

Supporting Information

Palladium(II)-Catalyzed Regioselective *Ortho*-C-H Bromination/Iodination of Arylacetamides *via* in situ Generated Imidic Acid as Directing group: Mechanistic Exploration

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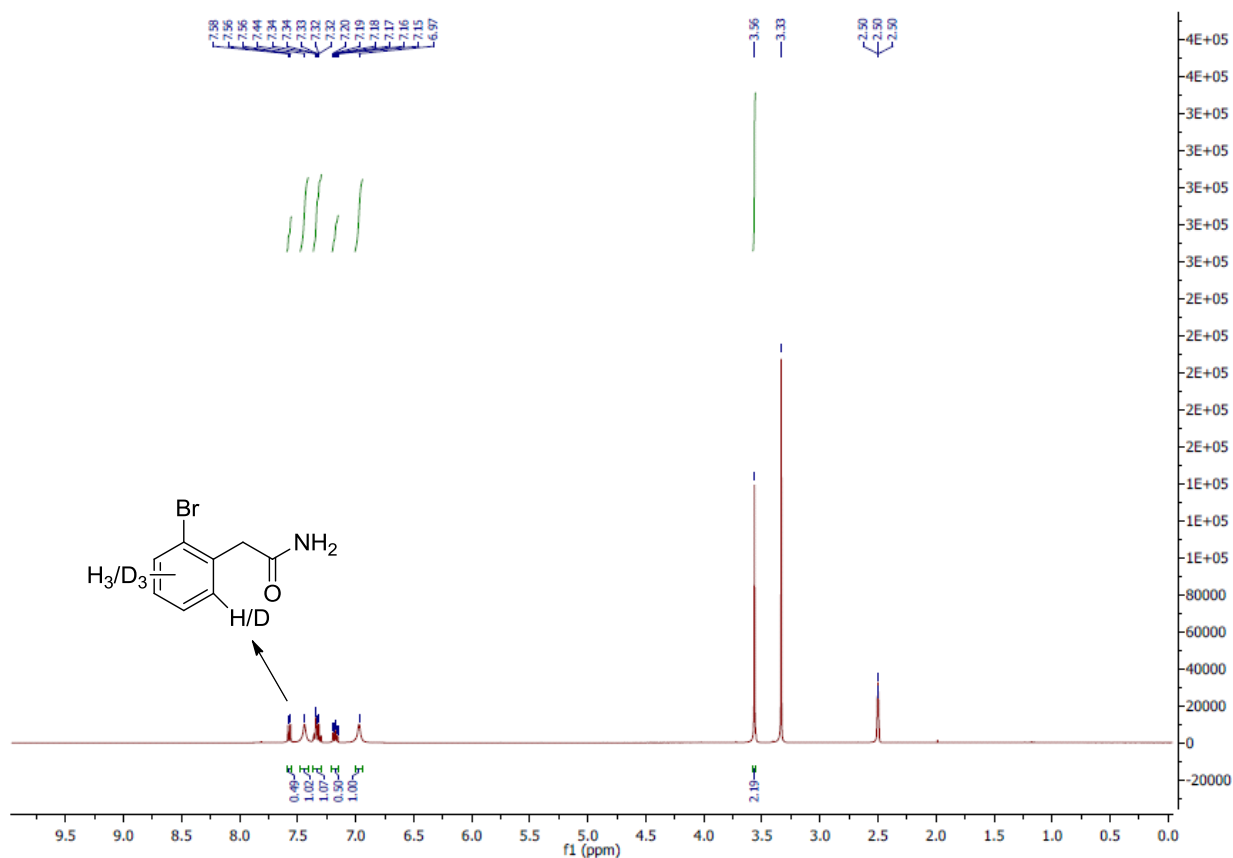
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1. Procedure for intermolecular competition experiment between 1b and 1j. A suspension of Pd(OAc)₂ (5.0 mol %, 2.4 mg), NBS (1.2 equiv, 43 mg), TFA (10.0 equiv, 150.0 μL), **1b** (0.2 mmol, 29.8 mg, 1.0 equiv), and **1j** (0.2 mmol, 36 mg, 1.0 equiv) was stirred in DCE (2.0 mL) for 24 h at 50 °C. After cooling to room temperature, the solvent was evaporated in vacuum. The reaction mixture was diluted with ethyl acetate, followed by neutralization with an aqueous solution of sodium bicarbonate. After extraction with ethyl acetate, the organic layer was washed with brine solution and dried over sodium sulfate. The combined organic layer was concentrated under vacuum. The crude mixture was purified by column chromatography using ethyl acetate/hexanes as eluent. Compound **2b** was isolated in 57% yield and **2j** was formed in trace amount.

2. Procedure for intermolecular competition experiment between 1a and 5: To a oven dried sealed tube, phenylacetamide (**1a**) (30 mg, 0.20 mmol), N-benzyl phenylacetamide (**5**) (45 mg, 0.20 mmol), Pd(OAc)₂ (2.4 mg, 0.05 mmol), NBS (43 mg, 0.24 mmol), TFA (10 equiv, 150 μL) and DCE (2.0 mL) was added. The mixture was stirred at 50 °C for 24 h. After cooling to room temperature, the solvent was evaporated in vacuum. The reaction mixture was diluted with ethyl acetate, followed by neutralization with an aqueous solution of sodium bicarbonate. After extraction with ethyl acetate, the organic layer was washed with brine solution and dried over sodium sulfate. The combined organic layer was concentrated under vacuum. The crude mixture was purified by column chromatography using ethyl acetate/hexanes as eluent. Compound **2a** was isolated in 38% yield and **4a** was formed in 28% amount.

3. Procedure for intermolecular competition experiment between 1a and 1a-D₅: To a oven dried sealed tube, following the general procedure, phenylacetamide (**1a**) (27 mg, 0.20 mmol), deuterated phenylacetamide (**1a-D₅**) (28 mg, 0.20 mmol), Pd(OAc)₂ (2.4 mg, 0.05 mmol),

NBS (43 mg, 0.24 mmol), TFA (10 equiv, 150 μ L) and DCE (2.0 mL) was added. The mixture was stirred at 50 $^{\circ}$ C for 2 h. After cooling to room temperature, the solvent was evaporated in vacuum. The reaction mixture was diluted with ethyl acetate, followed by neutralization with an aqueous solution of sodium bicarbonate. After extraction with ethyl acetate, the organic layer was washed with brine solution and dried over sodium sulfate. The combined organic layer was concentrated under vacuum. The crude mixture was purified by column chromatography using ethyl acetate/hexanes as eluent. The ratio of **1a** and **1a-D₅** was determined by 1 H NMR analysis, found to be $k_H/k_D \approx 1.0$.



4. Procedure for parallel experiment between **1a and **1a-D₅**:** Following the general procedure, two parallel reaction for phenylacetamide (**1a**) (27 mg, 0.25 mmol) and deuterated phenylacetamide (**1a-D₅**) (28 mg, 0.25 mmol), were performed. The mixture was stirred at 50

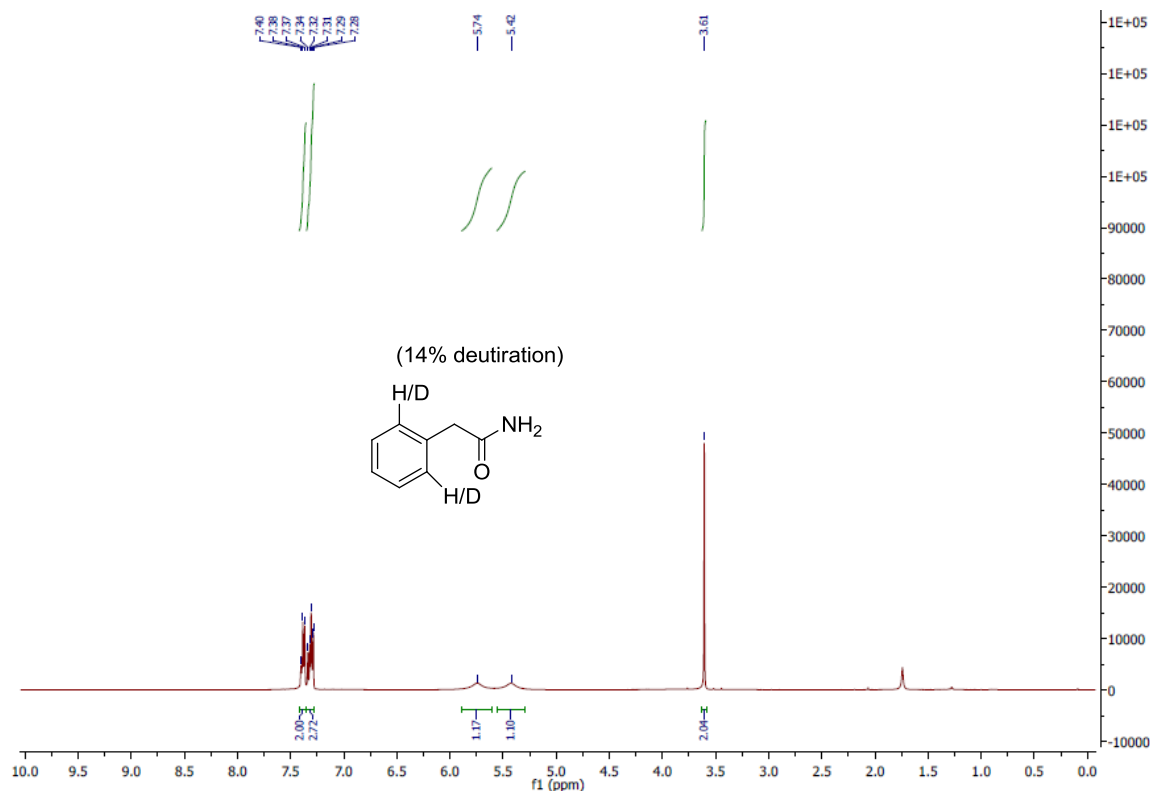
°C for 2 h. After cooling to room temperature, the solvent was evaporated in vacuum. The reaction mixture was diluted with ethyl acetate, followed by neutralization with an aqueous solution of sodium bicarbonate. After extraction with ethyl acetate, the organic layer was washed with brine solution and dried over sodium sulfate. The combined organic layer was concentrated under vacuum. The crude mixture was purified by column chromatography using ethyl acetate/hexanes as eluent. Product **2a** was isolated in 18% yield and **2a-d₄** was isolated in 14% yield.

5. Procedure for H/D exchange experiment without NBS in D₂O: In a oven dried sealed tube equipped with stirrer bar, was sequentially added phenylacetamide (**1a**) (0.25 mmol, 34.0 mg), Pd(OAc)₂ (5.0 mol%, 2.8 mg), D₂O (10.0 equiv, 50.0 μL) and TFA (10.0 equiv, 190.0 μL). Then 2.0 mL of DCE was added in the reaction mixture. The reaction was stirred at 50 °C for 24 h and the solvent was evaporated in vacuum. The reaction mixture was diluted with ethyl acetate, followed by neutralization with an aqueous solution of sodium bicarbonate. After extraction with ethyl acetate, the organic layer was washed with brine solution and dried over sodium sulfate. The combined organic layer was concentrated under vacuum. The crude mixture was purified by column chromatography using ethyl acetate/hexanes as eluent to give starting material in 90% yield without any deuterium exchange.

6. Procedure for H/D exchange experiment with NBS in D₂O: In a oven dried sealed tube equipped with stirrer bar, was sequentially added phenylacetamide (**1a**) (0.25 mmol, 34 mg), Pd(OAc)₂ (5.0 mol%, 2.8 mg), NBS (0.3 mmol, 53.4 mg), D₂O (10.0 equiv, 50.0 μL) and TFA (10.0 equiv, 190 μL). Then 2.0 mL of DCE was added in the reaction mixture. The reaction was stirred at 50 °C for 24 h and the solvent was evaporated in vacuum. The reaction mixture was diluted with ethyl acetate, followed by neutralization with an aqueous solution of sodium

bicarbonate. After extraction with ethyl acetate, the organic layer was washed with brine solution and dried over sodium sulfate. The combined organic layer was concentrated under vacuum. The crude mixture was purified by column chromatography using ethyl acetate/hexanes as eluent to give product **2a** in 30% yield without any deuterium exchange along with 55% of starting material **1a**.

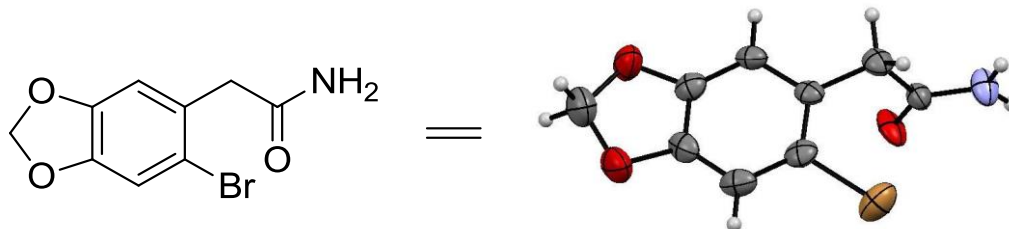
7. Procedure for H/D exchange experiment without NBS in CF₃COOD: In a oven dried sealed tube equipped with stirrer bar, was sequentially added phenylacetamide (**1a**) (0.25 mmol, 34 mg), Pd(OAc)₂ (5.0 mol%, 2.8 mg), D₂O (10.0 equiv, 50.0 μL) and CF₃COOD (10.0 equiv, 190.0 μL). Then 2.0 mL of DCE was added in the reaction mixture. The reaction was stirred at 50 °C for 24 h and the solvent was evaporated in vacuum. The reaction mixture was diluted with ethyl acetate, followed by neutralization with an aqueous solution of sodium bicarbonate. After extraction with ethyl acetate, the organic layer was washed with brine solution and dried over sodium sulfate. The combined organic layer was concentrated under vacuum. The crude mixture was purified by column chromatography using ethyl acetate/hexanes as eluent to give starting material in 90% yield. Deuterium incorporation was determined by ¹H NMR.



8. Procedure for H/D exchange experiment with NBS in CF₃COOD: In a oven dried sealed tube equipped with stirrer bar, was sequentially added phenylacetamide (**1a**) (0.25 mmol, 34 mg), Pd(OAc)₂ (5.0 mol%, 2.8 mg), NBS (0.3 mmol, 53.4 mg) and DCE (2.0 mL). Then CF₃COOD (10.0 equiv, 190.0 μL) was added in the reaction mixture. The reaction was stirred at 50 °C for 24 h and the solvent was evaporated in vacuum. The reaction mixture was diluted with ethyl acetate, followed by neutralization with an aqueous solution of sodium bicarbonate. After extraction with ethyl acetate, the organic layer was washed with brine solution and dried over sodium sulfate. The combined organic layer was concentrated under vacuum. The crude mixture was purified by column chromatography using ethyl acetate/hexanes as eluent to give product **2a** in 55% yield without any deuterium exchange.

9. XRD data

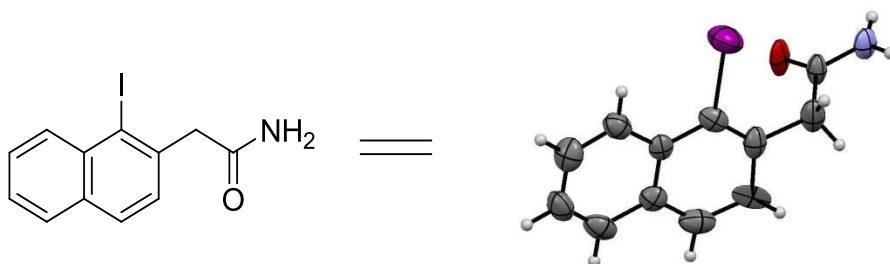
(a) XRD data of 2e (CCDC No. 1909226)



Chemical formula	$C_{88}BrNO_2$	
Formula weight	258.07 g/mol	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal size	0.300 x 0.300 x 0.300 mm	
Crystal system	Monoclinic	
Space group	$P1\ 21/c$	
Unit cell dimensions	$a = 11.507(4)$ Å	$\alpha = 90^\circ$
	$b = 4.8430(18)$ Å	$\beta = 100.591(9)^\circ$
	$c = 17.180(6)$ Å	$\gamma = 90^\circ$
Volume	$941.1(6)$ Å ³	
Z	4	
Density (calculated)	1.821 g/cm ³	
Absorption coefficient	4.346 mm ⁻¹	
F(000)	512	
Theta range for data collection	2.73 to 24.84°	
Index ranges	$-13 \leq h \leq 13, -5 \leq k \leq 5, -20 \leq l \leq 20$	
Reflections collected	9914	
Independent reflections	1617 [R(int) = 0.0923]	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/ (Sheldrick, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	1617 / 0 / 127	
Goodness-of-fit on F2	1.022	

Final R indices	1029 data; $I > 2\sigma(I)$	R1 = 0.0485, wR2 = 0.0749
	all data	R1 = 0.1020, wR2 = 0.0894
Weighting scheme	where $P = (F_o^2 + 2F_c^2)/3$	
Largest diff. peak and hole	0.395 and -0.374 $e\text{\AA}^{-3}$	
R.M.S. deviation from mean	0.089 $e\text{\AA}^{-3}$	

(b) XRD data of 3m (CCDC No. 1909424)



Chemical formula	C ₁₂ H ₁₀ INO	
Formula weight	311.11 g/mol	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal size	0.200 x 0.200 x 0.300 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 14.336(7) Å	α = 90°
	b = 4.975(2) Å	β = 106.346(13)°
	c = 16.193(8) Å	γ = 90°
Volume	1108.2(9) Å ³	
Z	4	
Density (calculated)	1.864 g/cm ³	
Absorption coefficient	2.861 mm ⁻¹	
F(000)	600	
Theta range for data collection	2.96 to 24.55°	
Index ranges	-16 ≤ h ≤ 16, -5 ≤ k ≤ 5, -18 ≤ l ≤ 18	
Reflections collected	15699	
Independent reflections	1844 [R(int) = 0.0857]	

Coverage of independent reflections	99.2%
Absorption correction	Multi-Scan
Max. and min. transmission	0.5980 and 0.4810
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick 2008)
Refinement method	Full-matrix least-squares on F ²
Refinement program	SHELXL-2014 (Sheldrick 2014)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	1844 / 0 / 136
Goodness-of-fit on F²	1.021
Final R indices	1121 data; I > 2 σ (I) R1 = 0.0533, wR2 = 0.1006 all data R1 = 0.1149, wR2 = 0.1204
Weighting scheme	$w = 1 / [\sigma^2(F_o^2) + (0.0499P)^2 + 3.3221P]$ where $P = (F_o^2 + 2F_c^2) / 3$
Largest diff. peak and hole	0.711 and -0.421 e \AA^{-3}
R.M.S. deviation from mean	0.109 e \AA^{-3}

Alert level A

PLAT213_ALERT_2_A Atom C12 has ADP max/min Ratio 12.2 prolat

Explanation: The high variation in ADP max/min ratio of C12 caused by large anisotropic thermal displacements.

10. Reaction monitoring by ¹H NMR experiment.

To gain insight into to reaction mechanism, the reaction of phenylacetamide (0.25 mmol) was performed, and ¹H NMR was recorded every 30 minutes after sequential addition of catalyst and reagents. Initially, phenylacetamide was stirred with 5 mol% of Pd(OAc)₂ in CDCl₃ for 30 min at 50 °C. No changes in NMR spectra was observed [Fig. 2(b)]. Then, we added 10.0 equiv of TFA to the reaction mixture and again stirred for 30 min at 50 °C. ¹H NMR spectrum shows the

formation of corresponding imidic acid [Fig. 2(c)]. Further, we added 1.2 equiv of NBS in reaction mixture and reaction was further stirred for 30 min. at 50 °C. Then, ^1H NMR of the crude reaction mixture was recorded and spectrum revealed that the formation of the desired product started within stipulated time [Fig. 2(d)].

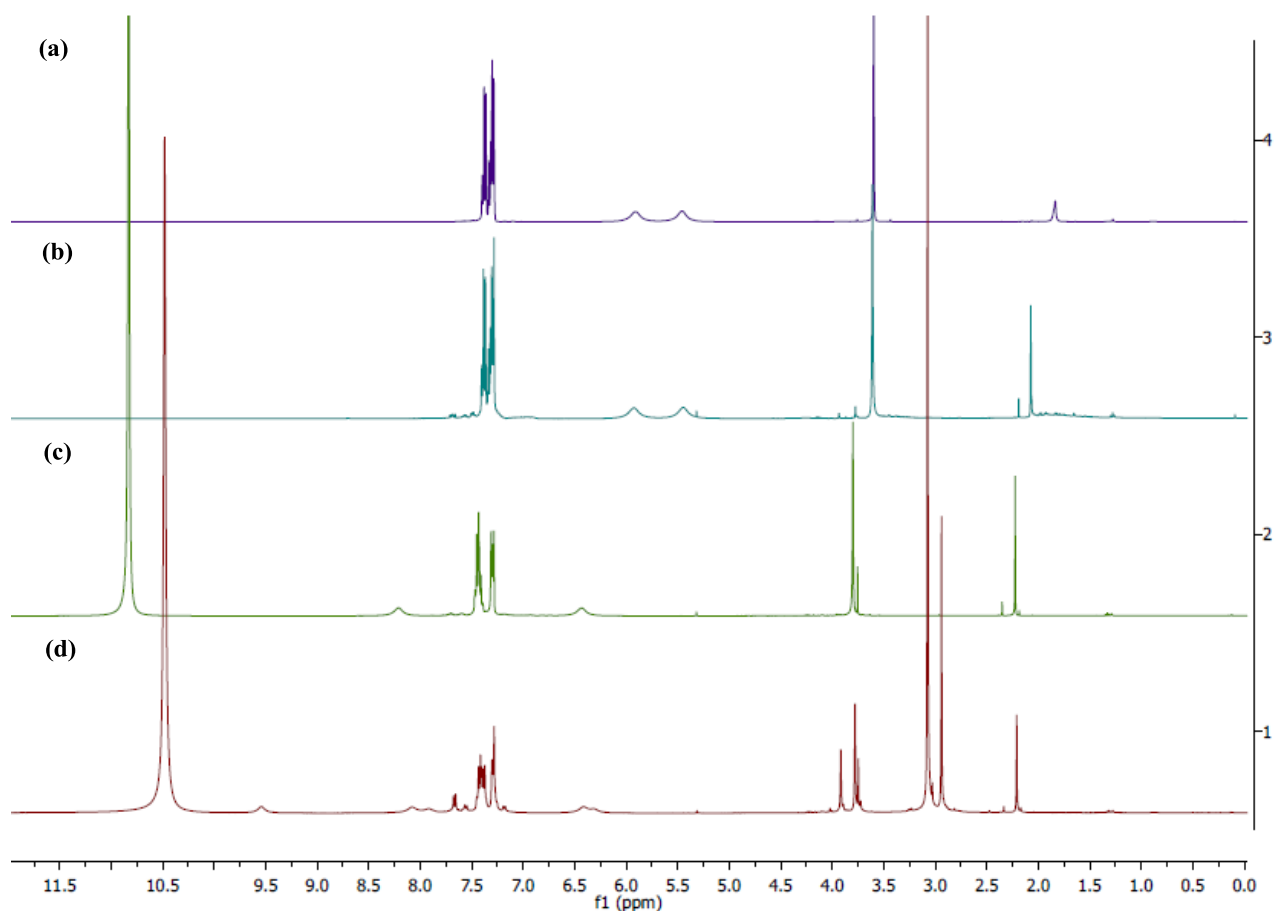


Figure 2. (a) ^1H NMR of pure **1a**. (b) ^1H NMR of **1a** with 5 mol % of $\text{Pd}(\text{OAc})_2$. (c) ^1H NMR of **1a** with $\text{Pd}(\text{OAc})_2$ and TFA (10.0 equiv). (d) ^1H NMR of **1a** with $\text{Pd}(\text{OAc})_2$, TFA (10.0 equiv) and NBS (1.2 equiv).

11. DFT details

Phenylacetamide tautomerizes to form imidic acid in the presence of trifluoroacetic acid. The imidic acid has three possible coordinating sites: (a) imidic nitrogen (=NH) (b) oxygen (c) nitrogen atom of amide to form a six-membered palladacycle intermediate. In reaction mixture, palladium trifluoroacetate may coordinate to these three possible sites resulting in chemical species **A**, **A'** and **A''** respectively. We have performed DFT calculation to find the relative free energy of **A**, **A'** and **A''** (Figure 1). DFT calculation revealed that formation of **A** is more exothermic than **A'** and exothermicity equals to $\Delta H = -3.78$ kcal/mole. In addition, the formation of **A'** is more exothermic than **A''** and $\Delta H = -3.84$ kcal/mole. The relative free energy change between **A** and **A'** is $\Delta G = 3.6$ kcal/mol, for **A'** and **A''** ΔG is 5.9 kcal/mole. These results conclude that formation of species **A** is more favored than **A'**, which prefer to form over **A''** in the reaction mixture.

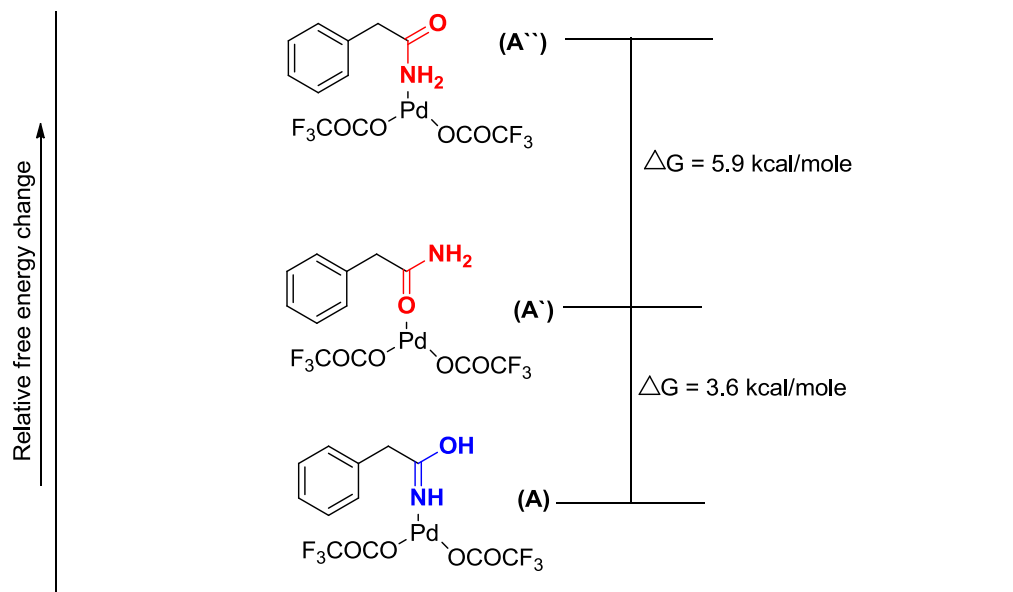


Figure S1. Coordination mode primary amide with Pd(TFA)₂ in reaction mixture.

Computational Details

All the calculations were carried out with Gaussian 16¹. All geometry optimizations were performed using B3LYP² level of theory of DFT method in gas phase. The LANL2DZ³ basis set with effective core potential (ECP) was used for Pd, and the 6-31G (d)⁴ basis set was used for all H, C, N, F, and O atoms. Frequency analysis was conducted at the same level of theory to verify that the stationary points are minima. Solvent effects were computed using the same DFT method and basis sets in ClCH₂CH₂Cl with the integral equation formalism for the polarizable continuum model (IEF-PCM)⁵ at 323.15 K. Frequency analysis were carried out at the same level to evaluate the zero-point vibrational energy and thermal corrections at 323.15 K. The relative Gibbs free energies are given in kcal/mol. Computed structures are visualized using GaussView0.5.⁶

Cartesian coordinates and Energy (in hartrees unit) of Complex A:

Symbol	X	Y	Z
C	-3.2791270	2.2049650	0.8524900
C	-2.0779420	2.7975330	0.4381090
C	-2.0285290	3.4252390	-0.8152130
C	-3.1564470	3.4594620	-1.6373640
C	-4.3492330	2.8678820	-1.2142190
C	-4.4085590	2.2404640	0.0324430
H	-3.3320050	1.7205930	1.8246550
H	-1.1051790	3.8961350	-1.1443410
H	-3.1044190	3.9529530	-2.6037730
H	-5.2284250	2.8977770	-1.8516430
H	-5.3336500	1.7807820	0.3686440
C	0.1036620	1.6125720	1.1215790

C	-0.8576390	2.7696520	1.3305920
H	-0.2602930	3.6816320	1.2107810
H	-1.1435160	2.7328590	2.3887310
C	3.4980090	0.0829960	0.1763680
O	3.3241570	0.4093050	1.3555130
O	2.6471610	-0.3408740	-0.6772160
C	-1.9944870	-1.6939390	-0.2947820
O	-0.9023750	-1.9982680	0.3276390
C	4.9246090	0.1811370	-0.4227670
O	-2.2043150	-0.7885770	-1.0912060
C	-3.1420460	-2.6604850	0.1013690
Pd	0.8153680	-1.0466340	-0.1211160
F	-2.8028040	-3.9394740	-0.1565150
F	-3.4089790	-2.5619580	1.4197140
F	-4.2658370	-2.3839850	-0.5726950
F	4.9331360	1.0271000	-1.4702680
F	5.8081180	0.6220700	0.4803640
F	5.3336500	-1.0260840	-0.8583740
O	1.1079890	1.6316990	1.9604210
N	-0.0688330	0.7188710	0.2011490
H	-0.9233790	0.7880910	-0.3525200
H	1.8556390	0.9920650	1.7299200

Absolute Free Energy: -1619.274784 Hartree

Absolute Enthalpy: -1619.175028 Hartree

Cartesian coordinates and Energy (in hartrees unit) of Complex A`

Symbol	X	Y	Z
C	1.1764720	3.9217080	-0.2554290
C	-0.0246230	3.1975970	-0.2067150
C	-1.2395410	3.8984530	-0.2538600
C	-1.2537140	5.2914860	-0.3483590
C	-0.0518070	6.0024860	-0.3965380
C	1.1636260	5.3147890	-0.3498540
H	2.1239980	3.3889180	-0.2284660
H	-2.1765320	3.3474080	-0.2258150
H	-2.2022410	5.8196130	-0.3896800
H	-0.0623250	7.0861400	-0.4733870
H	2.1017630	5.8610690	-0.3922690
C	-0.0043820	1.1212020	1.3012850
O	0.0025800	-0.1239690	1.5391340
N	-0.0060160	1.9510220	2.3382010
H	-0.0016530	1.5855070	3.2825710
H	-0.0120630	2.9527770	2.1972560
C	-0.0103930	1.6887710	-0.1020750
H	-0.8830170	1.2435680	-0.5979380
H	0.8697320	1.2596430	-0.5987840
C	2.7917040	-1.0733840	-0.4677900
O	2.5065120	-0.1542430	-1.2225020
O	2.0180520	-1.8235600	0.2452300
C	-2.7743580	-1.1093940	-0.4681270
O	-2.5012030	-0.1864200	-1.2224770

C	4.2783200	-1.4722020	-0.2617070
O	-1.9906570	-1.8510610	0.2427380
C	-4.2558910	-1.5256240	-0.2599990
Pd	0.0125890	-1.6665230	0.1552270
F	-4.6146580	-1.3792170	1.0320040
F	-5.0806920	-0.7784060	-1.0064340
F	-4.4435600	-2.8179840	-0.5960510
F	4.4797010	-2.7645560	-0.5894190
F	5.0925650	-0.7208420	-1.0154510
F	4.6389320	-1.3126670	1.0283170

Absolute Free Energy: -1619.269018 Hartree

Absolute Enthalpy: -1619.169002 Hartree

Cartesian coordinates and Energy (in hartrees unit) of Complex A⁺⁺

Symbol	X	Y	Z
C	3.9827900	-0.3679440	0.3491840
C	3.2108470	-1.5018270	0.6308640
C	3.7764050	-2.7745080	0.4653580
C	5.0942200	-2.9098960	0.0281790
C	5.8619540	-1.7746990	-0.2483050
C	5.3037610	-0.5055120	-0.0857880
H	3.5565390	0.6233680	0.4716220
H	3.1820590	-3.6587220	0.6800090
H	5.5218580	-3.9011950	-0.0937650
H	6.8889600	-1.8800950	-0.5865710
H	5.8941410	0.3817460	-0.2968380

C	0.8040740	-1.9843250	0.1368350
C	1.7726310	-1.3617200	1.1236410
H	1.6383090	-1.8952030	2.0696140
H	1.5294290	-0.3092840	1.2893700
C	-3.7786960	-1.4449830	-0.4336950
O	-4.6276820	-2.2602320	-0.7416690
O	-2.5174400	-1.5007210	-0.7387600
C	0.8606320	2.0198530	-0.4318710
O	-0.2238450	1.6889510	0.1737970
C	-4.2272870	-0.2494530	0.4565690
O	1.4974300	1.3984000	-1.2830670
C	1.4597860	3.3556010	0.0790810
Pd	-1.3192570	0.0526720	-0.2933840
F	2.0091360	4.0450660	-0.9306190
F	0.5573940	4.1380630	0.6856260
F	2.4366360	3.0731310	0.9724980
F	-5.4709520	0.1315310	0.2033600
F	-4.1102910	-0.5474370	1.7552000
F	-3.4213650	0.8764790	0.2459130
O	0.4549700	-3.1405760	0.1418110
N	0.3065800	-1.1005670	-0.9072860
H	0.9697970	-0.3650540	-1.2185010
H	-0.0405120	-1.6561010	-1.6933120

Absolute Free Energy: -1619.259533 Hartree

Absolute Enthalpy: -1619.162867 Hartree

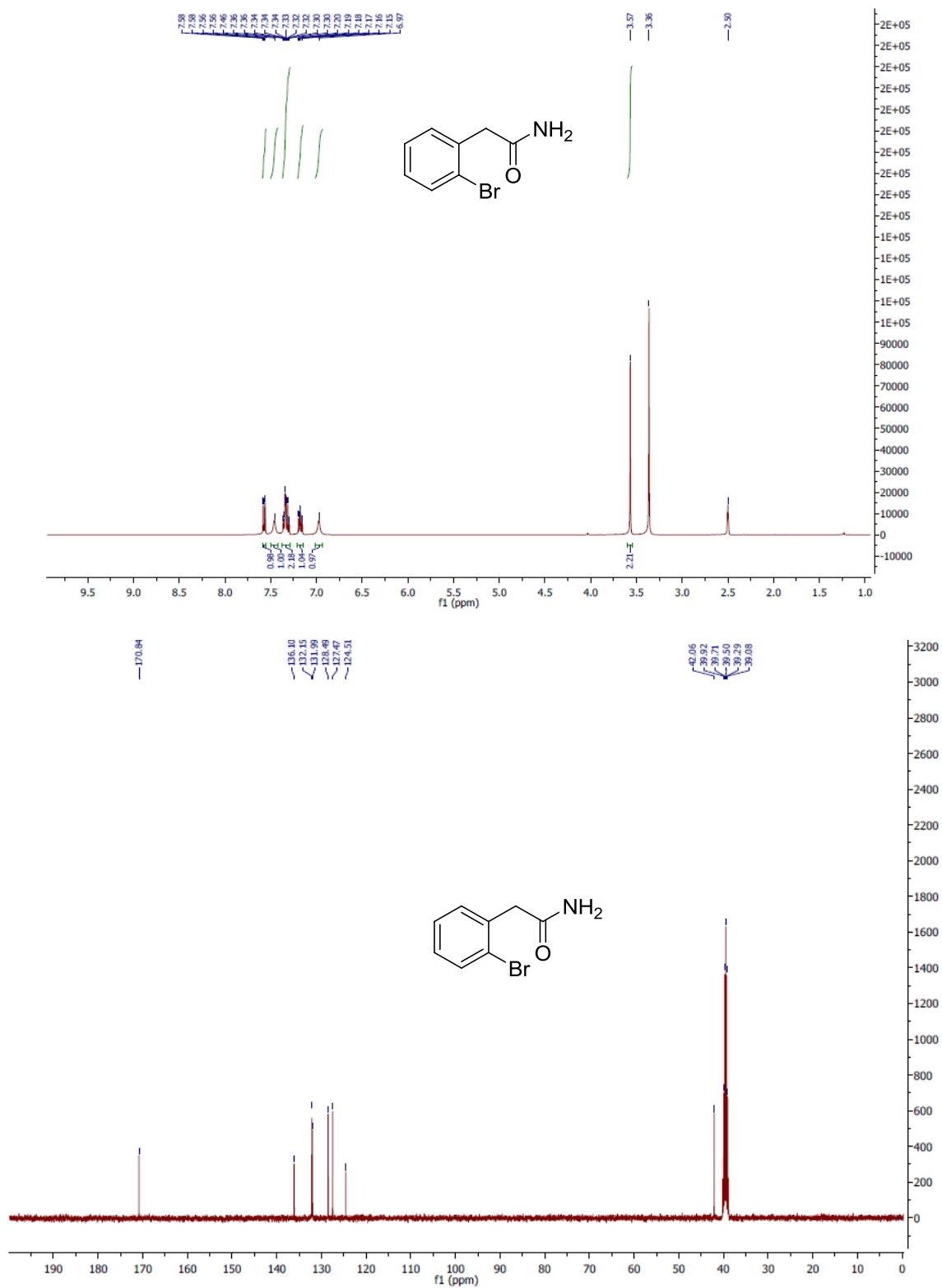
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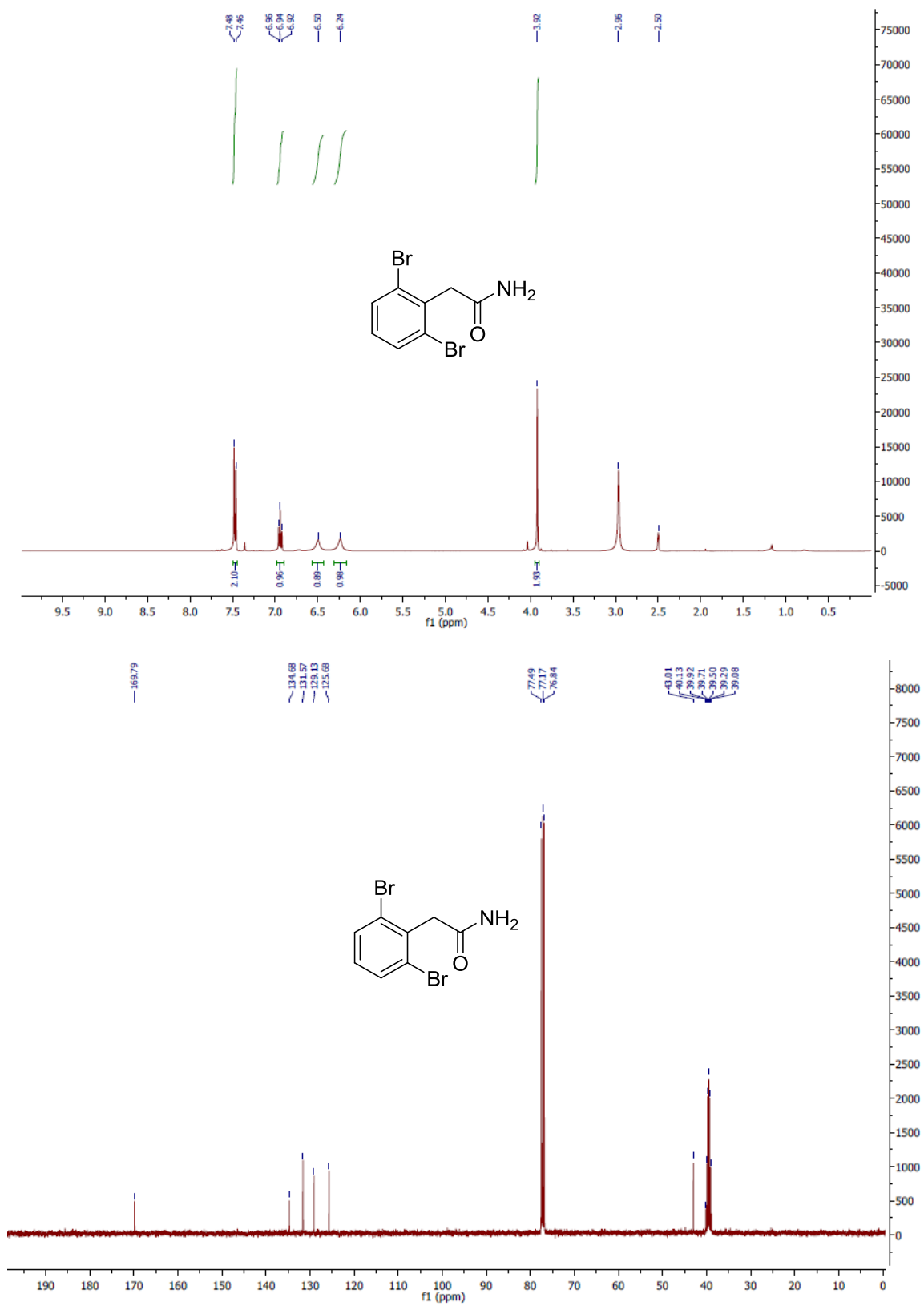
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13. NMR spectra

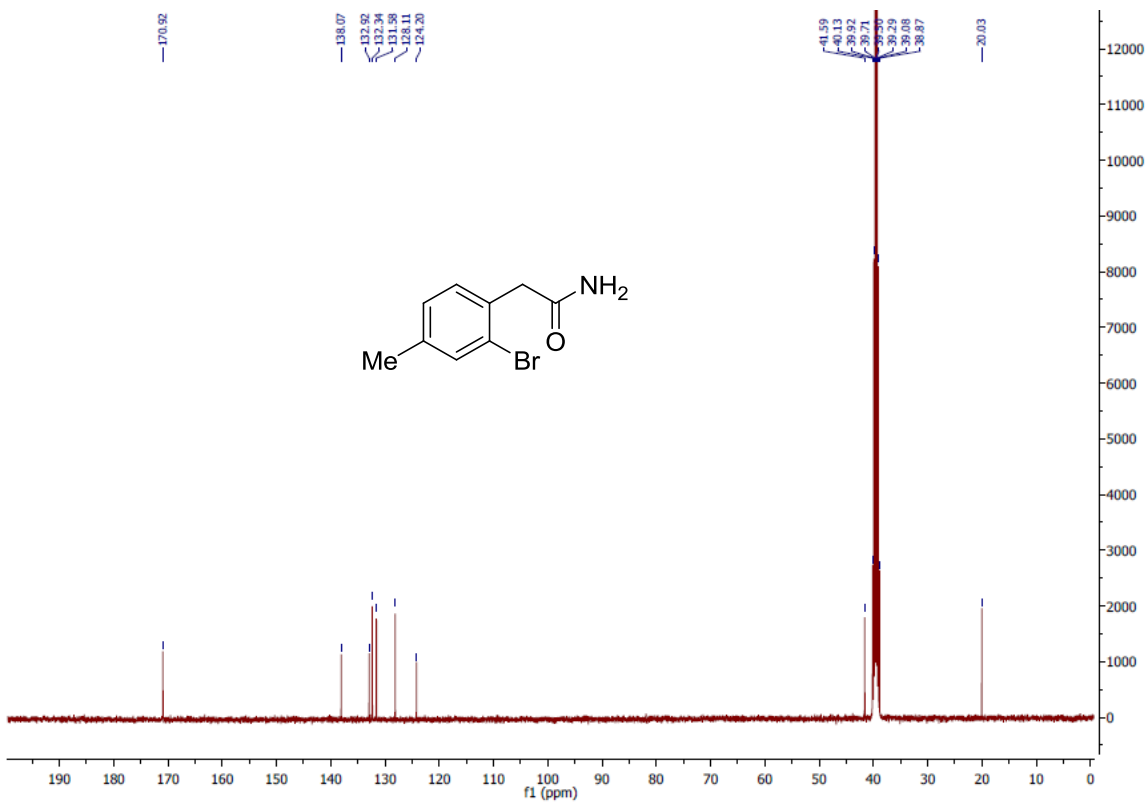
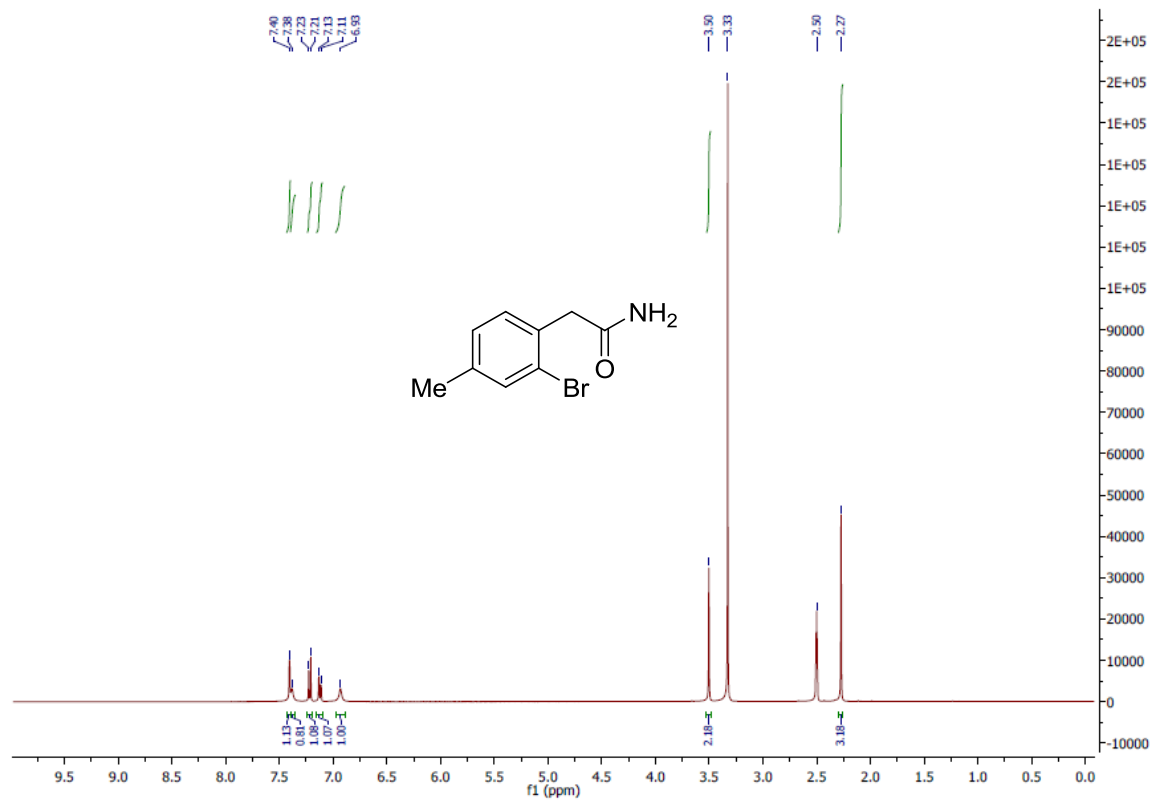
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2a**



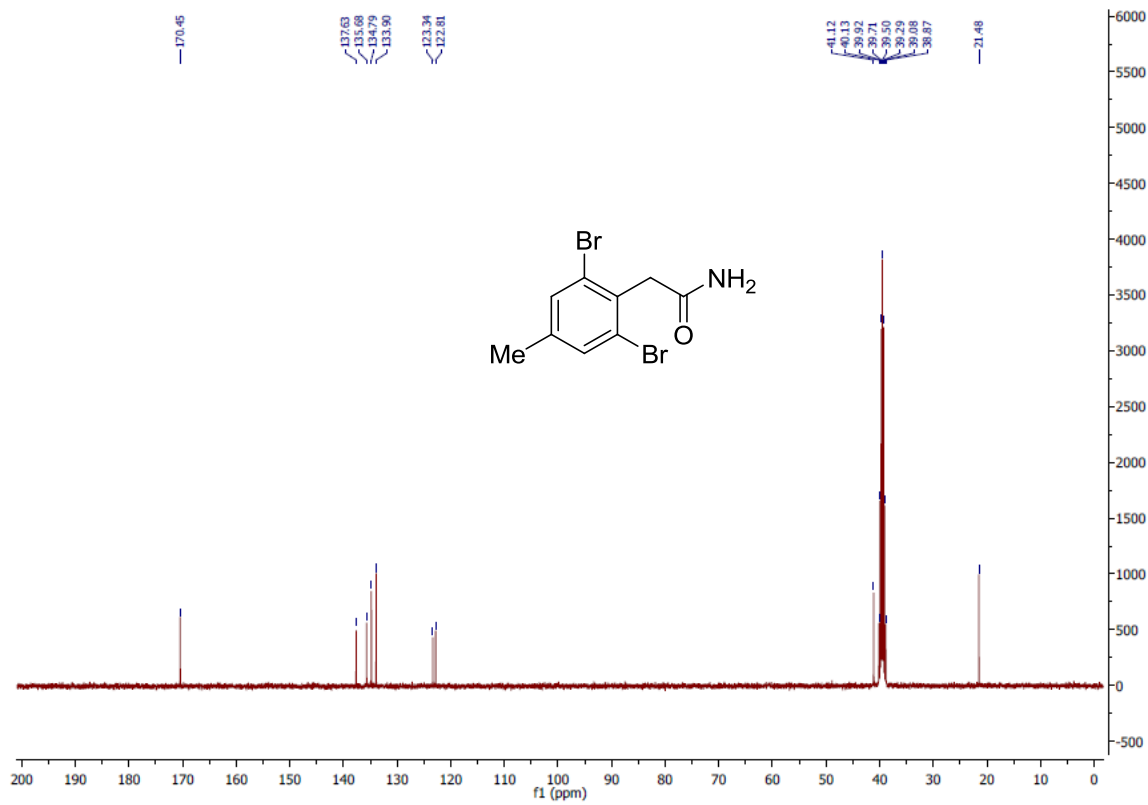
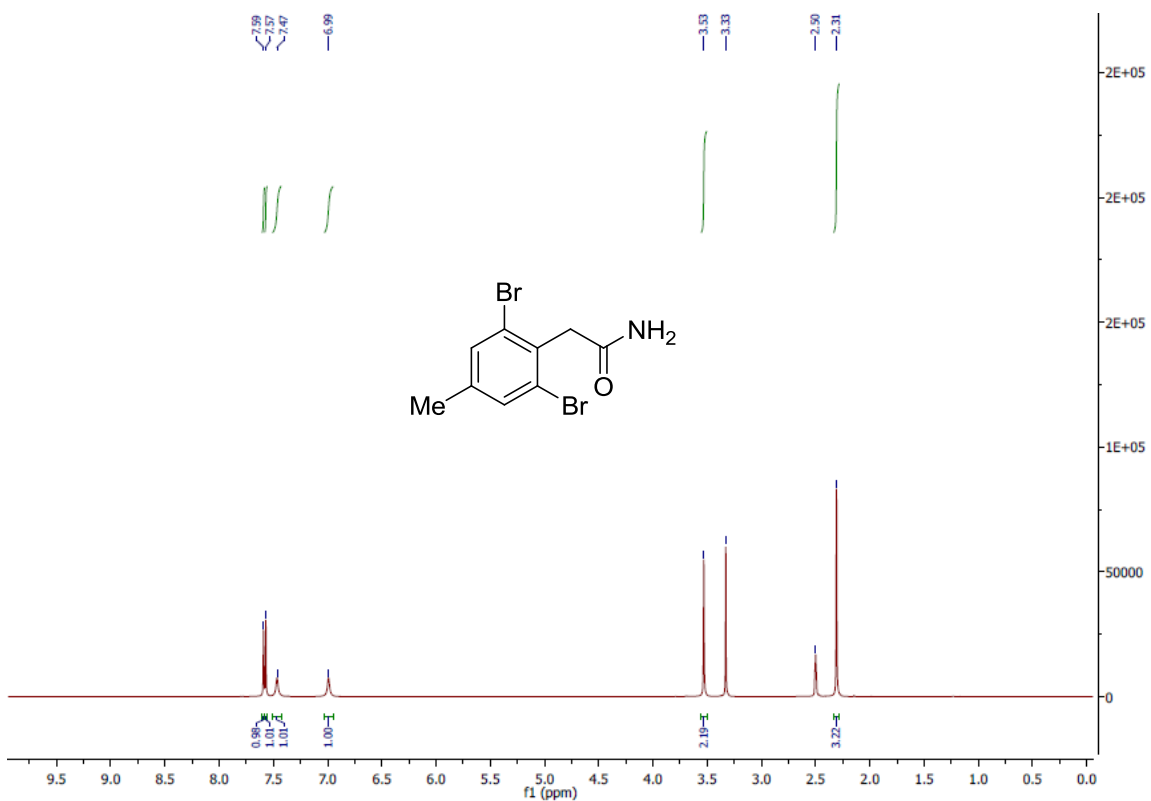
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2aa**



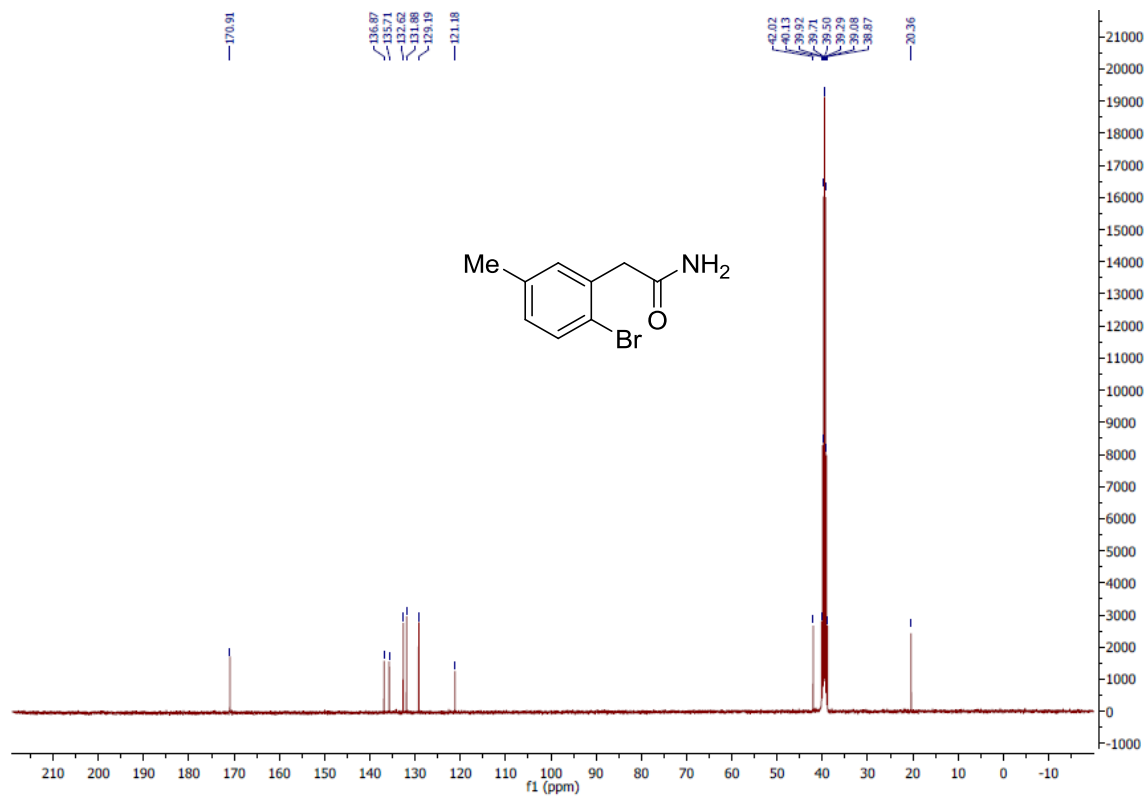
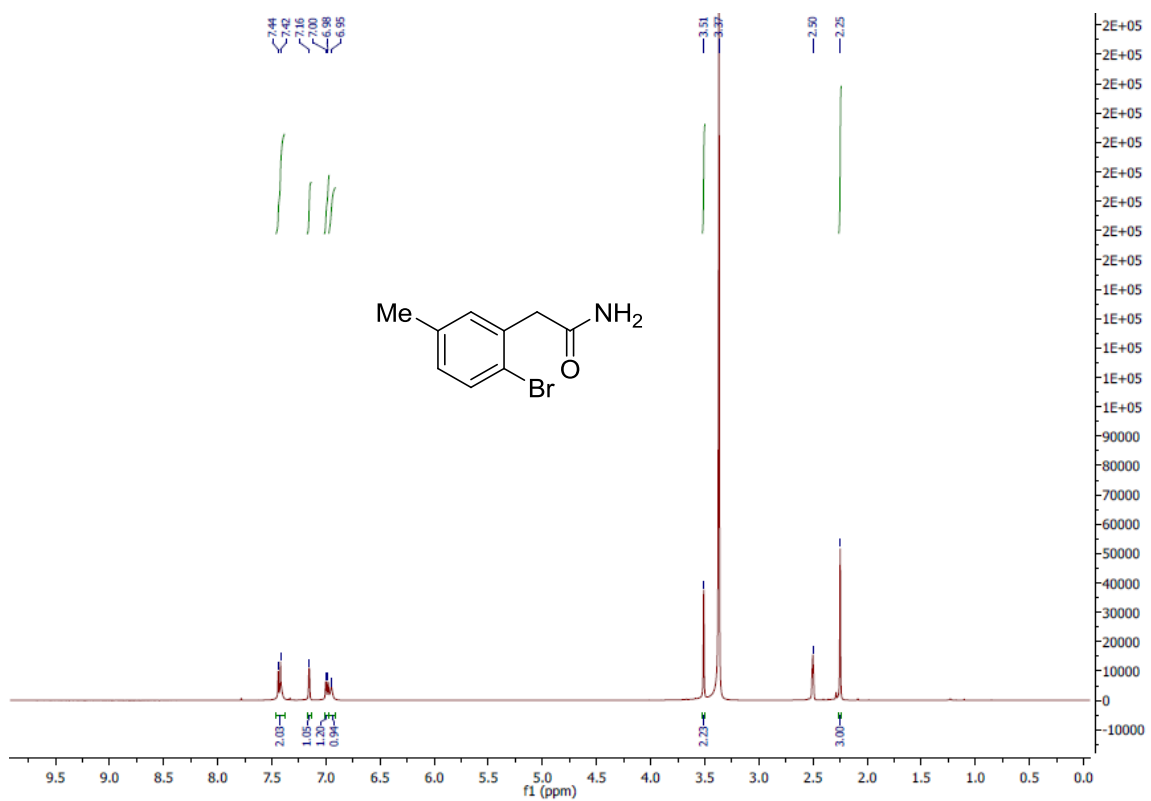
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2b**



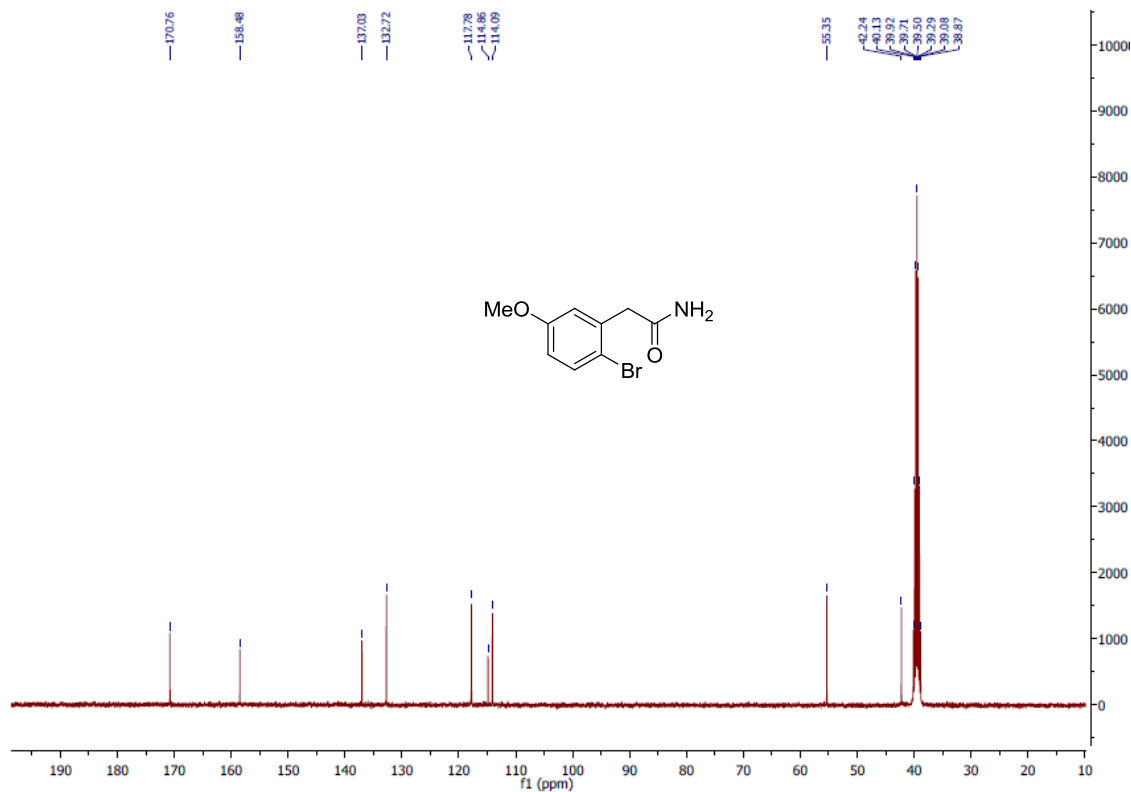
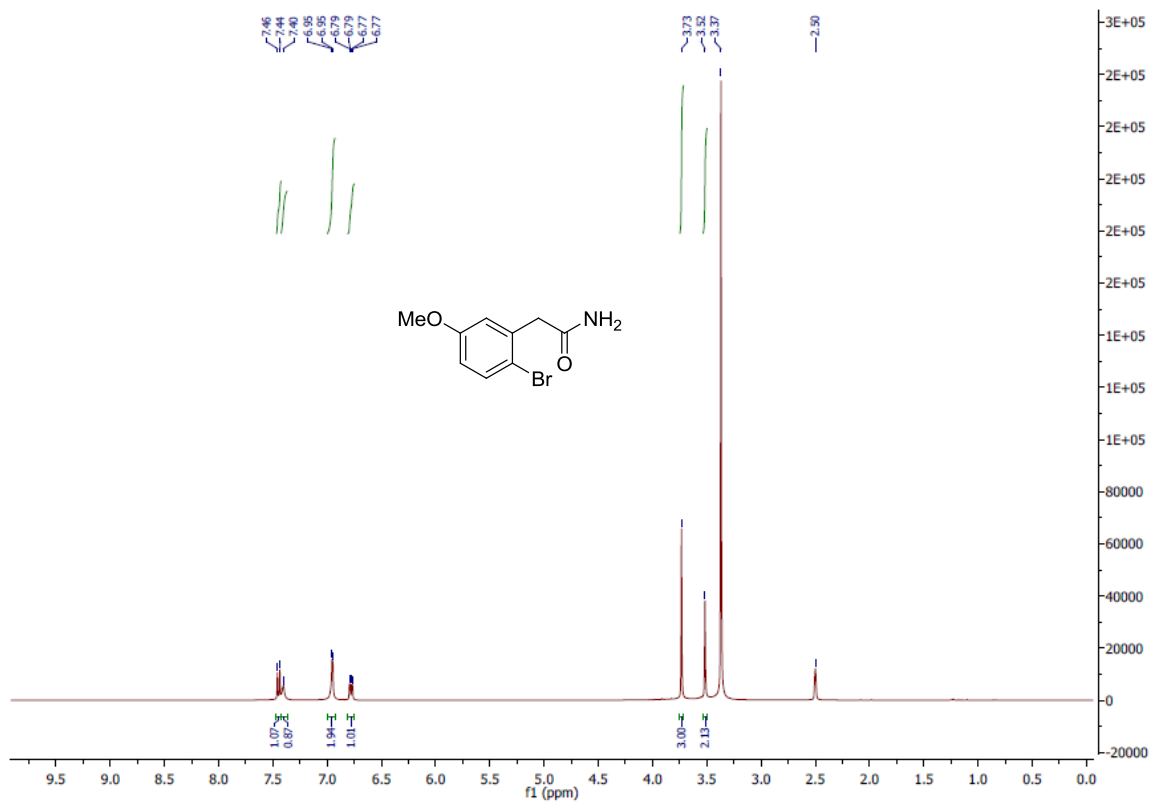
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2bb**



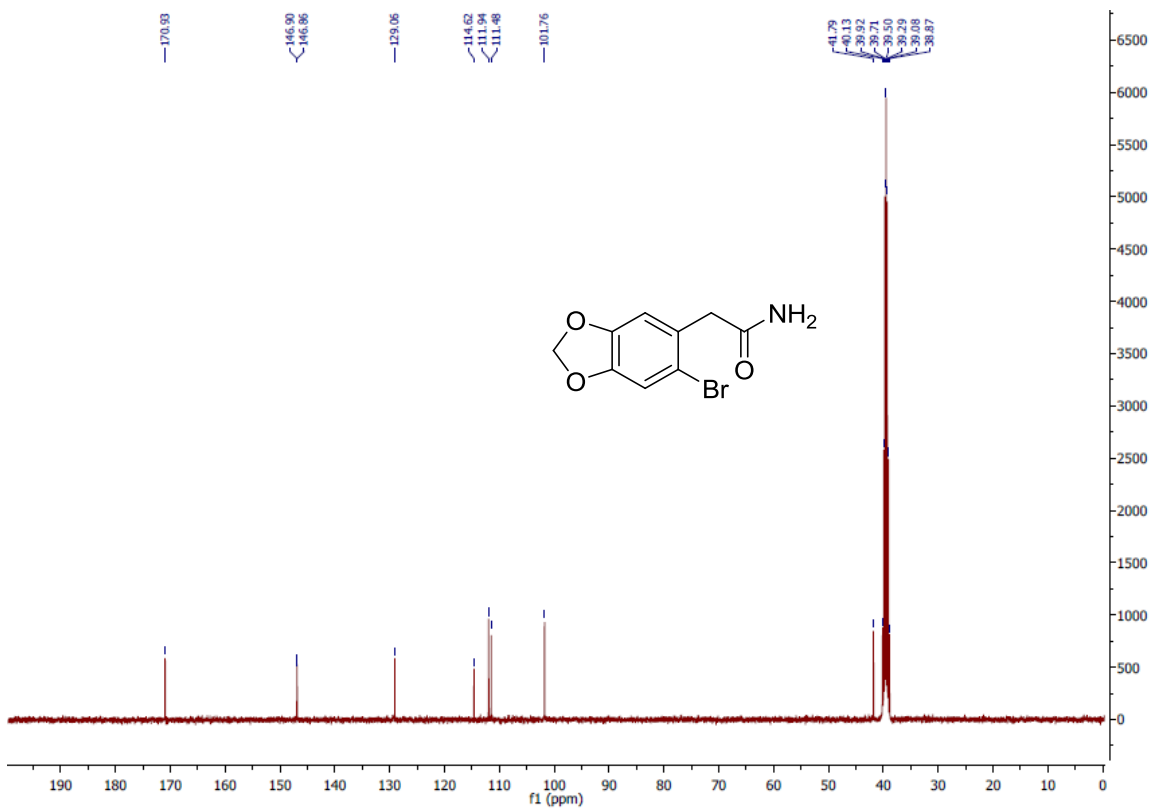
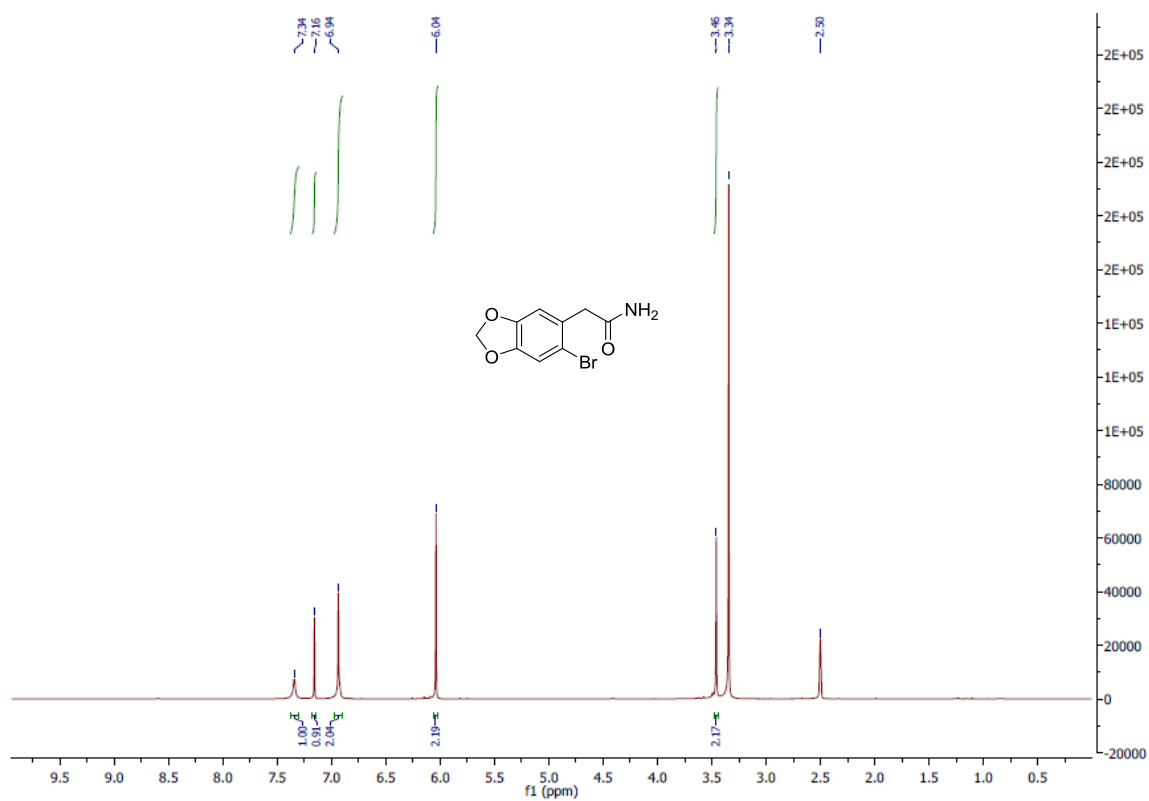
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2c**



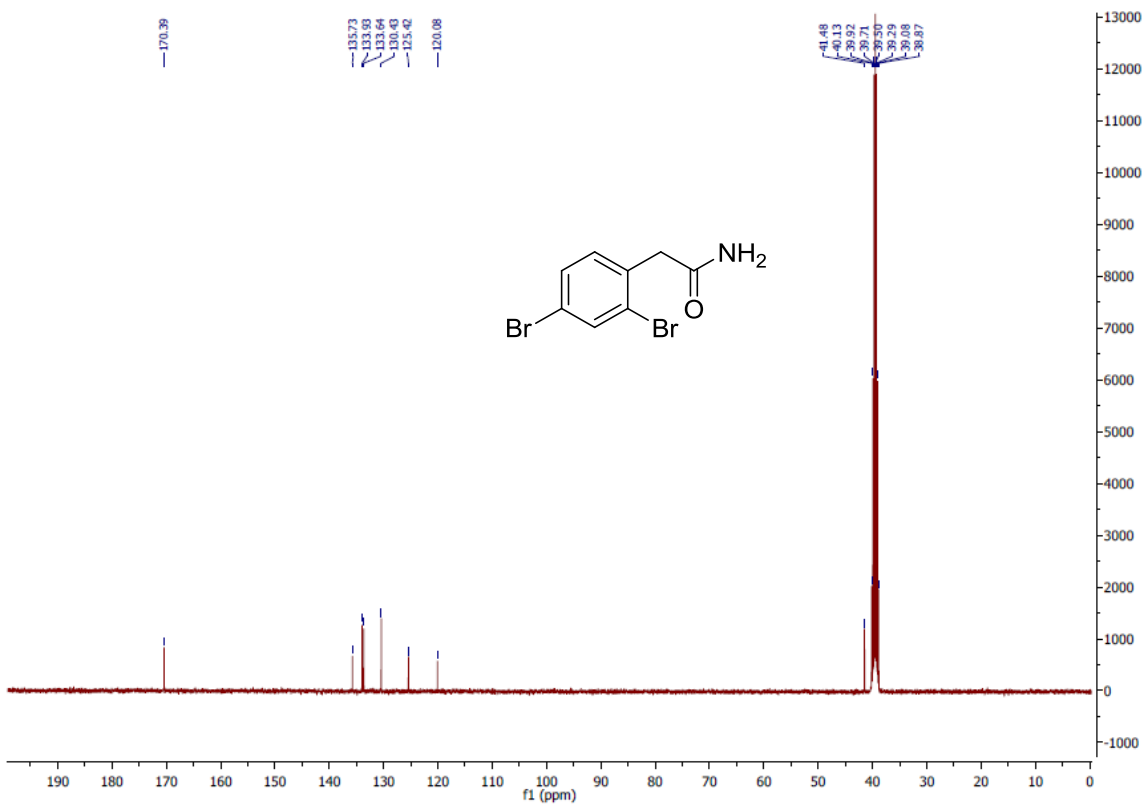
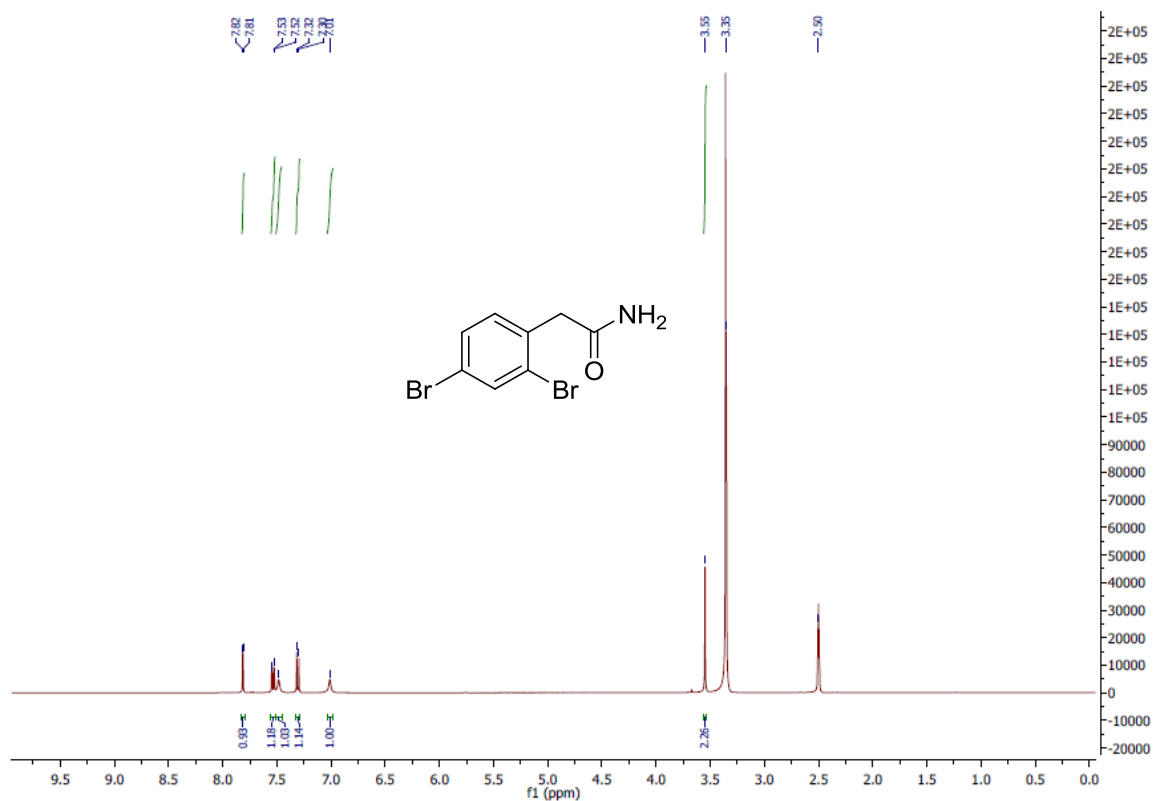
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2d**



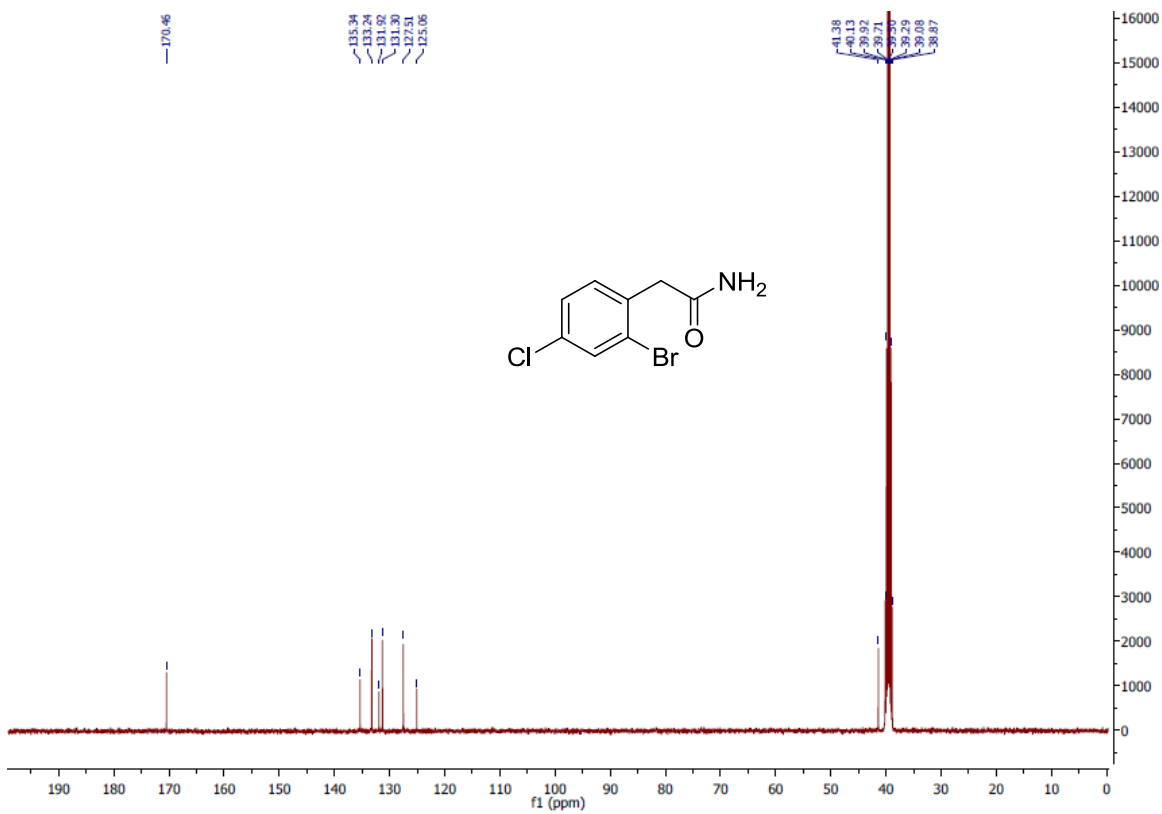
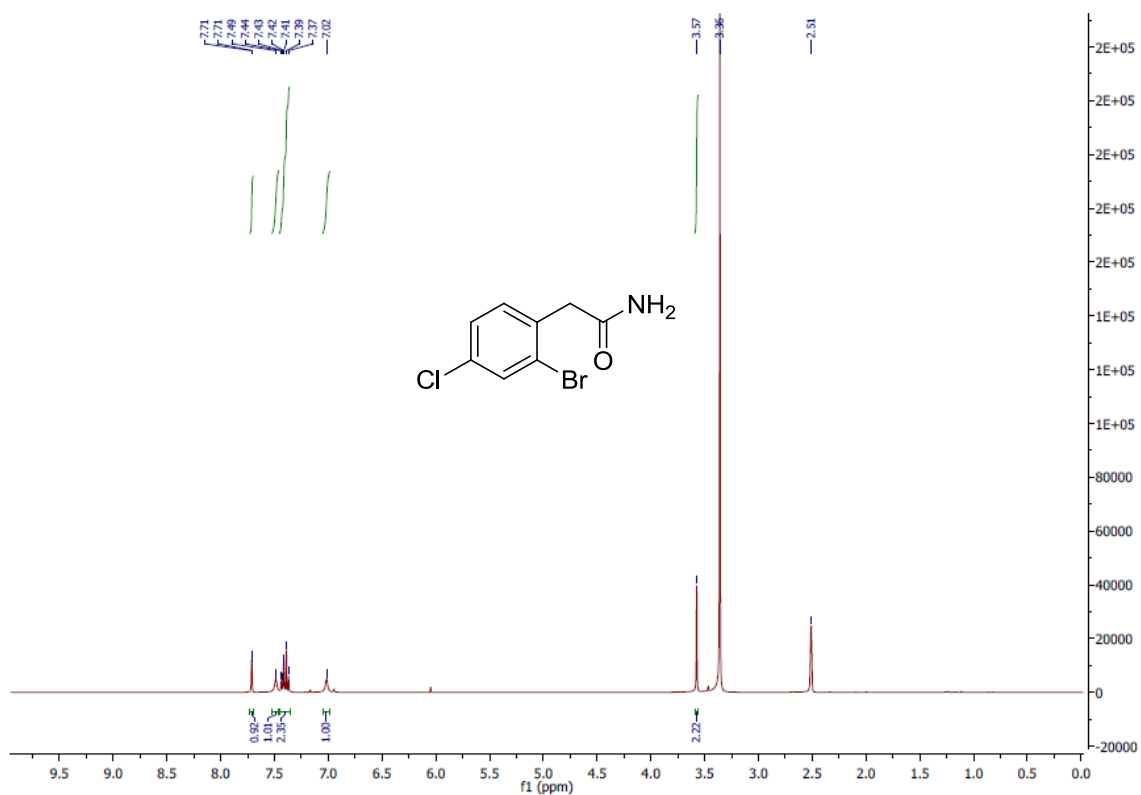
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2e**



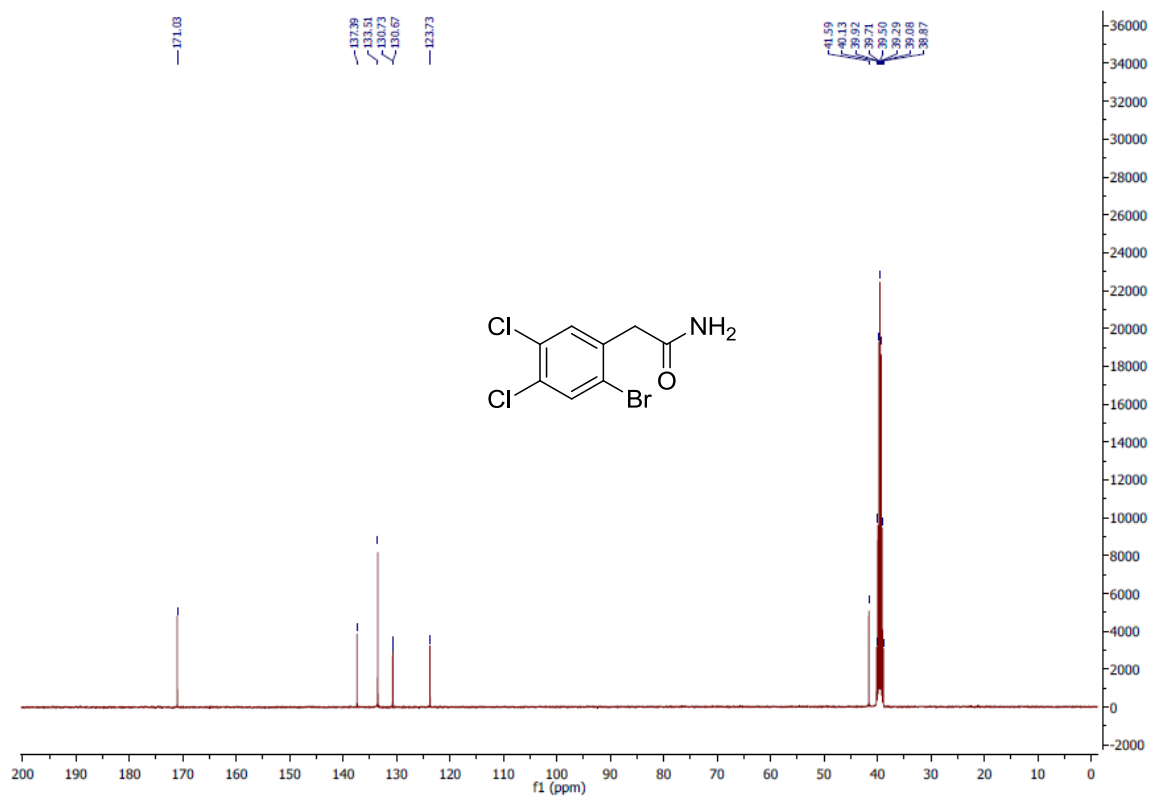
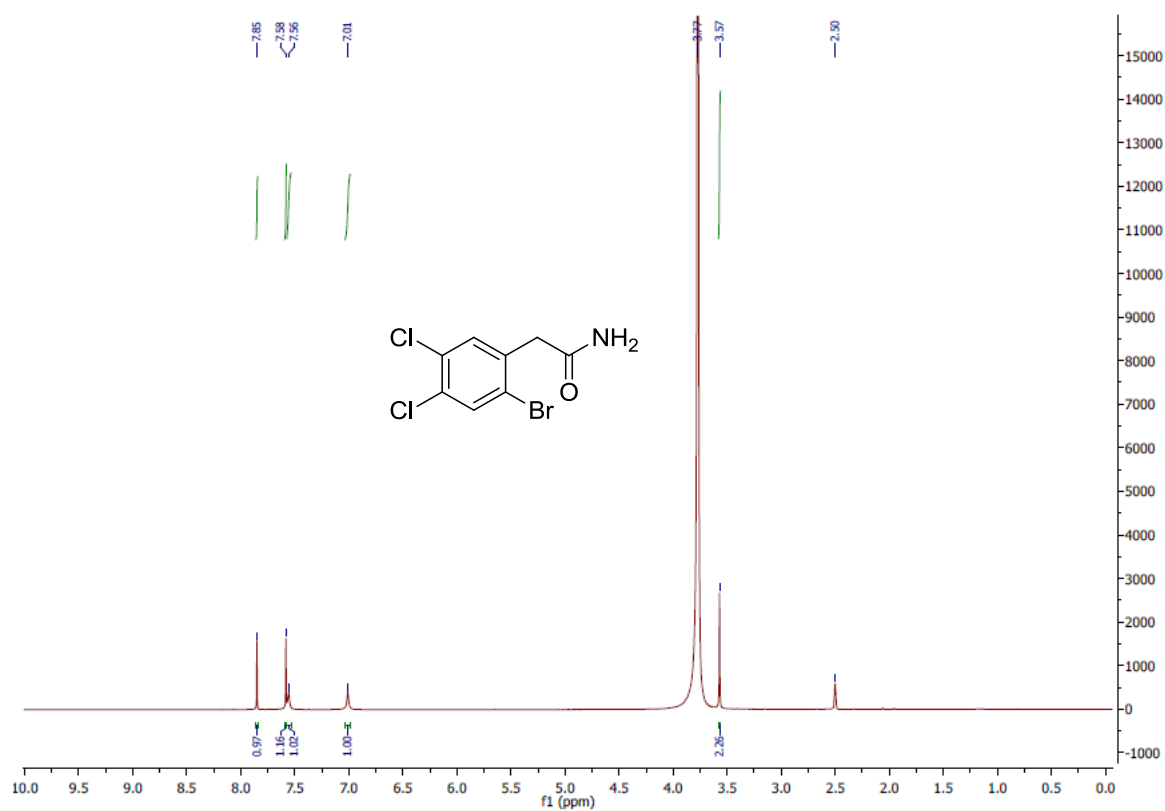
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2f**



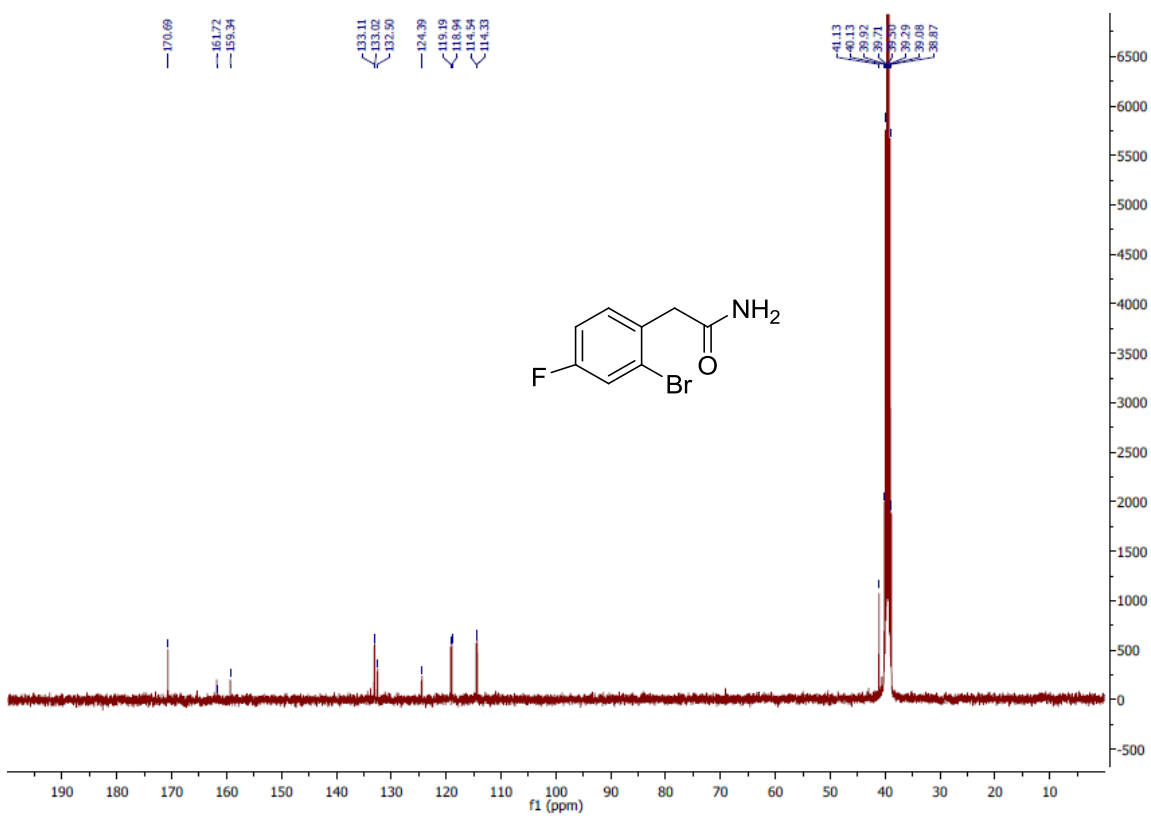
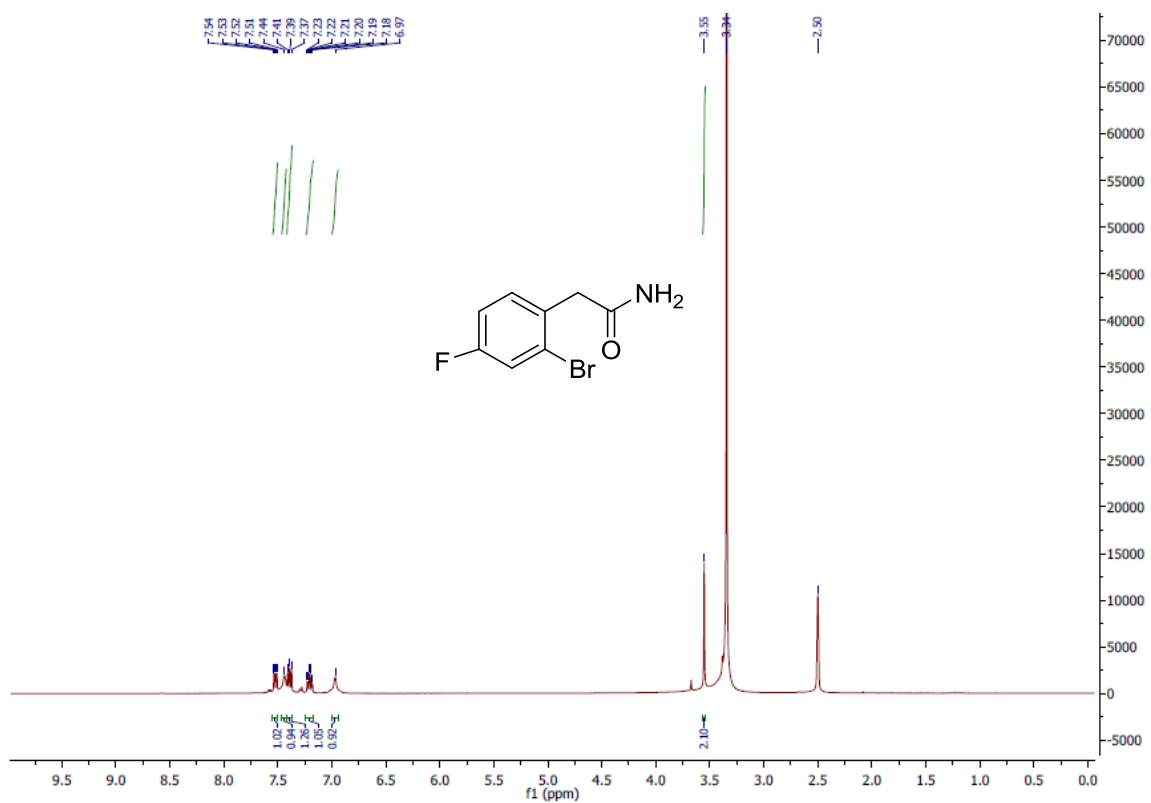
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2g**

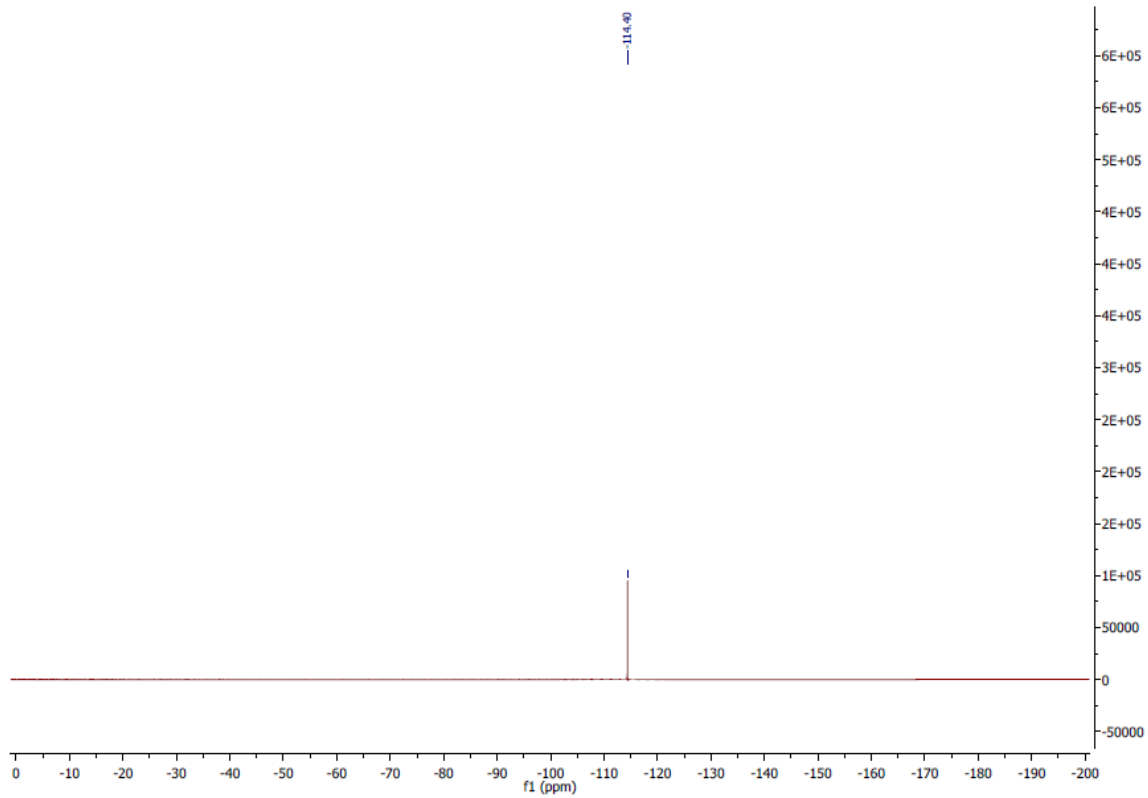


^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2h**

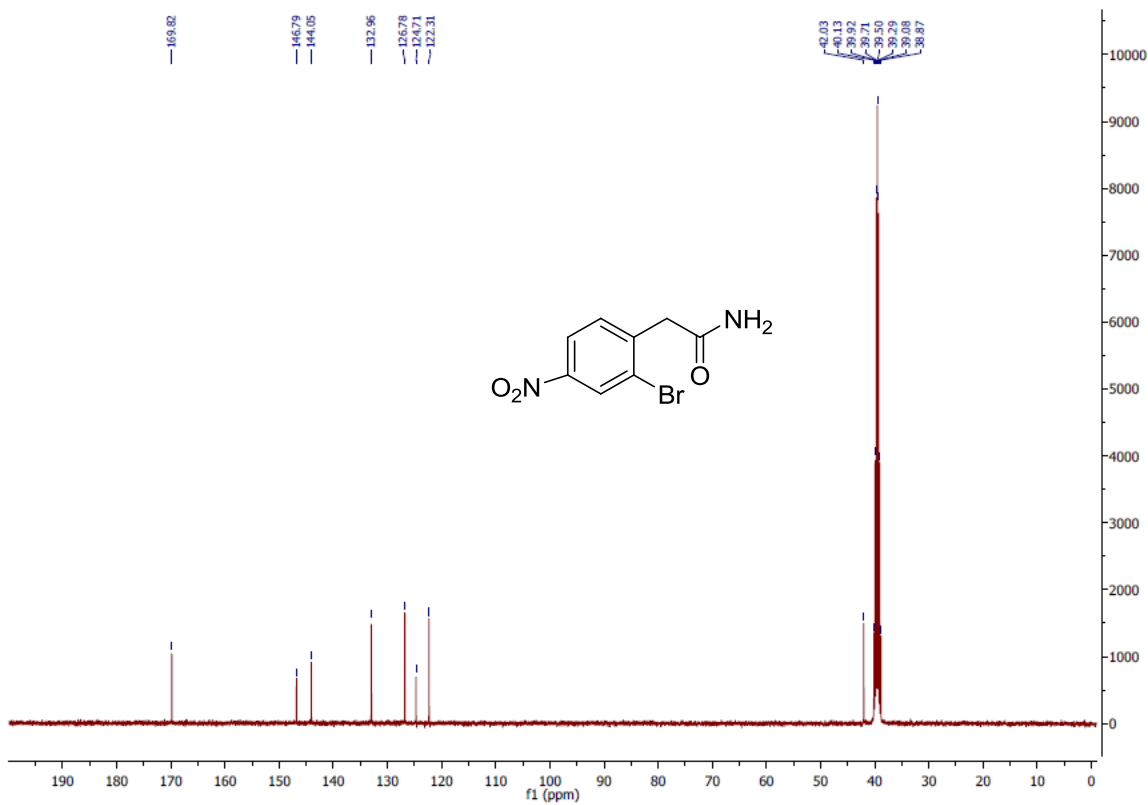
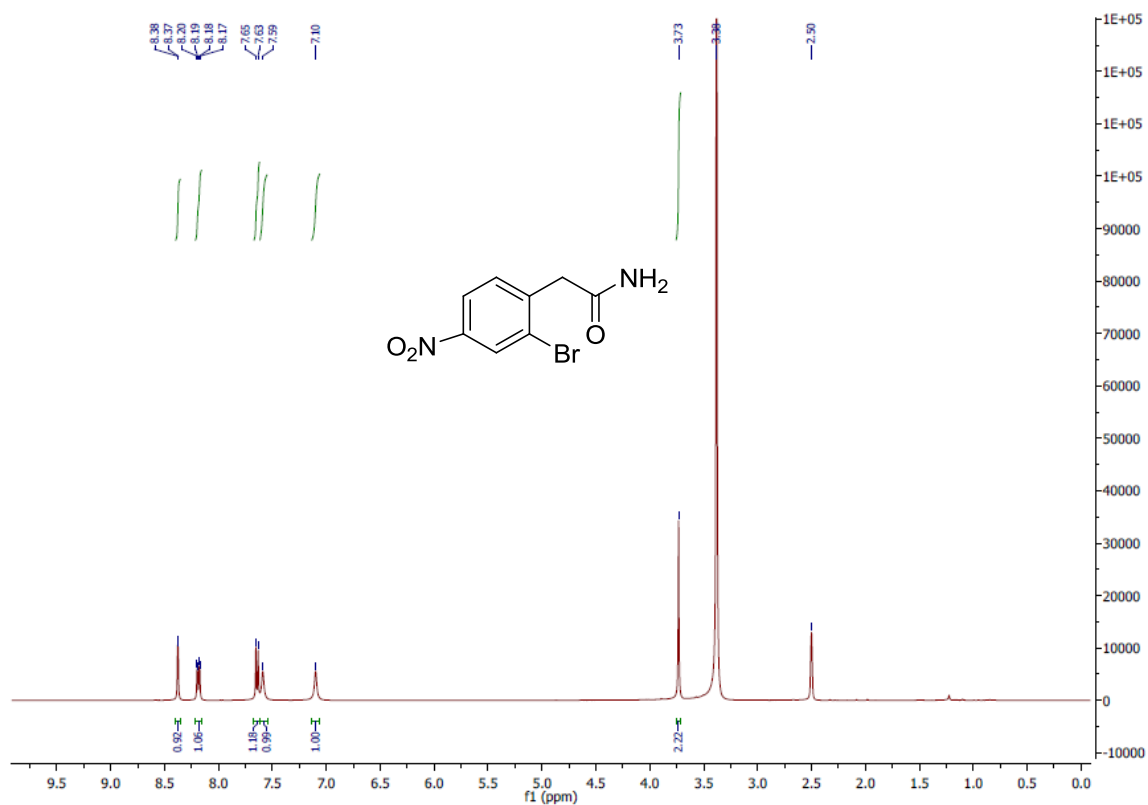


^1H , $^{13}\text{C}\{\text{H}\}$ and ^{19}F spectra of **2i**

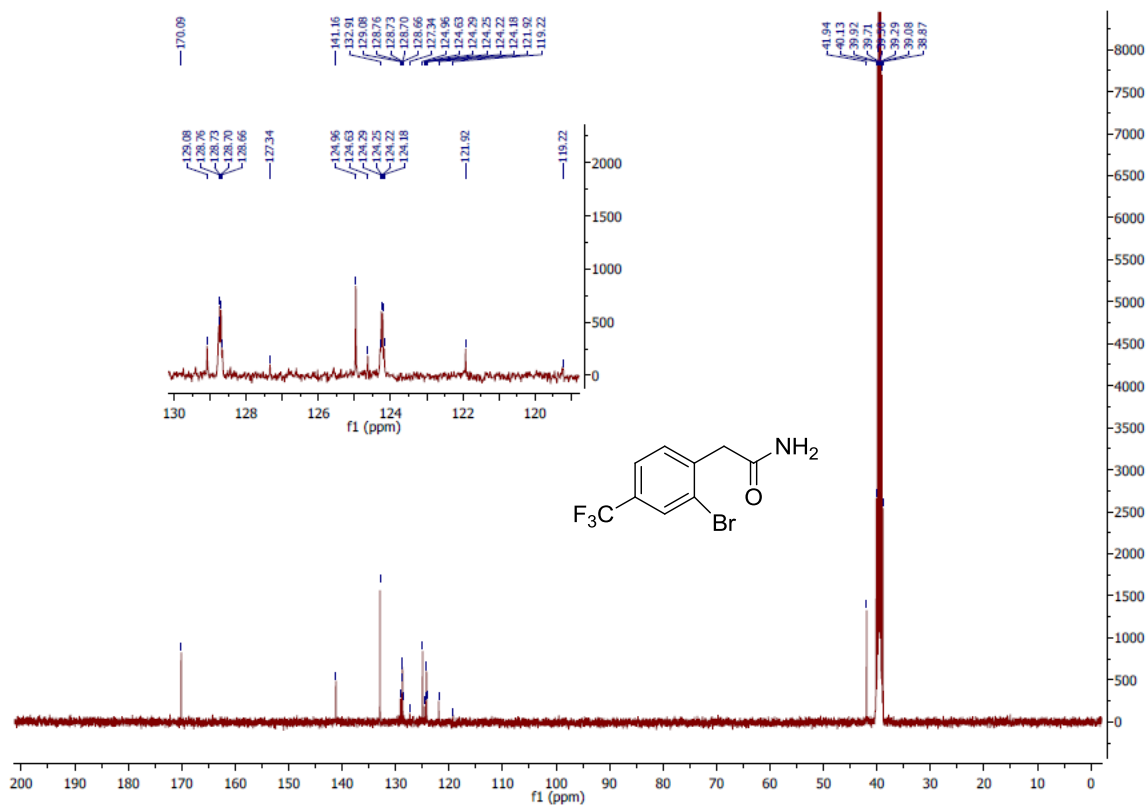
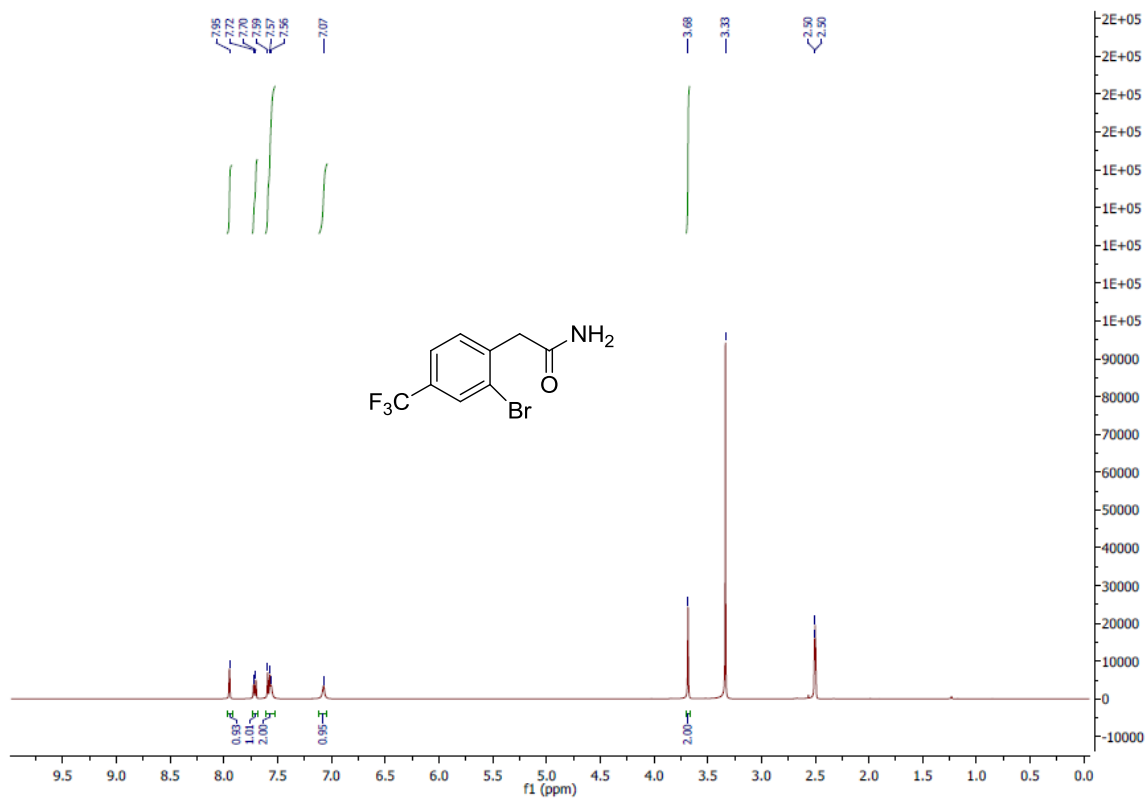


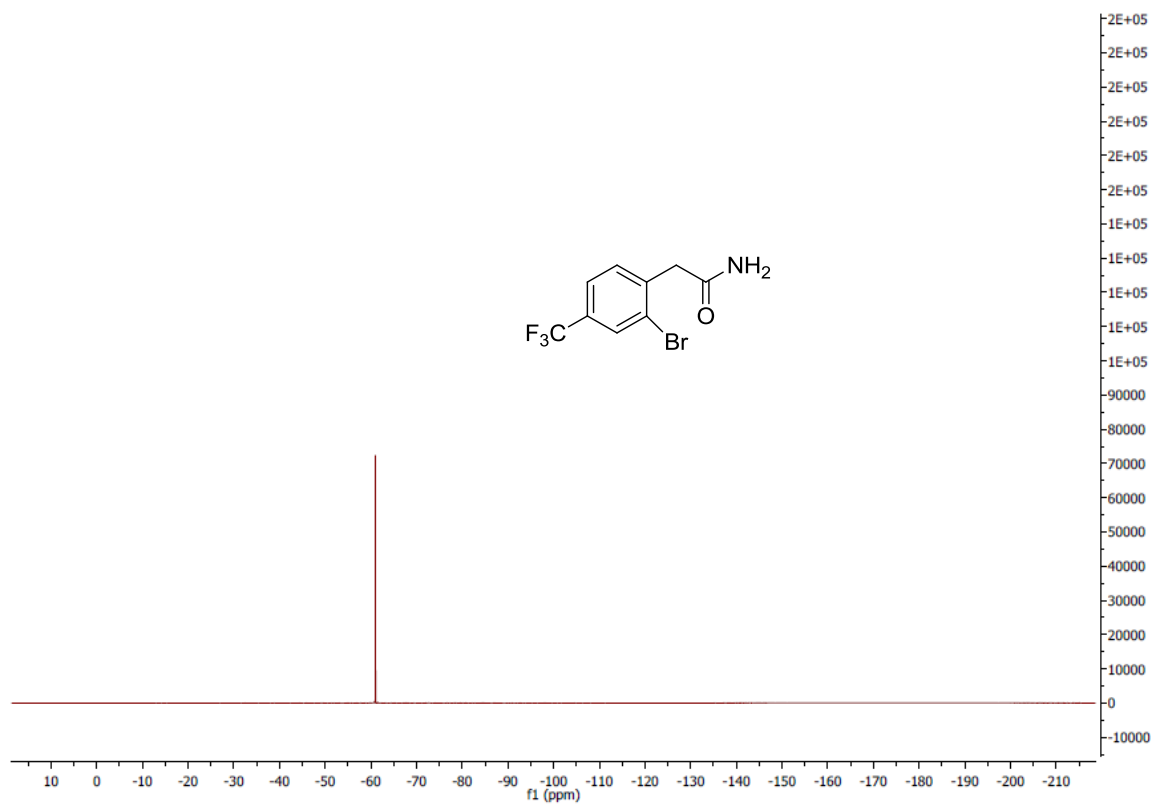


^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **2j**

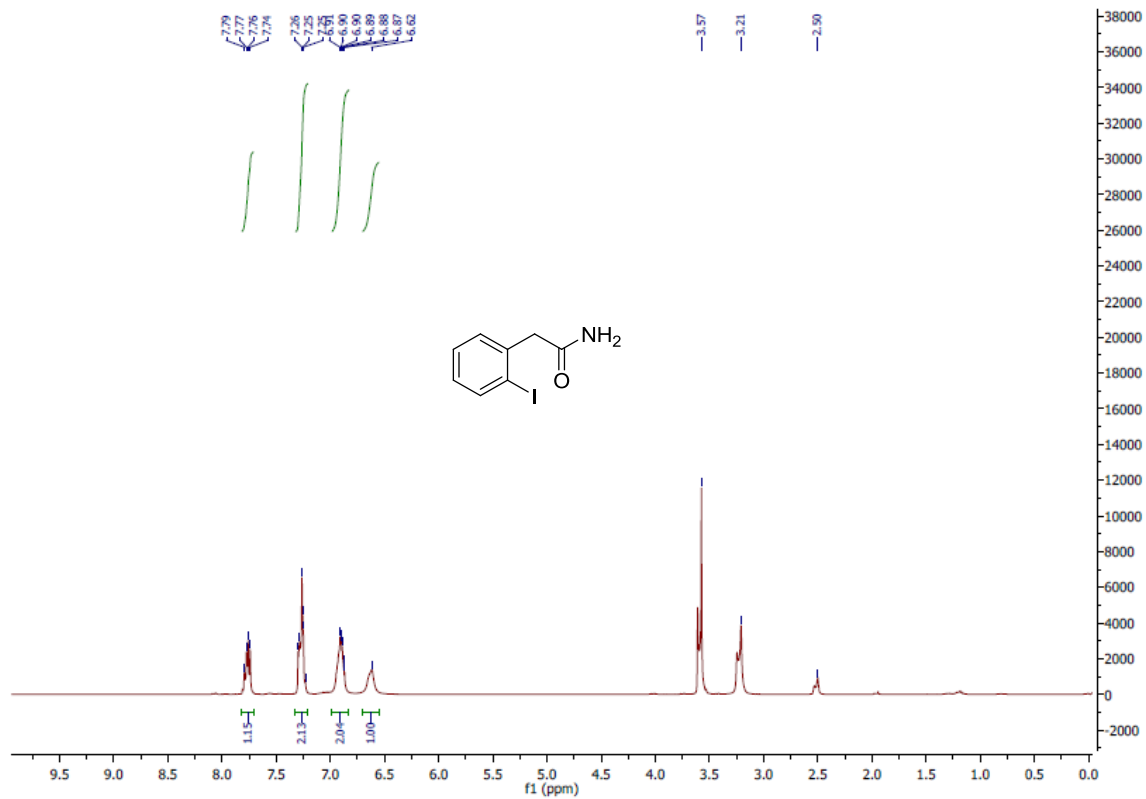


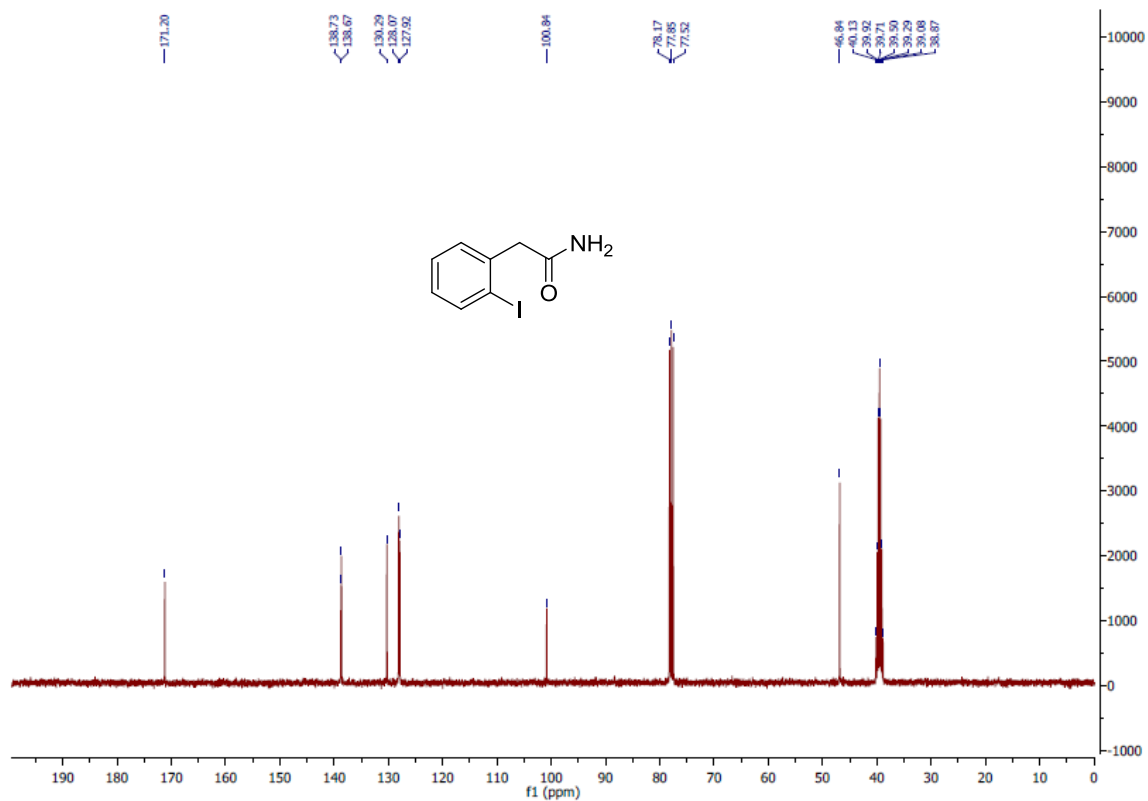
^1H , $^{13}\text{C}\{\text{H}\}$ and ^{19}F spectra of **2k**



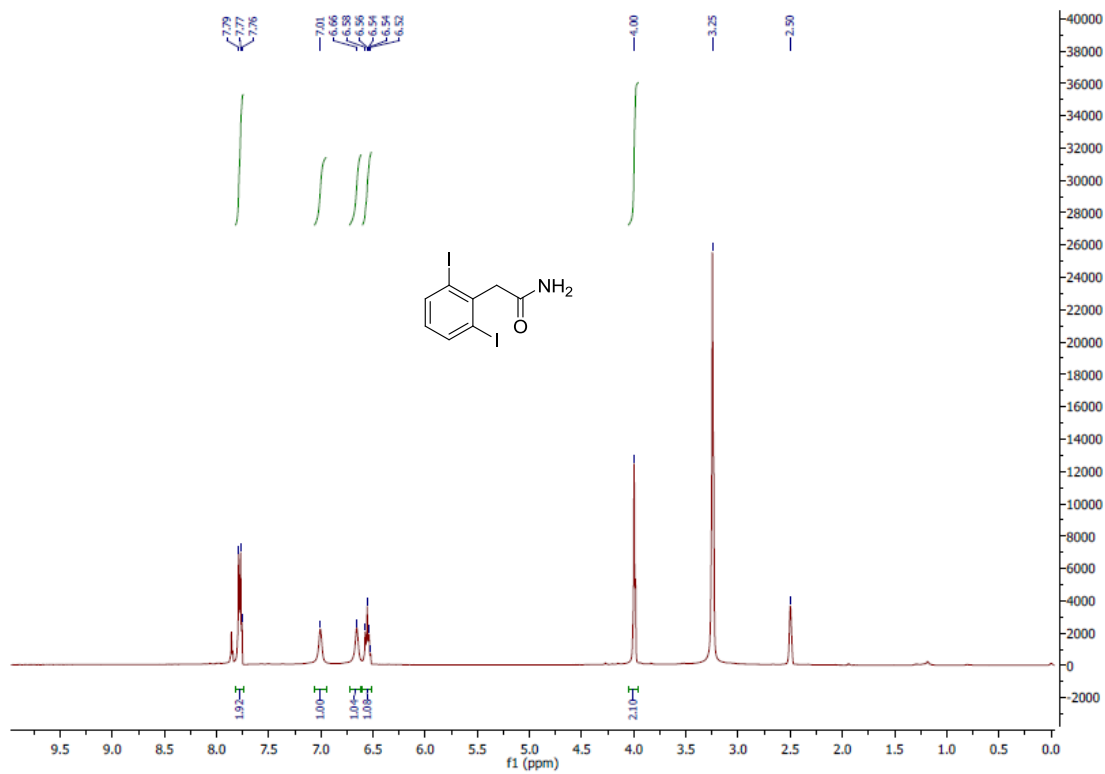


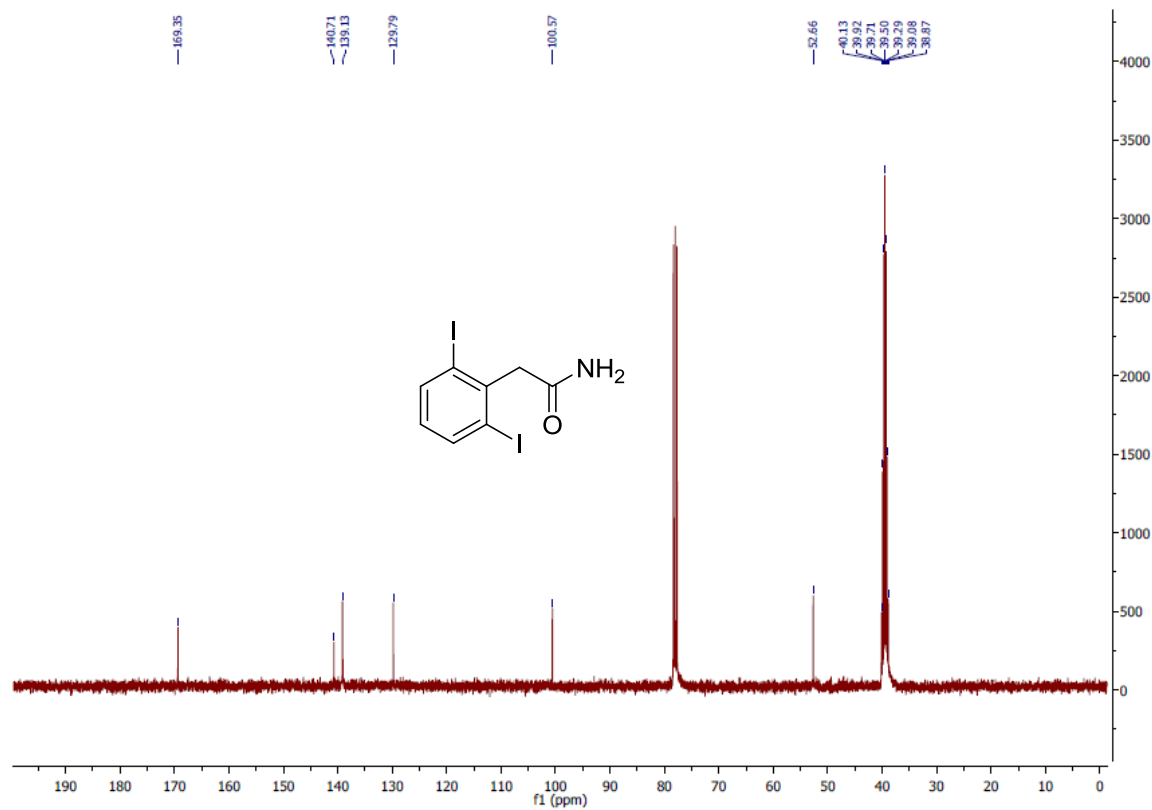
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **3a**



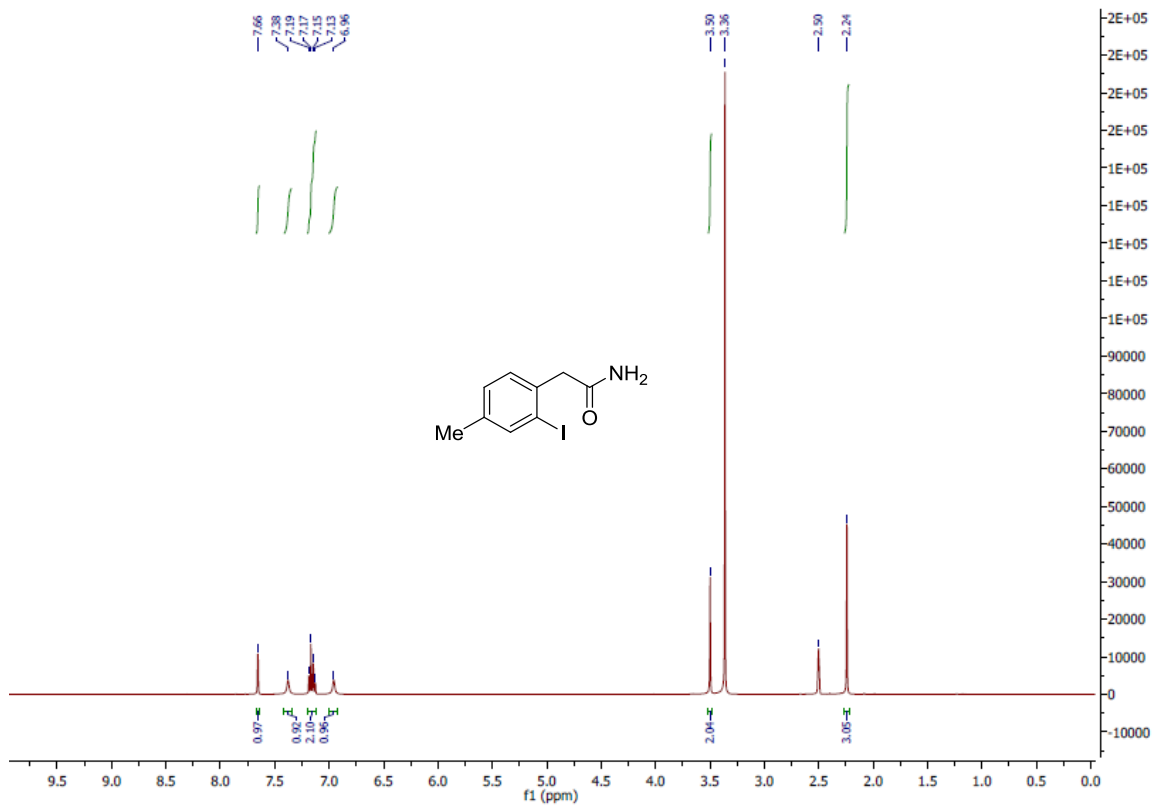


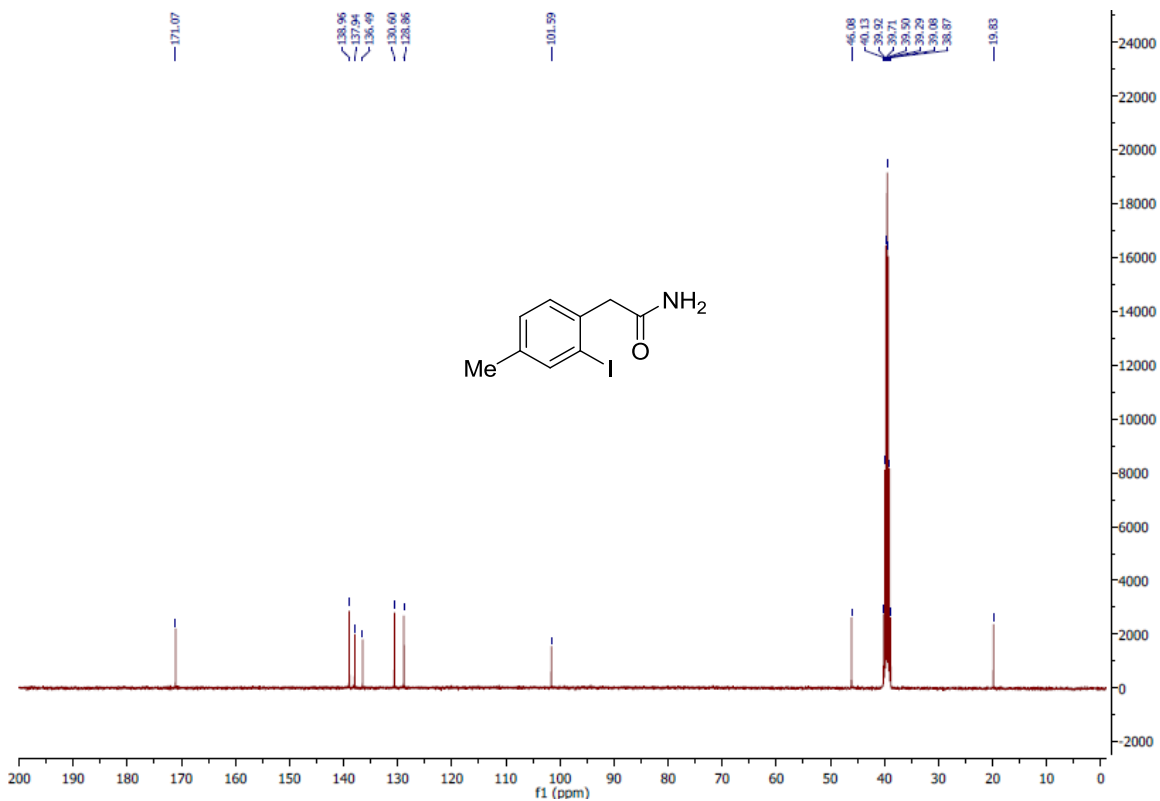
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **3aa**



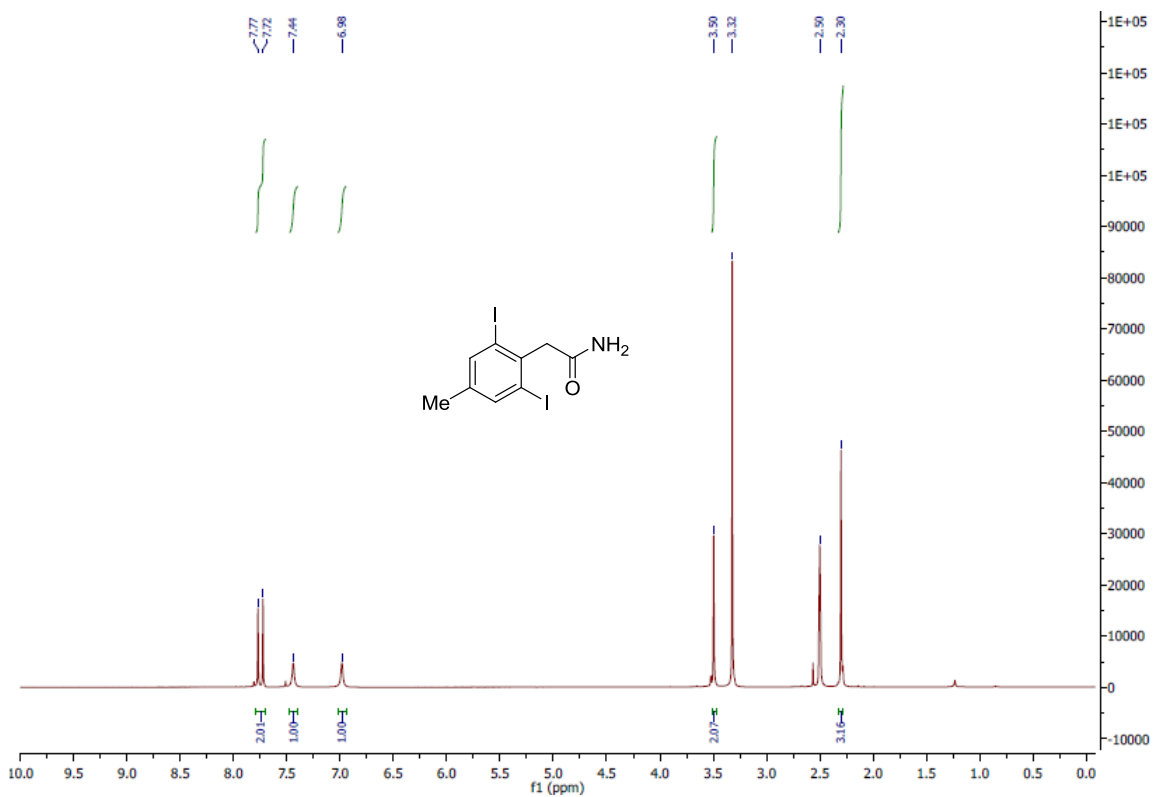


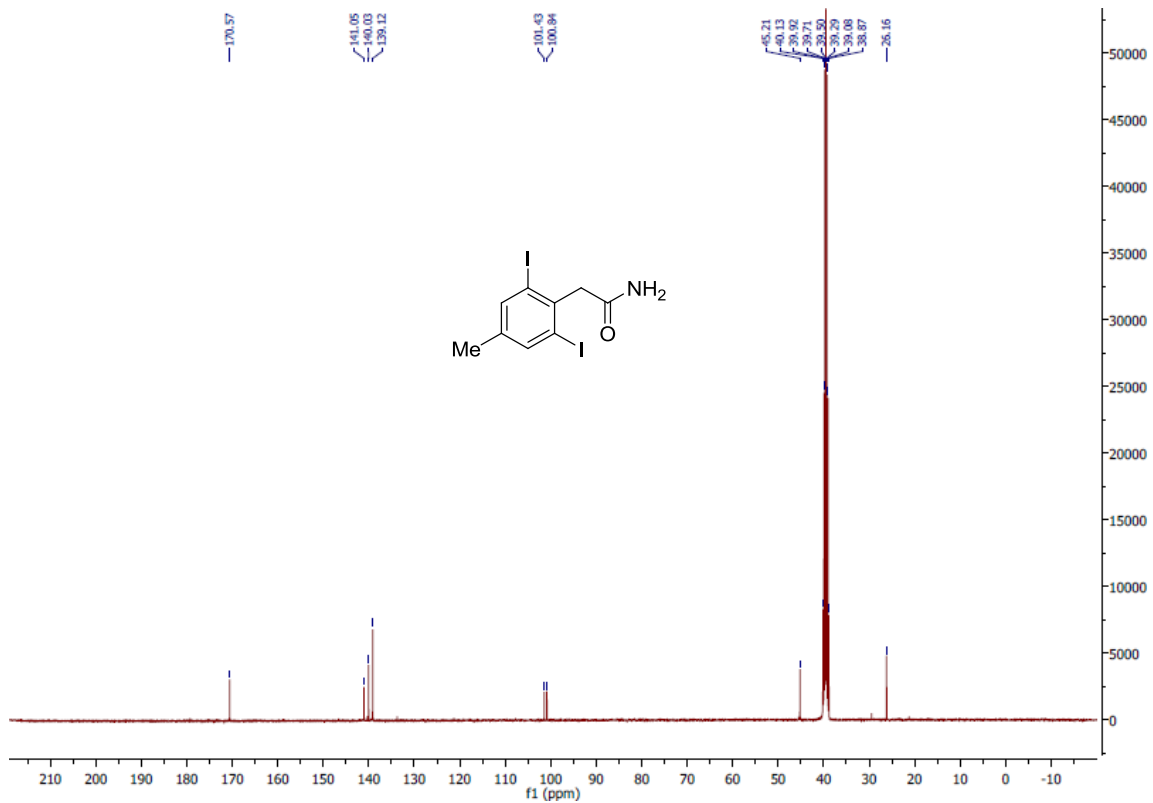
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **3b**



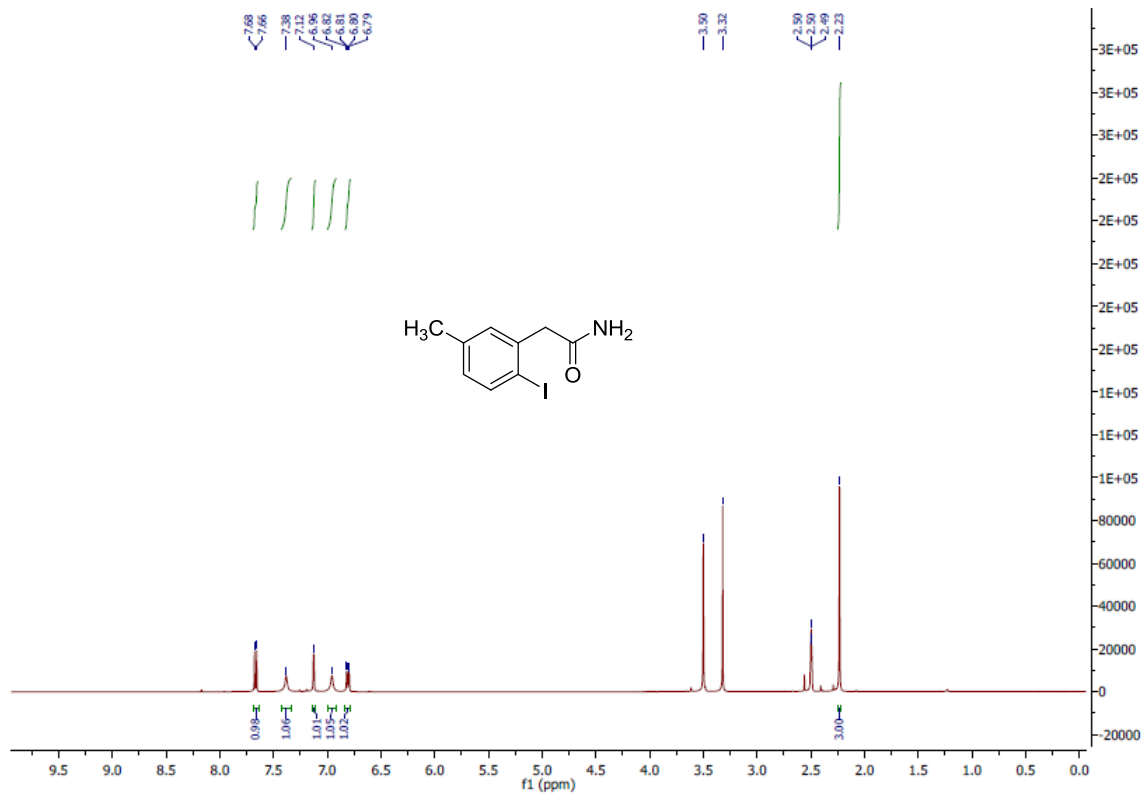


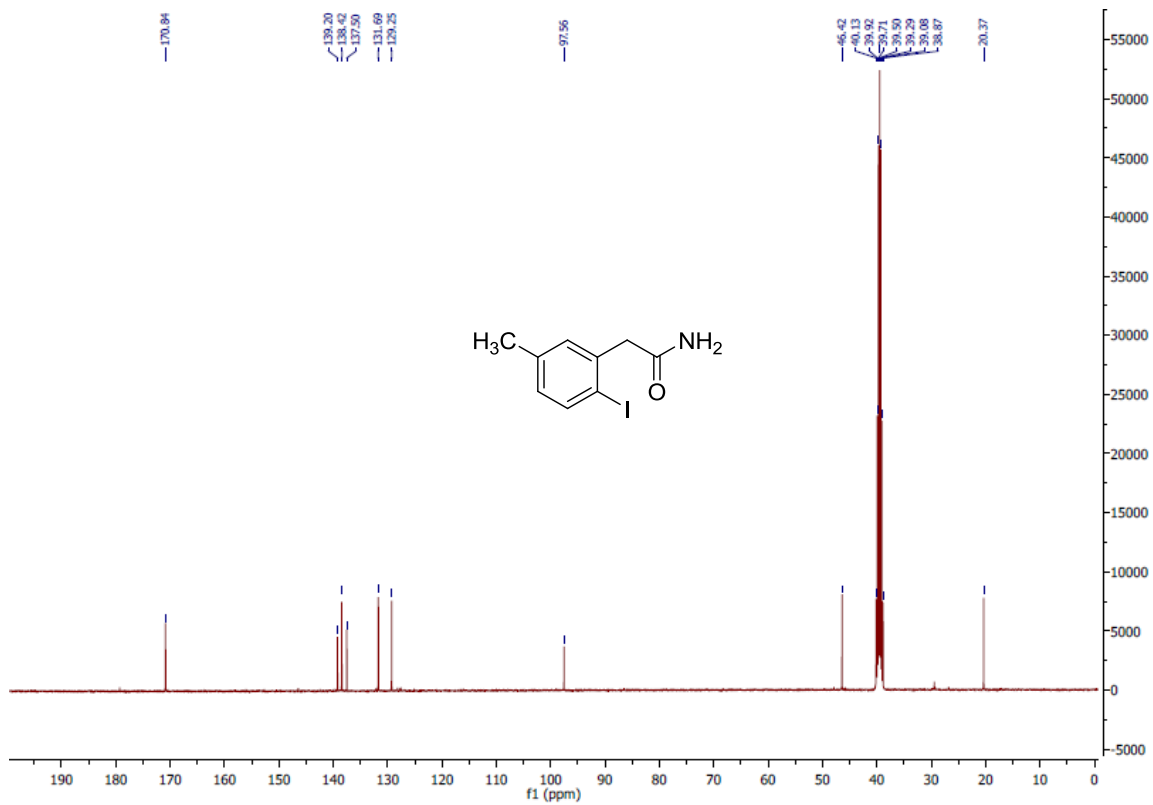
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **3bb**



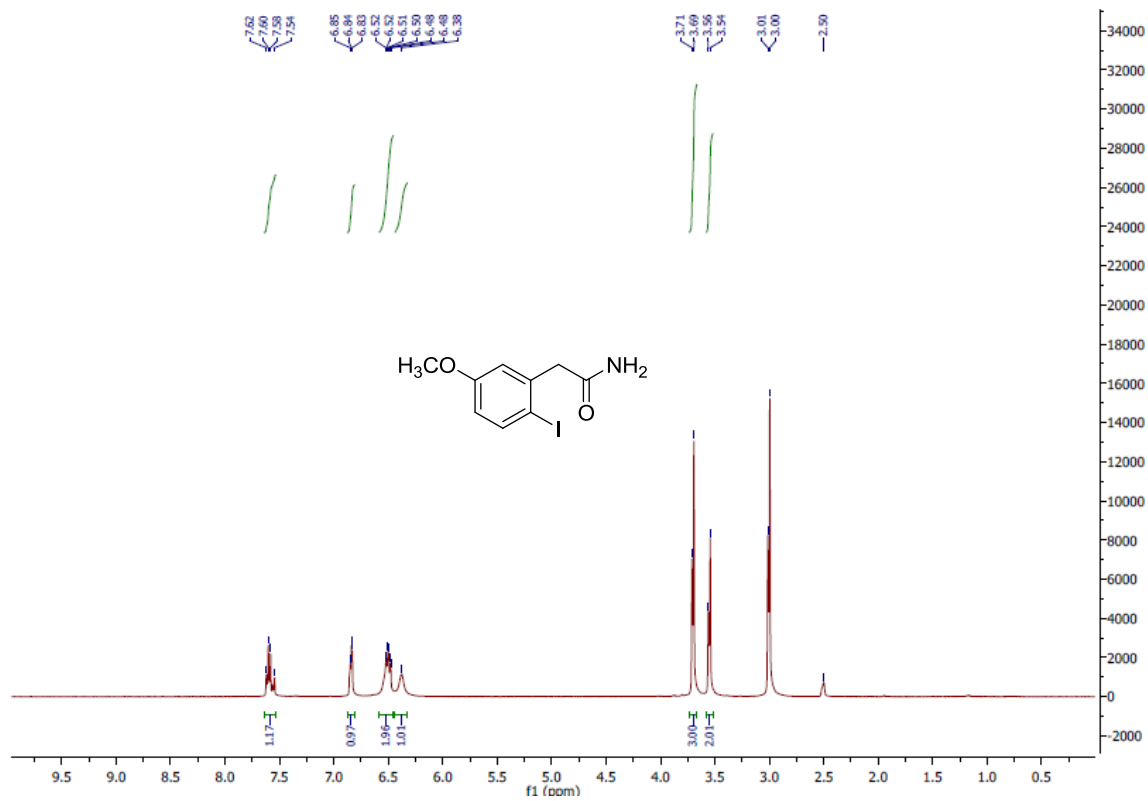


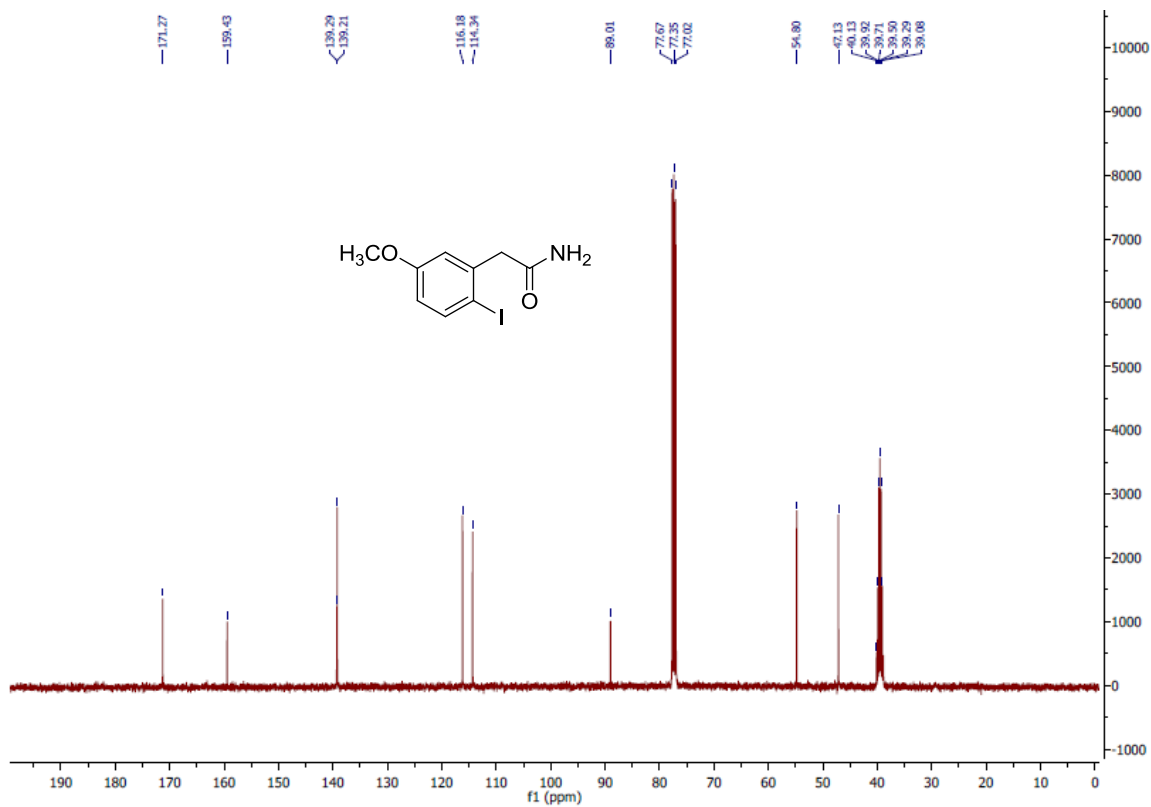
¹H and ¹³C{H} spectra of **3c**



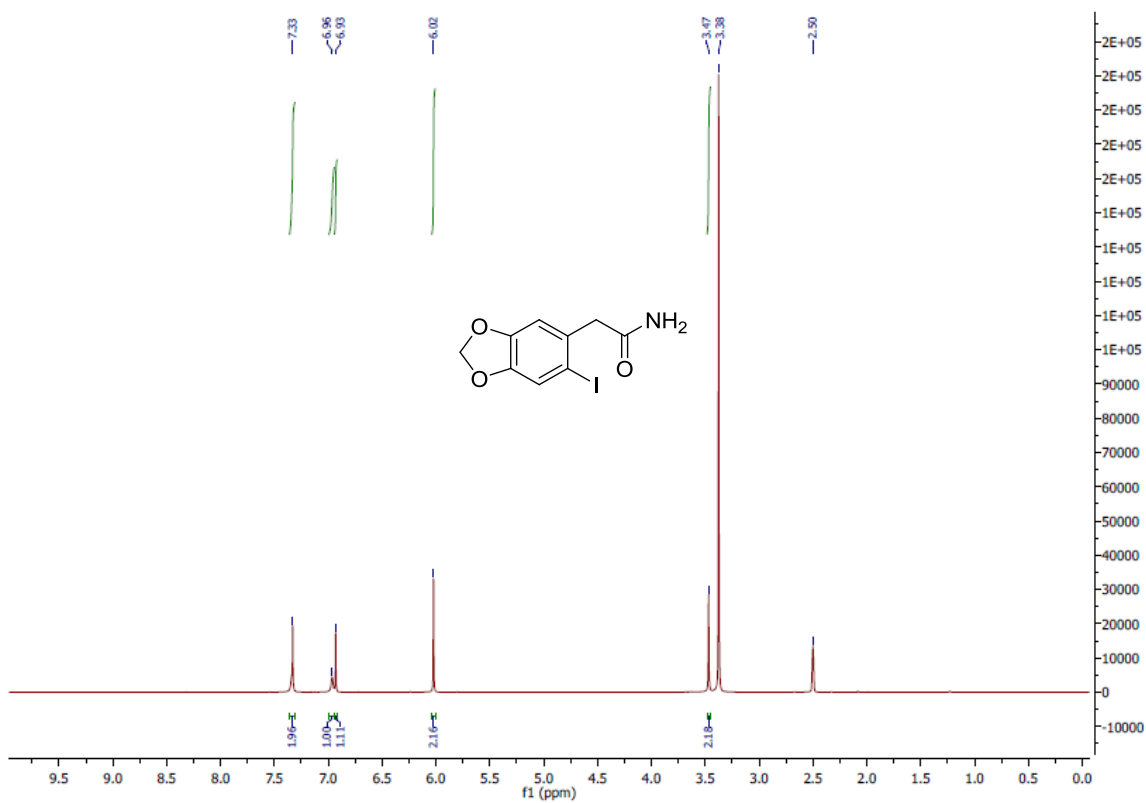


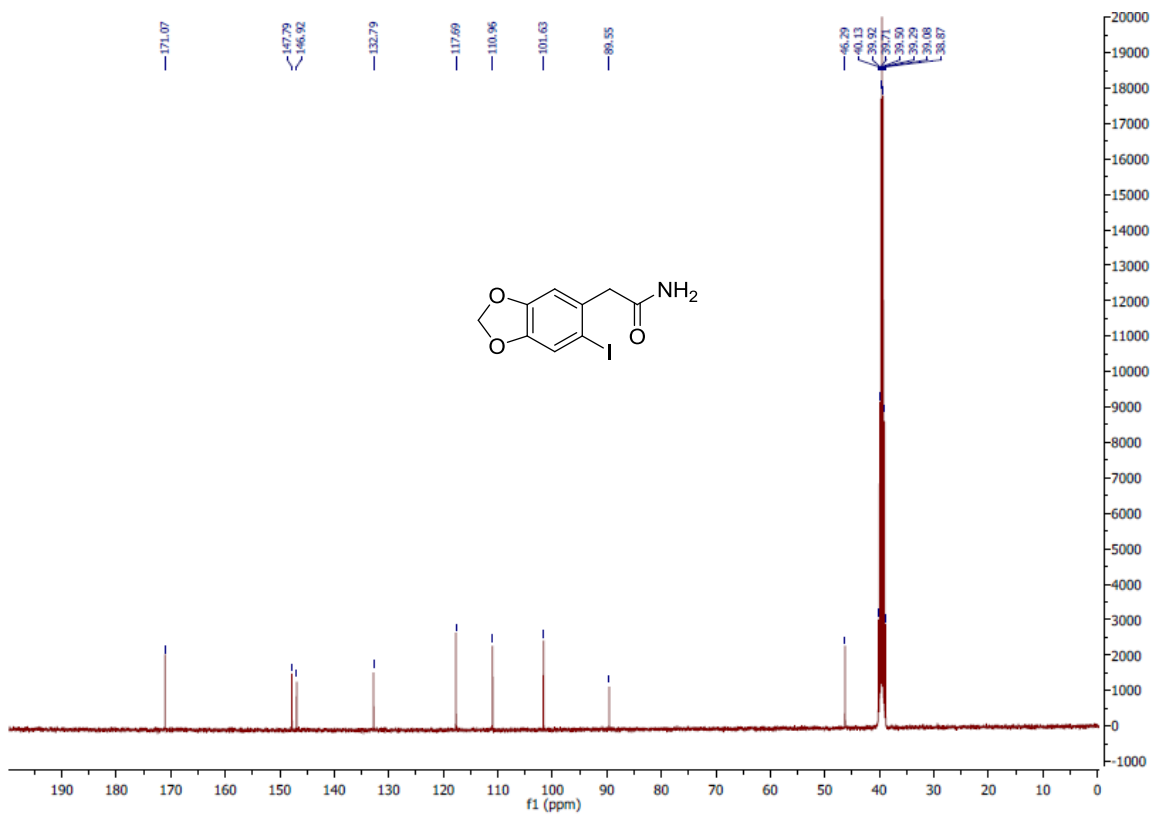
¹H and ¹³C{H} spectra of **3d**



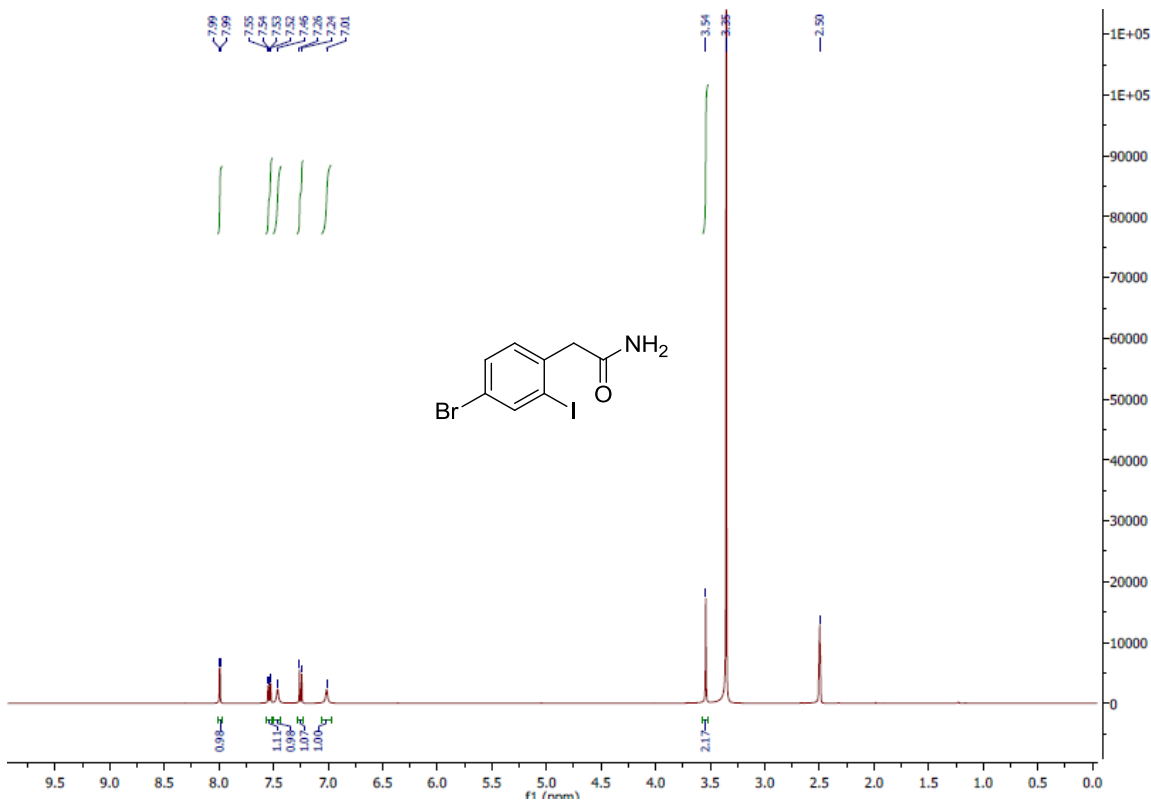


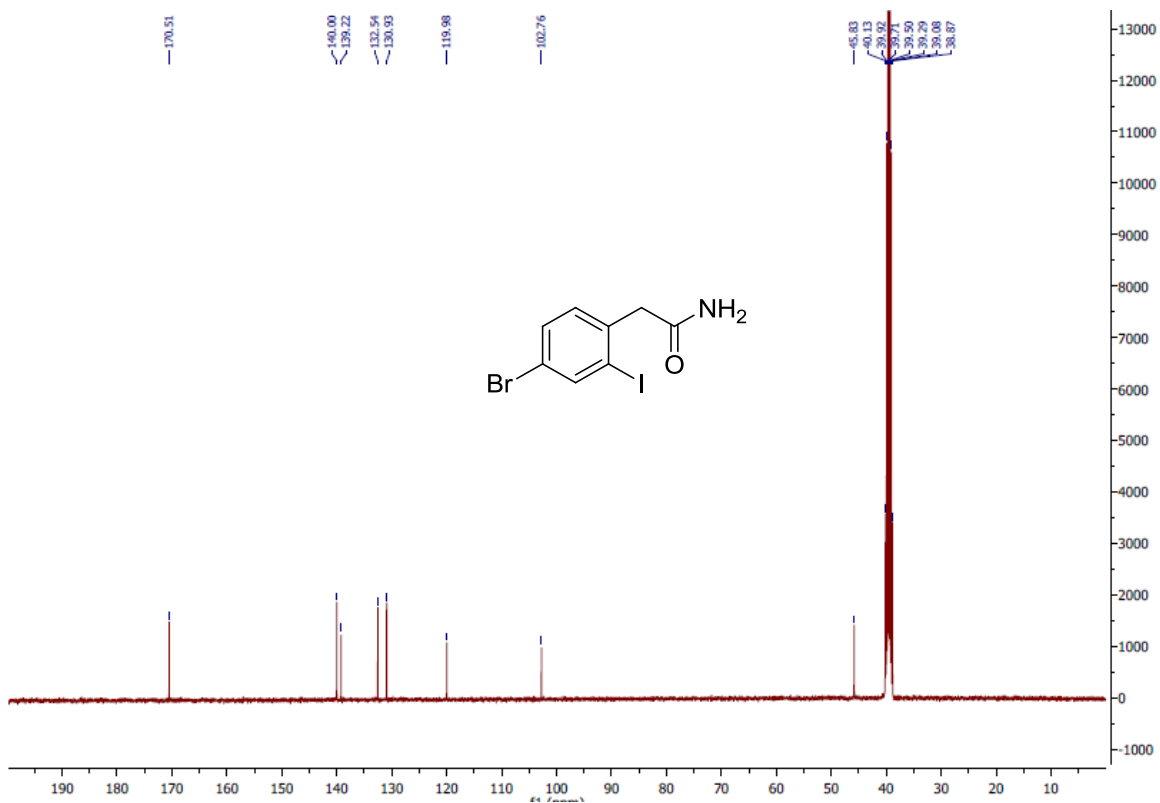
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **3e**



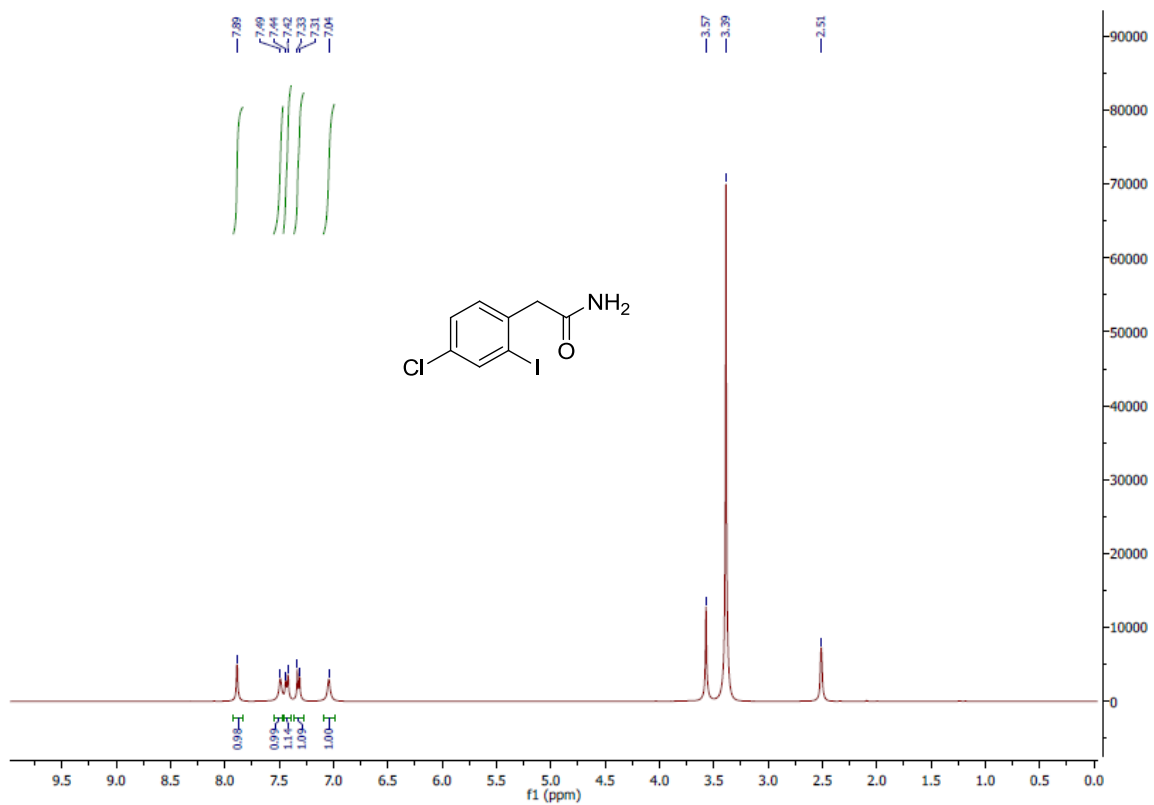


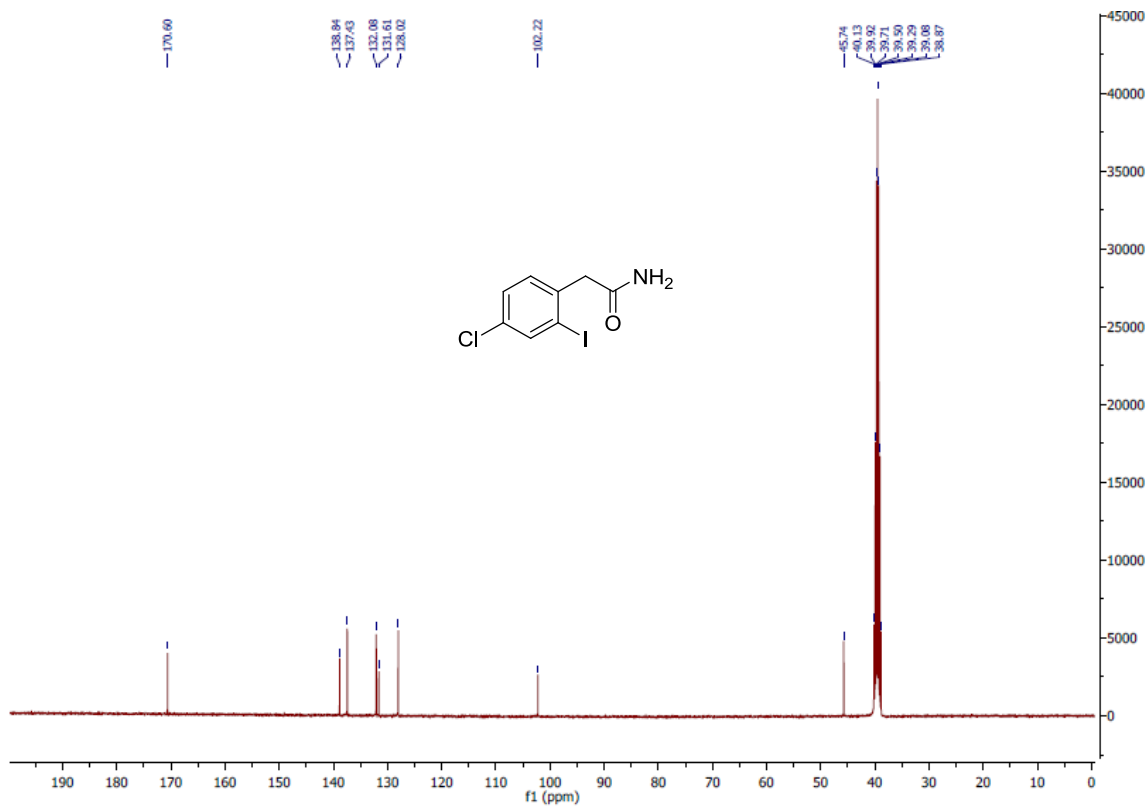
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **3f**



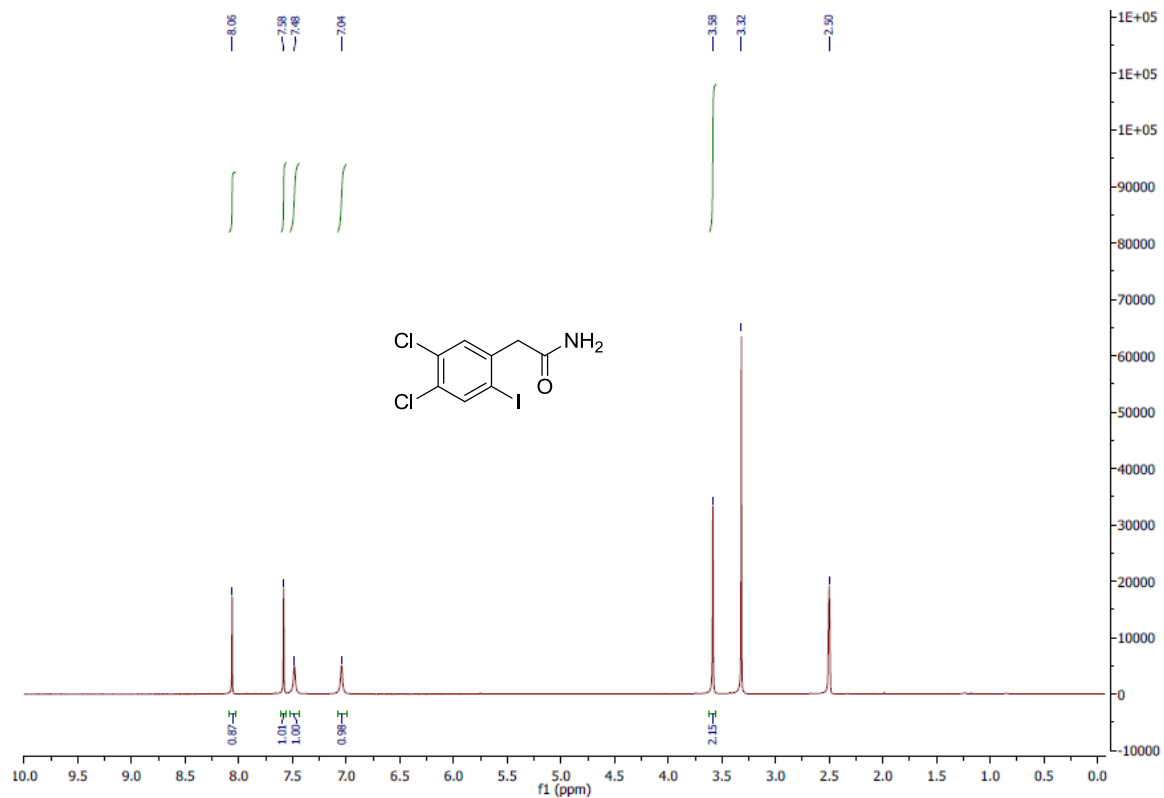


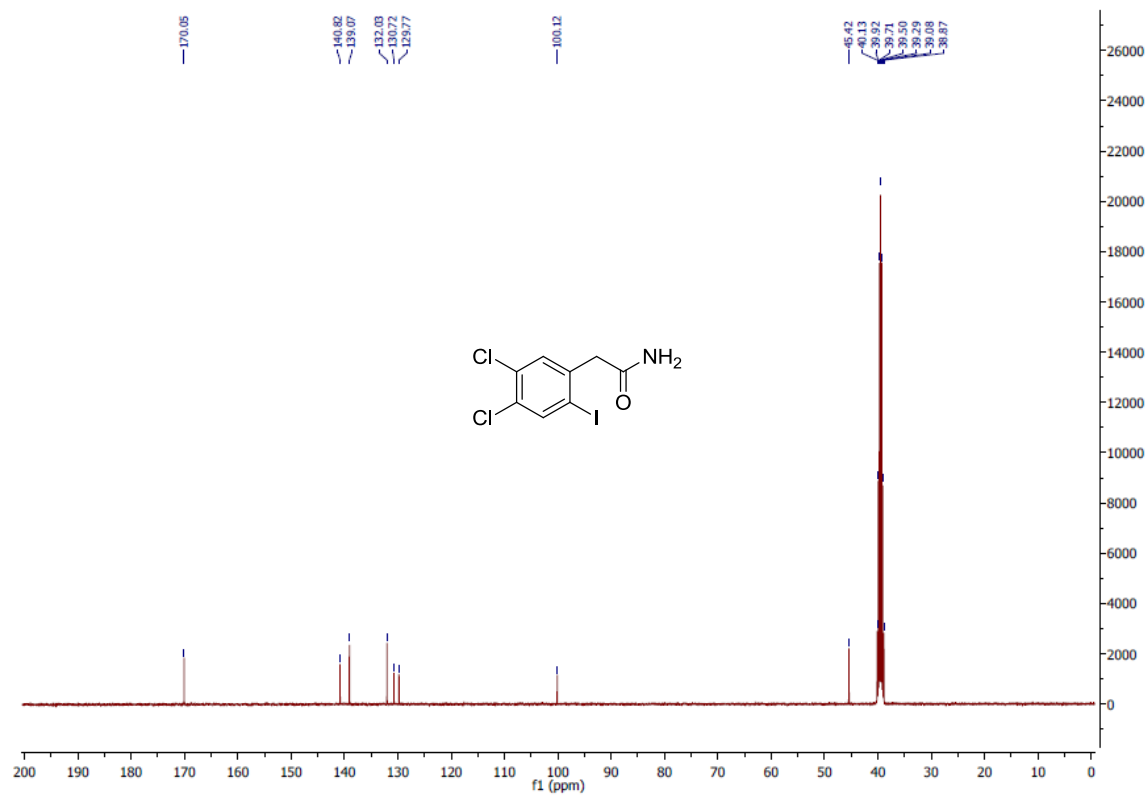
¹H and ¹³C{H} spectra of **3g**



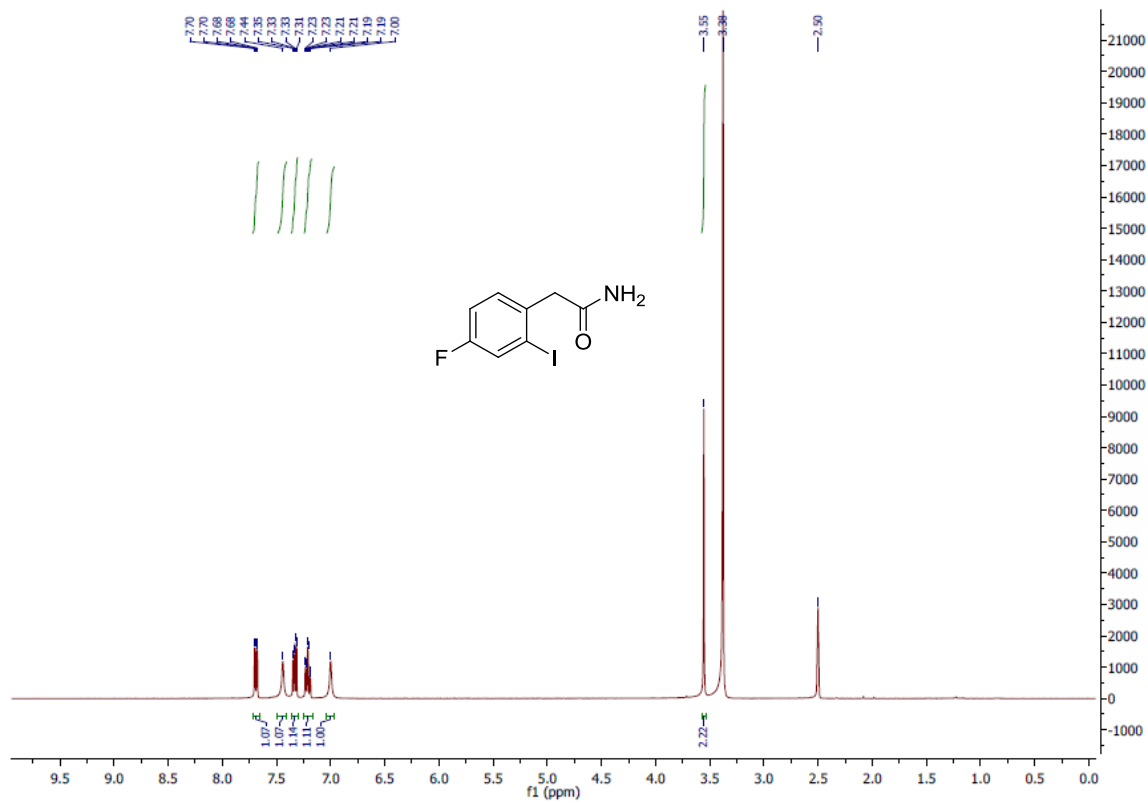


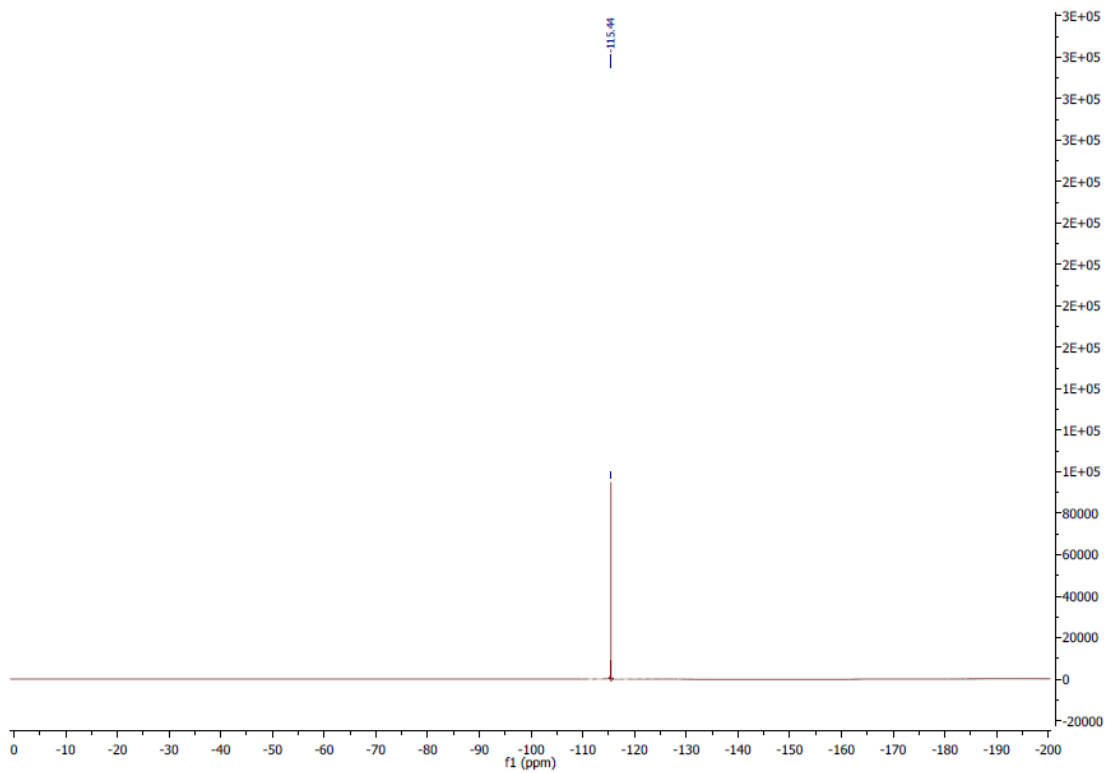
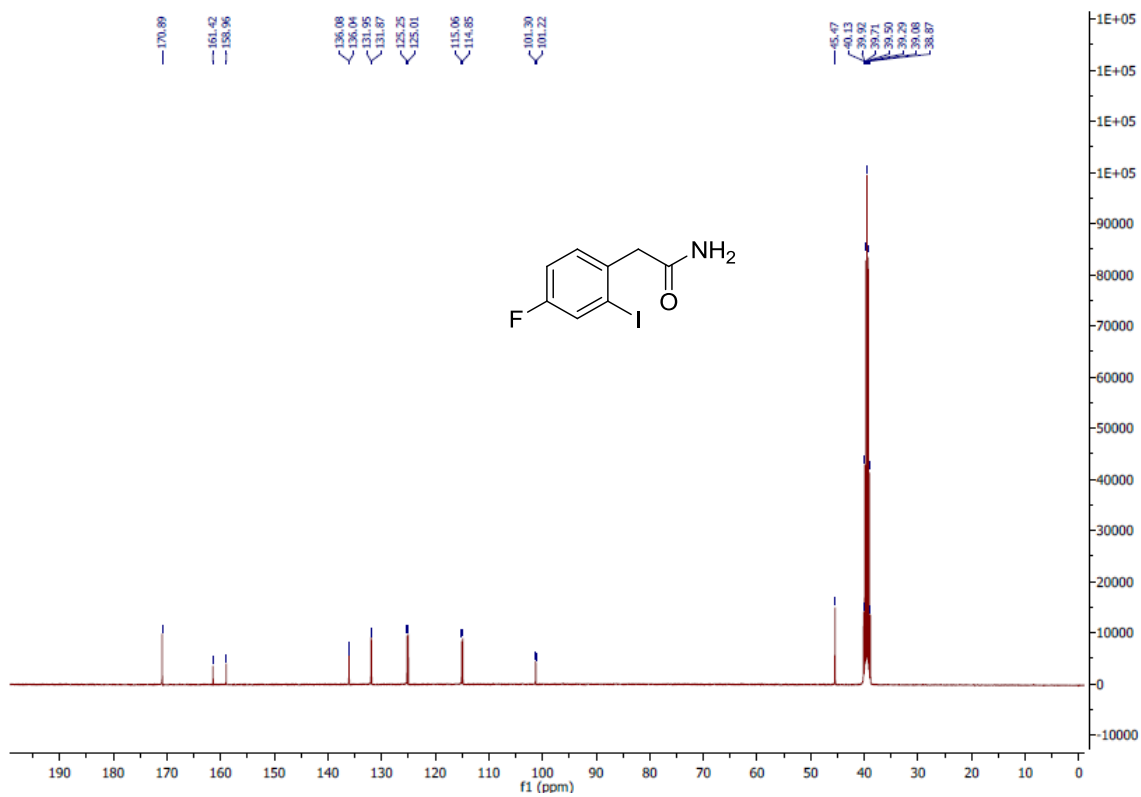
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **3h**



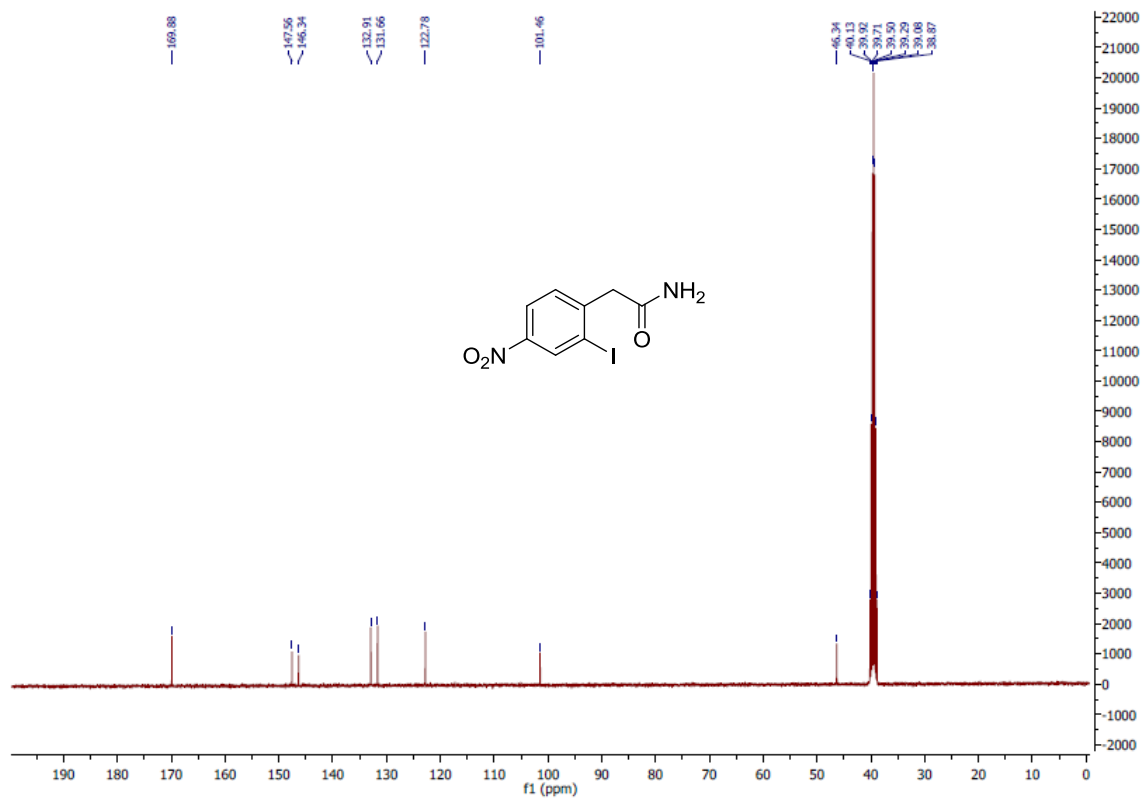
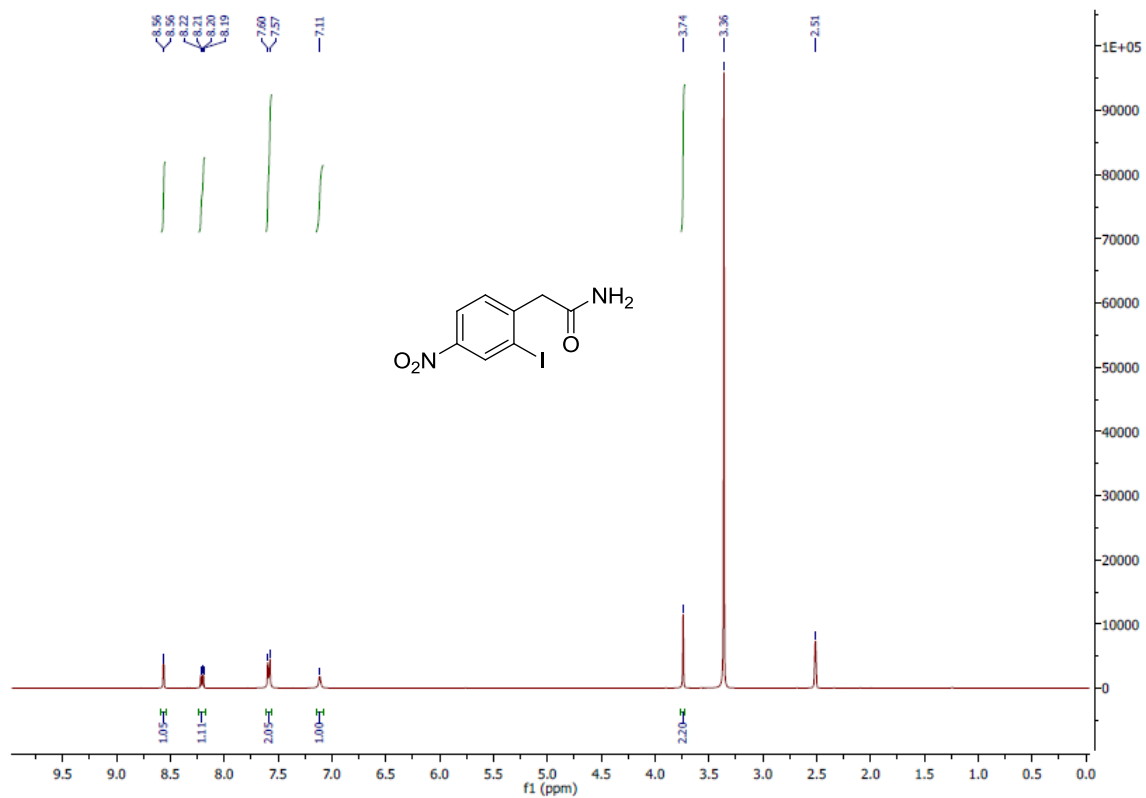


^1H $^{13}\text{C}\{\text{H}\}$, ^{19}F and spectra of **3i**

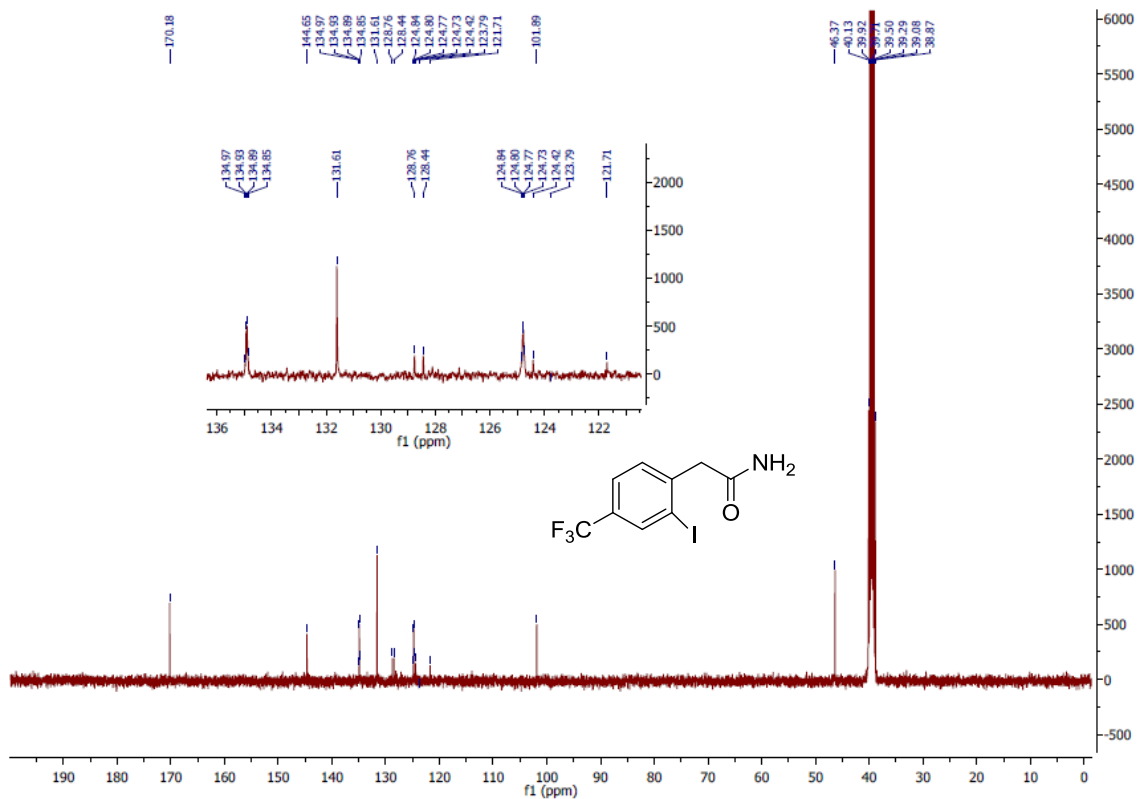
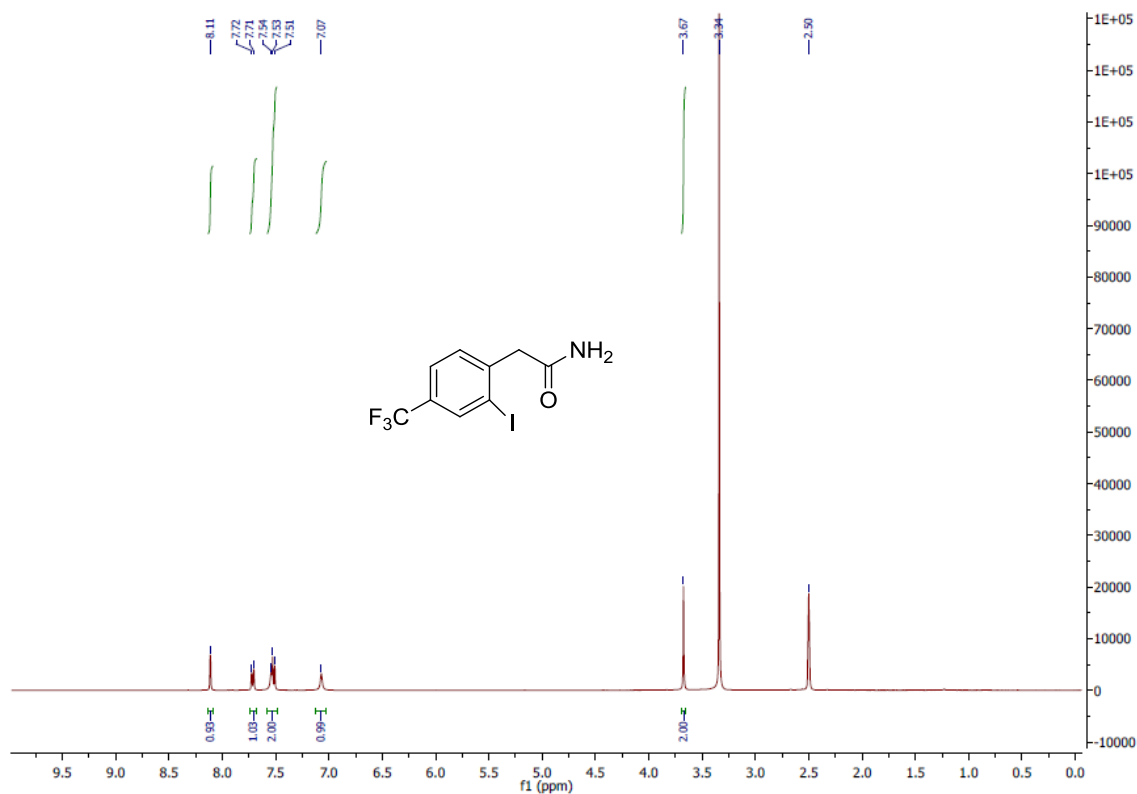


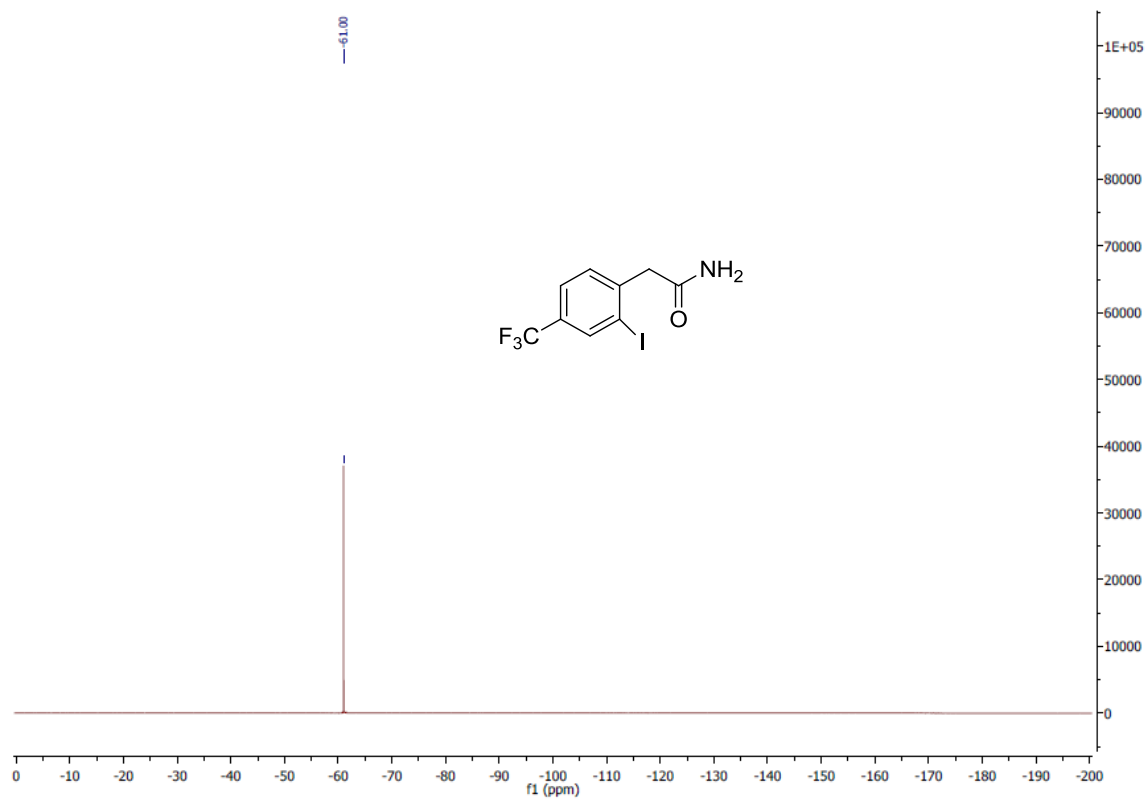


^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **3j**

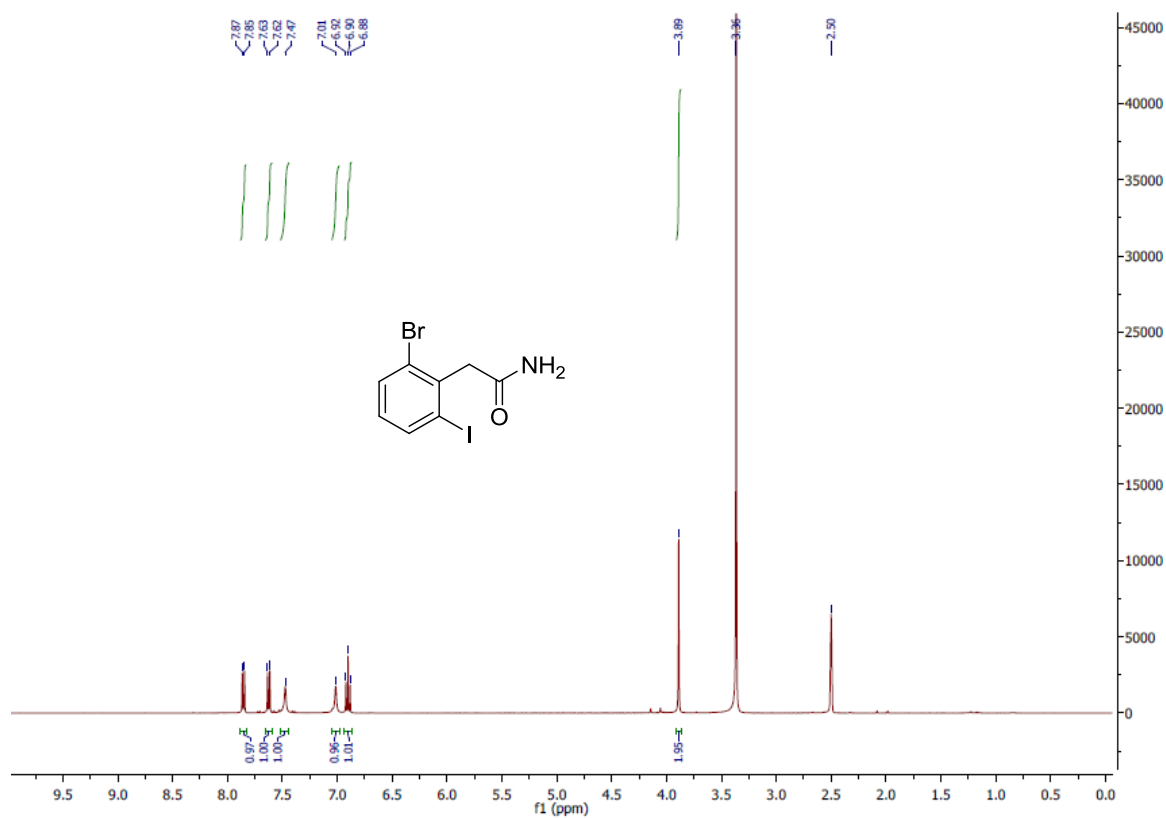


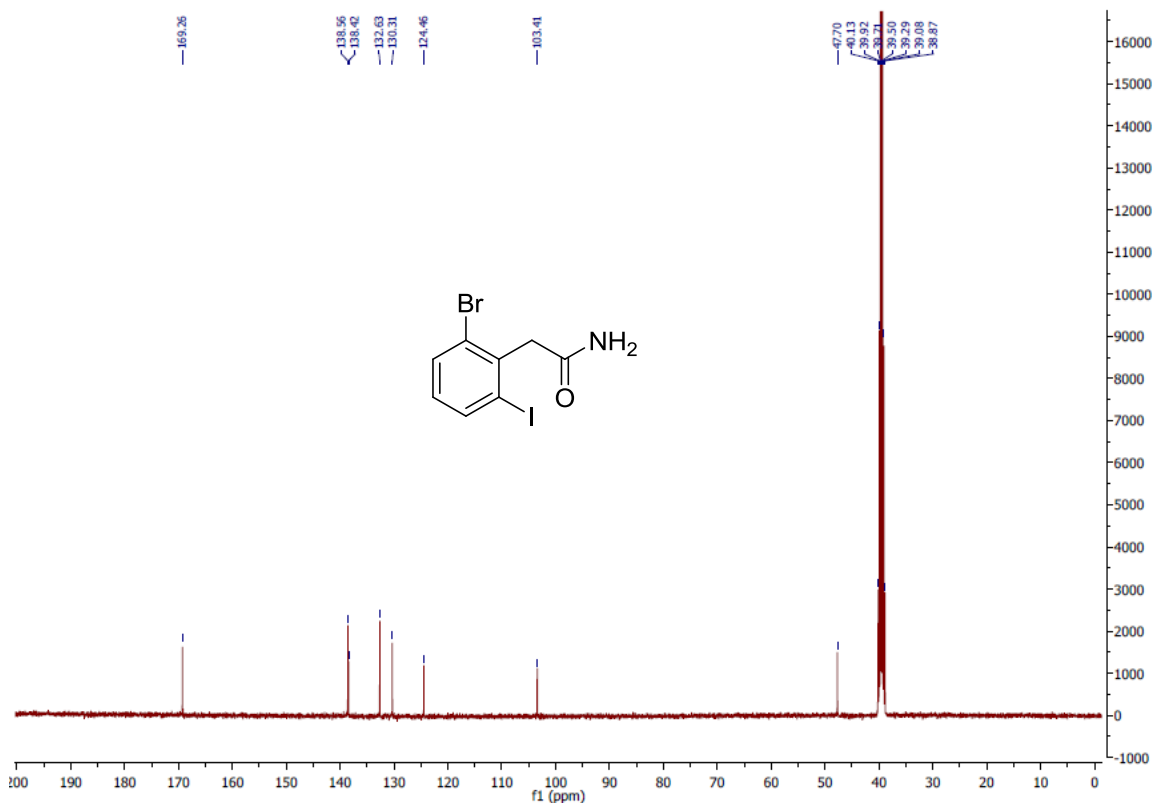
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **3k**



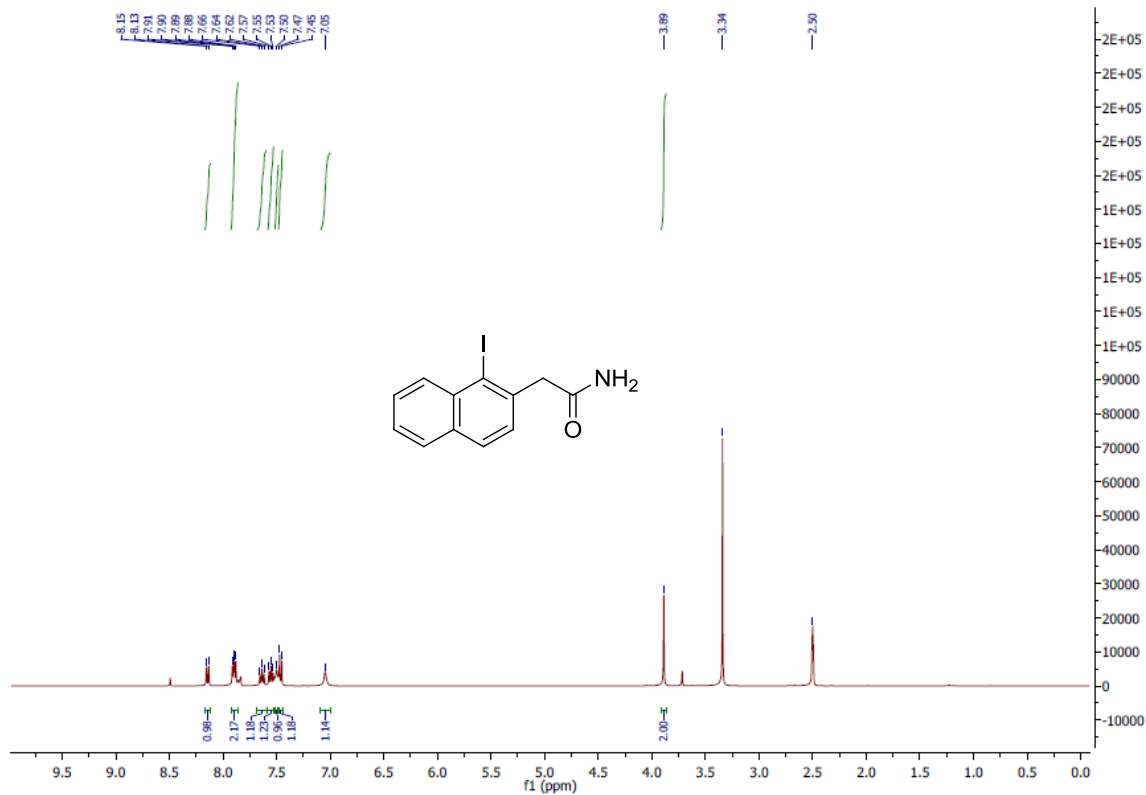


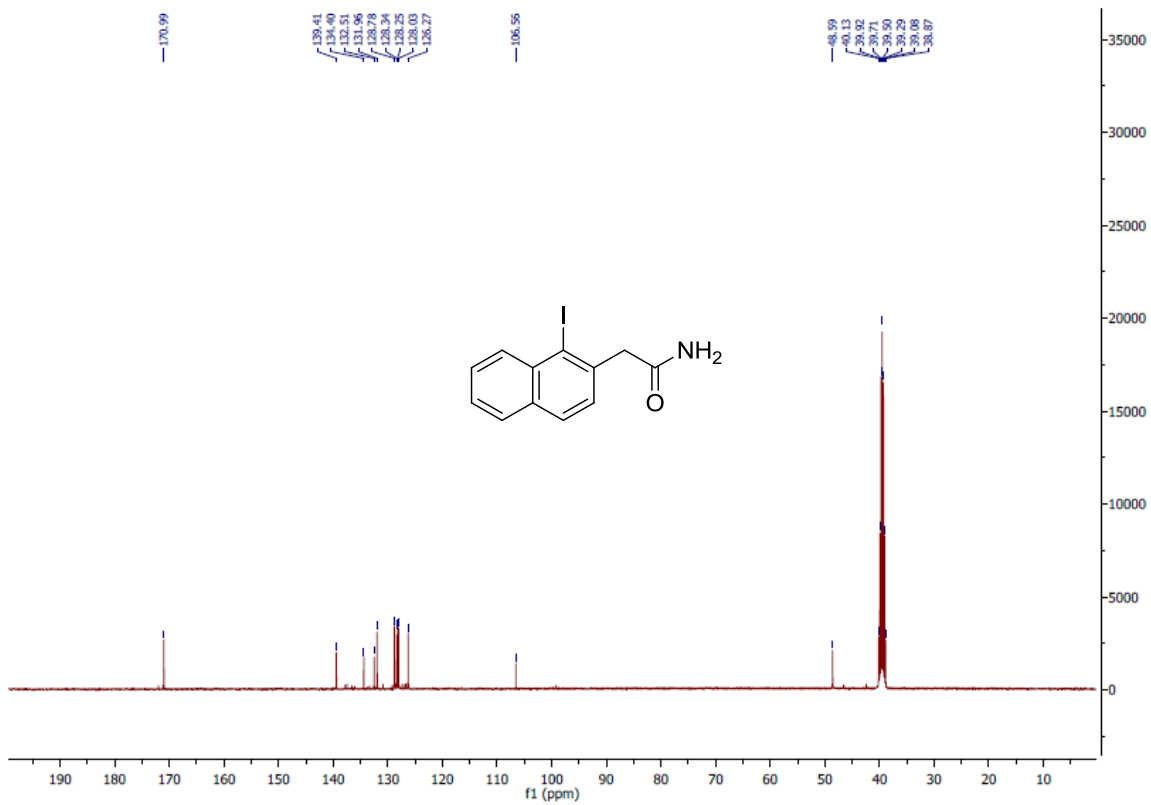
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **31**



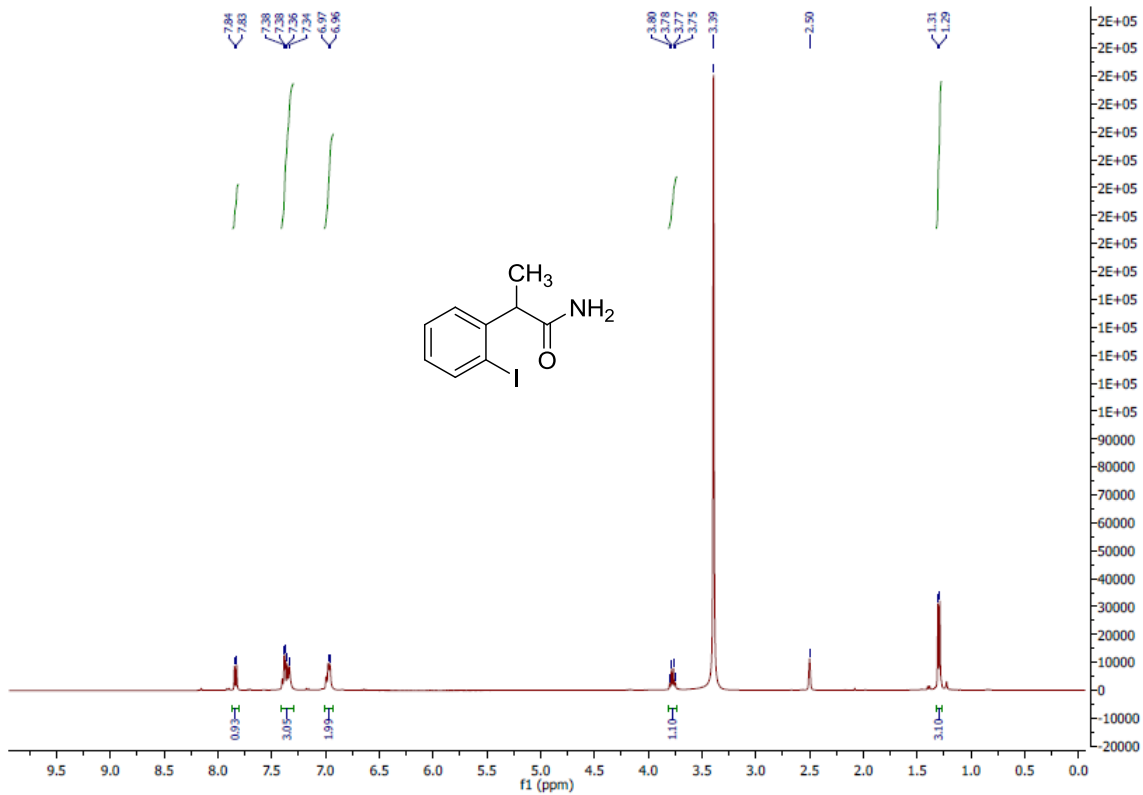


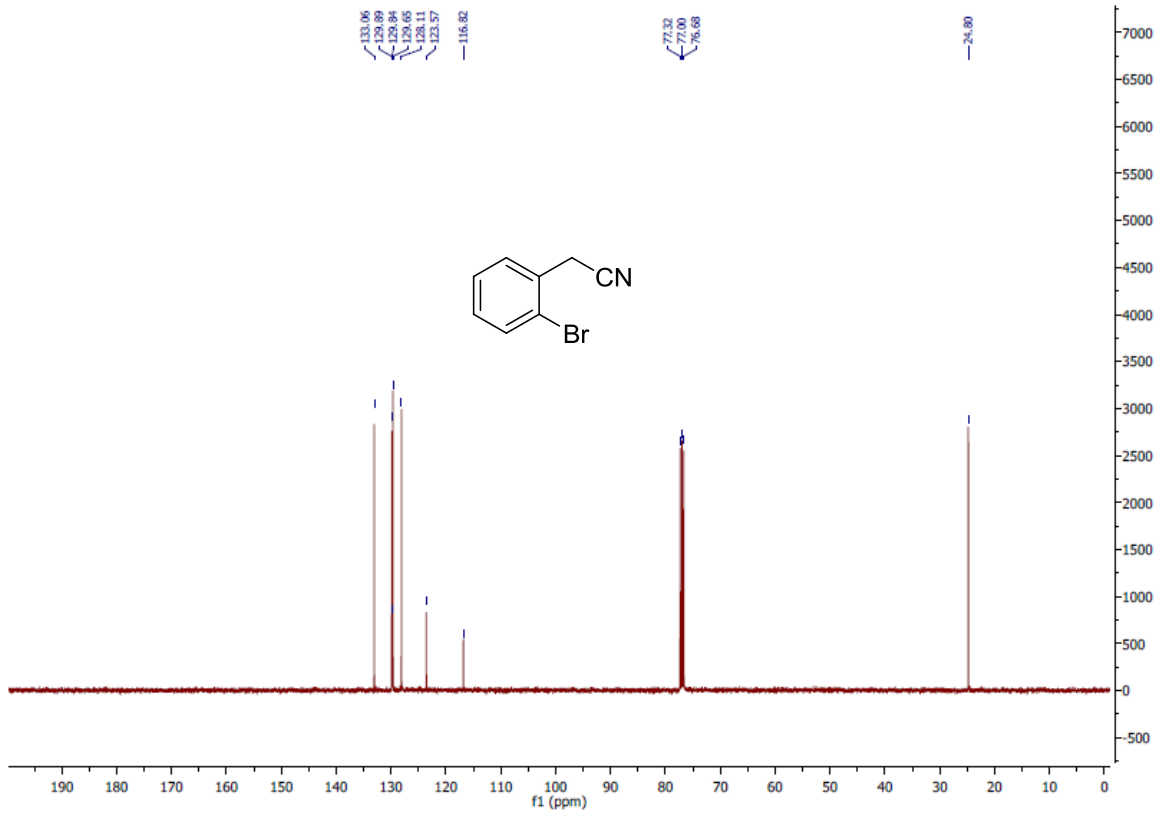
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **3m**



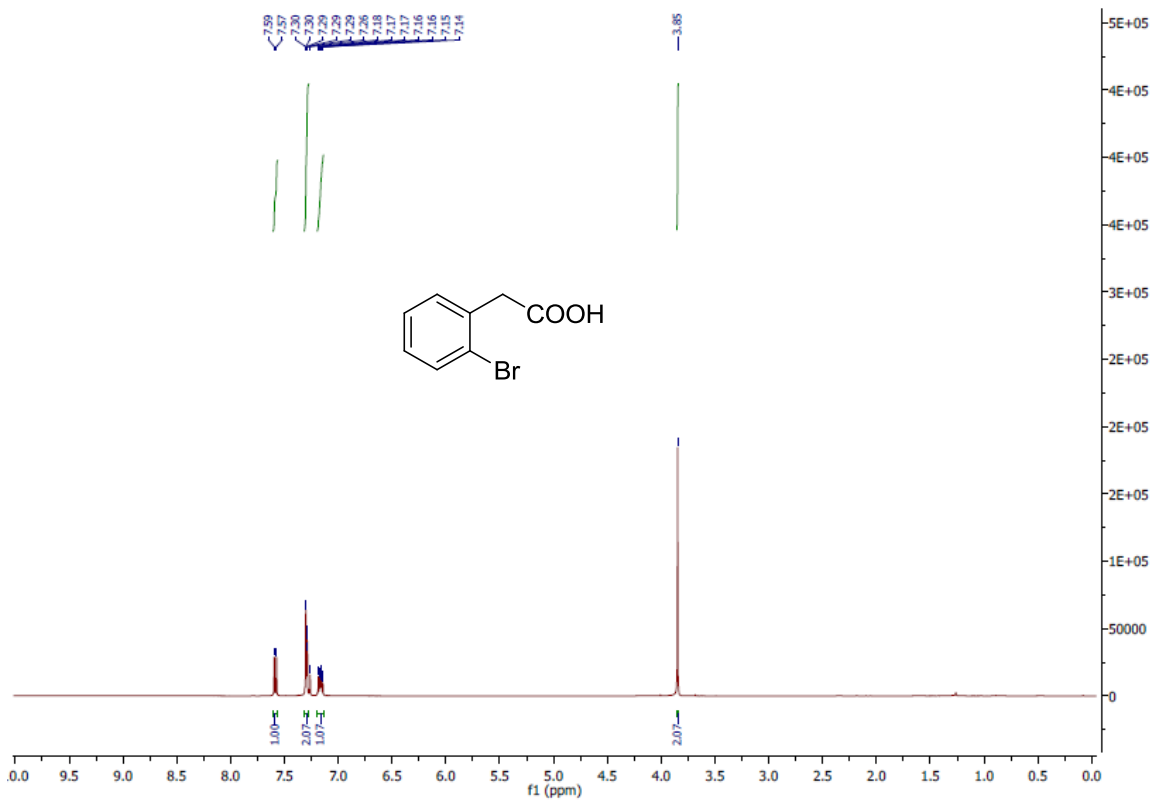


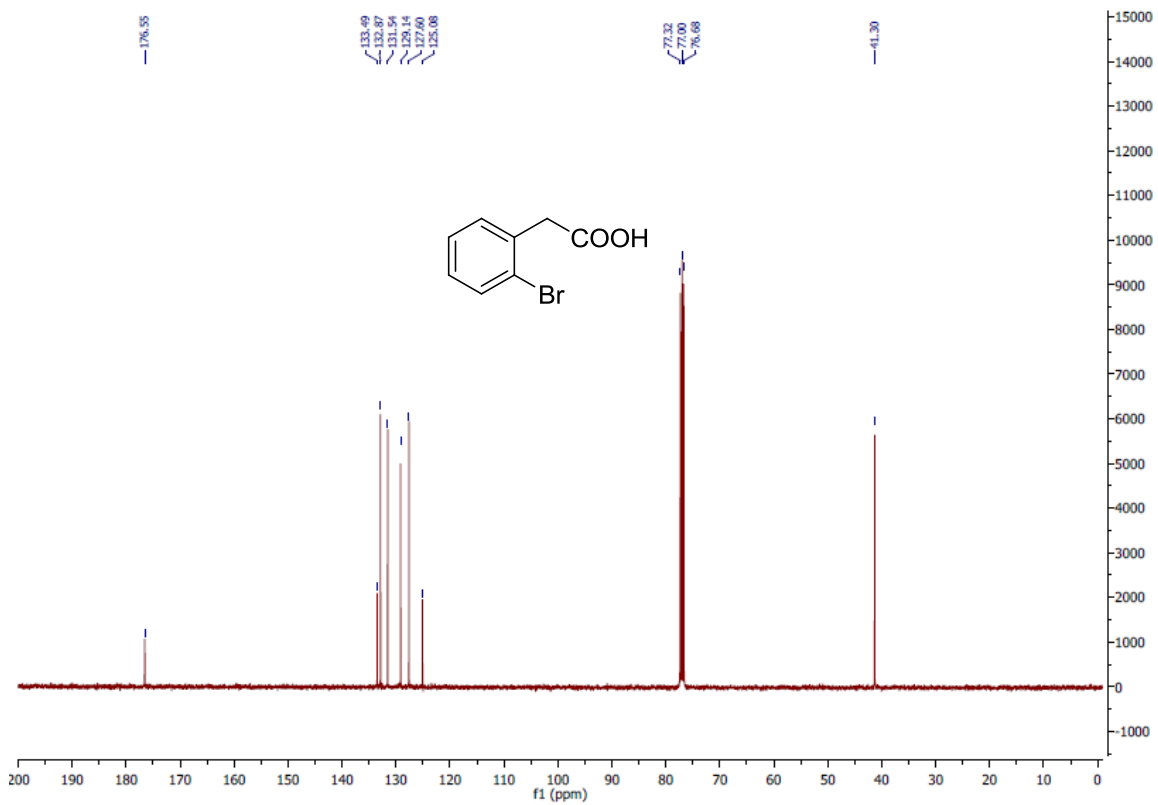
¹H and ¹³C{H} spectra of **3n**



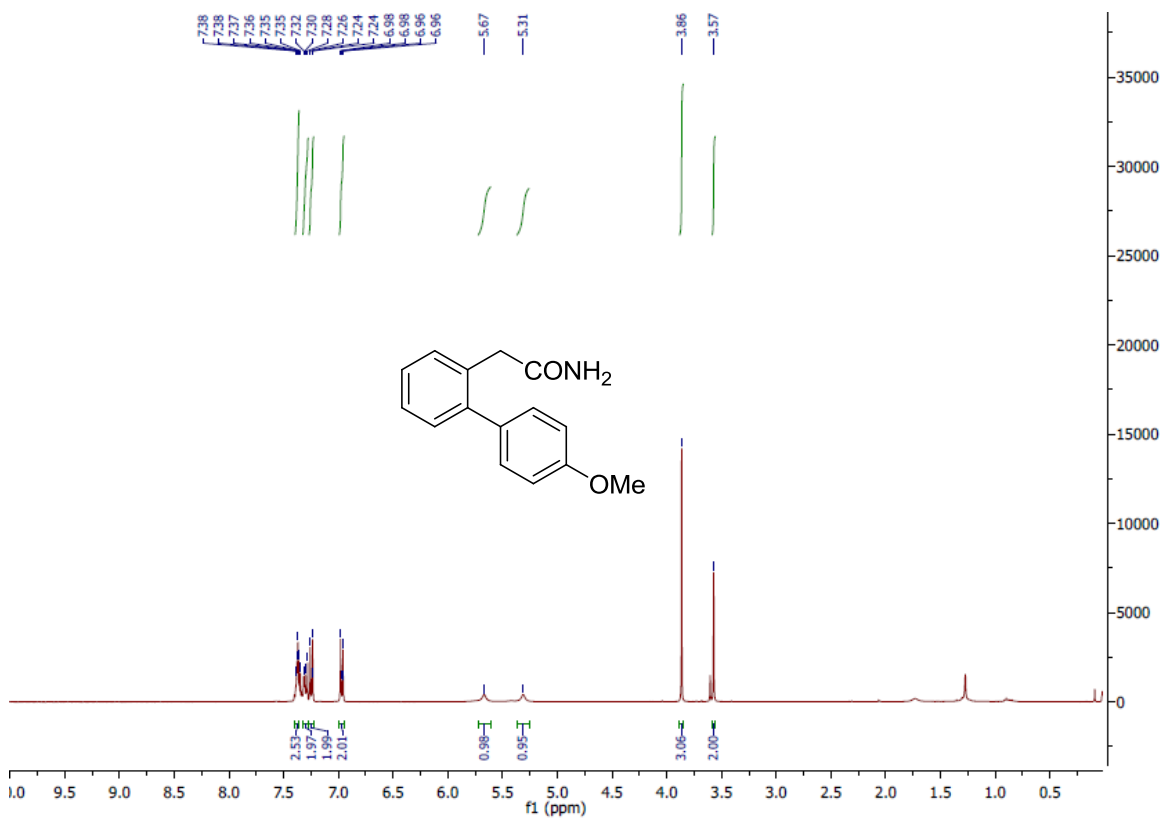


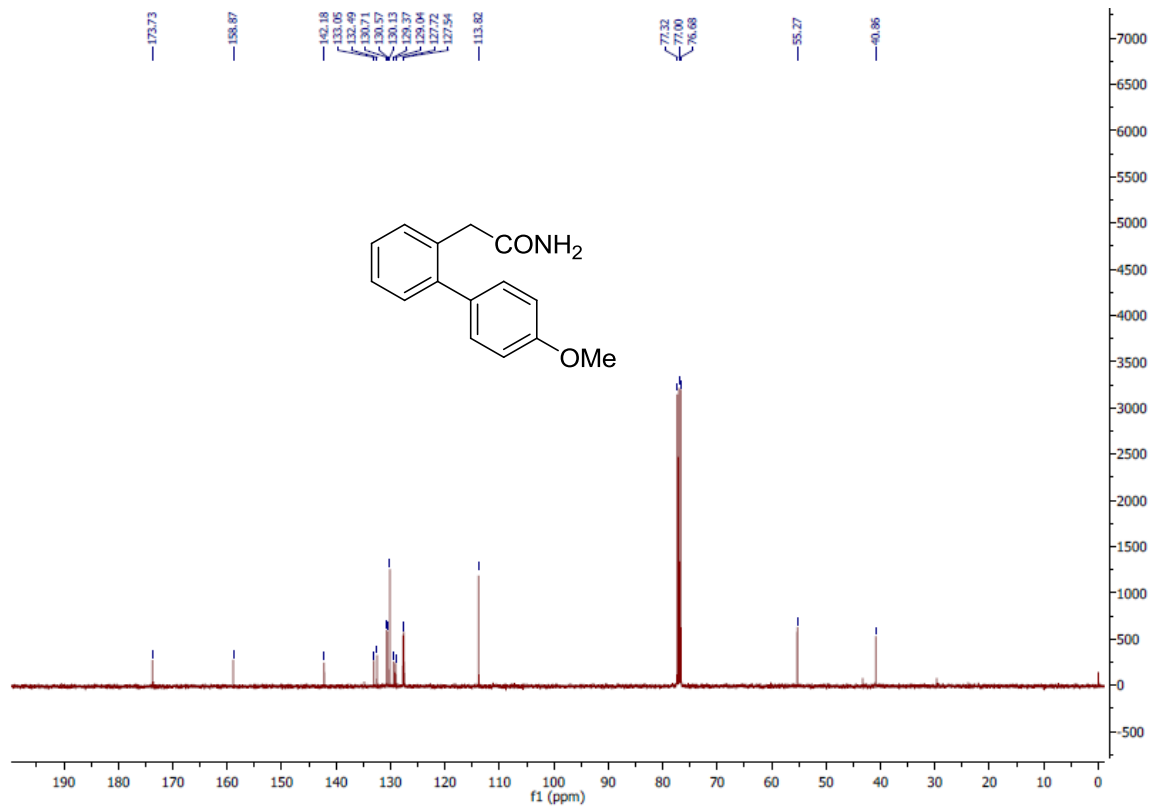
^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **4b**





^1H and $^{13}\text{C}\{\text{H}\}$ spectra of **4c**





¹H and ¹³C{H} spectra of 5a

