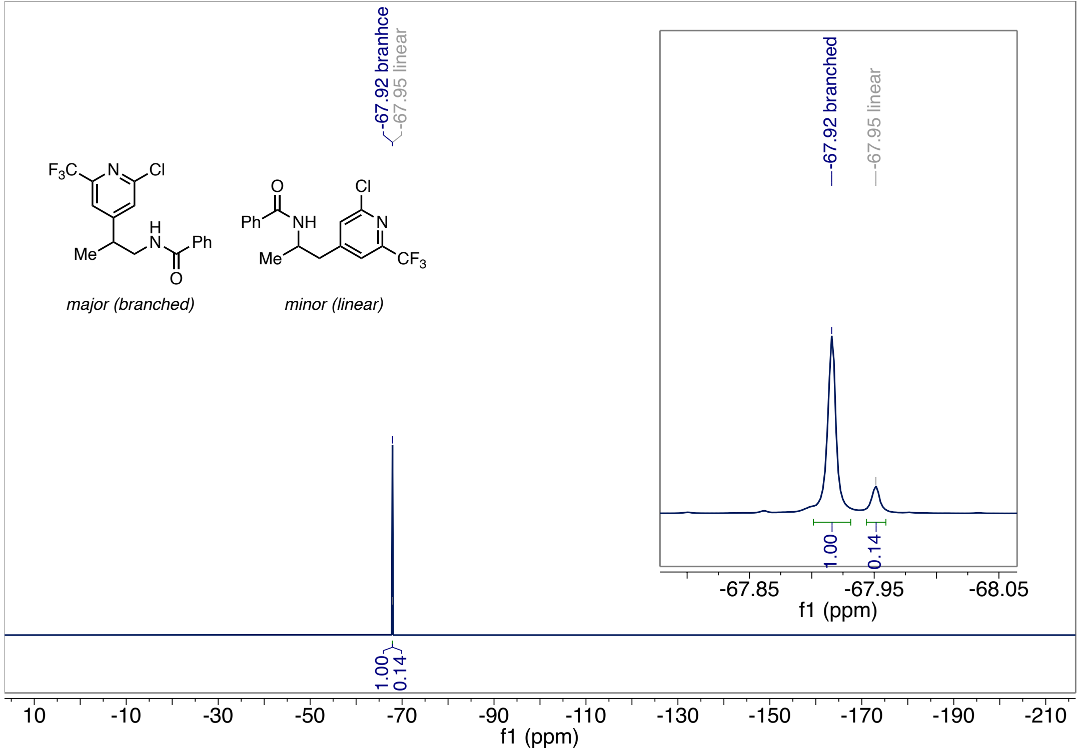
^{1}H NMR (600 MHz, CDCl$_3$) of *N*-(2-(2-chloro-6-(trifluoromethyl)pyridin-4-yl)propyl) benzamide (het-3), mixture of isomers (7:1):



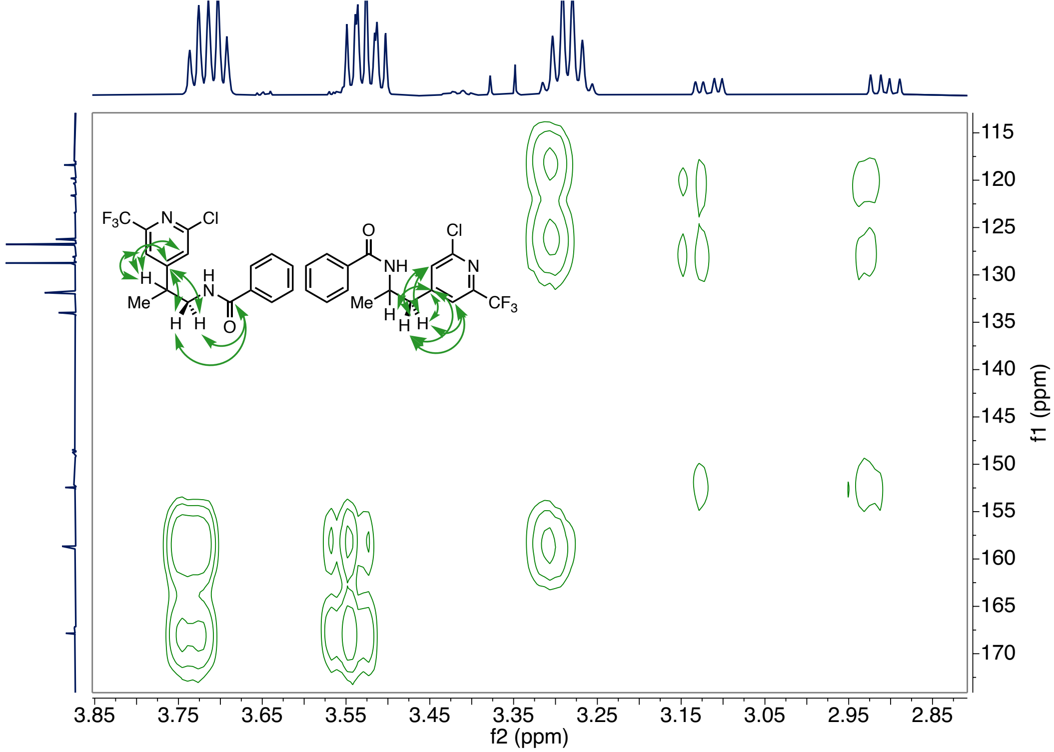
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of *N*-(2-(2-chloro-6-(trifluoromethyl)pyridin-4-yl)propyl) benzamide (het-3), mixture of isomers (7:1):



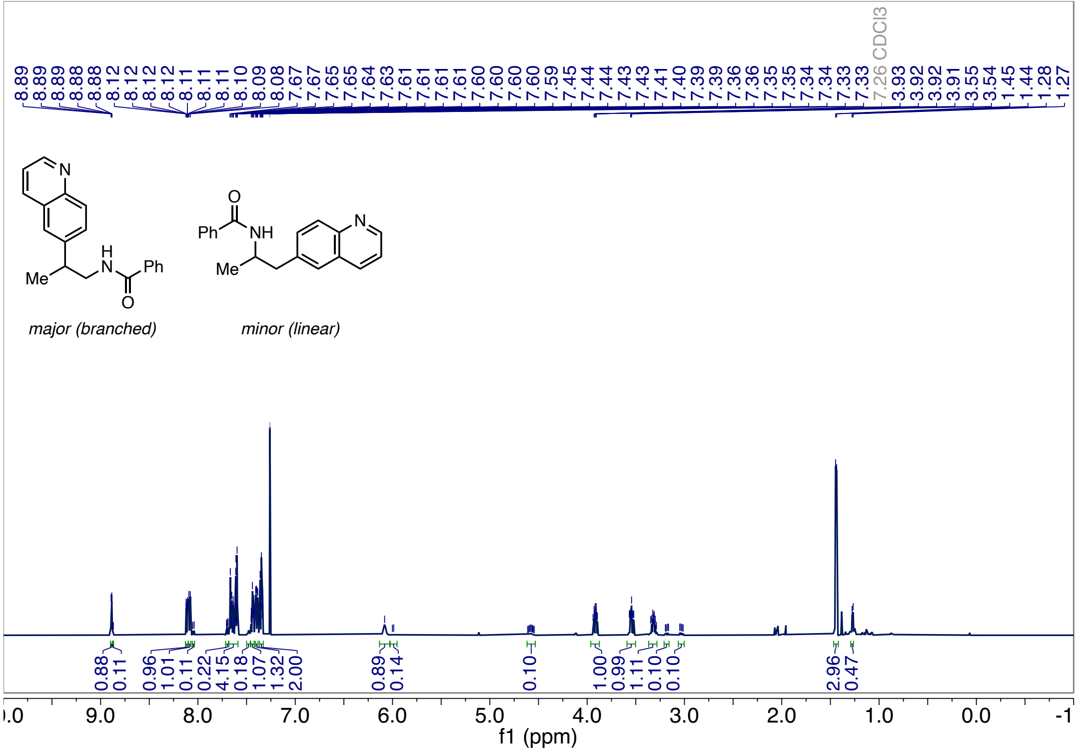
^{19}F NMR (565 MHz, CDCl$_3$) of *N*-(2-(2-chloro-6-(trifluoromethyl)pyridin-4-yl)propyl) benzamide (het-3), mixture of isomers (7:1):



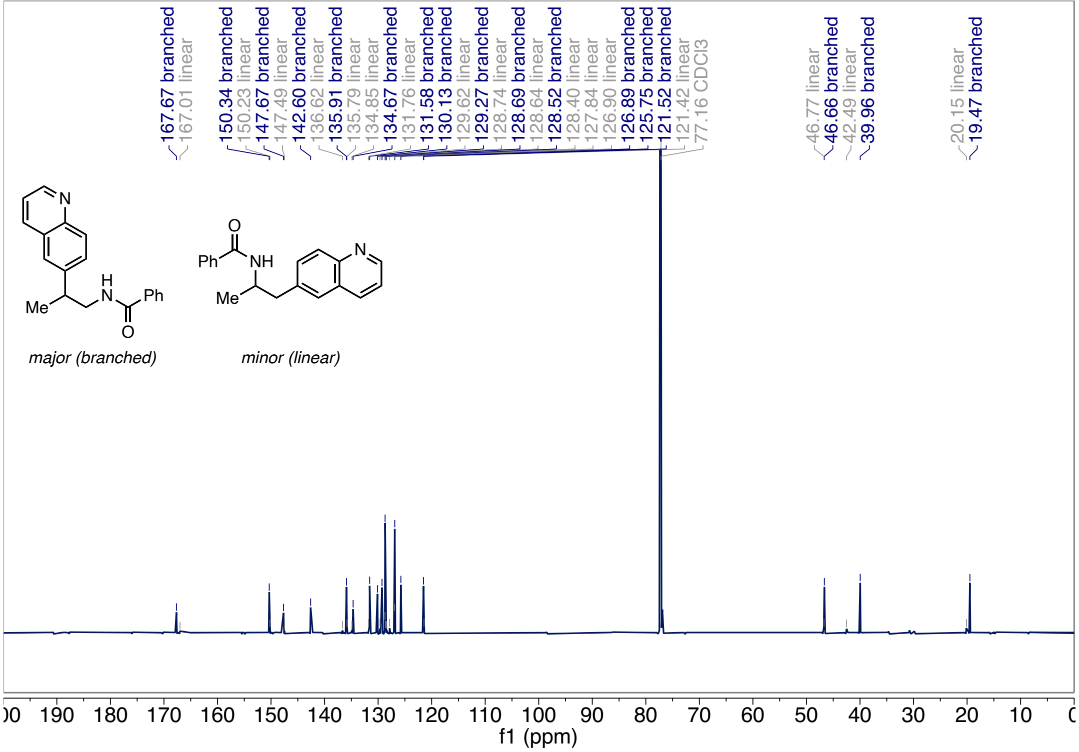
HMBC (600 MHz, CDCl$_3$) of *N*-(2-(2-chloro-6-(trifluoromethyl)pyridin-4-yl)propyl) benzamide (het-3), mixture of isomers (7:1):



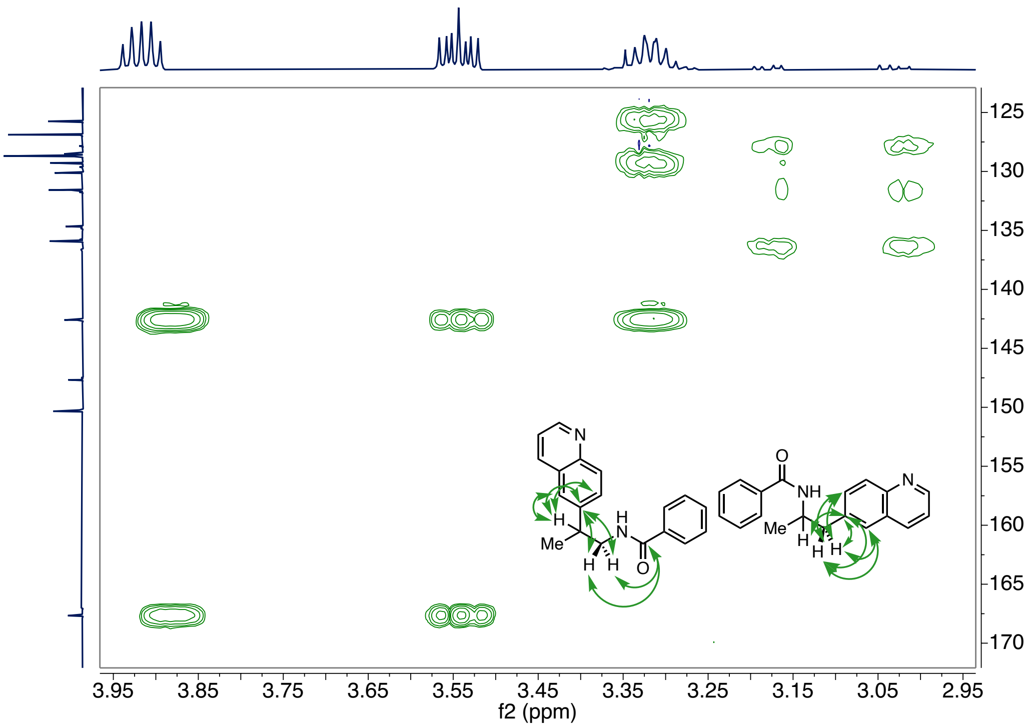
^{1}H NMR (600 MHz, CDCl$_3$) of *N*-(2-(quinolin-6-yl)propyl)benzamide (het-4), mixture of isomers (10:1):



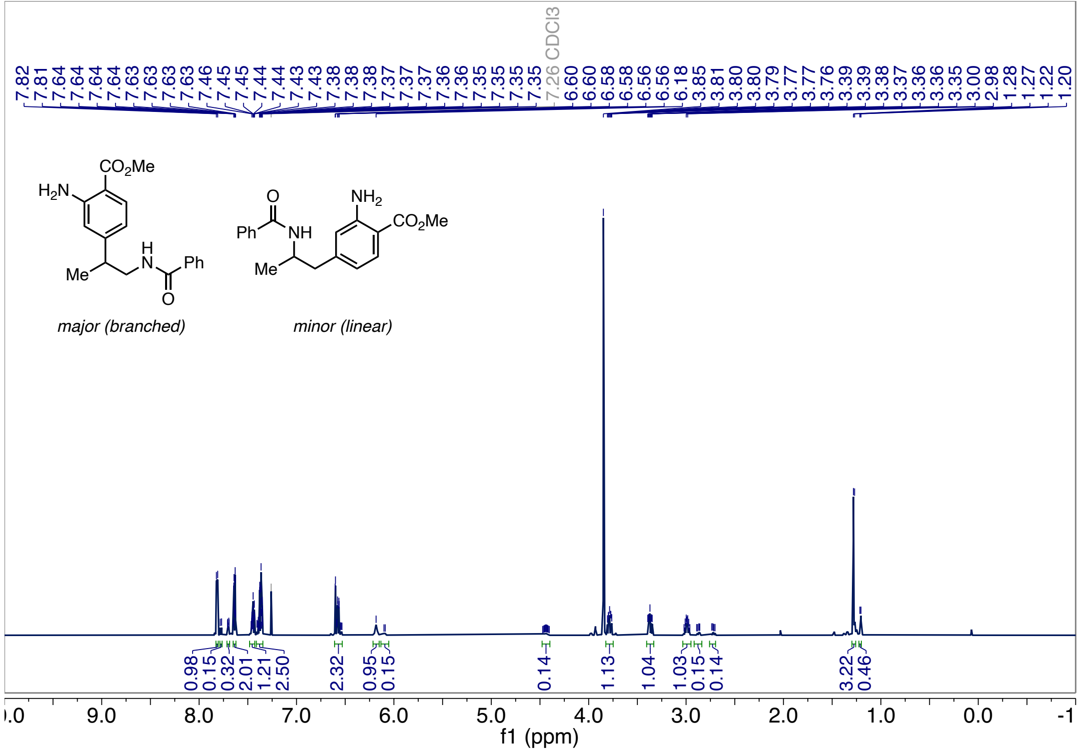
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of *N*-(2-(quinolin-6-yl)propyl)benzamide (het-4), mixture of isomers (10:1):



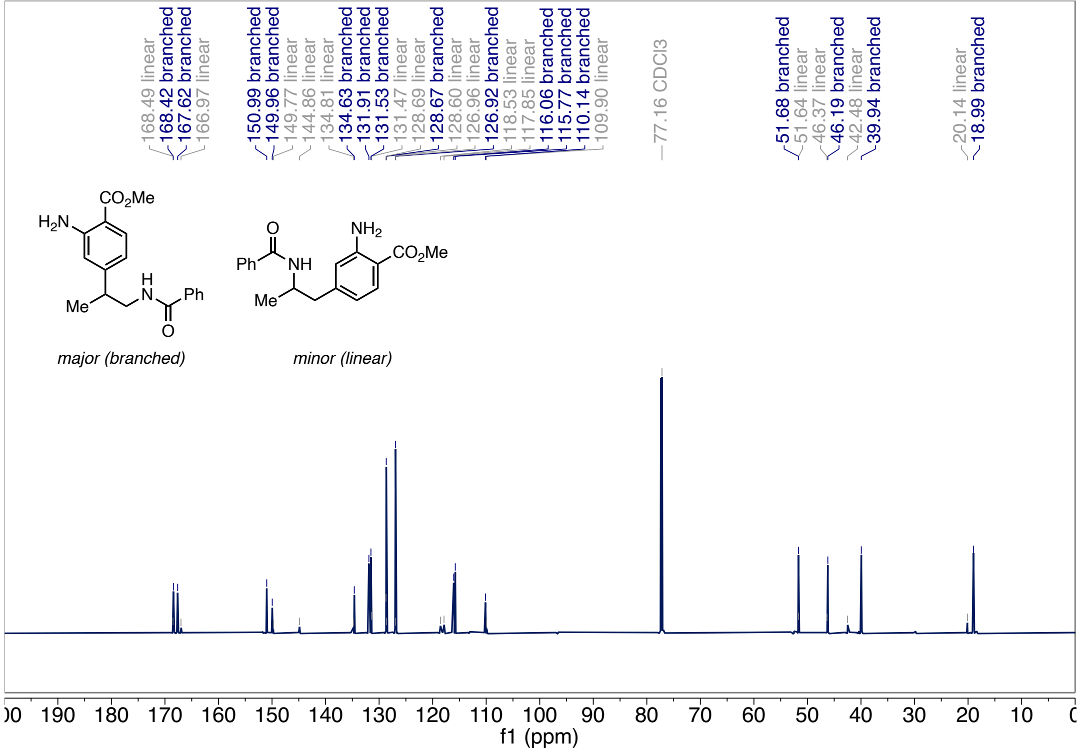
HMBC (600 MHz, CDCl$_3$) of *N*-(2-(quinolin-6-yl)propyl)benzamide (het-4), mixture of isomers (10:1):



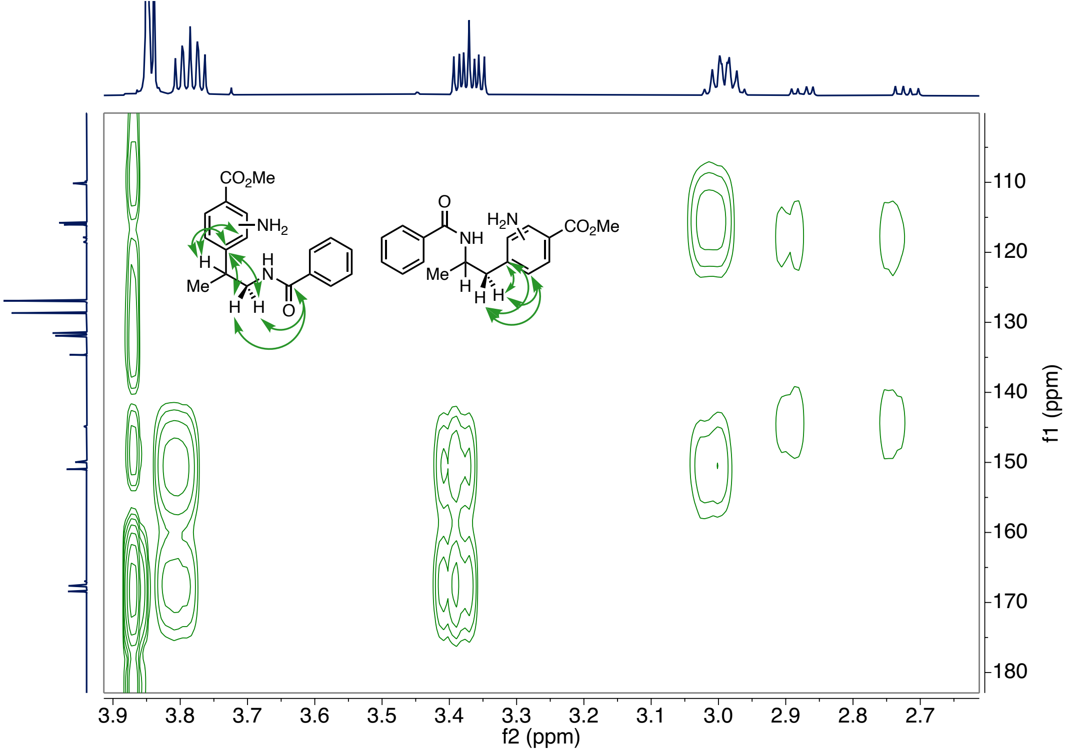
^{1}H NMR (600 MHz, CDCl$_3$) of methyl 2-amino-4-(1-benzamidopropan-2-yl)benzoate (I-2), mixture of isomers (7:1):



^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of methyl 2-amino-4-(1-benzamidopropan-2-yl)benzoate (I-2), mixture of isomers (7:1):

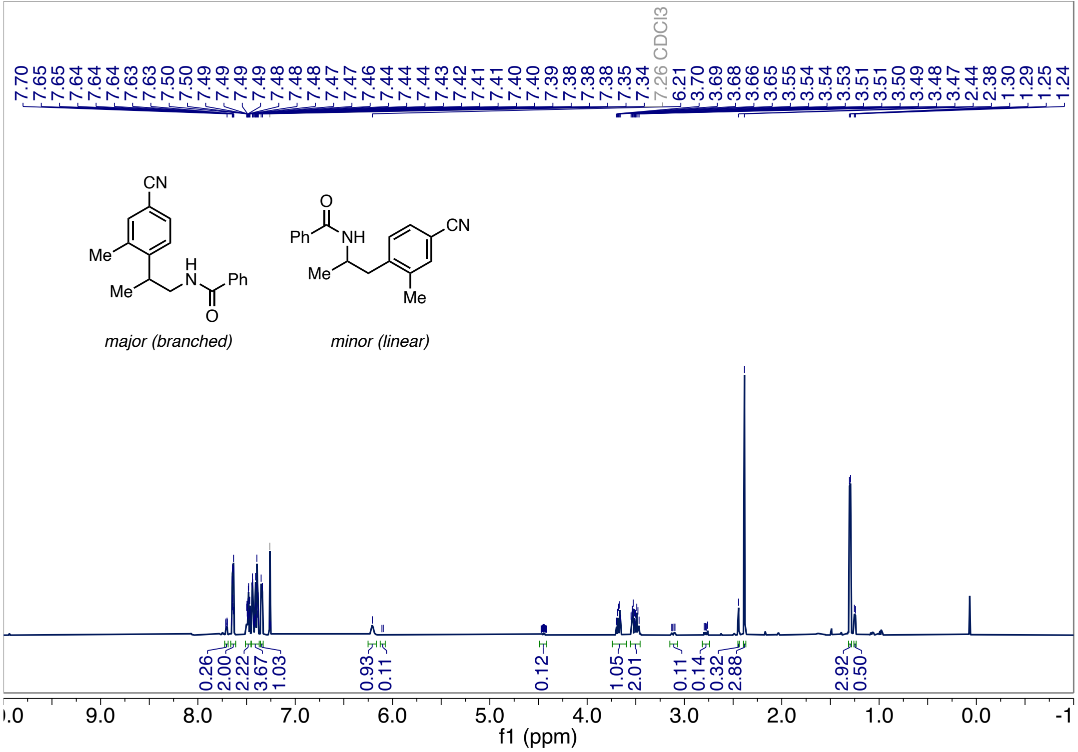


HMBC (600 MHz, $CDCl_3$) of methyl 2-amino-4-(1-benzamidopropan-2-yl)benzoate (I-2), mixture of isomers (7:1):

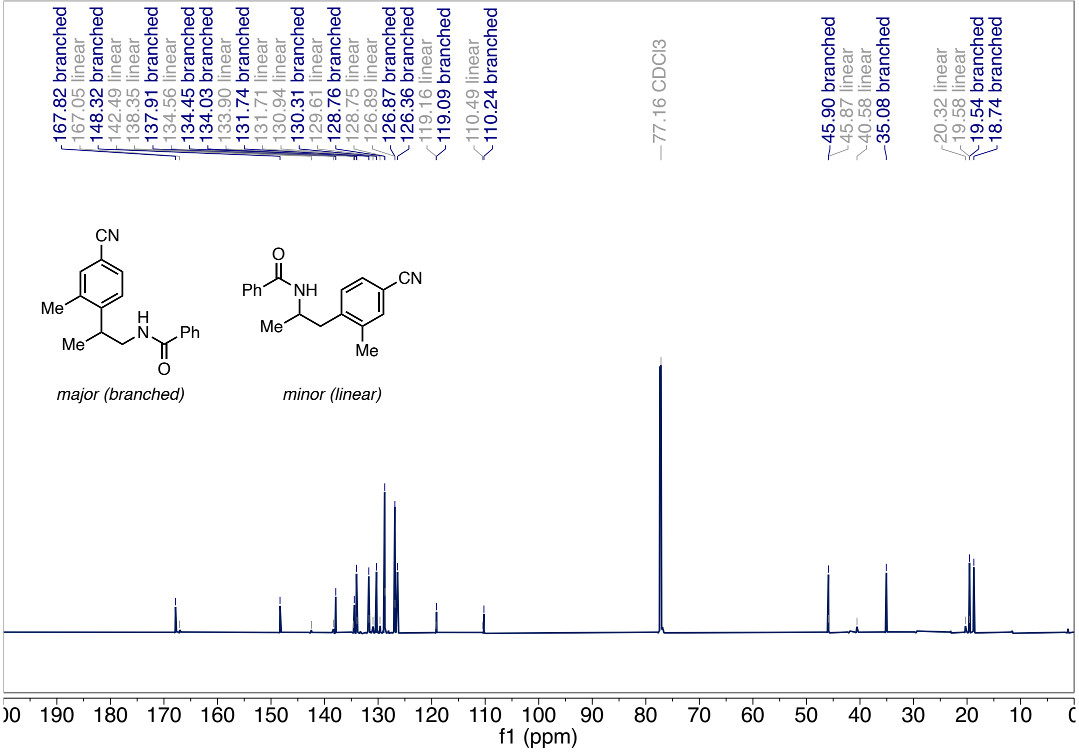


Only correlations necessary to establish branched/linear connectivity are identified.

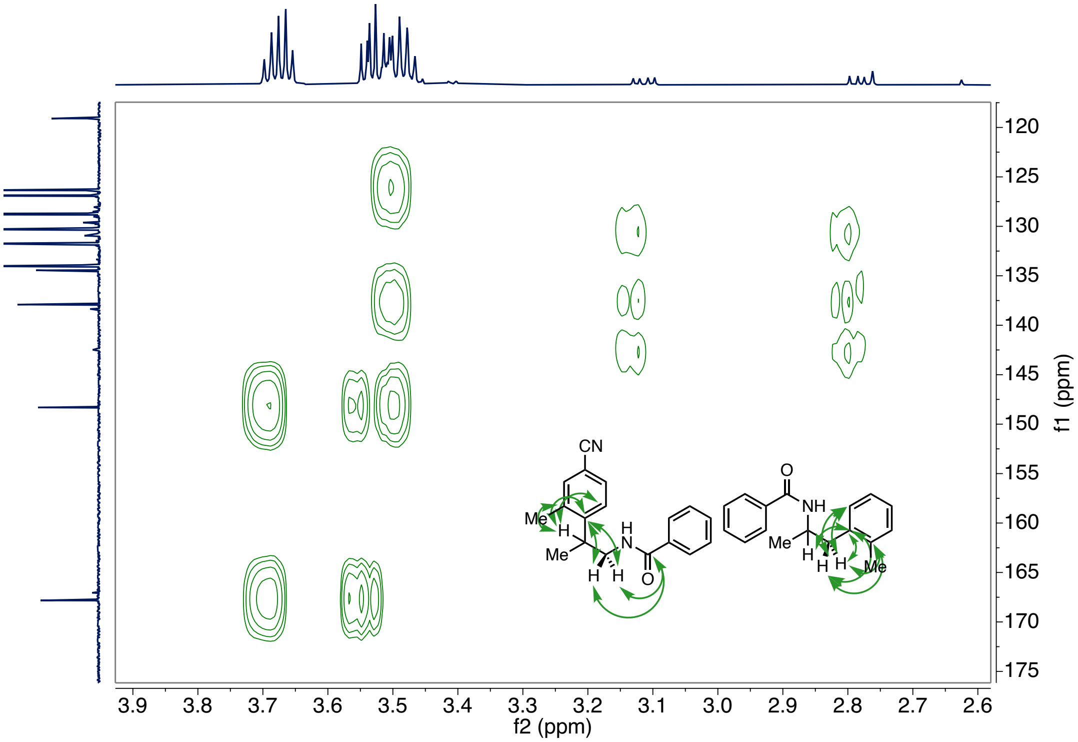
^{1}H NMR (600 MHz, CDCl$_3$) of *N*-(2-(4-cyano-2-methylphenyl)propyl)benzamide (L-2), mixture of isomers (9:1):



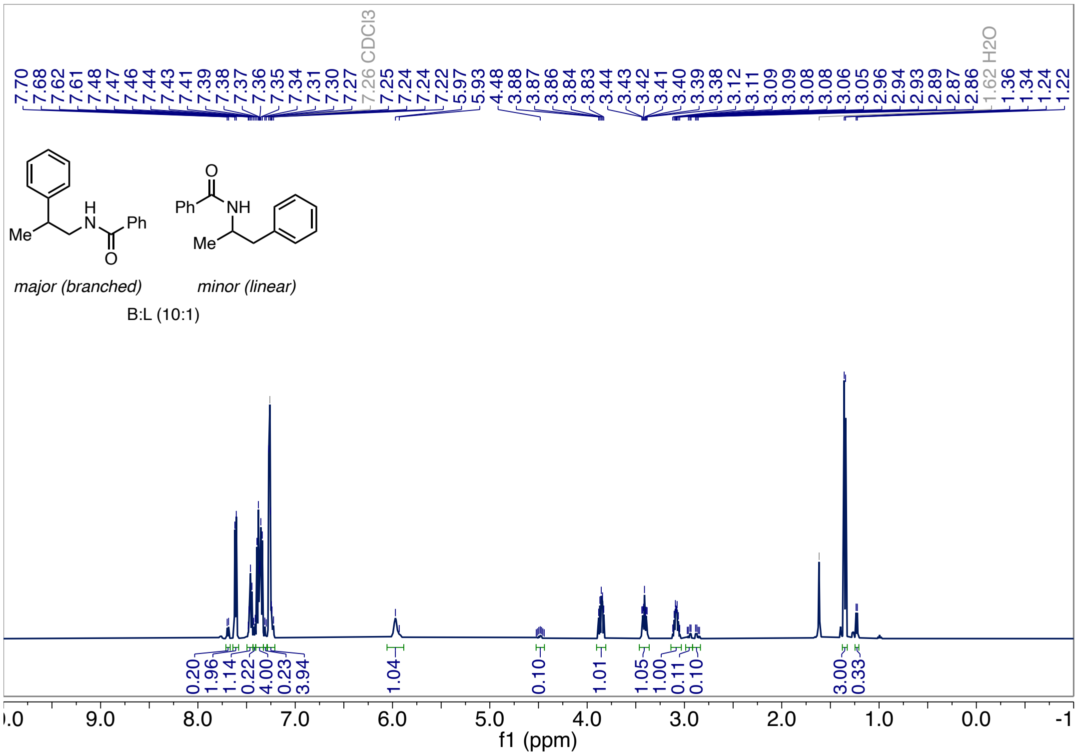
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of *N*-(2-(4-cyano-2-methylphenyl)propyl)benzamide (L-2), mixture of isomers (9:1):



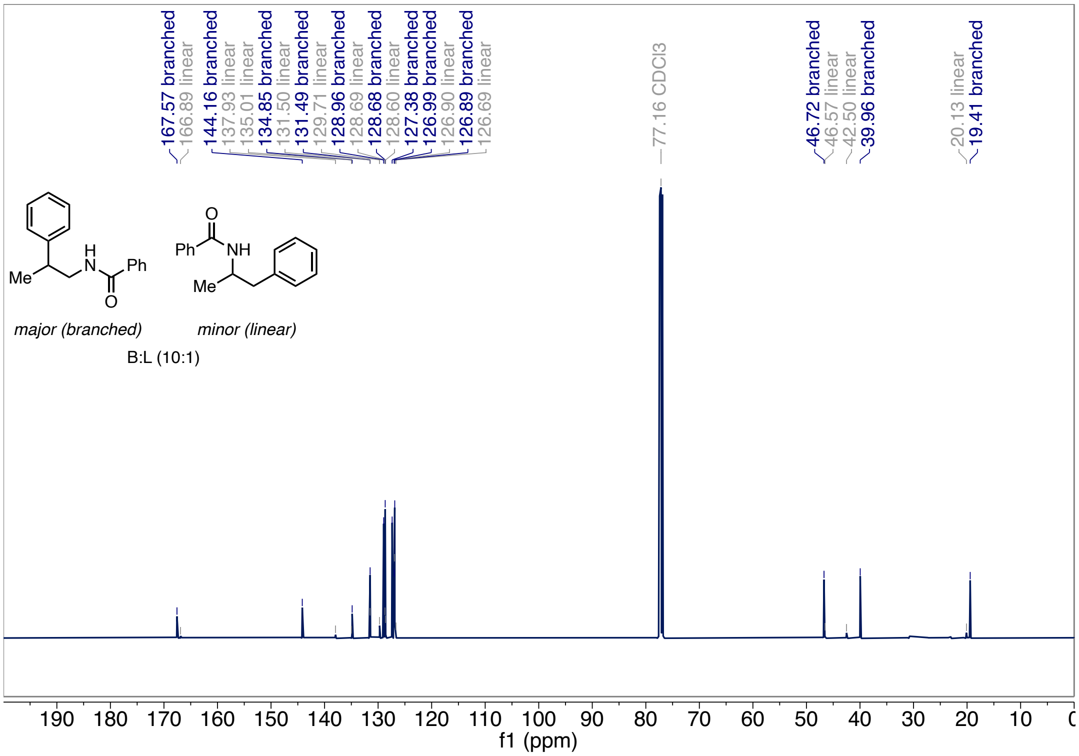
HMBC (600 MHz, CDCl$_3$) of *N*-(2-(4-cyano-2-methylphenyl)propyl)benzamide (L-2), mixture of isomers (9:1):



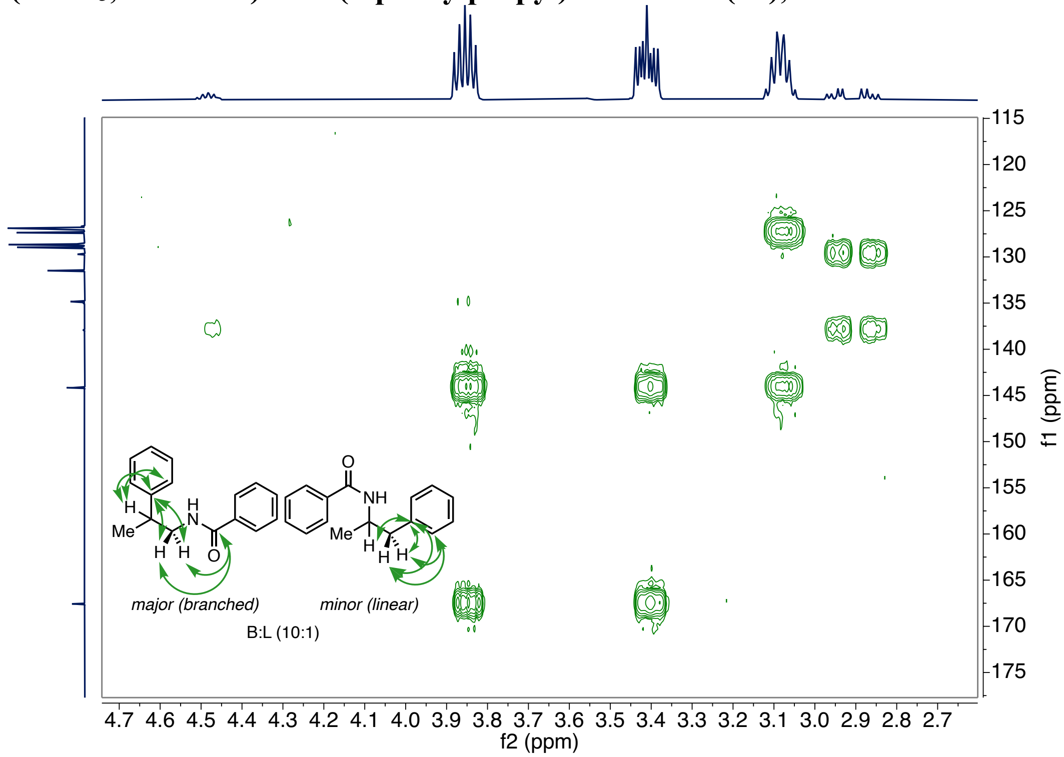
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-phenylpropyl)benzamide (1b), mixture of isomers (10:1):



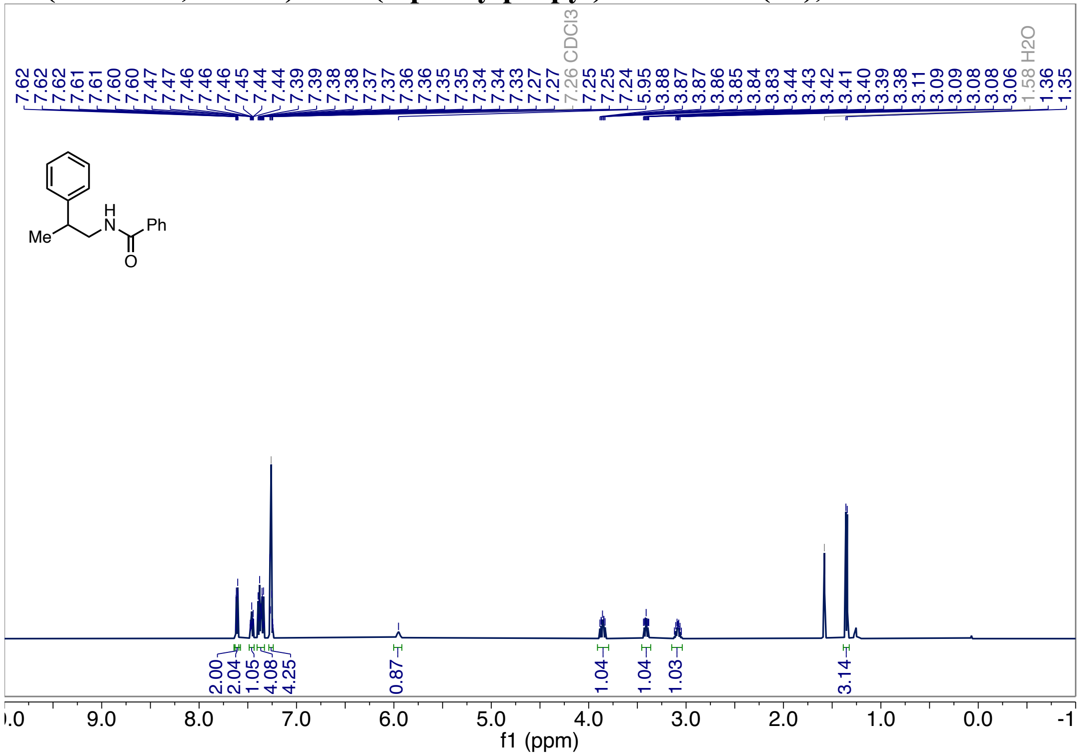
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-phenylpropyl)benzamide (1b), mixture of isomers (10:1):



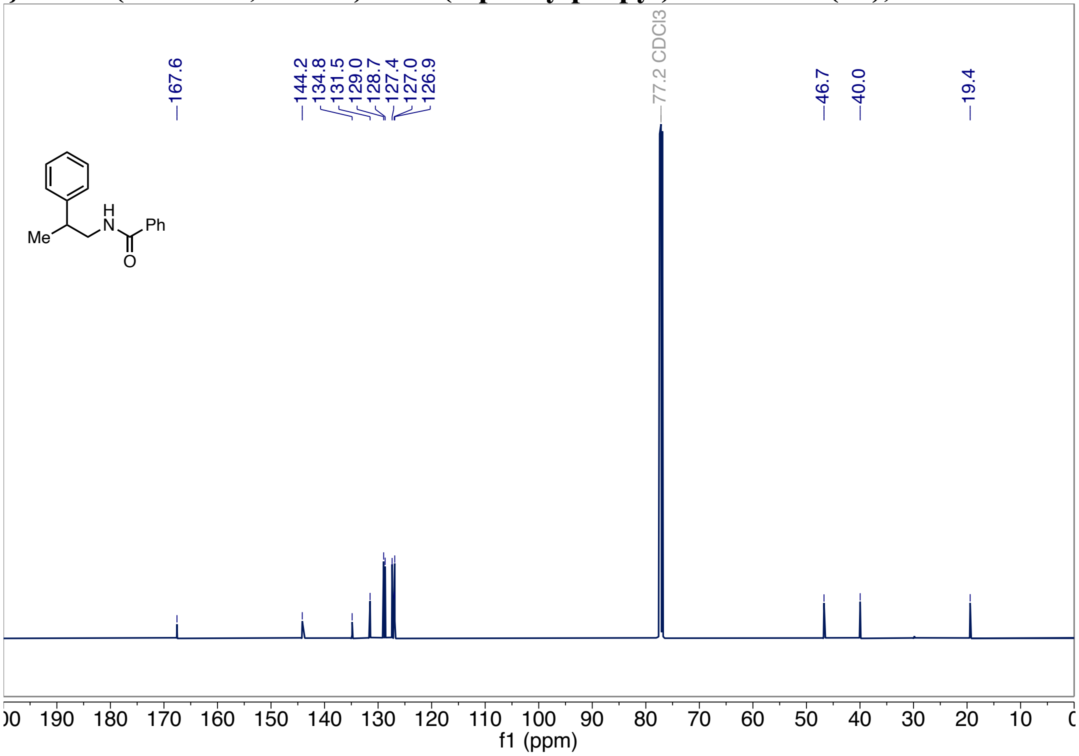
HMBC (CDCl$_3$, 500 MHz) of *N*-(2-phenylpropyl)benzamide (1b), mixture of isomers (10:1):



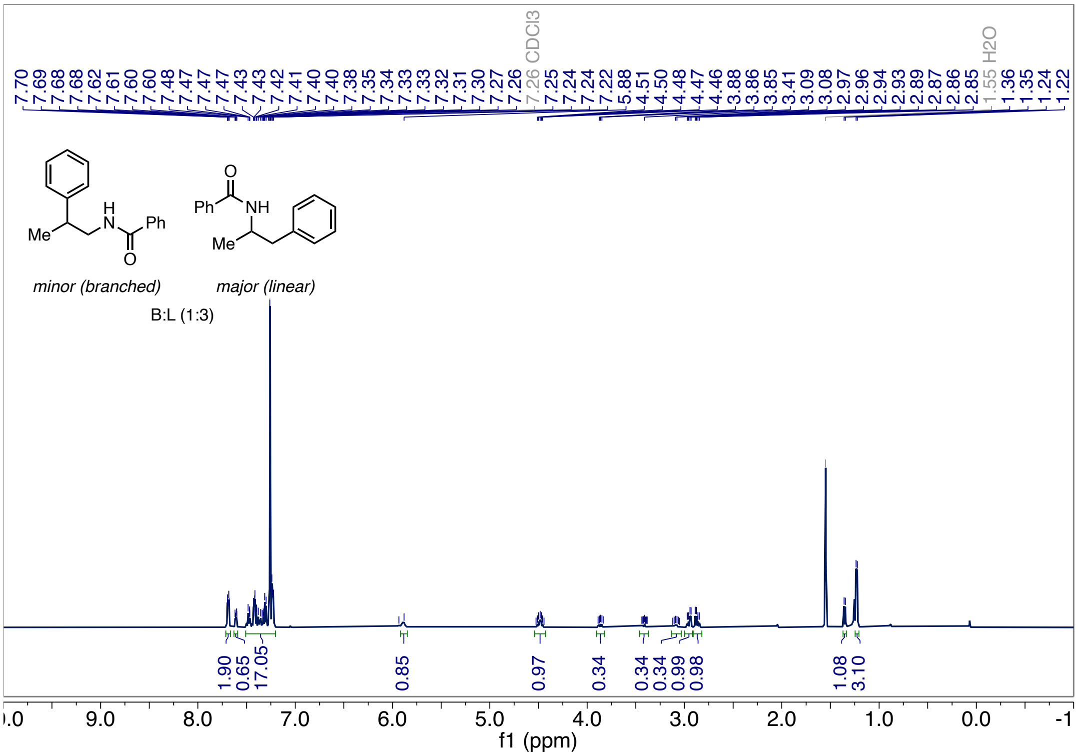
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-phenylpropyl)benzamide (1b), branched isomer:



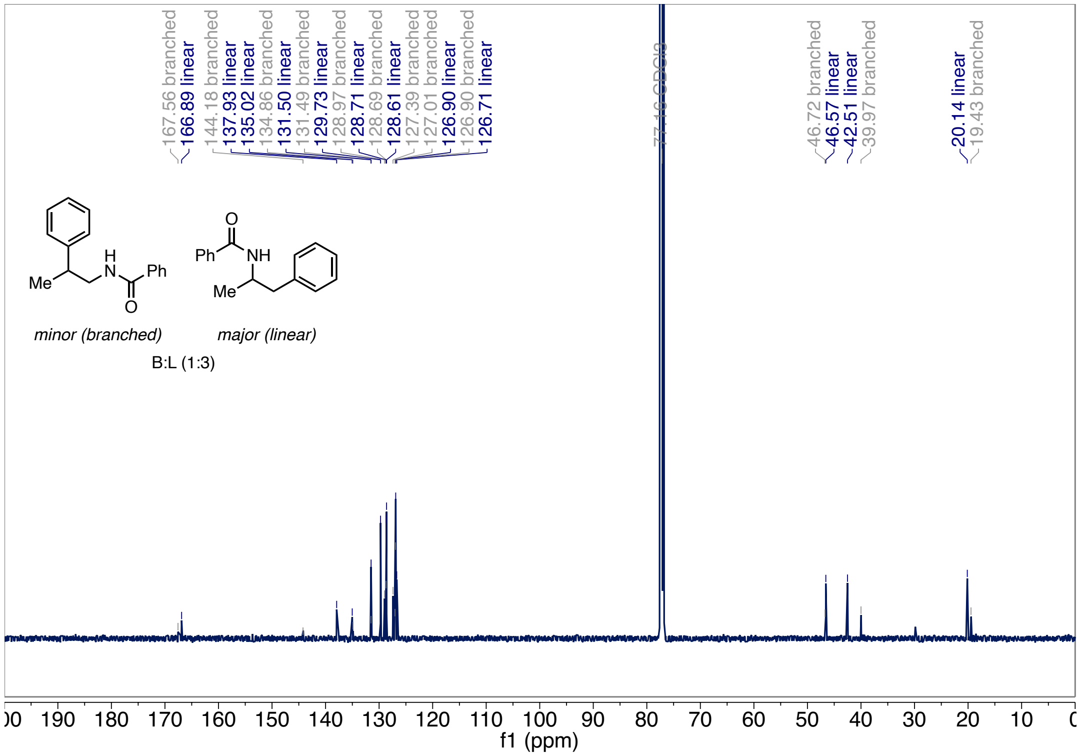
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) of *N*-(2-phenylpropyl)benzamide (1b), branched isomer:



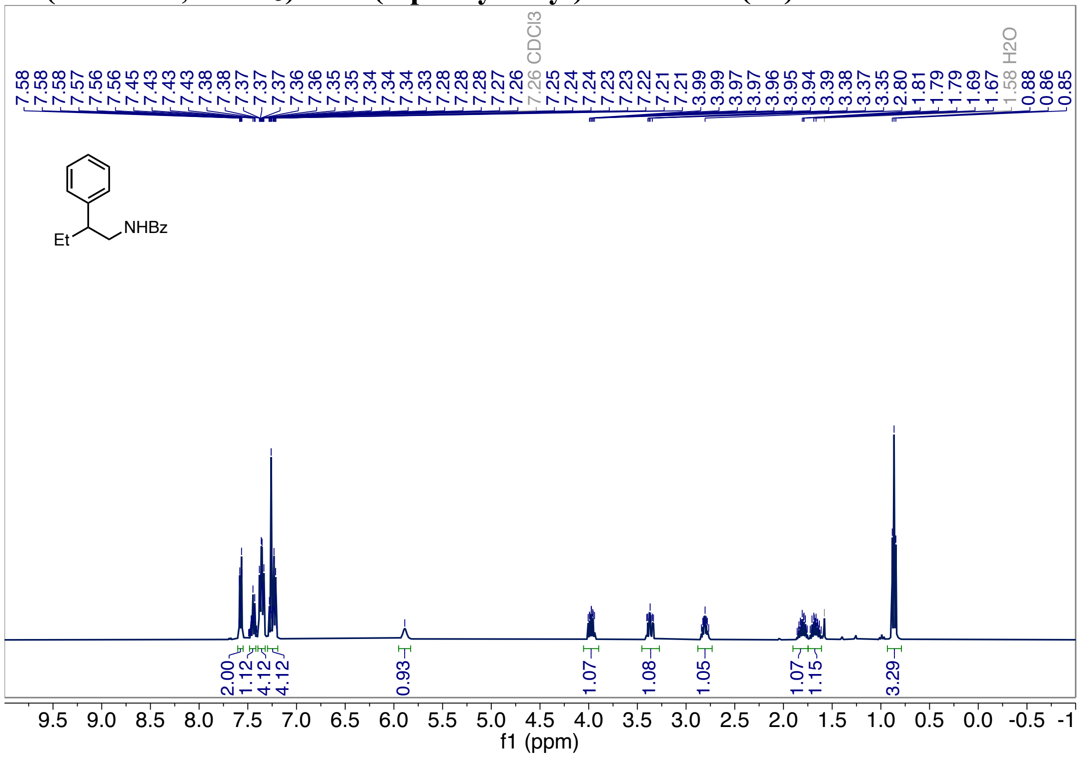
^1H NMR (500 MHz, $CDCl_3$) of *N*-(2-phenylpropyl)benzamide (1b), mixture of isomers (1:3):



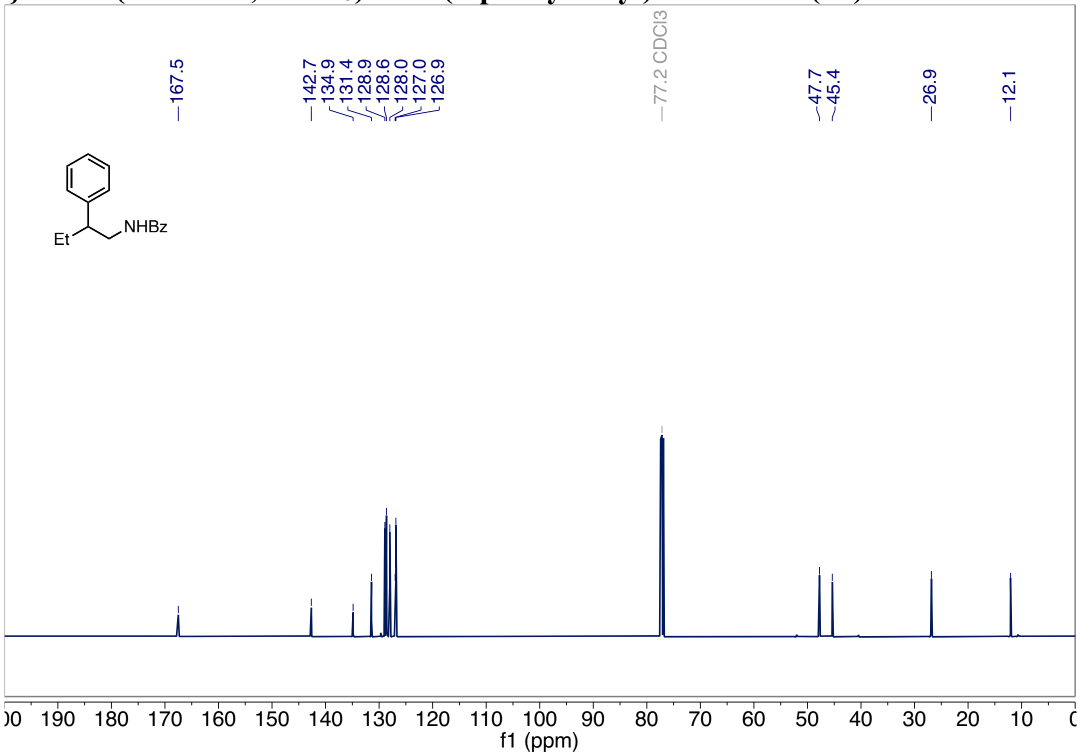
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-phenylpropyl)benzamide (1b), mixture of isomers (1:3):



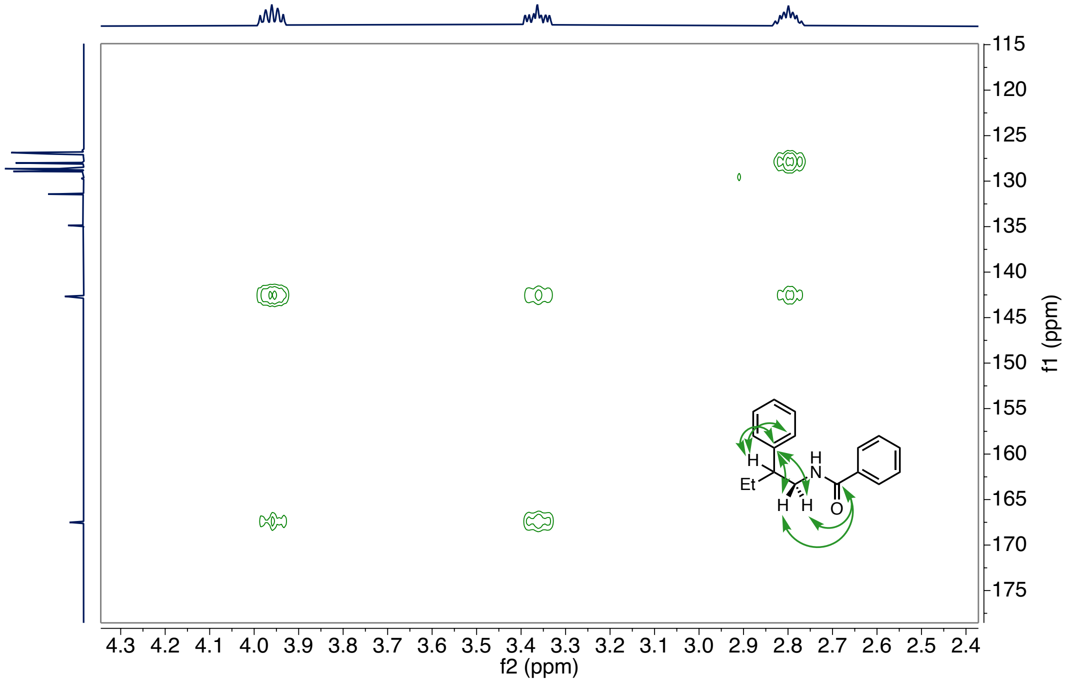
^{1}H NMR (400 MHz, CDCl$_3$) of *N*-(2-phenylbutyl)benzamide (2b):



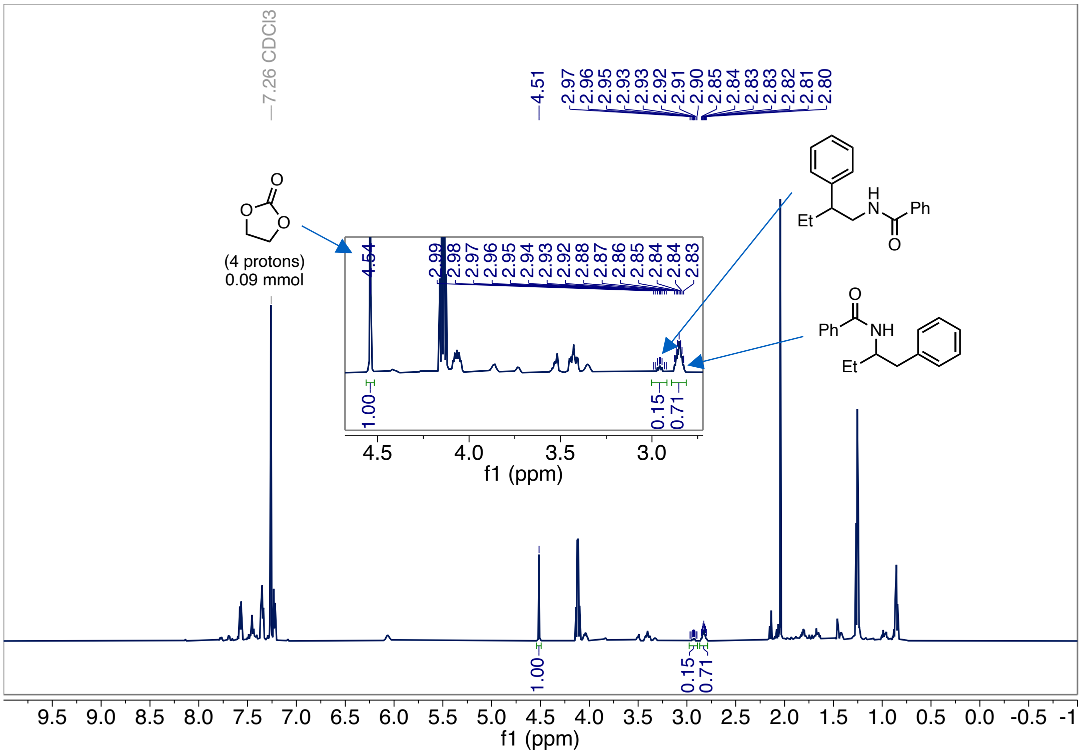
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-phenylbutyl)benzamide (2b):



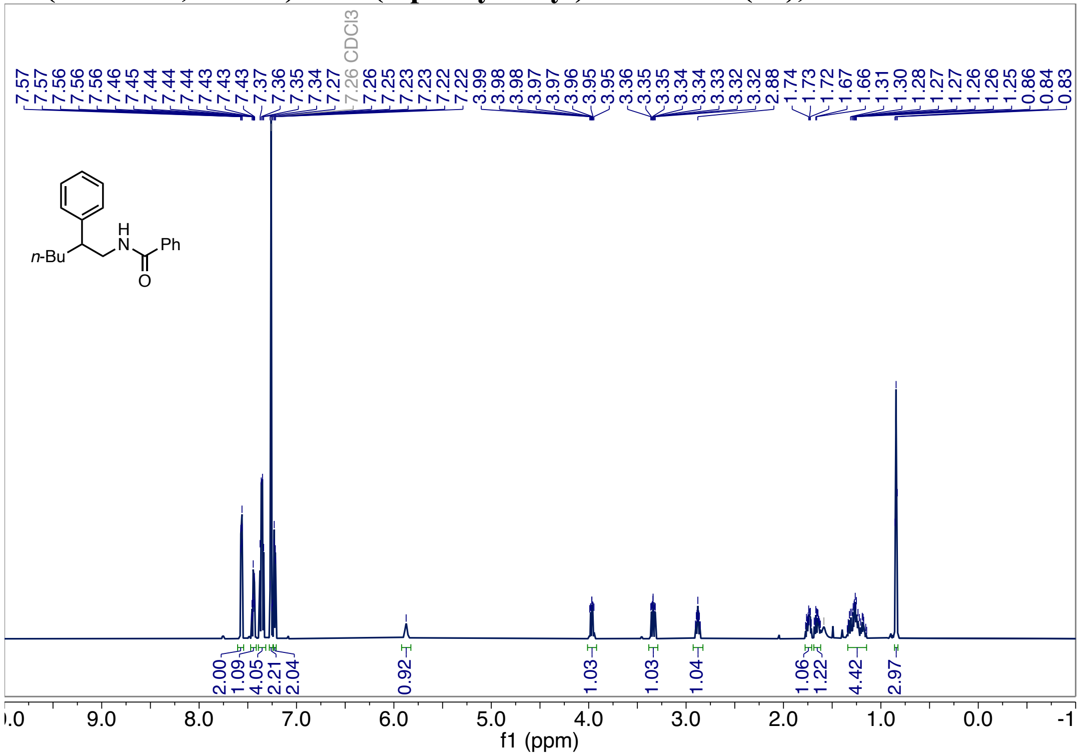
HMBC (CDCl$_3$, 500 MHz) of *N*-(2-phenylpropyl)benzamide (2b):



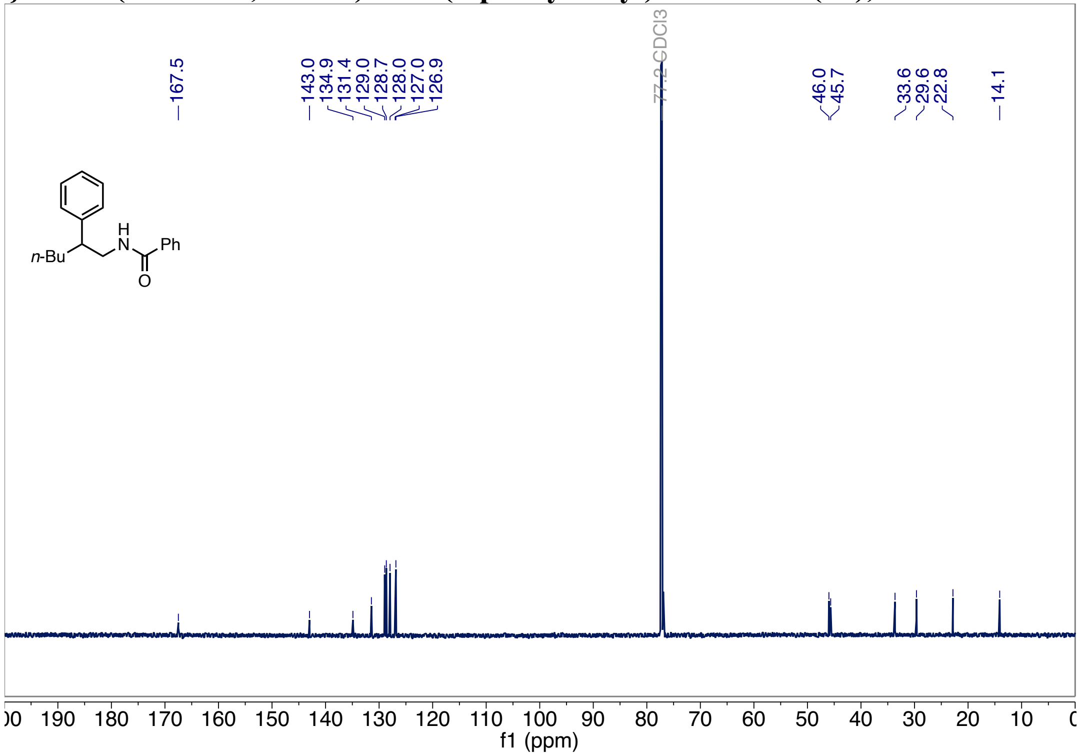
^{1}H NMR (600 MHz, CDCl$_3$) yield of *N*-(2-phenylbutyl)benzamide (2b) versus ethylene carbonate:



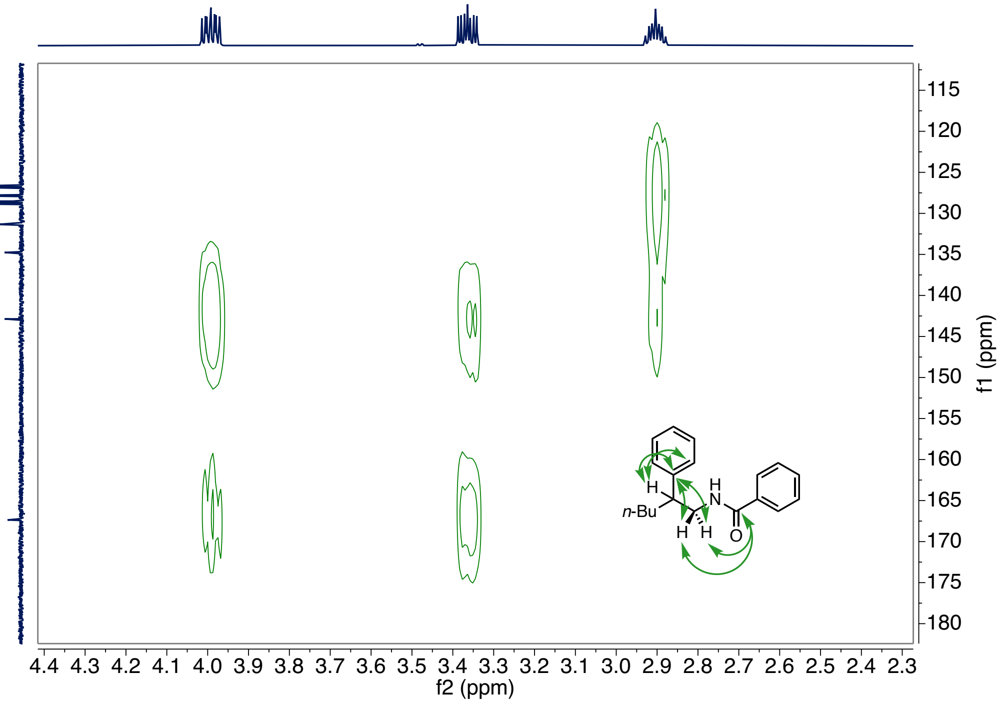
^{1}H NMR (600 MHz, CDCl$_3$) of *N*-(2-phenylhexyl)benzamide (3b), branched isomer:



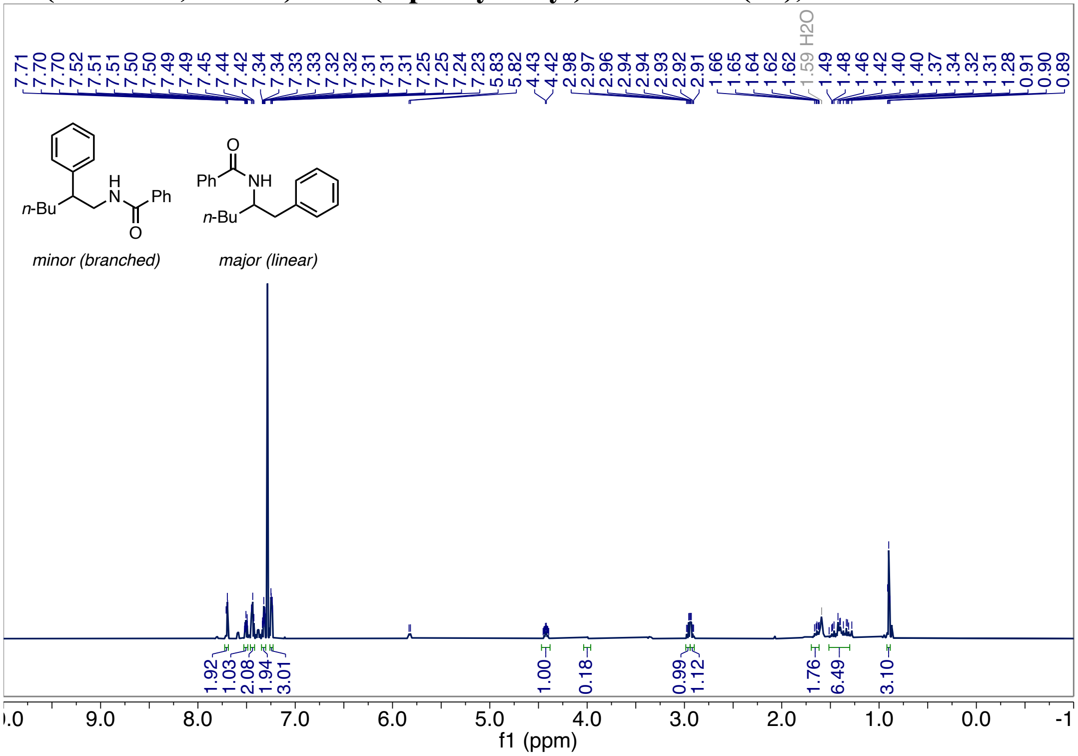
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of *N*-(2-phenylhexyl)benzamide (3b), branched isomer:



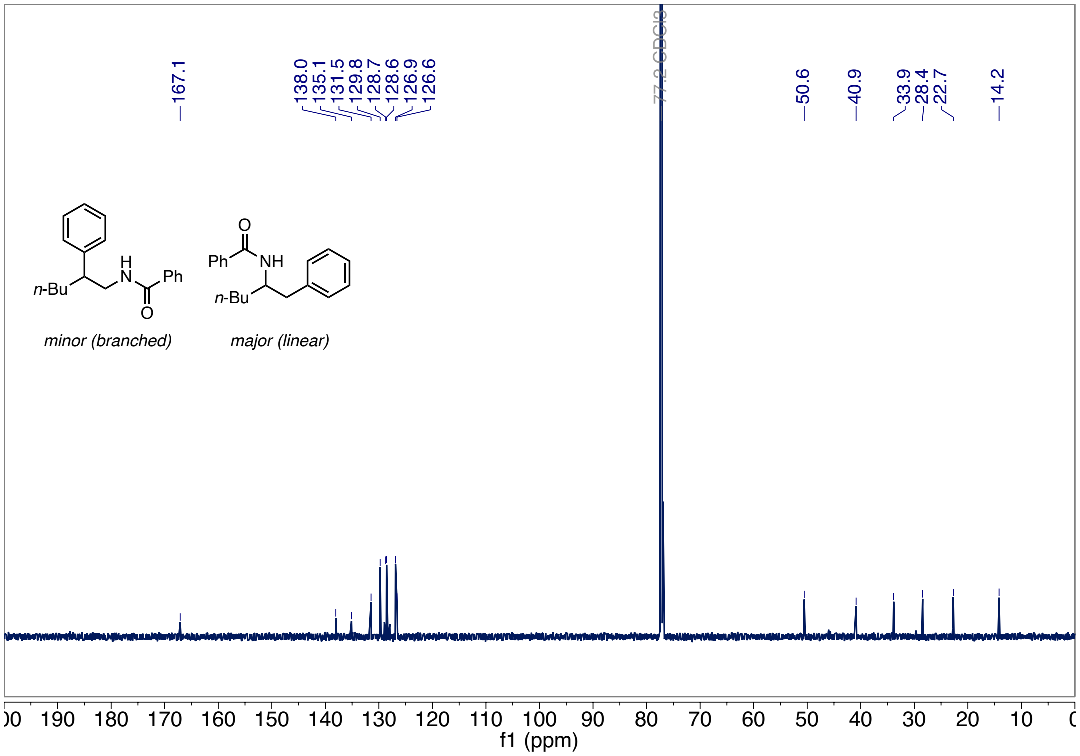
HMBC (600 MHz, $CDCl_3$) of *N*-(2-phenylhexyl)benzamide (3b), branched isomer:



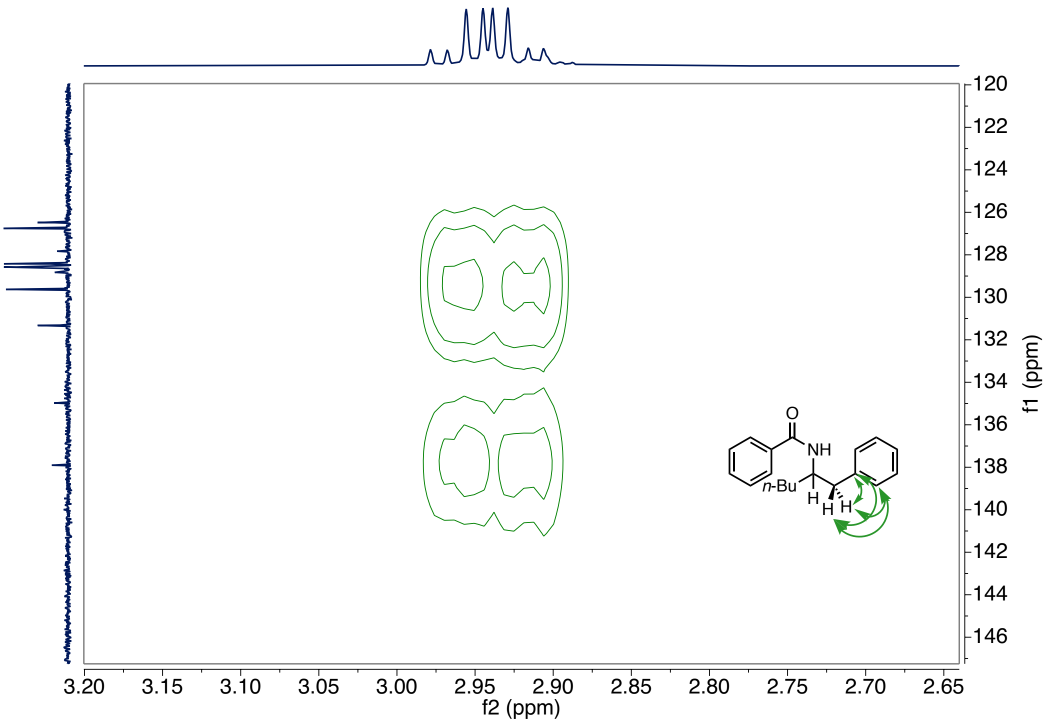
^{1}H NMR (600 MHz, $CDCl_3$) of *N*-(2-phenylhexyl)benzamide (3b), mixture of isomers (1:5):



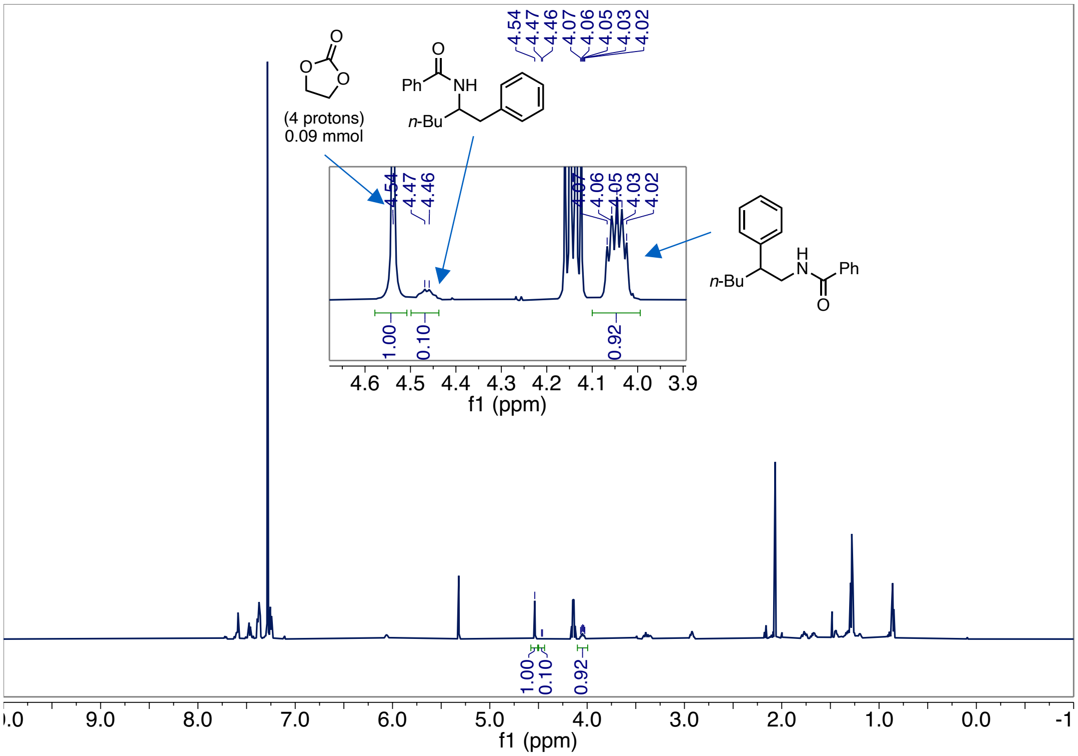
$^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) of *N*-(2-phenylhexyl)benzamide (3b), mixture of isomers (1:5):



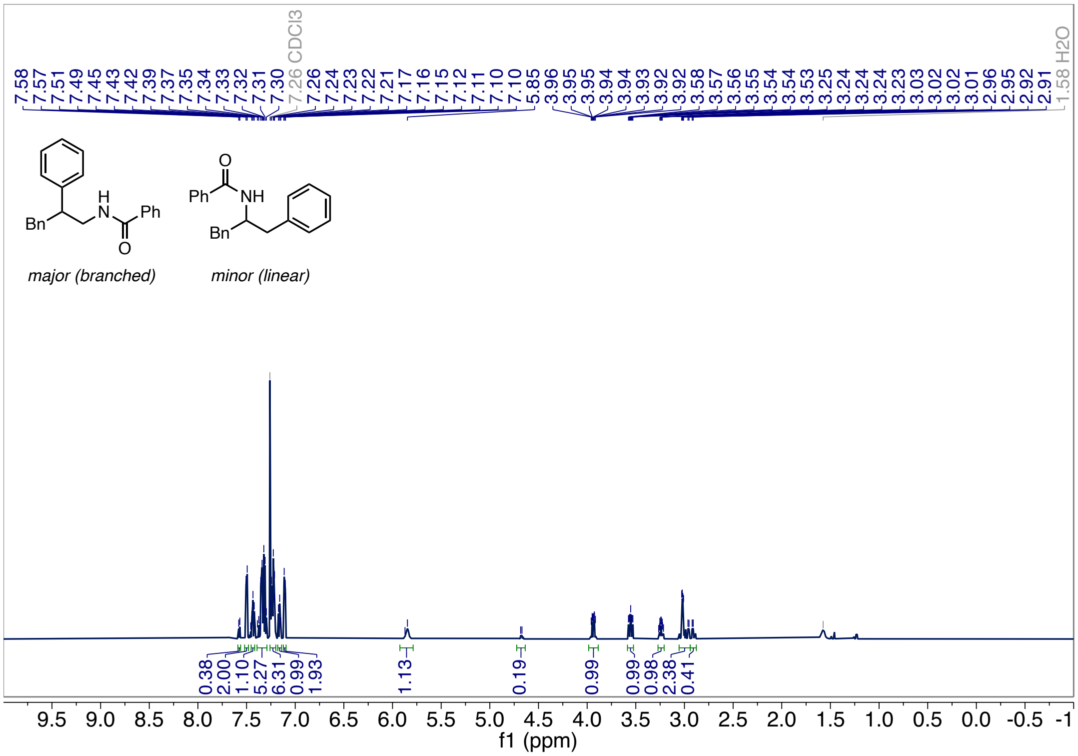
HMBC (600 MHz, $CDCl_3$) of *N*-(2-phenylhexyl)benzamide (3b), mixture of isomers (1:5):



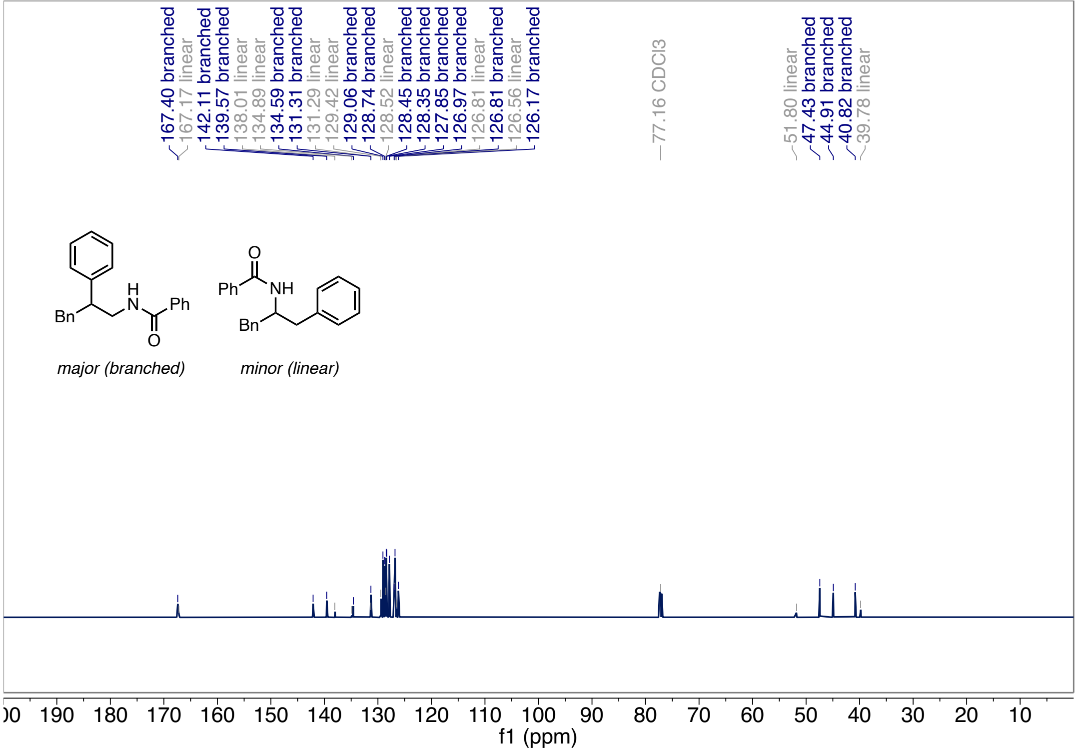
^{1}H NMR (600 MHz, CDCl$_3$) yield of *N*-(2-phenylhexyl)benzamide (3b) versus ethylene carbonate:



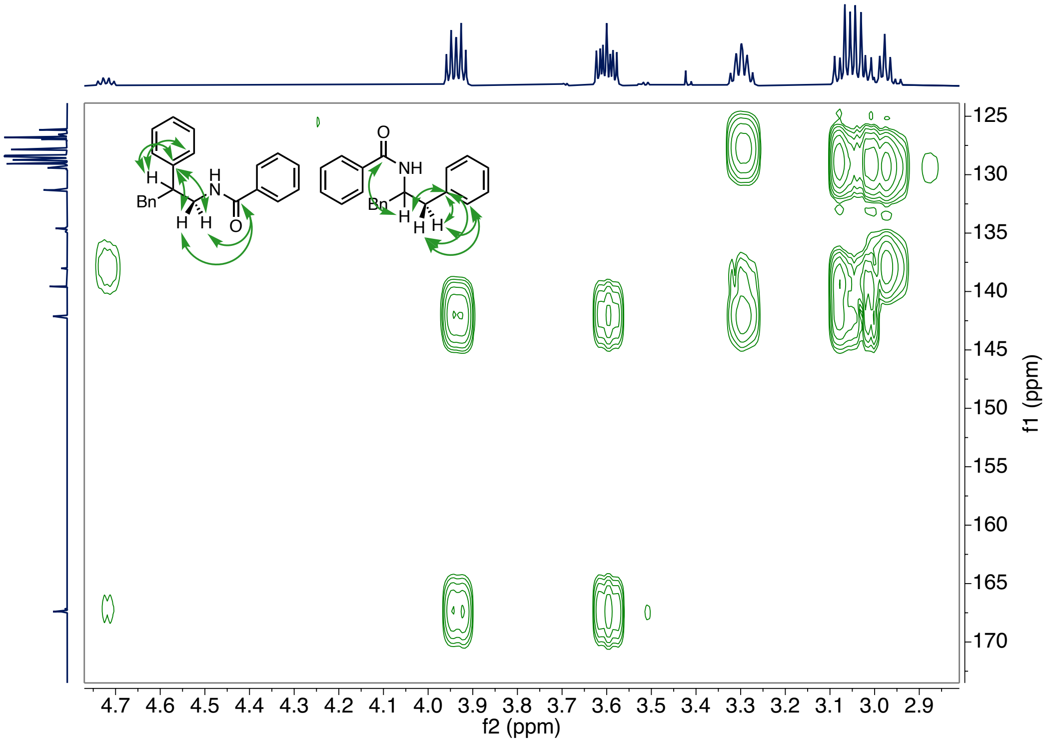
^{1}H NMR (600 MHz, CDCl$_3$) of *N*-(2,3-diphenylpropyl)benzamide (4b), mixture of isomers (5:1):



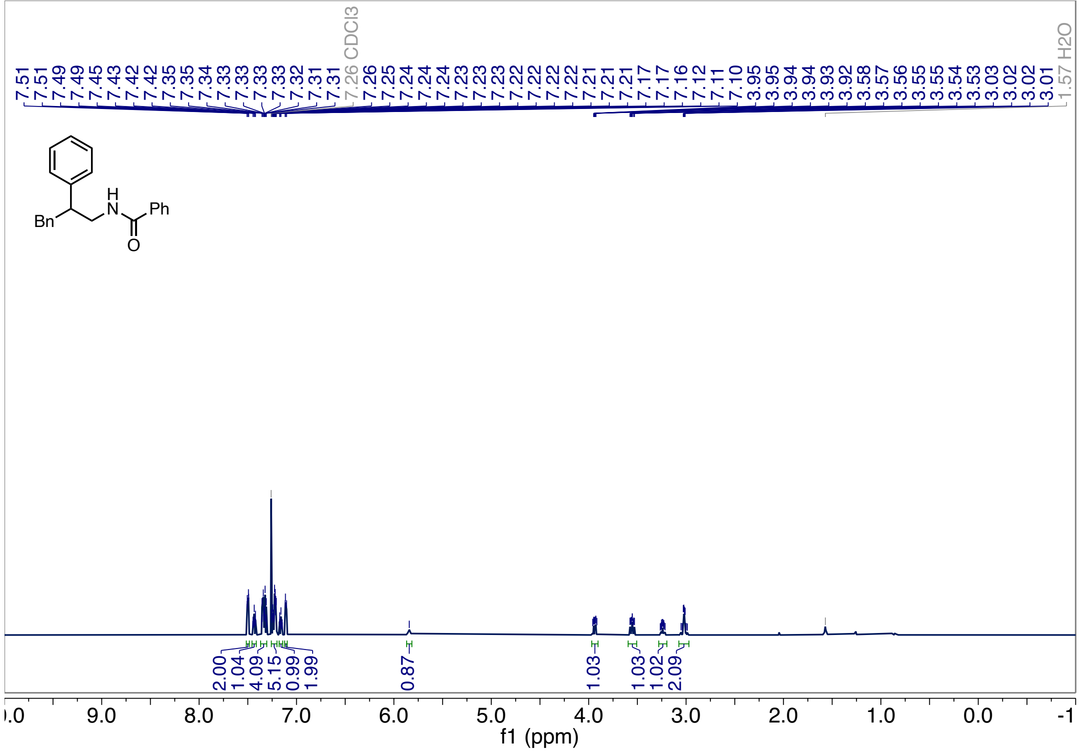
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of *N*-(2,3-diphenylpropyl)benzamide (4b), mixture of isomers (5:1):



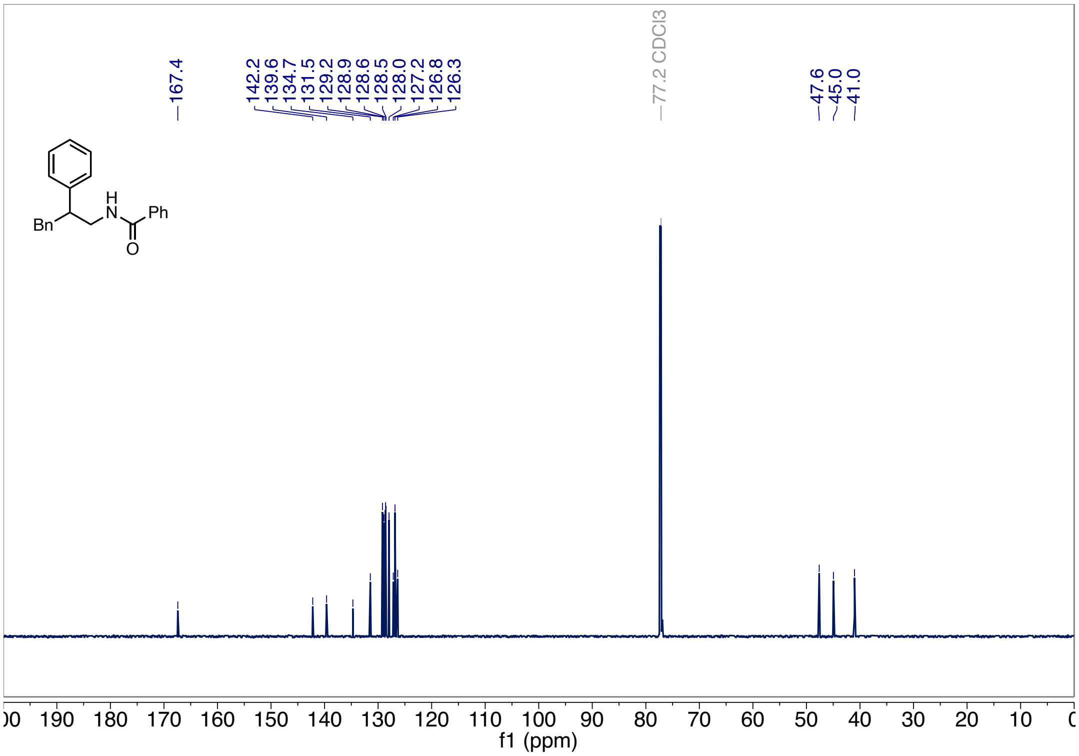
HMBC (600 MHz, $CDCl_3$) of *N*-(2,3-diphenylpropyl)benzamide (4b), mixture of isomers (5:1):



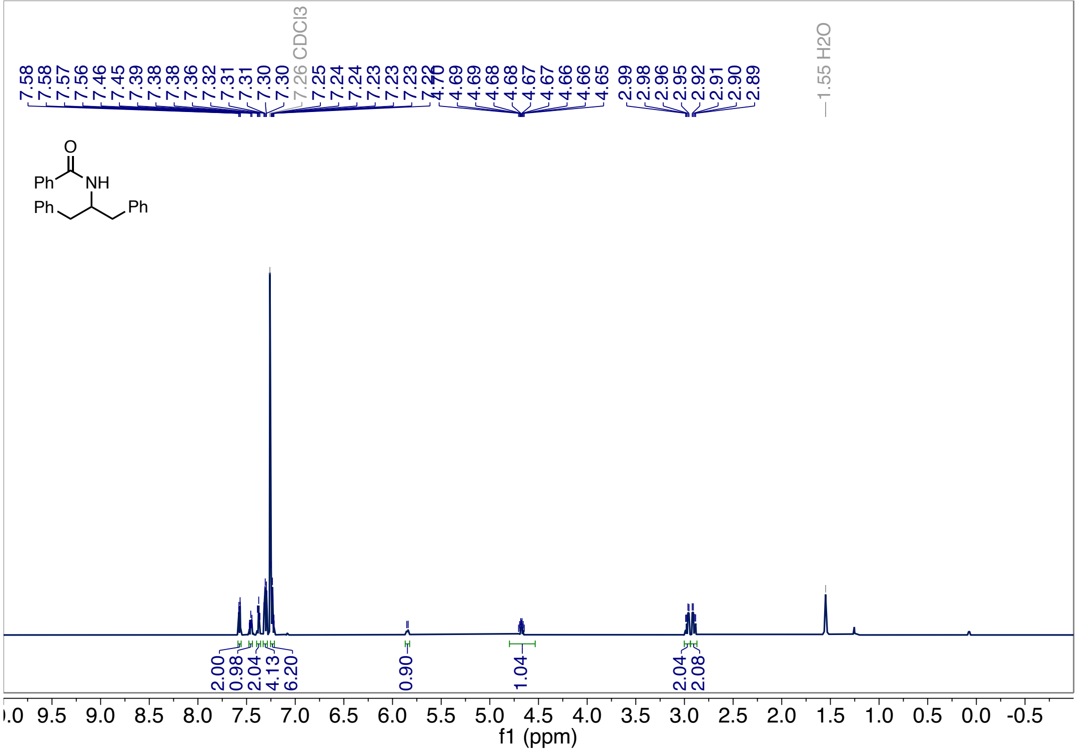
^{1}H NMR (600 MHz, $CDCl_3$) of *N*-(2,3-diphenylpropyl)benzamide (4b), branched isomer:



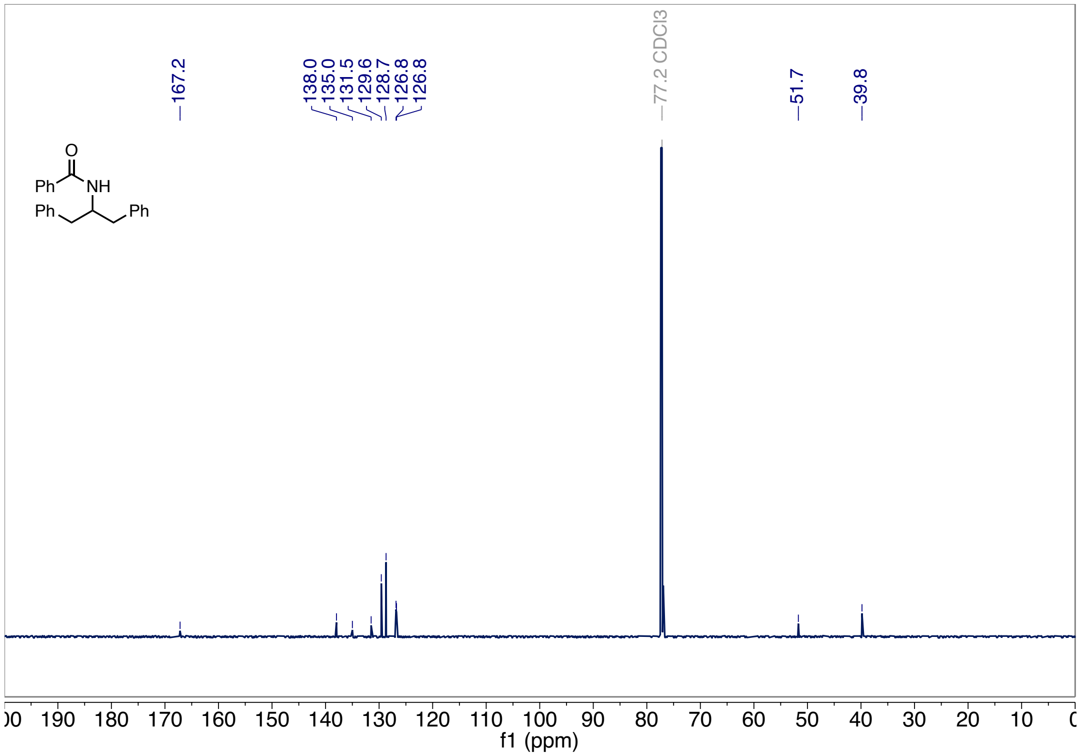
$^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) of *N*-(2,3-diphenylpropyl)benzamide (4b), branched isomer:



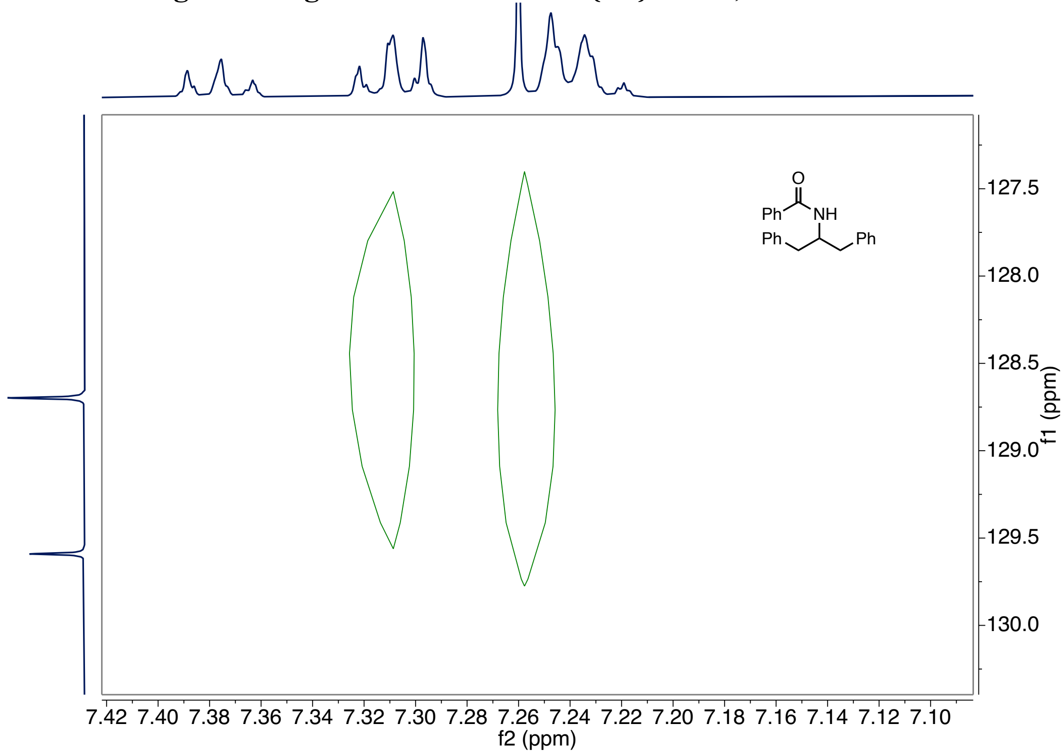
^1H NMR (600 MHz, $CDCl_3$) of *N*-(1,3-diphenylpropan-2-yl)benzamide (4b), linear isomer:



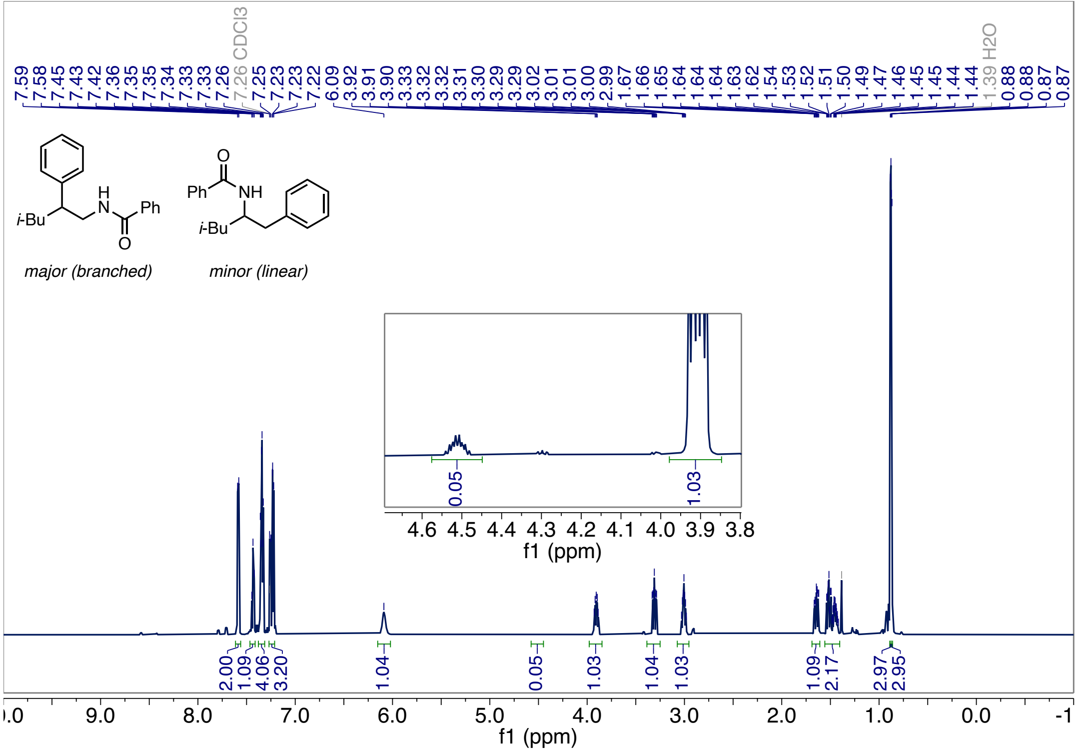
$^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) of *N*-(1,3-diphenylpropan-2-yl)benzamide (4b), linear isomer:



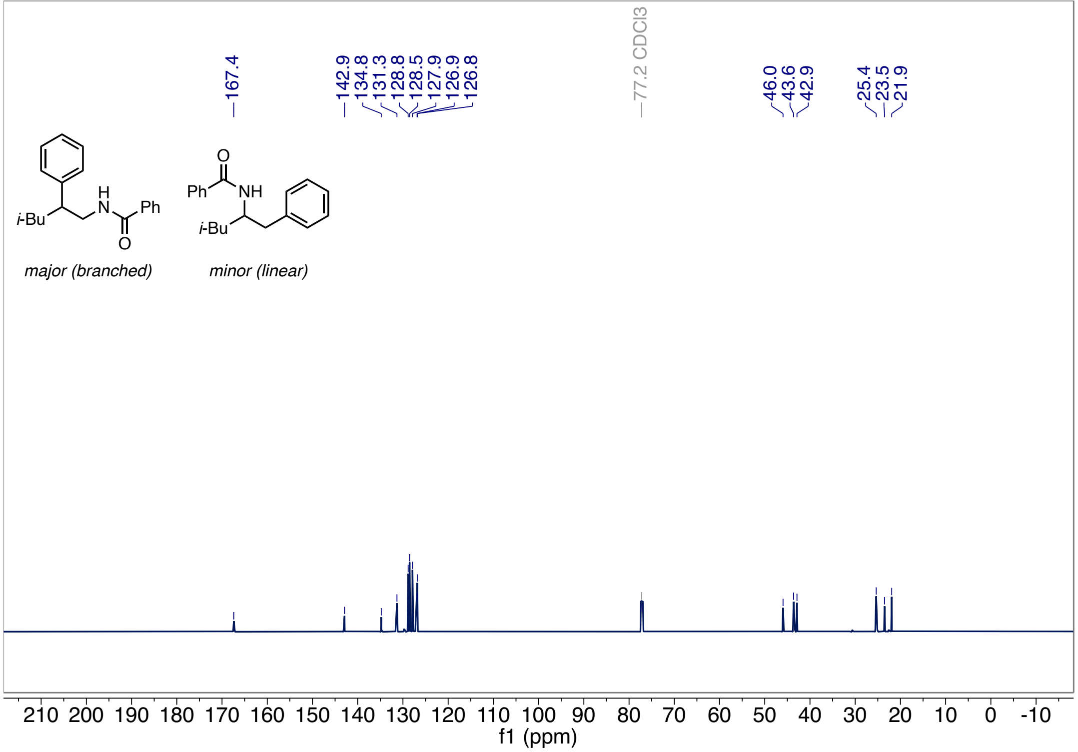
HSQC (600 MHz, $CDCl_3$) of *N*-(1,3-diphenylpropan-2-yl)benzamide (4b) to demonstrate two carbons contributing to the signal at δ 128.7 in $^{13}C\{^1H\}$ NMR, linear isomer:



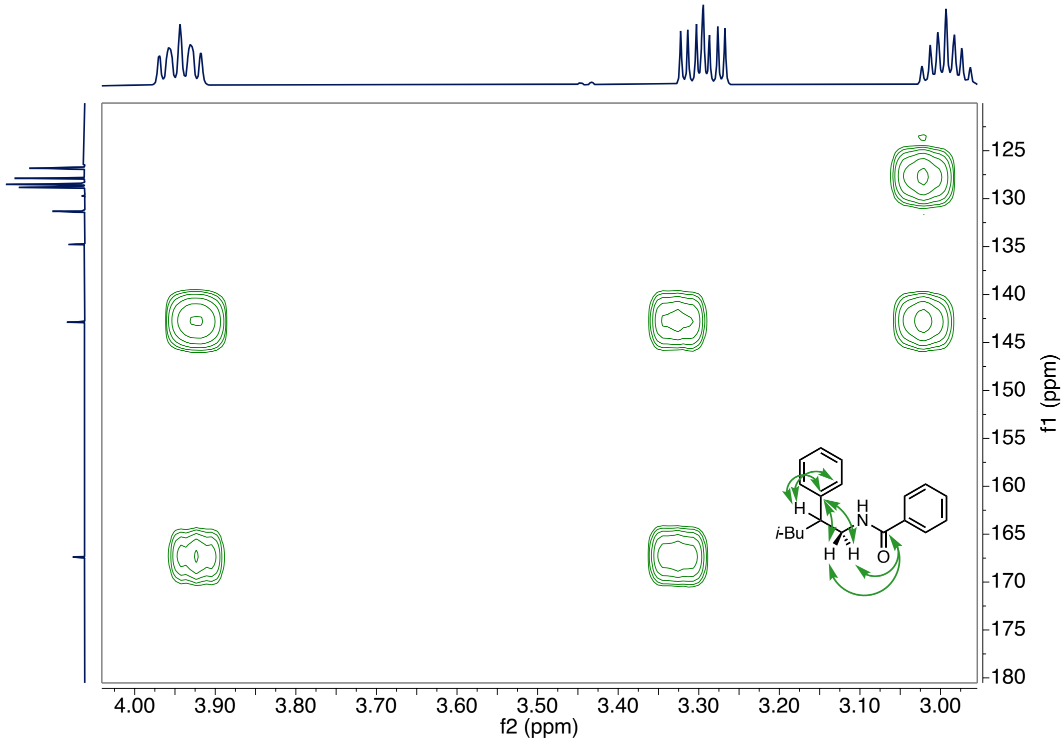
^{1}H NMR (600 MHz, CDCl$_3$) of N-(4-methyl-2-phenylpentyl)benzamide (5b), mixture of isomers (>20:1):



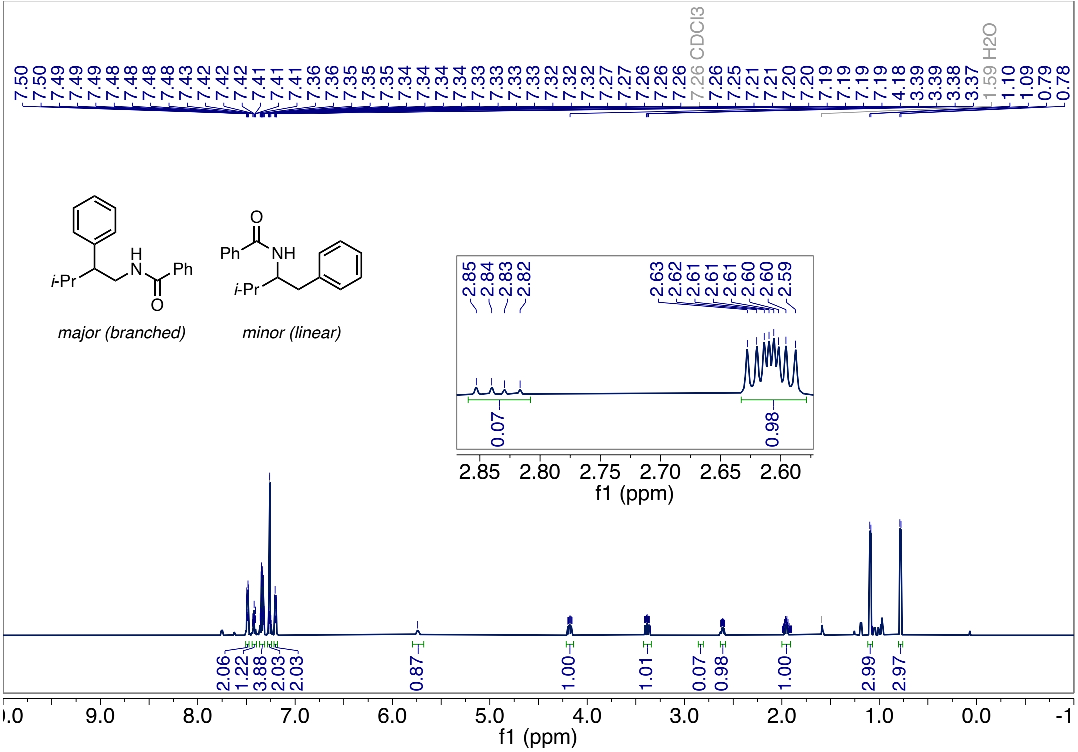
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of N-(4-methyl-2-phenylpentyl)benzamide (5b), mixture of isomers (>20:1):



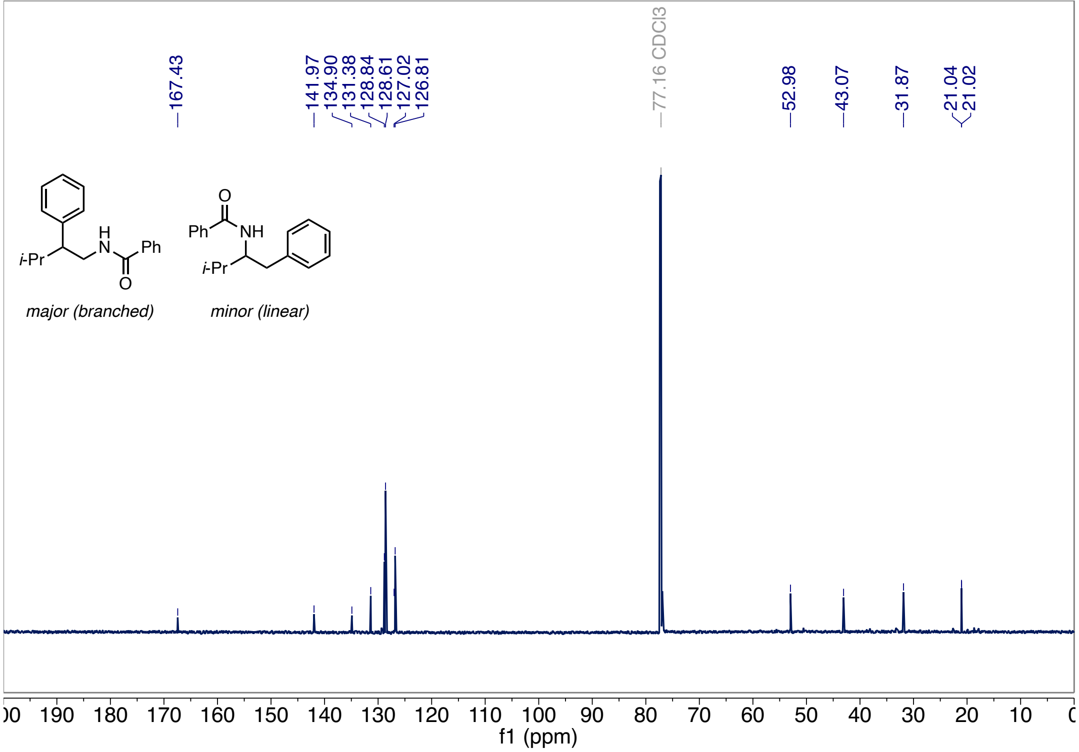
HMBC (600 MHz, CDCl$_3$) of N-(4-methyl-2-phenylpentyl)benzamide (5b), mixture of isomers (>20:1):



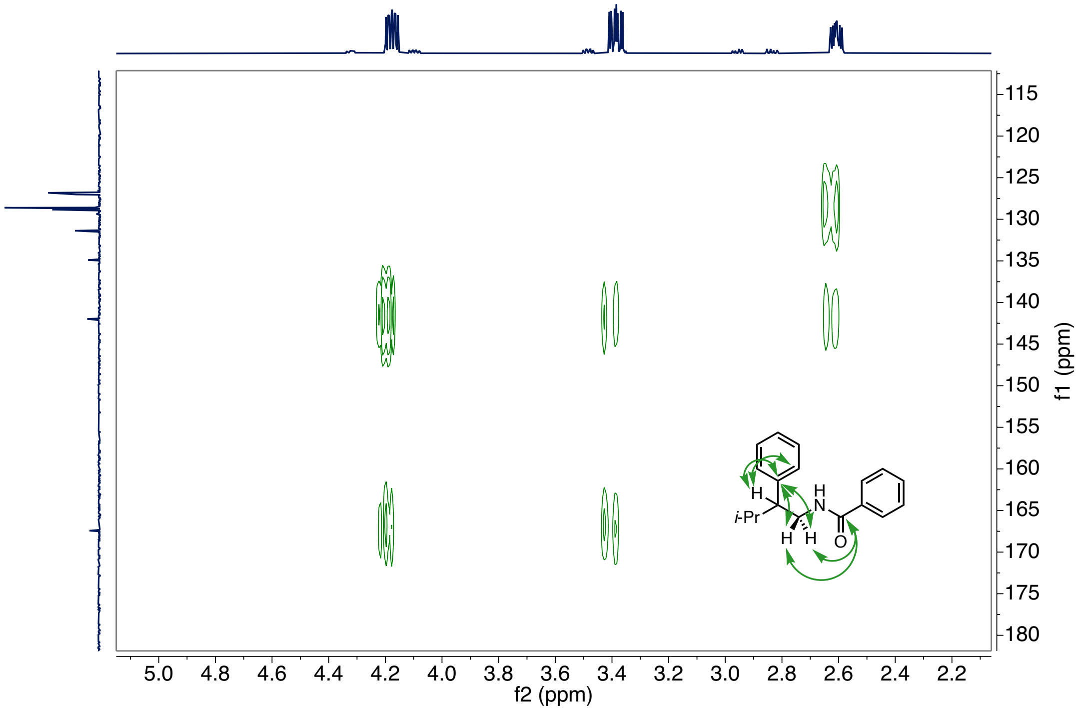
^{1}H NMR (600 MHz, CDCl$_3$) of *N*-(3-methyl-2-phenylbutyl)benzamide (6b), mixture of isomers (14:1):



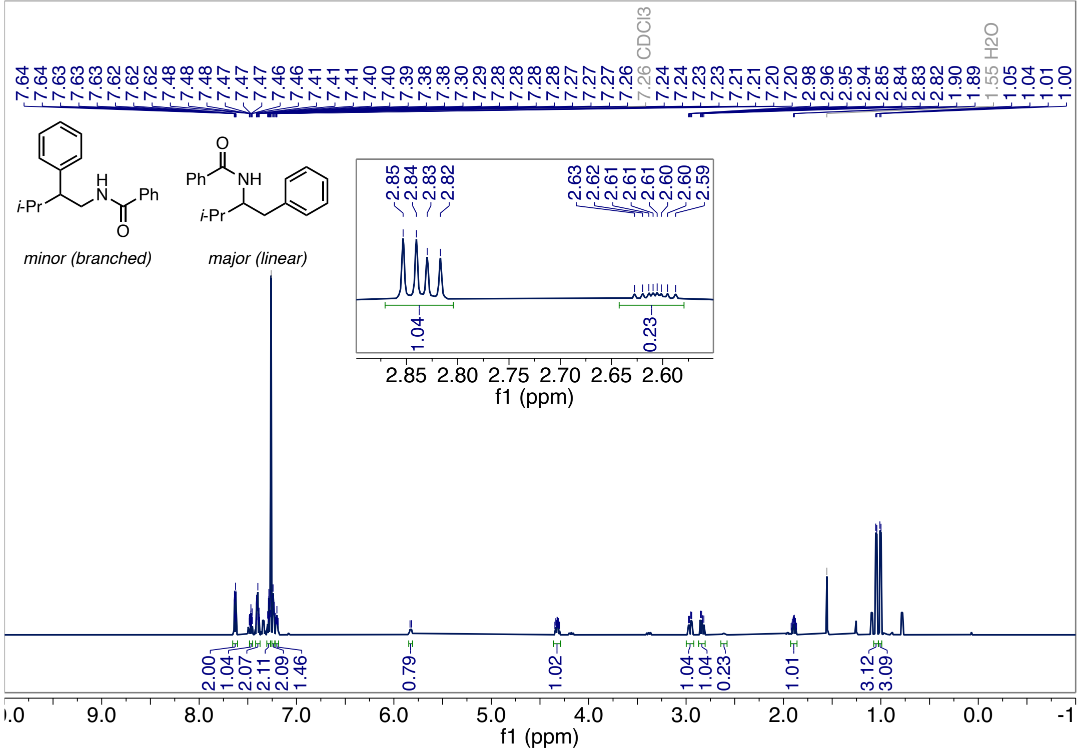
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(3-methyl-2-phenylbutyl)benzamide (6b), mixture of isomers (14:1):



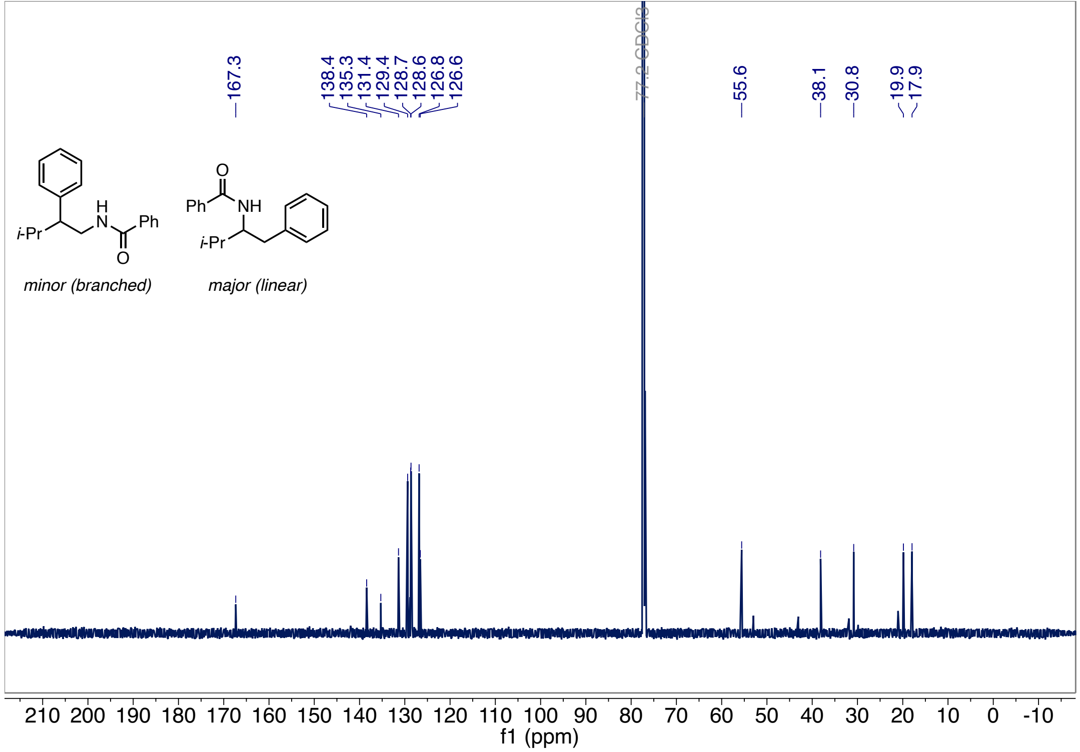
HMBC (600 MHz, $CDCl_3$) of *N*-(3-methyl-2-phenylbutyl)benzamide (6b), mixture of isomers (14:1):



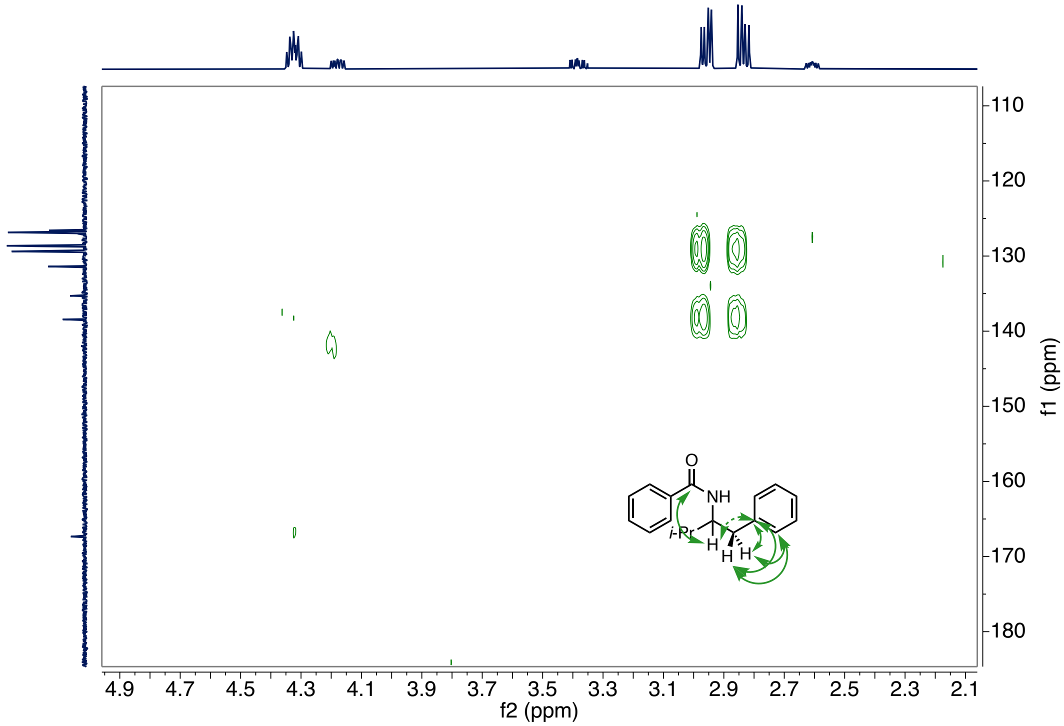
^1H NMR (600 MHz, $CDCl_3$) of *N*-(3-methyl-2-phenylbutyl)benzamide (6b), mixture of isomers (1:5):



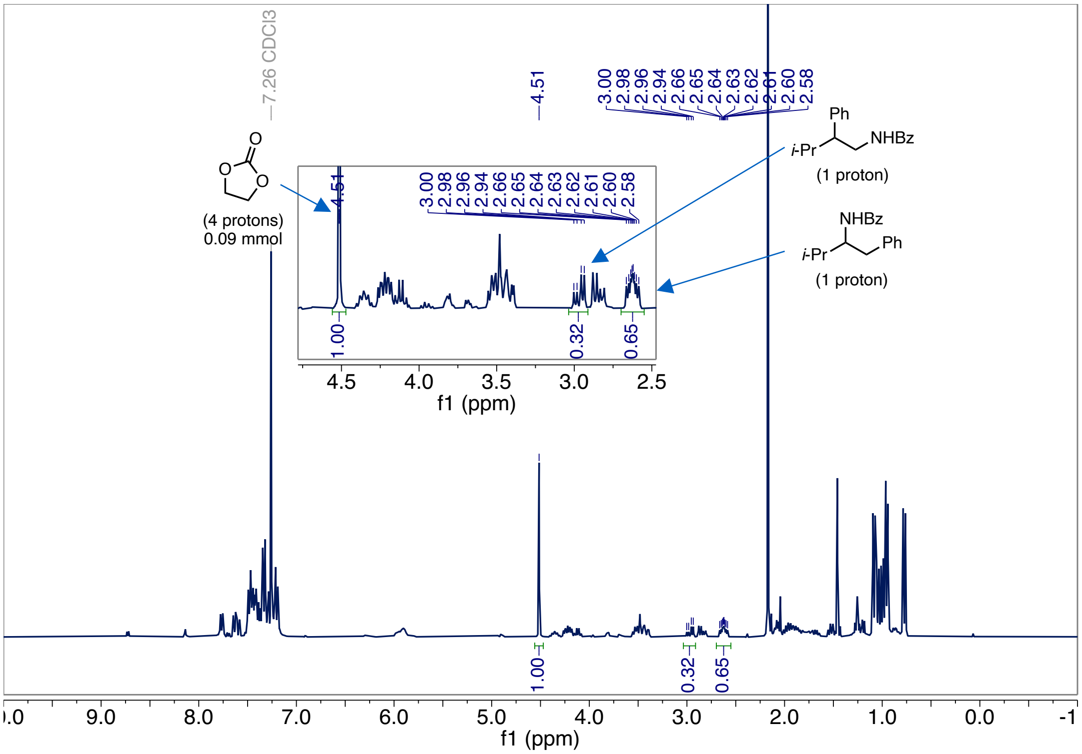
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) of *N*-(3-methyl-2-phenylbutyl)benzamide (6b), mixture of isomers (1:5):



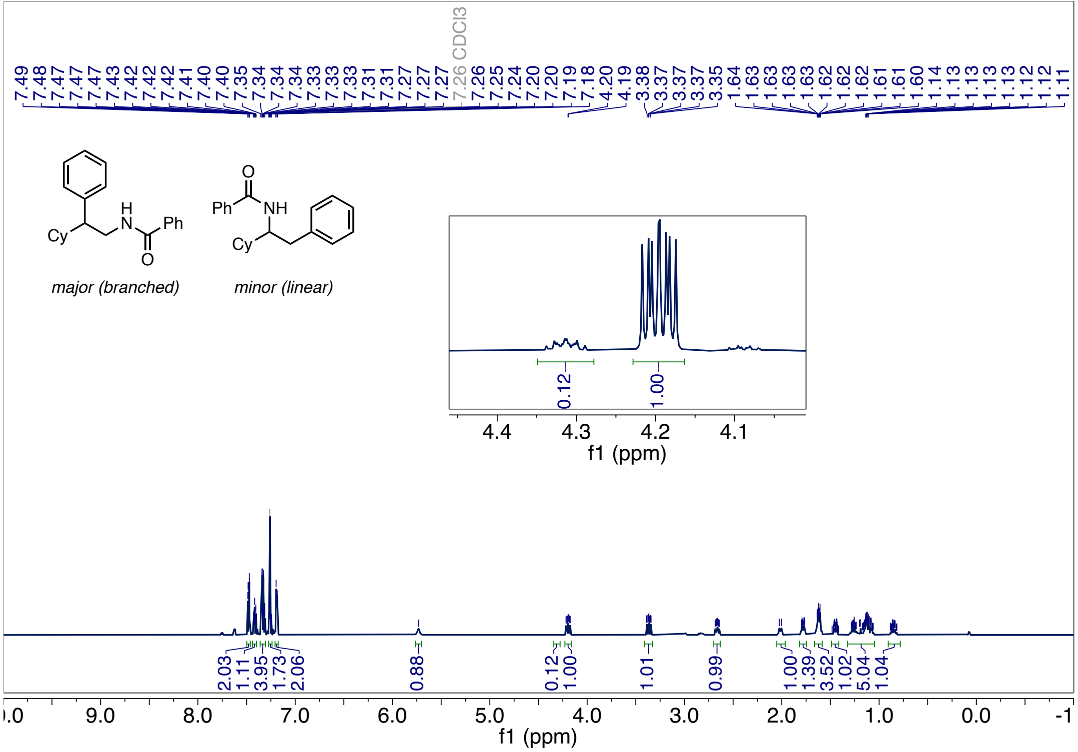
HMBC (600 MHz, $CDCl_3$) of *N*-(3-methyl-2-phenylbutyl)benzamide (6b), mixture of isomers (1:5):



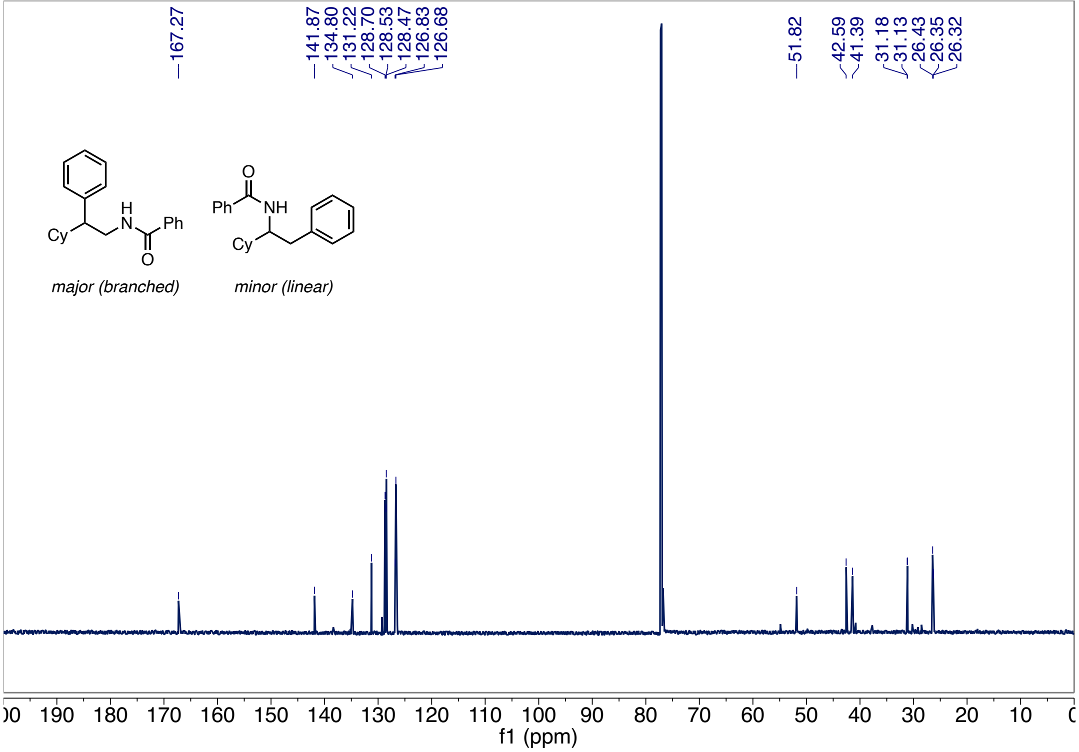
^{1}H NMR (500 MHz, CDCl$_3$) yield of *N*-(3-methyl-2-phenylbutyl)benzamide (6b) versus ethylene carbonate:



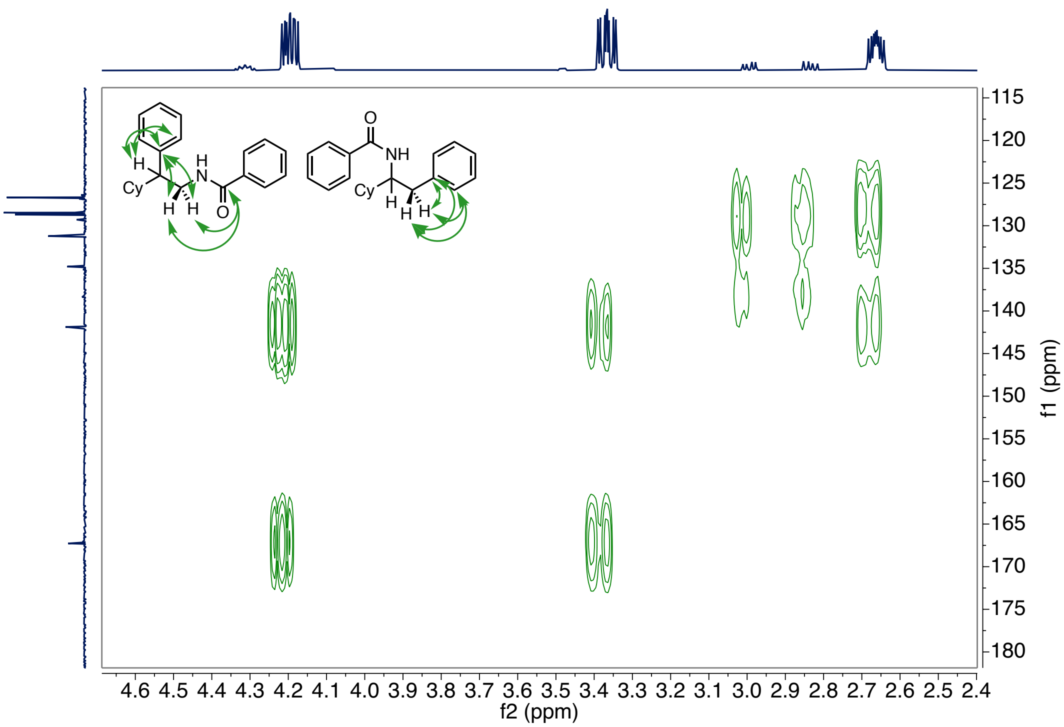
^{1}H NMR (600 MHz, CDCl$_3$) of *N*-(2-cyclohexyl-2-phenylethyl)benzamide (7b), mixture of isomers (10:1):



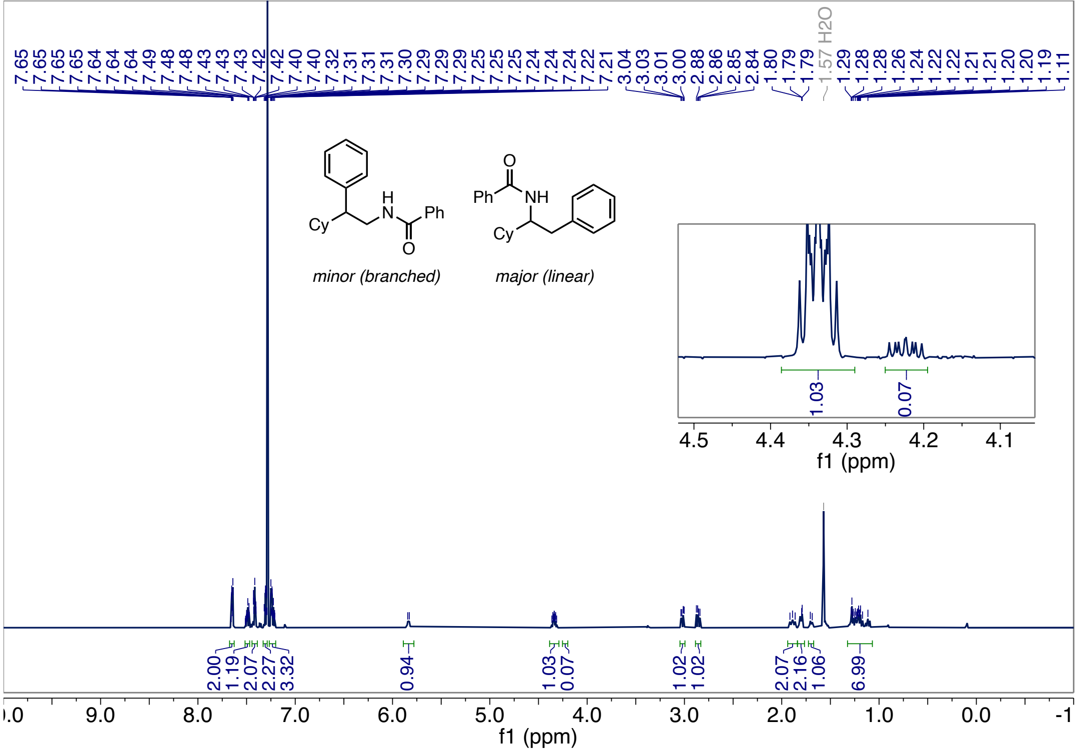
^{13}C{^{1}H} NMR (600 MHz, CDCl$_3$) of *N*-(2-cyclohexyl-2-phenylethyl)benzamide (7b), mixture of isomers (10:1):



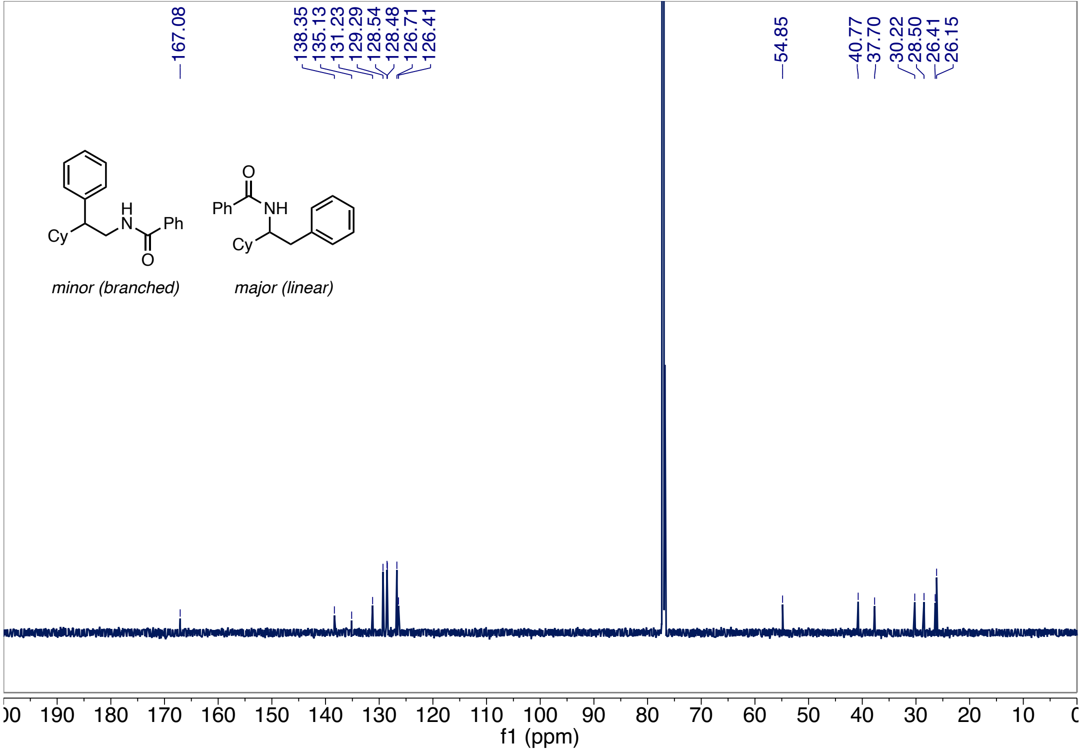
HMBC (600 MHz, CDCl₃) of *N*-(2-cyclohexyl-2-phenylethyl)benzamide (7b), mixture of isomers (10:1):



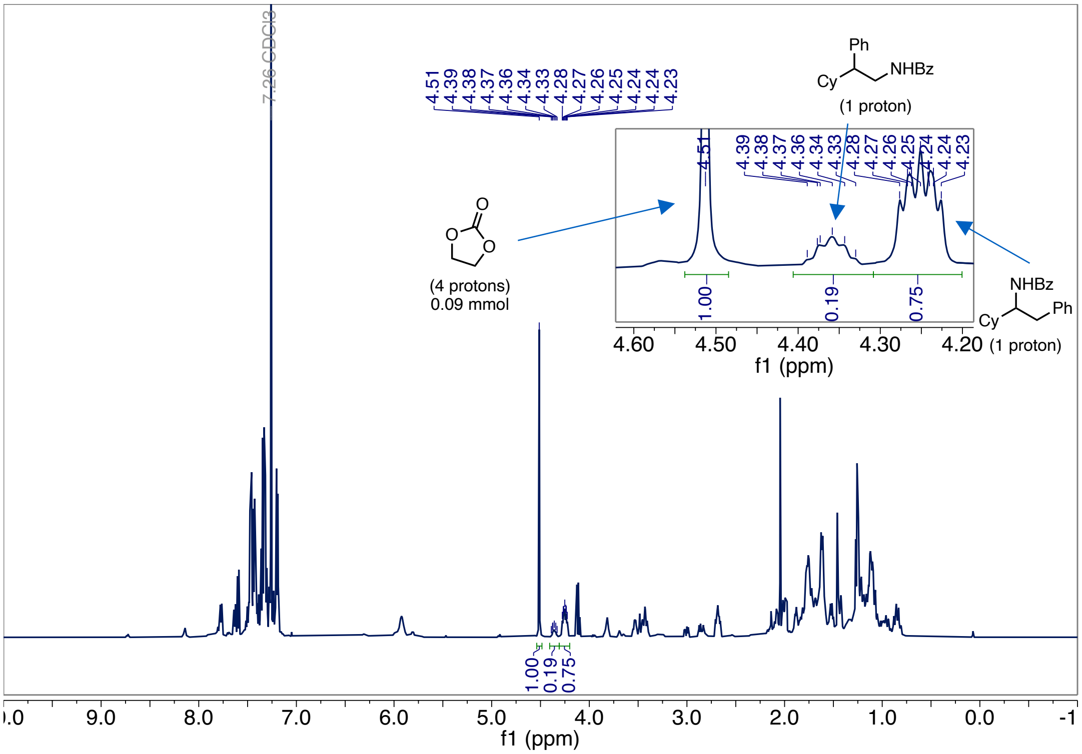
^{1}H NMR (600 MHz, CDCl₃) of *N*-(2-cyclohexyl-2-phenylethyl)benzamide (7b), mixture of isomers (1:15):



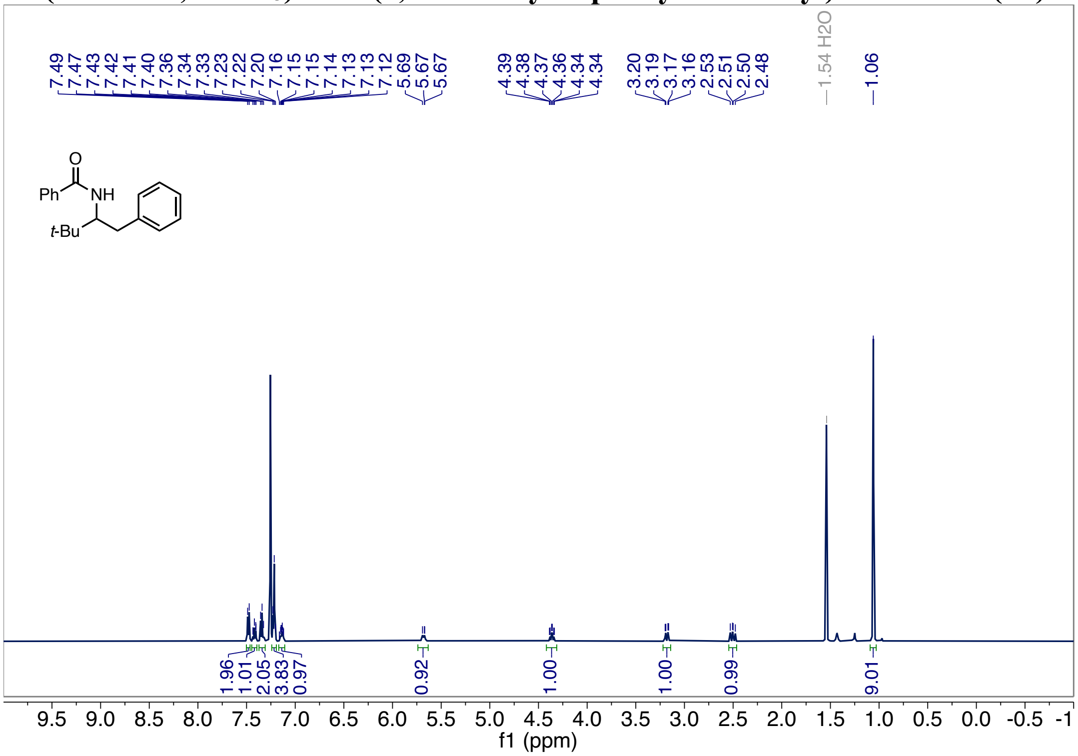
$^{13}C\{^1H\}$ NMR (600 MHz, $CDCl_3$) of *N*-(2-cyclohexyl-2-phenylethyl)benzamide (7b), mixture of isomers (1:15):



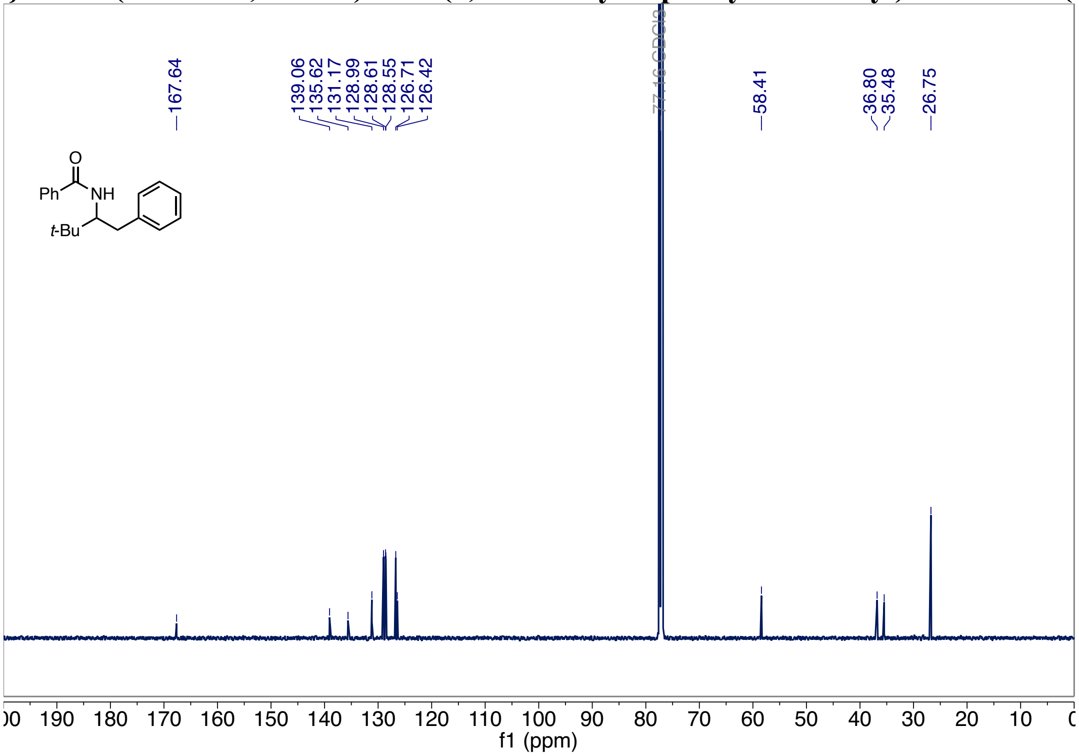
^1H NMR (600 MHz, $CDCl_3$) yield of *N*-(2-cyclohexyl-2-phenylethyl)benzamide (7b) versus ethylene carbonate:



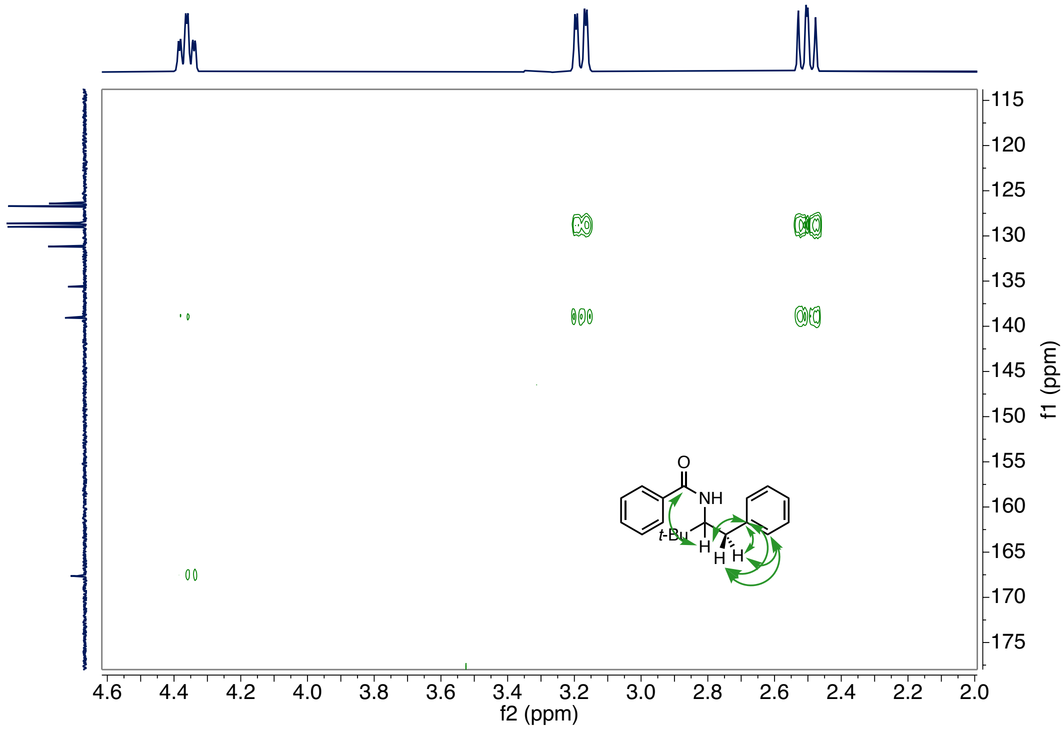
^{1}H NMR (500 MHz, $CDCl_3$) of *N*-(3,3-dimethyl-1-phenylbutan-2-yl)benzamide (8b):



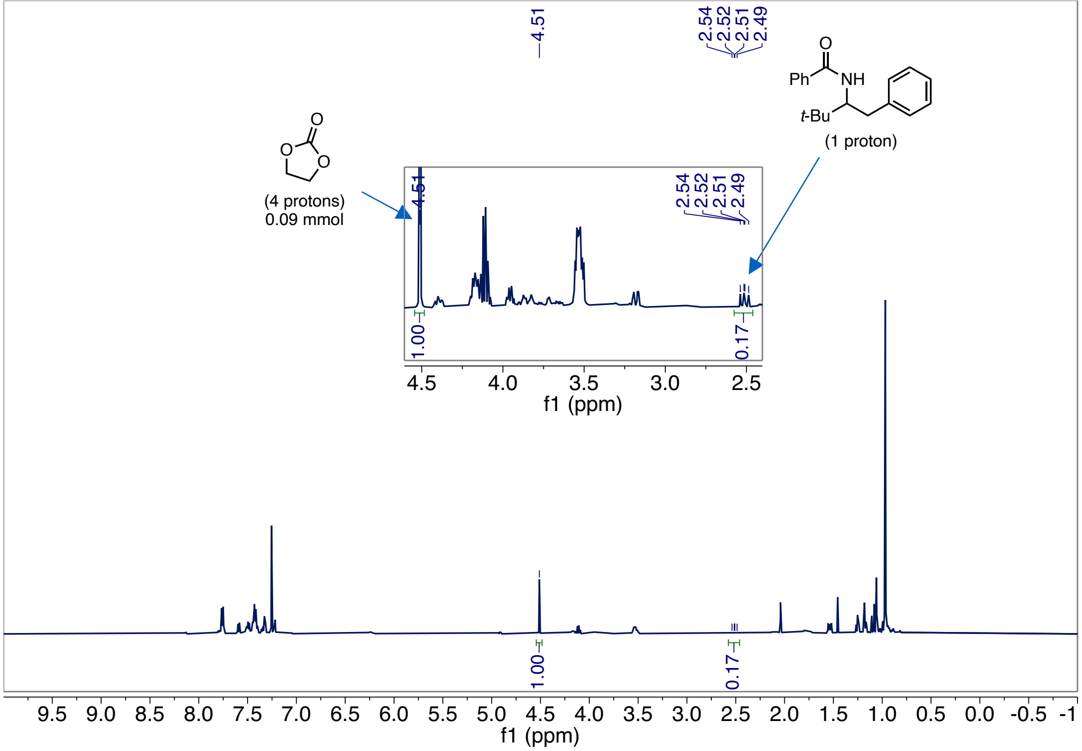
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) of *N*-(3,3-dimethyl-1-phenylbutan-2-yl)benzamide (8b):



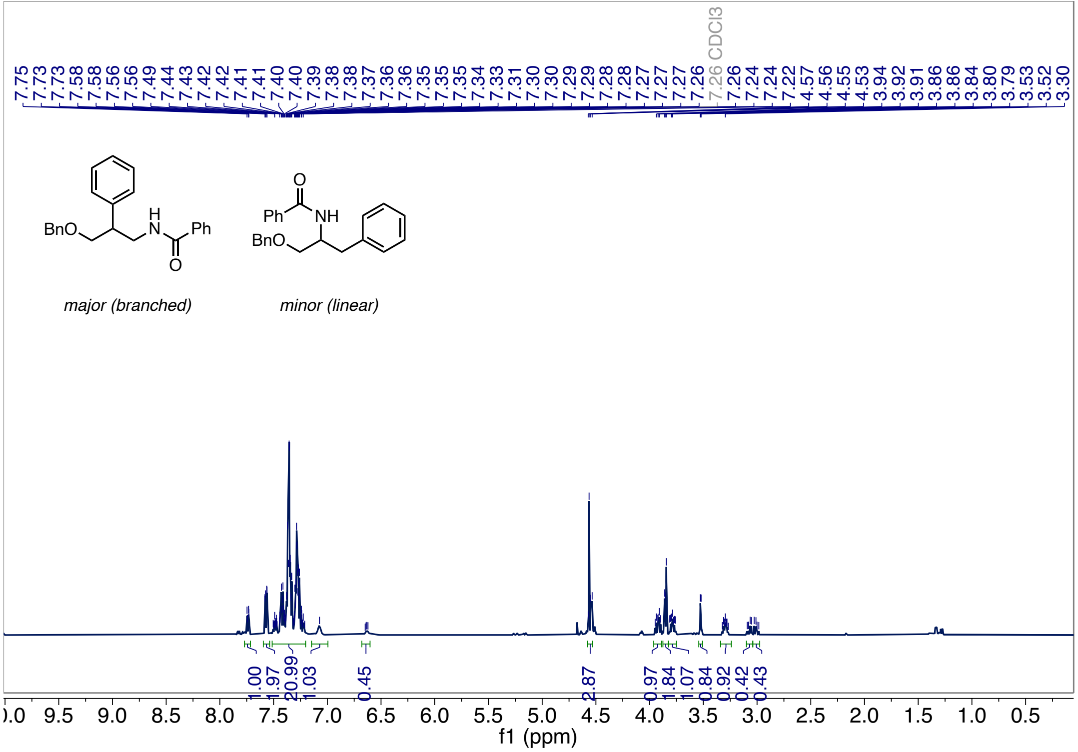
HMBC (500 MHz, CDCl₃) of *N*-(3,3-dimethyl-1-phenylbutan-2-yl)benzamide (8b):



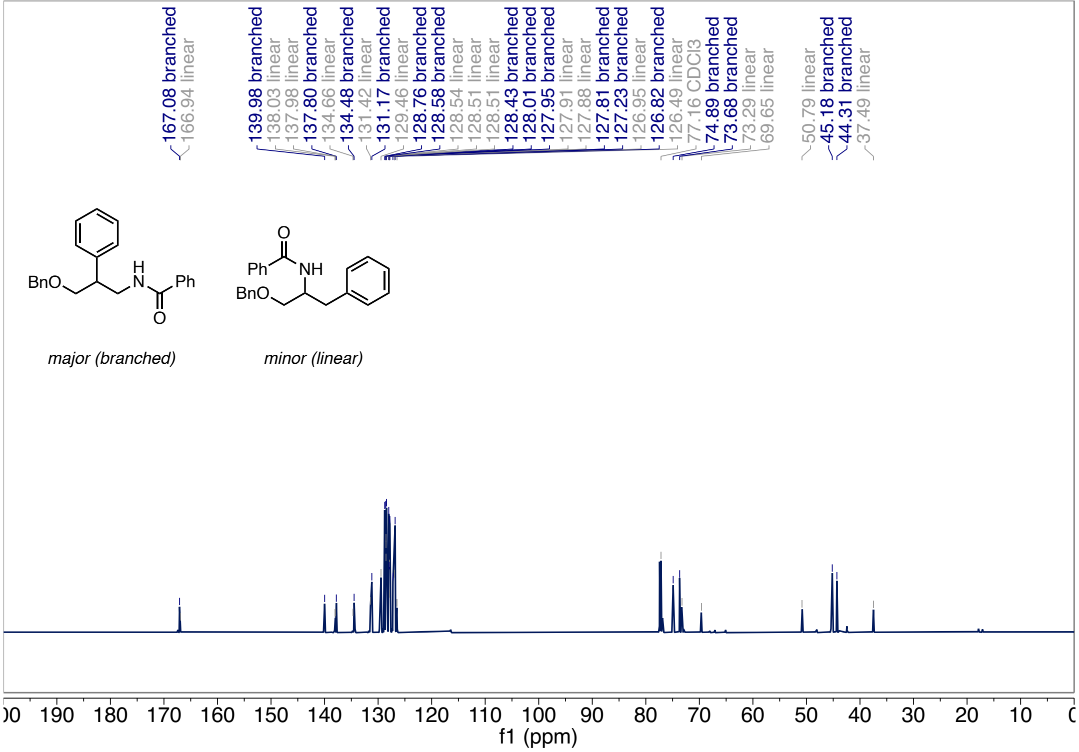
^{1}H NMR (500 MHz, CDCl₃) yield of *N*-(3,3-dimethyl-1-phenylbutan-2-yl)benzamide (8b) versus ethylene carbonate:



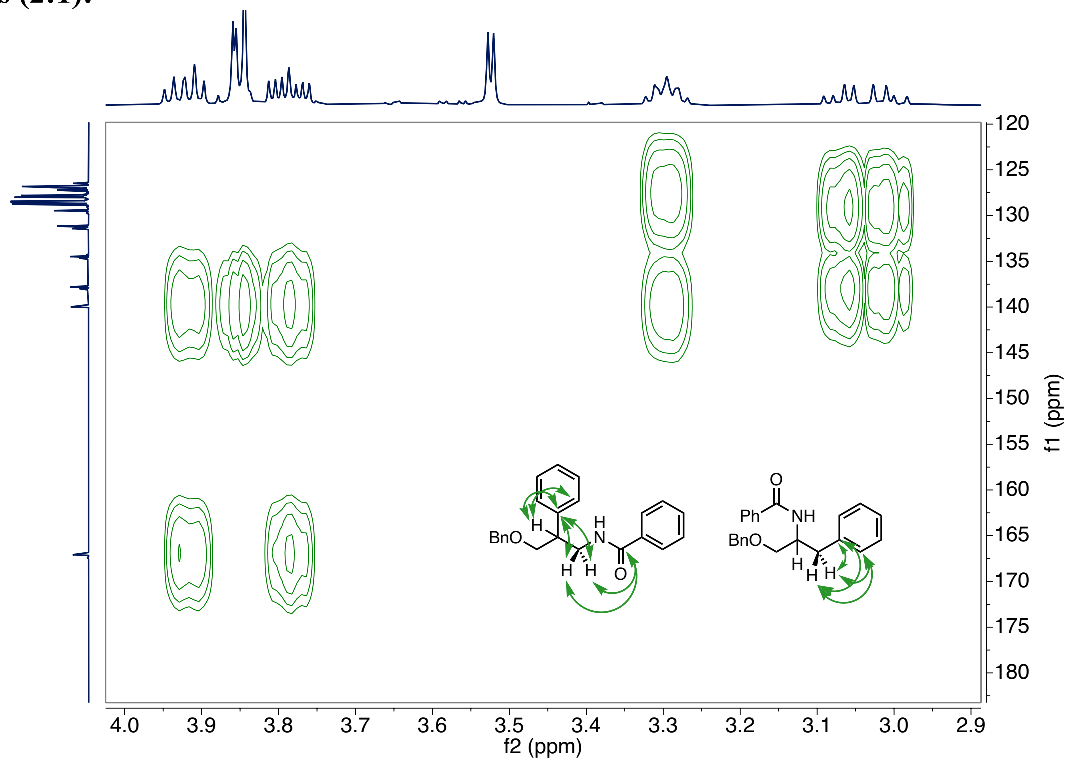
^{1}H NMR (500 MHz, $CDCl_3$) of *N*-(3-(benzyloxy)-2-phenylpropyl)benzamide (9b), mixture of isomers (2:1):



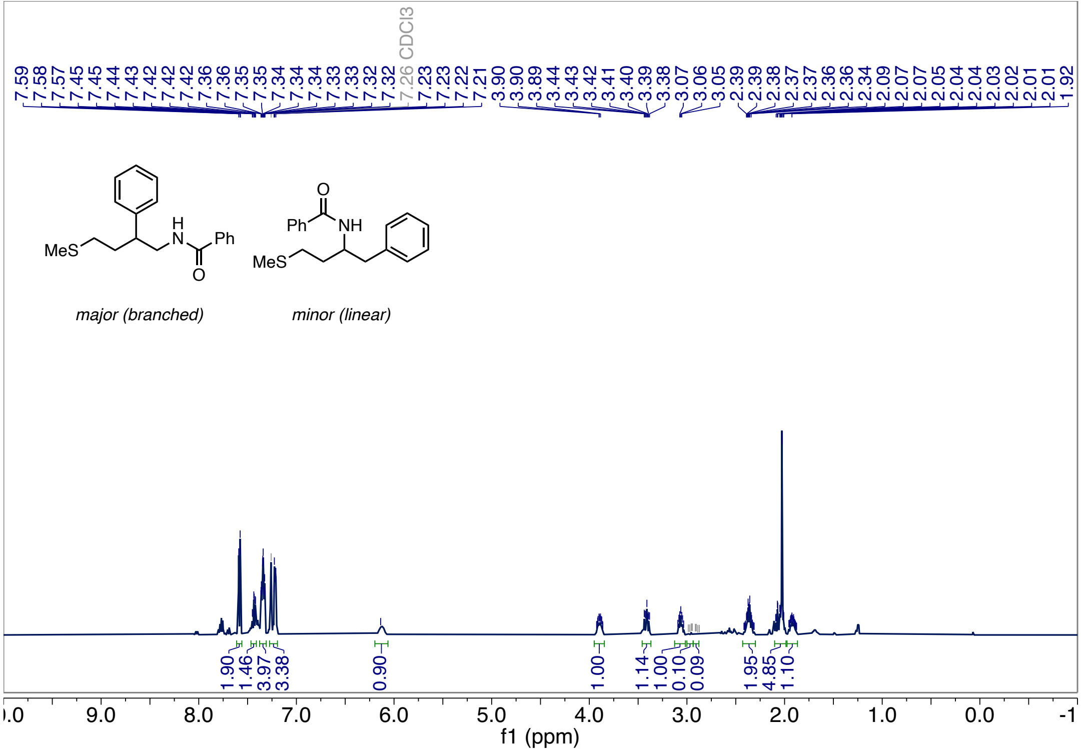
$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) of *N*-(3-(benzyloxy)-2-phenylpropyl)benzamide (9b), mixture of isomers (2:1):



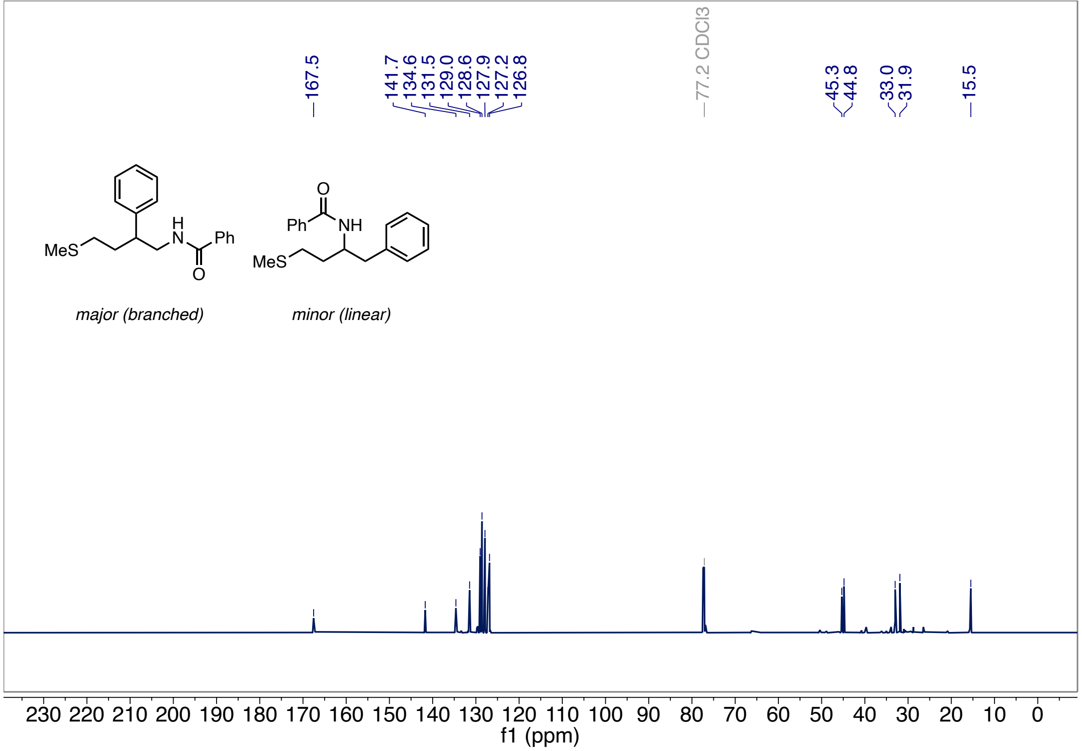
HMBC (600 MHz, CDCl$_3$) of *N*-(3-(benzyloxy)-2-phenylpropyl)benzamide (9b), mixture of isomers (2:1):



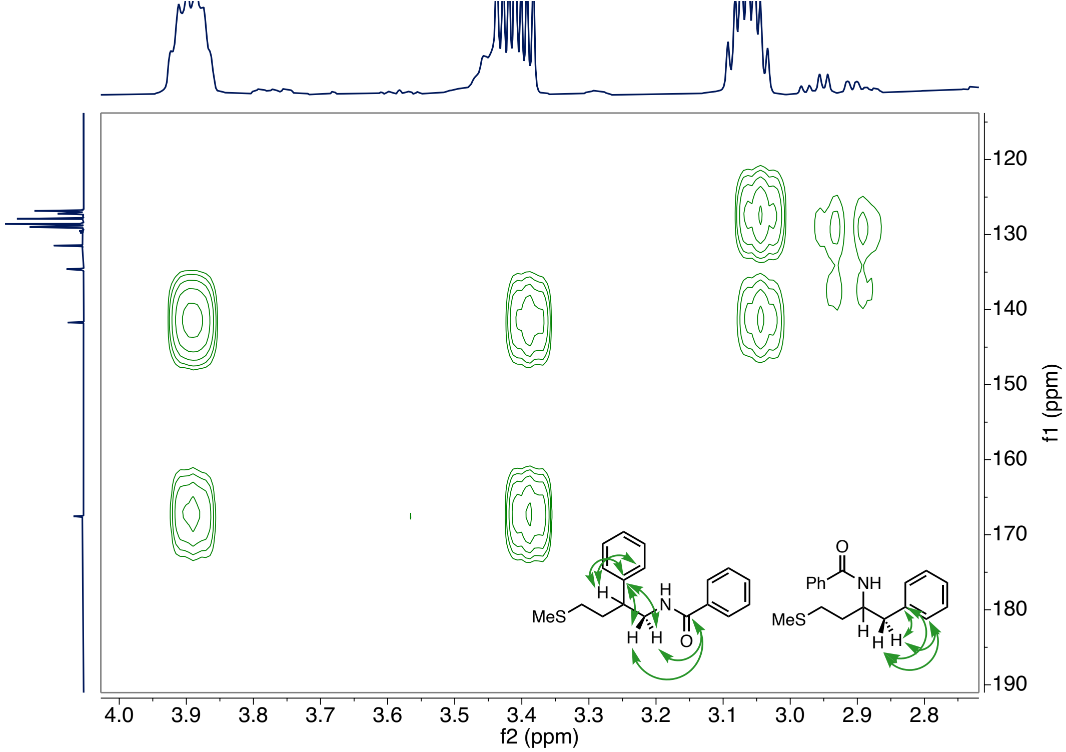
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(4-(methylthio)-2-phenylbutyl)benzamide (10b), mixture of isomers (10:1):



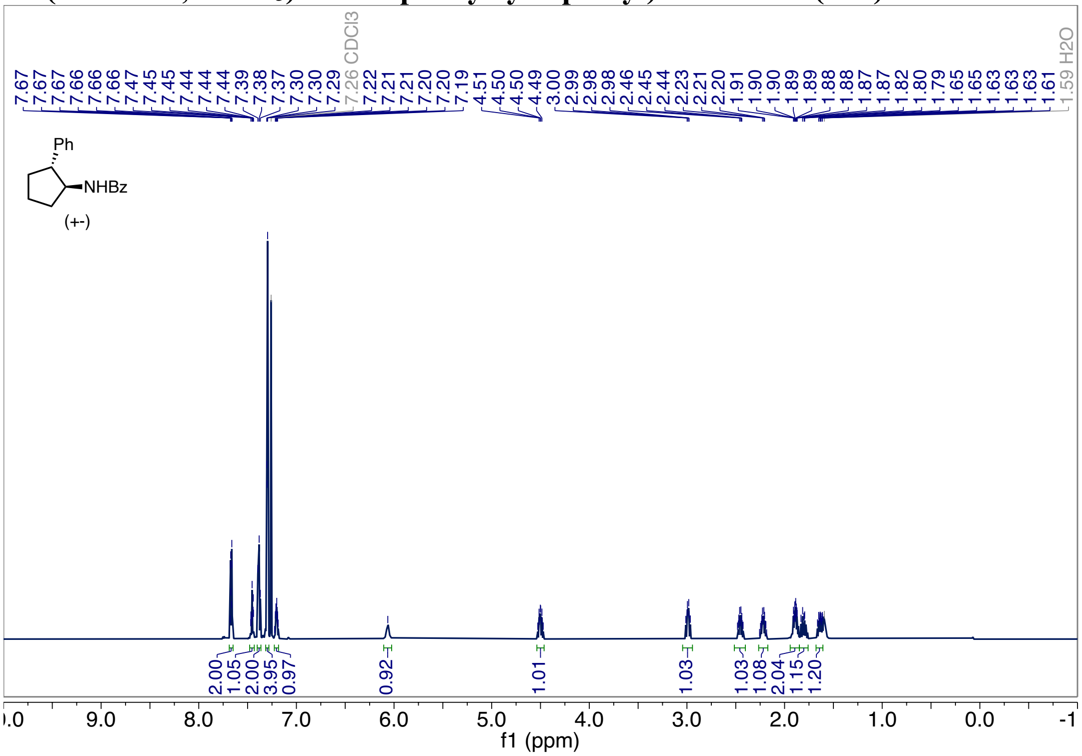
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(4-(methylthio)-2-phenylbutyl)benzamide (10b), mixture of isomers (10:1):



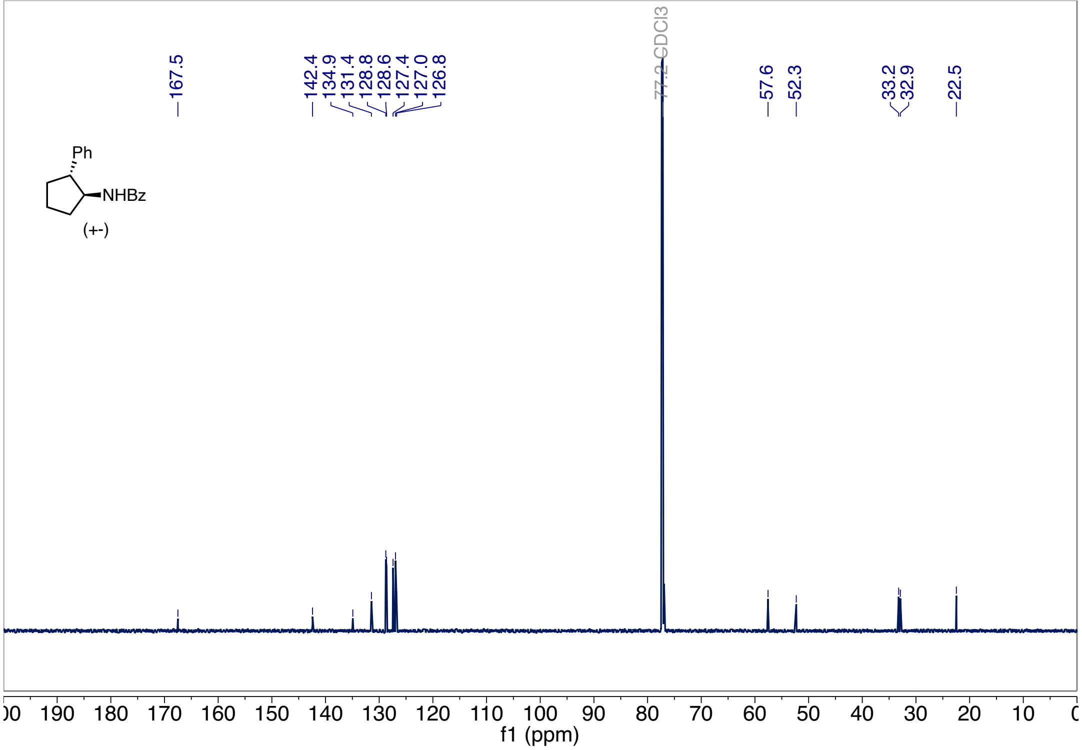
HMBC (600 MHz, CDCl$_3$) of *N*-(4-(methylthio)-2-phenylbutyl)benzamide (10b), mixture of isomers (10:1):



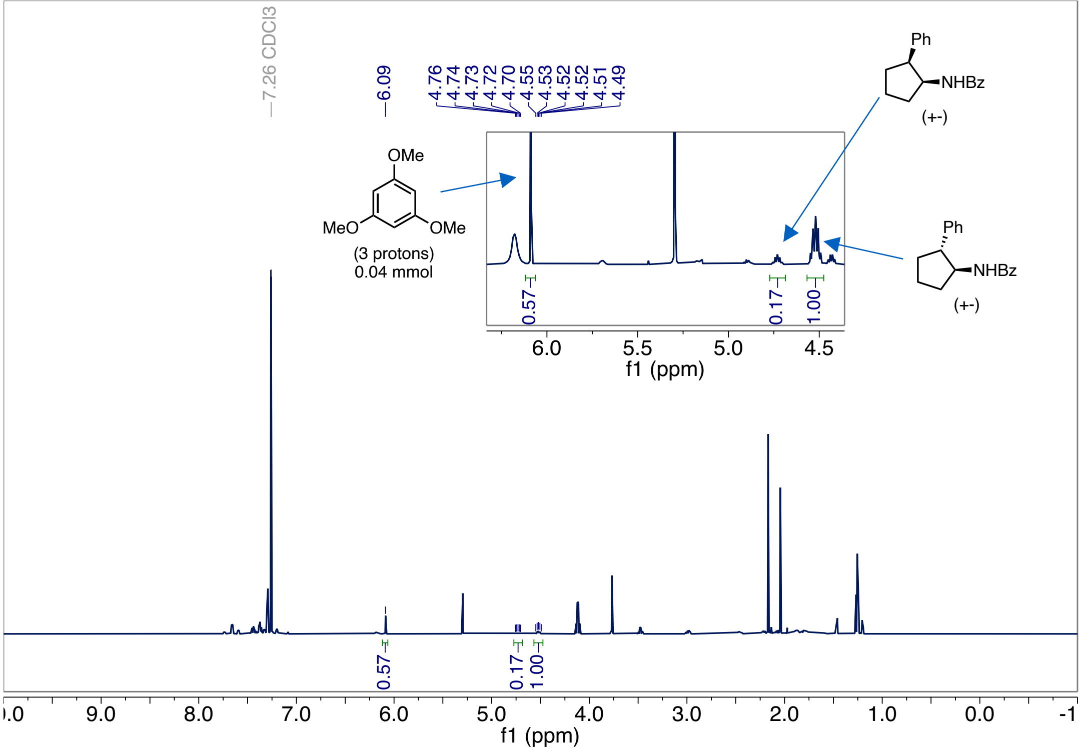
^{1}H NMR (600 MHz, $CDCl_3$) of *N*-2-phenylcyclopentyl)benzamide (11b):



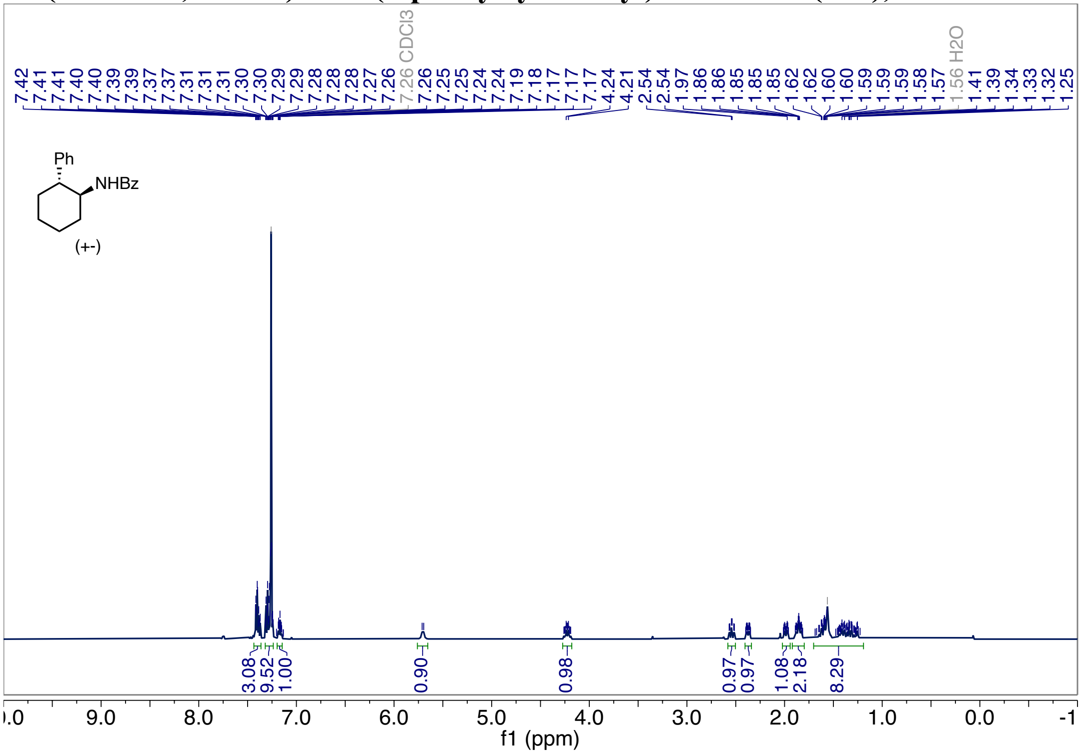
^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) of *N*-2-phenylcyclopentyl)benzamide (11b):



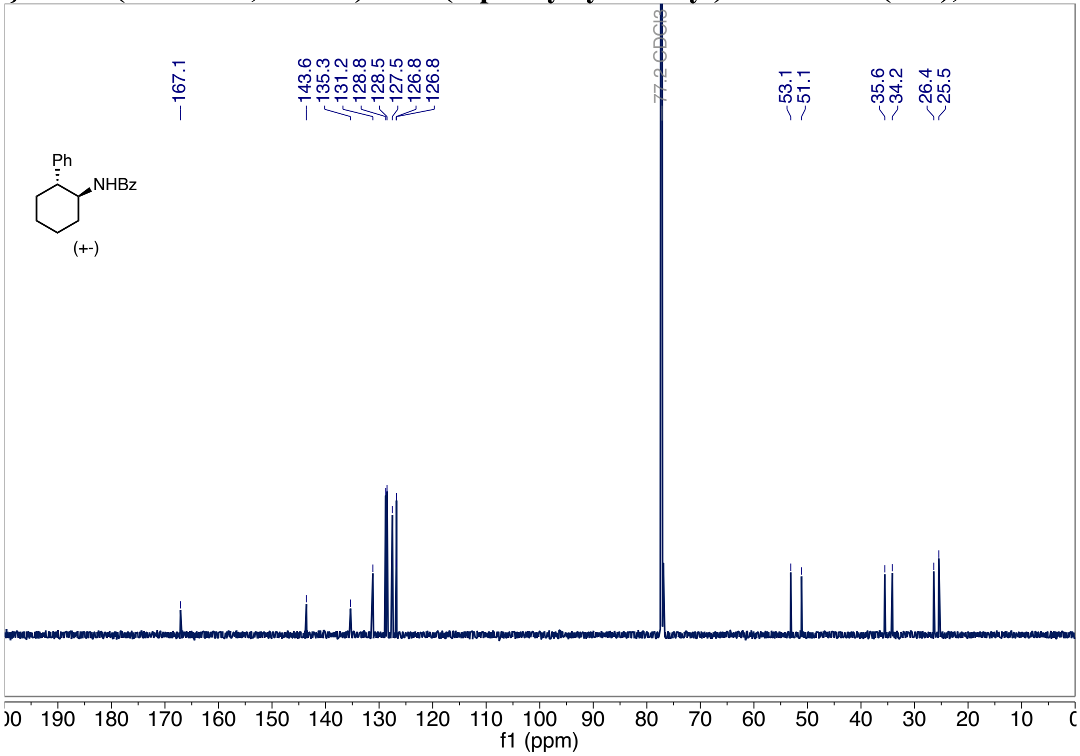
^{1}H NMR (600 MHz, $CDCl_3$) yield of *N*-2-phenylcyclopentyl)benzamide (11b) versus trimethoxy benzene:



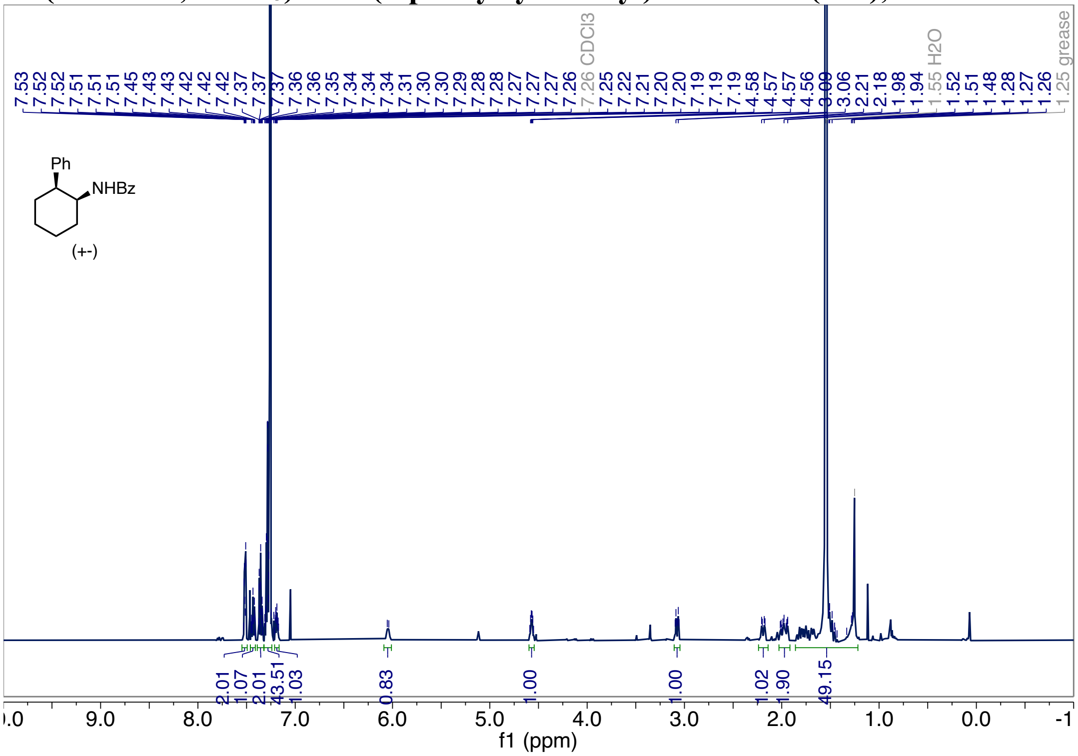
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-phenylcyclohexyl)benzamide (12b), trans isomer:



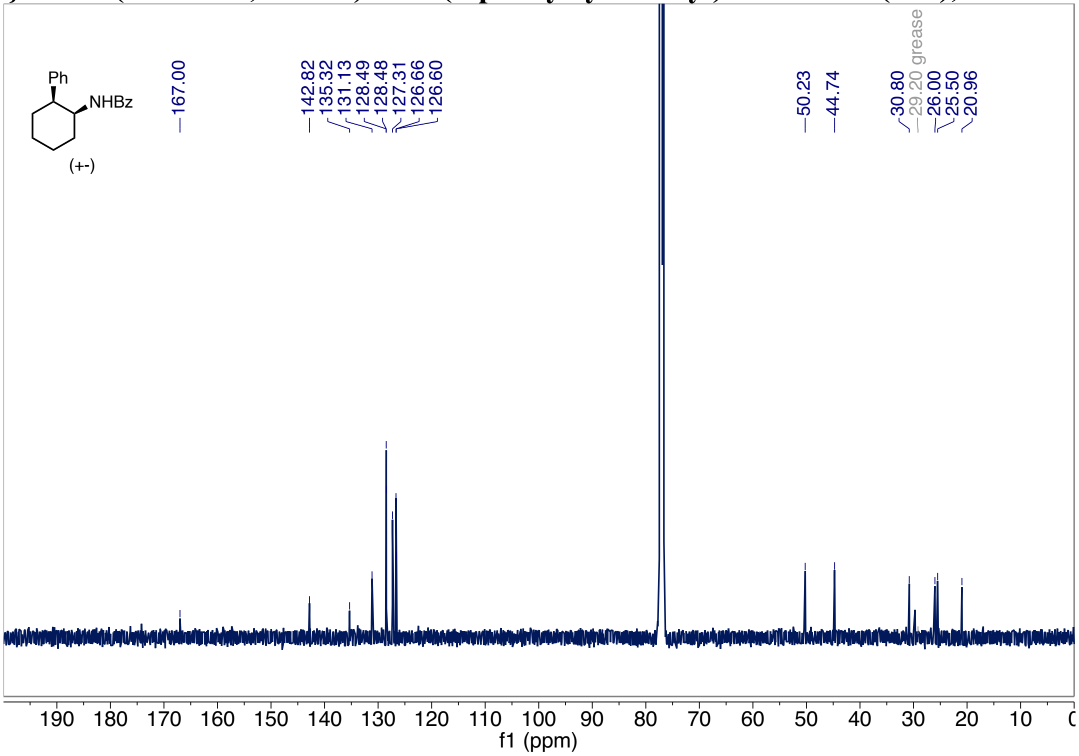
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of *N*-(2-phenylcyclohexyl)benzamide (12b), trans isomer:



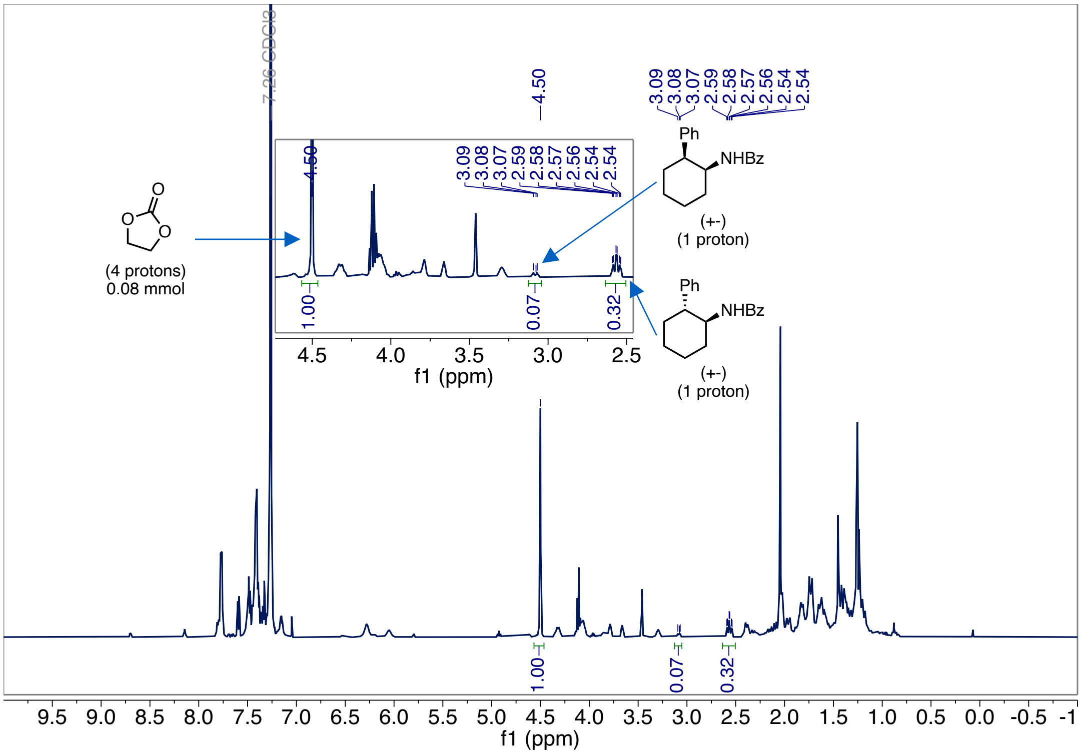
^{1}H NMR (500 MHz, CDCl$_3$) of *N*-(2-phenylcyclohexyl)benzamide (12b), cis isomer:



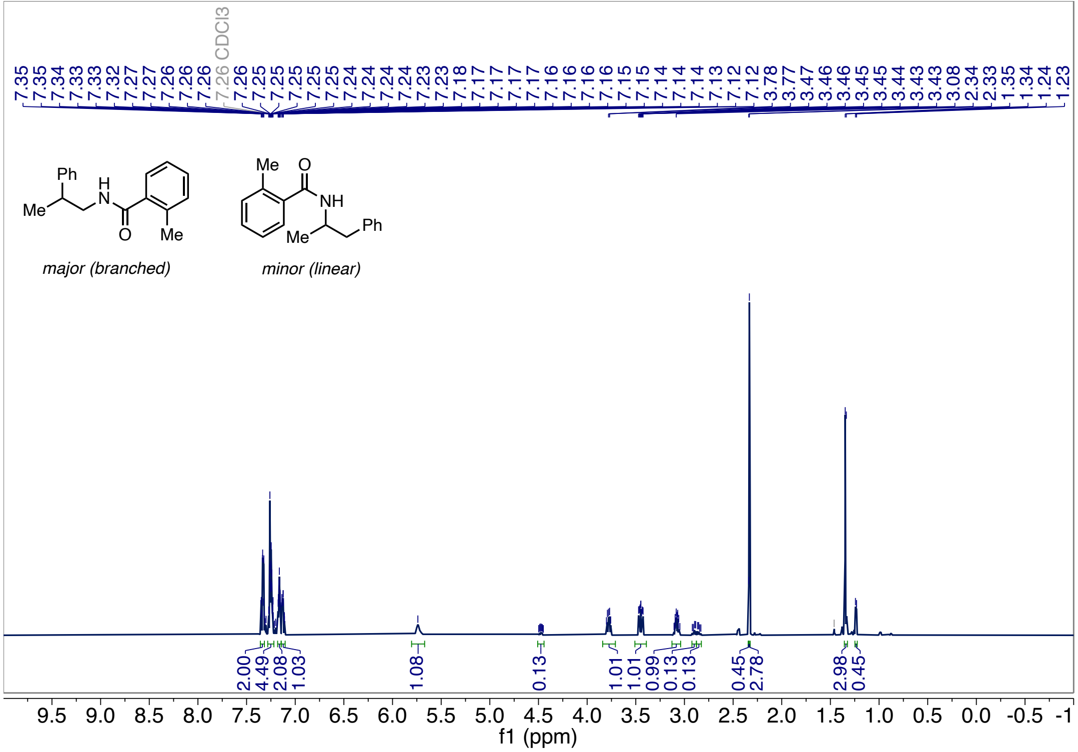
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of *N*-(2-phenylcyclohexyl)benzamide (12b), cis isomer:



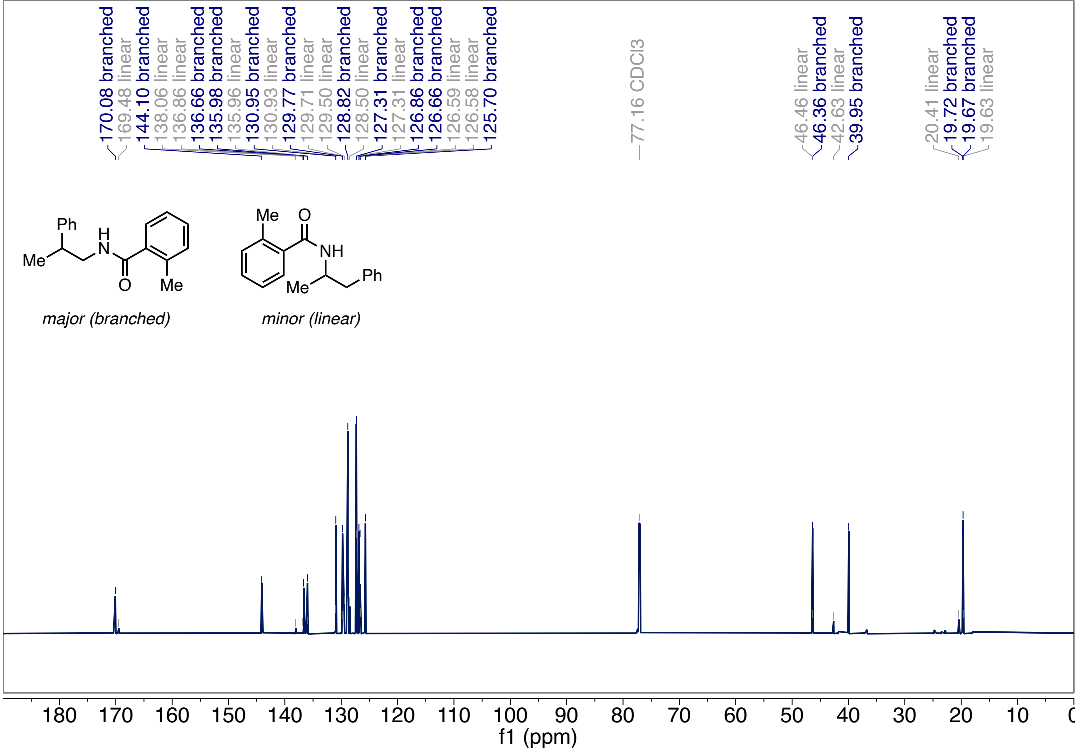
^{1}H NMR (500 MHz, CDCl$_3$) yield of *N*-(2-phenylcyclohexyl)benzamide (12b) versus ethylene carbonate:



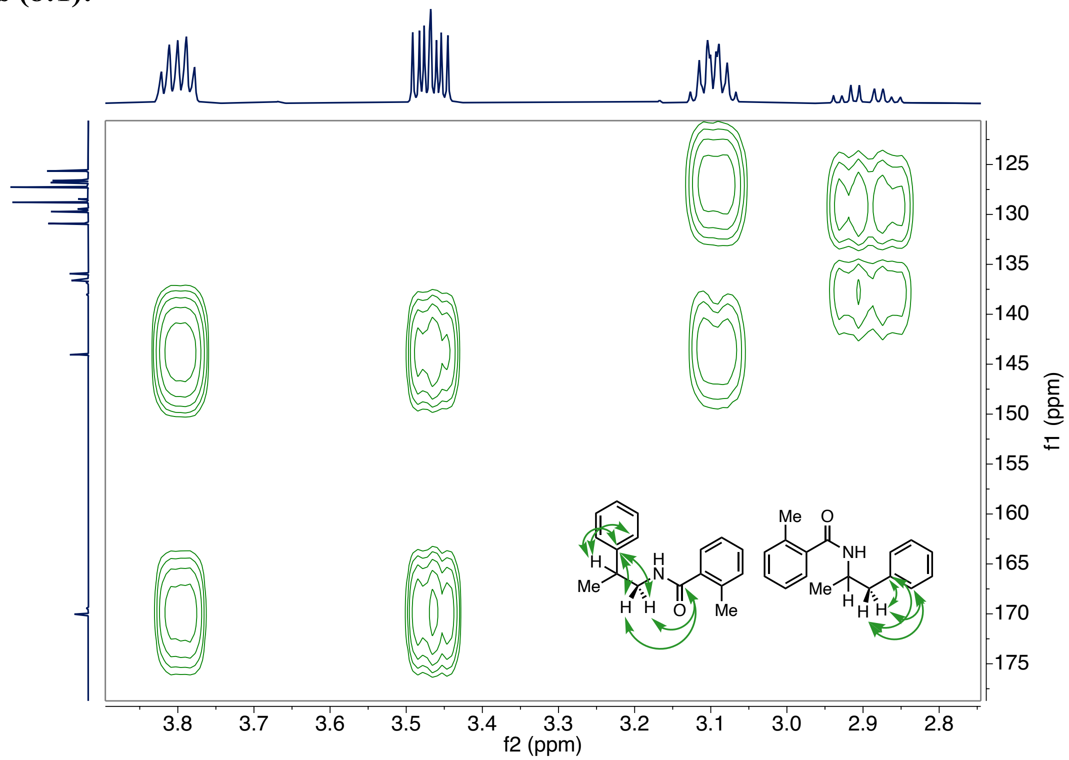
^{1}H NMR (600 MHz, CDCl3) of 2-methyl-*N*-(2-phenylpropyl)benzamide (13b), mixture of isomers (8:1):



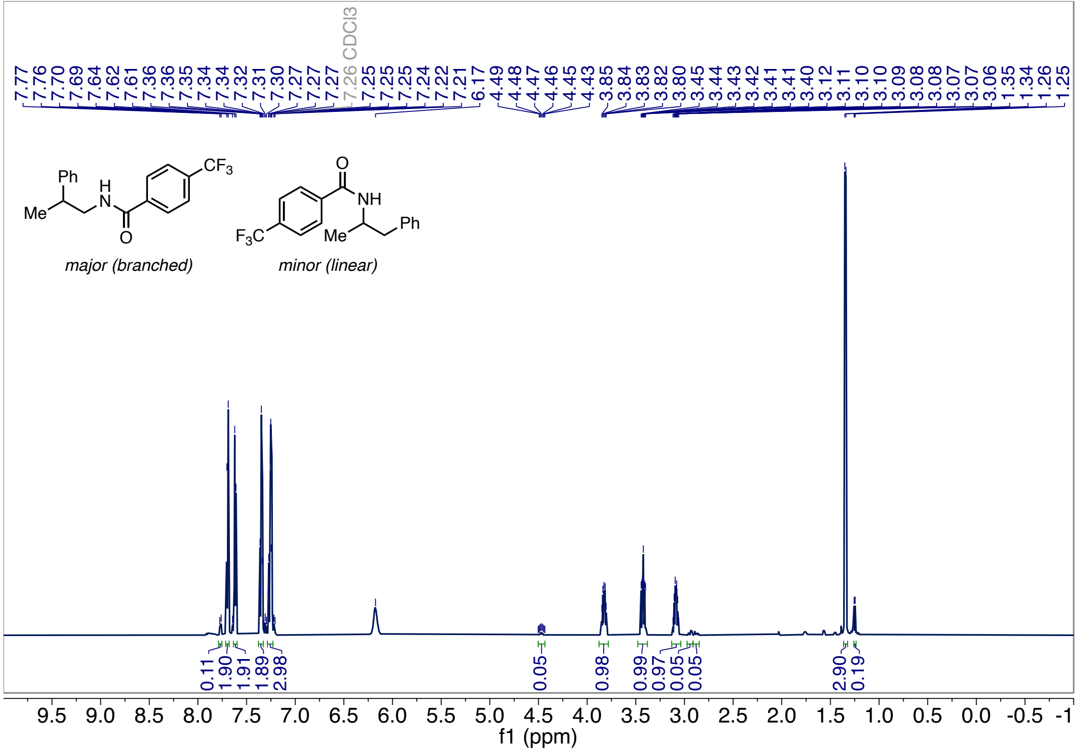
^{13}C NMR (151 MHz, CDCl3) of 2-methyl-*N*-(2-phenylpropyl)benzamide (13b), mixture of isomers (8:1):



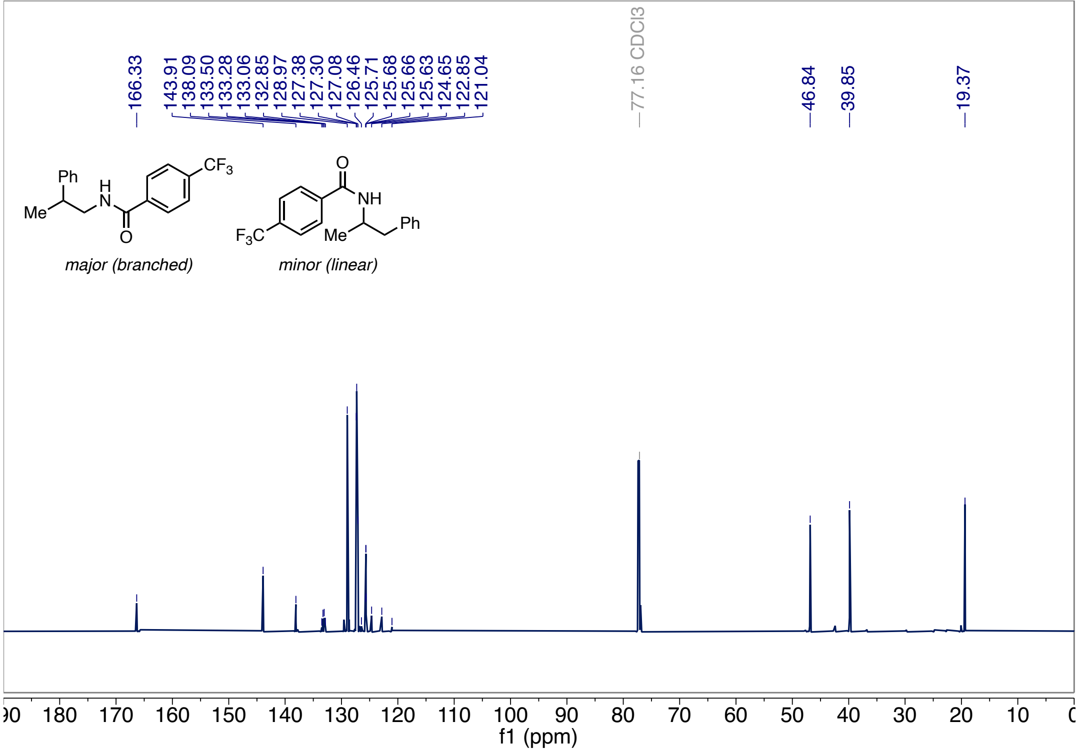
HMBC (600 MHz, CDCl3) of 2-methyl-*N*-(2-phenylpropyl)benzamide (13b), mixture of isomers (8:1):



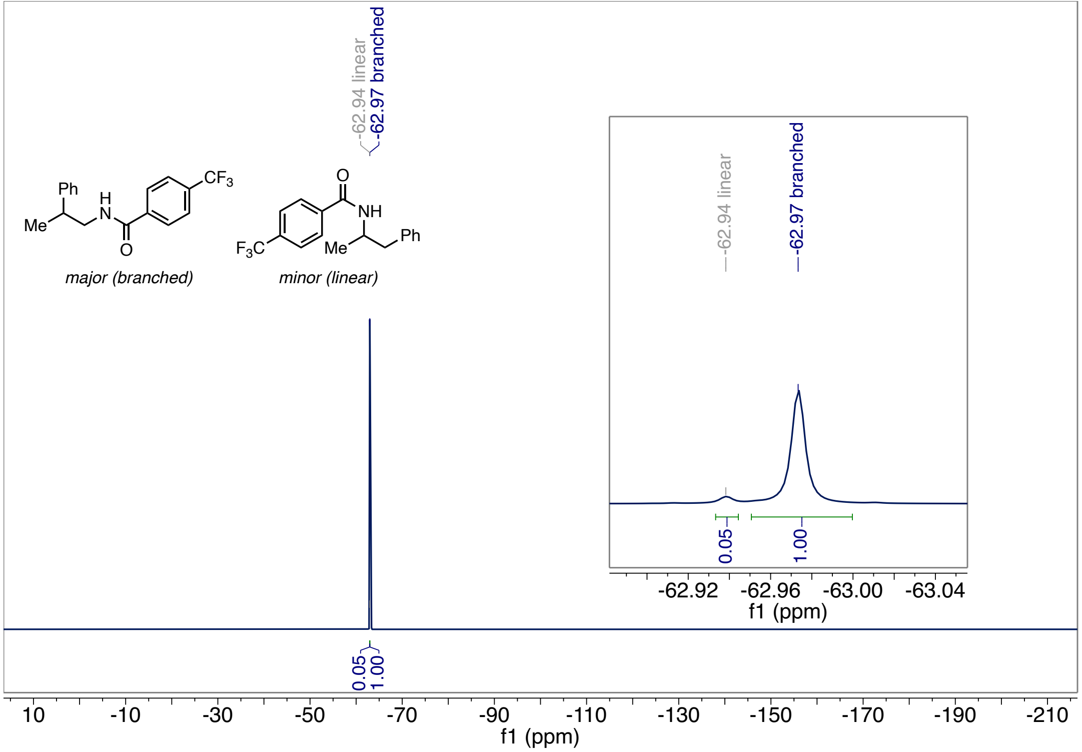
^{1}H NMR (600 MHz, CDCl3) of *N*-(2-phenylpropyl)-4-(trifluoromethyl)benzamide (14b), mixture of isomers (20:1):



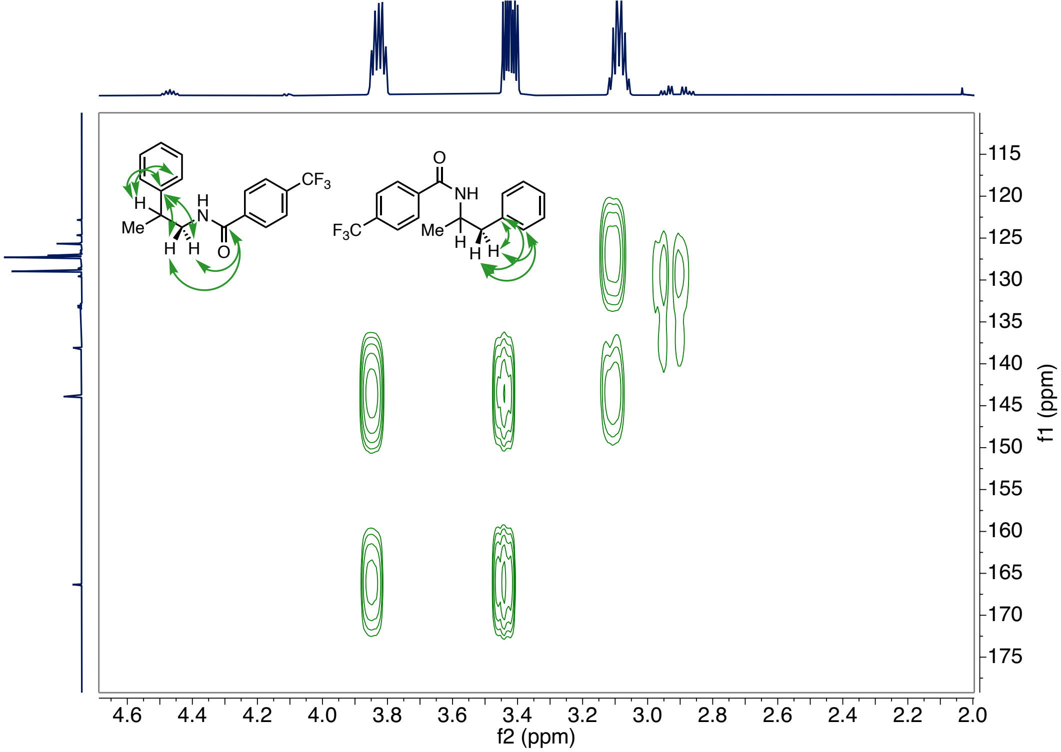
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of *N*-(2-phenylpropyl)-4-(trifluoromethyl)benzamide (14b), mixture of isomers (20:1):



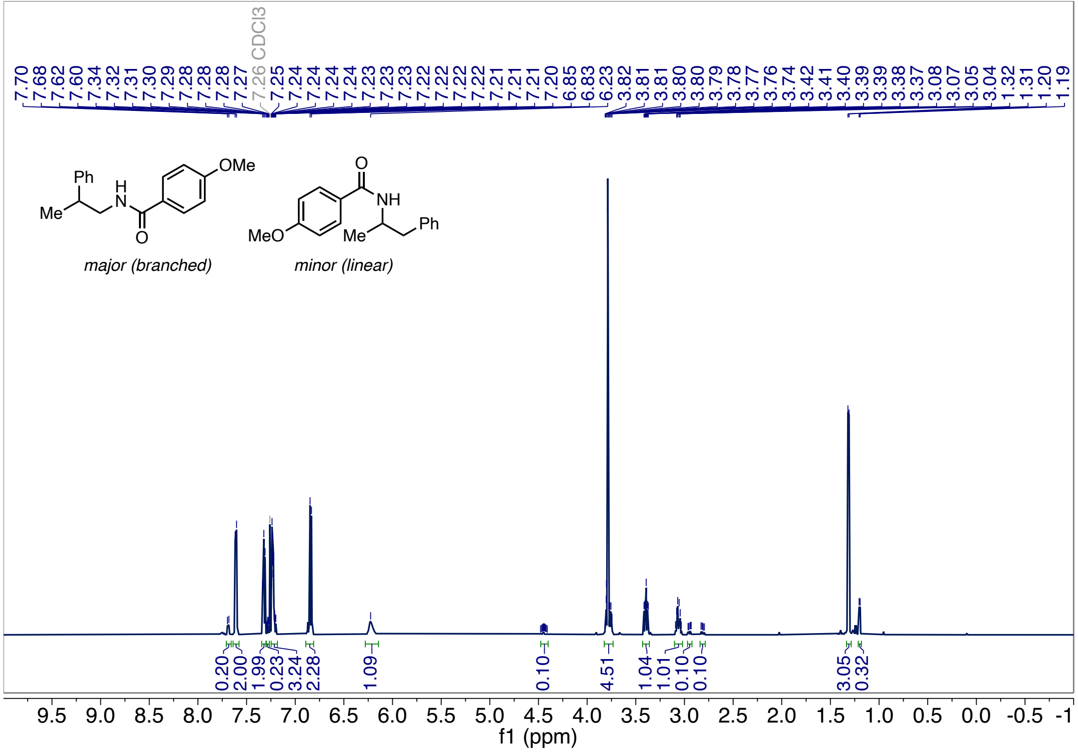
^{19}F NMR (565 MHz, CDCl3) of *N*-(2-phenylpropyl)-4-(trifluoromethyl)benzamide (14b), mixture of isomers (20:1):



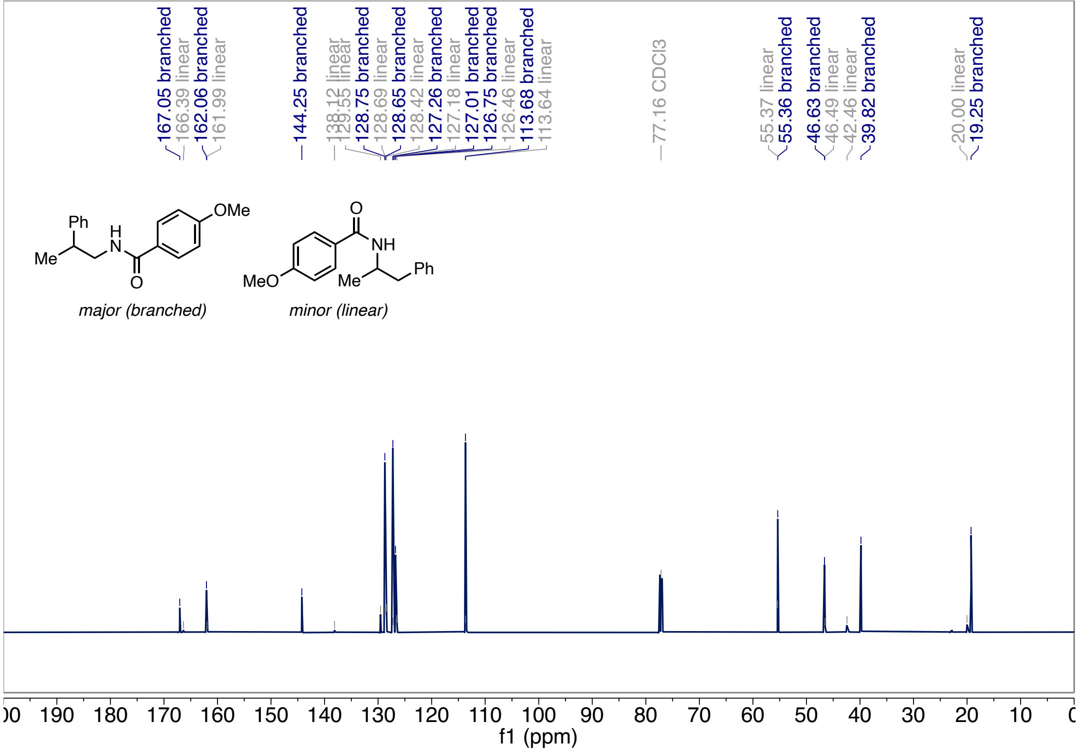
HMBC (600 MHz, CDCl3) of *N*-(2-phenylpropyl)-4-(trifluoromethyl)benzamide (14b), mixture of isomers (20:1):



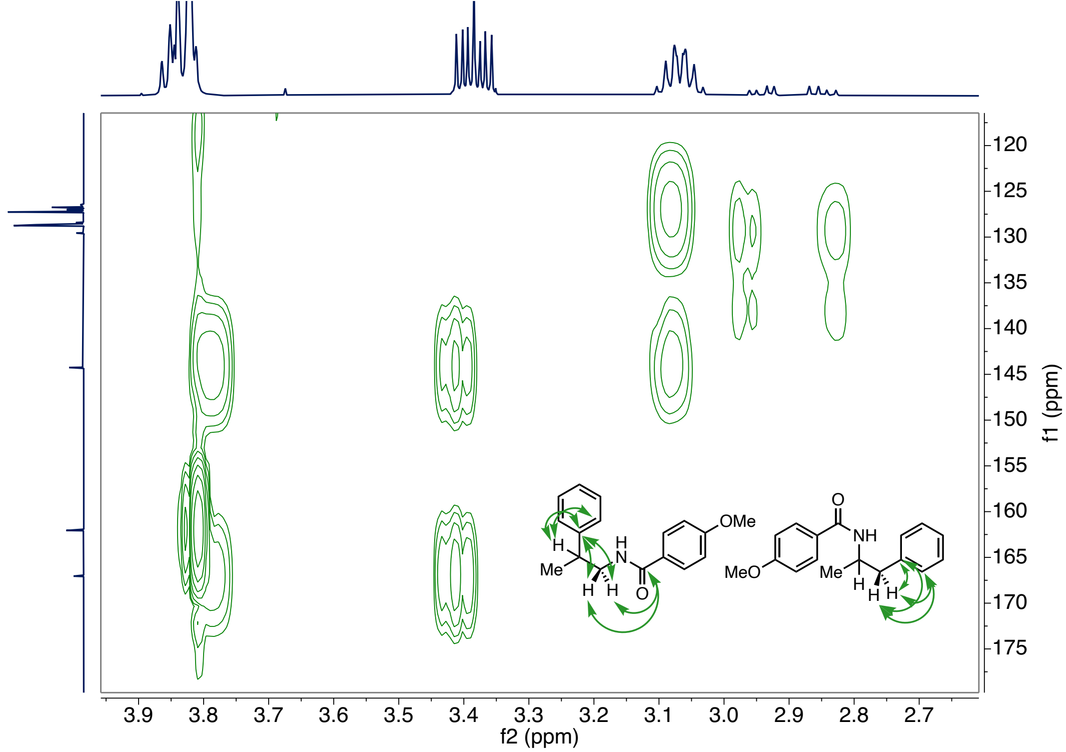
^{1}H NMR (600 MHz, CDCl$_3$) of 4-methoxy-N-(2-phenylpropyl)benzamide (15b), mixture of isomers (10:1):



^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of 4-methoxy-N-(2-phenylpropyl)benzamide (15b), mixture of isomers (10:1):

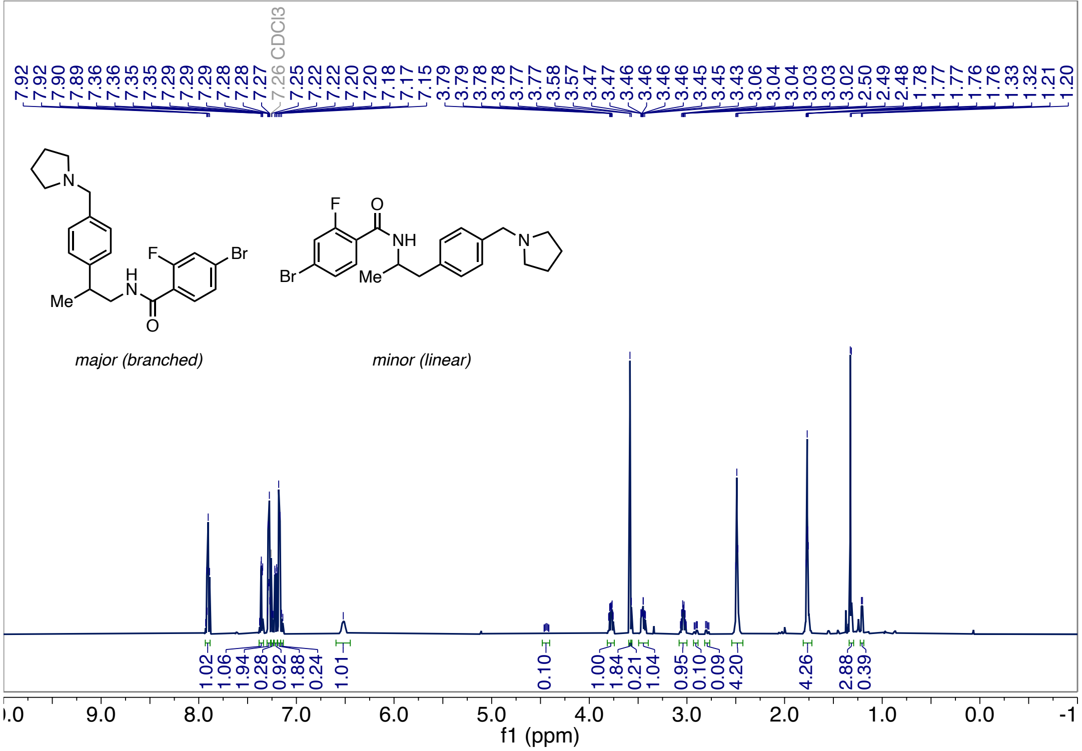


HMBC (600 MHz, $CDCl_3$) of 4-methoxy-N-(2-phenylpropyl)benzamide (15b), mixture of isomers (10:1):

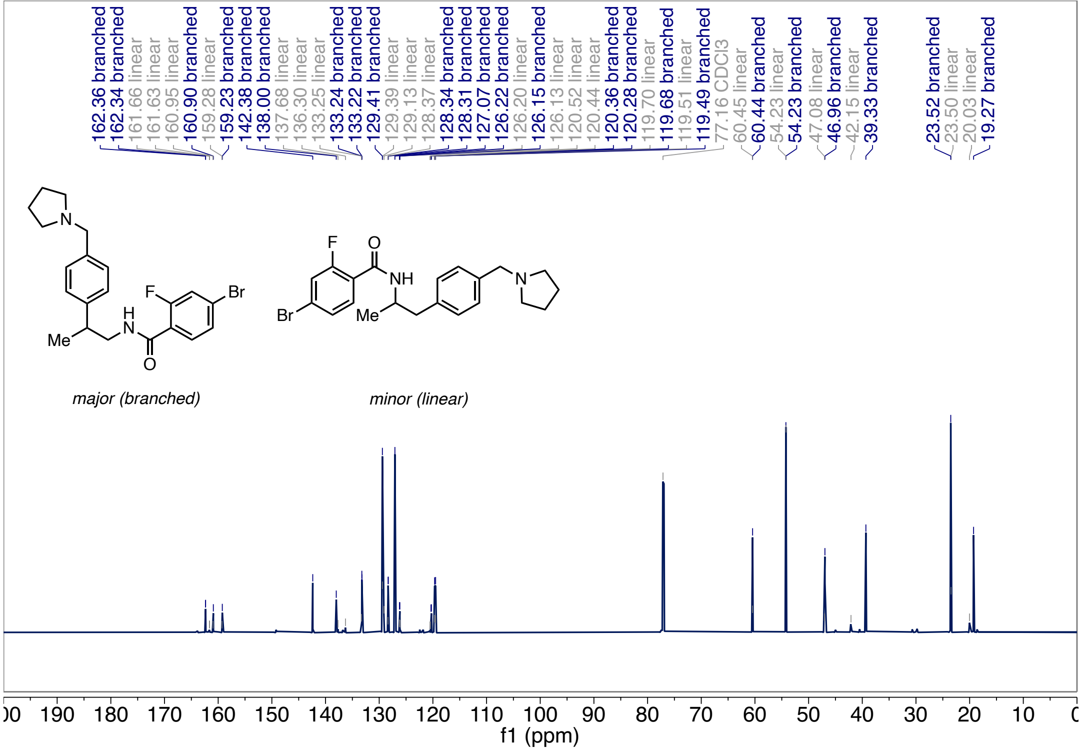


Only correlations necessary to establish branched/linear connectivity are identified.

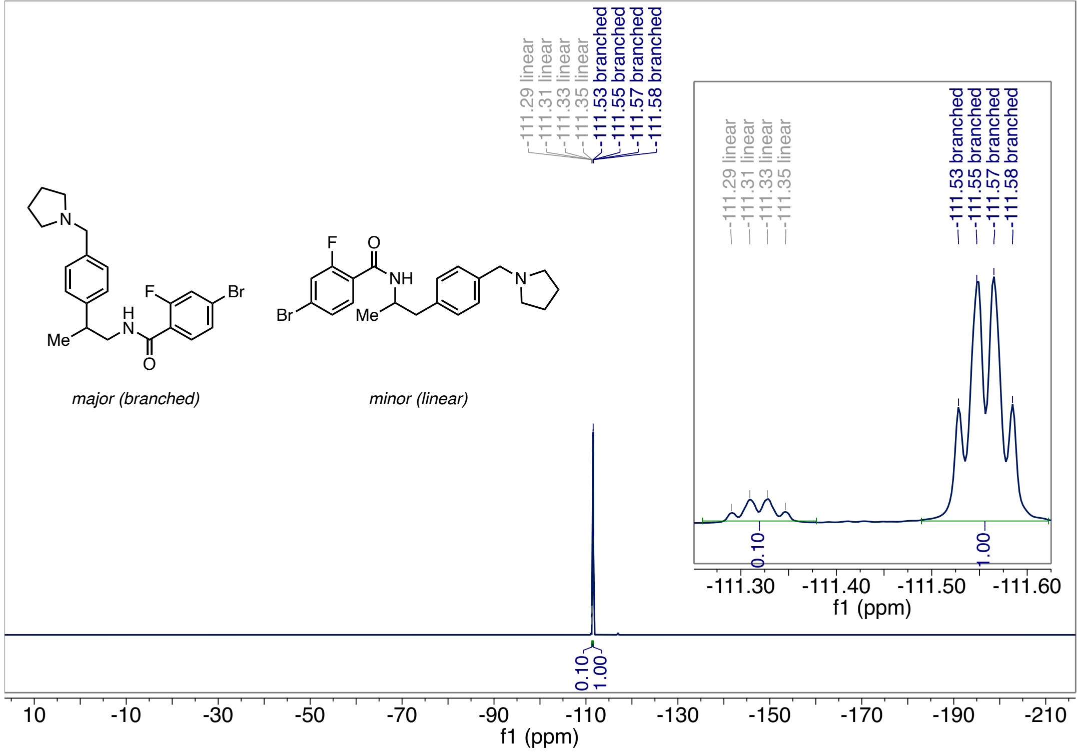
^{1}H NMR (600 MHz, CDCl$_3$) of 16b:



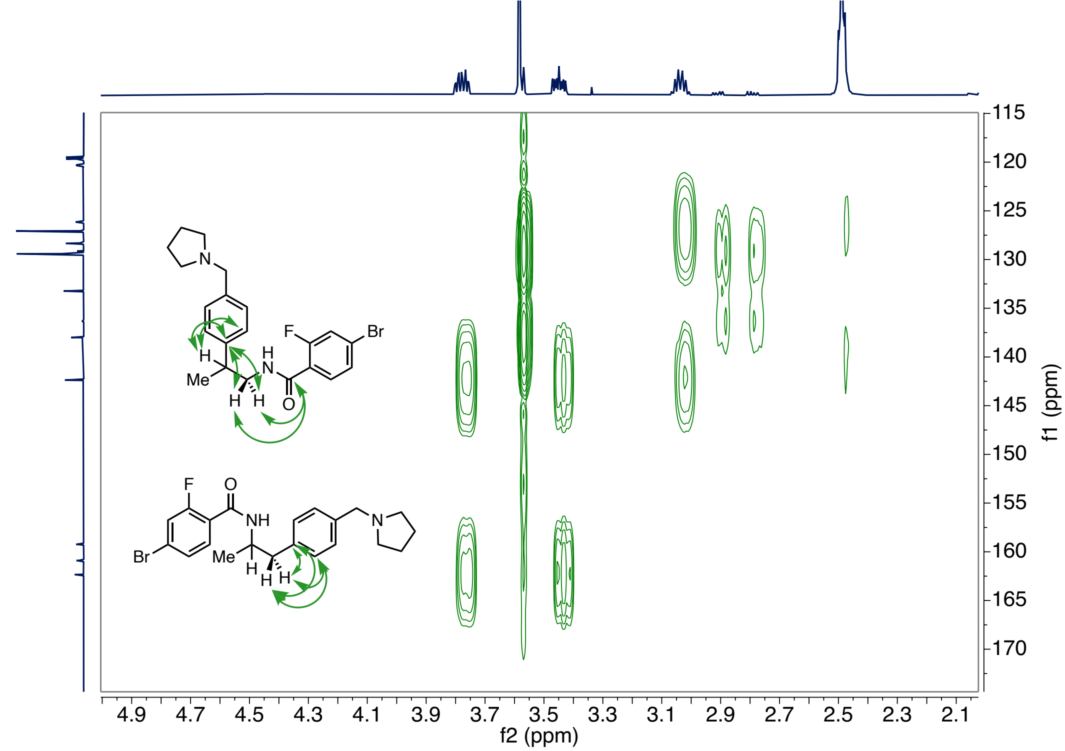
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) of 16b:



^{19}F NMR (565 MHz, CDCl$_3$) of 16b:

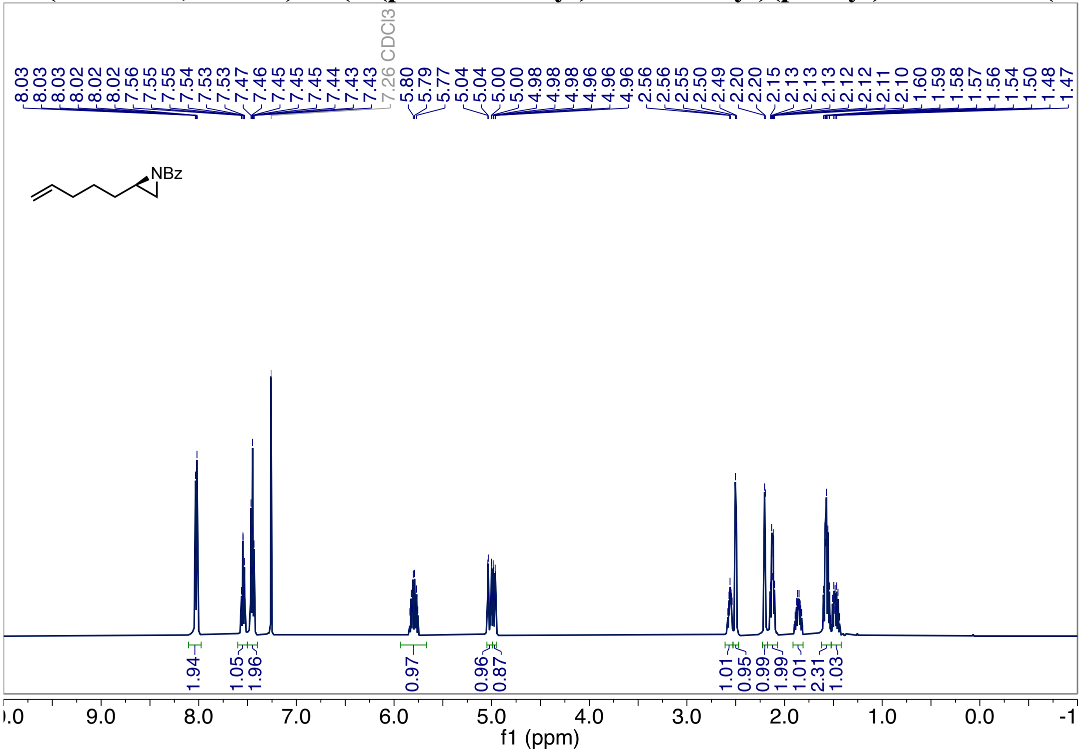


HMBC (600 MHz, CDCl$_3$) of 16b^{a}:

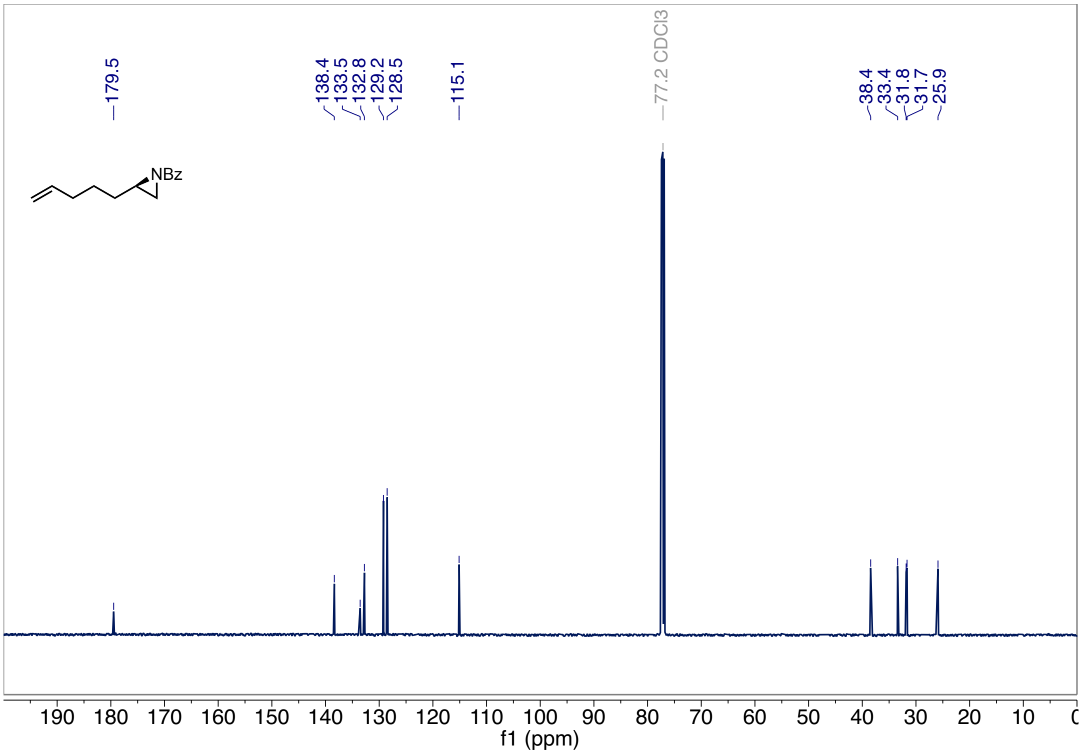


Only correlations necessary to establish branched/linear connectivity are identified.

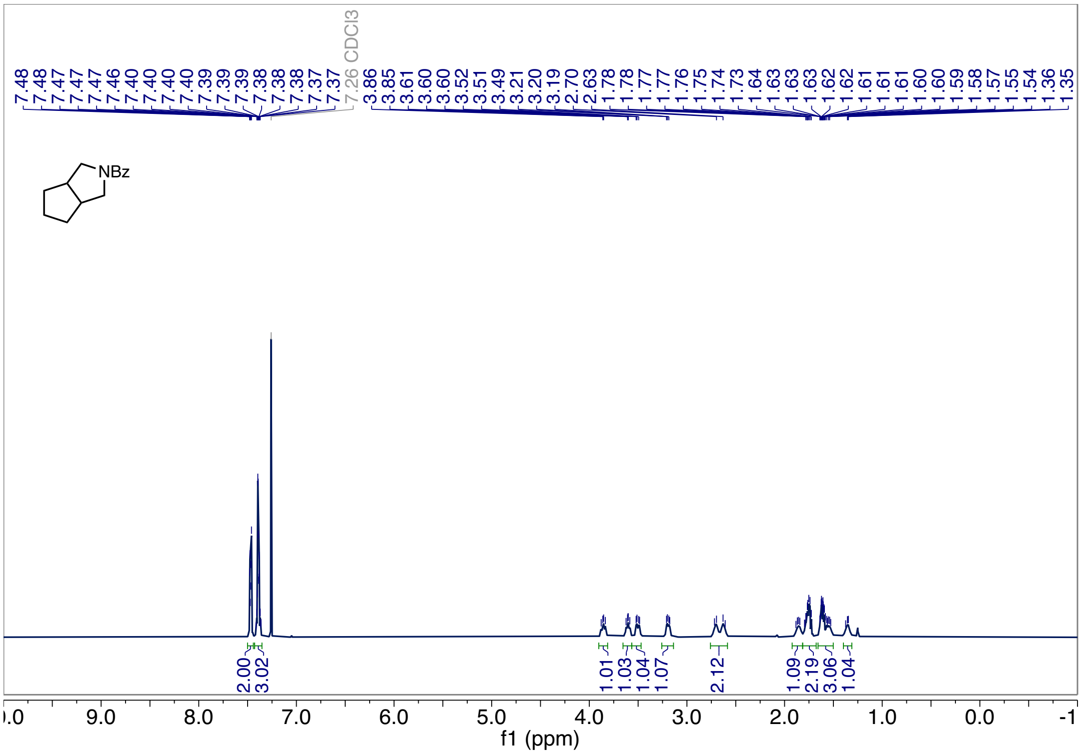
^{1}H NMR (500 MHz, CDCl$_3$) of (2-(pent-4-en-1-yl)aziridin-1-yl)(phenyl)methanone (17a):



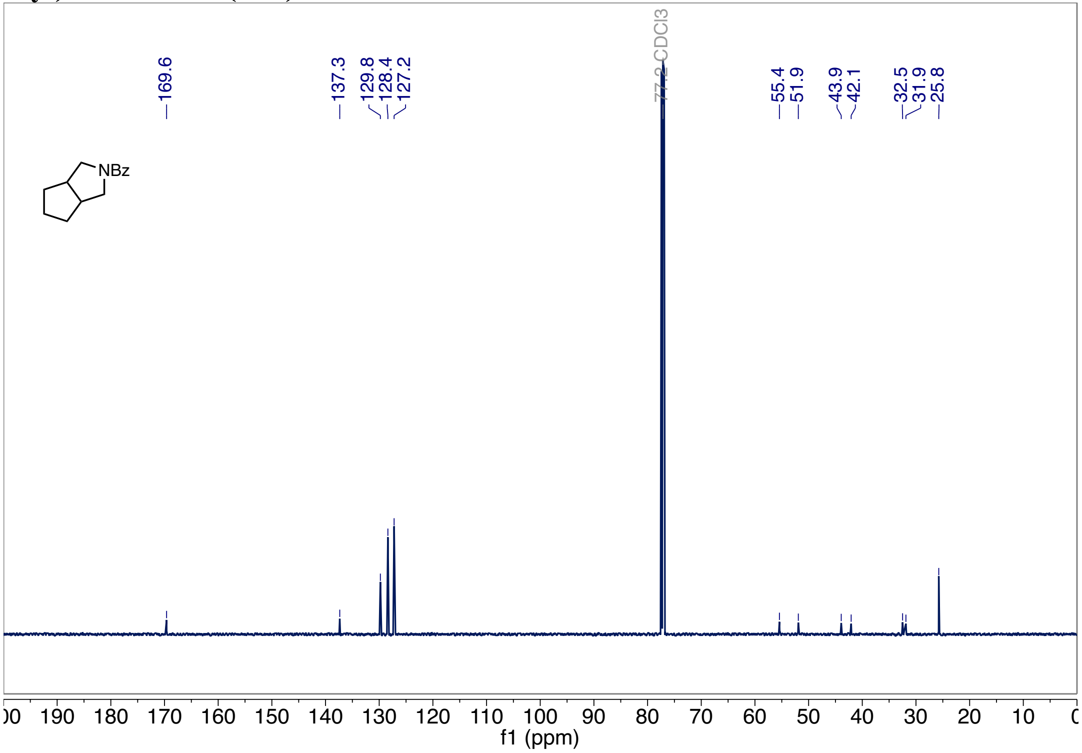
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of (2-(pent-4-en-1-yl)aziridin-1-yl)(phenyl)methanone (17a):



^{1}H NMR (500 MHz, CDCl$_3$) of (hexahydrocyclopenta[*c*]pyrrol-2(1*H*)-yl)(phenyl)methanone (17b):



^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$) of (hexahydrocyclopenta[*c*]pyrrol-2(1*H*)-yl)(phenyl)methanone (17b):



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12. Aryl Iodide SMILES

Cluster A

O=[N+]([O-])c1cccc(I)c1Br
COc1cc(I)cc(C=O)c1
COc1cc2ncnc(Nc3cccc(I)c3)c2cc1OC
Brc1c(I)ccc2ccccc12
O=Cc1ccc(Br)c(I)c1
Brc1cc(-n2c3ccccc3c3ccccc32)ccc1I
CSc1ncc(C(=O)O)c(=Nc2cccc(I)c2)[nH]1
Ic1cccc(Oc2ncccn2)c1
O=[N+]([O-])c1ccc(Br)c(I)c1
O=C(O)c1cccc(I)c1Br
O=C(O)c1ccc(Br)c(I)c1
OC(=Nc1cccc(I)c1)c1ccccc1
N#Cc1ccc(Br)c(I)c1
Clc1ccccc1I
FC(F)(F)c1cccc(I)c1Cl
O=C1c2cccc([N+](=O)[O-])c2C(=O)N1c1cccc(I)c1
Cc1ccc(N=C(O)c2ccccc2)cc1I
Cc1cc(Br)c(I)cc1C
O=[N+]([O-])c1ccccc1Oc1cccc(I)c1
COC(=O)c1ccc(Cl)c(I)c1
CC(C)c1ccc(I)c(Br)c1
Cc1cccc(C(O)=Nc2cccc(I)c2)c1
Cc1ccc(Br)c(I)c1
O=[N+]([O-])c1ccc(Cl)c(I)c1
O=[N+]([O-])c1cccc(C(O)=Nc2cccc(I)c2)c1
Oc1cc(I)ccc1-c1ccc(I)cc1O
Cc1cc(Cl)c(I)cc1C
OC(=NC1CC1)c1ccc(Cl)c(I)c1
Cc1cc(Cl)c(I)cc1C(=O)O
CC(C)(C)c1ccc(Br)c(I)c1
O=[N+]([O-])c1ccc(Cl)c(C(O)=Nc2cccc(I)c2)c1
O=C(Nc1cccc(I)c1)c1ccc([N+](=O)[O-])cc1
COC(=O)c1cc(O)cc(I)c1
Cc1ccc(I)c(Cl)c1
OCc1ccc(Br)c(I)c1
O=C(O)c1cccc(I)c1Cl
O=C(Nc1cccc(I)c1)c1cccs1
OC(=Nc1cccc(I)c1)c1ccccn1
Cc1ccc(N=C(O)c2ccc(N3CCOCC3)nc2)cc1I
COC(=O)c1ccc(Br)c(I)c1
O=C(Nc1cccc(I)c1)c1ccc(F)cc1

OCc1ccc(Cl)c(I)c1
OCc1ccc(I)c(Br)c1
Cc1ccc(I)c(Br)c1
CCc1ccc(I)c(Br)c1
CC(=O)c1ccc(Br)c(I)c1
N#Cc1ccc(Cl)c(I)c1
COC(=O)c1cc(I)c(Cl)cc1C
COC(=O)c1cc(I)cc(OC)c1
O=C(O)c1cc(O)cc(I)c1
FC(F)(F)c1ccc(Cl)c(I)c1
O=[N+]([O-])c1cccc(I)c1Cl
Cc1ccc(N=C(O)c2cnccn2)cc1I
N=C(O)c1ccc(Cl)c(I)c1
CCOC(=O)c1ccc(Cl)c(I)c1
Clc1cc(CBr)ccc1I
COC(=O)c1cc(I)c(Br)cc1C
CCOC(=O)c1cc(F)cc(I)c1
O=C(C=NO)Nc1cccc(I)c1
COC(=O)c1cc(N)cc(I)c1
Cc1cccc(I)c1Br
COc1cc(I)cc(C(=O)O)c1
N#Cc1cc(N)cc(I)c1
Brc1cc(-c2ccccc2)ccc1I
CS(=O)(=O)c1ncc(C(=N)O)c(=Nc2cccc(I)c2)[nH]1
FC(F)(F)c1ccc(Br)c(I)c1
Cc1ccc(Cl)c(I)c1
CC(C)(C)c1ccc(Cl)c(I)c1
OC(=Nc1cccc(I)c1)c1ccccc1F
CC(C)(C)c1ccc(I)c(Br)c1
O=[N+]([O-])c1cccc(-c2cn(-c3cccc(I)c3)nn2)c1
Clc1ccc(CBr)cc1I
COc1cccc(C(O)=Nc2cccc(I)c2)c1
O=C1C=CC(=O)N1c1cccc(I)c1
Ic1cccc(N=c2[nH]c(-c3ccccc3)nc3ccccc23)c1
CC(C)(C)OC(O)=Nc1cc(I)cc(C(=O)O)c1
O=C1c2ccc([N+](=O)[O-])cc2C(=O)N1c1cccc(I)c1
O=[N+]([O-])c1cc(F)cc(I)c1
CCOC(=O)c1cnc(SC)[nH]c1=Nc1cccc(I)c1
O=C(O)c1ccc(Cl)c(I)c1
N#Cc1cc(F)cc(I)c1

Cc1cccc(I)c1Cl
COC(=O)c1cccc(I)c1Cl
[N-]=[N+]=Nc1cccc(I)c1
O=C(O)c1cc(F)cc(I)c1
COC(=O)c1cccc(I)c1Br
O=Cc1cc(F)cc(I)c1
BrCc1cccc(I)c1Br
CSc1ncc(C(=N)O)c(=Nc2cccc(I)c2)[nH]1
O=[N+]([O-])c1ccccc1S(=O)(=O)Nc1cccc(I)c1
CON(C)C(=O)c1ccc(Cl)c(I)c1
CCOC(=O)c1cc(N)cc(I)c1
O=C(Nc1cccc(I)c1)c1ccco1
Cc1cc(Br)c(I)cc1C(=O)O
CC(C)(C)c1ccc(C(=O)Nc2cccc(I)c2)cc1
OC(=Nc1cccc(I)c1)c1cnccn1
OC(CN1CCCCC1)=Nc1cccc(I)c1
Nc1cc(I)cc([N+](=O)[O-])c1
OCc1cccc(I)c1Br
FC(F)(F)c1cccc(I)c1Br
Brc1ccccc1I
Cc1cc(=O)oc2cc(OCC(O)=Nc3cccc(I)c3)ccc12
OC(=Nc1cccc(I)c1)c1ccc2ccccc2c1
O=[N+]([O-])c1ccccc1C(O)=Nc1cccc(I)c1
Ic1cc2ccccc2cc1I
O=c1c2ccccc2sn1-c1cccc(I)c1
O=Cc1cccc(I)c1Br
Brc1cc2ccccc2cc1I
O=Cc1ccc(Cl)c(I)c1
S=C=Nc1cccc(I)c1
O=C(O)c1ccc(Cl)cc1NC(O)=Nc1cccc(I)c1
N#Cc1cccc(I)c1Br
Nc1cc(I)cc(C(=O)O)c1
CCOC(=O)C(=CNc1cccc(I)c1)C(=O)OCC
COc1cc(I)cc([N+](=O)[O-])c1
Cc1cc(Cl)c(I)cc1CO
CCOC(=O)c1cc(I)cc(OC)c1
OC(=Nc1cccc(I)c1)c1c(O)nc2ccccc2c1O
COC(=O)c1cc(F)cc(I)c1
Cc1ccc(N=C(O)c2ccnc(Cl)c2)cc1I
OC(=Nc1cccc(I)c1)c1ccccc1C(F)(F)F
Cc1ccc(N2C(=O)c3ccccc3C2=O)cc1I

Cluster B

Nc1c(F)cc(F)c(F)c1I
COc1cc(OC)c(C(C)=O)c(O)c1I
Oc1cc(OCc2ccccc2)ccc1I
O=C(O)c1cc(F)c(I)c(F)c1
COC(=O)c1cc(I)c(O)cc1OC
Fc1cc(F)c(I)c(F)c1
Nc1ccc(I)c(F)c1F
COCCCNS(=O)(=O)c1ccc(I)cc1
COc1cc(F)c(I)cc1OC
CCCCOc1ccc(I)c(F)c1F
O=C(O)c1c(F)cc(F)c(I)c1F
COc1ccc(F)c(I)c1OC
Fc1cc(F)c(I)cc1F
CON(C)C(=O)c1cccc(Cl)c1I
Oc1cc(F)c(Cl)cc1I
Nc1cc(F)c(I)cc1[N+](=O)[O-]
COc1cccc(O)c1I

Oc1cc(I)c(F)cc1F
Nc1cc(F)c(Br)cc1I
CC(O)=Nc1cc(F)c(I)c(F)c1
O=S(=O)(NCC1CCCO1)c1ccc(I)cc1
Nc1cc(F)c(Cl)cc1I
CC(C)NS(=O)(=O)c1ccc(I)cc1
FC(F)(F)c1cccc(Cl)c1I
COc1cc(N)c(I)cc1C(=O)O
O=S(=O)(c1ccc(I)cc1)N(Cc1ccccc1)Cc1ccccc1
Oc1cc(F)c(I)c(F)c1
COc1cc(Br)ccc1I
OCc1cc(F)c(I)c(F)c1
COc1ccc(F)c(F)c1I
CC(C)CNS(=O)(=O)c1ccc(I)cc1
OB(O)c1c(Br)ccc(I)c1F
COC(=O)c1cc(I)c(F)cc1F
N#Cc1cc(I)c(N)cc1Cl

N#Cc1c(N)ccc(I)c1F
COC(=O)c1cc(I)c(OC)cc1F
COC(=O)c1cc(I)c(O)cc1Cl
CCOc1cccc(F)c1I
COc1c(F)ccc(I)c1F
Cc1cc(I)c(F)cc1Cl
Nc1cc(Cl)ccc1I
O=C(Nc1ccc(I)cc1)c1cc2cc(Br)ccc2oc1=O
COc1ccc(C(=O)Oc2c(I)c(OC)cc(OC)c2C(C)=O)cc1
Fc1cc(Cl)c(Br)cc1I
O=S(=O)(NCCO)c1ccc(I)cc1
COc1cc(OC)c(I)c(OC)c1
FC(F)(F)Sc1ccc(I)cc1
COc1cc(F)c(F)cc1I
Nc1cc(Br)ccc1I
Nc1c(I)cc(Br)c(F)c1F

COC(=O)c1ccc(C)c(I)c1Cl
O=C(O)c1cc(I)c(F)c(F)c1F
N#Cc1cc(I)c(O)cc1F
COc1ccc(OC)c(I)c1F
COc1cc(N)c(I)cc1Cl
CN(C)c1ccc(I)c(F)c1
BrCc1cccc(Br)c1I
COc1cc(OC)c(I)cc1Cl
COC(=O)c1cc(I)c(N)cc1Cl
Nc1c(F)c(F)c(I)c(F)c1F
Oc1c(Br)ccc(I)c1F
Fc1ccc(I)c(F)c1Cl
N#Cc1cc(F)c(I)c(F)c1
COc1cc(I)c(N)cc1Br
Oc1cc(F)ccc1I
Nc1ccc(I)c(OC(F)(F)F)c1
O=C(O)CNS(=O)(=O)c1ccc(I)cc1
COc1cc(I)c(OC)cc1Cl
CC(O)=NCC1CN(c2ccc(I)c(F)c2)C(=O)O1
Oc1c(I)ccc(I)c1O
Nc1c(I)ccc(F)c1F
COC(=O)c1cc(N)c(I)c(O)c1
COc1cc(Cl)cc(C)c1I
COC(=O)c1cc(O)c(I)c(O)c1
Nc1cc(Br)c(Cl)cc1I
Nc1cc(Cl)c(Br)cc1I
Nc1cc(O)ccc1I
COc1cc(Br)c(F)cc1I
O=Cc1cc(I)c(O)cc1F
Fc1cc(I)c(F)cc1Cl
Nc1cc(F)c(F)c(F)c1I
Oc1cc(Br)cc(F)c1I
C#CC(C)(C)NS(=O)(=O)c1ccc(I)cc1
Cc1cc(Br)c(I)c(C(=O)O)c1
COc1cccc(N)c1I
Fc1c(F)c(I)c(F)c(F)c1I
Nc1cccc(F)c1I
COc1cc(N)ccc1I
CCOc1cc(Br)ccc1I
Fc1cc(F)c(I)cc1Cl
Fc1c(Br)cc(I)c(F)c1F
O=C(Nc1ccc(I)cc1)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Cc1cc(O)c(I)c(O)c1
O=C(O)c1cccc(Br)c1I
Cc1cc(C)c(I)c(Br)c1
Fc1cc(Cl)ccc1I
COc1ccc(I)c(F)c1
Oc1ccc(I)c(F)c1
Nc1cc(OC(F)(F)F)ccc1I
COc1cc(I)c(F)cc1F
Nc1cc(Br)c(F)cc1I
O=[N+]([O-])c1cc(I)c(F)c(F)c1F
Fc1c(I)ccc(Cl)c1Cl
C=CCNS(=O)(=O)c1ccc(I)cc1
COc1cc(N)c(I)cc1OC
Nc1ccc(I)c(F)c1
Cc1cccc(Br)c1I
Fc1ccc(Cl)c(F)c1I
Brc1ccc2ccccc2c1I
Cc1cc(Cl)cc(O)c1I
Cc1cc(I)c(O)cc1Cl
O=C(Nc1ccc(I)cc1)c1cc([N+](=O)[O-])ccc1Cl
O=C(Nc1ccc(I)cc1)c1ccc(Cl)cc1[N+](=O)[O-]
COc1cccc(OC)c1I
COc1cc(F)c(I)cc1C(=O)O
Cc1cc(I)c(N)cc1Cl
Nc1c(I)ccc(Br)c1Cl
COc1ccc(I)c(OC)c1OC
O=C1OC(CO)CN1c1ccc(I)c(F)c1
Nc1cc(I)c(F)cc1Cl
Nc1c(F)ccc(F)c1I
NNS(=O)(=O)c1ccc(I)cc1
Nc1cccc(O)c1I
COc1cc(F)c(C(=O)O)cc1I
COC(=O)c1ccc(N)c(I)c1O
Nc1cc(Cl)c(Cl)cc1I
COC(=O)c1cc(I)c(N)cc1OC
CC(C)(C)NS(=O)(=O)c1ccc(I)cc1
CC(C)C(NS(=O)(=O)c1ccc(I)cc1)C(=O)O
Cc1cc(I)c(F)cc1F
O=P(O)(O)c1ccc(I)cc1
Fc1c(I)ccc(I)c1F
Fc1c(I)ccc(Br)c1Cl
CCc1cc(F)c(I)c(F)c1
CC(C)(C)OC(=O)c1cc(I)c(F)cc1F
C[Si](C)(C)c1c(F)ccc(I)c1F
COc1c(I)ccc(I)c1OC
FC(F)(F)Oc1cc(Br)ccc1I
Oc1cc(Cl)ccc1I
OCc1cccc(Br)c1I
O=S(=O)(c1ccc(I)cc1)N1CCc2ccccc2C1
COc1cc(Br)c(Cl)cc1I
Cc1ccc(Oc2c(F)c(F)c(I)c(F)c2F)cc1
CCOc1cc(Cl)ccc1I
COC(=O)c1cccc(Br)c1I
Fc1ccc(F)c(I)c1F
COc1cc(Br)c(C(F)(F)F)cc1I
FC(F)(F)c1cccc(Br)c1I
OCc1cc(I)c(F)cc1F
Nc1cc(F)c(C(F)(F)F)cc1I
COc1ccc(I)c(N)c1
Nc1cc(F)ccc1I
Nc1cc(F)c(Br)c(F)c1I
O=[N+]([O-])c1ccc(F)c(I)c1F
O=S(=O)(NCc1ccccn1)c1ccc(I)cc1
O=C(Nc1ccc(I)cc1)c1cc2ccccc2oc1=O
COc1ccc(C=O)c(O)c1I
Nc1ccc(F)c(F)c1I
OB(O)c1cc(F)c(I)c(F)c1
COc1cc(C=O)c(I)c(OC)c1
COc1cc(Br)cc(OC)c1I
Fc1ccc(I)c(F)c1F
N#Cc1cc(I)c(N)cc1F
Nc1cc(Cl)c(F)cc1I
COc1ccc(Cl)c(F)c1I
COc1cc(C)c(I)c(OC)c1OC
O=C(O)c1c(F)c(F)c(F)c(F)c1I
COc1cc(N)c([N+](=O)[O-])cc1I
Fc1ccc(I)c(F)c1Br
Fc1ccc(I)c(F)c1OC(F)(F)F
CSc1ccc(F)c(I)c1F
Oc1ccc(I)c(F)c1F
COC(=O)c1cc(OC)cc(OC)c1I
Oc1cc(I)c(O)cc1I
O=[N+]([O-])c1ccc(Oc2c(F)c(F)c(I)c(F)c2F)cc1
Fc1cccc(F)c1I
COc1ccc(F)c(OC)c1I
COc1cc(N)c(C(=O)O)cc1I
COC(=O)c1cc(I)c(F)cc1OC
Nc1c(F)c(F)c(F)c(F)c1I
O=C(Nc1ccc(I)cc1)Nc1ccc([N+](=O)[O-])cc1
Oc1cccc(F)c1I
O=Cc1cc(F)c(I)c(F)c1
Nc1c(I)cc(F)c(F)c1F
Fc1ccc(I)c(F)c1
Nc1c(I)ccc(F)c1[N+](=O)[O-]
CN(C)S(=O)(=O)c1ccc(I)cc1
O=Cc1cc(I)c(F)cc1F
Fc1c(Cl)ccc(I)c1F
Nc1cc(Br)c(C(F)(F)F)cc1I
O=S(=O)(O)c1ccc(I)cc1
O=C(Nc1ccc(I)cc1)c1ccccc1[N+](=O)[O-]
CCOP(=O)(OCC)c1ccc(I)cc1
COc1cc(Br)cc(C)c1I
Oc1cc(F)c(F)cc1I
Fc1c(F)c(F)c(I)c(F)c1F
N#Cc1cccc(Br)c1I
Oc1cc(I)c(F)cc1Cl
CS(=O)(=O)c1ccc(I)cc1
COc1cc(O)c(C(=O)O)cc1I
COCCNS(=O)(=O)c1ccc(I)cc1
COc1cc(I)c(OC)cc1I
O=[N+]([O-])c1c(F)ccc(I)c1F
O=S(=O)(NC1CCCC1)c1ccc(I)cc1
CCOC(=O)c1cc(O)c(I)c(O)c1
FC(F)Oc1cc(Br)ccc1I
COc1c(Cl)ccc(I)c1F
Fc1c(I)ccc(Br)c1Br
Cc1cc(I)c(N)cc1Br
O=[N+]([O-])c1cc(I)c(F)cc1F
O=S(=O)(Oc1ccc(Cl)cc1)c1ccc(I)cc1
COc1cc(I)c(F)cc1Cl
CCNS(=O)(=O)c1ccc(I)cc1
FS(F)(F)(F)(F)c1ccc(I)cc1
Cc1cc(I)c(N)cc1O
Cc1cc(Cl)cc(N)c1I
COc1cc(OC)c(C(C)C)cc1I
O=S(=O)(NCc1ccccc1)c1ccc(I)cc1
COc1cc(Br)cc(F)c1I
O=S(=O)(NC1CC1)c1ccc(I)cc1
Fc1cc(OC(F)(F)F)ccc1I
O=C(O)c1cc(I)c(O)cc1O
NCC1CN(c2ccc(I)c(F)c2)C(=O)O1
Fc1cc(Br)ccc1I
Fc1cc(I)c(F)cc1Br
COc1cc(Br)c(C)cc1I
Oc1cccc(O)c1I
Fc1cc(F)c(CBr)cc1I
O=C(O)c1c(F)ccc(I)c1F
O=C(O)c1cc(O)c(I)c(O)c1
COc1ccc(I)c(OC)c1
COc1cc(C(=O)Nc2ccc(I)cc2)c([N+](=O)[O-])cc1OC
COc1ccc(C(C)=O)c(O)c1I
COc1ccc(I)c(O)c1
CCOc1cc(Cl)c(C#N)cc1I
N#Cc1cc(I)c(O)cc1Cl
Fc1ccc(Br)c(F)c1I
Nc1ccc(Cl)c(F)c1I
COC(=O)c1c(F)ccc(I)c1F
Fc1c(I)ccc(OCc2ccccc2)c1F
CCOC(=O)c1cccc(Br)c1I
Oc1c(I)ccc(F)c1F
COC(=O)c1cc(I)c(N(C)C)cc1O
COc1ccc(Br)c(F)c1I
O=C(O)c1cc(I)c(O)cc1F
CC(O)=NC[C@H]1CN(c2ccc(I)c(F)c2)C(=O)O1
CC(C)Oc1cc(Cl)ccc1I
Cc1ccc(F)c(I)c1F
CCOc1ccc(I)c(F)c1F
O=C(O)c1cccc(Cl)c1I
COc1ccc(I)c(OC)c1F
COc1cc(CO)c(I)c(OC)c1

Nc1ccc(Br)c(F)c1I
O=C(O)c1cc(I)c(F)cc1F
Cc1cccc(Cl)c1I
Nc1cc(I)ccc1I
Oc1cc(Br)ccc1I
COC(=O)c1cc(I)c(OC)cc1N
COc1cc(F)c(C=O)cc1I
CC(=O)c1c(F)ccc(I)c1F
N#Cc1cc(I)c(F)cc1F
COc1ccc(I)c(F)c1F
Cc1cc(I)c(N)cc1F
COc1cc(OC)c(C=O)cc1I
Cc1c(N)c(I)cc(Br)c1Cl
Fc1cc(I)ccc1I
Clc1ccc(I)c(OCc2ccccc2)c1
Nc1c(Br)cc(F)c(F)c1I
Fc1c(Br)ccc(I)c1F

Fc1c(Br)cc(Br)c(F)c1I
CNS(=O)(=O)c1ccc(I)cc1
Nc1cc(F)c(F)cc1I
NS(=O)(=O)c1ccc(I)cc1
Cc1c(F)ccc(I)c1F
Nc1ccc(F)c(I)c1F
Fc1cc(Br)c(Cl)cc1I
Cc1cc(Br)cc(F)c1I
Nc1cc(F)c(I)c(F)c1
COc1cc(Cl)ccc1I
COc1cc(OC)c(OC)cc1I
Cc1c(Br)ccc(I)c1F
Fc1cc(Br)cc(F)c1I
Nc1cc(F)c(I)cc1C(=O)O
COc1cc(F)ccc1I
O=S(=O)(NCc1ccncc1)c1ccc(I)cc1
Cc1cc(I)c(F)cc1N

CCC(C)NS(=O)(=O)c1ccc(I)cc1
CCCNS(=O)(=O)c1ccc(I)cc1
Fc1cc(F)c(I)cc1Br
CCOc1cc(F)c(I)c(F)c1
Cc1c(N)ccc(I)c1F
COc1cc(O)c(C=O)cc1I
Fc1cc(Cl)cc(F)c1I
Nc1ccc(I)c(F)c1[N+](=O)[O-]
COC(=O)c1cccc(Cl)c1I
COC(=O)c1cc(I)c(F)cc1N
COc1cc(I)c(OC)cc1Br
COc1cccc(F)c1I
NC[C@H]1CN(c2ccc(I)c(F)c2)C(=O)O1
Nc1cc(F)c(I)cc1F
Fc1cc(F)c(F)c(I)c1

Cluster C

Fc1cccc(COc2ccc(I)cc2)c1
FC(F)(F)Oc1ccc(Oc2ccc(I)cc2)cc1
Fc1ccccc1Oc1ccc(I)cc1
Fc1cc(Cl)cnc1Oc1ccc(I)cc1
NCCOc1ccc(I)cc1
OCCOc1ccc(I)cc1
Ic1ccc(OC2CCC2)cc1
CSCCOc1ccc(I)cc1
CC(=O)Oc1ccc(I)cc1
N#CCOc1ccc(I)cc1
O=C(O)CCCOc1ccc(I)cc1
Clc1ccc(Oc2ccc(I)cc2)cc1Cl
Cc1ccc(NC(=O)c2ccc(COc3ccc(I)cc3)o2)cc1F
Cc1ccc(Oc2ccc(I)cc2)c(C)c1
FC(F)(F)Oc1ccc(I)cc1
Ic1ccc(Oc2ccc(I)cc2)cc1
Cc1cc(C)cc(Oc2ccc(I)cc2)c1
O=C(O)c1cccc(N=C(O)COc2ccc(I)cc2)c1
Cc1ccc(S(=O)(=O)Oc2ccc(I)cc2)cc1
Ic1ccc(OC2CC2)cc1
O=C(Oc1ccc(I)cc1)N(c1ccccc1)c1ccccc1
CC(C)(C)OC(=O)N1C[C@@H](Oc2ccc(I)cc2)C[C@H]1C(=O)O
CC(O)=N[C@H]1[C@H](Oc2ccc(I)cc2)O[C@H](CO)[C@@H](O)[C@@H]1O
Ic1ccc(OCCN2CCCCC2)cc1
FC(F)C(F)(F)Oc1ccc(I)cc1
OC(COc1ccc(I)cc1)=NC1CCN(Cc2ccccc2)CC1
O=C(O)COc1ccc(I)cc1
NN=C(O)COc1ccc(I)cc1

N#Cc1ccc(COc2ccc(I)cc2)cc1
COc1ccc(COc2ccc(I)cc2)cc1
COC(=O)c1cccc(COc2ccc(I)cc2)c1
Ic1ccc(OCc2ccccc2)cc1
Oc1ccc(Oc2ccc(I)cc2)cc1
CC(C)(C)[Si](C)(C)Oc1ccc(I)cc1
O=C(O)c1ccc(Oc2ccc(I)cc2)cc1
COc1ccccc1Oc1ccc(I)cc1
NCC(O)COc1ccc(I)cc1
Nc1ccccc1Oc1ccc(I)cc1
Ic1ccc(OCC2CC2)cc1
CC(C)Oc1ccc(I)cc1
O=C(Cl)COc1ccc(I)cc1
C[C@H](Oc1ccc(I)cc1)C(=O)O
BrCCOc1ccc(I)cc1
CC(Oc1ccc(I)cc1)C(=O)O
FC(F)(F)COc1ccc(I)cc1
Ic1ccc(OCc2ccncc2)cc1
COc1ccc(Oc2ccc(I)cc2)cc1
Clc1ccc(COc2ccc(I)cc2)c(Cl)c1
CCOC(=O)COc1ccc(I)cc1
Fc1cccc(F)c1Oc1ccc(I)cc1
N#Cc1ccc(Oc2ccc(I)cc2)cc1
Ic1ccc(Oc2ccccc2)cc1
Oc1ccc(I)cc1
OC(COc1ccc(I)cc1)=NCC1CCCO1
N=C(O)COc1ccc(I)cc1
O=C(O)c1ccc(COc2ccc(I)cc2)cc1
COC(=O)COc1ccc(I)cc1

OC(COc1ccc(I)cc1)=NCCc1nc2ccccc2[nH]1
Fc1ccc(Oc2ccc(I)cc2)cc1
CCOc1ccc(I)cc1
Ic1ccc(OC2CCCCC2)cc1
COc1ccc(I)cc1
Clc1ccc(Oc2ccc(I)cc2)cc1
Cc1cccc(NC(=O)c2ccc(COc3ccc(I)cc3)o2)c1
O=C(Nc1ccc(F)c(F)c1)c1ccc(COc2ccc(I)cc2)o1
OCCNCCOc1ccc(I)cc1
COC(=O)c1ccc(COc2ccc(I)cc2)o1
Ic1ccc(OC2CCOCC2)cc1
N=C(O)c1cccc(COc2ccc(I)cc2)c1
COC(=O)c1ccc(Oc2ccc(I)cc2)cc1
FC(F)Oc1ccc(I)cc1
O=S(=O)(Oc1ccc(I)cc1)C(F)(F)F
C#CCOc1ccc(I)cc1
COCCOc1ccc(I)cc1
CC(C)(C)Oc1ccc(I)cc1
CCCCOc1ccc(I)cc1
OC(COc1ccc(I)cc1)=NCc1nc2ccccc2[nH]1
Ic1ccc(OC2CCCC2)cc1
Clc1ccc(COc2ccc(I)cc2)cc1
O=C(O)CCOc1ccc(I)cc1
Cc1ccc(Oc2ccc(I)cc2)cc1
Ic1ccc(OCc2cccnc2)cc1
COC(=O)c1ccc(C)c(NC(=O)c2ccc(COc3ccc(I)cc3)o2)c1

Cluster D

Cc1cc(C)cc(NC(=O)c2ccc(I)cc2)c1
NC(=O)c1ccc(I)cc1
O=C(O)/C=C/c1ccc(I)cc1
O=C(O)C=Cc1ccc(I)cc1
NNC(=O)c1ccc(I)cc1
Oc1nc(SCc2ccc(I)cc2)nc2ccccc12
O=Cc1ccc(I)cc1
COc1ccc(N=C(O)c2ccc(I)cc2)cc1
OC1=NC(=S)S/C1=C\c1ccc(I)cc1
O=C(/C=C/c1ccc([N+](=O)[O-])cc1)c1ccc(I)cc1
CC(C=O)c1ccc(I)cc1
O=C(NO)c1ccc(I)cc1
O=C(CC1OC(=O)c2ccccc21)c1ccc(I)cc1
Ic1ccc(/C=C/c2ccc(I)cc2)cc1
O=C(Nc1ccccc1O)c1ccc(I)cc1

Ic1ccc(CSc2nc3ccccc3[nH]2)cc1
Ic1ccc(-c2noc(-c3ccco3)n2)cc1
CCOC(=O)c1ccccc1C(=O)c1ccc(I)cc1
CC(=O)Cc1ccc(I)cc1
O=Cc1ccc(-c2ccc(I)cc2)cc1
O=C(NC1CCN(Cc2ccccc2)CC1)c1ccc(I)cc1
O=[N+]([O-])c1ccc(N=C(O)c2ccc(I)cc2)cc1
COc1ccccc1N1CCN(C(=O)c2ccc(I)cc2)CC1
O=C(CO)c1ccc(I)cc1
Ic1ccc(-c2nc(-c3ccccc3)no2)cc1
O=C(N=c1cc[nH]cc1)c1ccc(I)cc1
O=C(CC(=O)C(F)(F)F)c1ccc(I)cc1
OC1=NN=C(c2ccc(I)cc2)CC1
O=C(c1ccc(I)cc1)N(c1ccccn1)c1ccccn1
CC(C)c1ccc(N=C(O)c2ccc(I)cc2)cc1

COc1ccccc1CNC(=O)c1ccc(I)cc1
O=C(O)CCC(=O)c1ccc(I)cc1
O=C(Nc1cccc2ccccc12)c1ccc(I)cc1
CCNC(=O)c1ccc(I)cc1
COc1cccc(/C=C/C(=O)c2ccc(I)cc2)c1
Ic1ccc(-c2nc3ccccc3s2)cc1
O=C(c1ccc(I)cc1)c1ccccc1Cl
COc1ccccc1NC(=O)c1ccc(I)cc1
CCN1CCN(C(=O)c2ccc(I)cc2)CC1
Ic1ccc(-c2ncco2)cc1
OC1=NC(S)=N/C1=C\c1ccc(I)cc1
Oc1ncnc2ncc(-c3ccc(I)cc3)nc12
Ic1ccc(C#Cc2ccccc2)cc1
Ic1ccc(-c2nc3ncccc3o2)cc1
COc1ccc(C=CC(=O)c2ccc(I)cc2)cc1O

O=C(C(=O)c1ccc(I)cc1)c1ccccc1
O=C(Nc1ccccc1)c1ccc(I)cc1
CC(=O)c1ccc(-c2ccc(I)cc2)cc1
O=C(COC(=O)c1ccc(I)cc1)c1ccc(Br)cc1
O=C(C=Cc1cccs1)c1ccc(I)cc1
O=C(CCl)c1ccc(I)cc1
NCCNC(=O)c1ccc(I)cc1
O=C(OCc1ccc(I)cc1)c1ccc([N+](=O)[O-])cc1
O=C(c1ccc(Br)cc1)c1ccc(I)cc1
CC1(C)CC(=O)C2=C(C1)Nc1ccc3ccccc3c1C2c1ccc(I)cc1
CC(=Cc1ccc(I)cc1)C(=O)O
COc1cc(C=CC(=O)c2ccc(I)cc2)ccc1O
Ic1ccc(-c2nnc(CN3CCCCC3)o2)cc1
Cc1ccc(NC(=O)c2ccc(I)cc2)nc1
N#Cc1cccc(C(=O)c2ccc(I)cc2)c1
O=C(O)c1cc(-c2ccc(I)cc2)nc2ccccc12
Ic1ccc(-c2ccc(-c3ccc(I)cc3)cc2)cc1
O=C(CBr)c1ccc(I)cc1
O=C1N=C(O)/C(=C/c2ccc(I)cc2)S1
COc1ccc2nc(NC(=O)c3ccc(I)cc3)sc2c1
O=C(OCc1ccccc1)c1ccc(I)cc1
CC(O)=Nc1nc(-c2ccc(I)cc2)cs1
Ic1ccc(-c2ccno2)cc1
COC(=O)CNC(=O)c1ccc(I)cc1
O=C(c1ccc(I)cc1)n1nnc2ccccc21
CCN(CC)c1ccc(C=O)c(OCc2ccc(I)cc2)c1
O=C(C=Cc1ccsc1)c1ccc(I)cc1
CCOC(=O)c1ccc(C(=O)c2ccc(I)cc2)cc1
COc1ccccc1CC(=O)c1ccc(I)cc1
O=c1c(=Cc2ccc(I)cc2)sc2nc3ccccc3n12
Cc1cccc(N(c2ccccc2)c2ccc(-c3ccc(I)cc3)cc2)c1
O=C(O)CN1C(=O)/C(=C\c2ccc(-c3ccc(I)cc3)o2)SC1=S
CN1CCC(NC(=O)c2ccc(I)cc2)CC1
OC(=Nc1ccc(Br)cc1)c1ccc(I)cc1
Cc1cc(C)c(NC(=O)c2ccc(I)cc2)c(C)c1
O=C(Nc1cccc(Cl)c1)c1ccc(I)cc1
CN(C)CCNC(=O)c1ccc(I)cc1
O=C(O)/C(S)=C/c1ccc(I)cc1
COC(=O)c1ccccc1NC(=O)c1ccc(I)cc1
O=c1nc(-c2ccc(I)cc2)[nH]o1
O=C(Nc1ccccc1Cl)c1ccc(I)cc1
CC(C)(C)OC(=O)c1ccc(I)cc1
Ic1ccc(B2Nc3cccc4cccc(c34)N2)cc1
O=C(c1ccc(O)cc1)c1ccc(I)cc1
Nc1ccc(C(=O)c2ccc(I)cc2)cc1
CN1CCN(C(=O)c2ccc(I)cc2)CC1
O=C(Nc1ccccc1C(=O)O)c1ccc(N=C(O)c2ccc(I)cc2)cc1
Cc1cccc(NC(=O)c2ccc(I)cc2)n1
O=Cc1ccc(OCc2ccc(I)cc2)cc1
CCOC(=O)CC(=O)c1ccc(I)cc1
COc1ccc2oc(=O)c(-c3ccc(I)cc3)cc2c1
O=C(ON1C(=O)CCC1=O)c1ccc(I)cc1
CCOC(=O)CCCCC(=O)c1ccc(I)cc1
COC(=O)CC(=O)c1ccc(I)cc1
CN(C)/C=C/C(=O)c1ccc(I)cc1
Nc1cc(-c2ccc(I)cc2)no1
CCOC(=O)C1=C(C)NC(C)=C(C(=O)OCC)C1c1ccc(I)cc1

CC1(C)C(c2ccc(I)cc2)=[N+]([O-])C(C)(C)N1O
Cc1ccccc1NC(=O)c1ccc(I)cc1
Ic1ccc(-c2noc(-c3cccs3)n2)cc1
O=C(Nc1ncccc1O)c1ccc(I)cc1
Cc1cc(C)n2c1C(=C1C=CC(=[I+])C=C1)c1c(C)cc(C)n1[B-]2(F)F
N#CCCCCC(=O)c1ccc(I)cc1
Cc1ccc(C(=O)c2ccc(I)cc2)cc1
COc1cc(NC(=O)c2ccc(I)cc2)cc(OC)c1
O=C(O)c1ccc(I)cc1
N#CCCCC(=O)c1ccc(I)cc1
O=C(c1ccc(F)cc1)c1ccc(I)cc1
O=c1ccccn1Cc1ccc(I)cc1
O=C(CBr)CCc1ccc(I)cc1
O=C(O)C(=O)c1ccc(I)cc1
O=C(O)c1ccc(N=C(S)N=C(O)c2ccc(I)cc2)cc1
Cc1cccc(C(=O)c2ccc(I)cc2)c1
Cc1ccc(I)cc1Cc1ccc(-c2ccc(F)cc2)s1
Cc1nnc(-c2ccc(I)cc2)nn1
COc1cc(OC)c(OC)cc1C=CC(=O)c1ccc(I)cc1
O=c1/c(=C/c2ccc(I)cc2)sc2nc3ccccc3n12
ClC(=NNc1ccccc1)c1ccc(I)cc1
O=C(c1ccccc1)c1ccc(I)cc1
O=C(NC1CCN(Cc2ccccc2)C1)c1ccc(I)cc1
O=C(Nc1ccccc1F)c1ccc(I)cc1
O=Cc1ccc(-c2ccc(I)cc2)o1
CC1=NN(C(=O)c2ccc(I)cc2)C(C)(O)C1
Ic1ccc(-c2ccncc2)cc1
Cc1cccn2cc(-c3ccc(I)cc3)nc12
ClCc1nnc(-c2ccc(I)cc2)o1
O=C(Cc1ccc(I)cc1)C(F)(F)F
N#CCC(=O)c1ccc(I)cc1
CCOC(=O)CCC(=O)c1ccc(I)cc1
O=C(c1ccc(Cl)cc1)c1ccc(I)cc1
O=C(Nc1cccc(F)c1)c1ccc(I)cc1
O=c1oc2ccc(Cl)cc2cc1-c1ccc(I)cc1
Cc1cccc(NC(=O)c2ccc(I)cc2)c1
O=C(O)c1cccc(-c2ccc(I)cc2)c1
O=C(O)C(S)=Cc1ccc(I)cc1
O=C(O)c1cc(-c2ccc(I)cc2)nc2ccc(Br)cc12
Ic1ccc(CSc2nnc(-c3ccncc3)o2)cc1
O=C(Cc1ccccc1F)c1ccc(I)cc1
COc1cc(C=O)ccc1OCc1ccc(I)cc1
CCC(=O)Cc1ccc(I)cc1
O=C(C=Cc1ccc(I)cc1)c1ccc(B(O)O)cc1
O=c1oc2ccccc2cc1-c1ccc(I)cc1
CCN=c1cc(C)nc(N2CCN(C(=O)c3ccc(I)cc3)CC2)[nH]1
CN(C(=O)c1ccc(I)cc1)c1ccccc1
CCOC(=O)CCC(NC(=O)c1ccc(I)cc1)C(=O)OCC
N=C(O)c1ccccc1NC(=O)c1ccc(I)cc1
C=CCNC(=O)c1ccc(I)cc1
Ic1ccc(-c2cn3ccccc3n2)cc1
O=C(O)CCCCC(=O)c1ccc(I)cc1
N=c1[nH]c(-c2ccc(I)cc2)cs1
O=C(NCc1ccco1)c1ccc(I)cc1
O=C(O)CCCCCC(=O)c1ccc(I)cc1
COc1ccc(C(=O)c2ccc(I)cc2)cc1
O=Cc1cn(Cc2ccc(I)cc2)c2ccccc12
Cc1ccc(S(=O)(=O)CC(=O)c2ccc(I)cc2)cc1
OC1=NC(=S)SC1=Cc1ccc(I)cc1

O=C(Cc1ccccc1Cl)c1ccc(I)cc1
O=C(NCc1cccnc1)c1ccc(I)cc1
O=C(NC1CC1)c1ccc(I)cc1
CCOC(=O)Cc1csc(NC(=O)c2ccc(I)cc2)n1
Ic1ccc(/N=N/c2ccc(I)cc2)cc1
Cc1ccccc1C(=O)c1ccc(I)cc1
COC(=O)[C@@H]1CS[C@H](c2ccccc2Cl)N1C(=O)c1ccc(I)cc1
CCC(=O)c1ccc(I)cc1
Ic1ccc(-c2cc(-c3ccccc3)nc(-c3ccccc3)c2)cc1
O=C(O)c1ccc(-c2ccc(I)cc2)cc1
O=C(Cc1ccc(Cl)cc1)c1ccc(I)cc1
NC(=S)c1ccc(I)cc1
ON=Cc1ccc(I)cc1
CC(C)C(=O)c1ccc(I)cc1
O=C(Cc1ccccc1)c1ccc(I)cc1
CCOc1ccc(C(=O)c2ccc(I)cc2)cc1
OC(=Nc1ccc(Cl)cc1)c1ccc(I)cc1
CCSc1ccc2nc(-c3ccc(I)cc3)cn2c1
O=Cc1ccccc1OCc1ccc(I)cc1
CC(C)(C)OC(=O)CC(=O)c1ccc(I)cc1
O=C(O)c1cc(NC(=O)c2ccc(I)cc2)cc(C(=O)O)c1
O=C(Nc1cccnc1)c1ccc(I)cc1
Ic1ccc(-c2cnco2)cc1
N=c1nc(-c2ccc(I)cc2)[nH]c(=N)[nH]1
O=C(c1ccc(I)cc1)c1ccc(I)cc1
CC1(C)CC(=O)C2=C(C1)OC1=C(C(=O)CC(C)(C)C1)C2c1ccc(I)cc1
C=C(C(=O)OC)c1ccc(I)cc1
O=C(c1ccc(I)cc1)C(F)(F)F
CN=c1[nH]c(-c2ccc(I)cc2)cs1
COC(=O)C1=C(C)NC(C)=C(C(=O)OC)C1c1ccc(I)cc1
OC(=Nc1ccc(F)cc1)c1ccc(I)cc1
C=CCOC(=O)C1=C(C)NC(C)=C(C(=O)OCC=C)C1c1ccc(I)cc1
O=S(=O)(Cl)Cc1ccc(I)cc1
COc1ccc(CNC(=O)c2ccc(I)cc2)cc1
FC(F)(F)c1cc(-c2ccc(I)cc2)cc(C(F)(F)F)c1
CC(=O)c1ccc(I)cc1
Ic1ccc(-c2nc3ccccc3n2-c2ccccc2)cc1
O=C(NC1CCCCCC1)c1ccc(I)cc1
Nc1cc(-c2ccc(I)cc2)nn1-c1ccccc1
O=C(NC1CCCCC1)c1ccc(I)cc1
Cc1ccc(C(=O)O)cc1NC(=O)c1ccc(I)cc1
O=C(Cl)c1ccc(I)cc1
O=C(Nc1ccccn1)c1ccc(I)cc1
COc1ccc(C(O)=NN=C(O)c2ccc(I)cc2)cc1
COc1ccc(/C=C/C(=O)c2ccc(I)cc2)c(OC)c1OC
Ic1ccc(-c2nc3ccccc3nc2-c2ccccc2)cc1
CCN(CC)CCNC(=O)c1ccc(I)cc1
COc1ccc(C=CC(=O)c2ccc(I)cc2)cc1OC
Cc1ccc(-c2cc(-c3ccccc3)cc(-c3ccc(I)cc3)n2)cc1
O=C(NCCN1CCCCC1)c1ccc(I)cc1
CC(=O)CCc1ccc(I)cc1
O=C1N=C(O)CCC1(c1ccccc1)C1CCN(Cc2ccc(I)cc2)CC1
O=[N+]([O-])c1ccc(-c2ccc(I)cc2)cc1

Cluster E

COC(=O)CCc1ccc(I)cc1
Ic1ccc(CN2CCOCC2)cc1
CC(C)(C)OC(O)=N[C@@H](CC(=O)O)Cc1ccc(I)cc1

OCc1ccc(I)cc1CO
C=Cc1ccc(I)cc1
CC(NC1CC1)c1ccc(I)cc1
C=C(C)c1ccc(I)cc1

OCc1ccc(I)cc1
N#Cc1ccc(I)cc1
O=C(c1ccc(I)cc1)N1CCOCC1
OCC1CCN(Cc2ccc(I)cc2)CC1

CCCCCc1ccc(-c2ccc(I)cc2)cc1
Cc1ccc(I)cc1N=C(O)OC(C)(C)C
CCc1ccc(I)cc1C
FC[C@H]1N=C(c2ccccc2)O[C@@H]1c1ccc(I)cc1
Ic1ccc(Cc2ccc(I)cc2)cc1
OCc1ccc(I)cc1C(F)(F)F
CSCc1ccc(I)cc1
ClCc1ccc(I)cc1
CCCCc1ccc(I)cc1
COC(=O)C(N)Cc1ccc(I)cc1
CC(C)(C)OC(=O)N1CCN(Cc2ccc(I)cc2)CC1
Clc1ccc(-c2ccc(I)cc2)cc1
CC(C)(C)OC(=O)N1CCC[C@H]1c1ncc(-c2ccc(I)cc2)[nH]1
O=C(O)[C@H](Cc1ccc(I)cc1)N=C(O)OCc1ccccc1
CC(C)(C)OC(O)=NC(Cc1ccc(I)cc1)C(=O)O
Cc1cc(I)cc(C)c1C
Ic1ccc(C2CC2)cc1
OCCc1ccc(I)cc1
Ic1ccc(C2CCCCN2)cc1
CN1CCN(Cc2ccc(I)cc2)CC1
COC(=O)[C@@H](Cc1ccc(I)cc1)N=C(O)OC(C)(C)C
O=C(O)[C@@H](O)Cc1ccc(I)cc1
CC(C)(C)NC(=O)c1ccc(I)cc1
Cc1cc(I)ccc1C(F)(F)F
CC(C)(C)c1ccc(I)cc1
CCCC12COC(c3ccc(I)cc3)(OC1)OC2
O=C(NCCCn1ccnc1)c1ccc(I)cc1
Cc1cc(I)ccc1-c1ccccc1
Cc1ccc(I)cc1C(=N)O
CCOC(=O)Cc1ccc(I)cc1
NCc1ccc(I)cc1
Cc1cc(I)ccc1C(C)C
CC(C)(O)c1ccc(I)cc1
N=C(O)Cc1ccc(I)cc1
Cc1ccc(-c2ccc(I)cc2)cc1
Ic1ccc(COc2ccccn2)cc1
CCOC(=O)[C@H](Cc1ccc(I)cc1)N=C(O)OC(C)(C)C
CCCCc1ccc(-c2ccc(I)cc2)cc1
OC(c1ccc(I)cc1)(C(F)(F)F)C(F)(F)F
CSc1ccc(I)cc1
Cc1cc(I)cc(C(=O)O)c1C
CCCc1ccc(-c2ccc(I)cc2)cc1
Ic1ccc(Cn2ccnc2)cc1
O=C(NCC1CC1)c1ccc(I)cc1
CC1(C)COB(c2ccc(I)cc2)OC1
CC(C)N=C(O)Cc1ccc(I)cc1
CON(C)C(=O)c1ccc(I)cc1
CCOP(=O)(Cc1ccc(I)cc1)OCC
CN(C)C(=O)c1ccc(I)cc1
Ic1ccc(C2CCNCC2)cc1
NC(C(=O)O)c1ccc(I)cc1
CN(Cc1ccccc1)C(=O)c1ccc(I)cc1
CN(C)Cc1ccc(I)cc1
OC[C@H]1N=C(c2ccccc2)O[C@@H]1c1ccc(I)cc1
O=C(O)CCc1ccc(I)cc1
CC1CC(C)(C)OB(c2ccc(I)cc2)O1
FC(F)c1ccc(I)cc1
CC(C)(C)OC(=O)Cc1ccc(I)cc1
Cc1ccc(I)cc1CO[Si](C)(C)C(C)(C)C
CNC(=O)c1ccc(I)cc1
CC(C)c1ccc(I)cc1
Ic1ccc(Cn2cccc2)cc1
CN(C)c1ccc(-c2ccc(I)cc2)cc1
CC(C)(C)OC(O)=N[C@H](Cc1ccc(I)cc1)C(=O)O
CC(C)(C)[Si](C)(C)OCc1ccc(I)cc1
CC(C)NC(=O)c1ccc(I)cc1
N#CC(c1ccccc1)c1ccc(I)cc1
C[C@H](N)c1ccc(I)cc1
O=C(O)CCCc1ccc(I)cc1
O=C(O)CCCCCc1ccc(I)cc1
N[C@H](CC(=O)O)Cc1ccc(I)cc1
Ic1ccc(CN2CCCCC2)cc1
Ic1ccc(-c2ccccc2)cc1
CCc1cc(I)ccc1C
C=CCN(CC=C)C(=O)c1ccc(I)cc1
COCCNC(=O)c1ccc(I)cc1
O=C(Cl)Cc1ccc(I)cc1
NCCc1ccc(I)cc1
Brc1ccc(-c2ccc(I)cc2)cc1
CC(O)=NCCNC(=O)c1ccc(I)cc1
N#CC1(c2ccc(I)cc2)CC1
CC(Br)c1ccc(I)cc1
Ic1ccc(-c2cn3ccsc3n2)cc1
CC(C)(C)OC(O)=NCc1ccc(I)cc1
CC(C)(C)OC(O)=NNC(=O)c1ccc(I)cc1
Nc1ccc(-c2ccc(I)cc2)cc1
FC(F)(F)C(F)(c1ccc(I)cc1)C(F)(F)F
O=C(O)[C@H](Cc1ccc(I)cc1)N=CO
CCCCCCCCCCCCc1ccc(I)cc1
FC(F)(F)c1ccc(I)cc1CBr
Ic1ccc(CCN2CCOCC2)cc1
CC(N)c1ccc(I)cc1
COC(=O)Cc1ccc(I)cc1
Cc1cc(I)ccc1C(=O)O
O=C(O)C(Cc1ccc(I)cc1)N=C(O)OCc1ccccc1
CCN(CC)C(=O)c1ccc(I)cc1
N#CCc1ccc(I)cc1
Cc1ccc(I)cc1-c1cc(I)ccc1C
CCCCCCCc1ccc(I)cc1
NC1(c2ccc(I)cc2)CC1
Ic1ccc(CN2CCNCC2)cc1
CCCCCC1CCC(c2ccc(I)cc2)CC1
Ic1ccc(-c2ccc(I)cc2)cc1
CCc1ccc(I)cc1
NC(Cc1ccc(I)cc1)C(=O)O
CC(F)(F)c1ccc(I)cc1
Ic1ccc(CN2CCCC2)cc1
O=C(O)CCCCCCCCCCCCCCc1ccc(I)cc1
CC(C(=O)O)c1ccc(I)cc1
O=C(c1ccc(I)cc1)N1CCCC(c2nc3ccccc3s2)C1
FC(F)(F)c1ccc(I)cc1
CC[C@H](CO)NC(=O)c1ccc(I)cc1
O=C(c1ccc(I)cc1)N1CCCC1
O=C(O)C1(c2ccc(I)cc2)CC1
CCCc1ccc(I)cc1
N[C@H](CF)[C@H](O)c1ccc(I)cc1
Cc1cc(I)ccc1-c1ccc(I)cc1C
COC(=O)[C@H](Cc1ccc(I)cc1)N=C(O)OC(C)(C)C
Brc1cccc(-c2ccc(I)cc2)c1
COCc1ccc(I)cc1
CC(C)(C)OC(O)=N[C@H](CO)Cc1ccc(I)cc1
Cc1ccc(I)cc1CO
O=C(NC1CCOCC1)c1ccc(I)cc1
N=C(N)c1ccc(I)cc1
Cc1ccc(I)cc1C(F)(F)F
COc1ccc(-c2ccc(I)cc2)cc1
BrCc1ccc(I)cc1
N[C@@H](CC(=O)O)Cc1ccc(I)cc1
CC(C)(C)OC(O)=NC(CC(=O)O)Cc1ccc(I)cc1
CC(C)Cc1ccc(I)cc1
Sc1ccc(I)cc1
CCCCCc1ccc(I)cc1
C[Si](C)(C)C#Cc1ccc(I)cc1
Cc1ccc(I)cc1C
O=C(NCc1ccccc1)c1ccc(I)cc1
FC(F)(F)Cc1ccc(I)cc1
O=C(Cc1ccc(I)cc1)N1CCCCC1
CCN(CC)Cc1ccc(I)cc1
O=C(O)CCCCc1ccc(I)cc1
FC(F)(F)c1ccc(I)cc1C(F)(F)F
CCc1ccc(-c2ccc(I)cc2)cc1
CCOC(=O)c1ccc(I)cc1
OC(c1ccccc1)c1ccc(I)cc1
NNCc1ccc(I)cc1
CCCCCCc1ccc(I)cc1
SCc1ccc(I)cc1
Cc1ccc(I)cc1CBr
CC(C)(C)OC(O)=N[C@@H](Cc1ccc(I)cc1)C(=O)O
NCC1(c2ccc(I)cc2)CCCC1
O=C(OCc1ccc(I)cc1)c1ccccc1
OB(O)c1ccc(I)cc1
C#Cc1ccc(I)cc1
O=C(c1ccc(I)cc1)N1CCC(F)(F)CC1
CCOC(=O)C(Cc1ccc(I)cc1)N=C(O)OC(C)(C)C
O=c1nc(O)ccn1Cc1ccc(I)cc1
N[C@@H](C(=O)O)c1ccc(I)cc1
NC1(Cc2ccc(I)cc2)CC1
CC(C)N(C(=O)c1ccc(I)cc1)C(C)C
Cc1ccc(I)cc1
O=C(O)Cc1ccc(I)cc1
COC(=O)c1ccc(I)cc1C
Ic1ccc(P(c2ccccc2)c2ccccc2)cc1
C#CCNC(=O)c1ccc(I)cc1
CN(Cc1ccc(I)cc1)C(=O)OC(C)(C)C
O=C([O-])Cc1ccc(I)cc1
Ic1ccc([Si](c2ccccc2)(c2ccccc2)c2ccccc2)cc1
O=C(Cc1ccc(I)cc1)N1CCCC1
C[C@H](N=C(O)OC(C)(C)C)c1ccc(I)cc1
CCCNC(=O)c1ccc(I)cc1
N[C@@H](Cc1ccc(I)cc1)C(=O)O
CC(C)(C)c1ccc(-c2ccc(I)cc2)cc1
COC(=O)C1(c2ccc(I)cc2)CC1
Ic1ccc(Cc2ccccc2)cc1
CC1(c2ccc(I)cc2)N=C(O)N=C1O
COC(=O)C1C2CCC(CC1c1ccc(I)cc1)N2
COC(=O)c1ccc(I)cc1
CC(C)S(=O)(=O)N[C@H]1CCOC[C@@H]1c1ccc(I)cc1
O=C(Cc1ccc(I)cc1)N1CCOCC1
O=C(c1ccc(I)cc1)N(Cc1ccccc1)Cc1ccccc1
CC(C)(C)OC(=O)N1CCN(C(=O)c2ccc(I)cc2)CC1
N[C@H](Cc1ccc(I)cc1)C(=O)O
CC1(C)OB(c2ccc(I)cc2)OC1(C)C
Oc1ccc(-c2ccc(I)cc2)cc1
CC(O)=NC(Cc1ccc(I)cc1)C(=O)O
CC(O)c1ccc(I)cc1
Ic1ccc(C2=NCCC2)cc1
Cc1ccc(I)cc1C[C@H](N)C(=O)O
CC(C)S(=O)(=O)N[C@@H]1CCOC[C@H]1c1ccc(I)cc1
Ic1ccc(C2CCCCC2)cc1
Cc1cc(I)ccc1C#N
O=C1OCCC1N=C(O)Cc1ccc(I)cc1
CC(C)CNC(=O)c1ccc(I)cc1
C[C@H](O)c1ccc(I)cc1
CCOC(=O)C(c1ccc(I)cc1)P(=O)(OCC)OCC
Ic1ccc(-c2cn[nH]c2)cc1

Cluster F

O=C(Nc1ccc(I)cc1)c1cccc(I)c1
OC(=Nc1ccc(I)cc1)c1ccc(C(F)(F)F)cc1
COCCCN=C(O)Nc1ccc(I)cc1
O=[N+]([O-])c1cccc(N=C(O)Nc2ccc(I)cc2)c1
O=C(CCCN1C(=O)c2ccccc2C1=O)Nc1ccc(I)cc1
CC(C)C(=O)Nc1ccc(I)cc1
Cc1cc(C=O)c(C)n1-c1ccc(I)cc1
COc1ccc(Cl)cc1N=C(S)Nc1ccc(I)cc1
O=C(O)c1ccccc1Nc1ccc(I)cc1
O=C1Nc2ccccc2C1=Nc1ccc(I)cc1
Cc1cc(I)ccc1NC(O)=Nc1ccccc1
O=C(Nc1ccc(I)cc1C(=O)O)c1ccc(F)cc1
NN=C(O)CNc1ccc(I)cc1
O=C(O)C1C2CCC(O2)C1C(=O)Nc1ccc(I)cc1
CCOC(=O)C(=CNc1ccc(I)cc1C)C(=O)OCC
Cc1cc2c(n1-c1ccc(I)cc1)CC(C)(C)CC2=O
CC(C)=CC(=O)Nc1ccc(I)cc1
NN=C(S)Nc1ccc(I)cc1
O=C(Nc1ccc(I)cc1)c1cccnc1
CC(C)(C)c1ccc(OCC(=O)Nc2ccc(I)cc2)cc1
O=[N+]([O-])c1ccc(NC(=S)Nc2ccc(I)cc2)cc1
O=C1/C(=C\c2ccccc2O)C(O)=NN1c1ccc(I)cc1
O=C(CCCc1ccccc1)Nc1ccc(I)cc1
O=C1N(c2ccc(I)cc2)CCCC1(Cl)Cl
OC(=Nc1ccc(I)cc1)c1ccc2ccccc2n1
COC(=O)c1ccccc1N=C(O)Nc1ccc(I)cc1
CC(C)(C)c1ccc(-c2nn(CNc3ccc(I)cc3)c(=S)o2)cc1
Cc1cc(C(=O)Oc2ccc(I)cc2)ccc1[N+](=O)[O-]
O=C(Nc1ccc(I)cc1)c1ccccc1-c1ccccc1
CN(C)c1ccc(I)cc1Br
O=c1c(Oc2ccc(I)cc2)coc2cc(O)ccc12
O=C(Nc1ccc(I)cc1)c1c(F)cccc1F
O=C1c2ccccc2CN1c1ccc(I)cc1
O=C(Nc1ccc(I)cc1)C1CC(=O)N(C2CCCCC2)C1
CCOC(O)=NC(N=C(S)Nc1ccc(I)cc1)C(Cl)(Cl)Cl
CS(=O)(=O)Nc1ccc(I)cc1
O=C(O)c1cc(I)ccc1N=C(O)OCc1ccccc1
Cc1ccccc1C(=O)Nc1ccc(I)cc1
CC(C)C(O)=Nc1ccc(I)cc1C(=O)O
CC(Oc1ccccc1)C(=O)Nc1ccc(I)cc1
O=C1C(Cl)=C(Cl)C(=O)N1c1ccc(I)cc1
O=c1c(Oc2ccc(I)cc2)coc2cc(O)cc(O)c12
CC(O)=Nc1ccc(S(=O)(=O)Nc2ccc(I)cc2)cc1
O=C1/C(=C\c2cc(Br)ccc2O)C(O)=NN1c1ccc(I)cc1
O=C1CSC(=S)N1c1ccc(I)cc1
CC(=O)OCC(=O)Nc1ccc(I)cc1
O=C=Nc1ccc(I)cc1
O=S(=O)(Nc1ccc(I)cc1)c1ccccc1
Ic1ccc(-n2ccnn2)cc1
Cc1c(Cl)cccc1N=C(O)CN(c1ccc(I)cc1)S(C)(=O)=O
CCCCS(=O)(=O)Nc1ccc(I)cc1
O=C(O)c1ccccc1-c1ccccc1C(=O)Nc1ccc(I)cc1
CCOc1ccccc1N=C(O)Nc1ccc(I)cc1
O=C(CCNc1ccc(I)cc1)c1ccccc1
OC(=Nc1ccc(I)cc1)c1ccc(COc2ccccc2Br)o1
O=C(COc1ccc(I)cc1)Nc1ccc(C(=O)O)cc1
CC(Br)C(=O)N(C)c1ccc(I)cc1
Cc1cc(I)cc(C)c1NC(=O)c1ccccc1
COc1ccc(OC(C)C(=O)Nc2ccc(I)cc2)cc1
O=C(Nc1ccc(I)cc1)N(c1ccccc1)c1ccccc1
OC(=Nc1ccc(I)cc1)c1ccc(F)cc1
O=C(O)c1cccnc1Nc1ccc(I)cc1
CC(C)(C)OC(O)=Nc1ccc(I)cc1C(=O)O

O=C(O)C1CC=CCC1C(=O)Nc1ccc(I)cc1
CC(=O)Oc1ccc(C(O)=Nc2ccc(I)cc2)cc1
Cc1cc(I)ccc1NC(=O)CCl
O=C1C=CC(=O)N1c1ccc(I)cc1
Cc1cc(I)ccc1N=C(O)c1ccc2ccccc2n1
O=C(Nc1ccc(I)cc1)c1cccc([N+](=O)[O-])c1
CCCC(O)=NC(=S)Nc1ccc(I)cc1
CC(O)=NC(=S)Nc1ccc(I)cc1
Ic1ccc(N=c2c3ccccc3[nH]c3ccccc23)cc1
O=C1O[C@@H](CO)CN1c1ccc(I)cc1
CC(=O)/C(=C/Nc1ccc(I)cc1)c1ccccc1
O=[N+]([O-])c1cccc(N=C(S)Nc2ccc(I)cc2)c1
Cc1cc(C(=O)Nc2ccc(I)cc2)c(C)o1
CCOc1cc(OCC)c2c(=O)c(Oc3ccc(I)cc3)coc2c1
OC(=Nc1ccc(I)cc1)c1ccco1
S=C(Nc1ccc(I)cc1)Nc1ccc(I)cc1
CC(=O)N(C)c1ccc(I)cc1
O=C(Nc1ccc(I)cc1)C(F)(F)F
O=C(Oc1ccc(I)cc1)C1c2ccccc2Oc2ccccc21
N#CC(C#N)=NNc1ccc(I)cc1
COc1cccc2ccc(/C=C/c3cc(I)ccc3OC(C)=O)nc12
O=C(CC(Nc1ccc(I)cc1)c1ccccc1)c1ccccc1
CCN=C(S)Nc1ccc(I)cc1
OC(=NCc1ccco1)c1cc(I)ccc1N=C(O)c1cccc2ccccc12
O=C1c2ccccc2C(=O)N1CNc1ccc(I)cc1
OC(=Nc1cccc(Br)c1)Nc1ccc(I)cc1
Cc1cc(NC(=O)c2cccc([N+](=O)[O-])c2C)c(C)cc1I
CC(C)(C)c1ccc(S(=O)(=O)Nc2ccc(I)cc2)cc1
O=C(Nc1ccc(I)cc1)c1ccccc1Cl
O=C(Nc1ccc(I)cc1)OCc1ccccc1
CC(O)=Nc1ccc(I)cc1
O=[N+]([O-])c1ccc(C(O)=Nc2ccc(I)cc2)o1
O=C(O)C1CCCCC1C(=O)Nc1ccc(I)cc1
CN1CCN(c2ccc(I)cc2)CC1
Cn1c(=O)c(C(=O)Nc2ccc(I)cc2)c(O)c2ccccc21
OC(=NC(S)=Nc1ccc(I)cc1)c1ccc(Br)o1
O=C(Nc1ccc(I)cc1)c1ccc(Cl)cc1Cl
Oc1ccccc1/C=N/c1ccc(I)cc1
Oc1cccc(/C=N/c2ccc(I)cc2)c1O
O=[N+]([O-])c1ccc(O)c(/C=N/c2ccc(I)cc2)c1
CNc1ccc(I)cc1
O=C(CS(=O)(=O)c1ccccc1)Nc1ccc(I)cc1
O=S(=O)(Nc1ccc(I)cc1)c1ccc(F)cc1
CN(C(=O)OC(C)(C)C)c1ccc(I)cc1
CC(C)(Oc1ccc(Cl)cc1)C(=O)Nc1ccc(I)cc1
CCOc1ccc(NC(=O)Nc2ccc(I)cc2)cc1
CC(=O)Oc1ccccc1C(=O)Nc1ccc(I)cc1
O=C1N=C(O)CCN1c1ccc(I)cc1
Ic1ccc(-n2cnnn2)cc1
O=C(CSCc1c(F)cccc1Cl)Nc1ccc(I)cc1
O=C(CCc1ccccc1)Nc1ccc(I)cc1
O=S(=O)(Nc1ccc(I)cc1)c1ccc(Br)cc1
O=C(O)CCC(=O)Nc1ccc(I)cc1
Ic1ccc(N2CCNCC2)cc1
O=C1C2C3c4ccccc4C(c4ccccc43)C2C(=O)N1c1ccc(I)cc1
OC(=Nc1ccc(I)cc1)c1cccs1
O=C1/C(=C/c2ccccc2)C(O)=NN1c1ccc(I)cc1
O=C1c2cccc3cccc(c23)C(=O)N1c1ccc(I)cc1
O=[N+]([O-])c1ccccc1/C=N/c1ccc(I)cc1
SC(=NCc1ccco1)Nc1ccc(I)cc1
O=S(=O)(Nc1ccc(I)cc1)c1cccc2cccnc12
Cc1cc(Nc2ccc(I)cc2)n2ncnc2n1
CC(C)c1ccc(/C=C/C(O)=Nc2ccc(I)cc2Cl)cc1

CN(C)c1ccc(/N=N/c2ccc(I)cc2)cc1
CCN(CC)c1ccc(/C=C2/C(=O)N(c3ccc(I)cc3)N=C2O)c(O)c1
Cc1cc(I)ccc1NC1=CC(=O)CC(C)(C)C1
Cc1cn(C(=O)c2ccccc2)c(=S)n1-c1ccc(I)cc1
OC(=Nc1cccc2ccccc12)Nc1ccc(I)cc1
O=C(CN1CCOCC1)Nc1ccc(I)cc1
O=C(CCl)Nc1ccc(I)cc1
OC(=Nc1ccc(Cl)cc1)c1ccc(COc2ccc(I)cc2)o1
O=C(Nc1ccc(I)cc1)c1cccc(F)c1
O=C(Nc1ccc(I)cc1)c1cccc(C(F)(F)F)c1
O=[N+]([O-])c1ccc(Oc2ccc(I)cc2)cc1
OC(=Nc1ccc(I)cc1)c1ccc(I)cc1
Cc1cc(I)ccc1NC(=O)/C=C\C(=O)O
O=C(Nc1ccc(I)cc1)c1cccnc1Cl
CCCCCC(O)=NC(=S)Nc1ccc(I)cc1
Fc1ccc(NC(=S)Nc2ccc(I)cc2)cc1
CC(=O)Oc1cc(OC(C)=O)c2c(=O)c(Oc3ccc(I)cc3)coc2c1
O=C1CC(NCc2ccccc2)C(=O)N1c1ccc(I)cc1
Cc1cc(I)ccc1NC(=O)OC(C)(C)C
OC(=Nc1ccc(I)cc1)C(O)=Nc1ccc(I)cc1
O=C1CC(N2CCN(c3ccc(Cl)cc3)CC2)C(=O)N1c1ccc(I)cc1
COc1ccc(C(O)=Nc2ccc(I)cc2)cc1
OC(=NC1CCCCC1)Nc1ccc(I)cc1
C=CCn1c(CNc2ccc(I)cc2)nnc1SCC(=O)c1ccccc1
N#Cc1ccc(/C=N/c2ccc(I)cc2)cc1
O=C(Nc1ccc(I)cc1)c1c(O)nc2ccccc2c1O
Cc1cc(C)c(S(=O)(=O)Nc2ccc(I)cc2)c(C)c1
O=C(CSc1nc(O)c2ccccc2n1)Nc1ccc(I)cc1
O=C(CC1C=CCC1)Nc1ccc(I)cc1
O=C(O)c1cc(I)ccc1N=C(O)Cc1ccccc1
O=C(O)c1cc(S(=O)(=O)Nc2ccc(I)cc2)ccc1O
Cc1cc(I)cc(C(=O)O)c1N=C(O)C(F)(F)F
CC(O)=Nc1ccc(I)cc1C
O=C1CC(NC2CCCCC2)C(=O)N1c1ccc(I)cc1
Cc1cc(=O)n(-c2ccc(I)cc2)[nH]1
OC(=Nc1ccc(I)cc1)c1ccc(CN2CCOCC2)cc1
O=C(Nc1cccc([N+](=O)[O-])c1)c1ccc(COc2ccc(I)cc2)o1
O=c1oc2ccccc2c(Nc2ccc(I)cc2)c1[N+](=O)[O-]
CCS(=O)(=O)Nc1ccc(I)cc1
O=C(COc1ccc(I)cc1)c1ccc(Br)cc1
O=C(O)c1ccc(C(=O)Nc2ccc(I)cc2)c(C(=O)O)c1
O=C(Nc1ccc(I)cc1)c1ccccc1I
CCc1cc(I)ccc1N=C(O)c1ccc([N+](=O)[O-])o1
CCN(CC(=O)Nc1ccc(I)cc1)c1ccccc1
CN=C(S)Nc1ccc(I)cc1
O=C(Nc1ccc(I)cc1)N1CCCCC1
O=C(Nc1ccc(I)cc1)c1ccccn1
O=C(O)CCC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(I)cc2)cc1
Ic1ccc(Nc2ccc(I)cc2)cc1
Ic1ccc(/N=C/c2ccco2)cc1
O=[N+]([O-])c1cccc(S(=O)(=O)Nc2ccc(I)cc2)c1
N=C(O)Nc1ccc(I)cc1
O=C1/C(=C\c2cccs2)C(O)=NN1c1ccc(I)cc1
O=C(Nc1ccc(I)cc1)c1cnccn1
OC(=Nc1ccc(I)cc1)c1ccncc1
O=[N+]([O-])c1cc([N+](=O)[O-])c2cccnc2c1Nc1ccc(I)cc1
CC(C)(C)OC(=O)N1CCN(c2ccc(I)cc2)CC1
O=C(O)C1(C(=O)Nc2ccc(I)cc2)CC1
NS(=O)(=O)c1ccc(S(=O)(=O)Nc2ccc(I)cc2)cc1
O=C(Nc1ccc(I)cc1)Nc1ccc(I)cc1
O=C(Nc1ccc(I)cc1)C1CCCCC1

COc1cc2ncnc(Nc3ccc(I)cc3)c2cc1OC

Cc1cc(NC(=O)c2ccc(C)c([N+](=O)[O-])c2)c(C)cc1I

O=C(Nc1ccc(I)cc1)C1CCCO1

NC(=Nc1ccc(I)cc1)C(N)=Nc1ccc(I)cc1

O=C(Nc1ccc(I)cc1)N1CCOCC1

O=C(CCCCCCC(O)=NO)Nc1ccc(I)cc1

O=C1C(c2ccccc2)=C(Nc2ccc(I)cc2)c2ccccc21

CC(CC(=O)Nc1ccc(I)cc1)c1ccccc1

CCCC(=O)Nc1ccc(I)cc1

O=[N+]([O-])c1ccccc1S(=O)(=O)Nc1ccc(I)cc1

OC(CNc1ccc(I)cc1)Cn1c2ccccc2c2ccccc21

Ic1ccc(NCc2nnc3n2CCCCC3)cc1

Cc1cc(I)ccc1Nc1c(C(O)=NOCC2CC2)cc(F)c(F)c1F

CCCCC(O)=Nc1ccc(I)cc1C(=O)O

Ic1ccc(-n2cccn2)cc1

CCn1c(=O)c(C(=O)Nc2ccc(I)cc2)c(O)c2ccccc21

FC(F)(F)c1cnc(Oc2ccc(I)cc2)c(Cl)c1

O=S(=O)(Nc1ccc(I)cc1)c1cccc2ccccc12

CCCCC(=O)Nc1ccc(I)cc1

Cc1ccc(C(O)=Nc2ccc(I)cc2)cc1

O=[N+]([O-])c1ccc(S(=O)(=O)Nc2ccc(I)cc2)cc1

O=C1c2ccccc2C(O)(c2ccccc2)N1c1ccc(I)cc1

O=C1CCCCN1c1ccc(I)cc1

Nc1c(C(=O)O)cc(I)cc1C(=O)O

CCOC(=O)Nc1ccc(I)cc1

OC(=NCC1CC1)Nc1ccc(I)cc1

COC(=O)c1cccc(N=C(O)COc2ccc(I)cc2)c1

CC(C)=CC(=O)Nc1ccc(I)cc1C

O=S(=O)(Nc1ccc(I)cc1)c1ccc(Cl)cc1

Clc1ccc(/C=N/c2ccc(I)cc2)cc1

Cc1cc(C)c2[nH]c(C)cc(=Nc3ccc(I)cc3)c2c1

O=C(Nc1ccc(I)cc1)C1CC1

N#CCC(=O)Nc1ccc(I)cc1

OC(=Nc1ccc(Cl)c(Cl)c1)Nc1ccc(I)cc1

COc1cccc(C(=O)Nc2ccc(I)cc2)c1

N=C(S)Nc1ccc(I)cc1

O=[N+]([O-])c1ccc(Oc2ccc(I)cc2)nc1

Cc1oncc1C(=O)Nc1ccc(I)cc1

O=C(O)CCCC(=O)Nc1ccc(I)cc1

O=C(CSc1nc2ccc([N+](=O)[O-])cc2[nH]1)Nc1ccc(I)cc1

CC1=NN(c2ccc(I)cc2)C(=O)C1

CC(Cl)C(=O)Nc1ccc(I)cc1

COc1ccc(N(c2ccc(I)cc2)c2ccc(OC)cc2)cc1

O=C(Cc1c[nH]c2ccccc12)Nc1ccc(I)cc1

CC(O)=Nc1ccc(I)cc1C(F)(F)F

O=[N+]([O-])c1cccnc1Oc1ccc(I)cc1

CCCCn1c(=O)c(C(=O)Nc2ccc(I)cc2)c(O)c2ccccc21

O=[N+]([O-])c1ccc(/C=N/c2ccc(I)cc2)cc1

Ic1ccc(-n2cnnc2)cc1

N=C(O)CNc1ccc(I)cc1

Cc1ccc2ncnc(Nc3ccc(I)cc3)c2c1

Ic1ccc(Oc2ncccn2)cc1

O=[N+]([O-])c1cc(C(F)(F)F)cc([N+](=O)[O-])c1Oc1ccc(I)cc1

Brc1cnc(Oc2ccc(I)cc2)nc1

Ic1ccc(NC2CCCCC2)cc1

CCOC(=O)C(=CNc1ccc(I)cc1)C(=O)OCC

COc1ccc(S(=O)(=O)Nc2ccc(I)cc2)cc1

NNc1ccc(I)cc1

COc1ccc(S(=O)(=O)Nc2ccc(I)cc2)cc1OC

O=C(Cc1ccc(F)cc1F)Nc1ccc(I)cc1

Cc1cc(C(=O)Nc2ccc(I)cc2C(=O)O)ccc1[N+](=O)[O-]

COc1cccc(/C=N/c2ccc(I)cc2)c1O

O=C(Nc1ccc(I)cc1C(O)=NCCO)c1cccs1

OC(=NC(=S)Nc1ccc(I)cc1)c1ccccc1

O=C(Nc1ccc(I)cc1)C1CCN(C(=O)c2ccco2)CC1

Ic1ccc(N(c2ccccc2)c2ccccc2)cc1

Cn1nc(C2CC2)cc1C(O)=Nc1ccc(I)cc1

O=C1C=C(Nc2ccc(I)cc2)CCC1

Cc1cc(I)ccc1NC(O)=Nc1cccc2ccccc12

CC(C)(C)c1ccc(C(O)=Nc2ccc(I)cc2)cc1

OC1=NC(=S)N=C(O)C1=Cc1cccn1-c1ccc(I)cc1

NS(=O)(=O)c1ccc(NC(=S)Nc2ccc(I)cc2)cc1

Ic1ccc(N2CCOCC2)cc1

OC(=NOCC1CC1)c1ccc(F)c(F)c1Nc1ccc(I)cc1Cl

CC(C)(C)OC(=O)Nc1ccc(I)cc1

Cc1cc(I)ccc1Nc1c(C(=O)O)cc(F)c(F)c1F

O=C(COc1ccccc1C(O)=NCc1ccccc1)Nc1ccc(I)cc1

O=C(Nc1ccc(I)cc1)c1cc2cc(Cl)ccc2oc1=O

Ic1ccc(N=P(c2ccccc2)(c2ccccc2)c2ccccc2)cc1

OC(=Nc1ccccc1)Nc1ccc(I)cc1

CCOC(=O)c1ccc(NC(=O)Nc2ccc(I)cc2)cc1

O=C(O)c1ccccc1C(=O)Nc1ccc(I)cc1

Cc1nc2ccccc2c(=O)n1-c1ccc(I)cc1

Cc1ccc(/C=N/N=c2[nH]c3nonc3[nH]c2=Nc2ccc(I)cc2)o1

CC1=C(C)CC(C(=O)Nc2ccc(I)cc2)C(C(=O)O)C1

CCOC(=O)c1ccc(NC(=S)Nc2ccc(I)cc2)cc1

O=[N+]([O-])c1ccc(Nc2ccc(I)cc2)c([N+](=O)[O-])c1

CC1(C)CN(c2ccc(I)cc2)C1=O

NCCS(=O)(=O)Nc1ccc(I)cc1

CCc1ccc(S(=O)(=O)Nc2ccc(I)cc2)cc1

CCCCCC(=O)Nc1ccc(I)cc1

N=c1ncnc(Nc2ccc(I)cc2)[nH]1

CN(C)c1ccc(I)cc1

O=C(Nc1ccc(I)cc1)c1ccccc1F

O=C1C(N2CCOCC2)=CCCN1c1ccc(I)cc1

CCOC(=O)/C(C#N)=C/Nc1ccc(I)cc1

O=C(/C=C/c1ccccc1)Nc1ccc(I)cc1

CCN(CC)C(=O)Nc1ccc(I)cc1

CCOC(=O)c1c[nH]c2ccc(OCC)cc2c1=Nc1ccc(I)cc1

CC(=O)c1ccc(NC(=O)Nc2ccc(I)cc2)cc1

Ic1ccc(-n2c3ccccc3c3ccccc32)cc1

O=C(Nc1ccc(I)cc1)c1ccccc1C(F)(F)F

[N-]=[N+]=Nc1ccc(I)cc1

CCC(=O)Nc1ccc(I)cc1

O=C1SC(Nc2ccc(I)cc2)C(=O)N1c1ccccc1

O=Cc1ccccc1Oc1ccc(I)cc1

O=C(O)c1cc(I)ccc1N=C(O)c1ccccc1

SC(=Nc1ccccc1)Nc1ccc(I)cc1

O=[N+]([O-])c1ccc(C(O)=Nc2ccc(I)cc2)cc1

Ic1ccc(N2CCCCC2)cc1

Nc1ccc(I)cc1

CC(=O)CC(=O)Nc1ccc(I)cc1

O=S(=O)(Nc1ccc(I)cc1)c1cccs1

Cc1ccc(S(=O)(=O)N=C(O)Nc2ccc(I)cc2)cc1

Cc1ccc(S(=O)(=O)Nc2ccc(I)cc2)cc1

O=C(Nc1ccc(I)cc1)C(c1ccccc1)c1ccccc1

Ic1ccc(-n2cccc2)cc1

O=C(CCCCl)Nc1ccc(I)cc1

NCC(=O)Nc1ccc(I)cc1

O=C(O)CNc1ccc(I)cc1

Cc1nccn1-c1ccc(I)cc1

CCN(CC)c1ccc(/C=N/c2ccc(I)cc2)c(O)c1

O=C1OC(Nc2ccc(I)cc2)c2ccccc21

CS(=O)(=O)c1ccc(C(O)=Nc2ccc(I)cc2)cc1

Nc1ccc(S(=O)(=O)Nc2ccc(I)cc2)cc1

COCc1cc(C)nc2sc(C(=O)Nc3ccc(I)cc3)c(N)c12

O=Cc1ccc(OCC(=O)Nc2ccc(I)cc2)cc1

O=C(Nc1ccc(I)cc1C(=O)Nc1ccc(Cl)cc1)c1cccs1

Ic1ccc(N=c2ncnc3[nH][nH]cc2-3)cc1

S=C(Nc1ccc(Br)cc1)Nc1ccc(I)cc1

CC(C)(C)OC(O)=Nc1ccc(I)cc1[N+](=O)[O-]

Cc1c(C(=O)O)nnn1-c1ccc(I)cc1

COC(=O)c1ccccc1N=C(O)COc1ccc(I)cc1

Cc1ccc(C)n1-c1ccc(I)cc1

O=C(Nc1ccc(I)cc1)c1ccccc1

O=C1/C(=C\c2ccc(N3CCOCC3)cc2)C(O)=NN1c1ccc(I)cc1

CC(=O)c1cc(I)cc(C)c1NC(=O)C(F)(F)F

O=C1/C(=C\c2ccccc2)C(O)=NN1c1ccc(I)cc1

O=C(O)c1ccc(F)c(F)c1Nc1ccc(I)cc1Cl

CCOC(=O)CNc1ccc(I)cc1

O=Cc1cccn1-c1ccc(I)cc1

CC(=O)c1ccc(Oc2ccc(I)cc2)nc1

O=C(Cc1ccccc1)Nc1ccc(I)cc1

COCCN=C(O)Nc1ccc(I)cc1

Cc1cc(I)ccc1NC(=O)C(F)(F)F

Cc1cc(I)ccc1N1C(=O)C=CC1=O

OC(=Nc1ccc(I)cc1)c1ccc(Cl)cc1

Cluster G

O=C(O)c1c(F)cccc1I

Sc1cccc(I)c1

Cc1cc(N)cc(I)c1

CC(C)(C)OC(O)=Nc1cc(Br)cc(I)c1

Oc1cc(Br)cc(I)c1

N#Cc1c(F)cc(I)cc1F

Fc1cc(I)cc(F)c1I

Oc1cc(Cl)cc(I)c1

Cc1ccc(N=C(O)c2ccsc2)cc1I

OC(=NCc1ccccc1)c1ccc(F)cc1I

Nc1ccc(CO)c(I)c1

Cc1ccc(O)cc1I

CC(O)=Nc1ccc(S(=O)(=O)Nc2cccc(I)c2)cc1

Nc1cccc(I)c1C(=O)O

N=C(O)c1ccc(I)cc1F

Ic1cccc(OCc2ccccc2)c1

Fc1cccc(I)c1C(F)(F)F

Cc1cc(F)cc(I)c1C(=O)O

CN(C)CCOc1cccc(I)c1

CN(CCc1ccccn1)Cc1cccc(I)c1

COc1ccc(CO)c(I)c1

Cc1c(F)cc(F)cc1I

OCc1ccc(F)cc1I

N=C(O)c1ccc(I)cc1N

Cc1ccc(N=C(O)c2ccoc2)cc1I

Fc1cc(I)cc(F)c1Cl

Oc1cc(O)cc(I)c1

O=C(O)c1c(I)ccc(C(F)(F)F)c1F

NCc1ccc(I)cc1F

COC(=O)c1c(F)cccc1I

CN(C)c1cc(F)cc(I)c1

Ic1cccc(N2CCOCC2)c1

COc1cc(I)c(C(=O)O)c(OC)c1

CS(=O)(=O)Nc1cccc(I)c1

N#Cc1ccc(N)cc1I

OC(=Nc1cccc(I)c1)C(Cl)Cl

O=Cc1c(I)ccc(Br)c1F
Cc1ccc(C)n1-c1cccc(I)c1
CN=C(O)c1ccc(I)cc1F
N#CCc1ccc(I)cc1F
Cc1cc(O)cc(I)c1
COC(=O)c1c(O)cccc1I
O=C(O)c1c(F)cc(F)cc1I
OC(Cc1c[nH]c2ccccc12)=Nc1cccc(I)c1
Brc1cccc(I)c1
Cc1ccc(I)c(C(=O)O)c1F
Fc1cc(Cl)cc(I)c1
CC1(C)OB(c2c(F)cccc2I)OC1(C)C
Fc1ccc(N=C=S)c(I)c1
COc1cc(Br)cc(I)c1
N=C(O)Nc1cccc(I)c1
Cc1ccc(N)cc1I
O=[N+]([O-])c1c(F)cccc1I
CC(C)(C)OC(O)=Nc1ccc(F)cc1I
OB(O)c1c(F)cccc1I
COc1cc(Cl)cc(I)c1
Fc1cc(I)cc2ccccc12
O=Cc1c(I)ccc(Cl)c1F
Cc1ccc(N)c(C)c1I
CC(C)Oc1cccc(I)c1
CN(C)Cc1cccc(I)c1
O=C(O)c1c(O)cccc1I
OCc1ccc(I)cc1F
Cc1cccc(S(=O)(=O)Nc2cccc(I)c2)c1
Cc1cc(F)cc(I)c1
COc1cc(I)c([N+](=O)[O-])cc1Br
COCCN=C(O)Nc1cccc(I)c1
CCOC(=O)c1c(F)cccc1I
Oc1cc(F)cc(I)c1
OC(CCl)=Nc1cccc(I)c1
Cc1c(Br)cc(F)cc1I
Nc1ccc([N+](=O)[O-])c(I)c1
COc1ccc(C(=O)Cl)c(I)c1
COc1cc(I)cc(C(F)(F)F)c1
Ic1cccc(N2CCCC2)c1
COCCOc1cccc(I)c1
OC(=Nc1cccc(I)c1)OCc1ccccc1
CC(C)(C)OC(O)=Nc1c(F)cccc1I
COc1cc(I)c([N+](=O)[O-])cc1I
Cc1cc(C)c(I)cc1N
CNc1cccc(I)c1
OC(Cc1ccccc1)=Nc1cccc(I)c1
Cc1ccc(I)cc1F
Cc1ccc(S(=O)(=O)Nc2ccc(C)c(I)c2)cc1
O=S(=O)(Nc1cccc(I)c1)c1ccccc1
CC(C)(C)OC(O)=Nc1cccc(I)c1
OC(=NCC1CC1)Nc1cccc(I)c1
CCN(CC)CC(O)=Nc1cccc(I)c1
O=Cc1c(O)cccc1I
Cc1c(F)cccc1I
Fc1ccc(Oc2cccc(I)c2)cc1
Nc1cc(N)cc(I)c1
COc1cccc(I)c1C(=O)O
COc1cccc(I)c1C
O=C(O)Cc1ccc(F)cc1I
Ic1cccc(NCc2ccccc2)c1
OCc1c(F)cccc1I
C=C1[CH]C(I)=CC=C1.[Br-].[Zn+]
COC(=O)c1c(N)cccc1I
O=[N+]([O-])c1c(O)cccc1I
COc1ccc([N+](=O)[O-])c(I)c1
CCOc1cccc(I)c1
OCCOc1cccc(I)c1
OC(=Nc1cccc(I)c1)C(F)(F)F
Ic1cccc(-n2ccnn2)c1
CCCOc1cccc(I)c1
Cc1c(N)cc(Cl)cc1I
N#CCC(O)=Nc1cccc(I)c1
O=C(O)Cc1ccc(I)cc1F
Ic1cccc(CN2CCOCC2)c1
Nc1cccc(I)c1
CC(C)(C)[Si](C)(C)Oc1cccc(I)c1
OCc1ccc(I)cc1OCc1ccccc1
O=Cc1c(F)cccc1I
N#Cc1ccc(F)cc1I
Fc1cc(I)cc(C(F)F)c1
Cc1c(N)cccc1I
BrCCCOc1cccc(I)c1
Cn1c(=O)c2c(ncn2CC(O)=Nc2cccc(I)c2)n(C)c1=O
Cc1c(F)cc(I)cc1F
OCc1cc(F)cc(I)c1
CNc1cc(Br)cc(I)c1
COc1ccc(C(=O)O)c(I)c1
Nc1cc(I)cc(C(F)(F)F)c1
O=C(O)c1c(I)ccc(Br)c1F
CC(C)(C)OC(=O)N1CCN(c2cccc(I)c2)CC1
O=Cc1ccc(F)cc1I
COc1ccc(N=C(O)OC(C)(C)C)c(I)c1
Fc1ccc(CBr)c(I)c1
O=Cc1ccc(O)cc1I
N#Cc1c(I)ccc(Cl)c1F
O=C=Nc1cccc(I)c1
Fc1cc(I)ccc1C(F)(F)F
O=C(Cl)c1c(F)cccc1I
Fc1cc(I)cc(F)c1Br
CCOC(=O)COc1cccc(I)c1
Fc1cc(I)cc(OC(F)F)c1
COc1cccc(I)c1C#N
COC(=O)c1cc(Br)c(F)cc1I
Ic1cccc(NC2COC2)c1
Cc1cccc(N=C(O)Nc2cccc(I)c2)c1
CC(O)=Nc1cccc(I)c1
O=[N+]([O-])c1c(F)cc(F)cc1I
CN(C)c1cccc(I)c1
CC(O)=Nc1ccc(F)cc1I
O=C(O)c1ccc(OC(F)(F)F)cc1I
Fc1cccc(I)c1
CSc1cccc(I)c1
CC(O)=Nc1ccc(C)c(I)c1
Fc1cc(F)cc(I)c1
CCNc1ccc(F)cc1I
O=S(=O)(Nc1cccc(I)c1)c1cccs1
COc1cc(N)cc(I)c1
Cc1ccc(F)cc1I
O=C(O)c1c(F)cc(I)cc1F
CN=C(O)Nc1cccc(I)c1
COc1ccc(C(=N)O)c(I)c1
O=C(O)c1ccc(F)cc1I
COc1cccc(I)c1
COC(=O)c1cc([N+](=O)[O-])c(I)cc1O
N=C(O)c1c(F)cccc1I
O=C(O)COc1cccc(I)c1
CCCC(O)=Nc1ccc(F)cc1I
O=[N+]([O-])c1cc(Br)c(F)cc1I
COC(=O)c1ccc(F)cc1I
Fc1cc(I)cc(C(F)(F)F)c1
CC(=O)Oc1cccc(I)c1
Ic1cccc(N2CCCCC2)c1
Fc1cc(Br)cc(I)c1
Nc1cc(F)cc(I)c1
Nc1cc(Cl)cc(I)c1
N#Cc1c(F)cccc1I
COc1ccc(C#N)c(I)c1
COC(=O)c1ccc(N)cc1I
Nc1ccc(C(=O)O)c(I)c1
COc1cccc(I)c1N=C(O)OC(C)(C)C
COC(=O)c1ccc(OC)cc1I
COc1ccc(C=O)c(I)c1
BrCCOc1cccc(I)c1
FC(F)(F)Oc1cc(Br)cc(I)c1
Fc1cccc(I)c1CBr
Cc1ccc(N=C(O)CCl)cc1I
FC(F)(F)Oc1cccc(I)c1
CNc1ccc(OC)cc1I
Nc1c(O)cccc1I
COc1ccc(C)c(I)c1
Cc1ccc(I)c(C)c1N
FC(F)Oc1cccc(I)c1
Nc1cc(I)cc(CO)c1
O=C(O)c1c(I)ccc(Cl)c1F
CC(C)C(O)=Nc1cccc(I)c1
COc1cccc(I)c1C=O
O=[N+]([O-])c1ccc(F)cc1I
O=Cc1c(F)cc(I)cc1F
OCCCOc1cccc(I)c1
COc1ccc(C(C)=O)c(I)c1
Nc1cc(Br)cc(I)c1
Ic1cccc(CN2CCCCC2)c1
C#CCOc1cccc(I)c1
Oc1cc(I)cc(C(F)(F)F)c1
Ic1cccc(Oc2ccccc2)c1
COC(=O)c1c(I)cccc1OC
O=C(O)c1ccc(O)cc1I
O=[N+]([O-])c1ccc(O)cc1I
COc1cc(I)cc(OC)c1
Nc1ccccc1Oc1cccc(I)c1
OC(CCl)=Nc1ccc(F)cc1I
OB(O)c1ccc(I)cc1F
N#Cc1c(I)ccc(Br)c1F
OCc1c(F)cc(I)cc1F
Clc1cccc(I)c1
OC(=Nc1cccc(I)c1)C1CC1
Oc1cccc(I)c1
COc1cc(F)cc(I)c1
Fc1cc(I)cc(F)c1C(F)(F)F
Fc1cc(I)cc(CBr)c1
CC(C)Nc1cccc(I)c1
COc1cccc(I)c1[N+](=O)[O-]
N#CCc1ccc(F)cc1I
OC(=Nc1ccc(F)cc1I)c1ccccc1
Cc1ccc(OCc2ccccc2)cc1I
Fc1cc(I)ccc1CBr
O=S(=O)(Nc1cccc(I)c1)c1ccc(Cl)cc1
CCOC(=O)c1c(I)cccc1OC
OC(=NC1CCCC1)Nc1cccc(I)c1
O=[N+]([O-])c1c(F)cc(I)cc1F
COc1cccc(I)c1C(=N)O

Cluster H

Cc1ccc(OS(=O)(=O)c2ccc(I)cc2)cc1
O=S(=O)(Nc1ccccc1)c1ccc(I)cc1
O=C(O)c1ccc(I)c(C(F)(F)F)c1
O=S(=O)(c1ccc(I)cc1)N1CCOCC1
Cc1cc([N+](=O)[O-])ccc1I
CC(=O)c1ccc(I)c(C(F)(F)F)c1

O=S(=O)(NCCCN1CCOCC1)c1ccc(I)cc1
N=C(O)c1cc([N+](=O)[O-])ccc1I
O=S(=O)(NC(=Nc1ccccc1)c1ccccc1)c1ccc(I)cc1
O=[N+]([O-])c1ccc(I)cc1Cl
O=S(=O)(Oc1c(F)c(F)c(F)c(F)c1F)c1ccc(I)cc1
O=[N+]([O-])c1ccc(I)cc1
CCOC(=O)c1cc([N+](=O)[O-])ccc1I
COC(=O)c1cc(C(F)(F)F)ccc1I
O=S(=O)(c1ccc(I)cc1)N1CCCC1
O=S(=O)(F)c1ccc(I)cc1
Cc1cc([N+](=O)[O-])c(C)cc1I
O=S(=O)(Nc1ccccn1)c1ccc(I)cc1
COC(=O)c1ccc(I)c(C(F)(F)F)c1
COC(=O)c1cc(C#N)ccc1I
O=S(=O)(Nc1ncccn1)c1ccc(I)cc1
N#Cc1cc([N+](=O)[O-])ccc1I
N#Cc1ccc(I)c(C(F)(F)F)c1
O=S(=O)(NCCN1CCOCC1)c1ccc(I)cc1
C#CCN=C(O)c1cc([N+](=O)[O-])ccc1I
O=[N+]([O-])c1ccc(I)cc1C(F)(F)F
COC(=O)c1cc(S(=O)(=O)Cl)ccc1I
Cc1ccccc1NS(=O)(=O)c1ccc(I)cc1
O=S(=O)(Oc1cccc2ccccc12)c1ccc(I)cc1
N#Cc1ccc(I)c(C(=O)O)c1
COc1ccc(NS(=O)(=O)c2ccc(I)cc2)cc1
O=S(=O)(Cl)c1ccc(I)cc1
CC(C)(C)OC(=O)Cc1cc(I)ccc1[N+](=O)[O-]
O=C(O)c1cc([N+](=O)[O-])ccc1I
O=C(O)c1ccccc1NS(=O)(=O)c1ccc(I)cc1
CCN(CC)S(=O)(=O)c1ccc(I)cc1
O=[N+]([O-])c1ccc(I)cc1CO
O=[N+]([O-])c1ccc(-[n+]2nc(-c3ccccc3)nn2-c2ccc(I)cc2)cc1
O=Cc1cc(I)ccc1[N+](=O)[O-]
O=Cc1cc(C(F)(F)F)ccc1I
O=S(=O)(Cl)c1ccc(I)cc1Cl
COC(=O)c1ccc(I)c(C(=O)O)c1
CCN=c1cc(C)nc(N2CCN(S(=O)(=O)c3ccc(I)cc3)CC2)[nH]1
O=S(=O)(c1ccc(I)cc1)N1CCCCC1
Cc1ccc(NS(=O)(=O)c2ccc(I)cc2)cc1
COC(=O)c1cc([N+](=O)[O-])ccc1I
Cc1cc(I)ccc1[N+](=O)[O-]
CC(=O)c1ccc(NS(=O)(=O)c2ccc(I)cc2)cc1
O=c1[nH]c2ccccc2nc1CS(=O)(=O)c1ccc(I)cc1
O=S(=O)(NCc1ccc2c(c1)OCO2)c1ccc(I)cc1
O=S(c1ccc(I)cc1)c1ccc(I)cc1
CC1CCCCN1S(=O)(=O)c1ccc(I)cc1
O=[N+]([O-])c1ccc(I)cc1Br
CCc1nc(C)cn1S(=O)(=O)c1ccc(I)cc1
CN1CCN(S(=O)(=O)c2ccc(I)cc2)CC1
O=S(=O)(Nc1ccc(F)cc1)c1ccc(I)cc1
O=S(=O)(c1ccccc1)c1ccc(I)cc1
CCN1CCN(S(=O)(=O)c2ccc(I)cc2)CC1
O=[N+]([O-])c1ccc(I)c(C(F)(F)F)c1
O=C(c1ccccc1)c1ccc(NS(=O)(=O)c2ccc(I)cc2)cc1
O=[N+]([O-])c1ccc(OS(=O)(=O)c2ccc(I)cc2)cc1
CC(C)(C)OC(=O)c1cc([N+](=O)[O-])ccc1I
Cc1cccnc1NS(=O)(=O)c1ccc(I)cc1
O=C(O)c1ccc(I)c(C(=O)O)c1
O=C(O)c1ccc(NS(=O)(=O)c2ccc(I)cc2)cc1
Cc1cc([N+](=O)[O-])c(Cl)cc1I
CCCN(CCC)S(=O)(=O)c1ccc(I)cc1
O=C(O)c1cc(I)ccc1[N+](=O)[O-]
O=S(=O)(Nc1ccc(Br)cc1)c1ccc(I)cc1

Cluster I

FC(F)(F)c1cccc(I)c1
OC(=NCCc1cccs1)c1cccc(I)c1
CCOC(=O)c1ccc(I)cc1F
OC(c1ccccc1)c1cccc(I)c1
Nc1cc(I)ccc1C(=O)O
O/N=C/c1cccc(I)c1
Clc1cc(I)cc(Cl)c1Br
OC(=Nc1ccccc1F)c1cccc(I)c1
Cc1ccnc(NS(=O)(=O)c2ccc(NC(=O)c3cccc(I)c3)cc2)n1
CCOC(=O)c1cc(Br)cc(I)c1
CC(C)(C)c1cc(I)cc(C(C)(C)C)c1
CS(=O)(=O)c1cccc(I)c1
NCc1cccc(I)c1
Cc1ccc(C(=O)c2cccc(I)c2)cc1
N=C(O)c1cc(I)cc([N+](=O)[O-])c1
Ic1cccc(-c2nnc(-c3ccccc3)o2)c1
CCn1c2ccccc2c2cc(/C=N/N=C(O)c3cccc(I)c3)ccc21
O=S(=O)(O)c1cccc(I)c1
Ic1cccc(C2CCCC2)c1
O=C(Cl)Cc1cccc(I)c1
N=C(O)c1ccccc1N=C(O)c1cccc(I)c1
Cc1c(Br)cc(I)cc1C(=O)O
NS(=O)(=O)c1cccc(I)c1
O=Cc1ccc(I)cc1F
COc1cc(I)ccc1C(=O)O
N#Cc1ccc(I)cc1F
CC(C)c1cccc(I)c1
O=C(ON1C(=O)CCC1=O)c1cccc(I)c1
O=C(c1ccc(Br)cc1)c1cccc(I)c1
Cc1c(N=C(S)N=C(O)c2cccc(I)c2)c(=O)n(-c2ccccc2)n1C
CC(C)(C)OC(O)=NCc1cccc(I)c1
O=c1nc(-c2cccc(I)c2)[nH]o1
OC(=NN=C(O)c1ccccc1I)c1cccc(I)c1
Cc1ccc(/C=N/N=C(O)c2cccc(I)c2)o1
COC(=O)c1cccc(I)c1
Clc1ccc(=N/N=C/c2cccc(I)c2)[nH]n1
COC(=O)c1cc(C)cc(I)c1
BrCc1cc(Br)cc(I)c1
Cc1cc(C)cc(I)c1
Ic1cc(-c2ccccc2)cc(-c2ccccc2)c1
BrCc1cc(I)cc(CBr)c1
CC(C)(C)n1nc(Cc2cccc(I)c2)c2c(N)ncnc21
O=C(Oc1ccccc1[N+](=O)[O-])c1cccc(I)c1
OCc1cc(I)cc(CO)c1
O=C(Cl)c1cccc(I)c1
Cc1ccc(I)cc1C(=O)c1ccc(-c2ccc(F)cc2)s1
Cc1ccccc1N=C(O)c1cccc(I)c1
Cc1ccc(I)cc1C#N
CN1CCN(C(=O)c2cccc(I)c2)CC1
CC(=O)c1cccc(I)c1
N#Cc1cc(I)cc(C(F)(F)F)c1
C/C(=N\NS(=O)(=O)c1ccc(C)cc1)c1cccc(I)c1
COC(=O)c1ccc(I)cc1O
O=C(c1ccc(F)cc1)c1cccc(I)c1
COc1ccccc1N1CCN(C(=O)c2cccc(I)c2)CC1
O=C(O)c1cc(I)ccc1C(F)(F)F
Ic1cccc(-c2nc3ccccc3s2)c1
COc1ccc2nc(N=C(O)c3cccc(I)c3)sc2c1
COc1cc(I)ccc1C=O
NN=C(O)c1cccc(I)c1
CC(C)c1cc(Br)cc(I)c1
COc1ccc2c(c1)CCC1C2=NN(C(C)=O)C1c1cccc(I)c1
CN(C)C(=O)c1cccc(I)c1
OC(=Nc1ccc(Cl)c(C(F)(F)F)c1)c1cccc(I)c1
Cc1cc(Cl)cc(I)c1
CCOC(=O)c1cc(I)cc([N+](=O)[O-])c1
O=S(=O)(Cl)c1cccc(I)c1
O=[N+]([O-])c1cc(I)ccc1CO
OC(=Nc1ccc(Cl)c(-c2nc3ccccc3[nH]2)c1)c1cccc(I)c1
CC(C)(C)OC(=O)c1cc(Br)cc(I)c1
NCCc1cccc(I)c1
CC(C)C(=O)c1cccc(I)c1
BrCc1cccc(I)c1
O=[N+]([O-])c1ccc(I)cc1F
O=C(O)c1ccc(I)cc1[N+](=O)[O-]
COC(=O)C[C@@H](N)c1cccc(I)c1
FC(F)c1cc(Br)cc(I)c1
FS(F)(F)(F)(F)c1cccc(I)c1
COC(=O)c1cc(Cl)cc(I)c1
CCN=C(O)c1cccc(I)c1
COC(=O)c1cc(I)cc(Cl)c1C
Clc1cccc(-c2cccc(I)c2)c1
COC(=O)c1cc(I)ccc1C
O=C(c1ccccc1)c1cc2c(cc1N=C(O)c1cccc(I)c1)OCCO2
O=C(CBr)c1cccc(I)c1
Cc1cc(I)cc(/C=C/C#N)c1
CC(C)(C)N=C(O)c1cccc(I)c1
O=C(O)c1cc(I)cc(C(F)(F)F)c1
COC(=O)c1ccc(I)cc1OCc1ccccc1
O=C(c1cccc(I)c1)N1CCC(F)(F)CC1
Cc1c(I)ccc(C#N)c1Cl
CCOC(=O)Cc1cccc(I)c1
O=[N+]([O-])c1cc(I)cc([N+](=O)[O-])c1
OC(=Nc1cc(C(F)(F)F)ccc1N1CCCCC1)c1cccc(I)c1
N#CCc1cccc(I)c1
O=Cc1cc(I)cc(C(=O)O)c1
N#Cc1ccc(I)cc1Br
CC(C)(C)c1cc(Br)cc(I)c1
Cc1cc(I)cc(C(=O)O)c1
Ic1cccc(-c2nc3ncccc3o2)c1
Cc1cc(I)cc([N+](=O)[O-])c1
NC(Cc1cccc(I)c1)C(=O)O
Cc1cc([N+](=O)[O-])c(N)cc1I
O=C(O)CCc1cccc(I)c1
O=C(O)COCc1cccc(I)c1
Clc1cc(Br)cc(I)c1
O=C(O)C(O)c1cccc(I)c1
O=[N+]([O-])c1ccc(I)cc1O
C=Cc1cccc(I)c1
CC(C)(C)OC(O)=N[C@H](Cc1cccc(I)c1)C(=O)O
Cc1cc(I)cc(C)c1C=O
CN1CCN(C(=O)c2cc(Br)cc(I)c2)CC1
COC(=O)c1cc(I)ccc1CBr
O=[N+]([O-])c1cc(I)ccc1CBr
N#Cc1cc(Br)cc(I)c1
COC(OC)(OC)c1cccc(I)c1
N=C(O)c1cc(Cl)cc(I)c1
OC(=Nc1cccc(F)c1)c1cccc(I)c1

O=C(O)c1c(Cl)cc(Cl)cc1I
OC(=Nc1cc2c(cc1C(O)c1ccccc1)OCCO2)c1cccc(I)c1
N#Cc1cc(I)ccc1C(F)(F)F
COC(=O)c1ccc(I)cc1F
O=Cc1ccc(I)cc1Br
OCc1c(Cl)cc(I)cc1Cl
O=C(c1cccc(I)c1)C(F)(F)F
OC(=Nc1ccc(F)c(Cl)c1)c1cccc(I)c1
O=[N+]([O-])c1cc(I)cc(CO)c1
CCCCc1ccc(C(=O)c2cccc(I)c2)cc1
CC(C)(C)OC(=O)c1ccc(I)cc1Br
Cc1ccc(I)cc1C(=O)O
O=C(O)c1cccc(I)c1
Cc1cccc(C)c1N=C(O)c1cccc(I)c1
O=C(O)C(=O)c1cccc(I)c1
O=C(c1ccccc1)c1cccc(I)c1
O=Cc1cc(I)cc(CO)c1
CCOC(=O)CC(=O)c1cccc(I)c1
Ic1cccc(C2CC2)c1
O=C(Nc1ccc(Cl)cc1)c1cccc(I)c1
FCc1cccc(I)c1
CCOC(=O)c1ccccc1C(=O)c1cccc(I)c1
Ic1cccc(Cn2cccn2)c1
OC(=Nc1cccc(O)c1)c1cccc(I)c1
FC(F)(F)c1cc(I)cc(CBr)c1
CC(C)N(C(=O)c1cccc(I)c1)C(C)C
CN(Cc1ccccc1)C(=O)c1cccc(I)c1
O=Cc1ccc(OCc2cccc(I)c2)cc1
COC(=O)c1cc(I)cc(C(=O)OC)c1
N#CC1=C(N)Oc2cc(N)ccc2C1c1cccc(I)c1
COc1cc(I)ccc1C#N
Nc1ccc(NC(=O)c2cccc(I)c2)cc1
CCOC(=O)C1=C(C)NC(C)=C(C(=O)OCC)C1c1cccc(I)c1
CC1(C)OB(c2cc(Br)cc(I)c2)OC1(C)C
OC(=NC1CC1)c1cccc(I)c1
N#Cc1cccc(I)c1
CC(=O)SCc1cccc(I)c1
O=C(OCc1ccc(Br)cc1)c1cccc(I)c1
CCN(CC)C(=O)c1cccc(I)c1
O=C(NN=C(O)c1cccc(I)c1)c1ccco1
Ic1cccc(C2CCCN2)c1
COC(=O)c1ccc(I)cc1[N+](=O)[O-]
OCc1cc(Br)cc(I)c1
COC(=O)c1cc(Br)cc(I)c1
CC(C)(C)OC(=O)Cc1cccc(I)c1
OC1=Nc2c(ccc3ccccc23)C(c2cccc(I)c2)C1
COC(=O)CC(N)c1cccc(I)c1
CC(O)=NN=C(O)c1cccc(I)c1
CCOC(=O)c1ccc(I)cc1N
O=C(c1ccc(Cl)cc1)c1cccc(I)c1
OC(=NN=Cc1ccco1)c1cccc(I)c1
O=C(O)c1c(Cl)cc(I)cc1Cl
O=Cc1ccc(I)cc1Cl
N#Cc1cc(I)cc([N+](=O)[O-])c1
CNCc1cccc(I)c1
O=Cc1ccc(I)cc1[N+](=O)[O-]
Ic1cccc(-c2ccccc2)c1
CCCCc1cccc(I)c1
Cc1c([N+](=O)[O-])cc(I)cc1[N+](=O)[O-]
CC(C)(C)OC(O)=NN=C(O)c1cccc(I)c1
Ic1ccccc1
O=C1C(=O)N(Cc2cccc(I)c2)c2ccccc21
O=Cc1cc(I)cc(C(F)(F)F)c1
COC(=O)c1cc(I)cc(C2CC2)c1
Brc1cc(I)cc2ccccc12
O=C(O)c1cc(I)cc(C(=O)O)c1
O=C(O)C=Cc1cccc(I)c1
Cc1c(CC(=O)O)c(=O)oc2c(C)c(OCc3cccc(I)c3)ccc12
COC(=O)c1cc(I)cc(C=O)c1
CN(C)C(=O)c1cc(Br)cc(I)c1
N=C(S)c1cccc(I)c1
CC(=O)c1ccc(I)cc1F
CCc1cccc(I)c1
N=C(O)c1cc(Br)cc(I)c1
Cc1cc(I)cc(C#N)c1
FC(F)c1cccc(I)c1
COC(=O)c1ccc(I)cc1C(=O)OC
Brc1ccc(-c2cccc(I)c2)cc1
FC(F)(F)c1cc(Cl)cc(I)c1
N[C@@H](Cc1cccc(I)c1)C(=O)O
N#C/C(=C\c1cccc(I)c1)c1nc2ccccc2[nH]1
CC(C)CC(O)=Nc1ccc2oc(-c3cccc(I)c3)nc2c1
O=Cc1ccc(I)cc1O
COCCN=C(O)c1cccc(I)c1
O=C(O)c1cc(I)cc([N+](=O)[O-])c1
N[C@H](Cc1cccc(I)c1)C(=O)O
O=[N+]([O-])c1cc(Cl)cc(I)c1
OCc1cccc(I)c1
COC(=O)c1cc(I)cc(C(F)(F)F)c1
CNc1cc(I)ccc1C(=O)O
O=C(Oc1ccccc1)c1cccc(I)c1
Cc1cc(C)cc(N=C(O)c2cccc(I)c2)c1
CC(C)(C)OC(=O)c1ccc(I)cc1F
CNS(=O)(=O)c1cccc(I)c1
N#Cc1ccc(I)cc1Cl
Cc1cc(O)c(C2=NCCSC(c3cccc(I)c3)C2)c(=O)o1
O=C(O)Cc1cccc(I)c1
O=Cc1ccc(I)cc1C(F)(F)F
CN(C)C(=O)Cc1cccc(I)c1
OC(=NN=C(O)C1CCCC1)c1cccc(I)c1
Cc1c(Cl)cc(I)cc1C(=O)O
NC(CC(=O)O)c1cccc(I)c1
CCOC(=O)c1cc(I)ccc1C
COC(=O)c1ccc(I)cc1S(N)(=O)=O
O=C(Cc1cccc(I)c1)C(F)(F)F
CN=C(O)c1cccc(I)c1
O=Cc1c(Cl)cc(I)cc1Cl
COC(=O)c1ccc(I)cc1OC
CC(=O)c1cc(Br)cc(I)c1
O=C(c1cccc(I)c1)N1CCC(Cc2ccccc2)CC1
CC(C)(C)OC(=O)CC(=O)c1cccc(I)c1
Cc1c(-c2cccc(I)c2)[nH]c2cc3c(cc2c1=O)OCCO3
COC(=O)c1c(Cl)cc(I)cc1Cl
Ic1cccc(COCc2ccccc2)c1
Cc1c(C(=O)O)c(-c2cccc(I)c2)c(-c2ccc(Cl)cc2)n1C
O=Cc1cc(Br)cc(I)c1
OC(=Nc1nc2ccccc2[nH]1)c1cccc(I)c1
CCC(=O)c1cc2c(cc1N=C(O)c1cccc(I)c1)OCCO2
CC(C)(C)c1cccc(I)c1
Cc1cccc(I)c1
CCCCNCc1cccc(I)c1
O=Cc1ccc(I)cc1C(=O)O
N#Cc1ccc(I)cc1C(=O)O
OC(=NC12CC3CC(CC(C3)C1)C2)c1cccc(I)c1
N#Cc1cc(Cl)cc(I)c1
CCOC(=O)c1cccc(I)c1
O=C(O)c1ccc(I)cc1O
O=[N+]([O-])c1cccc(I)c1
COC(=O)c1ccc(I)cc1C(F)(F)F
N#Cc1ccc(I)cc1C#N
O=C(O)c1ccc(I)cc1F
Cc1ccc(-c2nc3ccccc3s2)cc1N=C(O)c1cccc(I)c1
OC(=Nc1ccccn1)c1cccc(I)c1
OC(=Nc1cccc2cccnc12)c1cccc(I)c1
CC(C)c1ccc(I)cc1[N+](=O)[O-]
CN(Cc1cccc(I)c1)C(=O)OC(C)(C)C
CCOC(=O)c1cc(Cl)nc(-c2cccc(I)c2)n1
Cc1ccc(I)cc1C(=O)Cl
Cc1c(Cl)cc(I)cc1Cl
OC(=N/N=C/c1cccc(O)c1O)c1cccc(I)c1
OC(=Nc1nc2ccccc2s1)c1cccc(I)c1
COc1cccc(C(O)=NN=C(O)c2cccc(I)c2)c1
Clc1cc(Cl)cc(I)c1
Cc1ccc(I)cc1[N+](=O)[O-]
OC(=NCc1ccccc1)c1cccc(I)c1
CSC(=CC(=O)c1cccc(I)c1)SC
CC(C)c1nnc(N=C(O)c2cccc(I)c2)s1
CC1(C)OB(c2cccc(I)c2)OC1(C)C
O=Cc1cc(I)cc(C=O)c1
CC(=O)c1cc2c(cc1N=C(O)c1cccc(I)c1)OCCO2
CCCN=C(O)c1cccc(I)c1
OC(=N/N=C/c1ccc(O)c(O)c1)c1cccc(I)c1
Ic1cccc(C2=Nc3cc4c(cc3C(c3ccccc3)O2)OCCO4)c1
CC(C)(C)OC(=O)c1cccc(I)c1
CCc1cc(Br)cc(I)c1
O=C(O)c1cc(Cl)cc(I)c1
O=C(O)CCCCN=C(O)c1cccc(I)c1
Cc1c(Br)cc(I)cc1Br
N=C(O)c1cccc(I)c1
Brc1cc(Br)cc(I)c1
COC(=O)Cc1cccc(I)c1
Clc1cc(I)cc(CBr)c1
Cc1cc(Br)cc(I)c1
OB(O)c1cccc(I)c1
O=Cc1ccccc1OCc1cccc(I)c1
COc1ccc(Cc2nnc(N=C(O)c3cccc(I)c3)s2)cc1
OC(=N/N=C/c1ccccc1O)c1cccc(I)c1
OCc1cc(Cl)cc(I)c1
O=C(OCc1ccccc1)c1cccc(I)c1
CCOC(=O)C1=C(C)NC2=C(C(=O)CCC2)C1c1cccc(I)c1
O=C(O)c1ccc(I)cc1C(=O)O
O=[N+]([O-])c1cc(I)cc(C(F)(F)F)c1
Cc1c(N=C(O)c2cccc(I)c2)c(=O)n(-c2ccccc2)n1C
O=C(O)c1cc(Br)cc(I)c1
FC(F)(F)c1cc(I)cc(C(F)(F)F)c1
CC(C)(C)Oc1ncc(-c2cccc(I)c2)c(OC(C)(C)C)n1
Cc1cccc(OCC(O)=N/N=C/c2cccc(I)c2)c1
CC(C)N=C(O)c1cccc(I)c1
Ic1cccc(-c2ccncc2)c1
N=C(O)Cc1cccc(I)c1
CC(=O)c1ccc(I)cc1O
O=C(c1cccc(I)c1)N1CCCC1
N#CCC(=O)c1cccc(I)c1
C[Si](C)(C)C#Cc1cccc(I)c1
Cc1cccc(C(=O)c2cccc(I)c2)c1
O=C(O)CCCCCN=C(O)c1cccc(I)c1
ON=C(O)c1cccc(I)c1
CC(C)(C)OC(O)=N[C@@H](Cc1cccc(I)c1)C(=O)O
COC(=O)c1cc(I)cc([N+](=O)[O-])c1
FC(F)(F)c1cc(Br)cc(I)c1
N#Cc1ccc(I)cc1C(F)(F)F
C=C(C)c1cccc(I)c1
CCCCN=C(O)c1cccc(I)c1
O=Cc1cccc(I)c1
CCCCOC(=O)C1=C(C)NC2=C(C(=O)CC(C)(C)C2)C1c1cccc(I)c1
O=C(O)c1cc(O)ccc1N=C(O)c1cccc(I)c1
Ic1cccc(COCCc2ccccc2)c1
CC(C)(C)n1nc(Cc2cccc(I)c2)c(C#N)c1N
COC(=O)c1cc(I)cc(Br)c1CBr

O=C(O)/C=C/c1cccc(I)c1
Ic1cccc(Cc2ccccc2)c1
O=C(O)c1ccc(I)cc1C(F)(F)F
Cc1ccc(I)cc1C=O
COC(=O)c1ccccc1N=C(O)c1cccc(I)c1
COc1cc(I)ccc1[N+](=O)[O-]
O=Cc1cc(Cl)cc(I)c1
OC(=NCCc1ccc(F)cc1)c1cccc(I)c1
ClCc1cccc(I)c1
Ic1cccc(Cn2cncn2)c1
OC(=Nc1ccccc1-c1nc2ccccc2s1)c1cccc(I)c1
O=C(c1cccc(I)c1)N1CCOCC1
COC(=O)c1cc(I)cc(C(=O)O)c1
COC(=O)c1ccc(I)cc1N
CN=C(O)c1cc(Br)cc(I)c1
COc1ccccc1N=C(O)c1cccc(I)c1
COc1cc(N=C(O)c2cccc(I)c2)cc(OC)c1
O=C(Nc1ccc(F)cc1)c1cccc(I)c1
O=C(O)c1ccc(I)cc1Cl
O=[N+]([O-])c1cc(Br)cc(I)c1
CC(C)Cc1cccc(I)c1
CS(=O)(=O)c1cc(I)cc(S(C)(=O)=O)c1
CON=C(O)c1cccc(I)c1
OCc1cc(-c2cccc(I)c2)on1
O=C(c1cccc(I)c1)N1CCCCC1
OC(=Nc1cc(Cl)ccc1O)c1cccc(I)c1
CC(Br)c1cccc(I)c1
O=C(O)c1cc(I)cc2ccccc12
O=[N+]([O-])c1cccc(N=C(O)c2cccc(I)c2)c1
OCc1cc(I)cc(C(F)(F)F)c1
COCCCN=C(O)c1cccc(I)c1
COC(=O)c1cc(I)cc(Br)c1C
O=C(c1cccc(I)c1)c1cccc(I)c1

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O=Cc1c(I)ccc(F)c1Cl
COc1ccc(I)cc1CN
FC(F)(F)Oc1ccc(I)cc1Br
COc1cc(I)cc(C(=O)O)c1OC
CCN=C(O)c1cc(OC)c(OC)cc1I
OCCON=C(O)c1ccc2cncn2c1Nc1ccc(I)cc1F
CCc1cc(OC)ccc1I
O=C(O)c1cc(F)c(F)cc1I
CC(C)(C)c1cc(I)ccc1N
CC(C)(C)OC(=O)N1CCN(C(=O)c2cc(I)ccc2O)CC1
Nc1cc(I)ccc1Br
FC(F)(F)Oc1ccc(I)cc1Cl
CCOC(=O)c1cc(I)ccc1OC
CN=C(O)c1cc(I)ccc1N
CC(O)c1cc(I)ccc1Br
Cc1cc(I)cc(C(=O)O)c1O
Nc1cc(I)ccc1Cl
O=Cc1cc(F)ccc1I
CC(O)=Nc1ccc(I)cc1Cl
Cc1cc(I)ccc1F
Nc1ccc(I)cc1F
COc1cc(I)cc([N+](=O)[O-])c1N
CCOC(=O)c1cc(OC)ccc1I
OB(O)c1cc(I)ccc1Br
COC(=O)c1cc(I)cc(F)c1N
Oc1ccc(I)c2ccccc12
Cc1cc(I)ccc1OCc1ccccc1
FC(F)(F)c1ccc(I)cc1Br
COC(=O)c1c(I)ccc(F)c1C
Cc1cc(I)cc(C)c1N
Nc1ccc(I)cc1C(=O)c1ccccc1
COc1cc(C)c(I)cc1C
CC(C)Oc1ccc(I)cc1C#N
COc1ccc(I)c(C=O)c1
CCOc1ccc(C(O)c2cc(I)ccc2Cl)cc1
N=C(O)c1cc(I)ccc1Cl
COc1ccc(I)c(C(C)C)c1
COc1cc(F)c(F)c(Nc2ccc(I)cc2F)c1[N+](=O)[O-]
Cc1cc(I)cc(C)c1Br
Clc1ccc(I)cc1Br
Nc1c(F)cc(I)cc1C(=O)O
CC(C)(C)OC(O)=Nc1ccc(I)cc1Cl
CCc1cc(I)ccc1Br
CC1(C)OB(c2cc(O)ccc2I)OC1(C)C
Cc1cc(O)c(C(=O)O)cc1I
O=C(O)c1ccc(I)cc1Br
CC(C)c1ccc(I)cc1N
Cc1cc(I)ccc1N
COc1cc(I)cc(C=O)c1O
COc1cc(I)ccc1O
CN1C(=O)/C(=C\c2cc(I)ccc2O)SC1=S
CCOCOc1cc(I)c(CCN=C(O)OC(C)(C)C)cc1OCOCC
Cc1cc(OC(F)(F)F)ccc1I
Cc1cc(C(O)=NOCCO)c(Nc2ccc(I)cc2F)n(C)c1=O
Cc1cc(N)ccc1I
CC(C)(C)OC(O)=NCCc1cc(O)c(O)cc1I
CC(C)(C)OC(O)=Nc1ccc(I)cc1F
COc1ccc(I)cc1C#N
COc1cc(I)c(C(=O)O)cc1OC
Cc1ccc(C(c2ccc(C)o2)c2cc(I)ccc2O)o1
Cc1cc(I)cc(F)c1Br
COc1ccc(I)c(B2OC(C)(C)C(C)(C)O2)c1
C[C@H](O)c1cc(F)ccc1I
N#CCc1cc(I)ccc1Br
Fc1c(Cl)cc(I)cc1C(F)(F)F
FC(F)(F)c1cc(I)ccc1Br
COc1ccc(I)cc1C(Nc1cc(C)ccn1)c1ccc2cccnc2c1O
Brc1ccc(I)cc1Br
Oc1c(F)cc(I)cc1F
OCc1ccc(I)cc1Br
COc1ccc(I)c(C(F)(F)F)c1
O=Cc1cc(O)ccc1I
Oc1ccc(I)cc1-c1cc(I)ccc1O
CC(C)(C)[Si](C)(C)Oc1ccc(I)c2ccccc12
COc1c(Br)cc(I)cc1Br
Brc1ccc(I)cc1C1OCCO1
N[C@@H](Cc1cc(I)ccc1Br)C(=O)O
CC(O)=Nc1cc(I)ccc1Cl
Fc1ccc(I)cc1
CC(C)(C)c1cc(I)cc(C=O)c1O
O=C(O)c1cc(O)ccc1I
C=Cc1ccc(I)cc1Cl
Nc1ccc(I)cc1CO
O=C(c1cc(I)ccc1F)C(F)(F)F
O=Cc1cc(I)ccc1F
CC(O)=Nc1ccc(I)cc1OC(F)(F)F
COc1cc(I)ccc1CO
Cc1c(F)ccc(I)c1C(=O)O
O=Cc1c(I)ccc(F)c1Br
N[C@@H](Cc1cc(I)ccc1F)C(=O)O
Fc1cc(I)ccc1Br
COc1ccc(I)c(C(=N)O)c1
COc1ccc(I)cc1C=O
CC(C)(C)OC(O)=Nc1cc(OCc2ccccc2)c2ccccc2c1I
COC(=O)c1ccc(I)cc1Br
Nc1ccc(I)cc1C=O
FC(F)(F)Oc1cc(I)ccc1Br
Cc1cc(OCc2ccccc2)ccc1I
Clc1ccc(I)cc1Cc1ccc(O[C@H]2CCOC2)cc1
Cc1cc(N)c([N+](=O)[O-])cc1I
Cc1cc(I)ccc1OC(C)C
COc1cc(I)c(CN=C(C)O)cc1OC
Cc1cc(I)cc(C)c1F
Fc1cc(I)ccc1Cl
CC(C)(C)OC(O)=NC(Cc1cc(I)ccc1F)C(=O)O
Cc1ccc(I)cc1Cl
CCOc1ccc(I)cc1C#N
Nc1ccc(I)c(C(=O)O)c1
O=[N+]([O-])c1c(F)cc(F)c(F)c1Nc1ccc(I)cc1F
Clc1ccc(I)cc1Cc1ccc(OC2CCOC2)cc1
COC(=O)c1cc(I)c(N=C(C)O)cc1OC
COC(=O)c1cc(I)ccc1N
COc1cc(C)c(I)cc1C(=O)O
COc1ccc(I)cc1N
N=C(O)c1ccc(I)cc1Br
Nc1c(F)cc(I)cc1Cl
O=C(O)c1cc(I)ccc1O
Fc1ccc(I)cc1Br
CCc1cc(O)ccc1I
Cc1c(I)ccc(F)c1C(=O)O
CC(C)c1cc(I)ccc1O
N#CC1(N=C(O)c2cc(I)ccc2Cl)CC1
CC(=O)c1cc(I)ccc1N
Cc1ccc(I)cc1O
CC(C)(C)c1cc(I)ccc1O
COc1c(F)cc(I)cc1F
COC(=O)c1cc(OC)c(OC)cc1I
COc1cc(I)ccc1N
Cc1cc(F)c(C(=O)O)cc1I
CCOc1ccc(Cc2cc(I)ccc2Cl)cc1
Cc1cc(N)c(F)cc1I
CC(C)CCOC(=O)c1cc(I)ccc1O
COC(=O)c1ccc(I)cc1Cl
CC(C)c1cc(O)ccc1I
COc1ccc(I)cc1C
Cc1ccc(I)cc1Br
O=C(O)c1cc(I)cc(Br)c1F
N=C(O)c1c(I)ccc(Br)c1F
Cc1cc(I)cc(N)c1N
N#Cc1cc(I)ccc1O
O=C(Cl)c1cc(I)ccc1F
Nc1ccc(I)cc1C(=O)O
COC(=O)c1cc(I)ccc1O
O=C=Nc1ccc(I)cc1Cl
CNc1ccc(I)cc1C(=O)O
Clc1ccc(I)cc1Cl
Oc1cc(I)ccc1Cl
COc1ccc(I)cc1Br
COc1cc(I)ccc1Br
Oc1ccc(I)cc1Br
Oc1c(Br)cc(I)cc1Br
COC(=O)c1cc(I)cc(C)c1N
OCc1cc(F)ccc1I
COc1ccc(I)cc1OCc1ccccc1
Cc1ccc(C)n1-c1ccc(I)cc1F

OC[C@@H](O)CON=C(O)c1ccc(F)c(F)c1Nc1ccc(I)cc1F
COc1cc(I)ccc1F
Clc1ccc(I)cc1CBr
Cc1c(O)ccc(I)c1C
COc1ccc(I)c(C)c1
O=C(O)c1cc(Br)c(F)cc1I
CC(C)Oc1ccc(I)cc1Br
COc1ccc(I)c(CC(=O)O)c1
COc1ccc(I)cc1Cl
Nc1ccc(I)cc1C(F)(F)F
Cc1cc(I)c(C)cc1N
Oc1ccc(Cc2cc(I)ccc2Cl)cc1
N=C(O)c1cc(I)ccc1F
Fc1ccc(I)c2ccccc12
COc1ccc(I)c(C#N)c1
O=C(O)c1cc(F)ccc1I
OC(=NC1CCCC1)c1cc(I)ccc1Cl
Oc1ccc(I)cc1C(F)(F)F
O=[N+]([O-])c1cc(I)ccc1OC(F)(F)F
Fc1ccc(I)c(C(F)(F)F)c1
OCc1cc(I)ccc1F
COc1ccc(I)cc1CO
NN=C(O)c1cc(I)ccc1O
Cc1cc(F)c(O)cc1I
COC(=O)c1cc(I)ccc1F
FC(F)c1cc(I)ccc1Br
OC(=NC1CC1)c1cc(I)ccc1Cl
Cc1cc(F)c(Br)cc1I
N=C(O)c1cc(F)c(F)cc1I
C=Cc1cc(I)ccc1OC
CN=C(O)c1cc(F)ccc1I
COc1c(Cl)cc(I)cc1Cl
Fc1c(Cl)cc(I)cc1Br
OCCON=C(O)c1ccc(F)c(F)c1Nc1ccc(I)cc1F
CC(O)=Nc1ccc(I)cc1F
Cc1cc(I)cc(C)c1O
OCc1cc(I)ccc1Cl
FC(F)(F)c1ccc(I)cc1Cl
OCc1ccc(I)cc1O
Cc1cc(I)ccc1O
CC(C)c1cc(I)ccc1Br
N#Cc1cc(F)ccc1I
C=CCOc1ccc(I)cc1C=O
CC(C)(C)c1cc(I)cc(Br)c1O
NS(=O)(=O)c1cc(I)ccc1Cl
Oc1cc(I)ccc1F
N#Cc1c(I)ccc(F)c1F
C[C@@H](O)c1cc(F)ccc1I
OCc1cc(I)cc(Cl)c1F
Cc1cc(N)c(C(=O)O)cc1I
COc1cc(I)c(Cc2nccc3cc(OC)c(OC)cc23)cc1OC
BrCc1cc(I)ccc1Br
CCOc1c(Cl)cc(I)cc1Cl
Clc1cc(I)ccc1CBr
COc1cc(I)ccc1I
Cc1ccc(I)cc1N
Fc1ccc(I)cc1CBr
COc1cc(I)ccc1OCc1ccccc1
COc1cc(I)cc(C(=O)O)c1N
CCCCCOC(=O)c1cc(I)ccc1O
COc1cc(I)c(CCN=C(C)O)cc1OC
FC(F)Oc1ccc(I)cc1Br
CC(C)(C)OC(O)=Nc1cc(I)ccc1Br
COc1ccc(I)cc1O
COC(=O)c1cc(F)c(F)cc1I
COc1cc(I)c(C=O)cc1OC
COC(=O)c1cc([N+](=O)[O-])c(F)c(F)c1Nc1ccc(I)cc1F

Cc1cc(I)cc(C)c1Cl
O=[N+]([O-])c1cc(I)ccc1O
N=C(O)c1cc(I)ccc1O
CC(C)COC(=O)c1cc(I)ccc1O
CCOC(=O)c1ccc(I)cc1Cl
CC(C)c1cc(I)ccc1F
COC(=O)c1cc(I)c(C)cc1OC
CC(C)OC(=O)c1cc(I)ccc1O
CCOc1ccc(I)cc1F
COc1ccc(I)c2ccccc12
COc1cc(I)ccc1N=C(O)OC(C)(C)C
COC(=O)c1cc(N)ccc1I
CC(C)(C)OC(O)=Nc1ccc(I)cc1O
CC(=O)Oc1ccc(I)cc1C(=O)O
Oc1c(Cl)cc(I)cc1Cl
CCOC(=O)c1cc(I)ccc1O
Oc1ccc(I)cc1-c1ccccc1
Nc1c(Cl)cc(I)cc1Cl
CCOc1ccc(I)cc1C
O=C(O)c1ccc(F)c(F)c1Nc1ccc(I)cc1F
OB(O)c1cc(I)ccc1F
OCc1ccc(I)cc1Cl
Fc1cc(I)ccc1OC(F)(F)F
Oc1ccc(I)cc1Cl
FC(F)c1ccc(I)cc1Br
CC(=O)c1cc(F)ccc1I
Sc1cc(I)ccc1Br
CC(C)Nc1ccc(I)cc1C(=O)O
O=S(=O)(Nc1cc(F)ccc1I)c1ccccc1
Fc1ccc(I)cc1Cl
ClCc1ccc(I)cc1Br
O=C(O)c1c(I)ccc(F)c1F
COc1ccc(I)c(C(=O)O)c1OC
CC(=O)c1cc(I)cc(C)c1N
Cc1cc(O)ccc1I
OC(=NC1CC1)Nc1ccc(I)cc1F
Cc1c(I)ccc(F)c1[N+](=O)[O-]
COC(=O)c1cc(I)ccc1OC
COC(=O)c1cc(OC)ccc1I
COc1ccc(I)cc1OC
Clc1cc(I)ccc1Br
Oc1ccc(I)cc1F
FC(F)(F)c1cc(I)ccc1Cl
CCc1cc(N)c(C(=O)OC)cc1I
COc1cc(I)cc(OC)c1OC
Ic1ccc(I)cc1
O=C(O)c1cc(I)cc(F)c1F
Nc1ccc(I)cc1[N+](=O)[O-]
O=[N+]([O-])c1cc(I)ccc1F
Nc1cc(I)ccc1O
COc1cc(I)c(CC(=O)O)cc1OC
Nc1ccc(I)cc1O
Cc1cc(I)ccc1OC(F)F
CC(C)(C)c1cc(O)ccc1I
COc1ccc(I)c(C(=O)O)c1F
Clc1ccc(I)cc1
OB(O)c1cc(OCc2ccccc2)ccc1I
Nc1ccc(I)c2ccccc12
CC(O)=Nc1cc(F)ccc1I
CCOC(=O)c1cc(I)ccc1F
N#CCC(=O)N(C(O)=Nc1ccc(I)cc1F)C1CC1
COc1ccc(I)c(CO)c1
COc1ccc(I)cc1[N+](=O)[O-]
CCc1cc(I)ccc1N
Nc1ccc(I)cc1Br
Nc1cc(I)ccc1CO
COc1ccc(I)c(C(=O)O)c1
CC(=O)Oc1ccc(I)cc1C(=O)Nc1ccc(Cl)cc1

Cc1cc(O)c(Cl)cc1I
Nc1ccc(I)cc1OC(F)(F)F
Nc1cc(I)ccc1F
Fc1ccc(I)cc1C(F)(F)F
Nc1c(Cl)cc(I)cc1[N+](=O)[O-]
CC(C)c1cc(I)cc(C(C)C)c1O
Fc1ccc(I)c(CBr)c1
Nc1cc(=O)n(C2CC2)c(=O)n1-c1ccc(I)cc1F
CCCCCCOC(=O)c1cc(I)ccc1O
Sc1ccc(I)cc1Cl
Cc1cc(I)ccc1Cl
COc1ccc(I)cc1F
CCOc1cc(I)ccc1F
CC(C)(C)OC(O)=Nc1ccc(I)cc1N
Fc1ccc(I)cc1F
O=C(O)c1cc(OC(F)(F)F)ccc1I
Nc1ccc(I)c(C(F)(F)F)c1
O=Cc1cc(I)ccc1O
Cc1cc(I)cc(Cl)c1N
COC(=O)c1cc(I)c(C)cc1O
ClCc1cc(I)ccc1Cl
COc1cc(I)c(C(=O)N(C)C)cc1OC
COC(=O)c1cc(I)c(C)cc1F
Cc1cc(Br)c(F)cc1I
O=C(O)c1cc(I)ccc1F
O=C(N/N=C/c1cc(I)ccc1O)c1ccncc1
COC(=O)c1cc(F)c(Br)cc1I
COC(=O)c1cc(I)c(C(F)(F)F)cc1N
FC(F)(F)Oc1cc(I)ccc1Cl
COc1cc(I)cc(OC)c1O
Cc1cc(F)ccc1I
Cc1cc(NC(=O)OC(C)(C)C)ccc1I
O=C(O)c1ccncc1Nc1ccc(I)cc1F
O=C(O)c1cc(Br)c(Cl)cc1I
CS(=O)(=O)Nc1ccc(I)cc1F
Nc1ccc(I)cc1Cl
CC(=O)c1cc(I)ccc1O
COc1cc(I)cc(C=O)c1OC
BrCc1ccc(I)cc1Br
CCOC(=O)c1c(I)ccc(F)c1C
OCc1cc(I)ccc1O
CCc1cc(I)cc(C)c1N
COC(=O)c1c(I)ccc(Br)c1F
COc1ccc(I)c(C)c1C
Fc1cc(I)cc(F)c1F
O=Cc1cc(I)cc(Br)c1F
COc1ccc2c(OC)ccc(I)c2c1
COc1cc(I)cc(OC)c1Br
N=C(O)c1cc(I)ccc1N
O=C(O)COc1ccc(I)cc1C(=O)O
Cc1cc(I)ccc1Br
CCN=C(O)c1cc(F)ccc1I
CCOc1ccc(I)cc1C(=O)OC
CNc1cc(=O)n(C2CC2)c(=O)n1-c1ccc(I)cc1F
COC(=O)c1cc(F)ccc1I
OCc1cc(I)ccc1Br
Cc1cc(F)cc(C(=O)O)c1I
COc1cc(I)ccc1C
CCCOC(=O)c1cc(I)ccc1O
O=C1CCCCN1c1ccc(I)cc1F
O=C(NC[C@H](O)CO)c1ccncc1Nc1ccc(I)cc1F
O=C(NC[C@@H](O)CO)c1ccncc1Nc1ccc(I)cc1F
O=C(O)c1c(I)ccc(F)c1Cl
CCOC(=O)c1cc(O)ccc1I
Nc1ccc(I)cc1N
OC(=NCc1ccccc1)c1cc(I)ccc1O
COc1cc(F)c(F)c(Nc2ccc(I)cc2F)c1N

CCCCCCCCC(O)=NCc1cc(OC)c(O)cc1I
CN(C)/C=N/c1cc(=O)n(C2CC2)c(=O)n1-c1ccc(I)cc1F
Fc1c(Cl)cc(I)cc1Cl
O=C(O)c1cc(I)cc(Cl)c1F
Nc1c(F)cc(I)cc1F
COC(O)=Nc1cc(F)c(Cl)cc1I
CCCCOC(=O)c1cc(I)ccc1O
COc1ccc(I)cc1C(=O)O
NN=C(O)c1cc(I)ccc1Cl
Oc1cc(I)ccc1Br
CC(C)(C)OC(=O)c1cc(I)ccc1O
Cc1c(N)ccc(I)c1C
Cc1cc(I)c(C)cc1O
Cc1cc(I)cc(C(=O)O)c1N
O=C(OCc1ccccc1)c1cc(I)ccc1O
COC(=O)c1cc(O)ccc1I
Brc1ccc(I)cc1
COc1cc(I)ccc1Cl
N#Cc1cc(I)ccc1N
COc1ccc(I)c(B(O)O)c1
CC(=O)c1cc(I)ccc1F
O=C(O)c1cc(I)ccc1N1CCOCC1
CC(C)(C)OC(=O)c1cc(I)ccc1N
CNc1ccc(I)cc1[N+](=O)[O-]
CCOC(=O)c1cc(I)ccc1N
N=C(O)c1cc(I)ccc1Br
Cc1cc(I)cc(C=O)c1O
COc1ccc(I)cc1OC(C)=O
COc1ccc(I)cc1N=C(O)OC(C)(C)C
Nc1c(Cl)cc(I)cc1C(=O)O
CON(C)C(=O)c1cc(F)ccc1I
O=[N+]([O-])c1cc(I)cc(Br)c1O
Cc1c(O)c2c(=O)n(C3CC3)c(=O)n(-c3ccc(I)cc3F)c2n(C)c1=O
N#Cc1cc(I)ccc1F
Cc1cc(I)cc([N+](=O)[O-])c1N
OCC(O)CON=C(O)c1ccc(F)c(F)c1Nc1ccc(I)cc1F
COc1ccc(I)c(C(O)=NC(C)C)c1

Cluster K

COc1cccc(CNc2ccccc2I)c1
Cc1c(C(O)=Nc2ccccc2I)cccc1[N+](=O)[O-]
N#Cc1ccc(C(=O)Nc2ccccc2I)cc1
COc1ccccc1I
CCOC(O)=Nc1ccc(C(F)(F)F)cc1I
O=[N+]([O-])c1ccccc1C(O)=Nc1ccccc1I
O=C(O)CCC(O)=Nc1ccccc1I
CCC(C(O)=Nc1ccccc1I)c1ccccc1
C=C1[CH]C=CC=C1I.[Br-].[Zn+]
Ic1ccccc1Oc1ccccc1
Ic1ccccc1OCc1ccccc1
N=C(S)Nc1ccccc1I
N#CC1=C(N)Oc2cc(O)c(/C=N/c3ccccc3I)cc2C1c1ccccc1
CN=C(O)Nc1ccccc1I
OC(=NC(S)=Nc1ccccc1I)c1cccnc1
CC(=O)Oc1ccccc1I
OC(Cc1ccccc1)=Nc1ccccc1I
COc1cccc(OC)c1C(O)=Nc1ccccc1I
CC(O)=Nc1ccc(C(F)(F)F)cc1I
O=S(=O)(Nc1ccccc1I)c1ccc(Cl)cc1
O=[N+]([O-])c1ccc(S(=O)(=O)Nc2ccccc2I)cc1
Ic1ccccc1N=c1c2ccccc2[nH]c2ccccc12
COc1c(C)cccc1I
FC(F)Oc1ccccc1I
Ic1ccccc1Nc1nc2nonc2[nH]c1=N/N=C/c1ccco1
COCOc1ccccc1I
NNc1ccccc1I
O=C1CCCCN1c1ccccc1I
CCC(CC)C(O)=Nc1ccccc1I
Clc1ccc(Oc2ccccc2I)c(Cl)c1
COc1ccc(S(=O)(=O)Nc2ccccc2I)cc1OC
OC(=Nc1ccccc1I)c1ccccc1F
CC(O)=Nc1ccc(S(=O)(=O)Nc2ccccc2I)cc1
Cc1ccc(S(=O)(=O)Nc2ccccc2I)cc1
CN(C)c1ccccc1I
COc1ccc(CC(O)=Nc2ccccc2I)cc1
Ic1ccccc1NCC1CC1
CCOc1ccc(C(=O)Nc2ccccc2I)cc1
OC(/C=C/c1ccccc1)=Nc1ccccc1I
Ic1ccccc1C1CCNCC1
O=C(Nc1ccccc1I)c1ccc([N+](=O)[O-])cc1
CN(C)CC(O)c1ccccc1I
O=C(Nc1ccccc1I)c1ccc(Cl)cc1
OC(CCC1CCCC1)=Nc1ccccc1I
Ic1ccccc1NCc1ccco1
Cc1ccccc1C(O)=Nc1ccccc1I
O=S(=O)(Nc1ccccc1I)c1ccc(Br)cc1
O=S(=O)(Nc1ccccc1I)c1cccc2nonc12
O=[N+]([O-])c1cc(C(O)=Nc2ccccc2I)cc([N+](=O)[O-])c1
OC(Cc1ccc(Cl)cc1)=Nc1ccccc1I
O=C1c2cc([N+](=O)[O-])cc3cc([N+](=O)[O-])cc(c23)C(=O)N1c1ccccc1I
OC(=Nc1ccccc1I)C1CCCC1
CCCN=C(O)Nc1ccccc1I
OC(=Nc1ccccc1I)Nc1ccc(Cl)cc1
OC(=Nc1ccccc1I)c1cccc(F)c1
O=S(=O)(Nc1ccccc1I)c1ccccc1C(F)(F)F
OC(=Nc1ccccc1I)C12CC3CC(CC(C3)C1)C2
O=C(Nc1ccccc1I)c1ccncc1
CCOc1ccccc1I
O=[N+]([O-])c1cccc(C(O)=Nc2ccccc2I)c1
CCOC(=O)C(=O)NNc1ccccc1I
OC(=Nc1ccccc1I)C1CC1
CC(N)c1ccccc1I
O=C(O)COc1ccccc1I
OC(=Nc1ccccc1I)c1cc(Cl)ccc1Cl
O=[N+]([O-])c1ccccc1S(=O)(=O)Nc1ccccc1I
O=S(=O)(Oc1ccccc1I)C(F)(F)F
Cc1nc2ccccc2c(=O)n1-c1ccccc1I
CNc1ccccc1I
O=C(COc1ccccc1I)c1ccc[nH]1
CC(C)(C)c1ccc(C(=O)Nc2ccccc2I)cc1
CC(C)(C)OC(=O)COc1ccccc1I
OC(=Nc1ccccc1I)C(F)(F)F
OC(=Nc1ccccc1I)c1ccccn1
CCC(O)=Nc1ccccc1I
OC(=Nc1ccccc1I)c1cc2ccccc2o1
COC(=O)c1ccccc1N=C(O)Nc1ccccc1I
O=C(Nc1ccccc1I)c1cccs1
OC(=Nc1ccccc1I)c1ccccc1
Ic1ccccc1CNC1CC1
CC(O)=Nc1ccccc1I
OC(=Nc1ccccc1I)c1ccccc1Cl
OC(Cc1c[nH]c2ccccc12)=Nc1ccccc1I
COCCOc1ccccc1I
Ic1ccccc1OC1CCOCC1
CCCC(O)=Nc1ccccc1I
Cc1cccc(C(O)=Nc2ccccc2I)c1
SC(=Nc1ccccc1)Nc1ccccc1I
O=C1C=CC(=O)N1c1ccccc1I
COc1ccccc1C(O)=Nc1ccccc1I
O=C1CSC(=S)N1c1ccccc1I
OC(=Nc1ccccc1I)c1cccnc1
OC(=Nc1ccccc1I)c1ccccc1Br
CS(=O)(=O)Nc1ccccc1I
C=CCN=C(O)Nc1ccccc1I
N#CCC(O)=Nc1ccccc1I
COc1ccccc1CC(O)=Nc1ccccc1I
O=C1c2ccccc2C(=O)N1c1ccccc1I
OC(=NC1CCCC1)Nc1ccccc1I
Ic1ccccc1NC1CCCC1
COc1ccc(C(=O)Nc2ccccc2I)cc1
O=C(O)CCNc1ccccc1I
Cc1cc(C)c(S(=O)(=O)Nc2ccccc2I)c(C)c1
CC(C)(C)OC(=O)CNc1ccccc1I
CCCOc1ccccc1I
CC(C)C(O)=Nc1ccccc1I
OC(=Nc1ccccc1I)C(F)(F)C(F)(F)C(F)(F)F
OC(=Nc1ccccc1I)c1cccc(Cl)c1
C=CC(O)=Nc1ccccc1I
COc1ccc(S(=O)(=O)Nc2ccccc2I)cc1
O=C=Nc1ccccc1I
OCCOc1ccccc1I
O=C1Nc2ccccc2C1=Nc1ccccc1I
OC(=Nc1ccccc1I)OCc1ccccc1
Ic1ccccc1CN1CCNCC1
Cc1ccc(C)n1-c1ccccc1I
COC(=O)c1ccccc1S(=O)(=O)Nc1ccccc1I
OC(=Nc1ccccc1I)c1cnccn1
Cc1c(C(O)=Nc2ccccc2I)oc2ccccc12
N#Cc1ccc(Oc2ccccc2I)c(Br)c1
O=S(=O)(Nc1ccccc1I)c1ccc(F)cc1
O=C(Nc1ccccc1I)c1ccc(F)cc1
C=C(COc1ccccc1I)C(=O)O
O=C1CC(Sc2nc3ccccc3s2)C(=O)N1c1ccccc1I
C#CCOc1ccccc1I
CCOC(=O)C(=CNc1ccccc1I)C(=O)OCC
Oc1ccccc1I
O=C(O)CCCC(O)=Nc1ccccc1I
CC(=O)N(/C=C1\Sc2ccccc2C1=O)c1ccccc1I
CC(Cl)C(O)=Nc1ccccc1I
CC(C(O)=Nc1ccccc1I)c1ccccc1
OC(CCc1ccccc1)=Nc1ccccc1I
S=C=Nc1ccccc1I
O=C(O)CCOc1ccccc1I
O=S(=O)(Nc1ccccc1I)c1ccc(C(F)(F)F)cc1
OC(Cc1cccs1)=Nc1ccccc1I
OC(=Nc1ccccc1I)c1cccc2ncccc12
Sc1ccccc1I
CNCc1ccccc1I
OC(CCl)=Nc1ccccc1I
COc1c(C)cc(C)cc1I
Oc1ccc(N=c2[nH]c3nonc3nc2Nc2ccccc2I)cc1
Ic1ccccc1CN1CCCCC1
Cc1ccc(C(=O)Nc2ccccc2I)cc1
Cc1ccc(C(=O)Nc2ccccc2I)cc1C
OC(=NNc1ccccc1I)C(O)(c1ccccc1)c1ccccc1
[C-]#[N+]c1ccccc1I
OC(=Nc1ccccc1)Nc1ccccc1I

CC(C)(C)OC(O)=Nc1ccccc1I
Ic1ccccc1CNC1CCCCC1
O=C(Nc1ccccc1I)c1ccco1
O=C(Nc1ccccc1I)c1ccc(Br)cc1
OC(=Nc1ccccc1I)c1ccccc1I
Ic1ccccc1-n1cccc1
OC(=Nc1ccccc1I)C1CCCO1
CC(C)(C)OC(=O)N(C(=O)OC(C)(C)C)c1ccccc1I
O=S(=O)(Nc1ccccc1I)c1ccccc1
Ic1ccccc1OC1CC1
Ic1ccccc1C1CCCN1
FC(F)(F)Oc1ccccc1I
OC(/C=C/c1ccco1)=Nc1ccccc1I
CC(C)(C)C(O)=Nc1ccccc1I
CCc1ccc(C(=O)Nc2ccccc2I)cc1
CC(C)Oc1ccccc1I
Ic1ccccc1NCc1cccs1
OC(=Nc1ccccc1I)c1ccccc1C(F)(F)F
CCOC(=O)c1ccc(NC(O)=Nc2ccccc2I)cc1
Fc1ccccc1CNc1ccccc1I
N#Cc1ccc(CNc2ccccc2I)cc1

Cluster L

COC(=O)c1cc(Br)cc(I)c1C
Cc1cc(I)c(C)cc1Cl
COC(=O)c1cc(C(C)(C)C)cc(C(=O)OC)c1I
Cc1c(Br)ccc(I)c1C
Cc1c(I)cccc1CC#N
Cc1c(I)ccc(Br)c1Cl
CC(C)(C)C(O)=Nc1ccc(Cl)cc1I
OCc1cc(Cl)ccc1I
Cc1c(Cl)cccc1I
N=C(S)Nc1ccc(Br)cc1I
O=Cc1c(Br)cccc1I
CCc1ccc(I)c(CC(=O)O)c1
N#Cc1ccc(Cl)cc1I
OC(=NCc1ccccc1)c1cc(Br)ccc1I
CCOC(=O)c1ccc(I)c(C)c1
Cc1cc(C#N)cc(C)c1I
ClCc1cc(Cl)ccc1I
Cc1cccc(C)c1I
Cc1c(I)cccc1CBr
CC(O)=Nc1cc(C)c(I)c(C)c1
COC(=O)c1c(C)cc(Br)cc1I
FC(F)(F)Oc1ccc(Br)cc1I
Cc1cc(C(F)(F)F)ccc1I
CCc1ccc(I)c(C)c1
COc1ccc(C(=O)Nc2ccc(Br)cc2I)cc1
CN=C(O)c1ccc(C)c(I)c1
N=C(O)c1cc(Br)ccc1I
Cc1c(C)c(I)c(C)c(C)c1I
Cc1cc(Br)c(C)c(I)c1
Cc1cccc(I)c1C(=O)O
OCc1cc(C(F)(F)F)ccc1I
Cc1cc(S(N)(=O)=O)ccc1I
Cc1cc(I)c(C(=O)O)cc1C
CCOC(=O)c1cccc(C)c1I
CN=C(O)c1cc(C)ccc1I
CC(C)c1cccc(C(C)C)c1I
N#CCc1cc(Br)ccc1I
Cc1c(I)cccc1C(=O)O
Cc1ccc(CCO)c(I)c1
O=C(O)Cc1c(Br)cccc1I
Cc1cc(F)cc(C)c1I
N#Cc1c(Cl)cccc1I
N=C(O)c1ccc(Cl)cc1I
Cc1cc(I)c(C)cc1Br
COC(=O)c1cc(Br)c(C)c(I)c1
Cc1ccc(C(=N)N)cc1I
C[C@@H](N=C(O)c1cc(Br)ccc1I)c1ccccc1
Cc1cc(O)cc(C)c1I
Cc1cccc(I)c1-c1c(C)cccc1I
CC(=O)Oc1cc(C)c(I)c(C)c1
OCc1cc(I)c(CO)cc1I
BrCc1cc(Br)ccc1I
Cc1cc(C(C)(C)C)cc(C)c1I
FC(F)Oc1ccc(Br)cc1I
O=C(O)c1cc(CO)ccc1I
COC(=O)c1c(I)ccc(C)c1Br
FC(F)(F)c1cc(Br)ccc1I
Cc1c(I)cccc1CO
Cc1ccc(C)c(I)c1
O=Cc1ccc(Cl)cc1I
Cc1cc(CO)ccc1I
CCc1c(Cl)cccc1I
COC(=O)c1c(C)cccc1I
OCc1c(Cl)cccc1I
Cc1ccc(I)c(C(O)=NC(C)C)c1
N#Cc1c(Br)cccc1I
Cc1cccc(I)c1CO
Cc1ccc(-c2ccccc2)c(I)c1
Cc1cc(C)c(C)c(I)c1C
Cc1c(Br)cc(C(=O)O)cc1I
Cc1cc(F)cc(CO)c1I
Cc1cc(C(=O)N(C)C)ccc1I
COc1cc(C)c(I)c(C)c1
N=C(O)c1cc(C(F)(F)F)ccc1I
CC(O)=Nc1cc(C)c(I)cc1C
Cc1c(F)cc(C(=O)O)cc1I
COC(=O)c1cccc(C)c1I
CC(C)N=C(O)c1cc(Br)ccc1I
Cc1ccc(I)c(CO)c1
Cc1cccc(CBr)c1I
O=C(O)c1c(I)cccc1C(F)(F)F
N#CC1(Cc2ccc(Br)cc2I)CCC1
Cc1cccc(CO)c1I
ClCc1ccc(Br)cc1I
Brc1ccc(OCc2ccccc2)c(I)c1
BrCc1ccc(Br)cc1I
Cc1c(F)cc(C(O)=NC2CC2)cc1I
OCc1ccc(C(F)(F)F)cc1I
Cc1cccc(C(=O)O)c1I
OCc1ccc(CO)c(I)c1
Cc1ccc(Br)cc1I
COC(=O)c1ccc(I)c(C)c1
COC(=O)c1cc(C)ccc1I
Cc1cc(-c2ccccc2)ccc1I
O=C(O)c1cc(Cl)ccc1I
COC(=O)c1cccc(I)c1C
N=C(O)c1cc(Cl)ccc1I
CNC(=O)c1ccc(I)c(C)c1
Cc1cccc(C(=N)O)c1I
Cc1ccc(I)c(C)c1
Cc1ccc(C(O)=NC2CC2)cc1I
Cc1cc(I)ccc1I
Cc1ccccc1N=C(O)c1c(C)cccc1I
Cc1ccc(CBr)cc1I
O=C(O)c1ccc(Br)cc1I
CC(C)N=C(O)c1cc(Cl)ccc1I
FC(F)(F)c1ccc(Br)cc1I
Cc1cc(Cl)cc(I)c1CBr
OCc1ccc(C(F)(F)F)c(I)c1
Cc1ccc(S(C)(=O)=O)cc1I
N#CCc1ccc(Br)cc1I
FC(F)(F)c1ccc(I)c(CBr)c1
Cc1cc(Br)cc(C)c1I
N#CC1(Cc2ccc(Br)cc2I)CC1
Cc1ccc(C(F)(F)F)cc1I
Cc1cc(I)c(C)cc1I
Cc1ccc(I)c(C(=O)O)c1Br
CC(C)(C)OC(=O)N(C(=O)OC(C)(C)C)c1ccc(Br)cc1I
Clc1ccc(-n2cnnn2)c(I)c1
CCc1cc(Br)ccc1I
OCc1ccc(Br)cc1I
COC(=O)c1c(Cl)cccc1I
CCN=C(O)c1cc(Br)ccc1I
Cc1ccc(C(=O)O)c(I)c1
CC(C)(C)OC(=O)c1ccc(Br)cc1I
NCc1cc(Cl)ccc1I
Ic1cc(C2CCCCC2)c(I)cc1C1CCCCC1
Cc1ccc(C)c(I)c1C
FC(F)(F)c1cc(CBr)ccc1I
O=C(Cl)c1ccc(Cl)cc1I
N#CCc1cc(C(F)(F)F)ccc1I
Cc1ccc(S(N)(=O)=O)cc1I
Cc1cc(Cl)ccc1I
Cc1ccc(C(C)(C)C)cc1I
CON=C(O)c1cc(C)ccc1I
Ic1c(-c2ccccc2)cccc1-c1ccccc1
O=C(O)c1c(Br)cccc1I
Cc1c(C)c(C)c(I)c(C)c1C
Clc1ccc(CBr)c(I)c1
CC(O)=Nc1ccc(Br)cc1I
CC(C)c1cc(Br)ccc1I
O=C(O)c1c(Cl)cccc1I
OCc1c(Br)cccc1I
CCc1ccc(C(C)(C)C(=O)O)cc1I
NCc1cc(Br)ccc1I
O=Cc1c(Cl)cccc1I
ClCc1cc(Br)ccc1I
Cc1c(I)cccc1C(F)(F)F
FC(F)(F)c1ccc(I)c(C(F)(F)F)c1
Clc1ccc(I)c(CBr)c1
COC(=O)c1cc(C)c(C)cc1I
COC(=O)CCN=C(O)c1cc(C)ccc1I
Cc1c(I)cccc1CC(=O)O
N#Cc1ccc(Br)cc1I
Cc1c(I)cc(Cl)cc1C(=O)O
CCOC(=O)c1cc(C)ccc1I
Cc1c(I)cc(Br)cc1C(=O)O
CC(=O)Oc1c(C)c(I)c(C)c(OC(C)=O)c1C
Cc1cc(C)c(I)cc1Br
Cc1ccc(C(O)=NN)cc1I
COC(=O)c1ccc(Cl)cc1I
Cc1ccc(CO)cc1I
CCc1cccc(CC)c1I
CC(C)(C)OC(O)=Nc1ccc(Br)cc1I
Cc1ccc(I)c(-c2ccccc2)c1
Cc1cc(Cl)cc(I)c1C(=O)O
Cc1cc(Cl)cc(C)c1I
COC(=O)c1cc(F)c(C)c(I)c1
Cc1ccc(C(=O)N2CCCC2)cc1I
Cc1ccc(C(=O)O)c(I)c1C

Cc1cc(C)c(I)c(C)c1Br
O=C(O)Cc1cc(Br)ccc1I
ClCc1ccc(CCl)c(I)c1
O=Cc1ccc(Br)cc1I
O=C(O)c1cc(Br)ccc1I
Cc1cccc(I)c1CBr
FC(F)(F)c1cc(Cl)ccc1I
CCN=C(O)c1cc(C)ccc1I
CC1(C)N=C(O)N(c2ccc(I)c(C(F)(F)F)c2)C1=O
Cc1c(F)cc([N+](=O)[O-])cc1I
FC(F)(F)c1ccc(Cl)cc1I
Cc1ccc(I)c(C(F)(F)F)c1
Cc1cccc(I)c1C
COC(=O)CCCN=C(O)c1cc(Br)ccc1I
O=C(O)Cc1ccc(Br)cc1I
CCc1cc(Cl)ccc1I
FC(F)(F)c1ccc(C(F)(F)F)c(I)c1
Cc1ccc(C(=N)O)cc1I
Cc1cc(N)cc(C)c1I
Cc1c(Cl)cc(Cl)cc1I
Nc1c(I)cc(Br)cc1C(=O)O
BrCc1c(Br)cccc1I
N=C(O)c1c(Cl)cccc1I
O=C(Cl)c1c(Cl)cccc1I
O=C(O)Cc1ccc(Cl)cc1I
CCOC(=O)c1ccc(Cl)cc1I
OCc1cc(Br)ccc1I
Clc1cccc(I)c1CBr
Cc1cc(Br)cc(I)c1C(=O)O
OCc1ccc(Cl)cc1I
COc1c(C)ccc(I)c1C
Cc1cc(Br)cc(C(=O)O)c1I
COc1c(Br)cccc1I
Cc1ccc(CO)c(I)c1
Cc1cc(C)c(I)c(C(=O)O)c1
Cc1cc(C#N)ccc1I
Cc1cc(Br)ccc1I
Cc1ccc(C(=O)N(C)C)cc1I
Cc1ccc(I)c(C(=O)O)c1
Clc1ccc(C2CC2)c(I)c1
Cc1cccc(C(=O)OC(C)(C)C)c1I
CCc1cc(Br)cc(C)c1I
O=C(O)c1cc(C(F)(F)F)ccc1I
Cc1c(I)cc(Br)cc1[N+](=O)[O-]
Cc1ccc(C#N)cc1I
O=C(O)Cc1cc(C(F)(F)F)ccc1I
Cc1c(Br)cccc1I
Cc1cc(C)c(I)c(C)c1
CCc1cccc(C)c1I
CCOC(=O)c1cc(Br)c(C)c(I)c1
COC(=O)c1ccc(Br)cc1I
COC(=O)c1c(Br)cccc1I
Cc1c(I)cc(Cl)cc1[N+](=O)[O-]
O=C(O)c1ccc(Cl)cc1I
Cc1cc(I)c(CO)cc1C
Brc1ccc(I)c(-c2ccccc2)c1
CCOC(=O)c1c(Cl)cccc1I
CC(C)c1ccc(I)c(C(C)C)c1
CCc1cc(Br)cc(CC)c1I
CC(C)c1ccc(Cl)cc1I
Cc1cccc(C(=O)N(C)C)c1I
COc1c(Cl)cccc1I
Cc1ccc(Cl)cc1I
CN=C(O)c1cccc(C)c1I
Cc1cc(-c2ccc(I)c(C)c2)ccc1I

Cluster M

Cc1nc(-c2ccc(CCN=C(O)c3ccccc3I)cc2)cs1
Ic1cccc2ccc3ccccc3c12
Cc1ccc(C(O)=Nc2sc3c(c2C(N)=O)CCCC3)cc1I
O=C(Cl)c1ccccc1I
O=C(O)c1cccc2cccc(I)c12
Ic1cccc2cc3cccc(I)c3cc12
CCOC(=O)c1ccccc1C(=O)c1ccccc1I
N#Cc1ccccc1I
Cc1cccc(I)c1C=O
CC(=O)Cc1ccccc1I
O=C(c1ccc(F)cc1)c1ccccc1I
COC(=O)c1cccc(I)c1CBr
Cc1c(I)cc([N+](=O)[O-])cc1[N+](=O)[O-]
Nc1cc2c(cc1C(=O)c1ccccc1I)OCCO2
CON(C)C(=O)c1ccc([N+](=O)[O-])cc1I
O=C(O)c1ccc(CBr)c(I)c1
Ic1ccccc1/C=C\c1ccccc1I
OC(=NCc1ccc2c(c1)OCO2)c1ccccc1I
O=C(Oc1ccc(C2CCCCC2)cc1)c1ccccc1I
COc1cc2nc(-c3ccccc3I)oc(=O)c2cc1OC
Cc1ccc(C(=O)Nc2ccc(Nc3ccccc3)cc2)cc1I
O=C(Nc1ccc(F)cc1)c1ccccc1N=C(O)c1ccccc1I
CC(C)(C)c1ccc(C(=O)O)cc1I
O=C(COC(=O)c1ccccc1I)c1ccc(-c2ccccc2)cc1
COC(=O)c1cccc2cccc(I)c12
N#Cc1cc(C(F)(F)F)ccc1I
Ic1ccccc1-c1nn2c(-c3ccccn3)nnc2s1
COC(=O)c1ccccc1N=C(O)c1ccccc1I
N#Cc1ccc2ccccc2c1I
CC(C)(C)C(=O)COC(=O)c1ccccc1I
CC(C)(C)OC(O)=Nc1ccc([N+](=O)[O-])cc1I
CC(=O)c1ccc(I)c(C)c1
OC1=NC(c2ccccc2)=C(c2nc3ccccc3[nH]2)C(c2ccccc2I)N1
N#Cc1cc2ccccc2cc1I
O=C(c1ccccc1I)N1CCN(c2ncccn2)CC1
COC(=O)c1cc(I)c(C)c([N+](=O)[O-])c1
O=C(O)c1cc2ccccc2cc1I
Cc1cccc(N=C(O)c2ccccc2I)n1
OC(=Nc1ccc(Cl)c(Cl)c1)c1ccccc1I
N=C(O)c1cccc(N=C(O)c2ccccc2I)c1
Ic1ccc2ccccc2c1
Cc1ccc(C(O)=NNC(=O)c2ccc(NC(=O)c3ccccc3)cc2)cc1I
Clc1ccc(-c2noc(-c3ccccc3I)n2)cc1
O=C(COC(=O)c1ccccc1I)c1ccccc1
Cc1cc(C)c(C=O)cc1I
Cc1ccc([N+](=O)[O-])cc1I
OC(=Nc1cccc(F)c1)c1ccccc1I
Cc1ccc(-c2csc(/C(C#N)=C/c3ccccc3I)n2)cc1
O=C(O)c1ccc(C(F)F)c(I)c1
O=C(c1ccccc1I)n1cccn1
COc1cc(N=C(O)c2ccccc2I)cc(OC)c1
Cc1cccc(C#N)c1I
O=S(=O)(Cl)Cc1ccccc1I
O=C(O)c1ccccc1I
OC(=N/N=C/c1cccc(Cl)c1Cl)c1ccccc1I
Cc1ccc(C(=O)c2ccccc2I)cc1
Nc1cccc2c(I)cccc12
N#Cc1c(N=C(O)c2ccccc2I)sc2c1CCCCC2
Cc1cc(I)c(C=O)cc1C
CCCCc1ccc(C(=O)c2ccccc2I)cc1
[N-]=[N+]=NCc1ccccc1I
CCOC(=O)c1ccc(C(F)(F)F)cc1I
COc1cccc2c(I)cccc12
O=C(CCc1ccccc1I)c1ccc2ccccc2c1
O=C(O)Cc1ccc([N+](=O)[O-])cc1I
O=C(Oc1cc(=O)oc2ccccc12)c1ccccc1I
Cc1ccc(I)c(C)c1[N+](=O)[O-]
CCc1ccc(C(=O)c2ccccc2I)cc1
CCOC(=O)c1sc(N=C(O)c2ccccc2I)c(C(=O)OC)c1C
Cc1ccc(C(O)=NN=C(O)C2CC2)cc1I
CCc1ccc(C(=O)OC)cc1I
O=c1oc(-c2ccccc2I)nc2cc(Cl)ccc12
Ic1ccc2ccc3ccccc3c2c1-c1ccccc1
Brc1ccc2cc(I)ccc2c1
O=[N+]([O-])c1ccc(N=C(O)C(F)(F)F)c(I)c1
O=C(c1ccccc1I)c1cn(CCCCCO)c2ccccc12
O=C(Nc1ccc(OCc2ccccc2)cc1)c1ccccc1I
CCN(CC)CCOC(=O)c1ccccc1I
Brc1cccc2cccc(I)c12
Cc1cc(C)cc(C(=O)c2ccccc2I)c1
Cc1c(I)cccc1[N+](=O)[O-]
[N-]=[N+]=Nc1cccc2c(I)cccc12
CC(=O)c1ccccc1I
COCCn1/c(=N/C(=O)c2ccccc2I)sc2ccccc21
COC(=O)c1ccc(C(C)C)c(I)c1
OC(=Nc1cccc(C(F)(F)F)c1)c1ccccc1I
COC(=O)c1ccc(C#N)c(I)c1
N#Cc1ccc([N+](=O)[O-])cc1I
O=C(c1ccccc1F)c1ccccc1I
Oc1nc2cc3c(cc2c(-c2ccccc2I)c1-c1ccccc1)OCCO3
CCCCCc1ccc(C(=O)c2ccccc2I)cc1
N#C/C=C/c1ccccc1I
Ic1ccccc1-c1nc2ccccc2[nH]1
N=C(S)c1ccccc1I
O=S(=O)(Cl)c1cccc2c(I)cccc12
CCCCCn1cc(C(=O)c2ccccc2I)c2ccccc21
CC(=O)c1ccc2ccccc2c1I
CCCc1ccc(C(=O)c2ccccc2I)cc1
N#Cc1cccc(C#N)c1I
CCOC(=O)c1cccc(N=C(O)c2ccccc2I)c1
Cc1ccc(N=C(O)c2ccccc2I)cc1F
CC(C)(C)c1ccc(C(=O)c2ccccc2I)cc1
CCOC(=O)c1ccc(C)c(I)c1
Cc1cccc(OC(=O)c2ccccc2I)c1
Cc1cc(C(=O)OC(C)(C)C)ccc1I
COC(=O)Cc1ccc(NC(=O)c2ccccc2I)cc1
Cc1cc(C)c(C(=O)O)cc1I
CON=C(O)c1ccc(C)c(I)c1
O=C(O)Cc1c(I)cccc1[N+](=O)[O-]
O=C(Nc1ccc(NC(=O)C2CC2)cc1)c1ccccc1I
O=Cc1ccccc1OCc1ccccc1I
Cc1ccc(C(O)=Nc2ccc(F)c(Cl)c2)cc1I
Cc1ccc(C(=O)OCc2ccccc2)cc1I
OC(=NN=C(O)c1ccccc1I)c1ccccc1I
O=Cc1ccc(C(F)(F)F)cc1I
O=C(c1ccccc1I)C(F)(F)F
O=[N+]([O-])c1ccc(NN=C(O)c2ccccc2I)cc1
Cc1ccc(I)c(C=O)c1
Cc1cc(C)cc(-c2c(I)ccc3ccc4ccccc4c23)c1
CC(=O)c1cccc(I)c1C
Cc1cc(C(=O)O)ccc1I
O=C(c1ccc(Br)cc1)c1ccccc1I
O=C(N/N=C/c1ccccc1I)c1ccncc1

Cc1cccc(C(=O)c2ccccc2I)c1
O=C(Nc1ccc(N2CCOCC2)cc1)c1ccccc1I
Ic1ccccc1-c1nc(-c2cccnc2)no1
O=C(COC(=O)c1ccccc1I)c1ccc([N+](=O)[O-])cc1
FC(F)(F)c1ccc(CBr)c(I)c1
OC(=Nc1cccc(Cl)c1)c1ccccc1I
O=C(O)CN1C(=O)/C(=C/c2ccccc2I)SC1=S
O=C(CBr)c1ccccc1I
OC(CSc1nc2ccccc2[nH]1)=N/N=C/c1ccccc1I
COc1cccc(CN=C(O)c2ccccc2I)c1
CN1CCN(C(=O)/C=C/c2ccccc2I)CC1
N#Cc1ccc(C(F)(F)F)cc1I
O=Cc1cccc(OCc2ccccc2I)c1
CC(C=O)c1ccccc1I
O=C(C=Cc1ccccc1I)c1ccccc1Cl
COC(=O)c1cccc(N=C(O)c2ccccc2I)c1
O=Cc1ccc([N+](=O)[O-])cc1I
Cc1csc2nc(-c3ccc(NC(=O)c4ccccc4I)cc3)cn12
O=C(Nc1ccc2oc(=O)ccc2c1)c1ccccc1I
Ic1ccccc1C=Nn1cnnc1
CC(C)c1ccc(C(=O)c2ccccc2I)cc1
CSc1ccccc1N=C(O)c1ccccc1I
C/C(=N\N=C(O)c1ccccc1I)c1ccc(N)cc1
CN(C)CCOC(=O)c1ccccc1I
Ic1ccc2ccc3cccc4ccc1c2c34
Ic1cccc2cccc(I)c12
Ic1cc2ccccc2c2ccccc12
Cc1ccc(C(O)=Nc2cccc([N+](=O)[O-])c2)cc1I
COc1ccc(C(=O)COC(=O)c2ccccc2I)cc1
Cc1cc(C)c([N+](=O)[O-])cc1I
COC(=O)c1ccc(CBr)c(I)c1
O=C(O)c1ccc(C(F)(F)F)cc1I
O=[N+]([O-])c1cccc(I)c1CBr
COc1ccccc1N=C(O)c1ccccc1I
O=Cc1ccc(C=O)c(I)c1
N#Cc1ccc(C(=O)O)c(I)c1
Ic1ccc2cc(I)ccc2c1
O/N=C/c1ccccc1I
Ic1ccccc1-c1nn2c(-c3ccncc3)nnc2s1
Cc1ccccc1C(=O)c1ccccc1I
COC(=O)c1ccc(C)cc1I
O=[N+]([O-])c1ccc(/C=N/N=C(O)c2ccccc2I)o1
CCn1c2ccccc2c2cc(N=C(O)c3ccccc3I)ccc21
Ic1cccc2c(I)cccc12
CC(=O)c1ccc(C(=O)O)c(I)c1
NS(=O)(=O)c1ccc(NC(=O)c2ccccc2I)cc1
N#Cc1ccc(NC(=O)c2ccccc2I)cc1
COC(=O)c1cccc(I)c1C(=O)OC
O=C(c1ccccc1I)n1cnc2ccccc21
O=C(c1cccc(F)c1)c1ccccc1I
N#CCCCC(=O)c1ccccc1I
OC(=Nc1ccc(F)c(Cl)c1)c1ccccc1I
Cc1ccc(C=O)cc1I
COC(=O)c1ccc(NC(=O)c2ccccc2I)cc1
Ic1ccc2c(ccc3ccccc32)c1
Cc1cccc(I)c1C#N
O=C1N=C(O)C(=Cc2ccccc2I)C(O)=N1
Fc1ccc2c(I)cccc2c1
Cc1ccc([N+](=O)[O-])c(C)c1I
CCN1C(=O)C(=Cc2ccccc2I)SC1=S
OCc1cccc2cccc(I)c12
O=C(O)c1ccc(C(F)(F)F)c(I)c1
O=C(c1ccccc1I)c1cc2c(cc1[N+](=O)[O-])OCCO2
CC(C)c1ccc(NC(=O)c2ccccc2I)cc1
CN(C(=O)c1ccccc1I)c1cccc2ccccc12
CCOC(=O)CC(=O)c1ccccc1I
N#CCC(=O)c1ccccc1I
OC(=Nc1cccc2cccnc12)c1ccccc1I
COC(=O)c1ccc(C(=O)OC)c(I)c1
Cc1cc(I)c(C)c([N+](=O)[O-])c1
Cc1ccc(C(=O)Nc2ccc(Cl)cc2)cc1I
N#CCc1c(I)cccc1[N+](=O)[O-]
N#Cc1cccc(C(F)(F)F)c1I
O=[N+]([O-])c1cccc(N=C(O)c2ccccc2I)c1
OC(=Nc1nccs1)c1ccccc1I
OC(=Nc1cccc(-c2nc3ccccc3s2)c1)c1ccccc1I
N#C/C(=C\c1ccccc1I)c1nc(-c2ccccc2)cs1
Cc1c(I)cc([N+](=O)[O-])cc1C(=O)O
Ic1cccc2ccccc12
Cc1ccc(C(=O)c2ccccc2I)cc1C
CCOC(=O)c1cc2ccccc2cc1I
COc1ccc(Cl)cc1N=C(O)c1ccccc1I
CCOC(=O)c1ccc(C#N)c(I)c1
O=C1OC(c2ccccc2I)=NC1=Cc1ccc(-n2cncn2)cc1
CCN(CC)S(=O)(=O)c1ccc(NC(=O)c2ccc(C)c(I)c2)cc1
O=C(O)c1ccc2cccc(I)c2c1
Ic1c2ccccc2cc2ccccc12
O=C(c1ccccc1)c1ccccc1I
O=C(ON1C(=O)c2ccccc2C1=O)c1ccccc1I
O=C(O)c1cc([N+](=O)[O-])cc2cccc(I)c12
COc1ccc(CC(=O)O)cc1SCc1ccccc1I
O=C(Cc1ccccc1)c1ccccc1I
OC1=Nc2c(cc(Br)c3ccccc23)C(c2ccccc2I)C1
CCON=C(O)c1ccc(C)c(I)c1
O=C(O)/C=C/c1ccccc1I
Ic1ccc2ccc(I)cc2c1
Cc1ccc(C(=O)Nc2ccc(S(=O)(=O)Nc3nccs3)cc2)cc1I
Oc1ccc(Cl)cc1/C=C/c1ccccc1I
O=C(c1ccccc1Cl)c1ccccc1I
CCOC(=O)c1c(-c2ccccc2)csc1N=C(O)c1ccccc1I
CC(=O)c1cc2c(cc1N=C(O)c1ccccc1I)OCCO2
O=[N+]([O-])c1ccc(CBr)c(I)c1
CCCc1ccc(C(=O)O)cc1I
CC(C)(C)OC(=O)N(C(=O)OC(C)(C)C)c1ccc([N+](=O)[O-])cc1I
Cc1ccc(C(=O)O)cc1I
COC(=O)CC(=O)c1ccccc1I
Oc1cccc2c(I)cccc12
COc1cccc(C=O)c1OCc1ccccc1I
OC(=Nc1ccccn1)c1ccccc1I
CCc1ccc(C(=O)O)cc1I
Cc1cc(C=O)c(C)cc1I
N#Cc1ccc(C(=O)O)cc1I
N=C(O)c1ccc([N+](=O)[O-])cc1I
Cc1c(I)ccc(N)c1C(=O)O
Oc1ccc2cccc(I)c2c1
O=C(OC(C(=O)c1ccccc1)c1ccccc1)c1ccccc1I
Cc1ccc(C(=O)Cl)cc1I
CN(C)C(=S)c1ccccc1I
O=C(c1ccc(Cl)cc1)c1ccccc1I
O=C(c1cccc(Cl)c1)c1ccccc1I
OC(=Nc1cccc2ccccc12)c1ccccc1I
Cc1cc(C=O)ccc1I
Oc1nnc(-c2ccccc2I)o1
Nc1cccc2cccc(I)c12
Cc1cc(C=O)cc(C)c1I
Cc1ccnc(N=C(O)c2ccccc2I)c1
N#Cc1ccc(CBr)c(I)c1
O=Cc1ccccc1I
N#Cc1c(N=C(O)c2ccccc2I)sc2c1CCCC2
CCOC(=O)c1ccc(NC(=O)c2ccccc2I)cc1
COC(=O)c1ccc([N+](=O)[O-])cc1I
Cc1c(I)cccc1C#N
O=C(O)c1cccc(I)c1C(=O)O
O=C(OCCN1CCOCC1)c1ccccc1I
Cc1ccc(C(=O)Nc2ccc([N+](=O)[O-])cc2C)cc1I
CC(=O)c1ccc(C)c(I)c1
COC(=O)c1ccc(C(C)=O)cc1I
COc1cccc(/C=N/N=C(O)c2ccccc2I)c1O
N=C(O)c1ccccc1N=C(O)c1ccccc1I
Cc1noc(-c2ccccc2I)n1
COC(=O)c1cc(I)c(C)cc1C
O=C1CCCC2=C1C(c1ccccc1I)c1c(ccc3ncccc13)N2
COC(=O)c1ccc(C(F)(F)F)cc1I
O=C(Nc1ccc(Cl)cc1)c1ccccc1I
Cc1c(I)cccc1C=O
CC(=O)c1ccc(NC(=O)c2ccccc2I)cc1
O=C(OCCN1CCCCC1)c1ccccc1I
COC(=O)c1ccc(C)c(I)c1
O=C(COC(=O)c1ccccc1I)c1ccc(Br)cc1
O=C(O)c1c(I)cccc1[N+](=O)[O-]
O=C(O)CCc1nnc(-c2ccccc2I)o1
Cc1ccc2ccccc2c1I
COc1cccc(N=C(O)c2ccccc2I)c1
Ic1ccc2c3ccccc3c3ccccc3c2c1
CC1(C)C(=O)OC(c2ccccc2I)C(C)(C)C1=O
O=[N+]([O-])c1ccc(CO)c(I)c1
O=C(OC1CCCCC1=O)c1ccccc1I
OC(=Nc1cccc(O)c1)c1ccccc1I
N=c1[nH]nc(-c2ccccc2I)s1
CC(C)(C)OC(=O)CC(=O)c1ccccc1I
OC(=Nc1cccc(-c2nnc(-c3ccco3)o2)c1)c1ccccc1I
O=C(O)c1ccc(C(=O)O)c(I)c1
O=C(c1ccccc1I)n1nnc2ccccc21
O=C(c1ccccc1I)c1cc2c(cc1N=C(O)Cc1ccccc1)OCCO2
BrCc1ccc(CBr)c(I)c1
O=C(c1ccccc1I)n1ccc2ccccc21
COC(=O)c1cc(C)c(I)c(C)c1
N#Cc1cccc(N=C(O)c2ccccc2I)c1
O=C(O)CN1C(=O)C(=Cc2ccccc2I)SC1=S
CCOC(=O)c1ccccc1N=C(O)c1ccccc1I
OC(=Nc1nc2ccccc2s1)c1ccccc1I
Cc1ccc(C(=O)Nc2ccc(S(=O)(=O)N3CCCC3)cc2)cc1I
Cc1ccc(S(=O)(=O)/N=C/c2ccccc2I)cc1
N#C/C(=C\c1ccccc1I)c1nc(-c2ccc(Br)cc2)cs1
CCOC(=O)C1C(O)=NC(SC)=C(C#N)C1c1ccccc1I
O=C(O)c1cccc(N=C(O)c2ccccc2I)c1
N#CC(C#N)=C1NC(N)=C(C#N)C(c2ccccc2I)=C1C#N
COC(=O)c1ccc(I)c(-c2ccccc2)c1
Cc1ccc(N=C(O)c2ccccc2I)c(C)c1
N#Cc1cccc(C(=O)O)c1I
Cc1ccc(N=C(O)c2ccccc2I)c([N+](=O)[O-])c1
Cc1cc(C(N)=O)cc(C)c1I
Cc1ccc(S(=O)(=O)Cl)cc1I
O=C(Nc1ccc(S(=O)(=O)Nc2nccs2)cc1)c1ccccc1I
O=C(O)c1ccc([N+](=O)[O-])cc1I
O=C(CCC1OCCCO1)c1ccccc1I
Ic1ccccc1-c1nn2c(-c3ccccc3)nnc2s1
Cc1c(N=C(O)c2ccccc2I)c(=O)n(-c2ccccc2)n1C
CCCCc1ccc(-c2csc(/C(C#N)=C/c3ccccc3I)n2)cc1
CCOC(=O)C1=C(C)NC2=C(C(=O)CC(C)(C)C2)C1c1ccccc1I
COC(=O)c1ccc(C(=O)O)cc1I
O=C(c1ccccc1I)c1cn(CCCCCF)c2ccccc12
Clc1ccc2cc(I)ccc2c1
Cc1cc(C(N)=O)ccc1I
CCOC(=O)C1=C(CCl)OC(N)=C(C#N)C1c1ccccc1I
Brc1cccc2c(I)cccc12

CC(C)c1ccc(C(=O)O)cc1I
CCn1c2ccccc2c2cc(/C=N/N=C(O)c3ccccc3I)ccc21
COC(=O)c1c(I)cccc1CBr

Cluster N

O=C(O)c1ccc(Cl)c(N=C(S)N=C(O)c2cc(I)ccc2Cl)c1
Clc1ccc(I)c(Cl)c1Cl
COC(=O)c1cc(Cl)c(I)cc1O
Clc1c(Br)ccc(I)c1Cl
Fc1cc(I)c(Cl)cc1Br
COc1cc(Cl)c(I)cc1N
Clc1c(Cl)c(Cl)c(I)c(Cl)c1Cl
Nc1cc(Br)c(I)c(Br)c1
O=[N+]([O-])c1ccc(I)c(Cl)c1
CCOC(=O)c1cc(Br)ccc1I
CS(=O)(=O)Nc1cc(C(F)(F)F)c(C#N)cc1I
COC(=O)c1ccc(I)c(Br)c1
N#Cc1cc(I)ccc1Cl
Brc1ccc(I)c2ccccc12
O=[N+]([O-])c1c(I)ccc(Br)c1Cl
Fc1c(Br)ccc(I)c1Cl
O=[N+]([O-])c1ccc(Cl)cc1I
O=C(c1cc(Cl)ccc1I)c1c(F)cccc1F
Clc1cc(Br)c(I)cc1Cl
O=[N+]([O-])c1ccc(I)c([N+](=O)[O-])c1
O=C(O)c1cc(I)c(Br)cc1F
N=C(O)c1cc(I)c(Br)c(F)c1N
CCNS(=O)(=O)c1ccccc1I
O=[N+]([O-])c1ccc(I)c(Br)c1
Cc1c(Br)ccc(I)c1Cl
FC(F)(F)c1cc(Cl)c(I)c(Br)c1
FC(F)(F)c1ccc(I)c(Br)c1
Fc1ccc(I)c(Br)c1
O=[N+]([O-])c1cc(CO)ccc1I
Oc1ccc(I)c(Cl)c1
CC(C)(C)c1ccc(I)c([N+](=O)[O-])c1
Brc1ccc(I)c(Br)c1Br
FC(F)(F)Oc1cc(Cl)c(I)c(Cl)c1
CC(C)c1ccc(I)c([N+](=O)[O-])c1
Fc1cc(Cl)c(I)c(C(F)(F)F)c1
Cc1cc(Cl)cc([N+](=O)[O-])c1I
Brc1ccc(I)c(Br)c1
O=[N+]([O-])c1cc(O)ccc1I
O=C(O)c1cc(I)c(C(=O)O)cc1I
Clc1cc(Cl)c(I)cc1Cl
COC(=O)c1ccc(I)c(Cl)c1
Nc1cc(Br)c(I)cc1Br
COC(=O)c1cc(I)c(C)cc1Br
Nc1ccc(Cl)c(I)c1
CC(=O)c1cc(Br)ccc1I
FC(F)(F)Oc1ccc(I)c(Br)c1
COC(=O)c1cc(I)c(Cl)cc1N
CCOC(=O)c1cc(I)ccc1Cl
N#Cc1cc(Br)ccc1I
Fc1cc(F)c(Br)c(I)c1Br
O=[N+]([O-])c1cccc(CBr)c1I
Nc1ccc(I)c(Br)c1
O=[N+]([O-])c1cc(Br)ccc1I
FC(F)(F)Oc1cccc(I)c1Cl
N#Cc1ccc(I)c([N+](=O)[O-])c1
COc1ccc(Cl)c(I)c1
O=S(=O)(Cl)c1ccc(Cl)cc1I
CCOC(=O)c1ccc(I)c(Br)c1
O=[N+]([O-])c1cc(Cl)cc(Cl)c1I
O=[N+]([O-])c1cc(Cl)ccc1I
Cc1ccc(I)c([N+](=O)[O-])c1
O=C(O)c1cc(Cl)cc(Cl)c1I
O=[N+]([O-])c1c(I)cccc1C(F)(F)F
O=C(c1ccc(F)cc1)c1cc(I)ccc1Cl
Cc1cc(Cl)c(I)c(Br)c1
COC(=O)c1cccc([N+](=O)[O-])c1I
O=C(O)c1cc(I)c(Cl)cc1F
Clc1cccc(Br)c1I
Oc1ccc(Cl)c(I)c1
O=C(c1ccc(O[C@H]2CCOC2)cc1)c1cc(I)ccc1Cl
CC(C)(C)c1cc(Br)c(I)c(Br)c1
O=[N+]([O-])c1ccc(Br)cc1I
COC(=O)c1cc(I)ccc1I
FC(F)(F)c1ccc(Cl)c(I)c1Cl
N#Cc1ccc(I)c(Cl)c1
CCOC(=O)c1ccc(I)c(Cl)c1
Cc1cc(I)c(Cl)cc1F
N#Cc1c(F)ccc(I)c1Cl
Clc1cccc(I)c1Br
OC(=Nc1ccccc1)c1cc(Br)ccc1I
Cc1ccc(-c2csc(N=C(O)c3cc(I)ccc3Cl)n2)cc1
O=Cc1cc(Cl)c(I)c(Cl)c1
COc1cc(Cl)c(I)cc1F
Fc1cc(Br)c(I)c(C(F)(F)F)c1
CS(=O)c1ccccc1I
Clc1ccc(I)c(Cl)c1
Cc1cc(Br)cc(Cl)c1I
CC(C)(C)OC(=O)c1cc(Cl)ccc1I
COc1cc(Br)c(I)c(Br)c1
Nc1ccc2oc(-c3cc(I)ccc3Cl)nc2c1
COC(=O)c1cc(I)c(N=C(C)O)cc1Cl
O=[N+]([O-])c1cccc(Br)c1I
O=C(Cl)c1cc(I)ccc1I
O=C(O)c1ccc(I)c(S(=O)(=O)Cl)c1
FC(F)(F)Oc1ccc(I)c(Cl)c1
Cc1cc(Cl)c(I)c(Cl)c1
Nc1cc(Cl)c(I)cc1F
O=C(O)c1cc(I)cc(Cl)c1Br
Clc1cccc(I)c1Cl
COC(=O)c1cc(I)c(Br)c(F)c1F
Clc1cc(Br)ccc1I
COc1cc(I)c(Cl)cc1C(=O)O
FC(F)(F)c1cc(Cl)c(I)c(Cl)c1
O=[N+]([O-])c1cc(Cl)c(I)c(Cl)c1
O=S(=O)(Cl)c1ccccc1I
Fc1cc(Br)c(I)cc1Cl
Fc1ccc(-c2ccc(Cc3cc(I)ccc3Cl)s2)cn1
COc1cc(Cl)c(I)cc1C(=O)O
CCOC(=O)c1cc(Cl)ccc1I
O=C(O)c1ccccc1N=C(S)N=C(O)c1cc(I)ccc1Cl
O=C(O)c1cc(I)ccc1Br
Cc1cc(Br)c(I)cc1Cl
O=[N+]([O-])c1cc(CBr)ccc1I
Oc1cccc(I)c1Br
Brc1ccc(Br)c(I)c1
CSc1cc(I)ccc1Br
OCc1cc(Cl)c(I)c(Cl)c1
O=Cc1cc(I)ccc1Cl
O=[N+]([O-])c1cccc(Cl)c1I
COC(=O)c1cc(I)c(Cl)cc1Cl
O=C(O)c1cc(Br)cc(C(=O)O)c1I
Oc1cc(Br)c(I)c(Br)c1
Nc1ccc(I)c(Cl)c1
COC(=O)c1cc(I)c(Cl)cc1F
COC(=O)c1cc(I)cc(Br)c1Cl
COC(=O)c1cc(I)ccc1Cl
O=C(O)c1cc(I)ccc1Cl
COc1ccc(I)c(Br)c1
Fc1cc(Cl)c(I)c(Cl)c1
O=C(O)c1ccc(I)c(S(=O)(=O)O)c1
Cc1cc(C)c(I)c([N+](=O)[O-])c1
O=S(=O)(Cl)c1cc(Cl)ccc1I
COc1cccc(I)c1Cl
Clc1cccc(Cl)c1I
Oc1cc(I)c(Br)cc1Cl
COc1ccc(I)c(S(=O)(=O)Cl)c1
COc1cccc(F)c1C(=O)c1cc(Cl)ccc1I
N#Cc1ccc(I)c(Br)c1
Cc1cc(Br)c(I)c([N+](=O)[O-])c1
N#Cc1cc(Cl)cc(Cl)c1I
Cc1cc(I)c(Cl)cc1Br
Fc1cc(Br)c(I)cc1F
Cc1ccc2nc(-c3cccc(N=C(O)c4cc(I)ccc4Cl)c3)oc2c1
O=C(O)c1cccc([N+](=O)[O-])c1I
O=C(Cl)c1cc(Br)ccc1I
Nc1ccc(I)c([N+](=O)[O-])c1
Cc1cc(I)cc(C(=O)O)c1Br
Cc1cc(I)c(Br)cc1Br
Cc1ccc([N+](=O)[O-])c(I)c1
COC(=O)c1cc(Cl)cc(Br)c1I
Clc1ccc(Br)cc1I
Fc1cc(I)c(Br)cc1Cl
Clc1cc(Cl)c(I)c(Cl)c1
COc1cc(Cl)c(I)c(Cl)c1
O=C(O)c1ccc(I)c([N+](=O)[O-])c1
CC(C)(C)OC(=O)c1cc(Br)ccc1I
COS(=O)(=O)c1ccccc1I
Oc1cccc(I)c1Cl
Clc1cc(Cl)c(I)c(Br)c1
Cc1cc(Cl)cc(Cl)c1I
O=C(O)c1cc(Cl)c(I)c(Cl)c1
Cc1cc(Br)c(I)c(Br)c1
Cc1cc(F)cc(Br)c1I
O=[N+]([O-])c1cc(I)ccc1Cl
O=[N+]([O-])c1cccc(CO)c1I
O=C(Cl)c1cc(I)ccc1Br
Fc1cc(Br)c(I)c(Br)c1
O=[N+]([O-])c1cc(C(F)(F)F)ccc1I
O=C(O)c1cc(Br)c(I)cc1F
Cc1c(F)ccc(I)c1Cl
Brc1cccc(Br)c1I
N#Cc1cc(Br)cc(Cl)c1I
COc1cc(Br)c(I)cc1OC
Fc1ccc(Cl)c(I)c1
COC(=O)c1cc(Br)ccc1I
Fc1ccc(Br)c(I)c1
O=[N+]([O-])c1cc(I)ccc1I
FC(F)(F)c1ccc(I)c(Cl)c1
Cc1cc(I)c([N+](=O)[O-])cc1C
O=[N+]([O-])c1ccccc1I
Clc1ccc(Cl)c(I)c1
COC(=O)c1cc(Br)cc([N+](=O)[O-])c1I
Cc1cccc(I)c1[N+](=O)[O-]
O=[N+]([O-])c1cc(Br)c(Cl)cc1I
COC(=O)c1cc(Cl)ccc1I
O=S(=O)(O)c1ccccc1I

Nc1ccc(I)c(Cl)c1Cl
Cc1cc(Br)cc([N+](=O)[O-])c1I
FC(F)(F)c1cc(I)ccc1I
Cc1cccc([N+](=O)[O-])c1I
COC(=O)c1cc(Br)c(I)cc1F
O=C=Nc1ccc(I)c(Cl)c1
Brc1cc(Br)c(I)c(Br)c1
O=Cc1cc(I)ccc1Br
O=C(Cl)c1cc(I)ccc1Cl
O=C(O)c1ccc(I)c(Br)c1
Clc1c(Br)cccc1I
CSc1ccc(Br)cc1I
O=Cc1ccc(I)c(Br)c1
COC(=O)c1cc(I)ccc1Br
Fc1cc(I)c(Br)c(F)c1Br
CCOC(=O)c1ccc(I)c([N+](=O)[O-])c1
CSc1ccc(I)c(C#N)c1
Sc1cc(Cl)ccc1I
Cc1cc([N+](=O)[O-])c(I)cc1Cl
Fc1cc(I)c(Br)c(F)c1F
CC(=O)c1cc(I)ccc1Br
NS(=O)(=O)c1ccccc1I
O=Cc1cc(I)c(Br)cc1F
O=Cc1cccc(Br)c1I
Clc1ccc(I)c(Br)c1Cl
N#Cc1cc(I)ccc1Br
O=[N+]([O-])c1cc(F)cc(Br)c1I
CCOc1ccc(C(=O)c2cc(I)ccc2Cl)cc1
O=C(O)c1cc(I)cc(Br)c1Cl
Fc1cccc(I)c1Cl
COc1cc(Cl)c(I)cc1NCC(=O)O
Cc1cc([N+](=O)[O-])c(C)c(Br)c1I
N=C(O)c1cccc([N+](=O)[O-])c1I
Clc1cc(Cl)c(Cl)c(I)c1
O=C(O)c1cc(I)ccc1I
Cc1c(N)ccc(I)c1Cl
CC(=O)c1ccc(I)c(Br)c1
COC(=O)c1ccc(I)c([N+](=O)[O-])c1
Nc1cc(Br)c(I)cc1C(=O)O
Clc1ccc(Br)c(I)c1
COc1cccc(I)c1Br
O=S(=O)(F)c1ccccc1I
Clc1ccc(I)c(Br)c1
Clc1ccc(Cl)c(I)c1Cl
Cc1ccc(Cl)c(I)c1Cl
COC(=O)c1cc(Br)cc(C(=O)OC)c1I
COC(=O)c1cc(Br)cc(C)c1I
C=CC(=O)N1CCN(C(=O)CNc2cc(I)c(Cl)cc2O)CC1
Cc1cc(Br)cc(Br)c1I
COc1cc(I)c(Cl)cc1Cl
Cc1ccc(I)c(Cl)c1Cl
Cc1c(Cl)ccc(I)c1Cl
COc1ccc(I)c([N+](=O)[O-])c1
Cc1cc(Br)c(I)cc1Br
O=Cc1c(F)ccc(I)c1Cl
O=[N+]([O-])c1c(Cl)cccc1I
Nc1cc(Cl)c(I)cc1C(=O)O
N#Cc1cccc([N+](=O)[O-])c1I
O=[N+]([O-])c1cccc([N+](=O)[O-])c1I
COc1ccc(Br)c(I)c1
O=C(O)c1cc([N+](=O)[O-])c(I)cc1Cl
COP(=S)(OC)Oc1cc(Cl)c(I)cc1Cl
CNS(=O)(=O)c1ccccc1I
Nc1ccc(I)c(Cl)c1F
O=C(O)c1cc(Cl)cc(I)c1Br
CC(C)(C)OC(=O)c1cc(I)ccc1Cl
O=Cc1cc(Cl)ccc1I
COc1cc(Cl)c(I)cc1[N+](=O)[O-]
CC(C)c1cc(Br)c(I)c(Br)c1
Nc1ccc(Cl)c(I)c1Cl
Nc1cc(Cl)c(I)c(Cl)c1
COc1ccc(Br)c(I)c1Br
COC(=O)c1cc(C)cc([N+](=O)[O-])c1I
N#Cc1cc(Cl)ccc1I
Cc1cc(Br)c(C(=O)O)cc1I
COc1cc(I)c(Cl)cc1Br
CN(C)c1ccc(I)c(Br)c1
Fc1c(Cl)ccc(I)c1Br
Nc1cccc(I)c1Br
Cc1ccc(S(=O)(=O)Cl)c(I)c1
O=[N+]([O-])c1cc(Br)c(I)c(Br)c1
Cc1cc(I)c(Br)cc1F
Brc1c(I)ccc(I)c1Br
Cc1ccc(S(N)(=O)=O)c(I)c1
N#Cc1cc(I)ccc1I
O=Cc1ccc(I)c(Cl)c1
Fc1cc(Cl)c(I)cc1Cl
Clc1cc(Br)cc(Cl)c1I
CC(C)Oc1ccc(I)c(Br)c1
COC(=O)c1cc(Cl)c(I)c(Cl)c1
CCOC(=O)CNc1cc(I)c(Cl)cc1OC
COc1ccc(I)c(S(=O)(=O)F)c1
Oc1ccc(I)c(Br)c1
Nc1cc(Cl)c(I)cc1N
CC(=O)c1cc(Cl)ccc1I
O=[N+]([O-])c1cc(F)ccc1I
O=Cc1ccc(I)c(Br)c1F
O=Cc1cc(Br)ccc1I
COC(=O)c1cc(I)c(C)cc1Cl
CSc1c(Cl)cccc1I
COC(=O)c1cc(Cl)c(I)cc1OC
O=[N+]([O-])c1ccc(-c2ccccc2)cc1I
O=[N+]([O-])c1cc2ccccc2cc1I
FC(F)(F)Oc1cccc(Br)c1I
O=C(O)c1cc(I)c(Cl)cc1Cl
Brc1cc(I)c(Br)cc1I
Clc1cc(Br)c(I)c(Br)c1
N=C(O)c1ccc(I)c([N+](=O)[O-])c1
COC(=O)c1cc(I)c(Cl)cc1OC
O=[N+]([O-])c1cc(OC(F)(F)F)ccc1I
Nc1ccc(Br)c(I)c1
COc1ccc(I)c(Cl)c1
CSc1cc(Br)ccc1I
O=C(O)c1cc(Cl)cc(Br)c1I
O=[N+]([O-])c1cc(I)ccc1Br
O=[N+]([O-])c1ccc(C(F)(F)F)cc1I
Fc1cccc(I)c1Br
Cc1cc(Br)c(I)c(Br)c1[N+](=O)[O-]
OCc1ccc(Cl)c(I)c1Cl
CCOC(=O)c1cc(I)ccc1Br
CC(O)=Nc1ccc(Cl)c(I)c1Cl
Nc1cc(I)c(Cl)cc1O
O=Cc1cccc([N+](=O)[O-])c1I
Fc1ccc(I)c(Cl)c1
Brc1cc(Br)c(I)cc1Br
O=[N+]([O-])c1c(Br)cccc1I
O=Cc1c(Cl)ccc(Cl)c1I
Nc1cc(Cl)c(I)cc1Cl
Oc1ccc(Br)c(I)c1
O=S(=O)(Cl)c1cc(I)ccc1Cl
Nc1cc(Cl)c(I)cc1[N+](=O)[O-]
Cc1cc(F)cc([N+](=O)[O-])c1I

Cluster O

OCc1ccccc1I
O=C(O)C(O)c1ccccc1I
CC(C)(C)c1ccccc1I
N#CC(O)c1ccccc1I
Cc1cccc(CN=C(O)c2ccccc2I)c1
OC(=NCc1cccs1)c1ccccc1I
CC1(C)OB(c2ccccc2I)OC1(C)C
CN=C(O)c1ccccc1I
CCc1ccc(NC(=O)c2ccccc2I)cc1
CCCCN(CCCC)C(=O)c1ccccc1I
O=C(c1ccccc1I)N1CCc2ccccc21
Cc1cccc(C)c1N=C(O)c1ccccc1I
OC(=NN1CCCCC1)c1ccccc1I
CCN(Cc1ccccc1)C(=O)c1ccccc1I
COc1ccc(CCN=C(O)c2ccccc2I)cc1OC
O=C(O)c1cccc(C(=O)O)c1I
COCCN=C(O)c1ccccc1I
C=CCN(CC=C)C(=O)c1ccccc1I
OC(=NC1CCCCC1)c1ccccc1I
Cc1cc(C)cc(N=C(O)c2ccccc2I)c1
OC(=NCCc1ccc(-n2cccn2)cc1)c1ccccc1I
O=C(O)CN=C(O)c1ccccc1I
COCCCN=C(O)c1ccccc1I
Ic1ccccc1-c1ccccc1
O=C(c1ccccc1I)N1CCCC1
OC(=Nc1cccc(Br)c1)c1ccccc1I
O=C(c1ccccc1I)N(Cc1ccccc1)Cc1ccccc1
BrC(c1ccccc1)c1ccccc1I
Cc1ccccc1CN=C(O)c1ccccc1I
Cc1cc(NC(=O)c2ccccc2I)on1
Cc1cccc(N=C(O)c2ccccc2I)c1
CC(C)(OSC(F)(F)F)c1ccccc1I
OC(=NC(c1ccccc1)c1ccccc1)c1ccccc1I
C=Cc1ccccc1I
CC(C)CN=C(O)c1ccccc1I
CCOC(=O)c1ccccc1I
OC(=NCCc1ccc(O)cc1)c1ccccc1I
CCCN=C(O)c1ccccc1I
CC(C)(C)OC(O)=N[C@@H](Cc1ccccc1I)C(=O)O
CSc1ccccc1I
N#CCN=C(O)c1ccccc1I
CCC(C)c1ccccc1N=C(O)c1ccccc1I
CCCCN=C(O)c1ccccc1I
CCCCCCCN=C(O)c1ccccc1I
Nc1ccccc1N=C(O)c1ccccc1I
COC(=O)C(N)c1ccccc1I
O=C(Nc1ccc(F)cc1)c1ccccc1I
Cc1ccc(NC(=O)c2ccccc2I)cc1
ClCc1ccccc1I
OC(=Nc1ccccc1F)c1ccccc1I
O=C(c1ccccc1I)N1CCNCC1
NC(Cc1ccccc1I)C(=O)O
CC(C)(C)OC(O)=NCc1ccccc1I
CN(C)CC(Cl)c1ccccc1I
OC(=NOCc1ccccc1)c1ccccc1I
Cc1cc(C)c(N=C(O)c2ccccc2I)c(C)c1
O=C1N=C(O)CCC1N=C(O)c1ccccc1I
OC(=Nc1ccc(Cl)cc1Cl)c1ccccc1I
Ic1ccccc1Cn1cncn1
O=C(Nc1ccc(Oc2ccccc2)cc1)c1ccccc1I
OC(=Nc1ccccc1Cl)c1ccccc1I
N#CCc1ccccc1I

O=C(Nc1ccc(O)cc1)c1ccccc1I
O=C(O)C1(c2ccccc2I)CC1
OC(=NCc1ccc(Br)cc1)c1ccccc1I
CC(C)(O)c1ccccc1I
CCCCCCN=C(O)c1ccccc1I
Cc1cccc(C(O)=NN=C(O)c2ccccc2I)c1
OC(c1ccccc1I)C(F)(F)F
COC(=O)C(O)c1ccccc1I
C[C@@H](N=C(O)c1ccccc1I)c1ccccc1
O=C(O)CCc1ccccc1I
SCCc1ccccc1I
O=C(O)c1ccccc1N=C(O)c1ccccc1I
COCc1ccccc1I
COC(=O)Cc1ccccc1I
CC(C)(C)OC(=O)c1ccccc1I
N=C(O)Cc1ccccc1I
CN(C)CCN=C(O)c1ccccc1I
C[Si](C)(C)OC(C#N)c1ccccc1I
COc1ccc(CN=C(O)c2ccccc2I)c(OC)c1
COc1ccc(N2CCN(C(=O)c3ccccc3I)CC2)cc1
CC(C)N=C(O)c1ccccc1I
CCOC(=O)CN=C(O)c1ccccc1I
OC(c1ccccc1)c1ccccc1I
CC(C)(C)OC(=O)N1CCN(C(=O)c2ccccc2I)CC1
CCCc1ccccc1I
COc1ccc(N(C)C(=O)c2ccccc2I)cc1
CCOC(=O)Cc1ccccc1I
C=CCN=C(O)c1ccccc1I
CCN(CC)CCN=C(O)c1ccccc1I
O=C(c1ccccc1I)N1CCCc2ccccc21
CCN(CC)C(=O)c1ccccc1I
N[C@H](Cc1ccccc1I)C(=O)O
CC(C)CCN=C(O)c1ccccc1I
O=C(O)c1cccc(C(F)(F)F)c1I
OC(=NCc1ccccc1)c1ccccc1I
OCCN=C(O)c1ccccc1I
CN1CCN(C(=O)c2ccccc2I)CC1
NCc1cccc(C(F)(F)F)c1I
CC(C)(C)N=C(O)c1ccccc1I
FC(F)(F)c1ccccc1I
OC(=NCc1ccc(C(F)(F)F)cc1)c1ccccc1I
CN(C(=O)c1ccccc1I)c1ccccc1
BrCc1ccccc1I
C=C(C(=O)OCC)c1ccccc1I
CCN=C(O)c1ccccc1I
O=C(c1ccccc1I)N1CCOCC1
OC(=Nc1ccccc1)c1ccccc1I
Cc1cc(=NC(=O)c2ccccc2I)[nH]o1
CCCCCN=C(O)c1ccccc1I
CCOc1ccc(NC(=O)c2ccccc2I)cc1
CC(O)=Nc1ccccc1N=C(O)c1ccccc1I
OC(=NCc1ccccc1Cl)c1ccccc1I
OC(=NCc1ccc(Cl)cc1)c1ccccc1I
CCc1ccccc1I
N[C@@H](Cc1ccccc1I)C(=O)O
CN(C)C(=O)COC(=O)c1ccccc1I
OB(O)c1ccccc1I
CC(C)c1ccccc1I
OC(=NCc1ccc(F)cc1)c1ccccc1I
O=P(c1ccccc1)(c1ccccc1)c1ccccc1I
O=C(O)Cc1ccccc1I
OC(=NCc1ccco1)c1ccccc1I
OC(=NC12CC3CC(CC(C3)C1)C2)c1ccccc1I
O=C([O-])CN=C(O)c1ccccc1I
O=C(Cl)Cc1ccccc1I
OC(=NCc1cc(F)cc(F)c1)c1ccccc1I
O=C(O)c1cccc(-c2ccccc2I)c1
OC(=Nc1cc(Cl)cc(Cl)c1)c1ccccc1I
Cc1ccc(N=C(O)c2ccccc2I)c(O)c1
Cc1ccc(N(C)C(=O)c2ccccc2I)cc1
CCN(C(=O)c1ccccc1I)c1ccccc1
CN(Cc1ccccc1)C(=O)c1ccccc1I
CN(C)C(=O)c1ccccc1I
OC(=NCC1CCCCC1)c1ccccc1I
Cc1ccc(CN=C(O)c2ccccc2I)cc1
O=C(N=c1cc[nH]cc1)c1ccccc1I
COC(OC)c1ccccc1I
C=C(C)c1ccccc1I
Cc1ccc(NC(=O)c2ccccc2I)cc1C
CP(C)(=O)c1ccccc1I
COC(=O)C1CCCCN1C(=O)c1ccccc1I
OC(=NCc1cccc(C(F)(F)F)c1)c1ccccc1I
COC(=O)C(N)Cc1ccccc1I
OC(=NC1CCCC1)c1ccccc1I
O=C(Nc1ccc(N2CCCC2)cc1)c1ccccc1I
Nc1ccc(NC(=O)c2ccccc2I)cc1
NS(=O)(=O)Cc1ccccc1I
COC(=O)c1ccccc1I
Cc1ccccc1I
OC(=NCC12CC3CC(CC(C3)C1)C2)c1ccccc1I
Ic1ccccc1-c1ccccc1I
OC(=NCCc1ccccc1)c1ccccc1I
OC(=NC1CC1)c1ccccc1I
O=C(c1ccccc1I)N1CCC(Cc2ccccc2)CC1
CN(Cc1ccccc1I)C(=O)OC(C)(C)C
O=C(c1ccccc1I)N1CCCCCC1
Brc1ccccc1-c1ccccc1I
CC(C)N(C(=O)c1ccccc1I)C(C)C
OCCc1ccccc1I
Ic1ccccc1C1CCOCC1
N=C(O)c1ccccc1I
COc1ccc(CN=C(O)c2ccccc2I)cc1
FC(F)c1ccccc1I
NCc1ccccc1I
N#CC(N)c1ccccc1I
O=C(Cc1ccccc1I)N=c1cc[nH]cc1
OC(CNCc1ccccc1I)c1ccccc1
Cc1ccccc1N=C(O)c1ccccc1I
COC(=O)C(CC(C)C)N=C(O)c1ccccc1I
C=C(C(=O)OC)c1ccccc1I
C#CCN=C(O)c1ccccc1I
COC(=O)C(CCSC)N=C(O)c1ccccc1I
OC(=NCc1ccccn1)c1ccccc1I
NN=C(O)c1ccccc1I
OC(=NCC1CC1)c1ccccc1I

Cluster P

Cc1ccc(I)c(F)c1
COc1cc(C(C)C)c(O)cc1I
COC(=O)c1cc(C)c(O)c(I)c1
Fc1c(I)ccc(C2OCCO2)c1F
Cc1cc(F)c(I)cc1[N+](=O)[O-]
O=[N+]([O-])c1cccc(O)c1I
Nc1c(I)cc(F)cc1[N+](=O)[O-]
Nc1ccc([N+](=O)[O-])cc1I
COc1ccc(S(=O)(=O)NCc2ccc3c(c2)OCO3)cc1I
COC(=O)c1cc(Br)cc(I)c1O
COC(=O)c1cc(Br)cc(I)c1N
CCN1C(=O)C(=Cc2ccc(O)c(I)c2)C(=O)N(CC)C1=S
OCc1cccc(F)c1I
O=Cc1cc(Br)cc(I)c1O
COc1cc(/C=N/NC(=O)c2cc3c(ccc4ccccc43)o2)cc(I)c1O
Oc1ccc(Cl)cc1I
CCOC(=O)c1ccc(N)c(I)c1
Fc1c(Cl)ccc(Cl)c1I
Nc1ccc(C(=O)O)cc1I
CCCCN=C(O)c1ccc(OC)c(I)c1
O=Cc1c(Br)ccc(I)c1F
COc1ccc(NCCO)cc1I
COc1cc([N+](=O)[O-])ccc1I
Cc1cc(N)c(I)cc1Cl
COc1cc(C=O)cc(I)c1OCc1ccc([N+](=O)[O-])cc1
Nc1cc(Br)cc(I)c1O
COc1cc(C(C)C)ccc1I
CCOc1cc(C)ccc1I
O=C(O)c1cc(Br)cc(I)c1F
O=Cc1ccc(F)c(F)c1I
N#Cc1ccc(O)c(I)c1
Fc1c(Cl)ccc(Br)c1I
Oc1c(I)cc(Br)cc1C(F)(F)F
CC(=O)c1ccc(I)c(O)c1
COc1cc(C=O)cc(I)c1OC(C)=O
COc1cc(C=O)cc(I)c1OC
CSc1ccc(N)c(I)c1
Fc1ccc(CBr)cc1I
COC(=O)c1cc(Br)cc(I)c1OC
O=C(O)c1ccc(I)c(O)c1
COc1c(I)cc([N+](=O)[O-])c2ccccc12
Fc1ccc(Cl)cc1I
CC(C)(C)OC(O)=Nc1cccc(F)c1I
Oc1c(Br)cc(F)cc1I
Cc1cc(O)c(I)cc1[N+](=O)[O-]
Oc1ccc2ccccc2c1I
COC(=O)c1cc(OC)c(I)cc1[N+](=O)[O-]
CC(C)(C)OC(O)=NCc1ccc(N)c(I)c1
NCc1ccc(I)c(F)c1Cl
COc1ccc(C(=O)Nc2ccc(S(N)(=O)=O)cc2)cc1I
COc1ccc(S(=O)(=O)NC(C)(C)C)cc1I
COc1c(I)cc(C(F)(F)F)cc1C(F)(F)F
Cc1cc(Br)cc(I)c1F
Nc1c(I)cc(Br)cc1[N+](=O)[O-]
Oc1cccc(I)c1O
O=Cc1ccc(I)c(F)c1F
Cc1cccc(O)c1I
COc1ccc(-c2ccccc2)cc1I
Fc1cc(C(F)(F)F)ccc1I
CC(=O)c1ccc(F)c(I)c1
O=Cc1c(Cl)ccc(I)c1F
CCOc1cc(C=O)cc(I)c1OC
O=Cc1cccc(I)c1F
CNc1ccc(C#N)cc1I
Fc1cccc(OC(F)F)c1I
CNc1ccc(C=O)cc1I
Oc1c(F)cccc1I
Nc1ccc(C(F)(F)F)cc1I
OCc1ccc(I)c(F)c1
O=Cc1cc([N+](=O)[O-])cc(I)c1O
N#Cc1cc(F)c(N)c(I)c1
Nc1ccc(Cl)cc1I
COC(=O)c1cc(I)c(F)cc1Cl
Cc1cccc(I)c1N

O=C(O)c1cc(I)c(F)cc1Cl
Oc1ccc(F)c(I)c1
O=C(O)Cc1ccc(O)c(I)c1
COc1ccc(/C=C2\SC(=S)N=C2O)cc1I
COC(=O)[C@H](Cc1ccc(OC)c(I)c1)N=C(O)OC(C)(C)C
COc1ccc(C(O)=Nc2ccccc2)cc1I
CCCc1ccc(N)c(I)c1
N#Cc1cc(I)c(N)c(C(F)(F)F)c1
COc1cc(C(=N)O)ccc1I
COc1cc(C=C2C(=O)OC(C)(c3ccccc3)OC2=O)cc(I)c1O
COc1cc(C=O)cc(I)c1OC(C)C
O=[N+]([O-])c1cc(I)c(Oc2ccccc2)c([N+](=O)[O-])c1
COc1ccc(S(=O)(=O)Nc2ccc(F)c(F)c2)cc1I
COc1cc(C(F)(F)F)c(Br)cc1I
Oc1cccc(Cl)c1I
CCCCOc1c(I)cc(C=O)cc1OC
N#CCc1ccc(N)c(I)c1
Nc1c(I)cccc1[N+](=O)[O-]
CCOc1ccc(C=O)cc1I
COCOc1cc(C)ccc1I
Oc1c(Cl)cccc1I
COc1cc(C(C)C)c(Oc2cnc(NC(CO)CO)[nH]c2=N)cc1I
O=Cc1cc(Cl)cc(I)c1O
C=C(C)COc1c(I)cc(C=O)cc1OC
O=C(c1ccc(I)c(F)c1)N1CCOCC1
O=Cc1cccc(I)c1O
Cc1cc(F)c(I)cc1C
O=C(O)c1cc(Cl)c(F)c(I)c1
Nc1cc(C(=O)O)ccc1I
O=[N+]([O-])c1cccc(F)c1I
COc1cc(C=O)c(OC)cc1I
CCCCOc1ccc(/C=C/C(=O)O)cc1I
Fc1ccc(Br)cc1I
Fc1cc(Cl)cc(Br)c1I
Cc1ccc(N)c(I)c1
CC(C)(C)c1ccc(O)c(I)c1
N#Cc1ccc(I)c(N)c1
OCc1ccc(F)c(F)c1I
Cc1noc(C)c1-c1cc(N)c(N)c(I)c1
Fc1cc(F)c(I)c(Cl)c1
N#Cc1cc(I)c(N)cc1C(F)(F)F
O=[N+]([O-])c1cccc(I)c1F
COc1cc(C(F)(F)F)ccc1I
COc1ccc2ccccc2c1I
Oc1c(I)cccc1C(F)(F)F
COc1ccc(C=O)c(I)c1OC
COC(=O)[C@@H](C)[C@H](c1ccc(I)c(O)c1)C1CC1
COC(=O)c1ccc(Oc2ccccc2)c(I)c1
Nc1cccc(Cl)c1I
COC(=O)c1ccc(N=C(O)C(F)(F)F)c(I)c1
CCOc1cc(C=O)cc(I)c1OCc1ccc([N+](=O)[O-])cc1
O=C(O)CCc1ccc(O)c(I)c1
COCOc1c(I)cccc1OC
CCOc1c(F)cccc1I
Nc1cc(C(F)(F)F)c(Cl)cc1I
CCOc1cc(C(C)(C)C)ccc1I
CC(=O)c1cc(Br)cc(I)c1N
N#Cc1cccc(I)c1N
O=Cc1cc(OC(F)(F)F)cc(I)c1O
COC(=O)c1ccc(I)c(N)c1
COC(=O)c1ccc(OC(F)F)c(I)c1
O=Cc1cc(C(=O)O)cc(I)c1O
COC(=O)c1cccc(I)c1N
COc1cc(I)c(OC)cc1C
CCOc1cc(C=O)cc(I)c1OCc1ccc(C)cc1
COc1ccc(C=O)cc1I
Cc1c(Br)ccc(N)c1I
Nc1ccc(-c2ccccc2)cc1I
CC(=O)c1ccc(N)c(I)c1
COC(=O)c1cc(Cl)cc(I)c1N
O=Cc1cc(OCc2ccccc2)c(I)c([N+](=O)[O-])c1
C=CCOc1c(I)cc(C=O)cc1OC
COc1ccc(/C=C(\C#N)c2nc3ccccc3[nH]2)cc1I
CC(=O)Oc1ccc(C(=O)O)cc1I
Fc1c(Cl)ccc(C(F)F)c1I
COC(=O)c1cc(Br)c(N)c(I)c1
COc1ccc(C=O)c(I)c1O
COc1c(C=O)ccc(I)c1F
CCOc1cc(C#N)cc(I)c1O
COc1ccc(C(=O)n2cnc3ccccc32)cc1I
Cc1cc(N)c(I)cc1F
CCOc1cc(C=O)cc(I)c1O
COc1ccc([N+](=O)[O-])cc1I
Fc1c(I)cc(Br)c2ccccc12
Nc1c(I)cc(C(F)(F)F)cc1[N+](=O)[O-]
O=C(O)c1ccc(I)c(F)c1
COc1cc(C(F)(F)F)c(F)cc1I
COc1cc(C=C2C(=O)c3ccccc3C2=O)cc(I)c1O
Cc1ccc(C#N)c(F)c1I
Fc1cc(F)c(F)c(I)c1
COc1ccc(F)cc1I
COc1cc(/C=N/O)cc(I)c1O
Fc1cc(CBr)ccc1I
Cc1ccc(F)c(I)c1
COc1cc(CNc2ccc(C)c(Cl)c2)cc(I)c1OC
N=C(S)N/N=C/c1ccc(O)c(I)c1
N#Cc1cc(F)c(O)c(I)c1
OCc1ccc(F)c(I)c1
Cc1cc(I)c(O)c([N+](=O)[O-])c1
COc1cc(C#N)cc(I)c1O
COc1cccc(I)c1N
CCOc1cc(C=O)cc(I)c1OCC
COc1cc(C#N)cc(I)c1OCC#N
Nc1c(Br)cc(Cl)cc1I
OCc1ccc(I)c(O)c1
Oc1ccc(Br)cc1I
OCc1cccc(I)c1F
COc1cc(C(C)C)c(Oc2c[nH]c(=N)[nH]c2=N)cc1I
Nc1c(I)cc([N+](=O)[O-])cc1C(F)(F)F
COc1cc(CO)ccc1I
COC(=O)c1ccc(N=C(C)O)c(I)c1
COc1ccc(C(F)(F)F)cc1I
COc1cccc(I)c1F
CC(C)c1ccc(N)c(I)c1
COc1cccc(CO)c1I
Nc1ccc(Br)cc1I
COc1cc(/C=C2/SC(=O)N=C2O)cc(I)c1O
Cc1cc(OC(=O)c2ccc(Br)o2)c(I)c(C)c1Cl
COC(=O)c1cc(C#N)cc(I)c1O
Cc1cc(C(=O)O)cc(I)c1O
Nc1c(I)cc(C(=O)O)cc1[N+](=O)[O-]
N#Cc1ccc(I)c(F)c1Cl
COc1ccc(/C=C/[N+](=O)[O-])cc1I
CCOc1c(I)cc(C=O)cc1OC
COc1cccc(C)c1I
Nc1cccc(I)c1N
Fc1ccc(C(F)(F)F)cc1I
COc1c(I)cc(Br)cc1C=O
COc1cccc(Cl)c1I
Nc1c(F)cc(Br)cc1I
Ic1c(OCc2ccccc2)cccc1OCc1ccccc1
Nc1cc(Cl)cc(Br)c1I
COc1ccc(OC)c(I)c1
COC(=O)c1cc(N)c(I)cc1OC
Oc1c(Cl)cc(Cl)cc1I
Nc1c(Cl)cccc1I
Fc1ccccc1I
Nc1ccc(Br)c(Cl)c1I
COc1cc(CC#N)cc(I)c1OC
O=[N+]([O-])c1ccc(I)c(O)c1
CCCCCCCCOc1ccc2cc(C(=O)O)ccc2c1I
COc1cc(Cl)cc(Cl)c1I
COc1cc(C=O)cc(I)c1OCc1ccccc1
COC(=O)c1cc(N)c(I)cc1C
COc1cc(C(=O)O)cc(I)c1O
O=[N+]([O-])c1ccc(O)c(I)c1
COc1cc(C=O)ccc1I
COC(=O)Cc1ccc(O)c(I)c1
Cc1cc(Cl)cc(I)c1O
COc1cc(C(=N)O)cc(I)c1OCc1ccccc1
CCOC(=O)COc1c(I)cc(C=O)cc1OC
CC(C)Oc1ccc(C(=O)O)cc1I
Oc1cc(C(F)(F)F)c(Br)cc1I
COc1ccc(N)cc1I
Nc1c(Cl)cc(Br)cc1I
Cc1cc(I)c(N)c([N+](=O)[O-])c1
CC(=O)c1cccc(I)c1F
CC(C)(C)OC(O)=Nc1ccc(Cl)c(F)c1I
N#Cc1cc(Br)cc(I)c1F
COc1cc2ccccc2cc1I
Nc1c(I)cc(Cl)cc1C(=O)O
CCOc1c(I)cc(Br)cc1C=O
COc1cccc([N+](=O)[O-])c1I
COC(=O)c1ccc(N2CCCCC2)c(I)c1
Nc1c(F)cc(C(F)(F)F)cc1I
Fc1c(Cl)cccc1I
Fc1cc(Br)c(F)c(Br)c1I
O=[N+]([O-])c1ccc(I)c(F)c1
Fc1c(Cl)cc(Br)cc1I
COc1cc(C(=N)O)cc(I)c1OC
N=C(O)c1ccc(I)c(O)c1
Nc1c(F)cc(Cl)cc1I
Nc1cc(C(F)(F)F)c(Br)cc1I
Nc1cc(CO)ccc1I
Oc1c(F)cc(Br)cc1I
Cc1cccc(N)c1I
O=C(O)c1cccc(F)c1I
COc1ccc(C(=O)Oc2ccccc2C(C)=O)cc1I
Cc1cc(F)c(I)cc1C(=O)O
COC(=O)CCc1ccc(O)c(I)c1
OC(c1ccc(I)c(F)c1)(C(F)(F)F)C(F)(F)F
Oc1c(F)cc(F)cc1I
Fc1cc(Br)cc(Cl)c1I
O=P(c1ccccc1)(c1ccccc1)c1ccc(I)c(F)c1
COc1cc([C@@H](O)C(C)(C)C)c([N+](=O)[O-])cc1I
COc1ccc(C(=O)O)cc1I
C#CCOc1c(I)cc(C=O)cc1OC
O=C(O)c1cc(Br)cc(I)c1O
N#Cc1ccc(N)c(I)c1
Fc1cccc(Br)c1I
CCOC(=O)c1ccc(I)c(OCC)c1
Nc1ccccc1I
O=C(O)c1ccc(I)c(OC(F)(F)F)c1
COc1cccc(C2=NC(C)(C)CO2)c1I
Nc1c(I)cc(F)cc1C(=O)O
Oc1cc(C(F)(F)F)ccc1I
COc1cc(C(C)C)c(OS(=O)(=O)c2ccc(C)cc2)cc1I
CCCOc1c(I)cc(C=O)cc1OC

Fc1cc(C2CC2)ccc1I
COc1c(F)cc(Br)cc1I
COc1cc(CO)cc(I)c1O
COc1ccc(N)c(I)c1
COC(=O)c1ccc(F)c(I)c1
COc1c(I)cc(-n2ccc(O)nc2=O)cc1C(C)(C)C
Nc1cc(F)c(I)c(Br)c1
Cc1cc(Br)cc(I)c1N
Oc1cc(Cl)cc(Cl)c1I
O=Cc1ccc(F)c(I)c1
O=C(O)c1ccc(F)c(F)c1I
COc1ccc(C(=O)Nc2ccc(S(=O)(=O)N3CCCC3)cc2)cc1I
Nc1c(F)cccc1I
O=[N+]([O-])c1cc(I)c(F)cc1Br
COc1cc(CO)cc(I)c1OCc1cccc(C(=O)O)c1
Cc1cc(Cl)cc(I)c1N
Nc1ccc(O)cc1I
COc1cccc(I)c1O
COC(=O)c1ccc(I)c(O)c1
Nc1c(Cl)cc(C(=O)O)cc1I
COC(=O)c1cc(C(F)(F)F)cc(I)c1N
Nc1cc(C(F)(F)F)ccc1I
N#Cc1cccc(F)c1I
O=C(O)c1c(Br)ccc(I)c1F
COC(=O)c1ccc(I)c(F)c1
Fc1c(Br)ccc(Cl)c1I
COc1c(I)ccc2ccccc12
CCOc1c(I)cc(C(=N)O)cc1OCc1ccccc1
COc1cc(/C=N/NC(=O)c2ccncc2)cc(I)c1O
Nc1c(I)cccc1C(=O)O
Oc1ccc(F)cc1I
COC(=O)c1cc(C)c(N)c(I)c1
Oc1c(Cl)cc(Br)cc1I
COc1cc(C=O)cc(I)c1OCc1ccc(C)cc1
Nc1cccc([N+](=O)[O-])c1I
COc1cc(C=O)cc(I)c1OCCO
CC(O)=Nc1cc(F)c(I)cc1C
COc1ccc(O)cc1I
Nc1ccc2ccccc2c1I
Cc1ccc(I)c(F)c1C
O=C(O)c1ccc(O)c(I)c1
COc1cc(C(O)C(C)(C)C)c([N+](=O)[O-])cc1I
COc1ccc(C(O)=NNC(=O)c2ccc(NC(=O)C(C)C)cc2)cc1I
COc1c(F)cccc1I
Fc1c(Br)cccc1I
Cc1ccc(I)c(F)c1F
CCCCc1ccc(N)c(I)c1
N#Cc1ccc(I)c(F)c1
Nc1c(Cl)cc(Cl)cc1I
CCOC(=O)c1cc(I)c(N)c([N+](=O)[O-])c1
COc1cc(C(=O)O)cc(I)c1OC
O=C(O)c1cccc(I)c1F
Cc1cc(F)c(I)c(Br)c1
COC(=O)c1cc(N)c(I)cc1CS(C)(=O)=O
Nc1ccc(OC(F)(F)F)c(Cl)c1I
COc1ccc(O)c(I)c1
COC(=O)C(C)(C)c1ccc(N)c(I)c1
Nc1cccc(Br)c1I
Nc1ccc(CC(=O)O)cc1I
COc1cccc(C(F)(F)F)c1I
COc1cc(Cl)cc(Br)c1I
COC(=O)c1cc(F)cc(I)c1N
CCOc1c(I)cc(C(=N)O)cc1OC
CC(C)Nc1ccccc1I
COC(=O)c1cc(I)c(F)cc1C
COc1ccc(C(O)=Nc2cccc([N+](=O)[O-])c2)cc1I
COc1cc(/C=C/c2ccc3cccc(OC)c3n2)cc(I)c1OC
Cc1cc(Cl)c(N)c(I)c1
CCOC(=O)c1ccc(O)c(I)c1
CCOC(=O)C1=C(C)N=C(O)NC1c1cc(I)c(O)c(OC)c1
CCc1ccc(N)c(I)c1
Nc1c(Cl)cc(C(F)(F)F)cc1I
COC(=O)c1ccc(I)c(OCc2ccccc2)c1
CC(C)(C)OC(O)=N[C@H](Cc1ccc(O)c(I)c1)C(=O)O
COc1cc(C)c(Cl)cc1I
CCN1C(=O)/C(=C\c2ccc(OCc3ccc(C(=O)O)cc3)c(I)c2)N=C1O
N#Cc1cc(Br)cc(I)c1O
Nc1cccc(C(=O)O)c1I
CC(C)(C)c1ccc(I)c(N)c1
COCOc1c(F)cccc1I
CCOC(=O)Cc1ccc(N)c(I)c1
N#Cc1ccc(I)c(O)c1
N[C@@H](Cc1cc(Cl)c(O)c(I)c1)C(=O)O
Cc1cc(C)c(N)c(I)c1
OCc1ccc(O)c(I)c1
Nc1ccc(O)c(I)c1
Nc1c(I)cc(Cl)cc1[N+](=O)[O-]
Cc1cccc(F)c1I
Oc1c(Br)cccc1I
COC(=O)c1cc(I)c(N)cc1C
COc1cc(/C=C/C(=O)O)cc(I)c1O
O=C(O)c1cccc(I)c1O
COc1cc(C=C2C(O)=NC(=S)N=C2O)cc(I)c1O
COc1cc(/C=C(\C#N)C(=O)c2ccc(O)c(O)c2)cc(I)c1O
Oc1cc(Br)cc(I)c1F
CCN(CC)S(=O)(=O)c1ccc(NC(=O)c2ccc(OC)c(I)c2)cc1
Nc1cccc(I)c1F
Cc1cc(F)c(N)c(I)c1
COc1ccc(C)cc1I
COc1cc(C)ccc1I
CC1(C)OB(c2cccc(I)c2F)OC1(C)C
O=[N+]([O-])c1ccc(F)c(I)c1
Nc1cc(C(F)(F)F)c(F)cc1I
COc1c(I)cccc1C(=O)OC(C)(C)C
Cc1ccc(I)c(O)c1
CCN1C(=O)/C(=C/c2cc(I)c(O)c(OC)c2)S/C1=N/c1ccccc1
COc1c(F)cc(F)cc1I
COc1cccc(I)c1OC
COC(=O)Cc1ccc(N)c(I)c1
Nc1cc(C(F)(F)F)cc(Br)c1I
COC(=O)c1ccc(I)c(N=C(C)O)c1
COc1cc(C(=O)O)ccc1I
COc1cc(C(C)=O)cc(I)c1O
O=Cc1ccc(OC(F)(F)F)c(I)c1
OC(=Nc1cccc(F)c1I)C(F)(F)F
COc1cc(C=C2C(=O)OC(c3ccccc3)OC2=O)cc(I)c1O
Cc1cc(C)c(I)c(N)c1
N#Cc1c(Br)ccc(I)c1F
COc1cc(C=O)cc(I)c1O
COC(=O)c1cc(I)c(N)c([N+](=O)[O-])c1
COC(=O)c1cc(F)c(N)c(I)c1
COc1cc(C2C(C#N)=C(N)OC3=C2C(=O)CC(C)(C)C3)cc(I)c1O
O=[N+]([O-])c1cccc(I)c1O
COc1cc(-c2cc(=O)c3cc(O)ccc3o2)cc(I)c1OC
O=C(O)c1ccc(F)c(I)c1
O=Cc1cc(I)c(O)c(OCc2ccccc2)c1
COc1cc(I)c(F)cc1C
COc1cc(-c2cc(=O)c3ccccc3o2)cc(I)c1O
COc1ccc(CO)cc1I
Fc1c(OCc2ccccc2)ccc(Br)c1I
O=Cc1cc(I)c(O)c([N+](=O)[O-])c1
COc1ccc2cc([C@H](C)C(=O)O)ccc2c1I
COc1ccc(C#N)cc1I
CNc1ccc([N+](=O)[O-])cc1I
O=C(N/N=C/c1cc(Br)cc(I)c1O)c1ccncc1
CCOC(=O)c1ccc(I)c(F)c1
O=C(O)Cc1ccc(I)c(F)c1
COc1ccc(C(C)=O)cc1I
Cc1cc(O)c(I)cc1Cl
O=Cc1ccc(O)c(I)c1
Fc1c(I)ccc(C(F)(F)F)c1F
O=C(O)c1c(F)ccc(F)c1I
Cc1ccc(I)c(N)c1
N[C@H](Cc1ccc(O)c(I)c1)C(=O)O
Nc1c(Br)cccc1I
Fc1cc(Br)cc(Br)c1I
COc1ccc(Br)cc1I
Oc1cc(F)cc(Br)c1I
Nc1c(Br)cc(OC(F)(F)F)cc1I
COc1cc(C#N)ccc1I
COC(=O)c1cc(Cl)c(N=C(C)O)c(I)c1O
Fc1cc(P(c2ccccc2)c2ccccc2)ccc1I
Fc1c(I)ccc2ccccc12
COC(=O)c1ccc(N)c(I)c1
FC(F)(F)c1ccc(OCc2ccccc2)c(I)c1
COc1c(Cl)cc(Br)cc1I
COC(=O)c1ccc(/N=C/c2cc(Cl)cc(I)c2O)cc1
Cc1cc(I)c(N)cc1C(F)(F)F
N#Cc1cc(Cl)c(N)c(I)c1
CCCOc1c(I)cc(C(=O)O)cc1OC
N#Cc1cc(I)c(O)c([N+](=O)[O-])c1
CSc1cccc(I)c1F
Fc1cccc(CBr)c1I
O=C(O)c1cc(Cl)cc(I)c1O
Cc1cc([N+](=O)[O-])cc(I)c1N
Oc1c(F)cc(Cl)cc1I
CCOC(=O)c1ccc(I)c(N)c1
Nc1cc(C(F)(F)F)c([N+](=O)[O-])cc1I
COc1cc(C=O)cc([N+](=O)[O-])c1I
O=C(O)c1ccc(I)c(F)c1F
COc1cc(C=O)cc(I)c1OCC(=O)O
COc1ccc(Cl)cc1I
Oc1ccc(OC(F)(F)F)cc1I
Oc1ccc2cc(Br)ccc2c1I
C=Cc1ccc(O)c(I)c1
CCOc1cc(C(=N)O)cc(I)c1OCC
CCCCCCCCOc1cc(C=O)c(OCCCCCCCC)cc1I
CCOC(=O)c1ccc(OC)c(I)c1
Cc1cc(N)c(I)cc1C#N
COc1cc(C(C)=O)ccc1I
Fc1cc(Br)c(I)c(F)c1F
Oc1ccc(O)c(I)c1
O=C(O)c1cccc(O)c1I
N#Cc1ccc(I)c(F)c1F
O=Cc1ccc(Cl)c(I)c1F
Oc1ccc(-c2ccccc2)cc1I
COc1cccc(C(=O)O)c1I
O=Cc1cccc(O)c1I
Fc1ccc(Br)c(Cl)c1I
CC(C)c1ccc(I)c(O)c1
Nc1ccc(OC(F)(F)F)cc1I
COc1ccc(F)c(I)c1
O=C(O)c1ccc(-n2cccn2)c(I)c1
O=[N+]([O-])c1cc(Br)cc(I)c1O
COc1ccc(Cl)c(Cl)c1I
COC(OC)c1ccnc(-c2ccc(I)c(F)c2)n1
Fc1cccc(OC(F)(F)F)c1I

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Nc1ccc(F)cc1I
N#Cc1ccc(F)c(I)c1Cl
COC(=O)c1c(C)ccc(F)c1I
Nc1c(I)cc(F)c(Br)c1F
COC(=O)c1cccc(N)c1I
CNc1ccc(C(=O)OC)cc1I
COc1cc(F)cc(Br)c1I
COC(=O)c1ccc(N)c(I)c1Cl
CC(O)=Nc1cc(C(=O)O)ccc1I
Nc1c(F)cc(F)cc1I
COC(=O)c1cccc(I)c1F
COC(=O)c1ccc(OC)c(I)c1
N[C@@H](Cc1ccc(O)c(I)c1)C(=O)O
COc1ccc(S(N)(=O)=O)cc1I
Fc1c(Br)cc(Cl)cc1I
Nc1cc([N+](=O)[O-])ccc1I
Cc1ccc(F)c(I)c1C(=O)O
COC(=O)c1cccc(F)c1I
COc1cc(OC)c(C(C)=O)c(OC(=O)c2ccc(OC)c(I)c2)c1
Nc1ccc(Cl)c(Cl)c1I
COC(=O)c1ccc(I)c(O)c1Cl
Nc1cccc(I)c1O
COc1cc(C(C)(C)C)ccc1I
Fc1cccc(Cl)c1I
Cc1cc(F)c(I)cc1O
O=[N+]([O-])c1ccc(Oc2ccccc2)c(I)c1
COc1ccc(OC)c(-c2c(C(C)C)cc(C(C)C)cc2C(C)C)c1I
O=Cc1ccc(I)c(O)c1
COc1cc(C(OC(C)=O)OC(C)=O)cc(I)c1OC(C)=O
Fc1ccc(F)c(I)c1
O=P(c1ccccc1)(c1ccccc1)c1cccc(F)c1I
Oc1cccc(I)c1F
Cc1cc(Br)c(N)c(I)c1
CC(C)(C)OC(O)=N[C@@H](Cc1ccc(O)c(I)c1)C(=O)O
CCOc1cc(/C=N/N=C(O)COc2ccc(C)cc2)cc(I)c1O
Nc1ccc(OC(F)F)cc1I
N#Cc1ccc(F)c(I)c1
N=C(O)c1cccc(F)c1I
COC(=O)c1cc(I)c(N)c(OC)c1
Oc1cccc(Br)c1I
N#Cc1ccc(-c2ccc(O)c(I)c2)cc1
COc1cc(C=O)cc(I)c1OCc1cccc(Cl)c1
Oc1c(I)cc(Cl)cc1-c1csnn1
CC(=O)c1cccc(I)c1O
C=CCNS(=O)(=O)c1ccc(OC)c(I)c1
COC(=O)c1c(F)ccc(F)c1I
COC(=O)c1ccc(O)c(I)c1
COc1c(F)cc(Cl)cc1I
Nc1cc(Br)cc(I)c1N
Cc1ccc(C(=O)O)c(F)c1I
Oc1ccc(C(F)(F)F)cc1I
COc1ccc(Oc2ccc(C[C@H](N=C(C)O)C(=N)O)cc2I)cc1
Fc1cc(F)c(I)c(Br)c1
COc1c(I)cccc1C(=O)O
COc1cc(/C=N/O)cc(I)c1OC
N#Cc1cc(Br)c(N)c(I)c1
Cc1ccc(O)c(I)c1
COc1cc(/C=C2/SC(=S)N(c3ccccc3C)C2=O)cc(I)c1O
COc1cc(C)c(C)cc1I
COC(=O)[C@@H](N)Cc1ccc(O)c(I)c1
O=Cc1cccc(F)c1I
Nc1ccc(N)c(I)c1
COC(=O)c1ccc(I)c(OC)c1
Cc1cccc(I)c1F
C=CCN(CC=C)C(=O)c1ccc(OC)c(I)c1
COc1cc(/C=N/N=C(O)c2cccc(F)c2)cc(I)c1O
CCOC(O)=Nc1ccc(F)c(F)c1I
N=C(O)c1ccc(I)c(F)c1
Nc1cc2ccccc2cc1I
COc1cc(C=O)cc(I)c1OC(=O)c1ccccc1
CC(C)c1ccc(I)c(F)c1
COC(=O)c1cccc(OC)c1I
Nc1ccc(CCO)cc1I
O=Cc1ccc(I)c(F)c1
CCOc1cc(/C=C/c2ccc3cccc(OC)c3n2)cc(I)c1OC(C)=O
Fc1cccc(I)c1F
COc1cccc(C#N)c1I
COc1cc(OC)c2c(=O)cc(-c3ccc(OC(C)C)c(I)c3)oc2c1
CC(C)(C)c1ccc(N)c(I)c1
Fc1c(Cl)ccc(-n2cc(C(F)(F)F)nn2)c1I
CC(=O)c1ccc(O)c(I)c1
Nc1c(Br)cc(C(F)(F)F)cc1I
COc1cc(Br)cc(Cl)c1I
Nc1ccc(F)c(I)c1
OC1=N/C(=C/c2ccc(O)c(I)c2)C(O)=N1
O=Cc1ccc(Br)c(I)c1F
Cc1cc(N)c(I)cc1C
COc1cc(/C=N/NC(=O)c2ccncc2)cc(I)c1OC
Fc1c(Cl)cc(C(F)(F)F)cc1I
N#Cc1cccc(I)c1F
CCOC(=O)c1cc(Br)c(N)c(I)c1
CC(C)(C)c1ccc(I)c(O)c1
Cc1cc(I)c(O)c(C(=O)O)c1
COc1ccc(-c2nc3ccccc3s2)cc1I
O=Cc1ccc(Cl)c(I)c1O
CC(=O)c1ccc(I)c(F)c1F
O=Cc1ccc(O)c(O)c1I
CCOc1cc(C=C2C(O)=NC(=S)N=C2O)cc(I)c1OC
Nc1cc(F)cc(Br)c1I
COc1cccc(Br)c1I
COc1c(C)cc([N+](=O)[O-])cc1I
OB(O)c1ccc(I)c(F)c1F
Fc1ccc(Cl)c(Br)c1I
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