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Supporting Information

A Modular Flow Design for the *meta*-Selective C–H Arylation of Anilines

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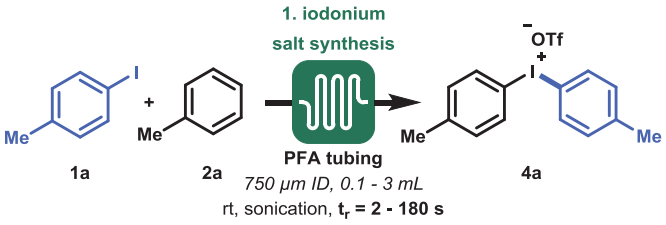
1. General information

All reagents and solvents were used as received without further purification, unless stated otherwise. Reagents and solvents were bought from Sigma Aldrich and TCI and if applicable, kept under argon atmosphere. Technical solvents were bought from VWR International and Biosolve, and are used as received. All capillary tubing and microfluidic fittings were purchased from IDEX Health & Science. Used syringes were of BD Discardit II® or NORM-JECT®, purchased from VWR Scientific. Syringe pumps were purchased from Chemix Inc. model Fusion 200 Touch. Product isolation was performed manually, using silica (60, F254, Merck™) or automatically by a Biotage® Isolera Four, with Biotage® SNAP KP-Sil 10 or 25 g flash chromatography cartridges. TLC analysis was performed using Silica on aluminum foils TLC plates (F254, Supelco Sigma-Aldrich™) with visualization under ultraviolet light (254 nm and 365 nm) or appropriate TLC staining. ^{1}H (400MHz), ^{13}C (100MHz) and ^{19}F (376 MHz) NMR spectra were recorded on ambient temperature using a Bruker-Avance 400 or Mercury 400. ^{1}H NMR spectra are reported in parts per million (ppm) downfield relative to $CDCl_3$ (7.26 ppm) and all ^{13}C NMR spectra are reported in ppm relative to $CDCl_3$ (77.2 ppm) unless stated otherwise. NMR spectra uses the following abbreviations to describe the multiplicity: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, h = hextet, hept = heptet, m = multiplet, dd = double doublet, td = triple doublet. NMR data was processed using the MestReNova 9.0.1 software package. Known products were characterized by comparing to the corresponding ^{1}H NMR and ^{13}C NMR from literature. GC analyses were performed on a GC-MS combination (Shimadzu GC-2010 Plus coupled to a Mass Spectrometer; Shimadzu GCMS-QP 2010 Ultra) with an auto sampler unit (AOC-20i, Shimadzu). Melting points were determined with a Buchi B-540 capillary melting point apparatus in open capillaries and are uncorrected. The names of all products were generated using the PerkinElmer ChemBioDraw Ultra v.12.0.2 software package.

2. Optimization of reaction conditions

2.1. Module 1: Diaryliodonium salts synthesis

Table S 1: Flow optimization of diaryliodonium salts synthesis



Entry	Reactor volume (mL)	Total flow rate (mL/min)	Isolated Yield (%)
1	3	1	68
2	1	1	73
3	0.1	1	72
4	0.1	3	82

[a]Reaction conditions: Syringe 1: 2.0 mmol of 4-iodotoluene (**1a**), 2.2 mmol of toluene (**2a**) in 10 mL DCE, syringe 2: 2.2 mmol *m*-CBPA in 10 mL of DCE, syringe 3: 4.0 mmol TfOH in 20 mL DCE, flow rate ratio for Syringe 1,2 and 3 respectively is (1:1:2).

A 3.0 mL PFA micro reactor coil (750 µm I.D.) was constructed and submerged, together with the connected cross-mixer, into a water bath. Reactions were performed under sonication to prevent possible blockage due to solids formation. 4-iodotoluene (**1a**) and toluene (**2a**) were used as model substrates. When operating the 3.0 mL reactor at a total flow rate of 1 mL/min (3 minutes residence time), 68% of the di-*p*-tolyliodonium triflate (**4a**) was acquired (see Table S1, entry 1). Decreasing the reactor volume to 0.1 mL resulted in a higher yield (entries 2-3). Finally, by increasing the flow rate to 3 mL/min, a steady flow was achieved and **4a** could be obtained in high yield (82%) within a residence time of 2 seconds (entry 4)

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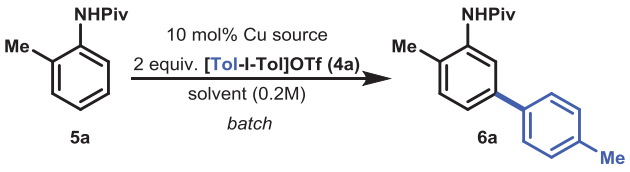
2.2. Module 2: Meta-selective C–H arylation of anilines

Table S 2: Initial optimization in batch[a]



Entry	Catalyst	T (°C)	Solvent	Reaction time	Isolated Yield (%)
1[b]	$Cu(OTf)_2$	70	DCE	24 h	79
2	Cu^0	70	DCE	4 h	74
3	Cu^0	70	1,4-doixane	4 h	71
4	Cu^0	70	THF	4 h	70
5	Cu^0	70	2-MeTHF	4 h	69
6	Cu^0	70	solvent[c]	4 h	n.d.
7	no cat.	80	DCE	24 h	19[d]
8	no cat.	90	DCE	24 h	36[d]
9	no cat.	100	DCE	24 h	45[d]
10	no cat.	110	DCE	24 h	34[d]

[a]reaction conditions: 1.0 mmol of *N*-(*o*-tolyl)pivalamide (**5a**), 2.0 equiv. di-*p*-tolyliodonium triflate (**4a**), and 10 mol % of catalyst in 5 ml of solvent; [b]Gaunt et al; [c]DMSO, NMP, DMF, i-PrOH, toluene; [d]conversion. N.d. = not detected.

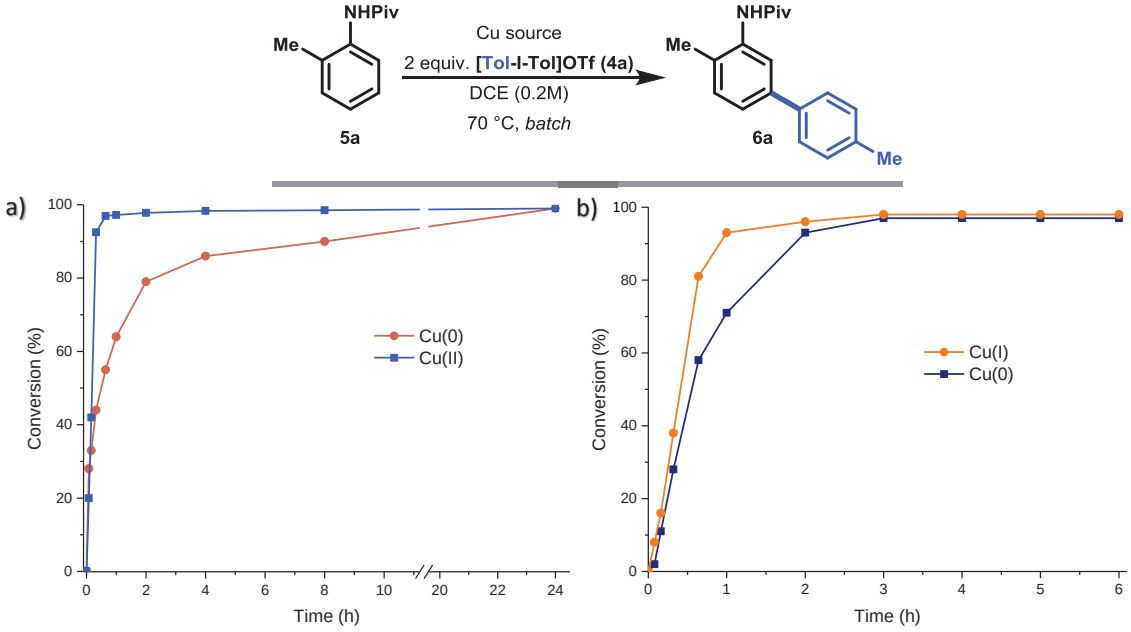
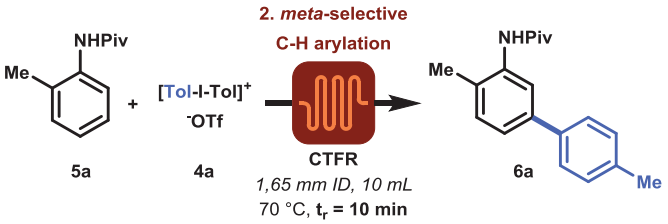


Figure S 1: a) Comparison between Cu(0) and Cu(II) as catalysts source (10 mol%) for the meta-selective C–H arylation of anilines, Cu(0) = copper powder, Cu(II) = $Cu(OTf)_2$. b) Comparison between activated/deactivated copper turnings as catalysts source (2 equiv.) for the meta-selective C–H arylation of anilines, Cu(0) = HCl treated copper turnings, Cu(I) = H_2O_2 treated copper turnings.

The readily available and cheap copper powder, as Cu(0) source, proved to be superior as compared to the previously used $Cu(OTf)_2$ catalyst (See Table S2, entries 1-2). Whereas, $Cu(OTf)_2$ needed about 24 h, the copper powder experiment reached reaction completion less than 2 hours (see Figure S1 a). In addition, conducting the reaction cyclic ether solvents 1,4-dioxane, THF and 2-MeTHF, resulted in overall similar yields (entries 3-5). Other solvents showed no reactivity towards the desired product (entry 6). Lastly, conducting the reaction under catalyst free conditions gave some conversion, although not more as 45% conversion was obtained after 24 hours at elevated temperatures (entries 7-10).

Next, following carefully the procedure steps as reported by Kappe *et al.*,[1] the activation and deactivation of the copper catalyst by surface treatment of copper turnings with HCl or H_2O_2 respectively was carried out. Conducting the reaction with either the activated or deactivated copper source resulted full conversion within 3 hours (see Figure S1b), proving that Cu(I) and Cu(0) are both suitable as pre-catalysts for the meta-selective C–H arylation reaction.

Table S 3: Flow optimization in a CTFR[a]

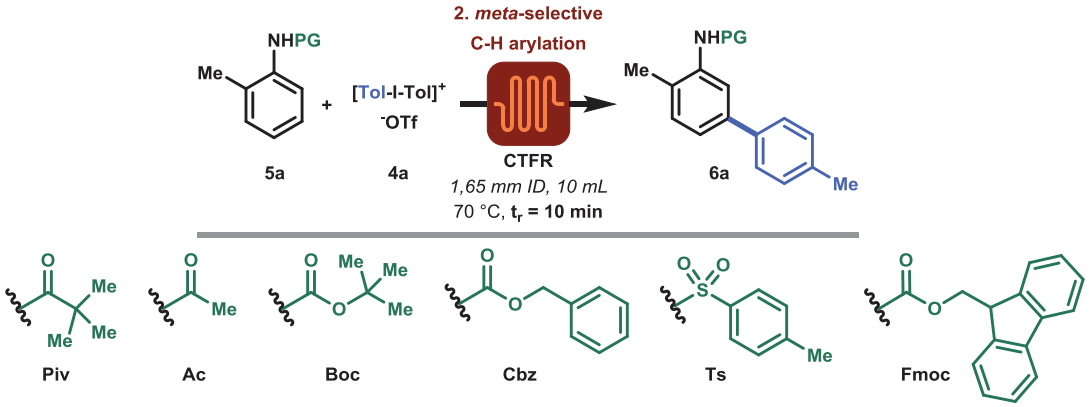


Entry	[Tol-I-Tol]OTf (equiv.)	Solvent	Residence time	Isolated Yield (%)
1	2.0	DCE	10 min	80
2[c]	2.0	1,4-dioxane	20 min	20
3[c]	2.0	THF	10 min	7
4	1.5	DCE	10 min	74
5	1.0	DCE	10 min	61

[a]reaction conditions: 0.5 mmol of *N*-(*o*-tolyl)pivalamide (**5a**), di-*p*-tolyliodonium triflate (**4a**) in 5 ml of solvent. Added to the CTFR via a 5 mL sample loop system with HPLC pump; [c]excessive copper leaching observed;

The desired product **6a** could be obtained in high yield (80%) within 10 minutes residence time (see Table S3, entry 1). Changing from DCE to more polar solvents, such as THF and 1,4-dioxane, resulted in lower yield and excessive copper leaching (entries 2-3). Moreover, decreasing the equivalents of **4a** resulted in decreased yields (entries 4-5).

Table S 4: Screening of protecting groups[a]



Entry	Protecting group	Isolated Yield (%)
1	Piv	80; 88[b]
2	Ac	52
3	Boc	n.d.[c]
4	Cbz	trace
5	Ts	n.d.
6	Fmoc	n.d.

[a]reaction conditions: 0.5 mmol of *N*-(*o*-tolyl)pivalamide (**5a**), 2.0 equiv. di-*p*-tolyliodonium triflate (**4a**) in 5 ml of solvent. Added to the CTFR via a 5 mL sample loop system with HPLC pump; [b]20 mL CTFR with 20 minutes residence time; [c]CO_2 formation, Boc is not stable under reaction conditions; n.d. = not detected.

Several other commonly used, directing groups were probed (See Table S4). However, the pivalamide outperformed all (entries 1-6). Finally, to push the reaction to completion, a 20 mL CTFR was constructed from fresh copper tubing, yielding 88% of the desired product **6a** within 20 minutes residence time.

2.3. Module 3: Inline extraction and phase separation

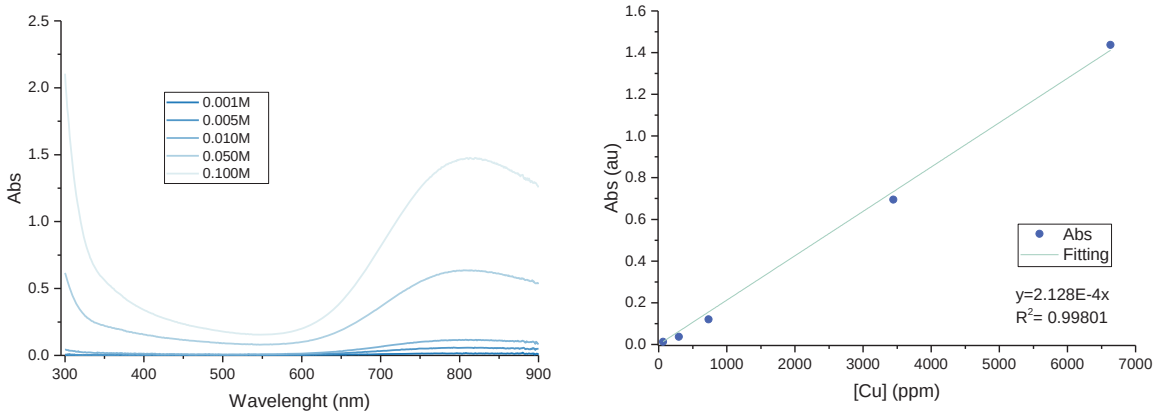


Figure S 2: A) Absorption spectra of $CuCl_2$ in the UV-VIS region. B) Calibration curve for $CuCl_2$ with UV-VIS at 810 nm.

First evaluation of copper content was performed by UV-VIS analysis in order to obtain an estimate before ICP analysis. Assuming that copper(II) chloride is formed during the calcination with aqua regia, different standard solutions of commercially available copper (II) chloride were measured, detecting a peak at 810 nm (Figure S2 A). Next, a calibration curve was plotted with the different absorptions measured at 810 nm (Figure S2 B). Finally, calcinated samples reported in Table S5 were analyzed with this method. As a result, the crude mixture corresponded to a concentration of 4733 ppm (entry 1, Table S5), while all the other samples were below the limit of detection.

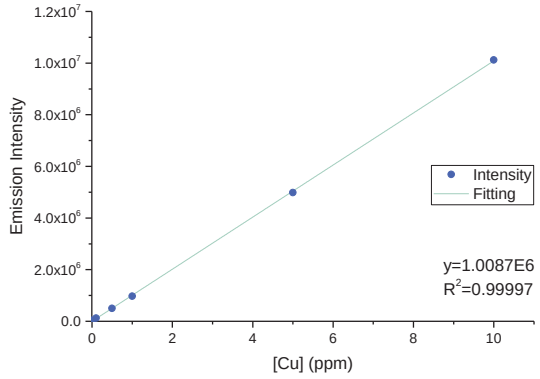
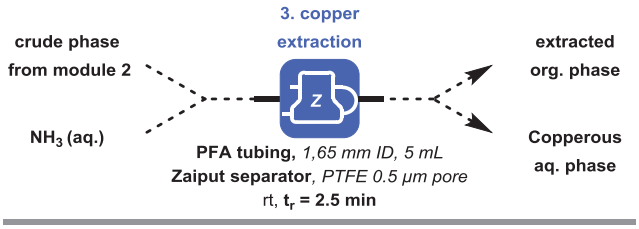


Figure S 3: Calibration curve for Cu content with ICP-OES analysis.

Next, ICP-OES analysis for copper content measurement were performed. Initially, a commercially available 1000 ppm copper standard was used to prepare standard solutions, which was used to plot a calibration curve (Figure S3). Next, the calcinated examples were properly diluted and analyzed. Notably comparable results were obtained for the crude sample with both the analytical methods (Table S5, entry 1), verifying the reliability of the developed UV-VIS method. Finally, the samples

after 1 and 3 inline extractions where successfully analyzed with ICP analysis, obtaining concentration <25 ppm in both cases (Table S5, entry 2-3).

Table S 5: Optimization of inline extraction and separation[a]



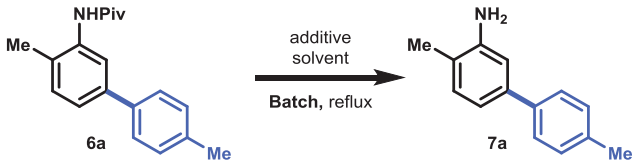
Entry	Number of extractions	Cu content (ppm)
Crude from module 2	no	4720; 4733 (UV-VIS)
Extracted org. phase	1	14.3
Extracted org. phase	3	6.3

[a]Crude phase from module 2 and NH_3 (32wt%) solution was pumped with syringe pump and mixed together in a T-mixer. A Zaiput membrane separator was connected at the end of the 5 mL PFA extraction coil. Cu content of organic phase was determined via ICP-OES analysis.

Module 3 was constructed out of a coiled 5 mL PFA tubing (1.65 mm I.D.) attached to a commercially available Zaitput liquid-liquid membrane separator (SEP-10). Conducting the extraction and separation at a total flow rate of 2 mL/min (2 x 1 mL/min) slug flow regime, copper content in the organic phase could be reduced from 4720 ppm (4733 ppm UV-VIS analysis) to 14.3 ppm (see Table S5, entries 1-2), as measured from ICP analysis. Conducted the inline extraction and separation of the crude 3 times, resulted in a residual copper content of 6.3 ppm in the organic phase (entry 3).

2.4. Module 4: Deprotection of anilines

Table S 6: Preliminary test reaction for the deprotection reaction in batch[a]

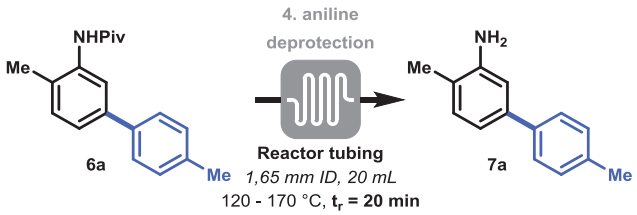


Entry	Solvent	additive	time until reaction completion
1	DCE	3 equiv. NaOH	nr
2	DCE	3 equiv. KOH	nr
3	DCE	3 equiv. *t*BuOK	nr
4	DCE	2 equiv. Cp_2ZrHCl	nr
5	DCE:THF (1:1)	2 equiv. Cp_2ZrHCl	nr
6	1M HCl	0.2 mL EtOH	60 h
7	1M HCl	2.0 equiv. $Zn(OAc)_2$	60 h
8	10M H_2SO_4 in 1,4-dioxane	-	nr
9	1M H_2SO_4 in 1,4-dioxane	10 mol % Cu(0)	9 h
10	1,4-dioxane	10 mol % Cu(0)	nr
11	HCl:1,4-dioxane (1:1)	10 mol % Cu(0)	6 h
12	HCl:1,4-dioxane (1:1)	-	6 h

[a]Reaction conditions: 0.5 mmol **6a** and additive in 2.5 mL of solvent, reaction was conducted under reflux conditions; nr = no reaction. Reaction completion was checked with TLC and GC-MS analysis.

Preliminary deprotection test reactions were carried out in order to gain some insight (Table S6). With the various conditions tried, conclusion was made that both an acidic environment (*e.g.,* 6M HCl) as well the use of 1,4-dioxane as solvent were crucial in order to obtain the desired product **7a** within a reasonable time frame (<10 h) (Table S6, entries 9-12)**.**

Table S 7: Optimization of the deprotection reaction in flow[a]



Entry	Reactor tubing	Organic phase	Aqueous phase	T (°C)	Isolated Yield (%)
1	stainless steel	DCE	H_2O	150	nr
2	stainless steel	DCE	1,4-dioxane:H_2O (3:1)	170	nr
3	stainless steel	DCE	1M H_2SO_4	150	nr[b,c]
4	PFA	DCE	H_2O	150	nr
5	PFA	DCE	1M HCl	150	nr
6	PFA	DCE	2M HCl	120	nr
7	PFA	DCE	1M TfOH	120	nr[c]
8	PFA	DCE	6M H_2SO_4	120	nr
9	PFA	DCE	H_2SO_4(95%):DMSO (2:1)	120	nr
10	PFA	DCE	2M NaOH	120	nr
11	PFA	1M KOH in EtOH	-	120	nr
12	PFA	TfOH:H_2O:1,4-dioxane (3:1:17)	-	130	trace
13	PFA	HCl:1,4-dioxane (1:1)	-	130	87
14	**PFA**	**HCl:1,4-dioxane (1:1)**	**-**	**130**	**94**[d]

[a]Reaction conditions: 0.5 mmol **6a** in 5.0 mL of solvent, added to the stainless steel reactor via HPLC pumps with a 5.0 mL sample loop system with 175 psi BPR, for the PFA reactor via syringe pumps with 140 psi BPR; [b]excessive iron leaching; [c]clogging of reactor; [d]40 min residence time, full conversion, isolated yields after extraction procedure (see 4.4); nr = no reaction.

With preliminary results in hand from the batch reactions (Table S6), a flow setup was constructed in order to fully explore the deprotection conditions for module 4. At first a 20 mL stainless steel reactor (1.65 mm I.D.) was constructed and submerged in an thermostatic oil bath. A 175 psi back pressure was attached in order to easily and safely operate the deprotection at superheated conditions. However, the use of a stainless steel reactor did not lead to any desired results (Table S7, entries 1-3). In particular, the expected iron leaching, while using acidic conditions, turn out to be problematic (entry 3). Therefore, another more inert reactor was constructed out of 20 mL PFA tubing (1.65 mm I.D.) with a 140 psi back pressure regulator and check valve. We started out with a two phase continuous-flow system whereas **6a** was dissolved in DCE and pumped to the reactor via syringe pump. In a T-mixer the organic phase (containing **6a**) was mixed with an aqueous phase obtaining a slug flow regime. However conducting the reaction at 120 °C, no desired product (**7a**)

was observed using various aqueous solutions (see Table S6, entries 4-10). In addition, carrying out the reactor in a basic (1M KOH) ethanol single phase system, still no reactivity was observed (entry 11). However, using triflic acid:water:1,4-dioxane (3:1:17) resulted in traces of the desired deprotected aniline **7a** (entry 12). Eventually, opting to use HCl (37 wt%) as acid in 1,4-dioxane in a 1:1 ratio, a satisfying yield of 87% **7a** was obtained within 20 minutes residence time (entry 13). Finally, full conversion was achieved by doubling the residence time (40 minutes residence time), acquiring **7a** in a near quantitative manner (entry 14).

3. Module pictures and schematics

3.1. Module 1: Flow reactor for the diaryliodonium salt synthesis

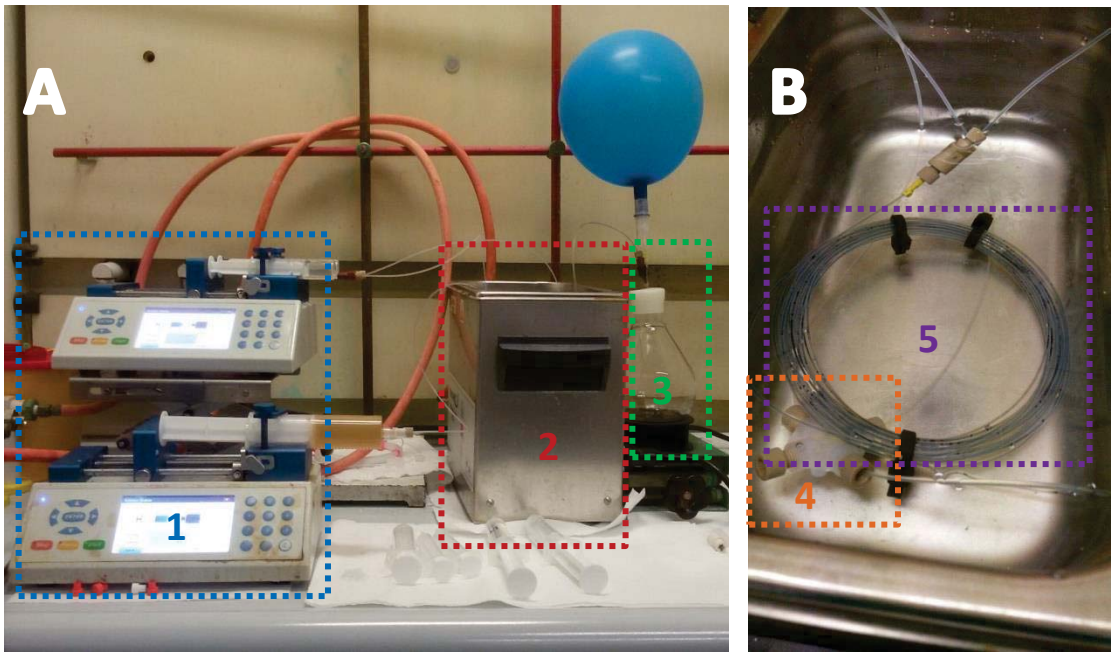
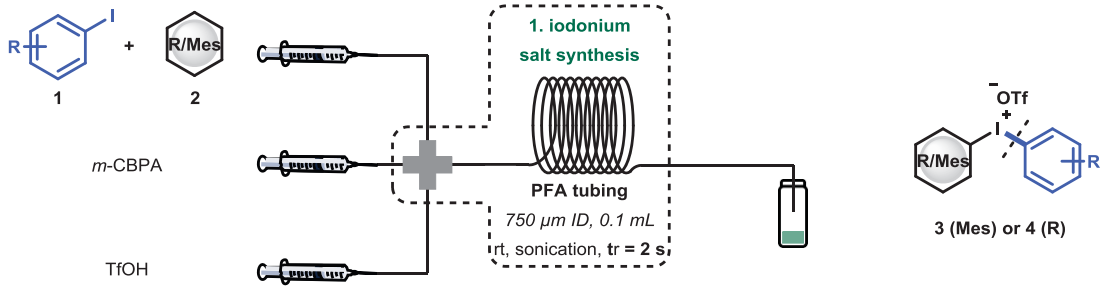


Figure S 4: A) Setup of module 1: 1. Syringe pumps, 2. Sonication bath, 3. Collection flask under argon B) Microreactor and cross-mixer submerged in the sonication bath: 4. Cross-mixer, 5. PFA coil.



Scheme S 1: Schematic representation of module 1.

3.2. Module 2: Flow reactor for the meta-selective C–H arylation of anilines

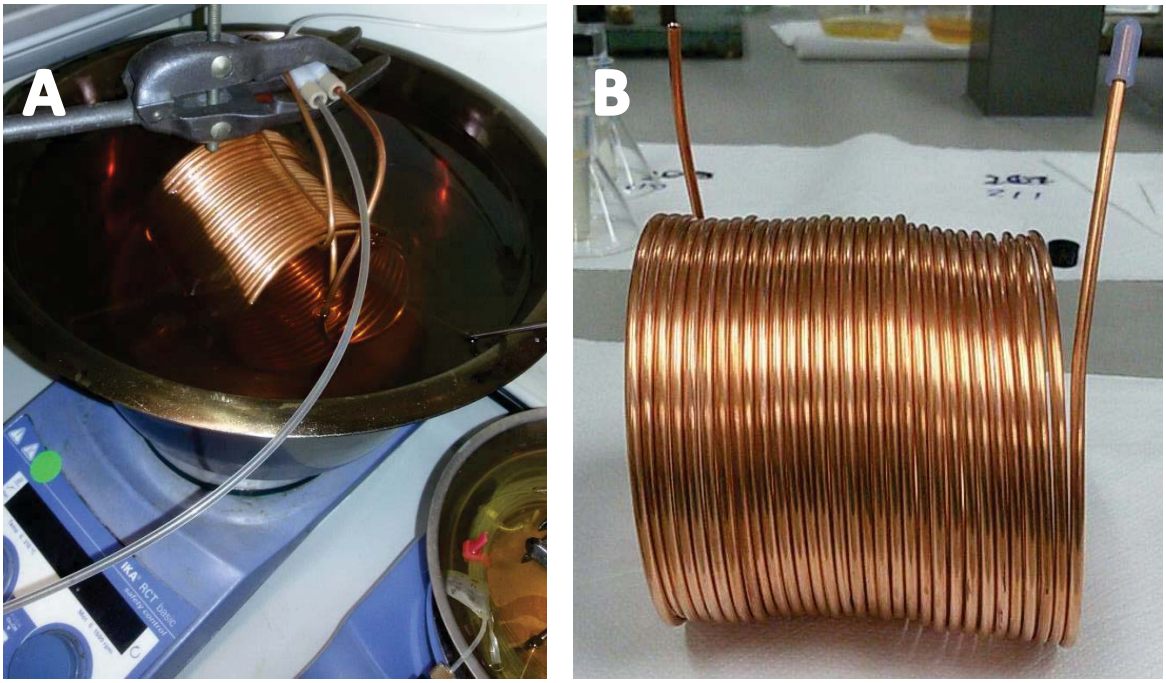
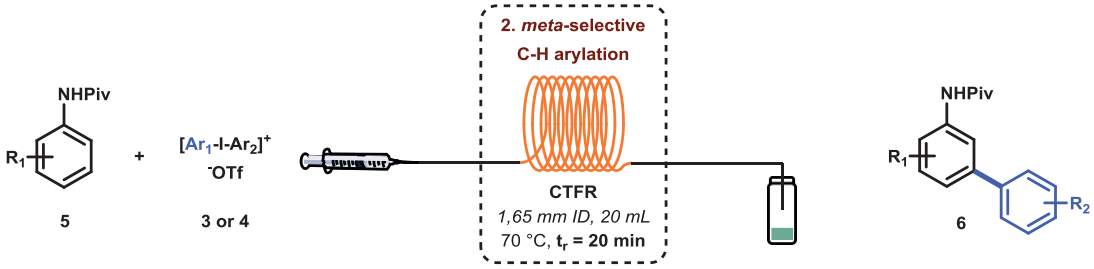


Figure S 5: A) Setup of module 2. B) Coiled copper tubing.



Scheme S 2: Schematic representation of module 2.

3.3. Module 3: Inline extraction and phase separation setup

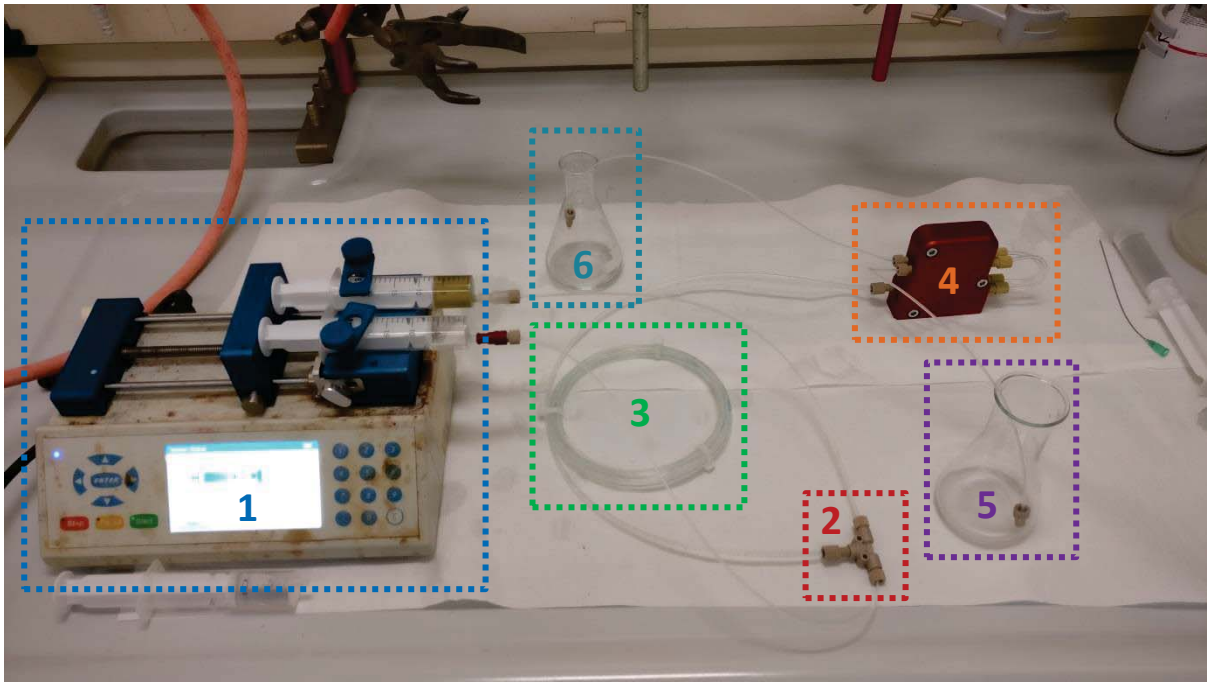
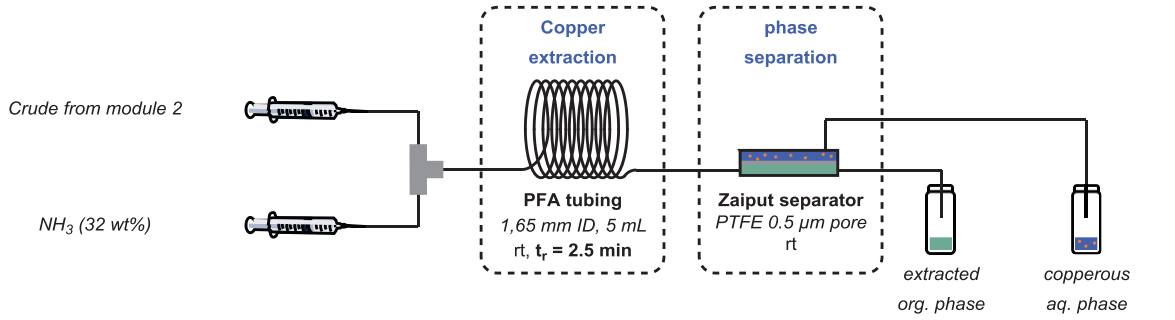


Figure S 6: Setup of module 3: 1. Syringe pump, 2. T-mixer, 3. PFA extraction coil, 4. Zaiput liquid-liquid membrane separator, 5. Collection flask of organic phase, 6. Collection flask of aqueous phase .



Scheme S 3: Schematic representation of module 3.

3.4. Module 4: Flow reactor for the deprotection of anilines

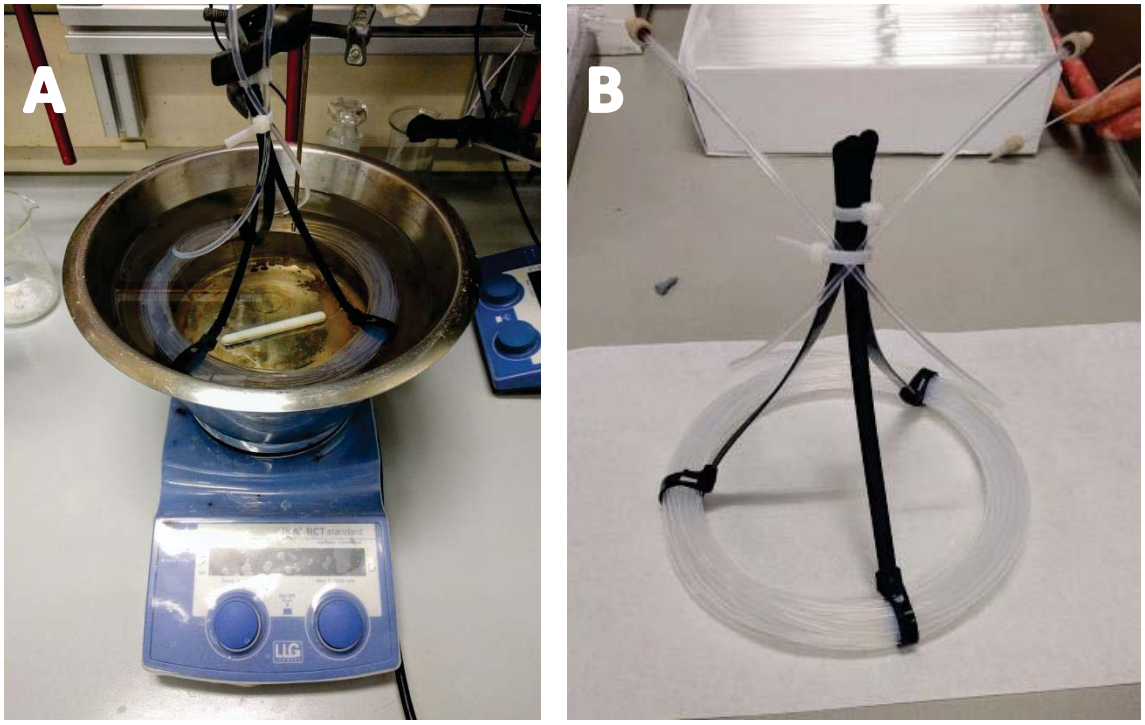
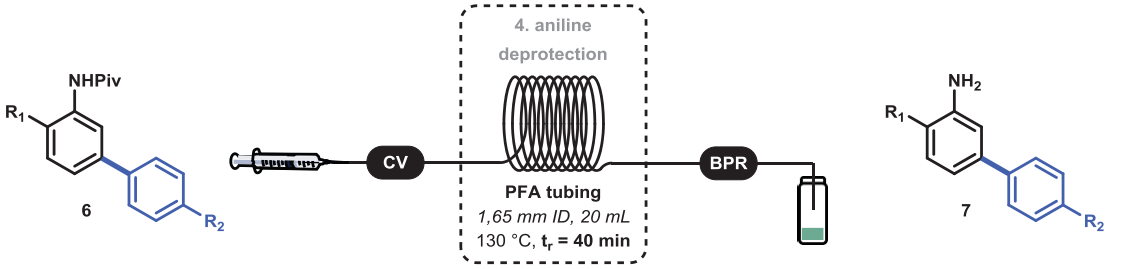


Figure S 7: A) Setup of module 4. B) Coiled PFA tubing.



Scheme S 4: Schematic representation of module 4, CV = check valve, BPR = back pressure regulator.

4. General procedures

4.1. Module 1: Diaryliodonium salts synthesis

A 25 mL oven-dried volumetric flask was charged with 4-iodotoluene (**1a**, 1.09 g, 5.0 mmol) and toluene (**2a,** 506 mg, 5.5 mmol). Next, a second 25 mL oven-dried volumetric flask was charged with *meta*-chloroperbenzoic acid (≤ 77%) (1.24 g, 5.5 mmol). Both the flasks were fitted with a septum and were degassed by alternating vacuum and argon backfill. Anhydrous dichloroethane was added via syringe to make a 25.0 mL solution in both flasks. Both the solutions were charged in 30 mL NORM-JECT® syringes and were fitted to a single syringe pump. After, a 50 mL oven-dried volumetric flask was charged with around 20 mL dichloroethane. The flask was fitted with a septum and was degassed by alternating vacuum and argon backfill. Trifluoromethanesulfonic acid (1.50 g, 10.0 mmol) was added carefully with a syringe and anhydrous dichloroethane was added via syringe to make a 50.0 mL solution. The solution was charged in a 60 mL NORM-JECT® syringe and fitted to a second syringe pump. All syringes were connected to a PEEK cross-mixer (500 µm I.D.) and subsequently connected to the inlet of the 0.1 mL PFA capillary tubing (750 µm I.D.). The cross-mixer and microreactor were submerged in a sonication bath and sonication was applied during operation. First syringe pump (containing 2 syringes) was operated at 2x 0.75 mL/min and the second syringe pump was operated at 1.5 mL/min (total 3 mL/min flow rate, 2 seconds residence time). The outlet of the reactor was fitted to an argon filled round bottom flask with septum via a needle connection. An argon filled balloon was attached in order to ensure a constant pressure. The reaction mixture was evaporated under reduced pressure at the rotavap. Residue was dissolved in diethyl ether and evaporated again at the rotavap. This procedure was repeated three times. Then, the residue was dissolved in a minimum amount of acetone, followed by addition of diethyl ether until cloudy solution was obtained. Next, the resulted mixture was kept in the freezer (-26 °C) overnight. Formed crystals were filtered off and washed with a minimum of diethyl ether. The final product was weighted and characterized by ^{1}H NMR, ^{13}C NMR, ^{19}F NMR (if applicable) and melting point analysis.

4.2. Module 2: Meta-selective C-H arylation of anilines

A 5 mL oven-dried volumetric flask was charged with *N*-(*o*-tolyl)pivalamide (**5a**, 95 mg, 0.5 mmol) and di-*p*-tolyliodonium triflate (**4a,** 458 mg, 1.0 mmol). The flask was fitted with a septum and was degassed by alternating vacuum and argon backfill. Anhydrous dichloroethane was added via syringe to make a 5.0 mL solution. The solution was charged in a 10 mL BD Discardit II® syringe. Next, the syringe was fitted to a syringe pump and connected to the inlet of the 20 mL CTFR. The CTFR was

submerged into a thermostatic oil bath and kept at 70 °C during operation. The outlet of the CTFR was fitted to an Erlenmeyer collection flask. The syringe pump was operated at a flow rate of 1.0 mL/min (20 minutes residence time). Three extra syringes of each 10 mL anhydrous dichloroethane were pumped after the sample (1.0 mL/min) in order to collect the complete sample. The resulted reaction mixture was monitored using TLC and/or GC-MS. The organic mixture was diluted in DCM and was introduced into a separation funnel. The organic phase was washed with 2x saturated aqueous NaHCO3 and 1x with brine solution sequentially. Aqueous phase was backwashed once with DCM. Collected organic phase was dried over MgSO4, filtered and concentrated under reduced pressure. Purification by flash chromatography on silica afforded the product. The final product was weighted and characterized by ^{1}H NMR, ^{13}C NMR, ^{19}F NMR (if applicable), HRMS and melting point analysis (if applicable).

4.3. Module 3: Inline extraction and phase separation

5.0 mL of the crude mixture from module 2 was loaded into a 10 mL BD Discardit II® syringe. Another, 10 mL syringe was prepared with 5.0 mL of ammonia (32wt%) solution. Both syringes were fitted to a syringe pump and connected to a PEEK T-mixer (1.0 mm I.D.) which in turn was connected to the 5 mL PFA extraction coil (1.65 mm I.D.). Both syringes were pumped with a flow rate of 1 mL/min (total 2 mL/min flow rate). Upon merging the two stream in the T-mixer, a slug flow (Taylor flow) regime was obtained which remained stable throughout the extraction coil. The extraction could be monitored visually due to complexation of Cu with ammonia (aqueous slugs turn deep blue). At the end of the extraction coil, a Zaiput liquid-liquid membrane separator (SEP-10) was attached, equipped with a PTFE 0.5 µm pore size membrane. The organic and aqueous phase were successfully separated and collected in separate Erlenmeyer flasks. The organic phase was calcinated at 200 °C with an aqua regia solution. The resulting solid residues were washed 3 times with distilled water. Finally, ICP-OES analysis was carried out. A calibration curve was prepared with the copper standard solution 1000 ppm purchased from VWR Scientific.

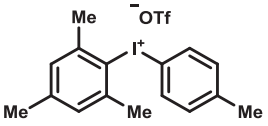
4.4. Module 4: Deprotection of anilines

A 5 mL oven-dried volumetric flask was charged with *N*-(4,4'-dimethyl-[1,1'-biphenyl]-3-yl)pivalamide (**6a**, 141 mg, 0.5 mmol) and HCl (37 wt%):1,4-dioxane (1:1) mixture was added via syringe to make a 5.0 mL solution. The solution was charged in a 10 mL BD Discardit II® syringe. Next, the syringe was fitted to a syringe pump and connected to the inlet of the 20 mL PFA deprotection coil (1.65 mm I.D.). The reactor was submerged into a thermostatic oil bath and kept at 130 °C

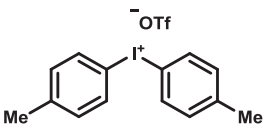
during operation. The outlet of the reactor was fitted to an Erlenmeyer collection flask. The syringe pump was operated at a flow rate of 0.5 mL/min (40 minutes residence time). Three extra syringes of each 10 mL anhydrous 1,4-dioxane were pumped after the sample in order to collect the complete sample. The resulted reaction mixture was monitored using TLC and/or GC-MS. The organic mixture was diluted in ethyl acetate and was introduced into a separation funnel. The organic phase was washed with aqueous 1M NaOH solution. Next the organic phase was extracted at least 3x with aqueous 1M HCl solution until al desired product 4,4'-dimethyl-[1,1'-biphenyl]-3-amine (**7a**) was extracted to the aqueous phase (monitored by TLC ninhydrin stain to detect the primary amine functionality). Finally, the aqueous phase was made basic by careful addition of NaOH pellets, and ethyl acetate was added in order to back-extract **7a** to the organic phase. The collected organic phase was dried over MgSO4, filtered and concentrated under reduced pressure in order to obtain the desired product. The final product was weighted and characterized by ^{1}H NMR, ^{13}C NMR, ^{19}F NMR (if applicable), HRMS and melting point analysis (if applicable).

5. Characterization data

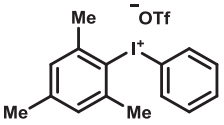
5.1. Diaryliodonium salts



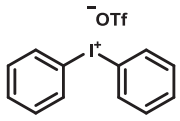
mesityl(p-tolyl)iodonium trifluoromethanesulfonate (**3a**).[2] Purification by recrystallization in diethyl ether to afford the product as white solids. Mp. 181-183 °C (Lit. 183-184 °C)[2]. ^{1}H NMR (400 MHz, DMSO-d6) δ 7.87 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.1 Hz, 2H), 7.21 (s, 2H), 2.60 (s, 6H), 2.33 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 143.0, 142.2, 141.4, 134.5, 132.5, 129.7, 122.7, 110.9, 26.3, 20.8, 20.5.



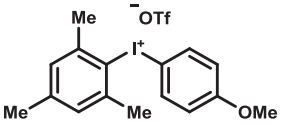
di-p-tolyliodonium trifluoromethanesulfonate (**4a**).[3] Purification by recrystallization in diethyl ether to afford the product as grey solids. Mp. 131-133 °C (Lit. 121-123 °C)[3]. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.82 (d, J = 8.4 Hz, 4H), 7.26 (d, J = 8.2 Hz, 2H), 2.41 (s, 6H). ^{13}C NMR (100 MHz, CDCl3) δ 144.0, 135.0, 133.4, 109.7, 21.6.



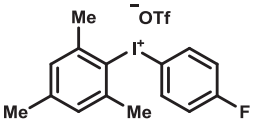
mesityl(phenyl)iodonium trifluoromethanesulfonate (**3b**).[4] Purification by recrystallization in diethyl ether to afford the product as off white solids. Mp. 148-150 °C (Lit. 137-138 °C)[4]. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.74 – 7.63 (m, 2H), 7.59 – 7.49 (m, 1H), 7.42 (dd, J = 8.4, 7.3 Hz, 2H), 7.11 (s, 2H), 2.63 (s, 6H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 144.8, 142.7, 133.0, 132.5, 132.0, 130.6, 122.0, 120.3, 118.9, 111.8, 27.28, 21.3.



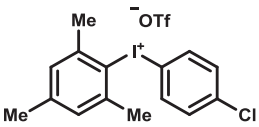
diphenyliodonium trifluoromethanesulfonate (**4b**).[5] Purification by recrystallization in diethyl ether to afford the product as off white solids. Mp. 169-173 °C (Lit. 172-174 °C)[5]. ^{1}H NMR (400 MHz, DMSO-d6) δ 8.25 (d, J = 7.4 Hz, 4H), 7.67 (t, J = 7.4 Hz, 2H), 7.53 (t, J = 7.8 Hz, 4H). ^{13}C NMR (101 MHz, DMSO) δ 135.2, 132.1, 131.8, 116.5.



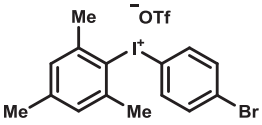
mesityl(4-methoxyphenyl)iodonium trifluoromethanesulfonate (**3c**).[4] Purification by recrystallization in diethyl ether to afford the product as dark grey solids. Mp. 148-150 °C (Lit. 150-152 °C)[4]. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.69 – 7.57 (m, 2H), 7.10 (s, 2H), 6.98 – 6.85 (m, 2H), 3.82 (s, 3H), 2.64 (s, 6H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 162.8, 144.7, 142.4, 135.5, 130.6, 121.0, 118.3, 99.9, 55.9, 27.2, 21.3.



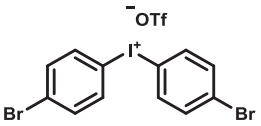
(4-fluorophenyl)(mesityl)iodonium trifluoromethanesulfonate (**3d**).[4] Purification by recrystallization in diethyl ether to afford the product as grey solids. Mp. 173-176 °C (Lit. 177-178 °C)[4]. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.73 (dd, J = 8.5, 4.7 Hz, 2H), 7.10 (d, J = 4.9 Hz, 4H), 2.63 (s, 6H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 164.7 (d, J = 255.0 Hz), 144.6, 142.5, 135.7 (d, J = 8.7 Hz), 130.5, 121.9, 121.2, 119.8 (d, J = 22.9 Hz), 118.7, 105.3 (d, J = 3.4 Hz), 27.2, 21.3. ^{19}F NMR (376 MHz, Chloroform-d) δ -78.40, -106.01 (ddd, J = 12.8, 8.2, 4.7 Hz).



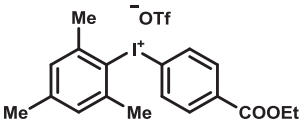
(4-chlorophenyl)(mesityl)iodonium trifluoromethanesulfonate (**3e**).[4] Purification by recrystallization in diethyl ether to afford the product as light grey solids. Mp. 161-163 °C (Lit. 132-133 °C)[4]. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.67 – 7.60 (m, 2H), 7.40 – 7.34 (m, 2H), 7.11 (s, 2H), 2.62 (s, 6H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 144.8, 142.6, 138.9, 134.4, 132.5, 130.6, 120.9, 108.9, 27.2, 15.4.



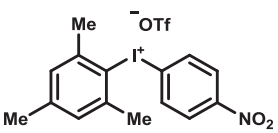
(4-bromophenyl)(mesityl)iodonium trifluoromethanesulfonate (**3f**).[2] Purification by recrystallization in diethyl ether to afford the product as light grey solids. Mp. 187-190 °C (Lit. 179-180 °C)[2]. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.57 (d, J = 8.8 Hz, 1H), 7.50 (d, J = 8.8 Hz, 1H), 7.09 (s, 1H), 2.61 (s, 2H), 2.34 (s, 1H). ^{13}C NMR (101 MHz, CDCl3) δ 144.6, 142.6, 135.3, 134.6, 130.5, 126.9, 121.9, 120.9, 118.7, 109.9, 27.2, 21.2.



bis(4-bromophenyl)iodonium trifluoromethanesulfonate (**4f**).[6] Purification by recrystallization in diethyl ether to afford the product as white solids. Mp. 183-188 °C (Lit. 185-190 °C)[6]. ^{1}H NMR (400 MHz, DMSO-d6) δ 8.17 (d, J = 8.6 Hz, 4H), 7.77 (d, J = 8.6 Hz, 4H). ^{13}C NMR (101 MHz, DMSO-d6) δ 137.0, 134.7, 126.3, 115.4.

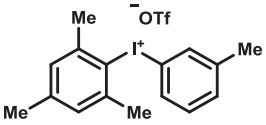


(4-(ethoxycarbonyl)phenyl)(mesityl)iodonium triflate (**3g**).[4] Purification by recrystallization in diethyl ether to afford the product as grey solids. Mp. 173-175 °C (Lit. 178-179 °C)[4]. ^{1}H NMR (399 MHz, Chloroform-d) δ 8.01 (d, J = 8.6 Hz, 2H), 7.76 (d, J = 8.7 Hz, 2H), 7.11 (d, J = 1.0 Hz, 2H), 4.36 (q, J = 7.1 Hz, 2H), 2.61 (s, 6H), 2.36 (s, 3H), 1.36 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 164.9, 144.7, 142.7, 133.7, 132.9, 132.8, 130.5, 121.9, 120.7, 118.7, 116.5, 62.0, 27.2, 21.3, 14.3.

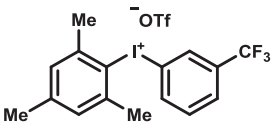


mesityl(4-nitrophenyl)iodonium trifluoromethanesulfonate (**3h**).[4] Purification by recrystallization in diethyl ether to afford the product as grey solids. Mp. 197-200 °C (Lit. 208 °C)[4]. ^{1}H NMR (399 MHz, DMSO-d6) δ

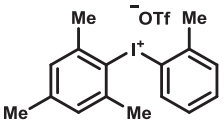
8.26 (d, J = 8.4 Hz, 2H), 8.22 – 8.12 (m, 2H), 7.26 (s, 2H), 2.59 (s, 6H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 149.3, 143.6, 141.8, 135.5, 130.0, 126.2, 122.8, 120.7, 26.3, 20.5.



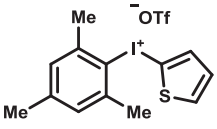
mesityl(m-tolyl)iodonium trifluoromethanesulfonate (**3i**).[2] Purification by recrystallization in diethyl ether to afford the product as off white solids. Mp. 169-171 °C (Lit. 171-172 °C)[2]. ^{1}H NMR (399 MHz, Chloroform-d) δ 7.58 (s, 1H), 7.39 (d, J = 7.9 Hz, 1H), 7.33 (d, J = 7.5 Hz, 1H), 7.26 (t, J = 7.8 Hz, 1H), 7.10 (s, 2H), 2.62 (s, 6H), 2.35 (s, 6H). ^{13}C NMR (100 MHz, CDCl3) δ 144.6, 143.3, 142.7, 133.6, 132.9, 132.1, 130.5, 129.9, 122.1, 120.2, 118.9, 111.6, 27.3, 21.5, 21.3.



mesityl(3-(trifluoromethyl)phenyl)iodonium trifluoromethanesulfonate (**3j**).[4] Purification by recrystallization in diethyl ether to afford the product as brown solids. Mp. 180-182 °C (Lit. 181-183 °C)[4]. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.94 (d, J = 8.4 Hz, 1H), 7.91 (s, 1H), 7.77 (d, J = 7.8 Hz, 1H), 7.54 (t, J = 8.0 Hz, 1H), 7.12 (s, 2H), 2.63 (s, 6H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 144.9, 142.7, 136.6, 134.3 (t, J = 34.2 Hz), 132.5, 130.6, 129.8 (t, J = 3.9 Hz), 128.6 (d, J = 3.7 Hz), 122.9 (d, J = 214.1 Hz), 121.0, 119.9 (d, J = 260.4 Hz), 112.1, 27.2, 21.3. ^{19}F NMR (376 MHz, CDCl3) δ -63.05, -78.53.

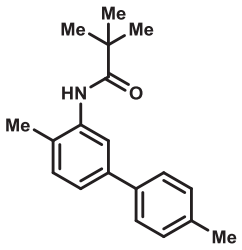


mesityl(o-tolyl)iodonium trifluoromethanesulfonate (**3k**).[4] Purification by recrystallization in diethyl ether to afford the product as white solids. Mp. 170-172 °C (Lit. 167-168 °C)[4]. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.50 – 7.38 (m, 3H), 7.17 (td, J = 7.7, 7.1, 2.0 Hz, 1H), 7.11 (s, 2H), 2.60 (s, 9H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 144.8, 142.7, 140.4, 133.7, 132.7, 132.6, 130.9, 123.0, 122.1, 119.7, 118.9, 115.8, 27.1, 25.0, 21.2.

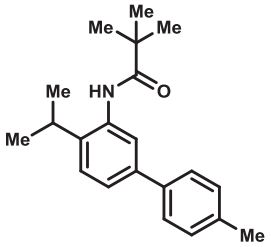


mesityl(thiophen-2-yl)iodonium trifluoromethanesulfonate (**3l**). Purification by recrystallization in diethyl ether to afford the product as light brown solids. Mp. 160-162 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.73 (dd, J = 3.8, 1.2 Hz, 1H), 7.61 (dd, J = 5.4, 1.2 Hz, 1H), 7.11 – 7.04 (m, 3H), 2.73 (s, 6H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 144.5, 141.7, 139.7, 135.8, 130.3, 129.8, 125.6, 94.5, 27.2, 21.2.

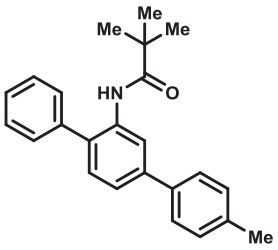
5.2. Meta-arylated pivalamides



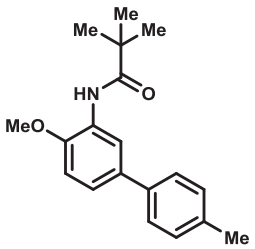
N-(4,4'-dimethyl-[1,1'-biphenyl]-3-yl)pivalamide (**6a**).[7] Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as white solids. Mp. 164-168 °C (Lit. 163 °C)[7]. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.18 (d, J = 1.8 Hz, 1H), 7.51 (d, J = 8.2 Hz, 2H), 7.30 (dd, J = 7.8, 1.9 Hz, 2H), 7.24 – 7.18 (m, 3H), 2.38 (s, 3H), 2.29 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.6, 140.0, 137.9, 137.1, 136.3, 130.8, 129.5, 127.3, 127.0, 123.3, 121.2, 40.0, 27.9, 21.2, 17.5. HRMS (ESI) calculated for $C_{19}H_{24}NO$ $[M+H]^+$: 282.1853, found: 282.1851.



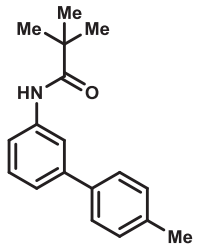
N-(4-isopropyl-4'-methyl-[1,1'-biphenyl]-3-yl)pivalamide (**6b**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as white solids. Mp. 190-194 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.10 (d, J = 1.5 Hz, 1H), 7.53 (d, J = 8.0 Hz, 2H), 7.46 – 7.37 (m, 2H), 7.33 (d, J = 8.1 Hz, 1H), 7.22 (d, J = 7.9 Hz, 2H), 3.01 (hept, J = 6.9 Hz, 1H), 2.39 (s, 3H), 1.37 (s, 9H), 1.32 (s, 3H), 1.31 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 176.8, 139.5, 138.2, 137.8, 137.0, 134.9, 129.4, 127.0, 125.9, 124.0, 122.6, 39.9, 28.1, 27.8, 22.9, 21.2. HRMS (ESI) calculated for $C_{21}H_{28}NO$ $[M+H]^+$: 310.2166, found: 310.2166.



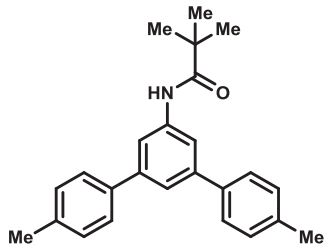
N-(4''-methyl-[1,1':4',1''-terphenyl]-2'-yl)pivalamide (**6c**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as white solids. Mp. 128-130 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.74 (s, 1H), 7.64 (d, J = 8.1 Hz, 2H), 7.59 – 7.55 (m, 1H), 7.55 – 7.51 (m, 2H), 7.49 – 7.46 (m, 1H), 7.44 (dt, J = 8.1, 1.9 Hz, 3H), 7.33 (d, J = 7.9 Hz, 1H), 7.29 (s, 1H), 2.43 (s, 3H), 1.16 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.5, 141.5, 138.0, 137.7, 137.4, 135.6, 130.9, 130.2, 129.5, 129.5, 129.2, 128.2, 127.2, 122.4, 119.4, 40.0, 27.5, 21.3. HRMS (ESI) calculated for $C_{24}H_{26}NO$ $[M+H]^+$: 344.2009, found: 344.2003.



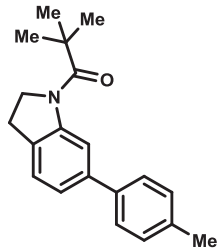
N-(4-methoxy-4'-methyl-[1,1'-biphenyl]-3-yl)pivalamide (**6d**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:2) to afford the product as white solids. Mp. 100-105 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.75 (d, J = 2.3 Hz, 1H), 8.15 (s, 1H), 7.51 (d, J = 8.1 Hz, 2H), 7.26 (dd, J = 8.5, 2.2 Hz, 1H), 7.19 (d, J = 7.9 Hz, 2H), 6.93 (d, J = 8.4 Hz, 1H), 3.93 (s, 3H), 2.37 (s, 3H), 1.34 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.8, 147.4, 137.9, 136.6, 134.3, 129.4, 128.2, 126.9, 121.7, 118.4, 110.1, 56.2, 40.2, 27.8, 21.2. HRMS (ESI) calculated for $C_{19}H_{24}NO_2$ $[M+H]^+$: 298.1802, found: 298.1802.



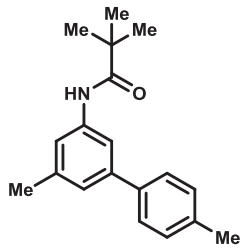
N-(4'-methyl-[1,1'-biphenyl]-3-yl)pivalamide (**6e**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as white solids. Mp. 129-135 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.80 (t, J = 1.9 Hz, 1H), 7.50 (d, J = 8.2 Hz, 2H), 7.49 – 7.45 (m, 1H), 7.40 – 7.30 (m, 3H), 7.23 (d, J = 7.9 Hz, 2H), 2.39 (s, 3H), 1.34 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.8, 142.2, 138.5, 137.9, 137.4, 129.6, 129.4, 127.1, 122.9, 118.7, 118.6, 39.8, 27.8, 21.3. HRMS (ESI) calculated for $C_{18}H_{22}NO$ $[M+H]^+$: 268.1696, found: 268.1690.



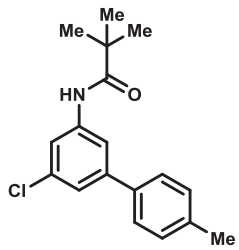
N-(4,4''-dimethyl-[1,1':3',1''-terphenyl]-5'-yl)pivalamide (**6e'**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as white solids. Mp. 187-192 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.74 (d, J = 1.6 Hz, 2H), 7.57 – 7.52 (m, 5H), 7.44 (s, 1H), 7.26 – 7.22 (m, 4H), 2.40 (s, 6H), 1.36 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.8, 142.6, 138.9, 138.0, 137.5, 129.6, 127.2, 121.8, 117.3, 39.9, 27.8, 21.3. HRMS (ESI) calculated for $C_{25}H_{28}NO$ $[M+H]^+$: 358.2166, found: 358.2172.



2,2-dimethyl-1-(6-(p-tolyl)indolin-1-yl)propan-1-one (**6f**). Purification by flash chromatography on silica: Cy:EtOAc (20:1) to afford the product as a colorless oil. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.56 (s, 1H), 7.53 (d, J = 8.0 Hz, 2H), 7.25 – 7.14 (m, 4H), 4.23 (t, J = 8.1 Hz, 2H), 3.11 (t, J = 8.2 Hz, 2H), 2.37 (s, 3H), 1.38 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.7, 145.4, 140.6, 138.4, 136.8, 129.8, 129.3, 127.1, 124.4, 122.5, 117.1, 49.9, 40.3, 29.1, 27.8, 21.1. HRMS (ESI) calculated for $C_{20}H_{24}NO$ $[M+H]^+$: 294.1853, found: 294.1858.

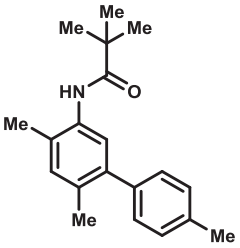


N-(4',5-dimethyl-[1,1'-biphenyl]-3-yl)pivalamide (**6g**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as yellow solids. Mp. 152-157 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.56 (t, J = 1.9 Hz, 1H), 7.49 (d, J = 8.1 Hz, 2H), 7.39 (d, J = 2.0 Hz, 2H), 7.22 (d, J = 7.8 Hz, 2H), 7.16 – 7.14 (m, 1H), 2.39 (s, 6H), 1.34 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.8, 142.0, 139.3, 138.5, 138.0, 137.3, 129.5, 127.1, 123.8, 119.3, 115.8, 39.8, 27.8, 21.7, 21.3. HRMS (ESI) calculated for $C_{19}H_{24}NO$ $[M+H]^+$: 282.1853, found: 282.1855.

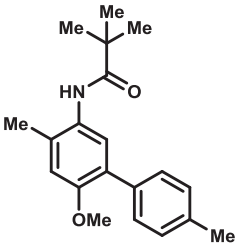


N-(5-chloro-4'-methyl-[1,1'-biphenyl]-3-yl)pivalamide (**6h**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as off white solids. Mp. 142-145 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.61 (dt, J = 7.5, 1.9 Hz, 2H), 7.48 – 7.44 (m, 2H), 7.38 (s, 1H), 7.30 (t, J = 1.7 Hz,

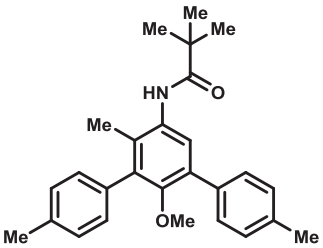
1H), 7.25 – 7.21 (m, 2H), 2.39 (s, 3H), 1.33 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.9, 143.5, 139.5, 138.1, 136.6, 135.0, 129.7, 127.1, 122.9, 118.5, 116.7, 39.9, 27.7, 27.7, 21.3. HRMS (ESI) calculated for $C_{18}H_{21}NO$ $[M+H]^+$: 302.1306, found: 302.1304.



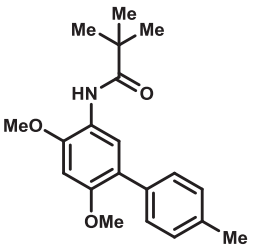
N-(4,4',6-trimethyl-[1,1'-biphenyl]-3-yl)pivalamide (**6i**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as white solids. Mp. 139-141 °C. ^{1}H NMR (399 MHz, Chloroform-d) δ 7.64 (s, 1H), 7.20 (q, J = 8.2 Hz, 5H), 7.08 (s, 1H), 2.38 (s, 3H), 2.25 (s, 3H), 2.22 (s, 3H), 1.33 (s, 9H). ^{13}C NMR (100 MHz, CDCl3) δ 176.6, 140.4, 138.6, 136.4, 133.5, 132.4, 132.3, 129.3, 128.8, 128.4, 125.0, 39.7, 27.9, 21.3, 20.1, 17.4. HRMS (ESI) calculated for $C_{20}H_{26}NO$ $[M+H]^+$: 296.2009, found: 296.2004.



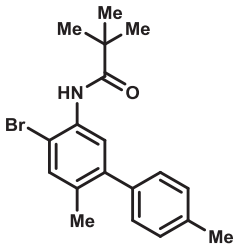
N-(6-methoxy-4,4'-dimethyl-[1,1'-biphenyl]-3-yl)pivalamide (**6j**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:2) to afford the product as white solids. Mp. 115-117 °C. ^{1}H NMR (399 MHz, Chloroform-d) δ 7.55 (s, 1H), 7.42 (d, J = 8.1 Hz, 2H), 7.18 (d, J = 7.9 Hz, 2H), 7.10 (s, 1H), 6.79 (s, 1H), 3.77 (s, 3H), 2.37 (s, 3H), 2.27 (s, 3H), 1.34 (s, 9H). ^{13}C NMR (100 MHz, CDCl3) δ 176.8, 154.2, 136.7, 135.1, 131.3, 129.5, 129.0, 128.8, 128.7, 127.2, 113.5, 56.0, 39.6, 27.9, 21.3, 18.1. HRMS (ESI) calculated for $C_{20}H_{26}NO_2$ $[M+H]^+$: 312.1958, found: 312.1957.



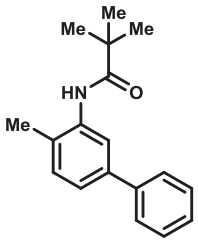
N-(2'-methoxy-4,4',4''-trimethyl-[1,1':3',1''-terphenyl]-5'-yl)pivalamide (**6j'**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as white solids. Mp. 176-180 °C. ^{1}H NMR (399 MHz, Chloroform-d) δ 7.71 (s, 1H), 7.53 (d, J = 7.6 Hz, 2H), 7.25 – 7.09 (m, 7H), 3.07 (s, 3H), 2.42 (s, 3H), 2.38 (s, 3H), 1.99 (s, 3H), 1.35 (s, 9H). ^{13}C NMR (100 MHz, CDCl3) δ 176.9, 152.9, 137.2, 136.8, 136.7, 135.4, 134.9, 132.9, 131.7, 129.8, 129.5, 129.2, 129.0, 129.0, 125.9, 60.5, 39.7, 27.9, 21.4, 21.3, 15.4. HRMS (ESI) calculated for $C_{27}H_{32}NO_2$ $[M+H]^+$: 402.2420, found: 402.2438.



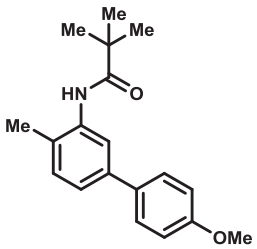
N-(4,6-dimethoxy-4'-methyl-[1,1'-biphenyl]-3-yl)pivalamide (**6k**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:2) to afford the product as a colorless oil. ^{1}H NMR (399 MHz, Chloroform-d) δ 8.39 (s, 1H), 7.89 (s, 1H), 7.44 (d, J = 8.1 Hz, 2H), 7.16 (d, J = 7.9 Hz, 2H), 6.57 (s, 1H), 3.94 (s, 3H), 3.78 (s, 3H), 2.36 (s, 3H), 1.32 (s, 9H). ^{13}C NMR (100 MHz, CDCl3) δ 176.3, 153.0, 148.5, 136.2, 135.2, 129.5, 128.7, 123.2, 122.7, 121.5, 96.2, 56.4, 56.2, 40.0, 27.8, 21.3. HRMS (ESI) calculated for $C_{20}H_{26}NO_3$ $[M+H]^+$: 328.1907, found: 328.1919.



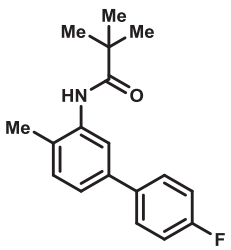
N-(4-bromo-4',6-dimethyl-[1,1'-biphenyl]-3-yl)pivalamide (**6l**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as off white solids. Mp. 119-122 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.26 (s, 1H), 7.92 (s, 1H), 7.43 (s, 1H), 7.22 – 7.17 (m, 4H), 2.38 (s, 3H), 2.22 (s, 3H), 1.34 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.7, 142.3, 137.8, 136.9, 133.5, 133.3, 132.7, 129.1, 128.9, 123.3, 112.2, 40.2, 27.7, 21.3, 20.0. HRMS (ESI) calculated for $C_{19}H_{23}BrNO$ $[M+H]^+$: 360.0958, found: 360.0965.



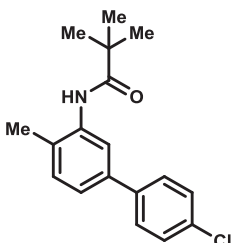
N-(4-methyl-[1,1'-biphenyl]-3-yl)pivalamide (**6m**).[7] Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as yellow solids. Mp. 112-114 °C (Lit.: Mp. 109-110 °C).[7]. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.21 (d, J = 1.8 Hz, 1H), 7.64 – 7.59 (m, 2H), 7.41 (t, J = 7.5 Hz, 2H), 7.35 – 7.27 (m, 3H), 7.24 (d, J = 7.8 Hz, 1H), 2.30 (s, 3H), 1.37 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.7, 140.8, 140.1, 136.4, 130.9, 128.8, 127.5, 127.3, 127.2, 123.5, 121.5, 40.0, 27.9, 17.5. HRMS (ESI) calculated for $C_{18}H_{22}NO$ $[M+H]^+$: 268.1696, found: 268.1690.



N-(4'-methoxy-4-methyl-[1,1'-biphenyl]-3-yl)pivalamide (**6n**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:2) to afford the product as brown solids. Mp. 122-126 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.16 (d, J = 1.7 Hz, 1H), 7.55 (d, J = 8.8 Hz, 2H), 7.32 – 7.25 (m, 2H), 7.21 (d, J = 7.9 Hz, 1H), 6.94 (d, J = 8.8 Hz, 2H), 3.84 (s, 3H), 2.28 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.7, 159.2, 139.7, 136.3, 133.4, 130.8, 128.2, 126.9, 123.1, 121.0, 114.2, 40.0, 27.9, 17.4. HRMS (ESI) calculated for $C_{19}H_{24}NO_2$ $[M+H]^+$: 298.1802, found: 298.1799.

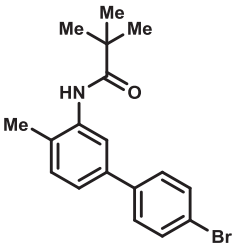


N-(4'-fluoro-4-methyl-[1,1'-biphenyl]-3-yl)pivalamide (**6o**).[8] Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as off white solids. Mp. 113-114 °C. (Lit.: Mp. 107-109 °C).[8]. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.19 (d, J = 1.5 Hz, 1H), 7.56 (dd, J = 8.8, 5.3 Hz, 2H), 7.31 (s, 1H), 7.27 – 7.19 (m, 2H), 7.08 (t, J = 8.7 Hz, 2H), 2.29 (s, 3H), 1.37 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.7, 162.6 (d, J = 246 Hz) , 139.1, 136.9 (d, J = 2.8 Hz), 136.4, 130.9, 128.8 (d, J = 8.0 Hz), 127.3, 123.3, 121.2, 115.6 (d, J = 21.4 Hz), 40.0, 27.9, 17.4. ^{19}F NMR (376 MHz, Chloroform-d) δ -115.95 – -116.06 (m). HRMS (ESI) calculated for $C_{18}H_{21}FNO$ $[M+H]^+$: 286.1602, found: 286.1604.

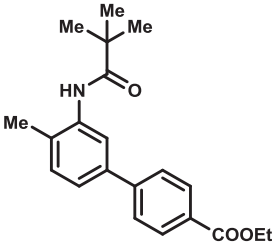


N-(4'-chloro-4-methyl-[1,1'-biphenyl]-3-yl)pivalamide (**6p**).[8] Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product

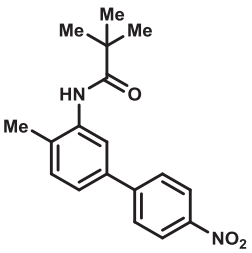
as yellow solids. Mp. 145-148 °C. (Lit.: Mp. 148 °C).[8]. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.18 (d, J = 1.7 Hz, 1H), 7.53 (d, J = 8.6 Hz, 2H), 7.40 – 7.31 (m, 3H), 7.29 – 7.20 (m, 2H), 2.28 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.8, 139.2, 138.7, 136.5, 133.3, 130.9, 128.9, 128.4, 127.9, 123.2, 121.2, 39.9, 27.8, 17.4. HRMS (ESI) calculated for $C_{18}H_{21}ClNO$ $[M+H]^+$: 302.1306, found: 302.1317.



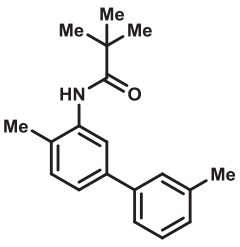
N-(4'-bromo-4-methyl-[1,1'-biphenyl]-3-yl)pivalamide (**6q**).[8] Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as white solids. Mp. 160-162 °C. (Lit.: Mp. 141-142 °C).[8]. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.16 (d, J = 1.7 Hz, 1H), 7.55 – 7.43 (m, 4H), 7.36 (s, 1H), 7.28 – 7.19 (m, 2H), 2.28 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.8, 139.6, 138.6, 136.4, 131.8, 130.9, 128.7, 128.1, 123.2, 121.4, 121.2, 39.9, 27.8, 17.4.. HRMS (ESI) calculated for $C_{18}H_{21}BrNO$ $[M+H]^+$: 346.0801, found: 346.0816.



ethyl 4'-methyl-3'-pivalamido-[1,1'-biphenyl]-4-carboxylate (**6r**).[7] Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:2) to afford the product as yellow solids. Mp. 119-120 °C. (Lit.: Mp. 111-112 °C).[7]. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.25 (d, J = 1.9 Hz, 1H), 8.07 (d, J = 8.5 Hz, 2H), 7.67 (d, J = 8.5 Hz, 2H), 7.33 (dd, J = 7.9, 2.0 Hz, 2H), 7.26 (d, J = 7.8 Hz, 1H), 4.39 (q, J = 7.1 Hz, 2H), 2.30 (s, 3H), 1.41 (t, J = 7.1 Hz, 3H), 1.36 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.8, 166.7, 145.1, 138.8, 136.6, 131.0, 130.1, 129.2, 128.5, 127.0, 123.6, 121.5, 61.0, 40.0, 27.8, 17.5, 14.5. HRMS (ESI) calculated for $C_{21}H_{26}NO_3$ $[M+H]^+$: 340.1907, found: 340.1906.

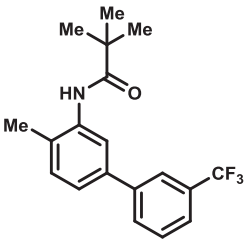


N-(4-methyl-4'-nitro-[1,1'-biphenyl]-3-yl)pivalamide (**6s**). Purification by flash chromatography on silica: Cy:EtOAc (4:1) to afford the product as a yellow oil. ^{1}H NMR (399 MHz, Chloroform-d) δ 8.33 (d, J = 1.8 Hz, 1H), 8.25 (d, J = 8.9 Hz, 2H), 7.75 (d, J = 8.9 Hz, 2H), 7.41 – 7.27 (m, 3H), 2.32 (s, 3H), 1.37 (s, 9H). ^{13}C NMR (100 MHz, CDCl3) δ 176.9, 147.2, 147.1, 137.5, 136.8, 131.2, 128.9, 127.8, 124.1, 123.5, 121.3, 40.1, 27.8, 17.5. HRMS (ESI) calculated for $C_{18}H_{21}N_2O_3$ $[M+H]^+$: 313.1547, found: 313.1551.

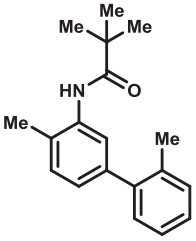


N-(3',4-dimethyl-[1,1'-biphenyl]-3-yl)pivalamide (**6t**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as off white solids. Mp. 126-129 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.19 (d, J = 1.8 Hz, 1H), 7.46 – 7.37 (m, 2H), 7.35 – 7.27 (m, 3H), 7.23 (d, J = 7.9 Hz, 1H), 7.17 – 7.10 (m, 1H), 2.40 (s, 3H), 2.29 (s, 3H), 1.37 (s, 9H). ^{13}C NMR (101

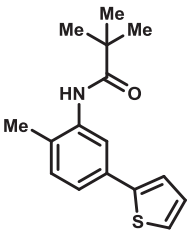
MHz, CDCl3) δ 176.7, 159.2, 139.7, 136.3, 133.4, 130.8, 128.2, 126.9, 123.1, 121.0, 114.2, 55.5, 40.0, 27.9, 17.4. HRMS (ESI) calculated for $C_{19}H_{24}NO$ $[M+H]^+$: 282.1853, found: 282.1846.



N-(4-methyl-3'-(trifluoromethyl)-[1,1'-biphenyl]-3-yl)pivalamide (**6u**).[7] Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as orange solids. Mp. 77-83 °C (Lit.: Mp. 60-62 °C).[7] ^{1}H NMR (400 MHz, Chloroform-d) δ 8.23 (d, J = 1.8 Hz, 1H), 7.82 (s, 1H), 7.79 (d, J = 7.7 Hz, 1H), 7.57 (d, J = 7.9 Hz, 1H), 7.52 (t, J = 7.7 Hz, 1H), 7.39 – 7.31 (m, 1H), 7.31 – 7.26 (m, 2H), 2.31 (s, 3H), 1.37 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.8, 141.7, 138.7, 136.6, 131.1 (q, J = 31.9 Hz), 130.7, 129.3, 128.3, 124.1 (q, J = 272 Hz), 124.0 (q, J = 3.8 Hz), 123.9 (q, J = 3.8 Hz), 123.5, 121.4, 40.0, 27.9, 17.5. ^{19}F NMR (376 MHz, CDCl3) δ -62.51. HRMS (ESI) calculated for $C_{19}H_{21}F_3NO$ $[M+H]^+$: 336.1570, found: 336.1555.

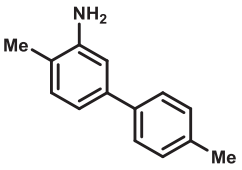


N-(2',4-dimethyl-[1,1'-biphenyl]-3-yl)pivalamide (**6v**).[7] Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:1) to afford the product as off white solids. Mp. 122-125 °C (Lit.: Mp. 115-116 °C).[7] ^{1}H NMR (400 MHz, Chloroform-d) δ 7.87 (d, J = 1.8 Hz, 1H), 7.29 (s, 1H), 7.26 – 7.19 (m, 5H), 7.05 (dd, J = 7.7, 1.8 Hz, 1H), 2.31 (d, J = 2.2 Hz, 6H), 1.35 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 176.6, 141.5, 140.7, 135.6, 135.5, 130.3, 130.2, 130.0, 127.3, 127.2, 125.8, 123.9, 39.9, 27.9, 20.7, 17.5. HRMS (ESI) calculated for $C_{19}H_{24}FNO$ $[M+H]^+$: 282.1853, found: 282.1858.

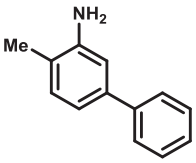


N-(2-methyl-5-(thiophen-2-yl)phenyl)pivalamide (**6w**). Purification by flash chromatography on silica: Cy:DCM:EtOAc (30:70:2) to afford the product as yellow solids. Mp. 107-113 °C. ^{1}H NMR (399 MHz, Chloroform-d) δ 8.23 (d, J = 1.9 Hz, 1H), 7.34 – 7.27 (m, 3H), 7.24 (d, J = 5.1 Hz, 1H), 7.17 (d, J = 7.9 Hz, 1H), 7.05 (t, J = 4.4 Hz, 1H), 2.26 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (100 MHz, CDCl3) δ 176.7, 144.2, 136.5, 133.4, 130.9, 128.0, 127.8, 124.7, 123.3, 122.5, 120.1, 40.0, 27.9, 17.5. HRMS (ESI) calculated for $C_{16}H_{20}NOS$ $[M+H]^+$: 274.1260, found: 274.1258.

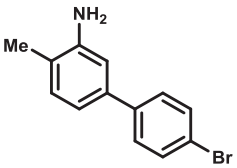
5.3. Meta-arylated anilines



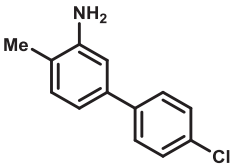
4,4'-dimethyl-[1,1'-biphenyl]-3-amine (**7a**).[9] Purification by extraction procedure (see 4.4) to afford the product as orange solids. Mp. 101-102 °C (Lit.: Mp. 104-105 °C)[9]. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.49 (d, J = 8.1 Hz, 2H), 7.25 (d, J = 8.0 Hz, 2H), 7.13 (d, J = 7.7 Hz, 1H), 6.97 (dd, J = 7.7, 1.7 Hz, 1H), 6.92 (d, J = 1.7 Hz, 1H), 3.66 (s, 2H), 2.41 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 144.9, 140.2, 138.6, 136.8, 130.9, 129.4, 126.9, 121.4, 117.5, 113.6, 21.2, 17.2. HRMS (ESI) calculated for $C_{14}H_{16}N$ $[M+H]^+$: 198.1277, found: 198.1277.



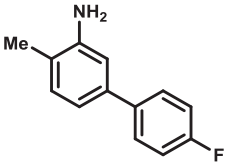
4-methyl-[1,1'-biphenyl]-3-amine (**7b**).[7] Purification by extraction procedure (see 4.4) to afford the product a yellow oil. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.56 (dd, J = 8.2, 1.1 Hz, 2H), 7.41 (t, J = 7.6 Hz, 2H), 7.35 – 7.28 (m, 1H), 7.13 (d, J = 7.6 Hz, 1H), 7.02 – 6.91 (m, 2H), 3.83 (s, 2H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 144.4, 141.4, 140.4, 131.0, 128.9, 128.7, 127.1, 122.0, 118.0, 114.1, 17.2. HRMS (ESI) calculated for $C_{13}H_{14}N$ $[M+H]^+$: 184.1121, found: 184.1121.



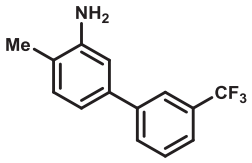
4'-bromo-4-methyl-[1,1'-biphenyl]-3-amine (**7c**). Purification by extraction procedure (see 4.4) to afford the product as yellow solids. Mp. 106-108 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.52 (d, J = 8.6 Hz, 2H), 7.42 (d, J = 8.6 Hz, 2H), 7.12 (d, J = 7.7 Hz, 1H), 6.96 – 6.81 (m, 2H), 3.67 (s, 2H), 2.21 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 145.0, 140.4, 139.1, 131.8, 131.1, 128.7, 122.1, 121.2, 117.4, 113.4, 17.2. HRMS (ESI) calculated for $C_{13}H_{13}BrN$ $[M+H]^+$: 262.0226, found: 262.0231.



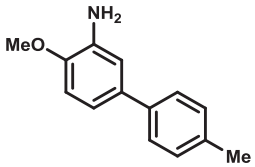
4'-chloro-4-methyl-[1,1'-biphenyl]-3-amine (**7d**). Purification by extraction procedure (see 4.4) to afford the product as orange solids. Mp. 93-95 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.50 – 7.45 (m, 2H), 7.39 – 7.34 (m, 2H), 7.12 (d, J = 7.6 Hz, 1H), 6.94 – 6.86 (m, 2H), 3.57 (s, 2H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 144.7, 139.9, 139.1, 133.1, 131.1, 128.9, 128.3, 122.2, 117.7, 113.7, 17.2.



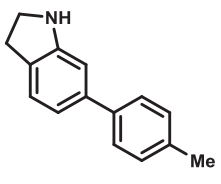
4'-fluoro-4-methyl-[1,1'-biphenyl]-3-amine (**7e**). Purification by extraction procedure (see 4.4) to afford the product as yellow solids. Mp. 72-74 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.53 – 7.48 (m, 2H), 7.13 – 7.06 (m, 3H), 6.94 – 6.86 (m, 2H), 3.99 (s, 2H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 162.4 (d, J = 245.6 Hz), 144.5, 139.4, 137.5, 131.1, 128.6 (d, J = 8.0 Hz), 122.0, 117.9, 115.6 (d, J = 21.3 Hz), 113.9, 17.2. ^{19}F NMR (376 MHz, Chloroform-d) δ -115.85 – -117.40 (m).



4-methyl-3'-(trifluoromethyl)-[1,1'-biphenyl]-3-amine (**7f**). Purification by extraction procedure (see 4.4) to afford the product as off white solids. Mp. 228-232 °C. ^{1}H NMR (399 MHz, Methanol-d4) δ 7.93 – 7.85 (m, 2H), 7.67 (d, J = 6.1 Hz, 2H), 7.60 – 7.49 (m, 2H), 7.45 (d, J = 7.9 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, Methanol-d4) δ 141.7, 140.4, 133.6, 132.6 (q, J = 42.6 Hz), 132.6, 131.6, 131.1, 128.3 (q, J = 272.0 Hz), 128.0, 125.6 (q, J = 3.8 Hz), 124.4 (q, J = 3.8 Hz), 122.1, 27.9, 16.8. ^{19}F NMR (376 MHz, Methanol-d4) δ -64.18.



4-methoxy-4'-methyl-[1,1'-biphenyl]-3-amine (**7g**). Purification by extraction procedure (see 4.4) to afford the product as orange solids. Mp. 108-112 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.43 (d, J = 8.1 Hz, 2H), 7.21 (d, J = 7.9 Hz, 2H), 6.95 (dd, J = 6.2, 2.1 Hz, 2H), 6.85 (d, J = 8.9 Hz, 1H), 3.89 (s, 3H), 3.79 (s, 2H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 146.9, 138.5, 137.0, 136.4, 134.4, 129.4, 126.8, 117.2, 113.8, 110.8, 55.8, 21.2. HRMS (ESI) calculated for $C_{14}H_{16}NO$ $[M+H]^{+}$: 214.1227, found: 214.1225.



6-(p-tolyl)indoline (**7h**). Purification by extraction procedure (see 4.4) to afford the product as brown solids. Mp. 162-165 °C. ^{1}H NMR (399 MHz, Chloroform-d) δ 7.46 (d, J = 8.1 Hz, 2H), 7.20 (dd, J = 17.7, 7.7 Hz, 3H), 6.96 (dd, J = 7.6, 1.1 Hz, 1H), 6.90 (s, 1H), 3.88 (s, 1H), 3.62 (t, J = 8.3 Hz, 2H), 3.08 (t, J = 8.3 Hz, 2H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 151.8, 140.9, 139.0, 136.8, 129.4, 128.6, 127.1, 124.9, 118.3, 108.5, 47.7, 29.7, 21.2.

6. References

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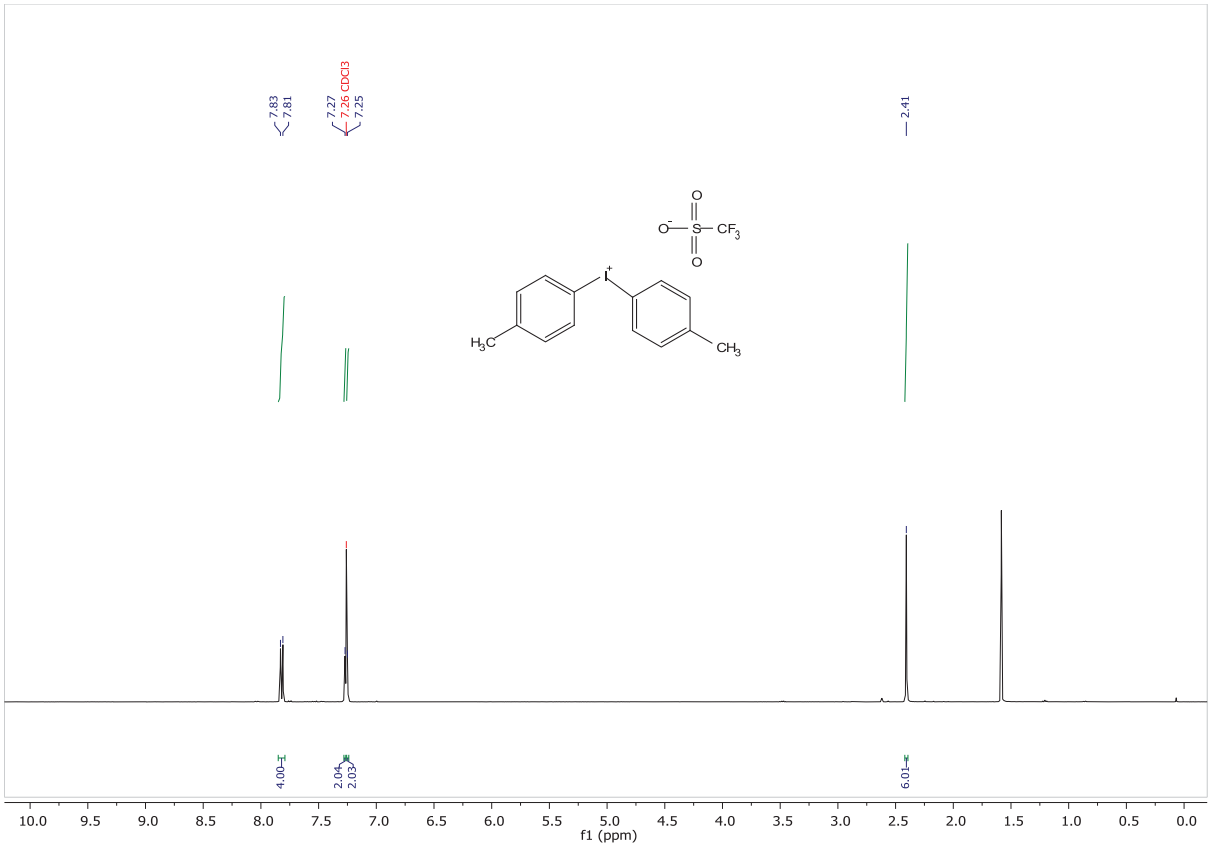
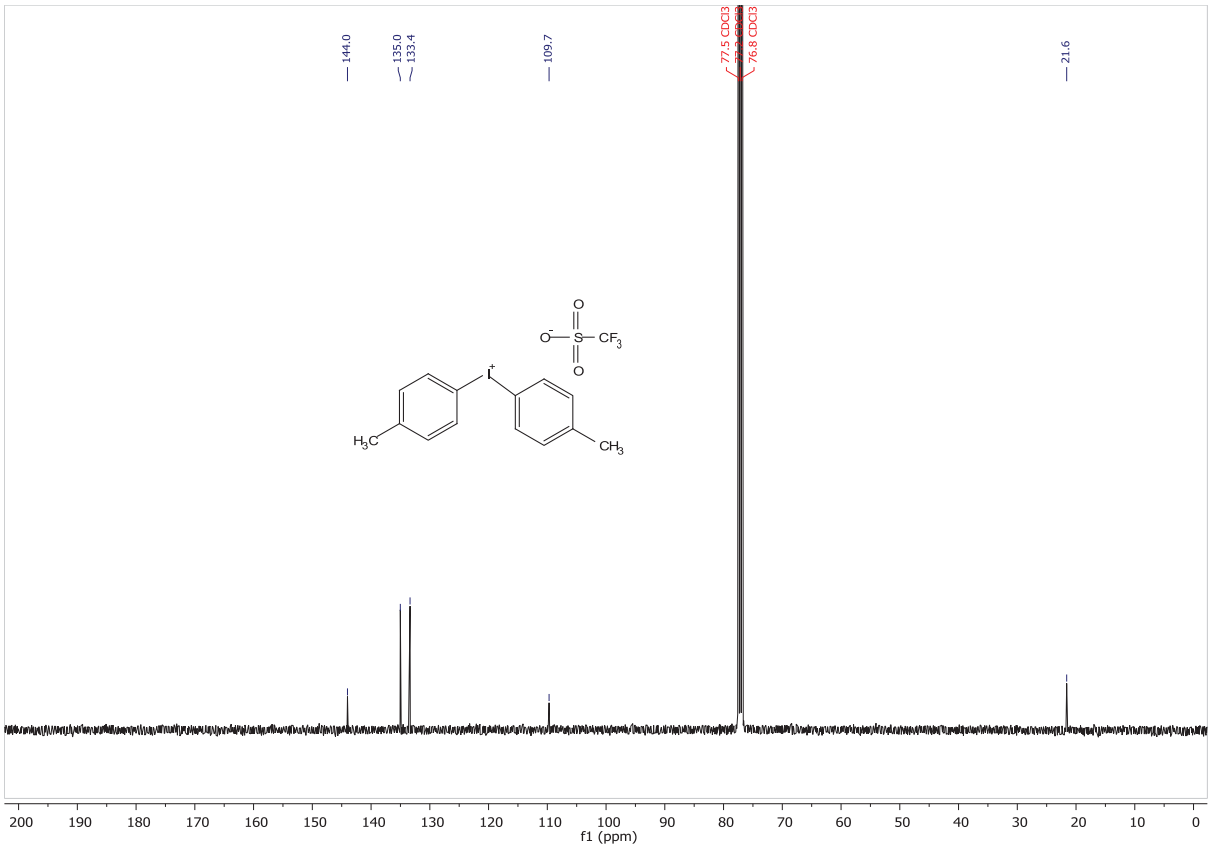
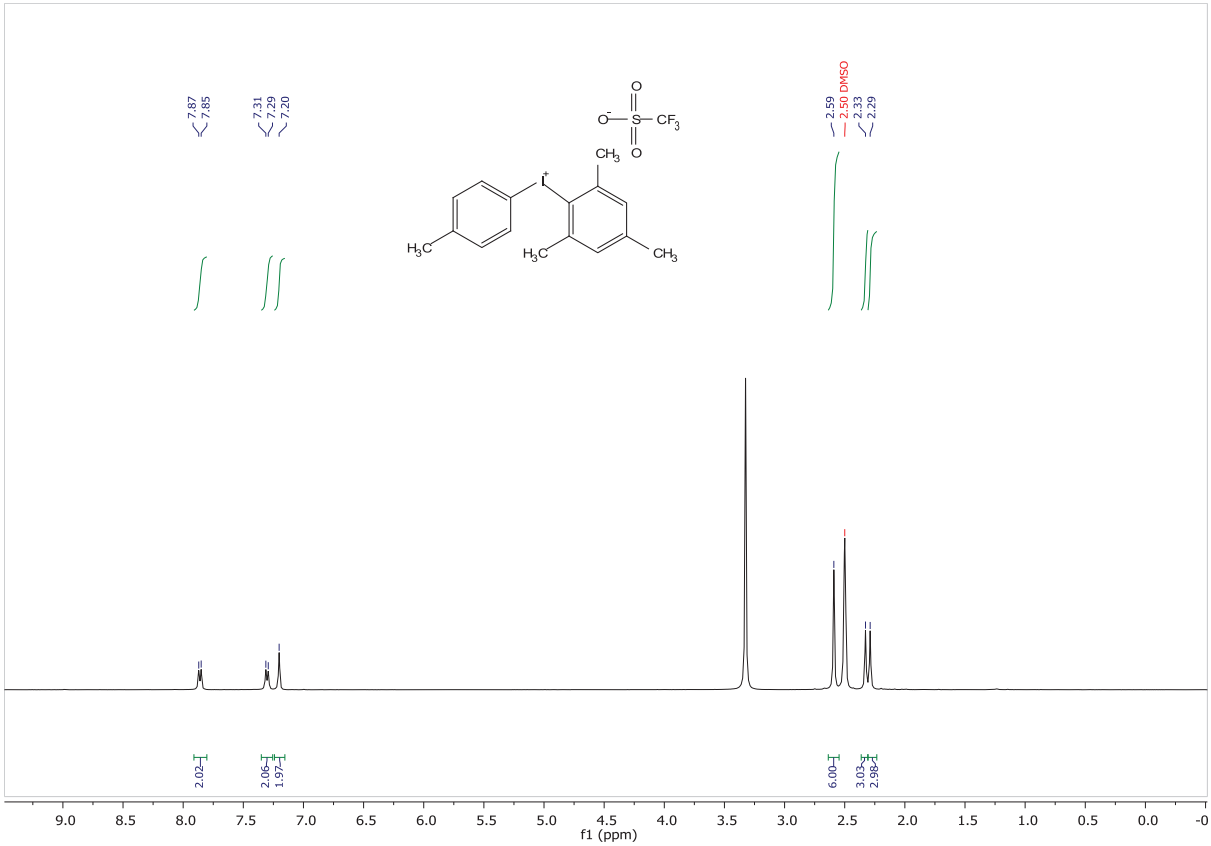
7. NMR spectra



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7.85
7.31
7.29
7.20
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2.33
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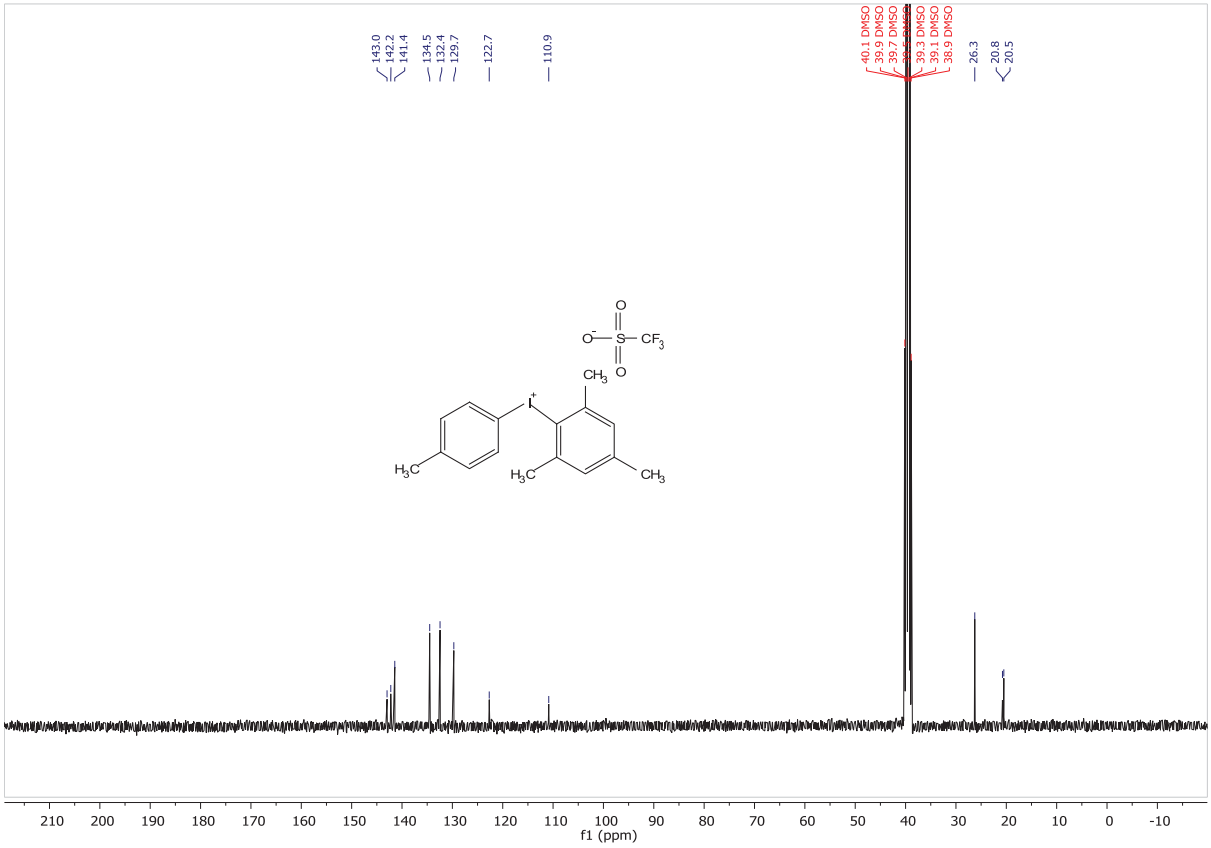
6.00
3.03
2.98
f1 (ppm)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142.2
141.4
134.5
132.4
129.7
122.7
110.9
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39.9 DMSO
39.7 DMSO
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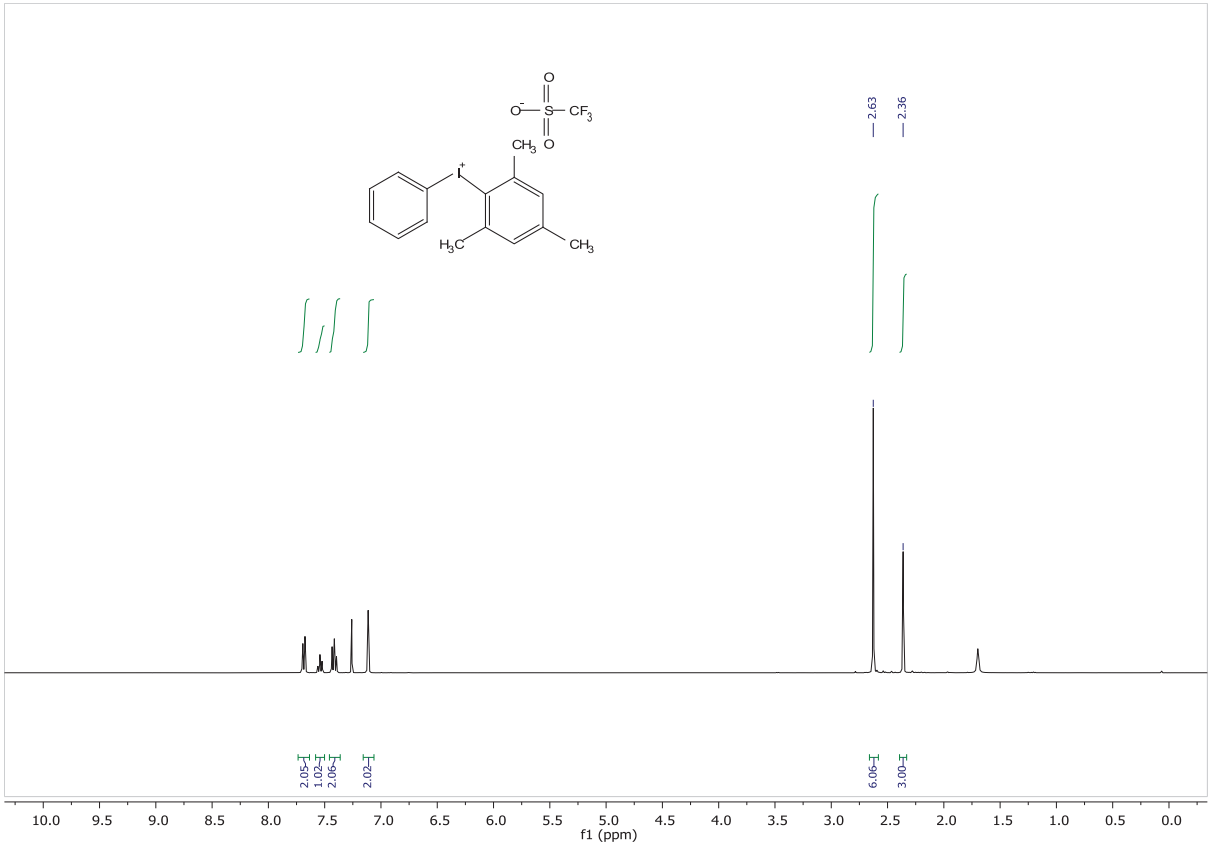
38.9 DMSO
26.3
20.8
20.5
f1 (ppm)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1.02
2.06
2.02
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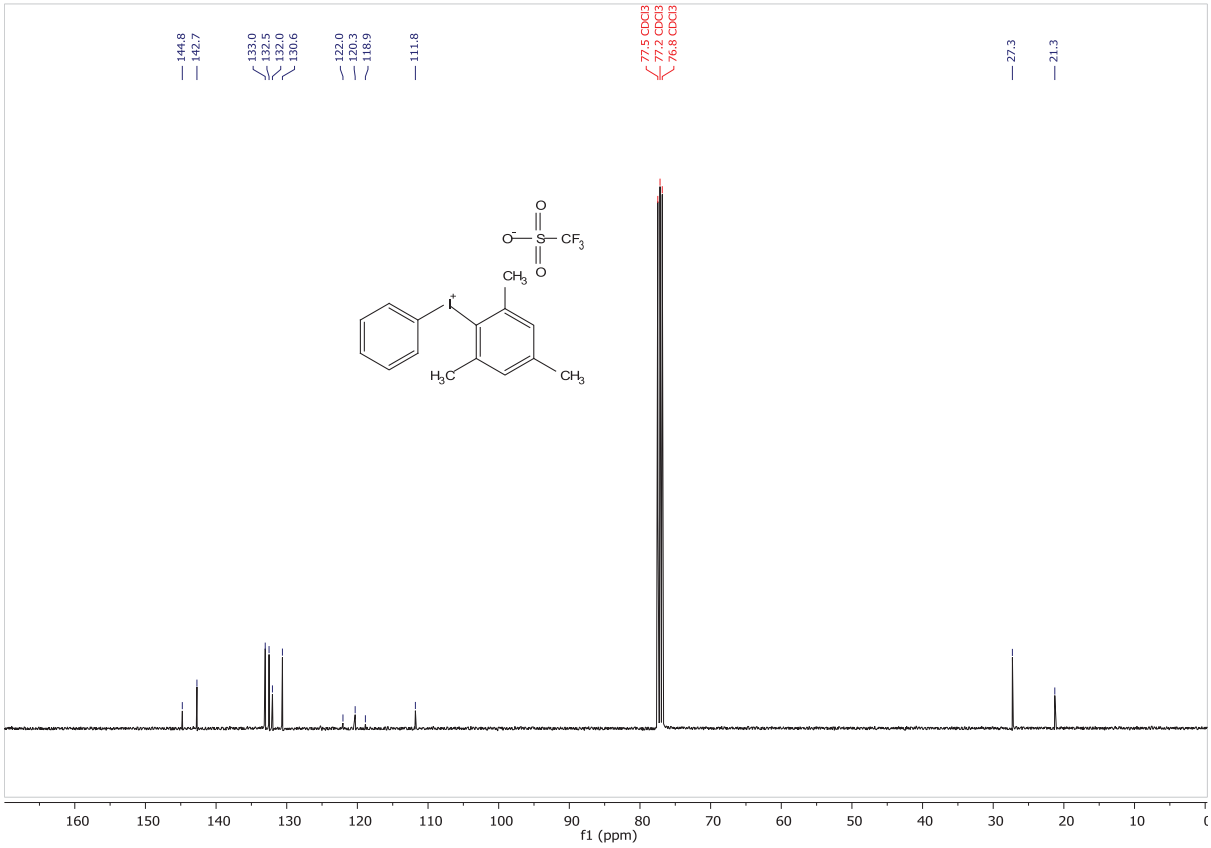
3.00
f1 (ppm)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142.7
133.0
132.5
132.0
130.6
122.0
120.3
118.9
111.8
77.5 CDCl3
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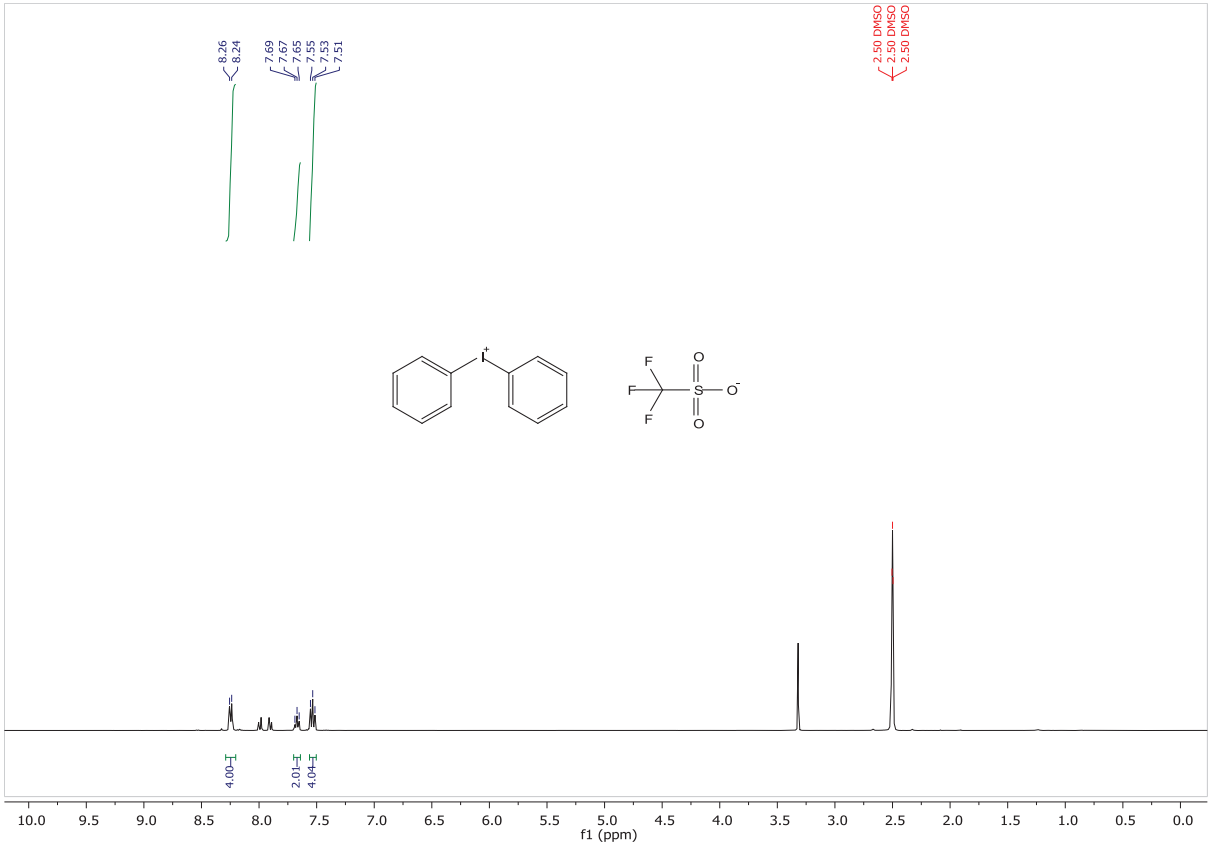
76.8 CDCl3
27.3
21.3
f1 (ppm)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8.24
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7.67
7.65
7.55
7.53
7.51
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2.50 DMSO
2.50 DMSO
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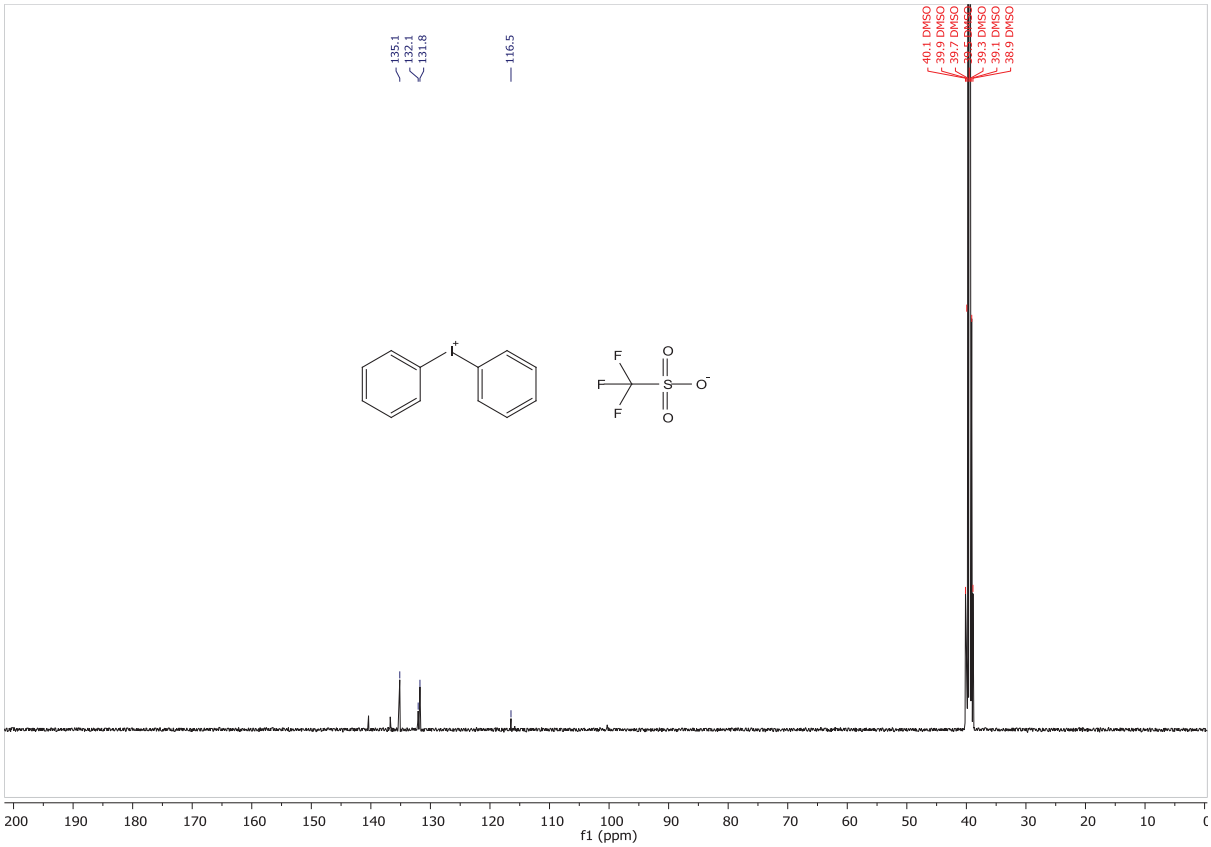
2.01
4.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.1
131.8
116.5
40.1 DMSO
39.9 DMSO
39.7 DMSO
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39.1 DMSO
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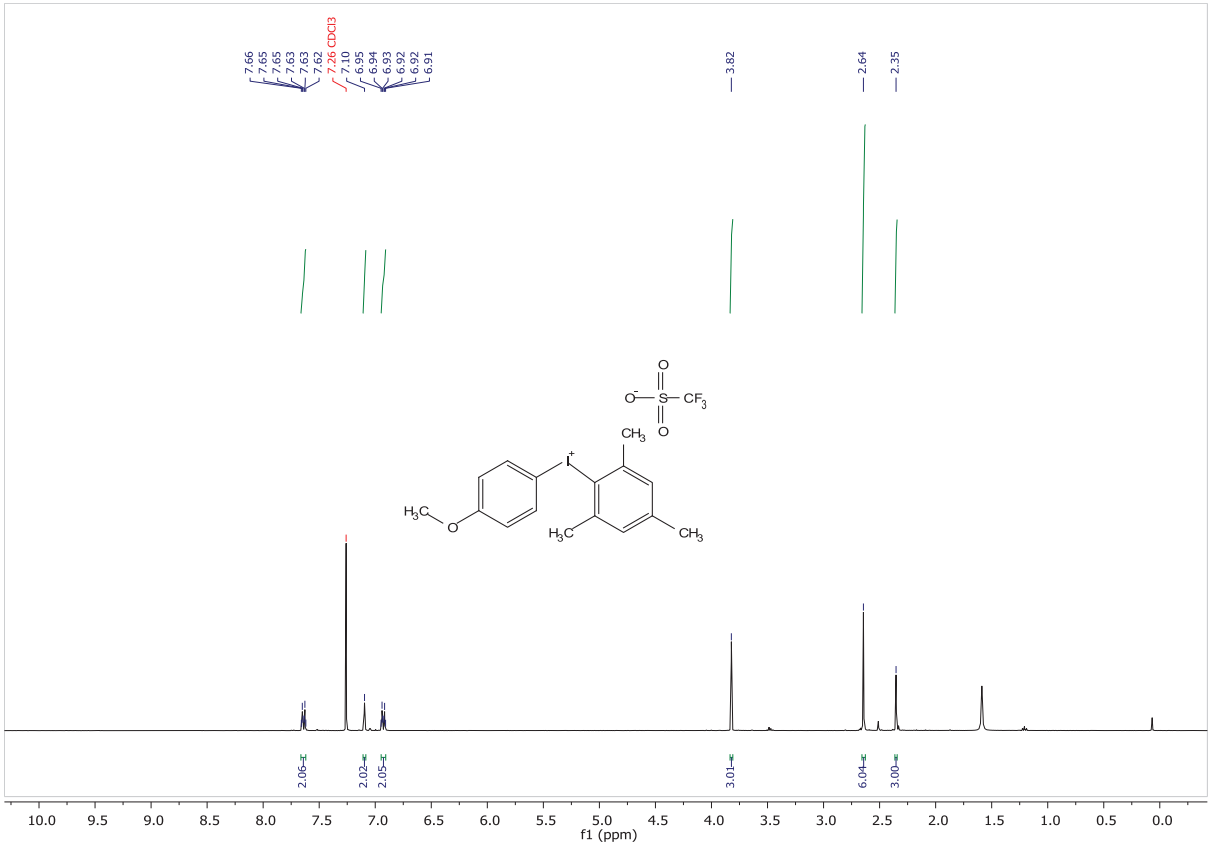
f1 (ppm)


7.66
7.65
7.65
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7.63
7.62
7.26 CDCl3
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6.95
6.94
6.93
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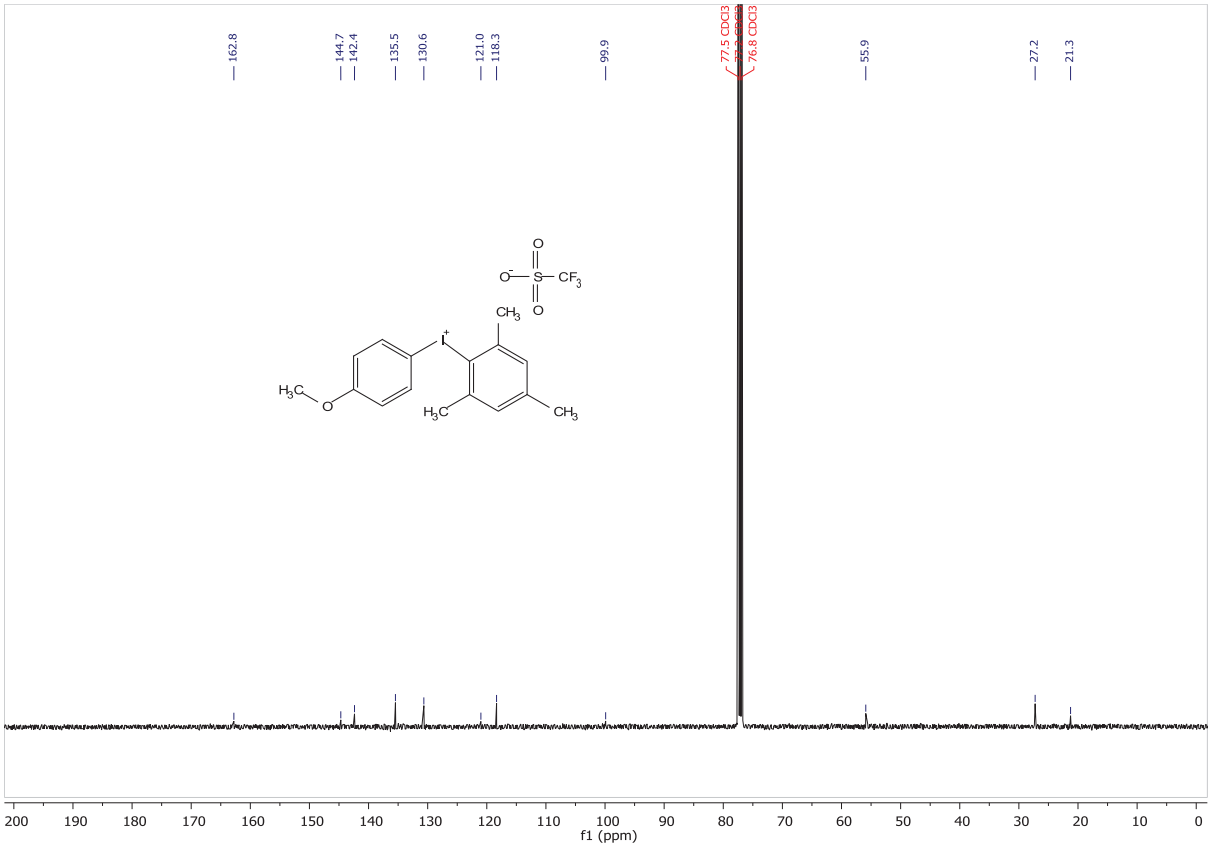
2.05
3.01
6.04
3.00
f1 (ppm)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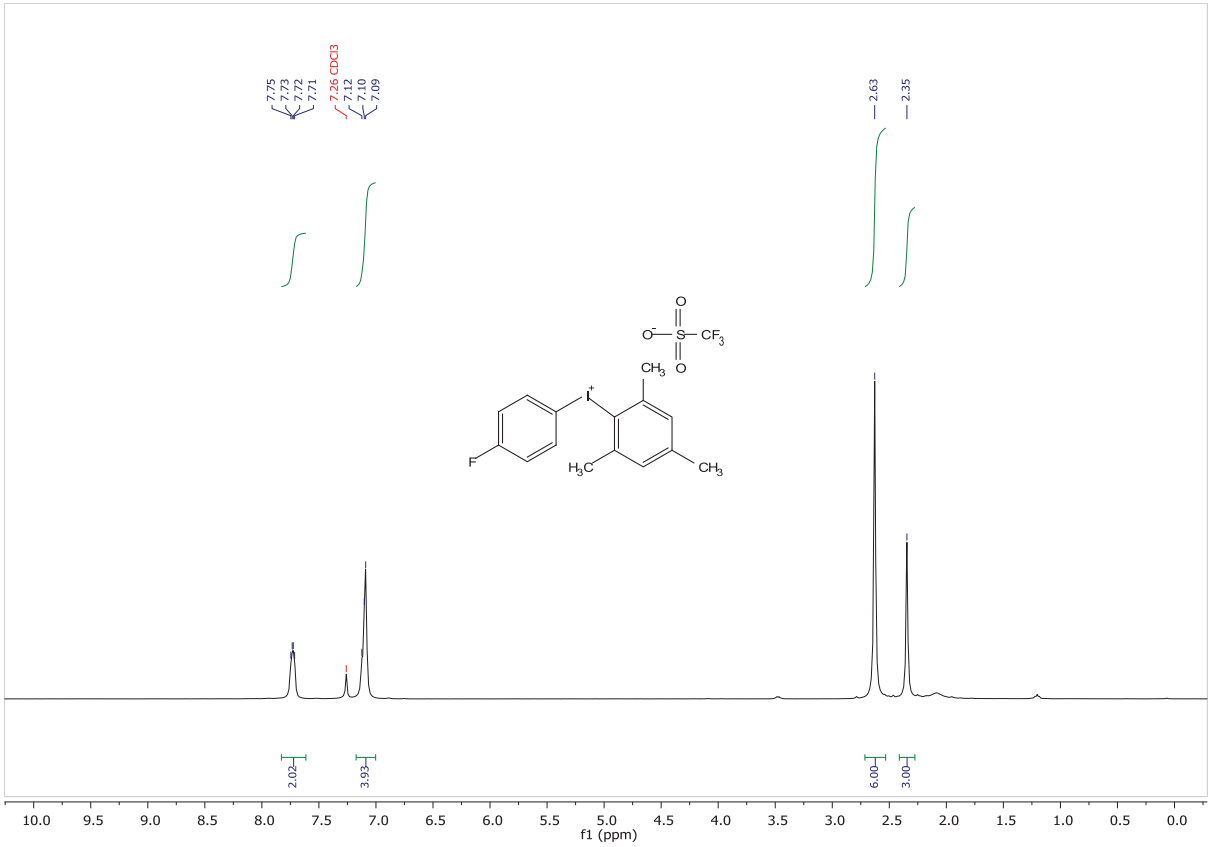
27.2
21.3
f1 (ppm)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7.71
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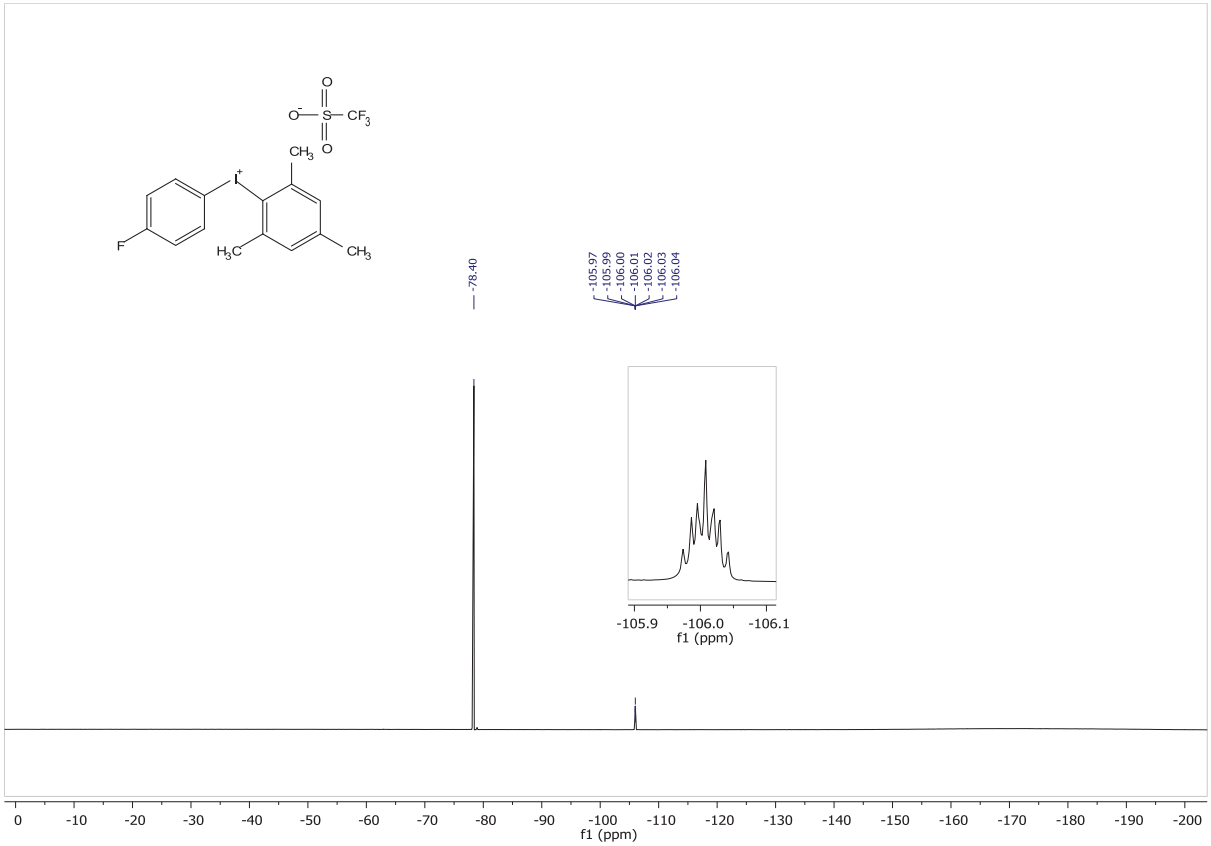
7.12
7.10
7.09
2.63
2.35
2.02
3.93
6.00
3.00
f1 (ppm)


165.9
163.4
144.6
142.5
135.8
135.7
130.5
121.9
121.2
119.9
119.6
118.7
105.3
105.2
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
27.2
21.3
f1 (ppm)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-106.03
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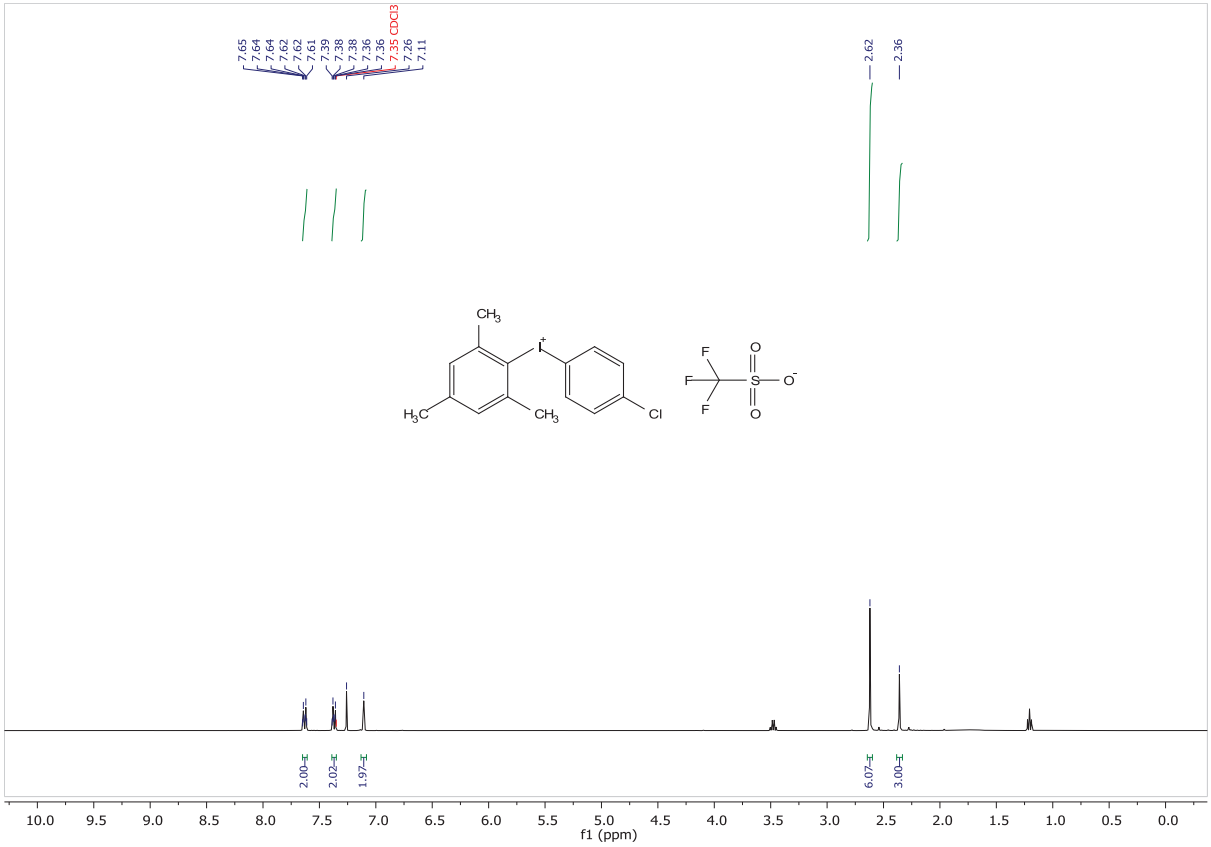
-105.9
-106.0
-106.1
f1 (ppm)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)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7.64
7.62
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7.36
7.36
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7.26
7.11
2.62
2.36
CH3
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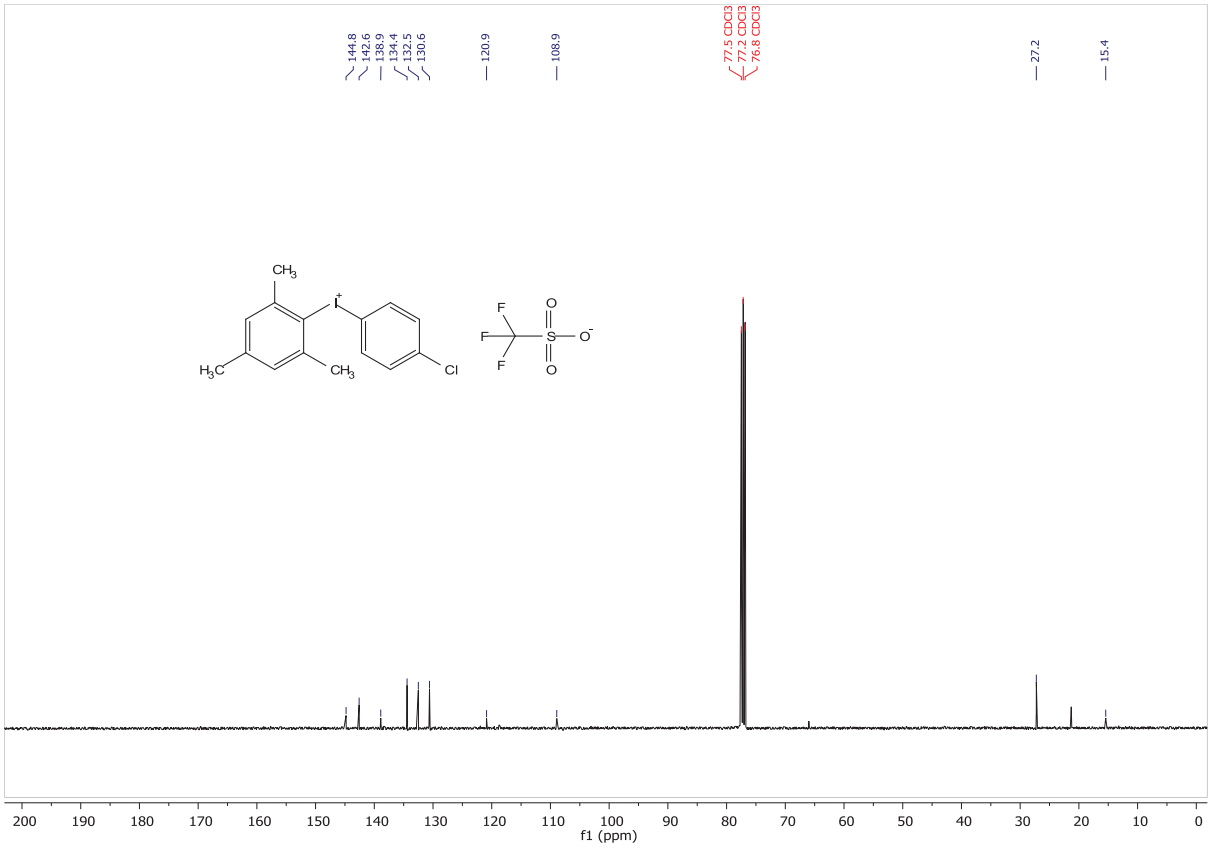
2.02
1.97
6.07
3.00
f1 (ppm)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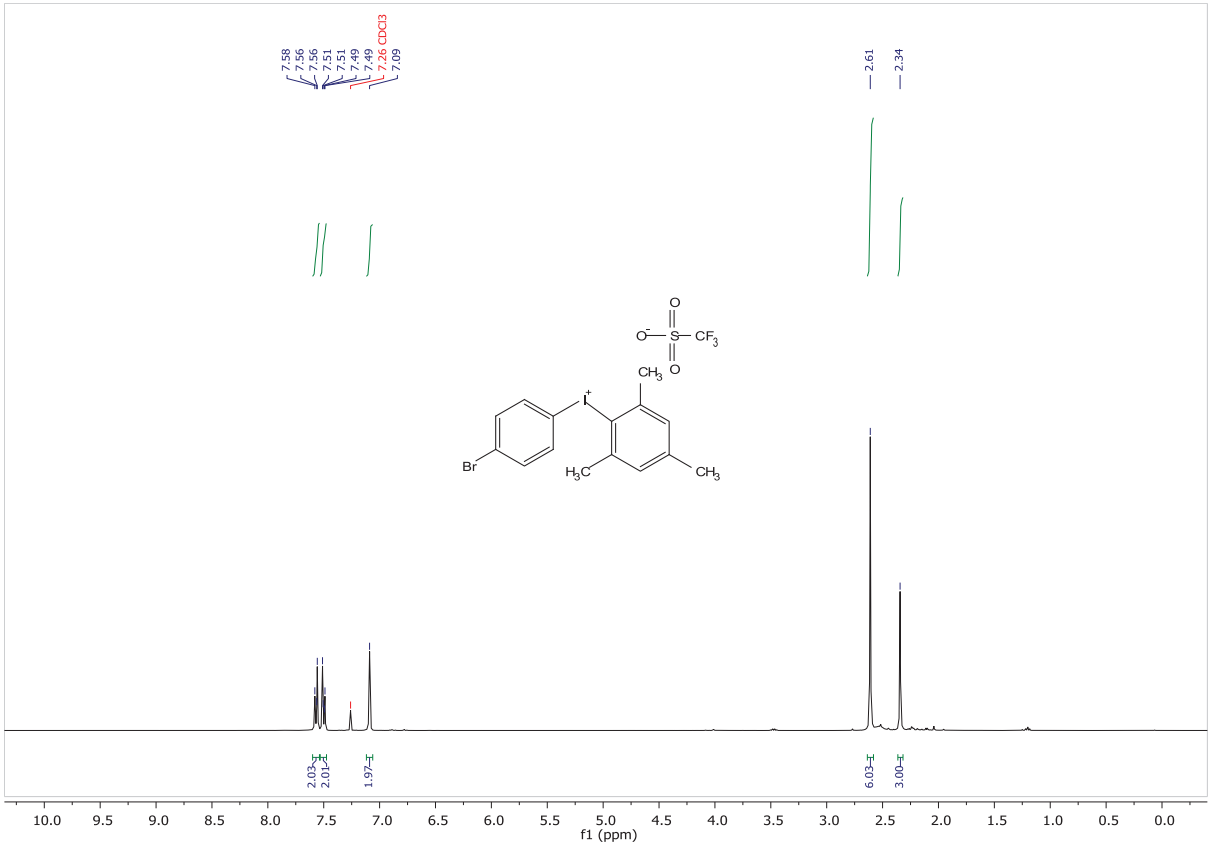
15.4
CH3
I+
H3C
CH3
Cl
F
F
F
O
S
O
O-
f1 (ppm)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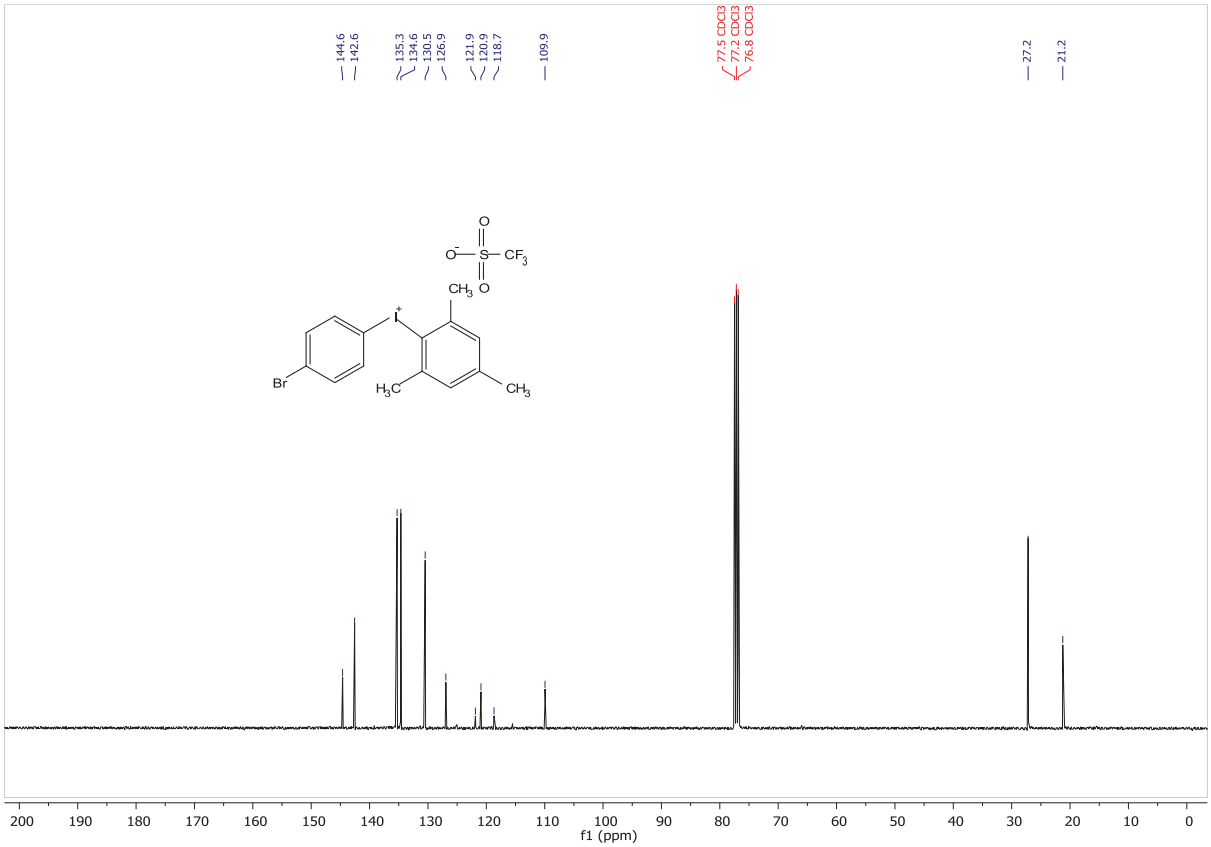
7.49
7.26 CDCl3
7.09
2.61
2.34
2.03
2.01
1.97
6.03
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.3
134.6
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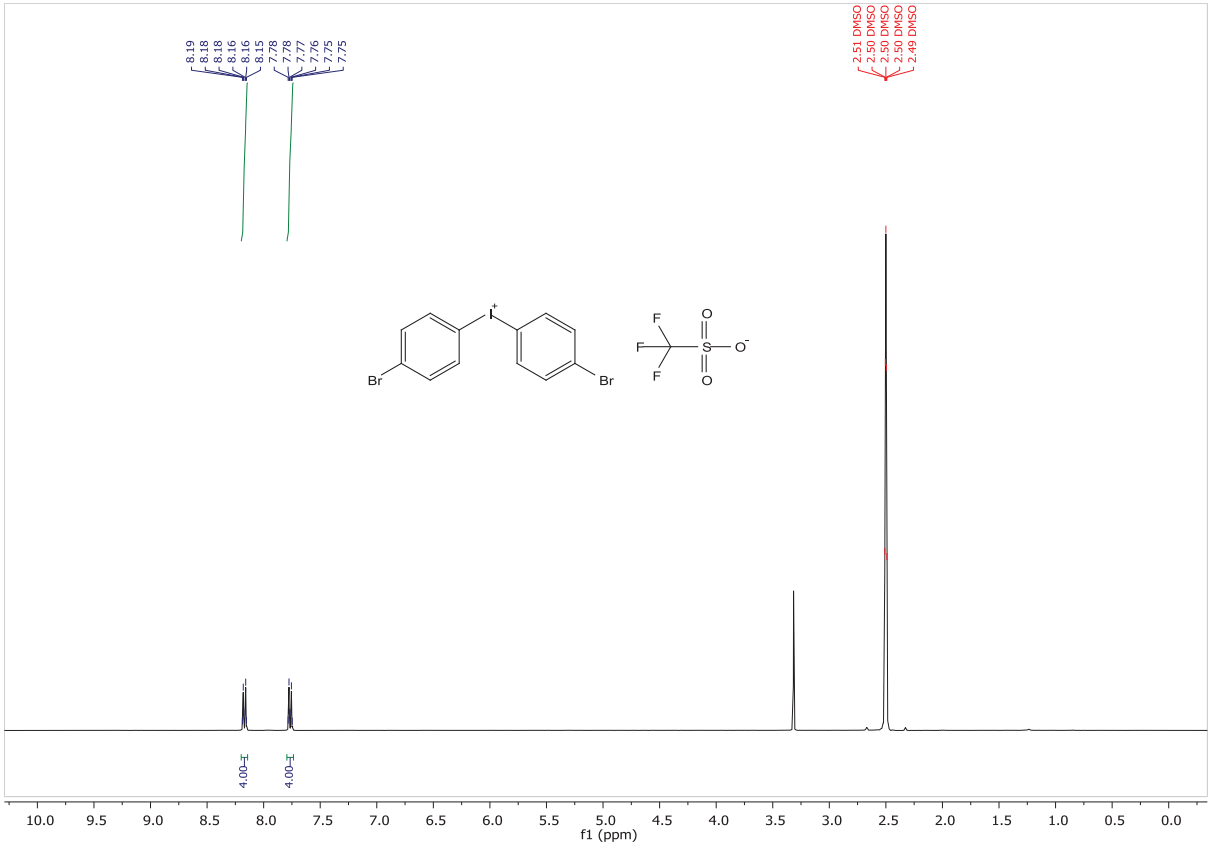
121.9
120.9
118.7
109.9
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
27.2
21.2
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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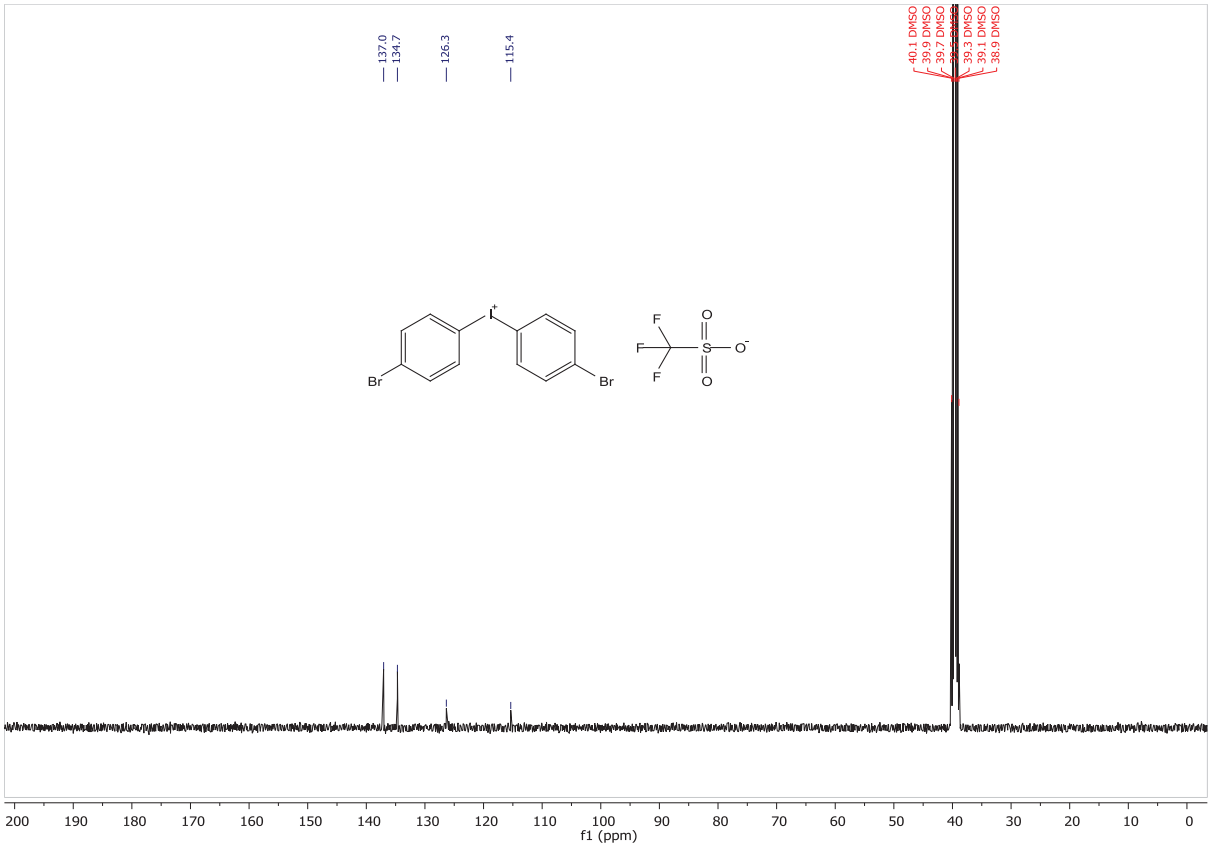
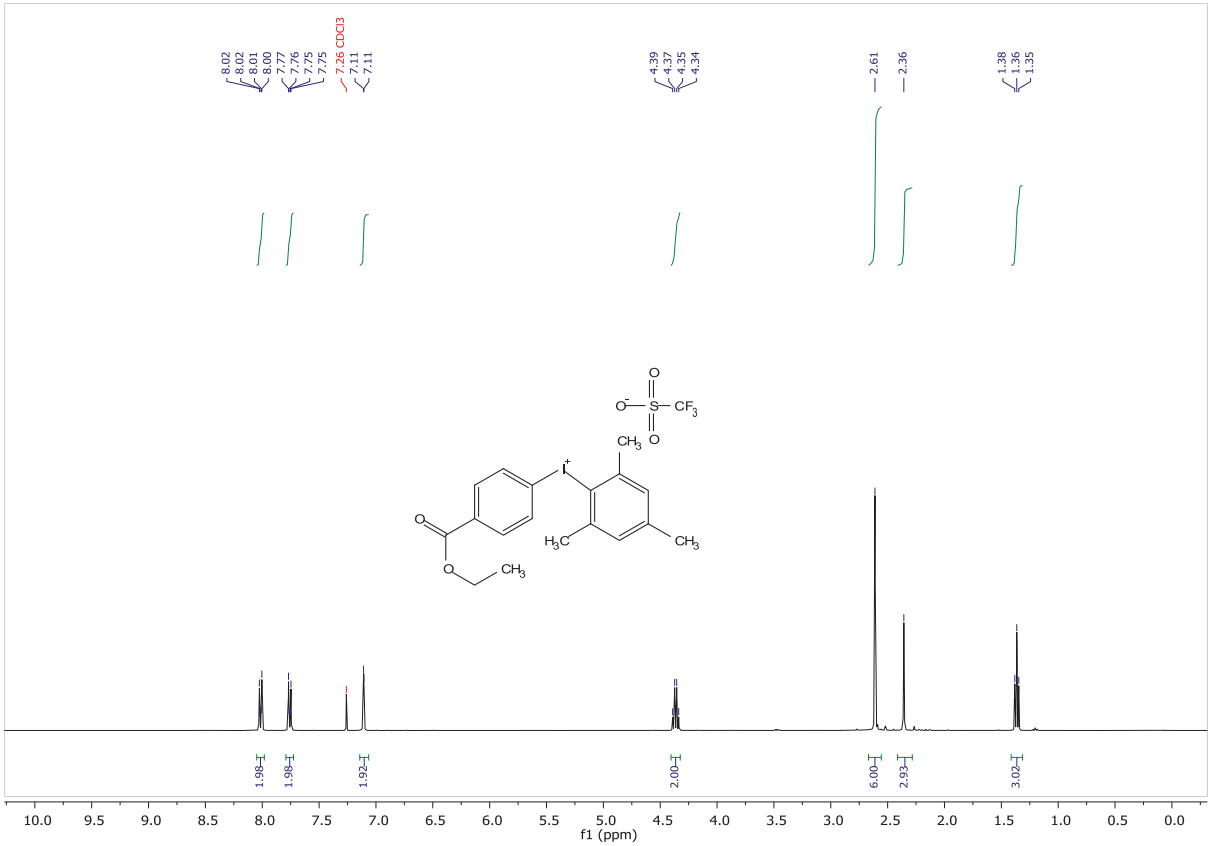
8.18
8.18
8.16
8.16
8.15
7.78
7.78
7.77
7.76
7.75
7.75
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.50 DMSO
2.49 DMSO
Br
Br
F
F
F
O
S
O
O
4.00
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


137.0
134.7
126.3
115.4
40.1 DMSO
39.9 DMSO
39.7 DMSO
39.5 DMSO
39.3 DMSO
39.1 DMSO
38.9 DMSO
Br
Br
F
F
F
O
S
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.02
8.01
8.00
7.77
7.76
7.75
7.75
7.26 CDCl3
7.11
7.11
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4.37
4.35
4.34
2.61
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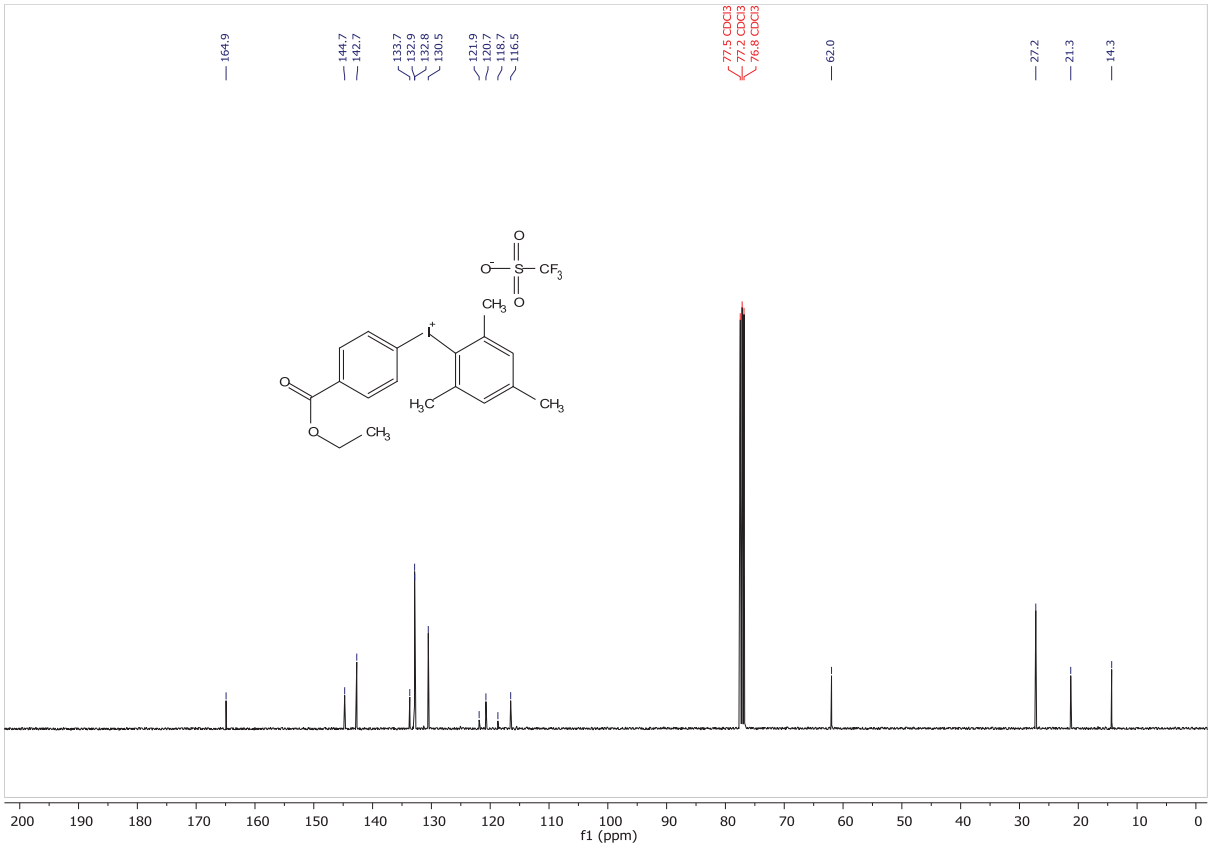
2.00
6.00
2.93
3.02
f1 (ppm)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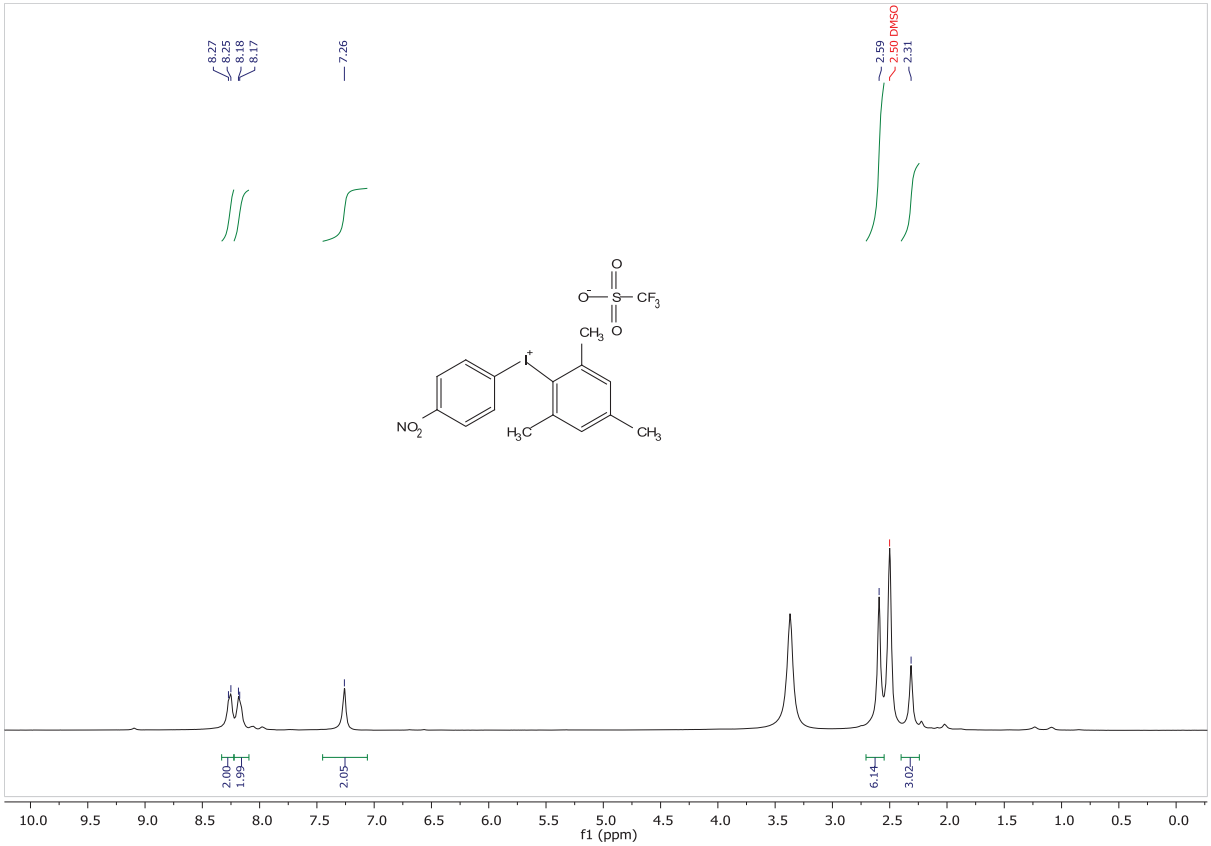
142.7
133.7
132.9
132.8
130.5
121.9
120.7
118.7
116.5
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
62.0
27.2
21.3
14.3
f1 (ppm)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8.25
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8.17
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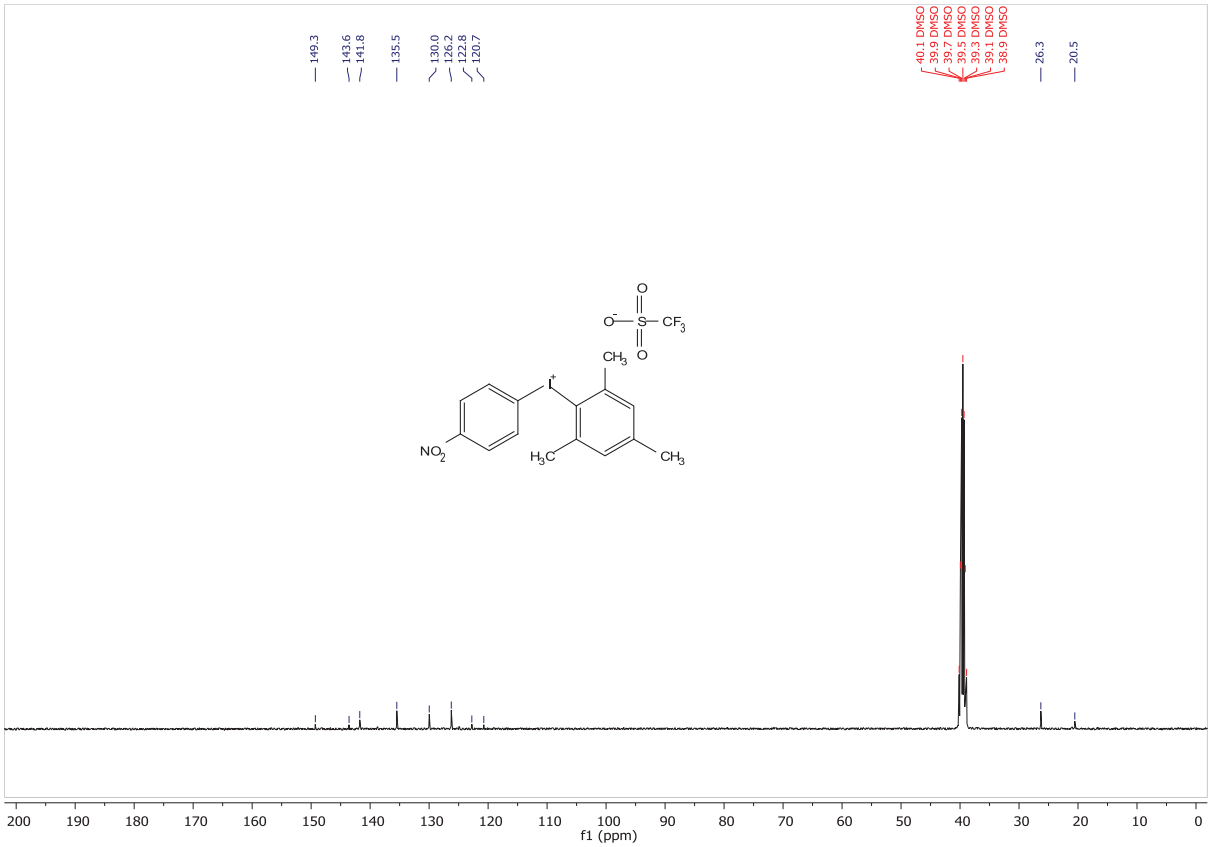
2.31
2.00
1.99
2.05
6.14
3.02
f1 (ppm)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143.6
141.8
135.5
130.0
126.2
122.8
120.7
40.1 DMSO
39.9 DMSO
39.7 DMSO
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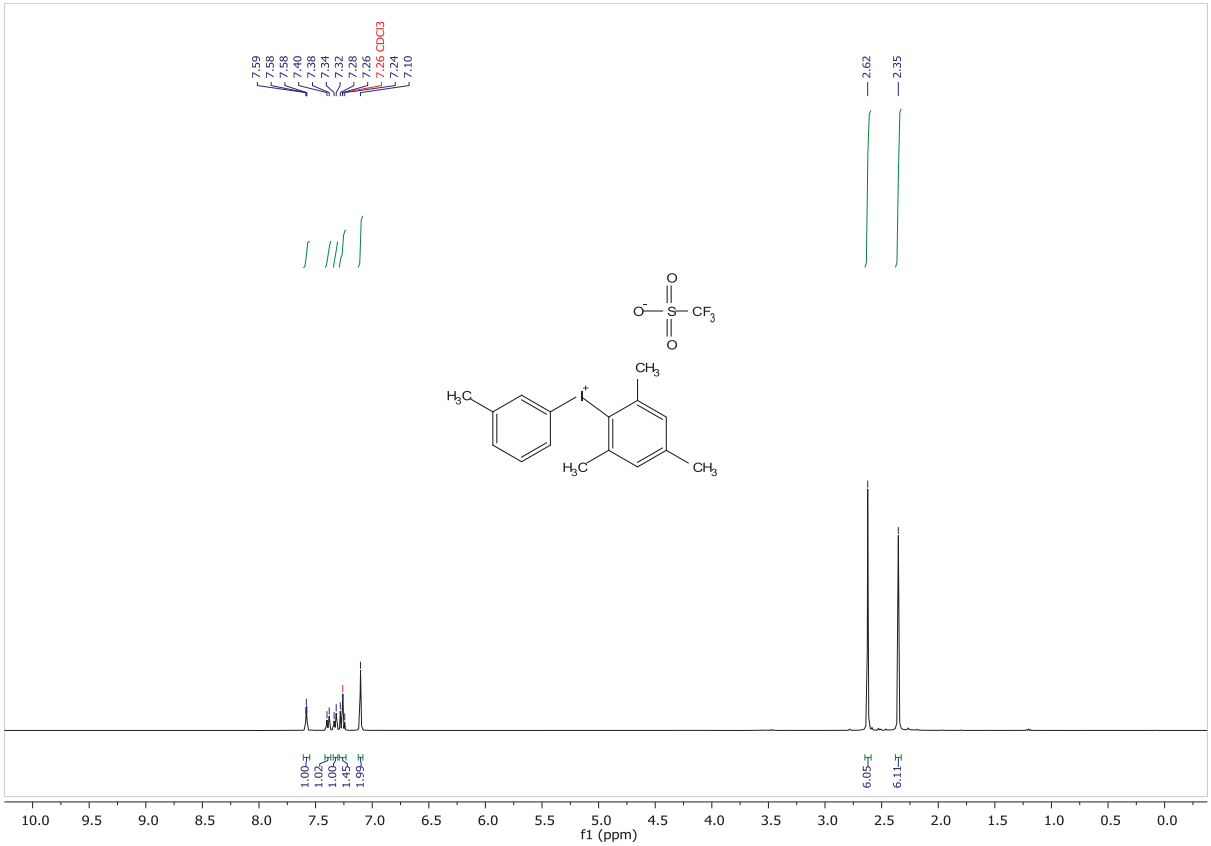
39.1 DMSO
38.9 DMSO
26.3
20.5
f1 (ppm)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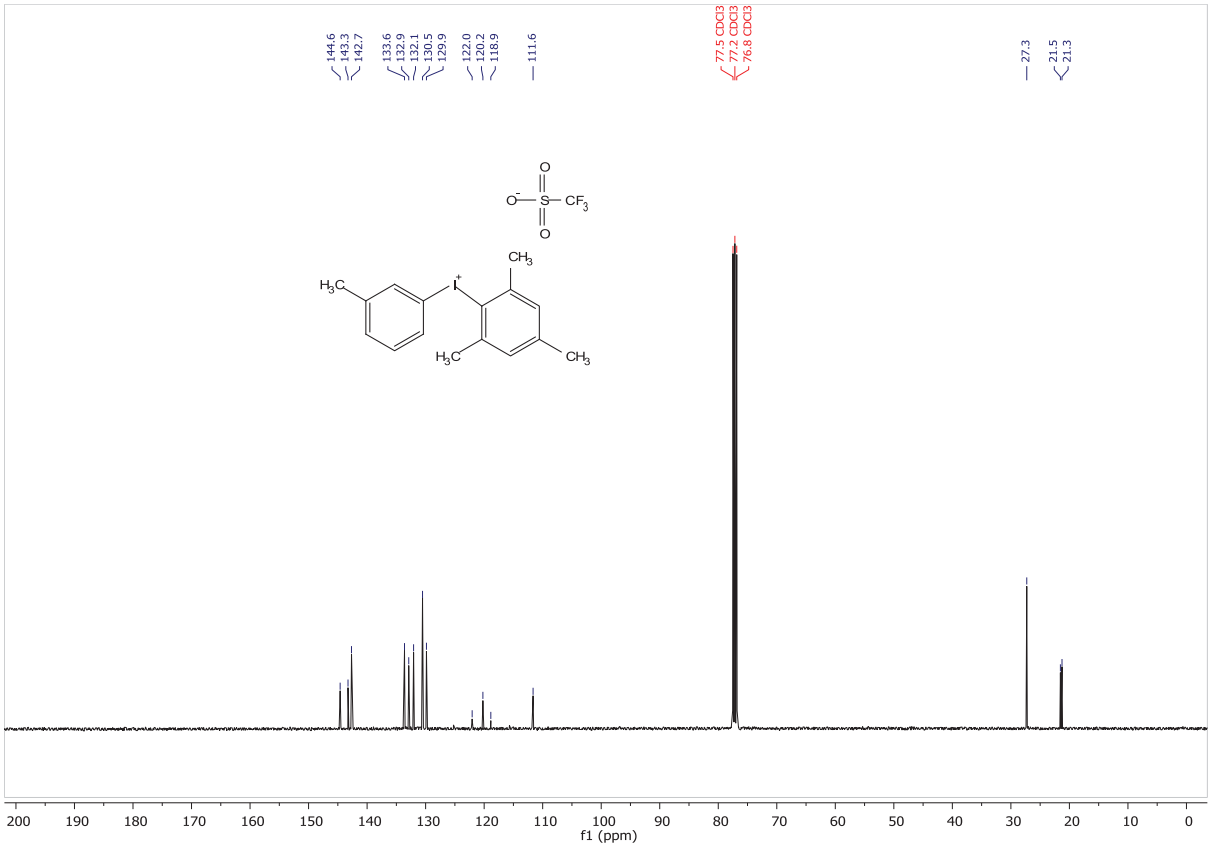
7.58
7.40
7.38
7.34
7.32
7.28
7.26
7.26 CDCl3
7.24
7.10
2.62
2.35
1.00
1.02
1.00
1.45
1.99
6.05
6.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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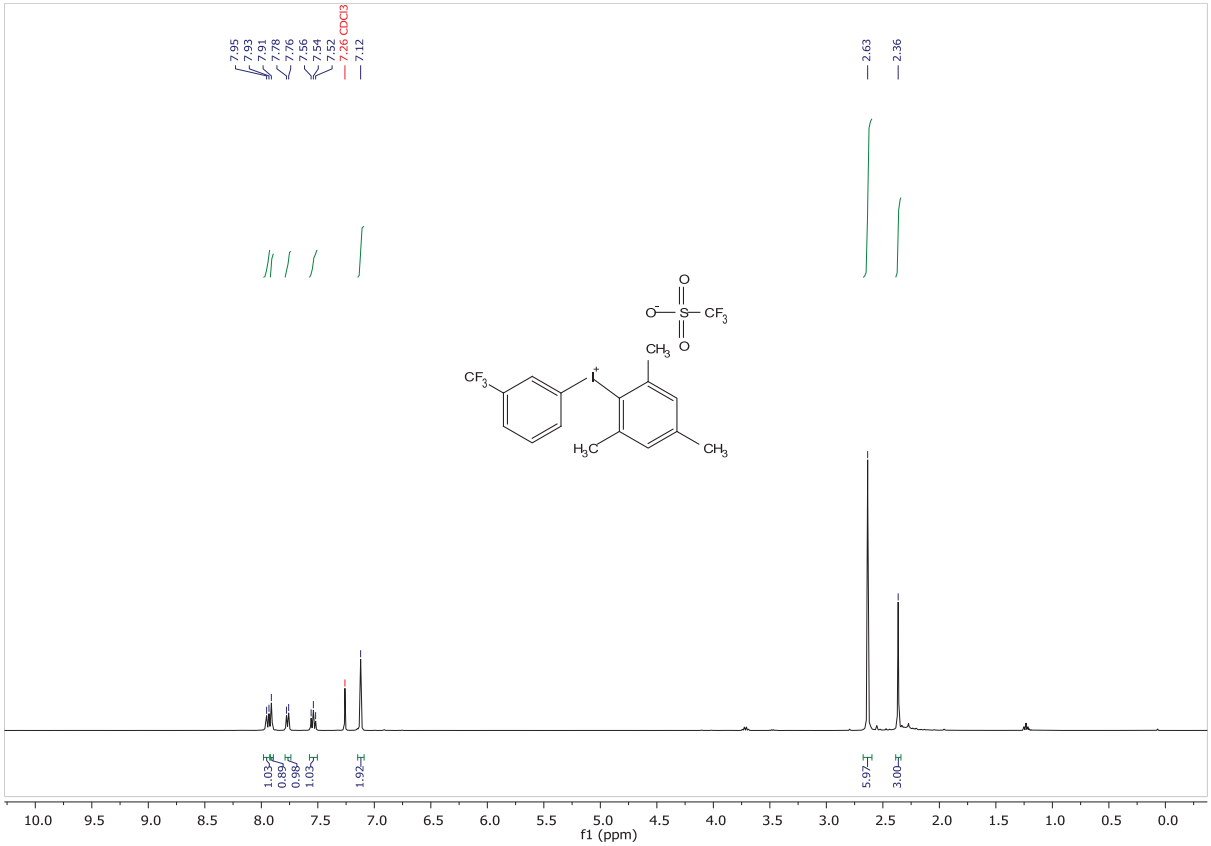
143.3
142.7
133.6
132.9
132.1
130.5
129.9
122.0
120.2
118.9
111.6
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
27.3
21.5
21.3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.93
7.91
7.78
7.76
7.56
7.54
7.52
7.26 CDCl3
7.12
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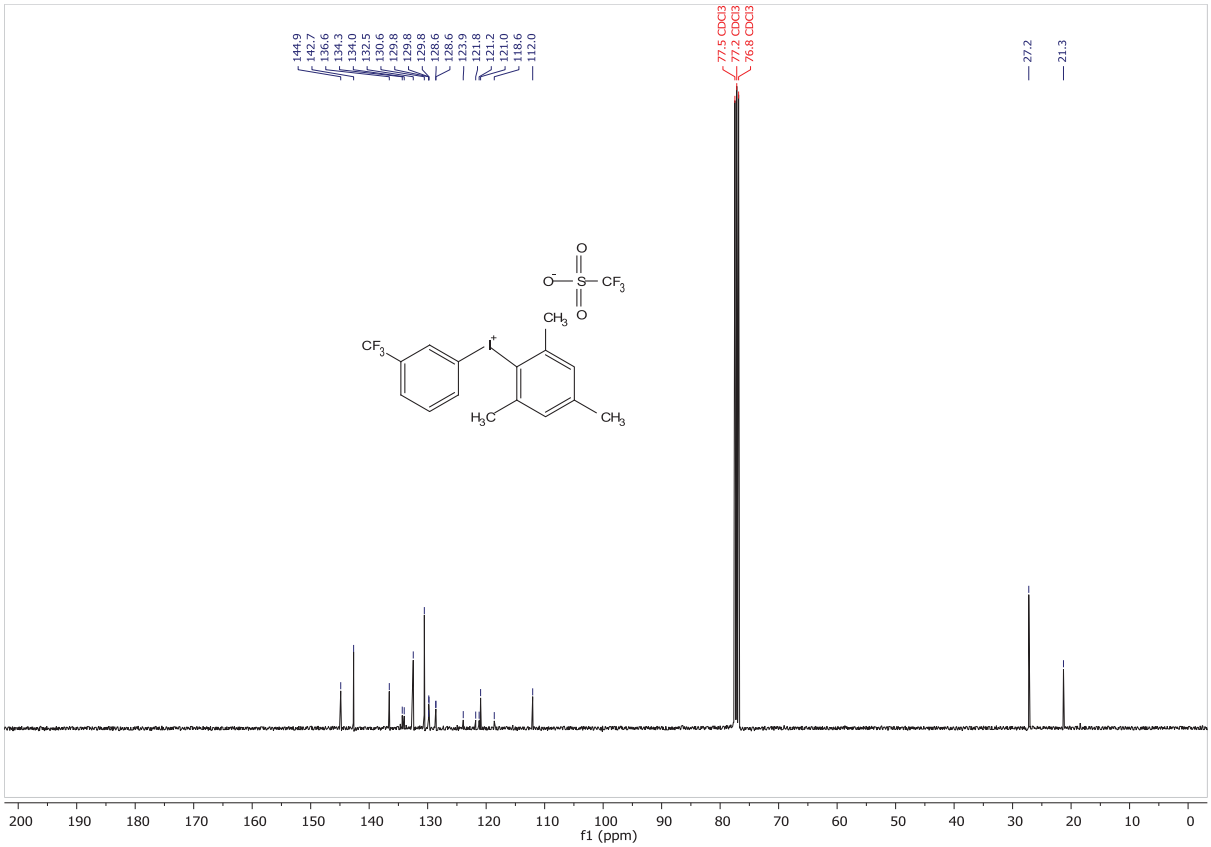
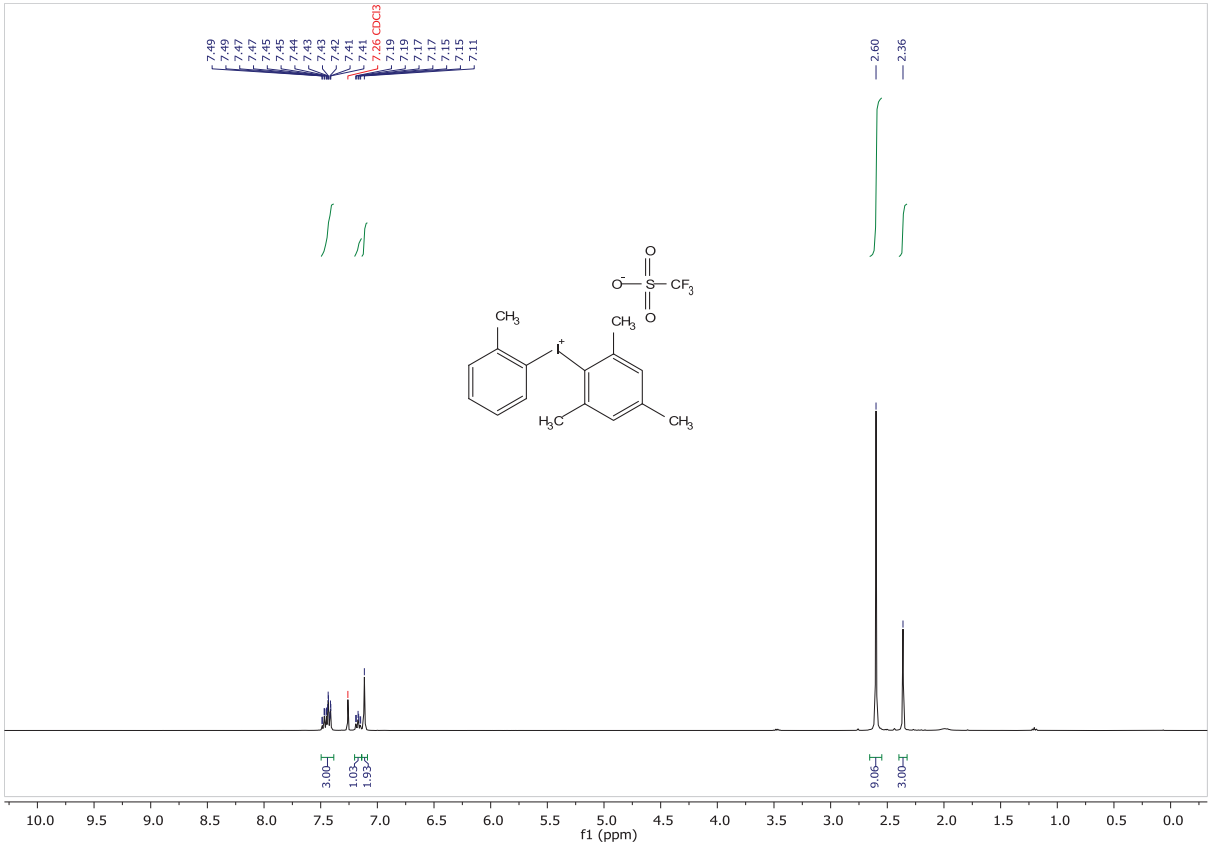
2.36
1.03
0.89
0.98
1.03
1.92
5.97
3.00
f1 (ppm)


144.9
142.7
136.6
134.3
134.0
132.5
130.6
129.8
129.8
129.8
128.6
128.6
123.9
121.8
121.2
121.0
118.6
112.0
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
27.2
21.3
f1 (ppm)


-63.05
-78.53
O
O⁻
S
CF3
O
CH3
CF3
I+
H3C
CH3
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)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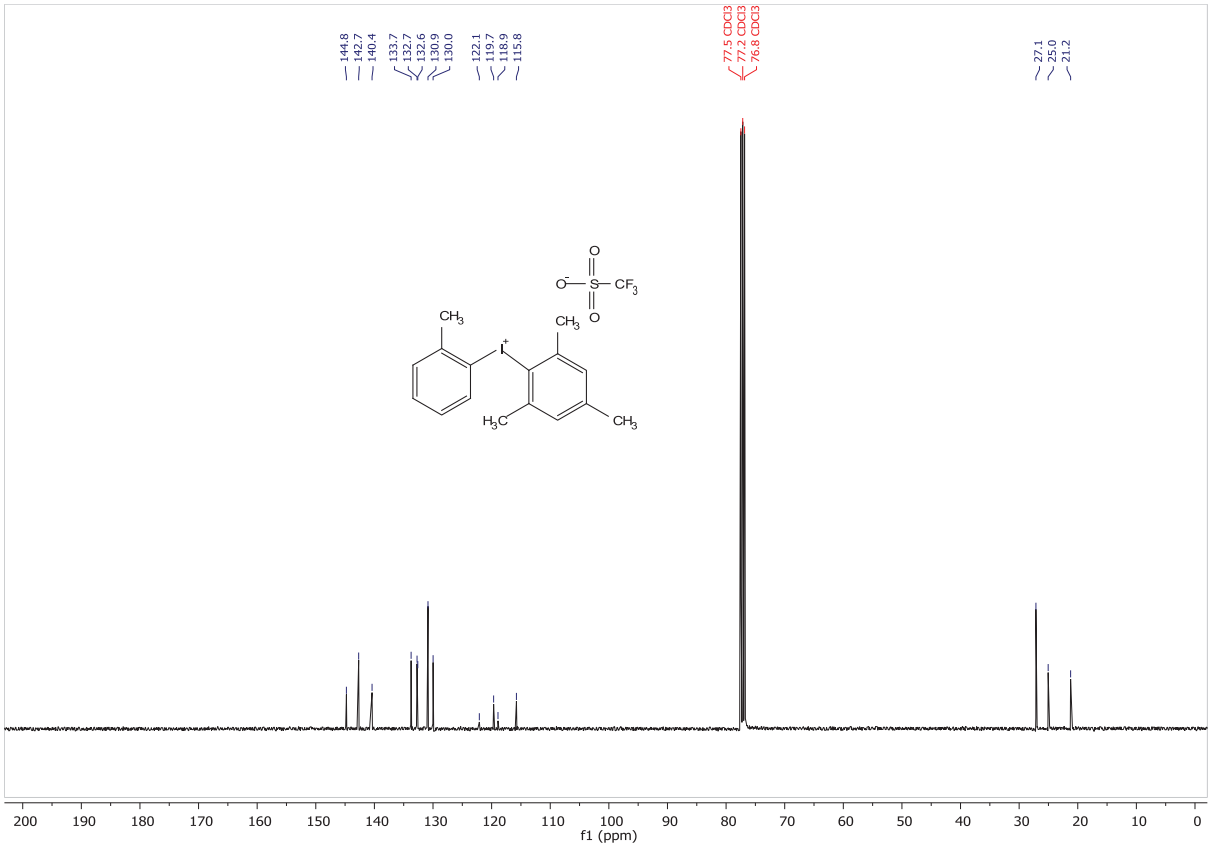
7.45
7.44
7.43
7.43
7.41
7.41
7.26 CDCl3
7.19
7.19
7.17
7.17
7.15
7.15
7.11
2.60
2.36
3.00
1.03
1.93
9.06
3.00
f1 (ppm)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142.7
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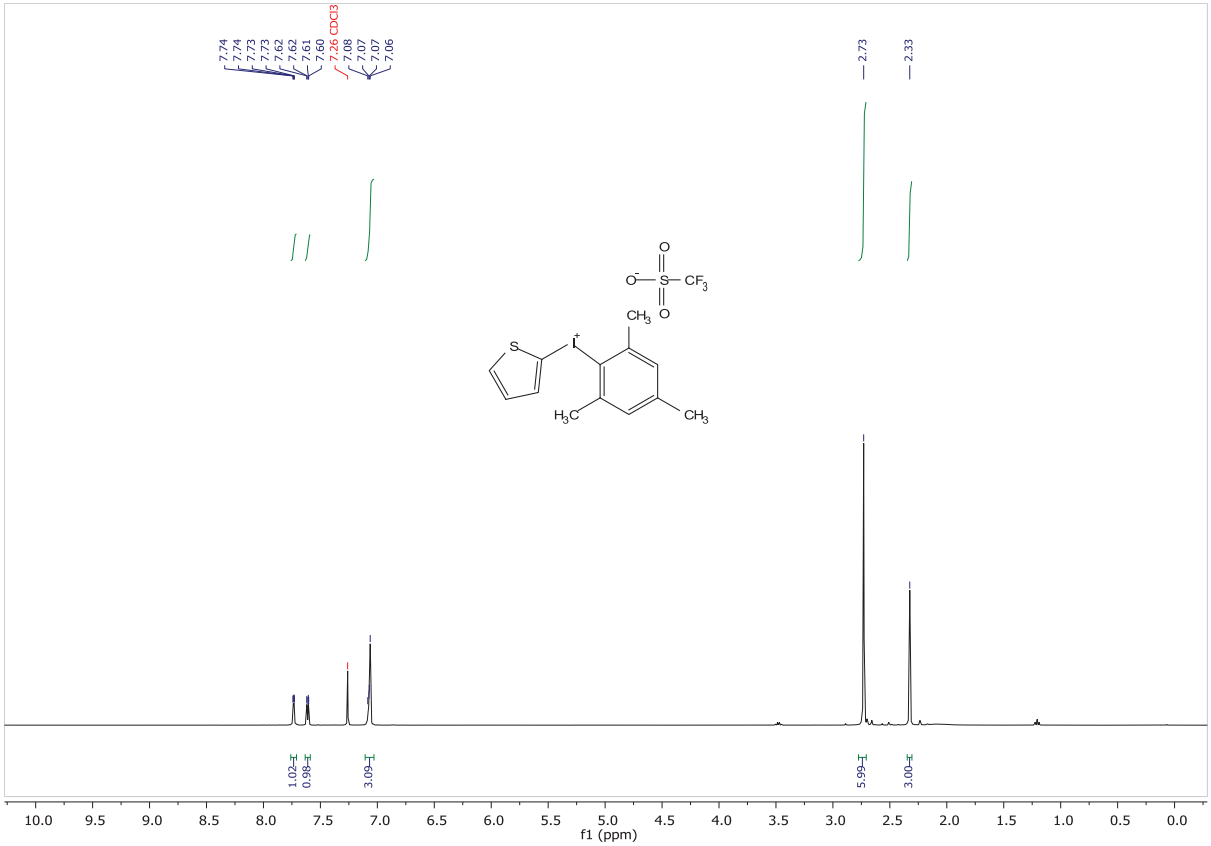
133.7
132.7
132.6
130.9
130.0
122.1
119.7
118.9
115.8
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
27.1
25.0
21.2
f1 (ppm)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7.60
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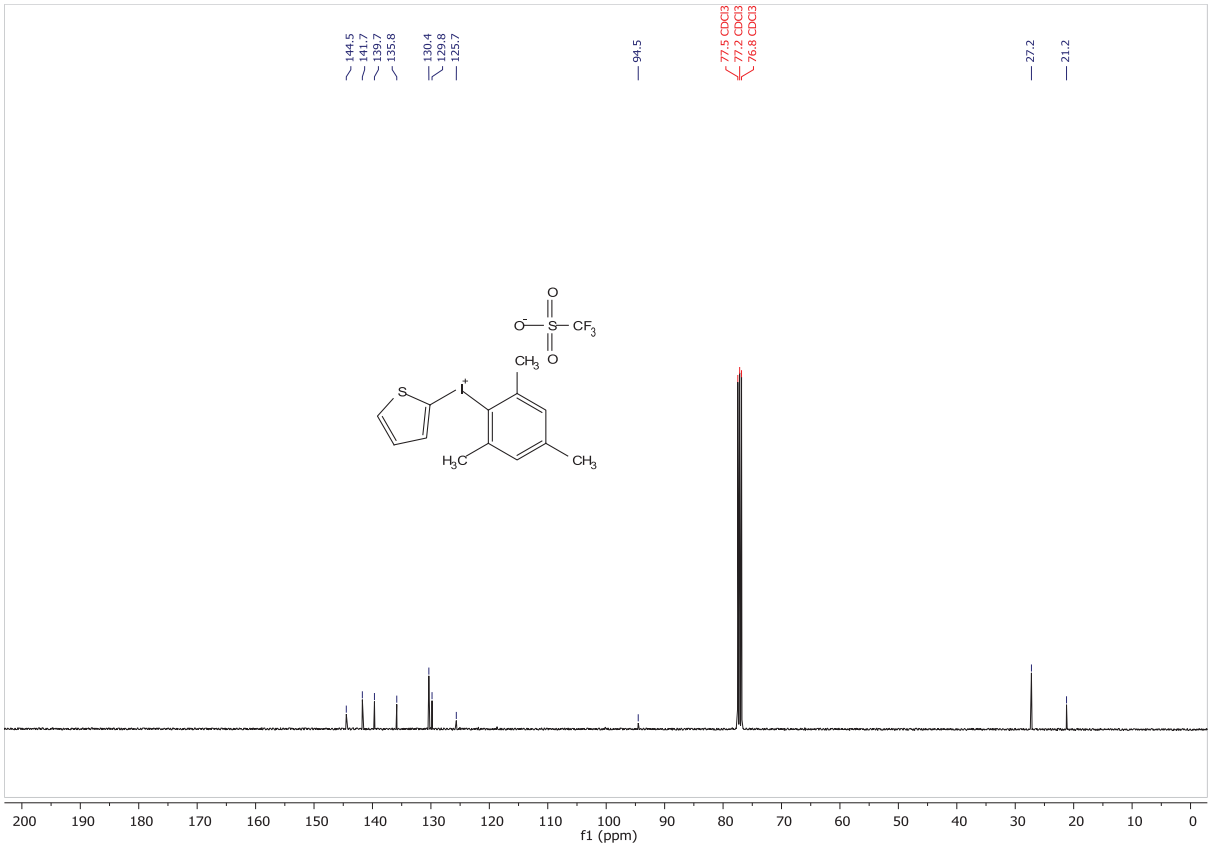
7.08
7.07
7.07
7.06
2.73
2.33
1.02
0.98
3.09
5.99
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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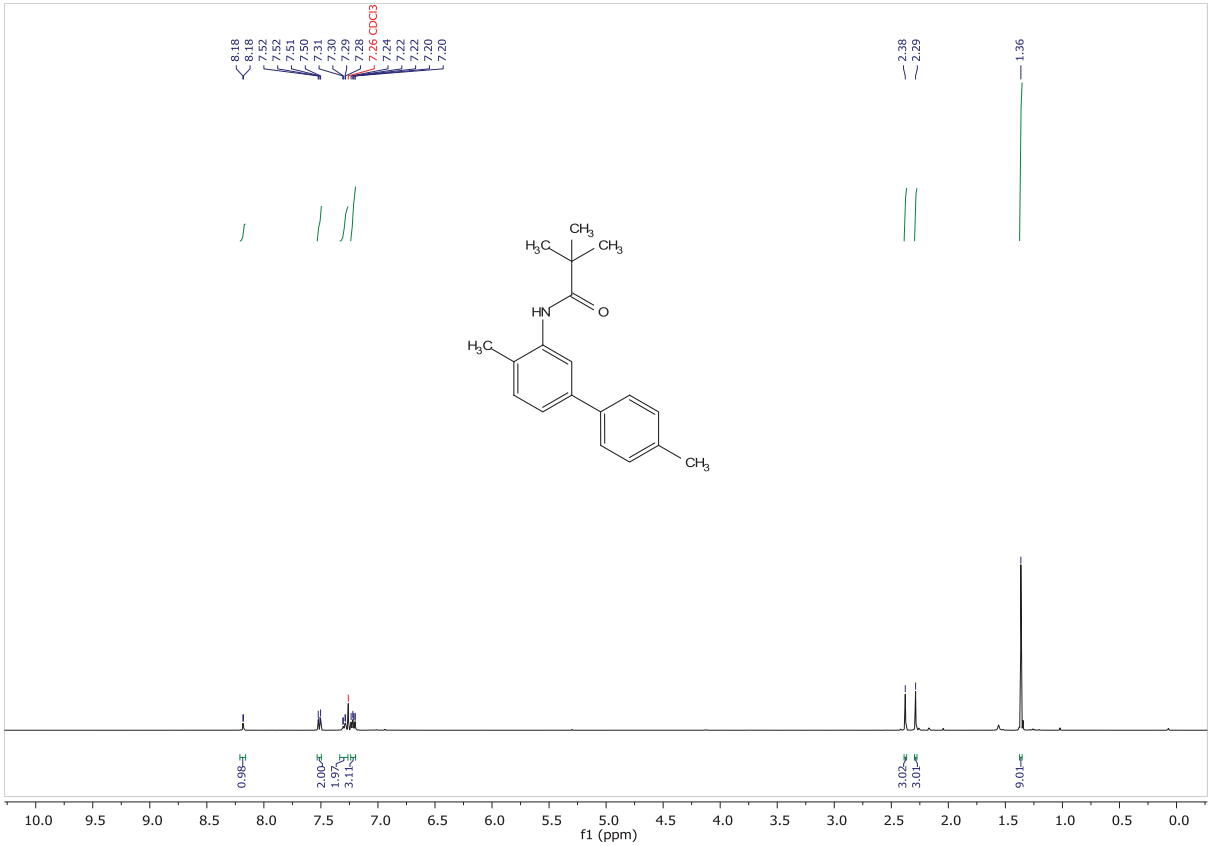
139.7
135.8
130.4
129.8
125.7
94.5
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
27.2
21.2
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.28
7.26 CDCl3
7.24
7.22
7.22
7.20
7.20
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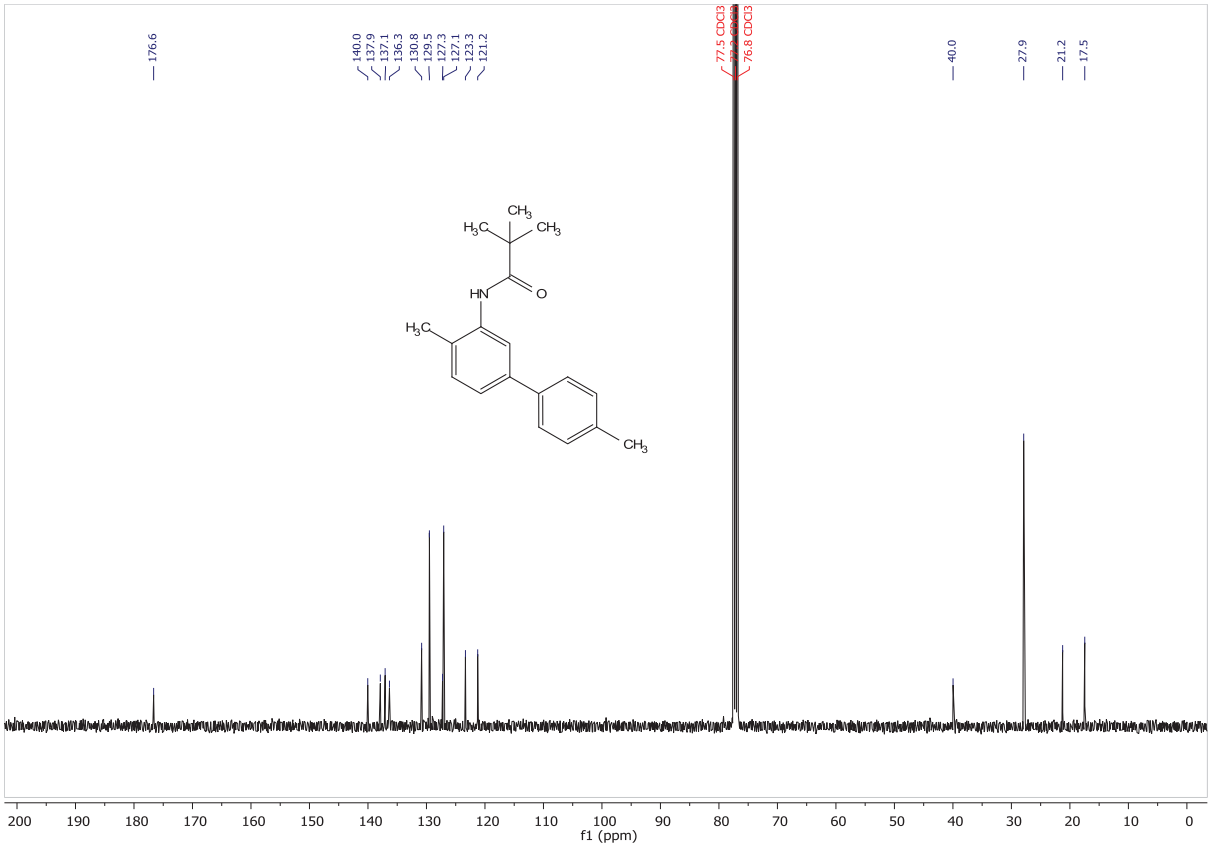
2.29
1.36
0.98
2.00
1.97
3.11
3.02
3.01
9.01
f1 (ppm)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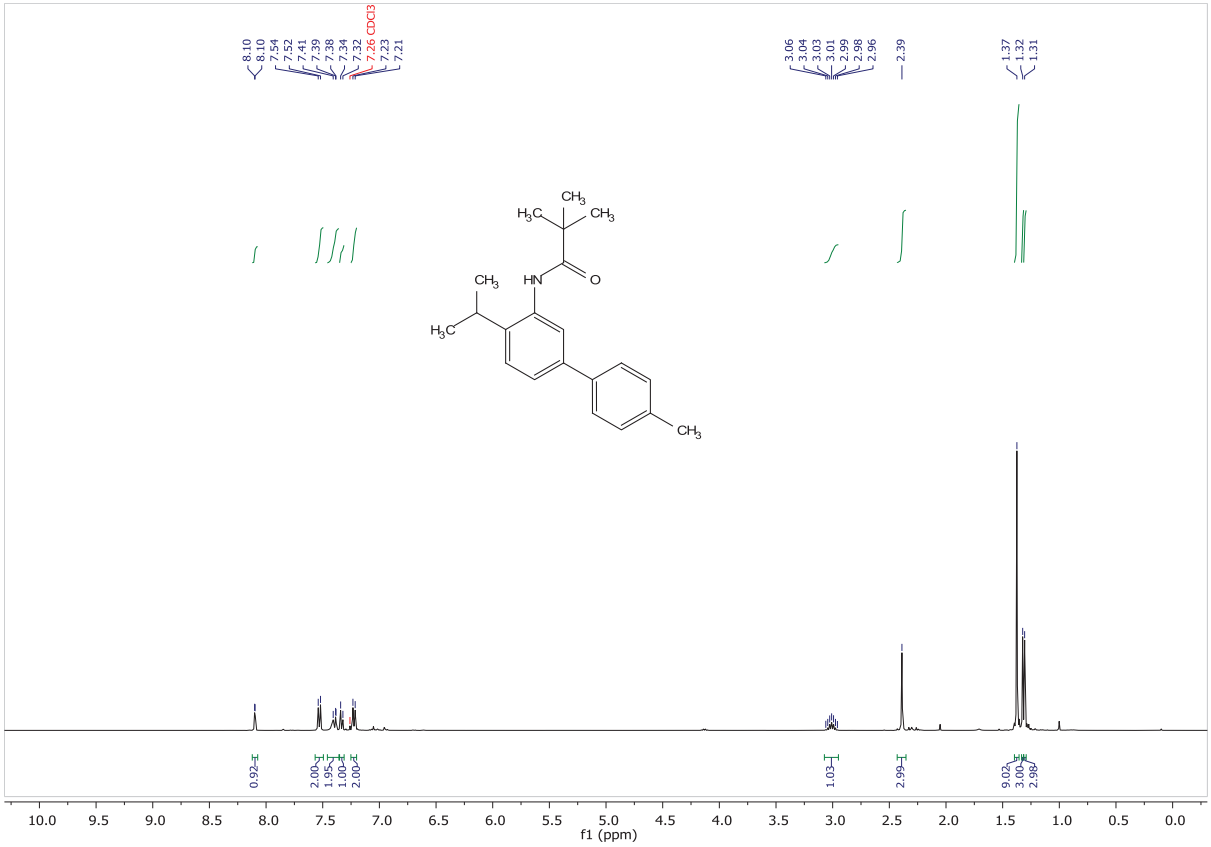
137.9
137.1
136.3
130.8
129.5
127.3
127.1
123.3
121.2
77.5 CDCl3
76.8 CDCl3
40.0
27.9
21.2
17.5
f1 (ppm)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7.34
7.32
7.26 CDCl3
7.23
7.21
3.06
3.04
3.03
3.01
2.99
2.98
2.96
2.39
1.37
1.32
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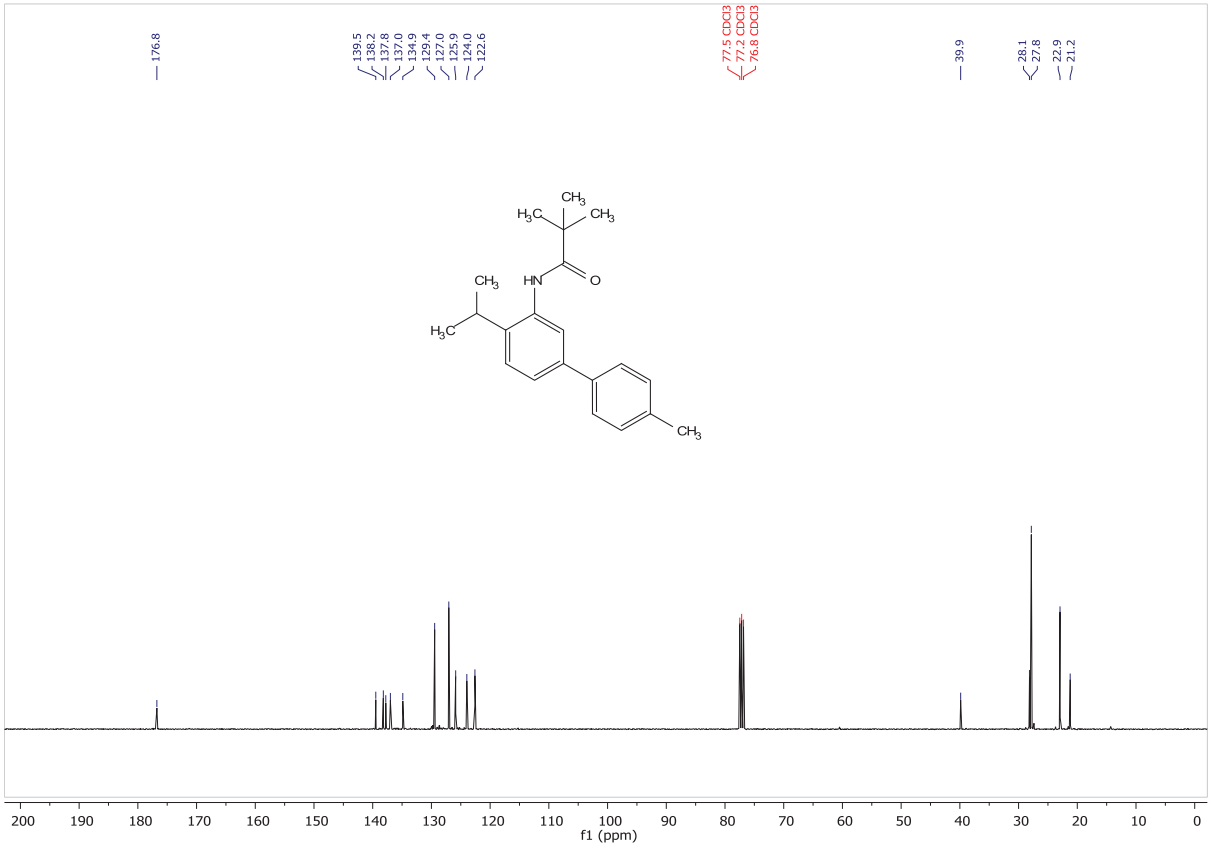
2.00
1.03
2.99
9.02
3.00
2.98
f1 (ppm)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134.9
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127.0
125.9
124.0
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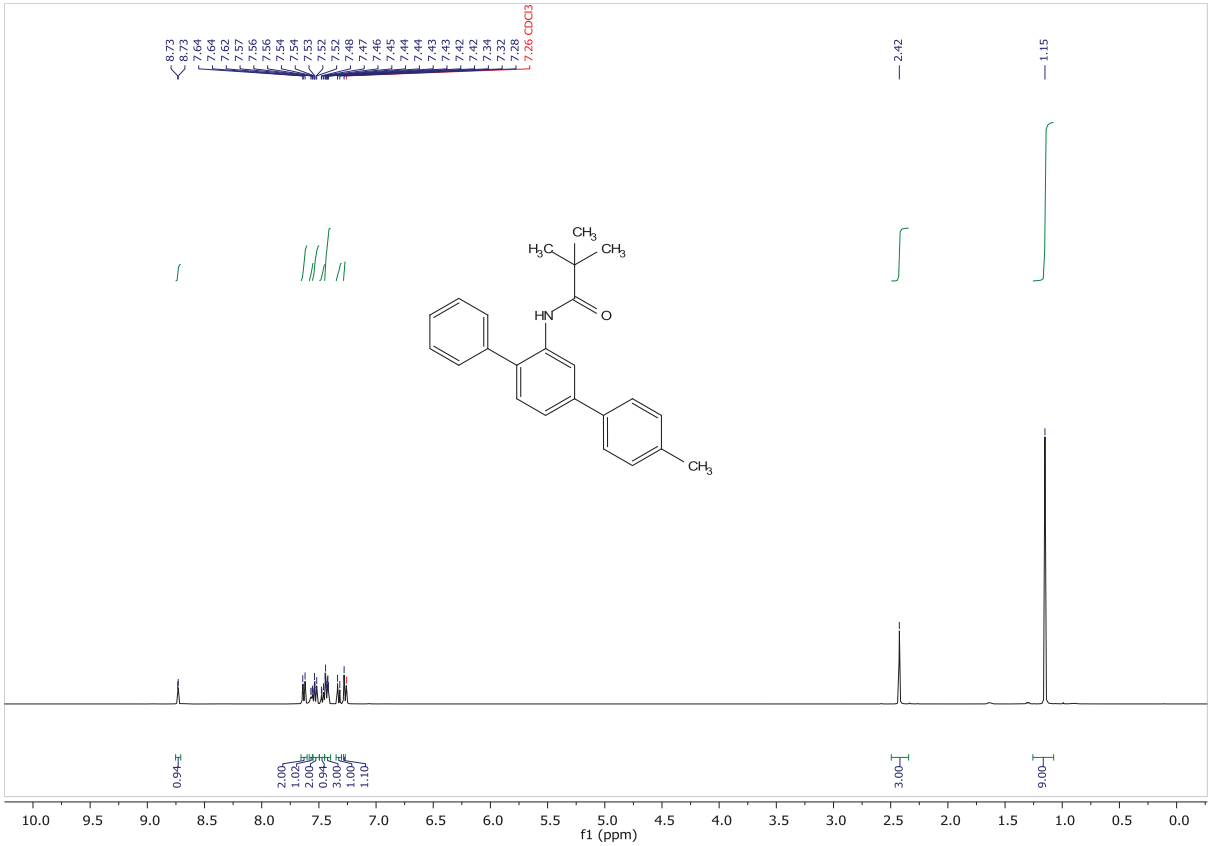
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
39.9
28.1
27.8
22.9
21.2
f1 (ppm)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7.47
7.46
7.45
7.44
7.44
7.43
7.43
7.42
7.42
7.34
7.32
7.28
7.26 CDCl3
2.42
1.15
CH3
H3C
CH3
HN
O
CH3
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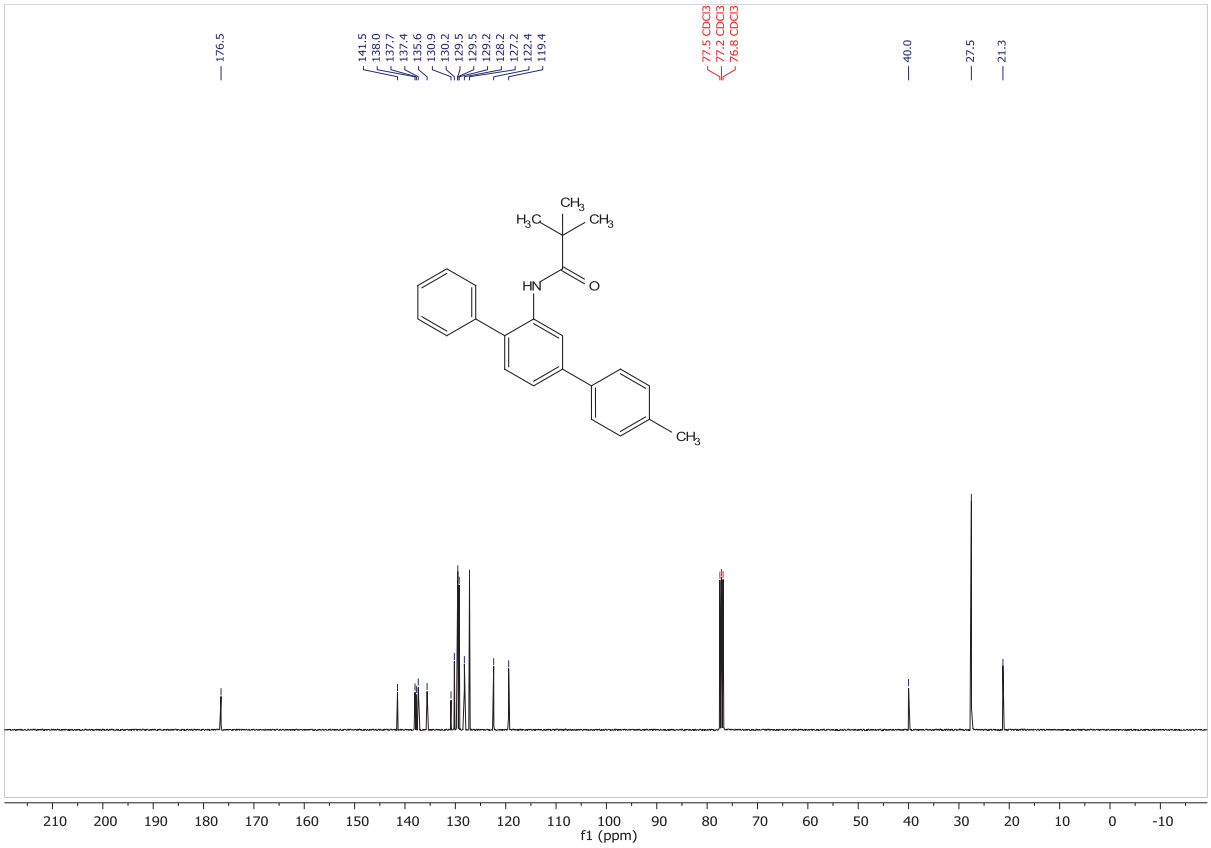
1.02
2.00
0.94
3.00
1.00
1.10
3.00
9.00
f1 (ppm)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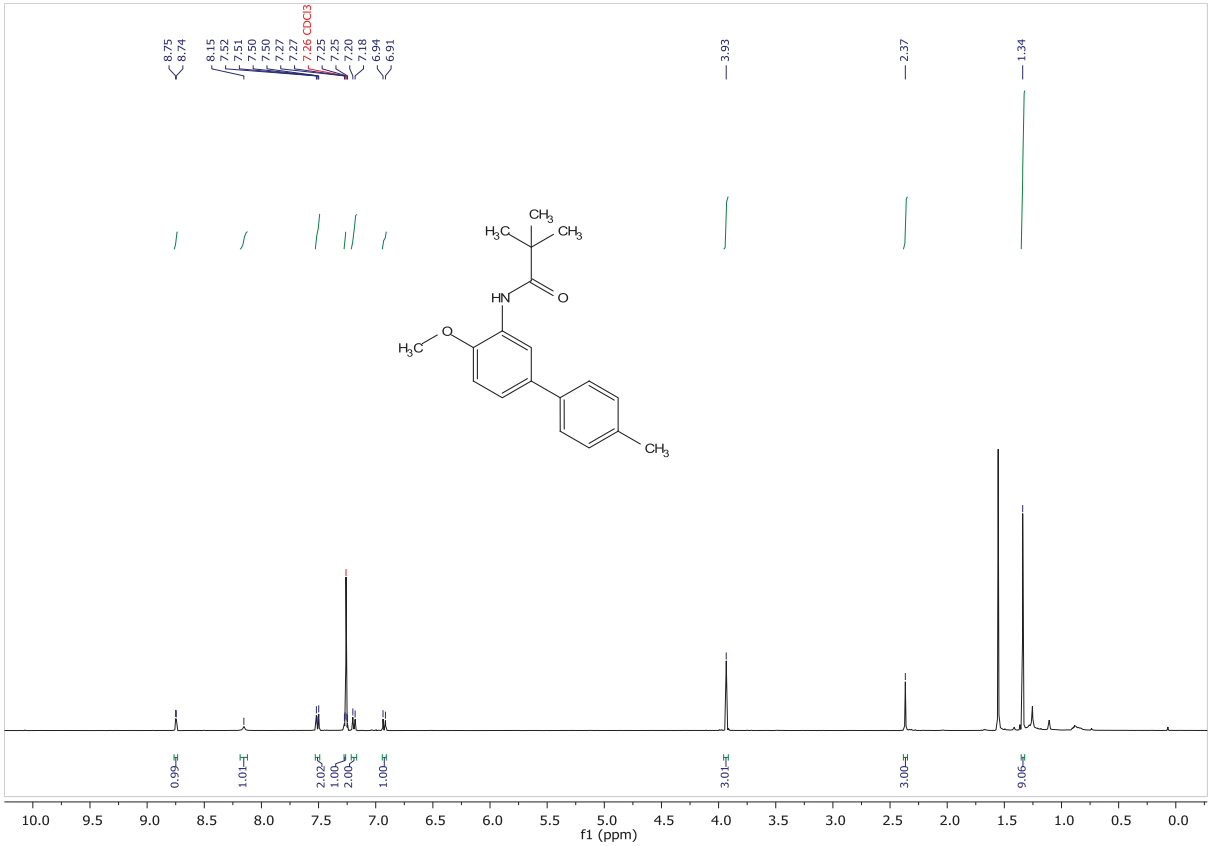
130.2
129.5
129.5
129.2
128.2
127.2
122.4
119.4
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
40.0
27.5
21.3
CH3
H3C
CH3
HN
O
CH3
f1 (ppm)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7.50
7.27
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7.25
7.20
7.18
6.94
6.91
3.93
2.37
1.34
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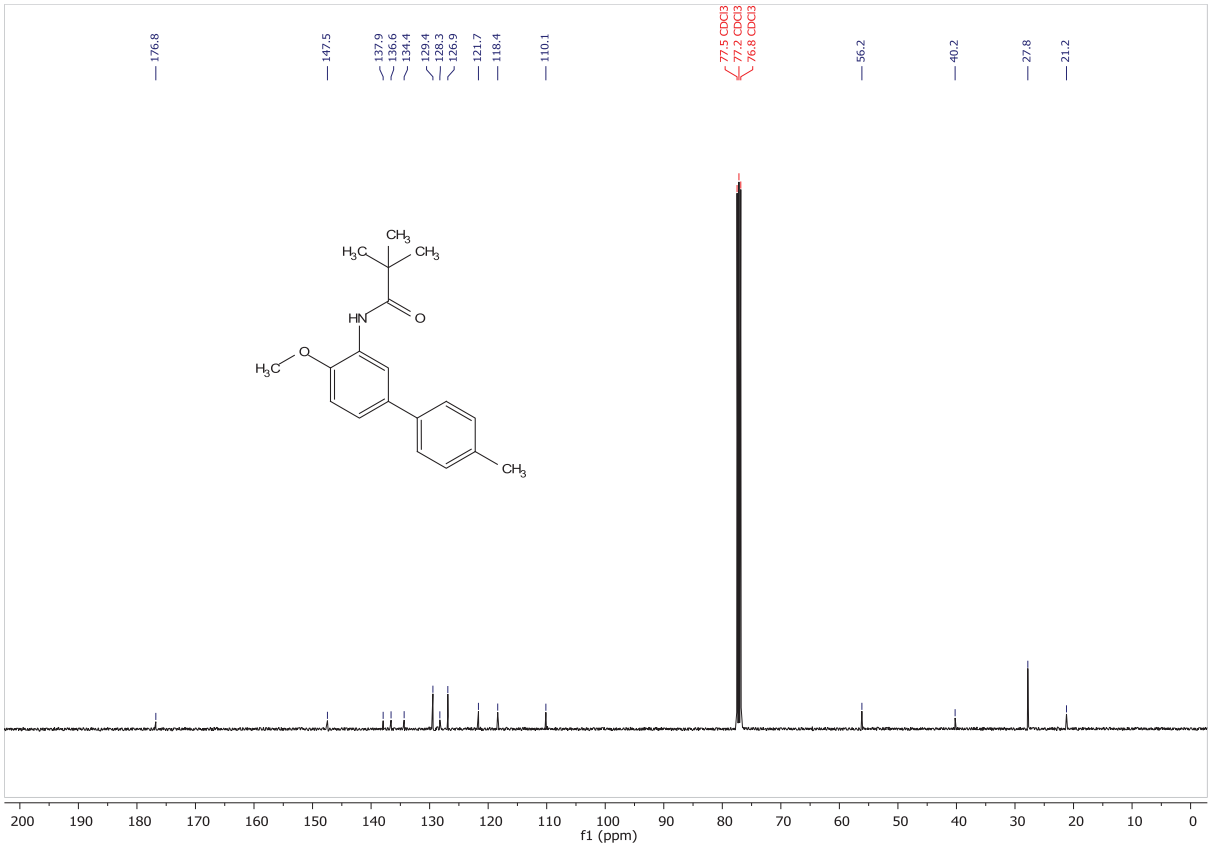
1.01
2.02
1.00
2.00
1.00
3.01
3.00
9.06
f1 (ppm)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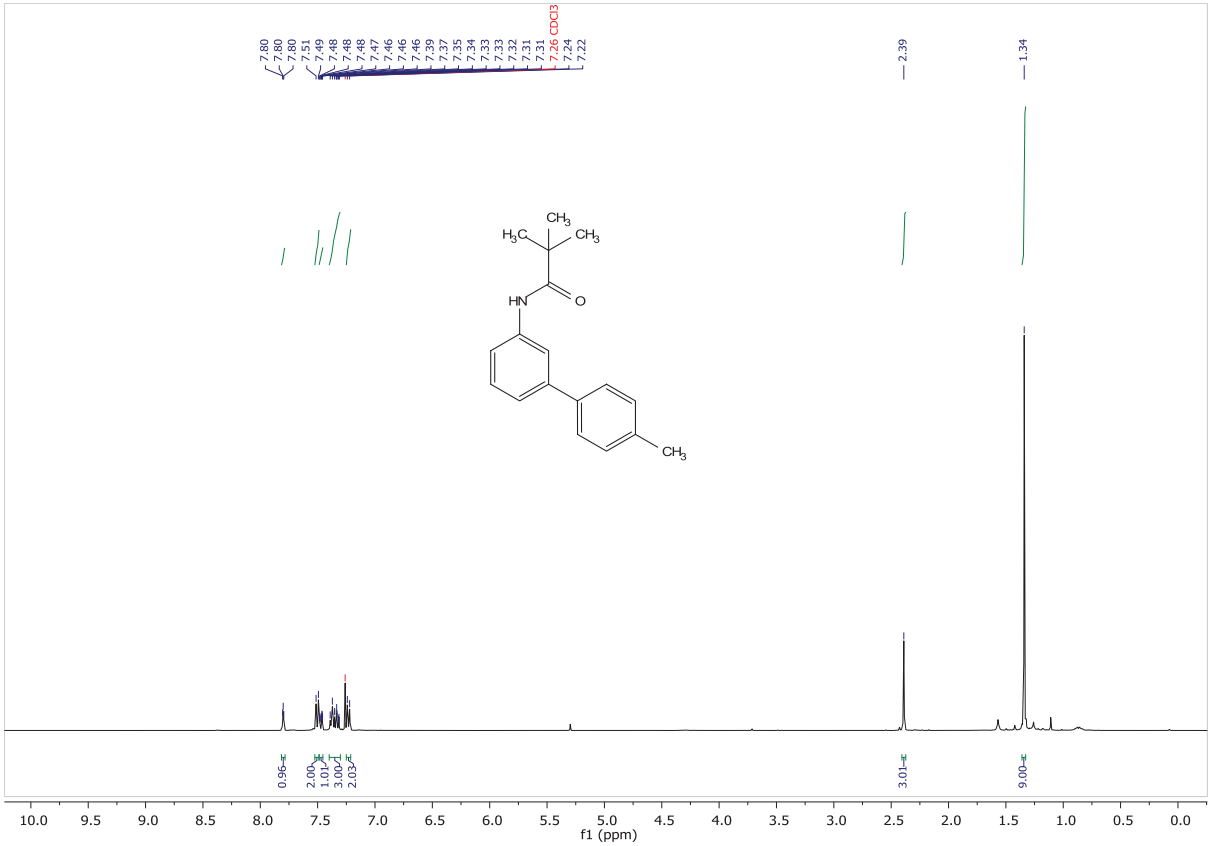
147.5
137.9
136.6
134.4
129.4
128.3
126.9
121.7
118.4
110.1
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
56.2
40.2
27.8
21.2
f1 (ppm)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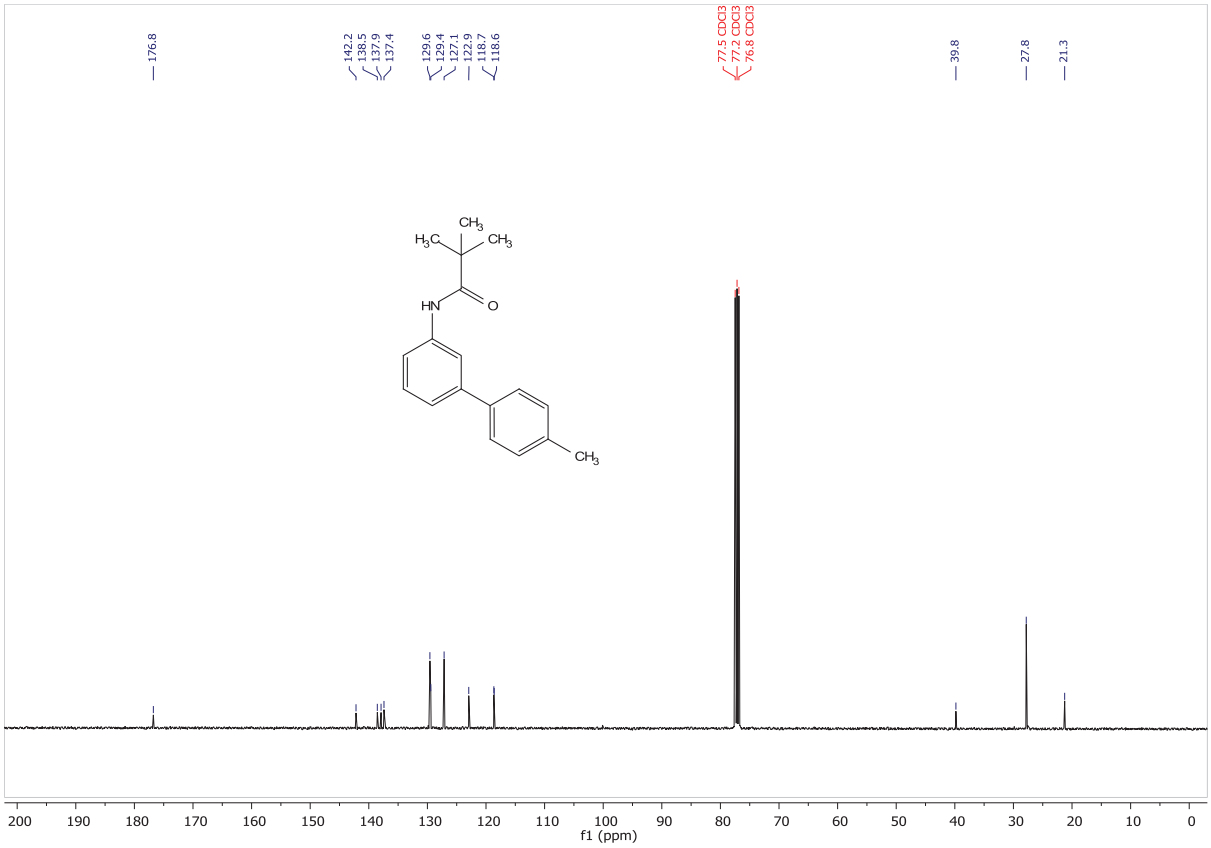
7.32
7.31
7.31
7.26 CDCl3
7.24
7.22
2.39
1.34
CH3
H3C
CH3
HN
O
CH3
0.96
2.00
1.01
3.00
2.03
3.01
9.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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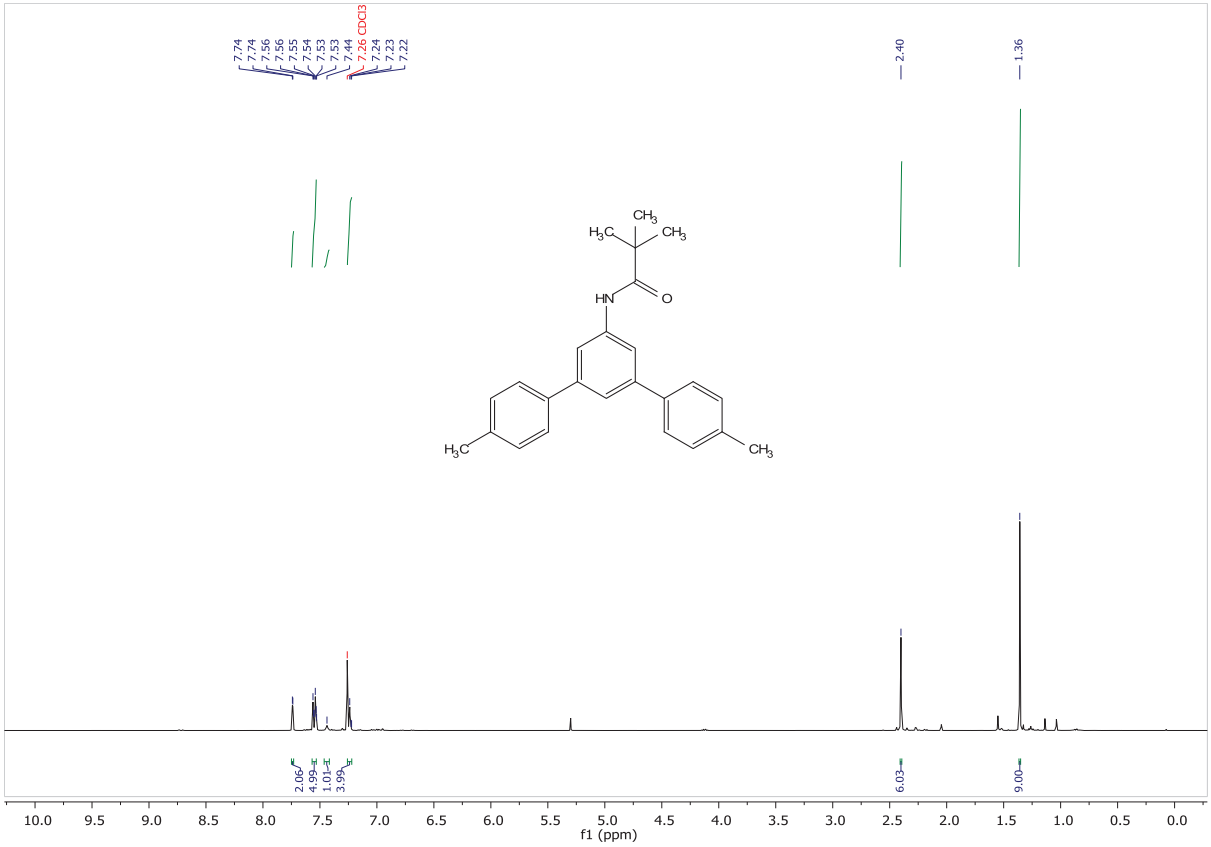
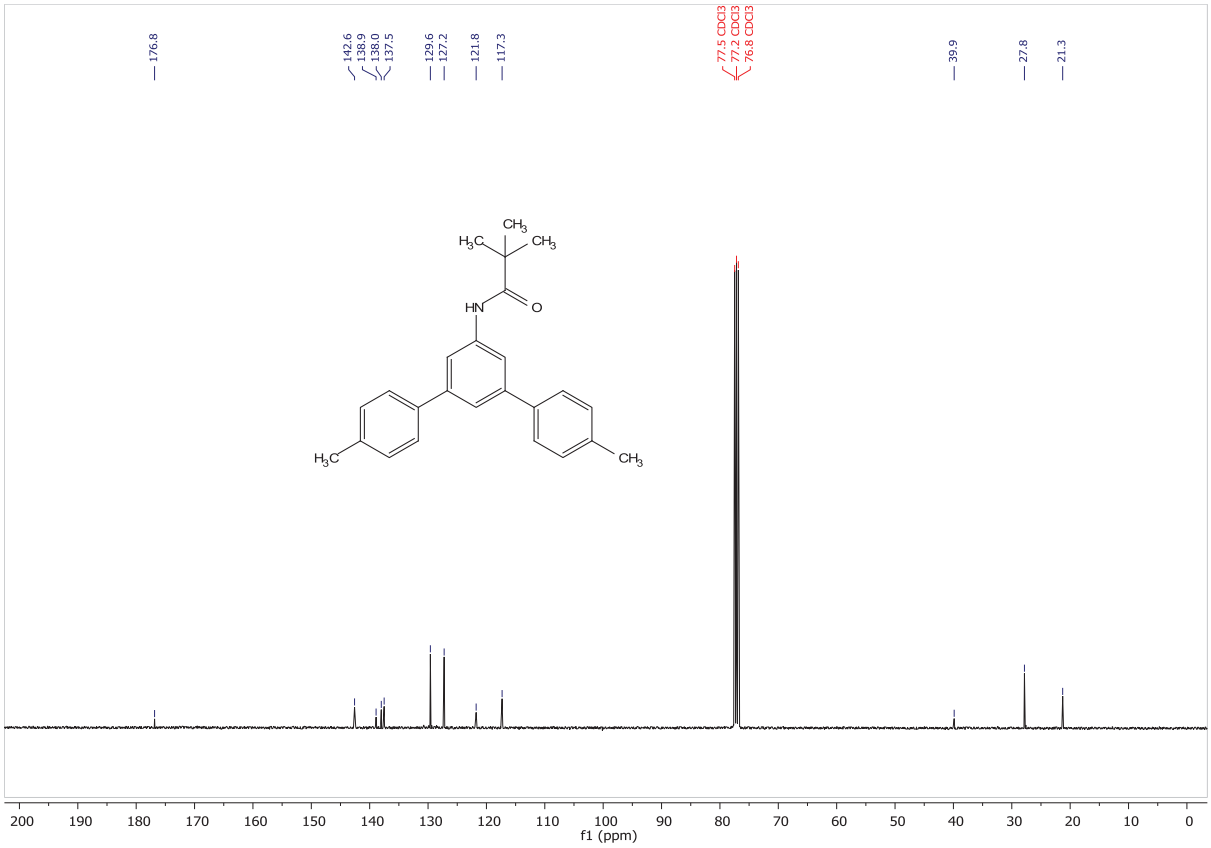
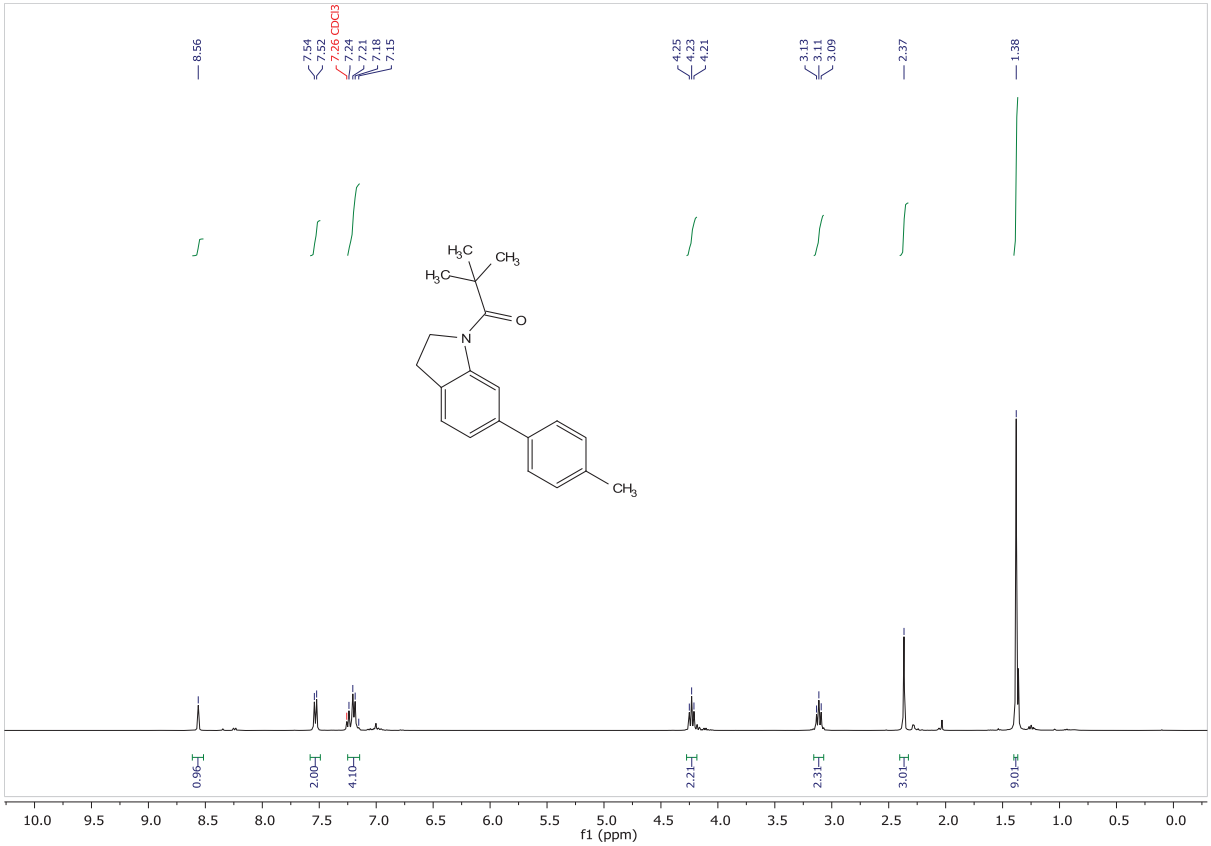
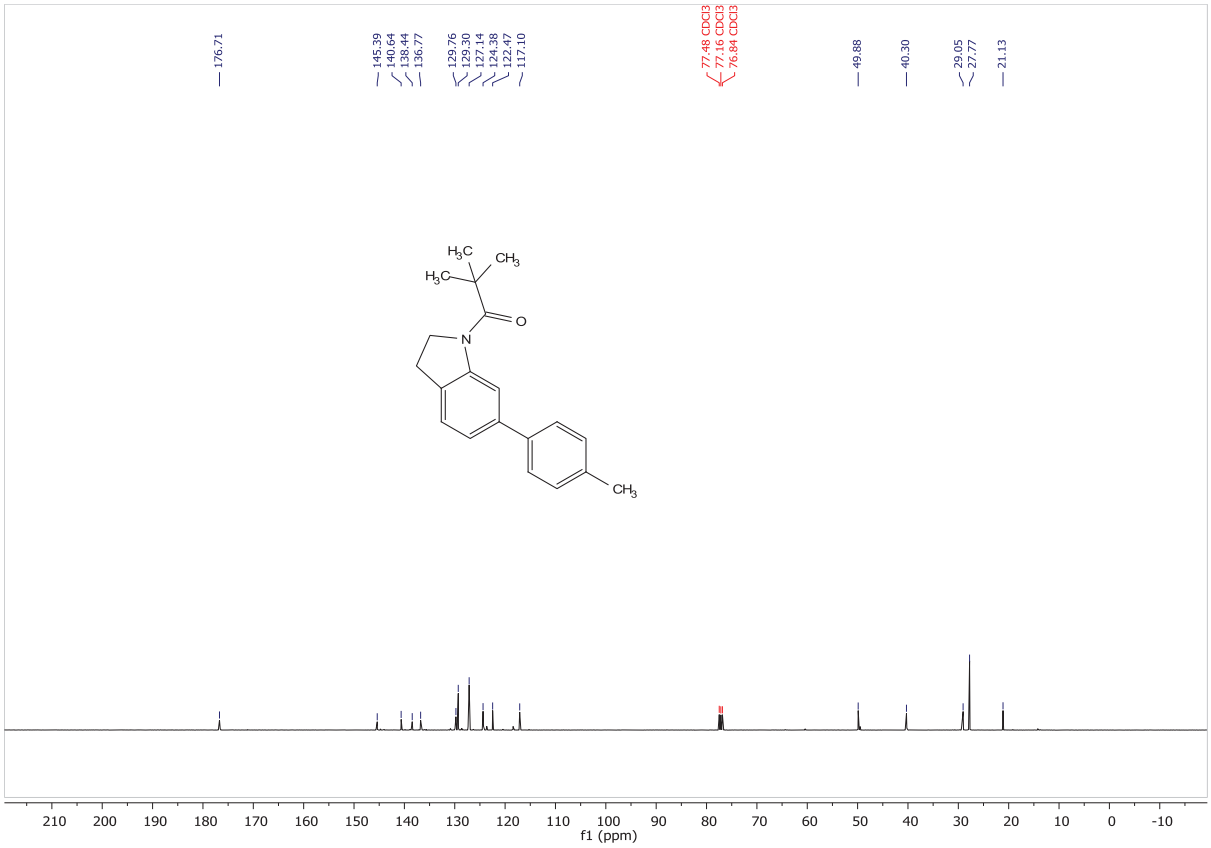
137.9
137.4
129.6
129.4
127.1
122.9
118.7
118.6
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
39.8
27.8
21.3
CH3
H3C
CH3
HN
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.74
7.74
7.56
7.56
7.55
7.54
7.53
7.53
7.44
7.26 CDCl3
7.24
7.23
7.22
2.40
1.36
CH3
H3C
CH3
HN
O
H3C
CH3
2.06
4.99
1.01
3.99
6.03
9.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


176.8
142.6
138.9
138.0
137.5
129.6
127.2
121.8
117.3
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
39.9
27.8
21.3
CH3
H3C
CH3
HN
O
H3C
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.56
7.54
7.52
7.26 CDCl3
7.24
7.21
7.18
7.15
4.25
4.23
4.21
3.13
3.11
3.09
2.37
1.38
0.96
2.00
4.10
2.21
2.31
3.01
9.01
f1 (ppm)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129.76
129.30
127.14
124.38
122.47
117.10
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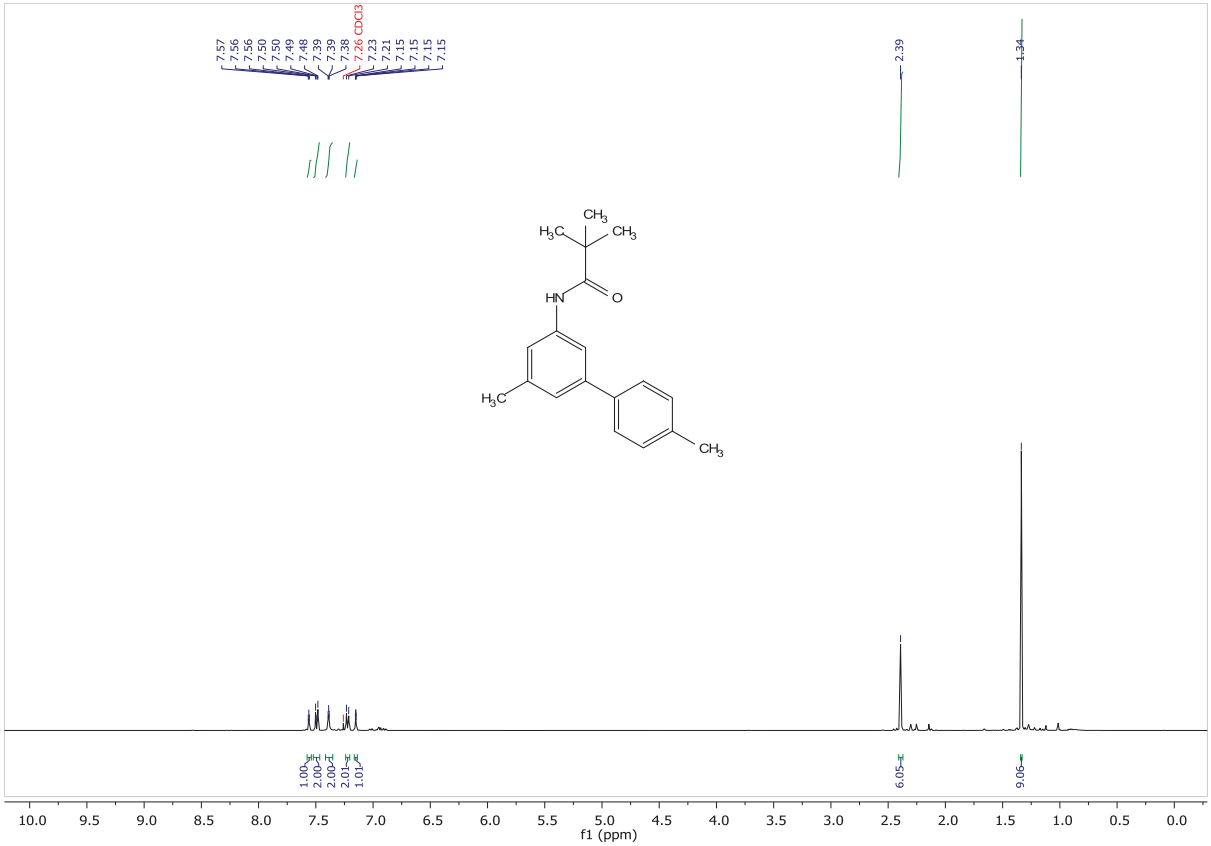
77.16 CDCl3
76.84 CDCl3
49.88
40.30
29.05
27.77
21.13
f1 (ppm)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7.56
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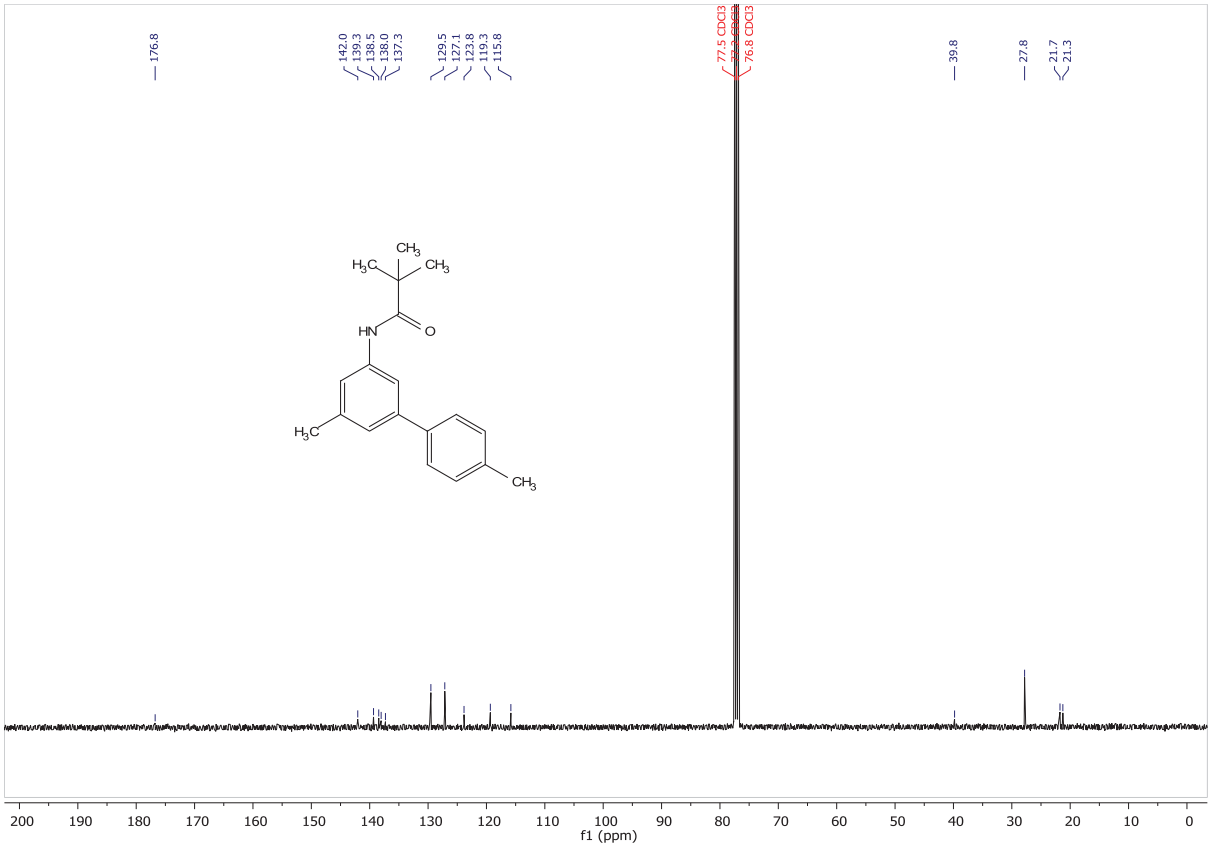
7.48
7.39
7.39
7.38
7.26 CDCl3
7.23
7.21
7.15
7.15
7.15
7.15
2.39
1.34
CH3
H3C
CH3
HN
O
H3C
CH3
1.00
2.00
2.00
2.01
1.01
6.05
9.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.5
127.1
123.8
119.3
115.8
77.5 CDCl3
76.8 CDCl3
39.8
27.8
21.7
21.3
CH3
H3C
CH3
HN
O
H3C
CH3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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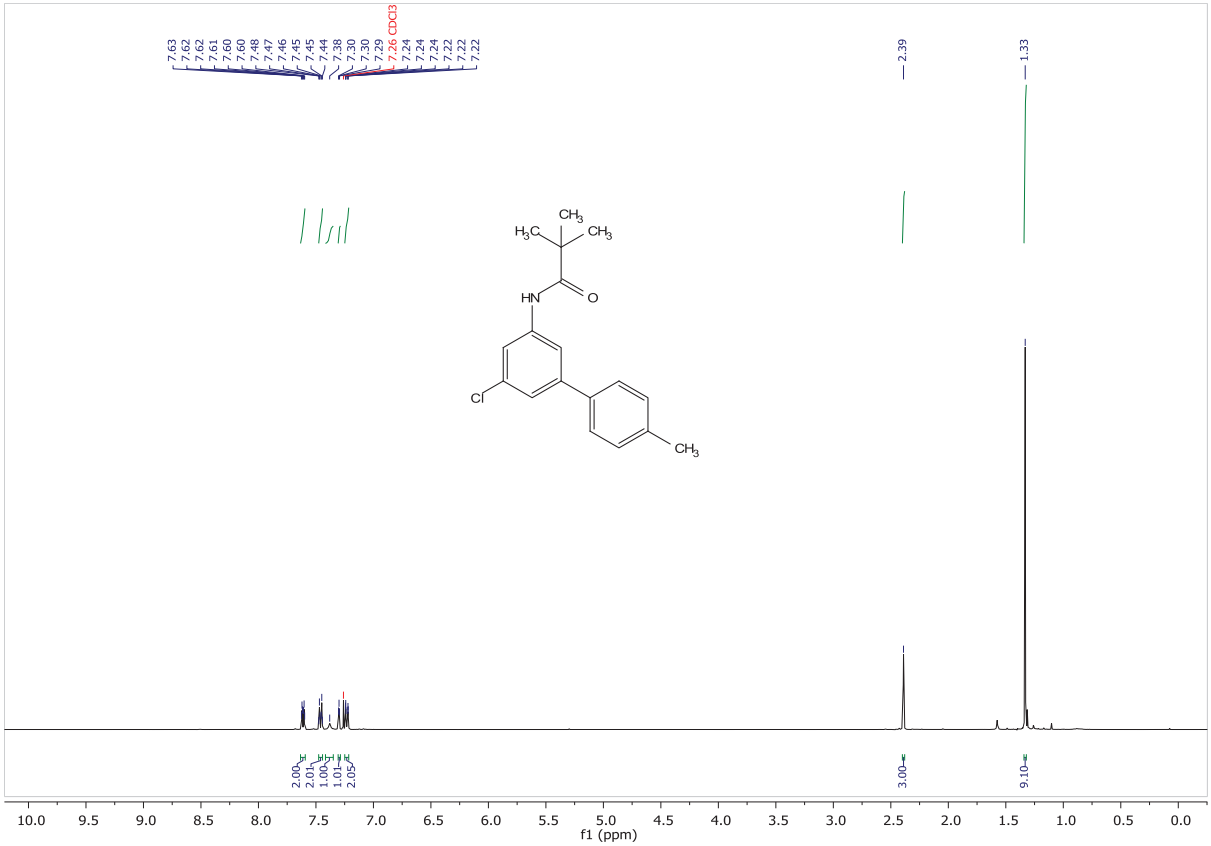
50
40
30
20
10
0
f1 (ppm)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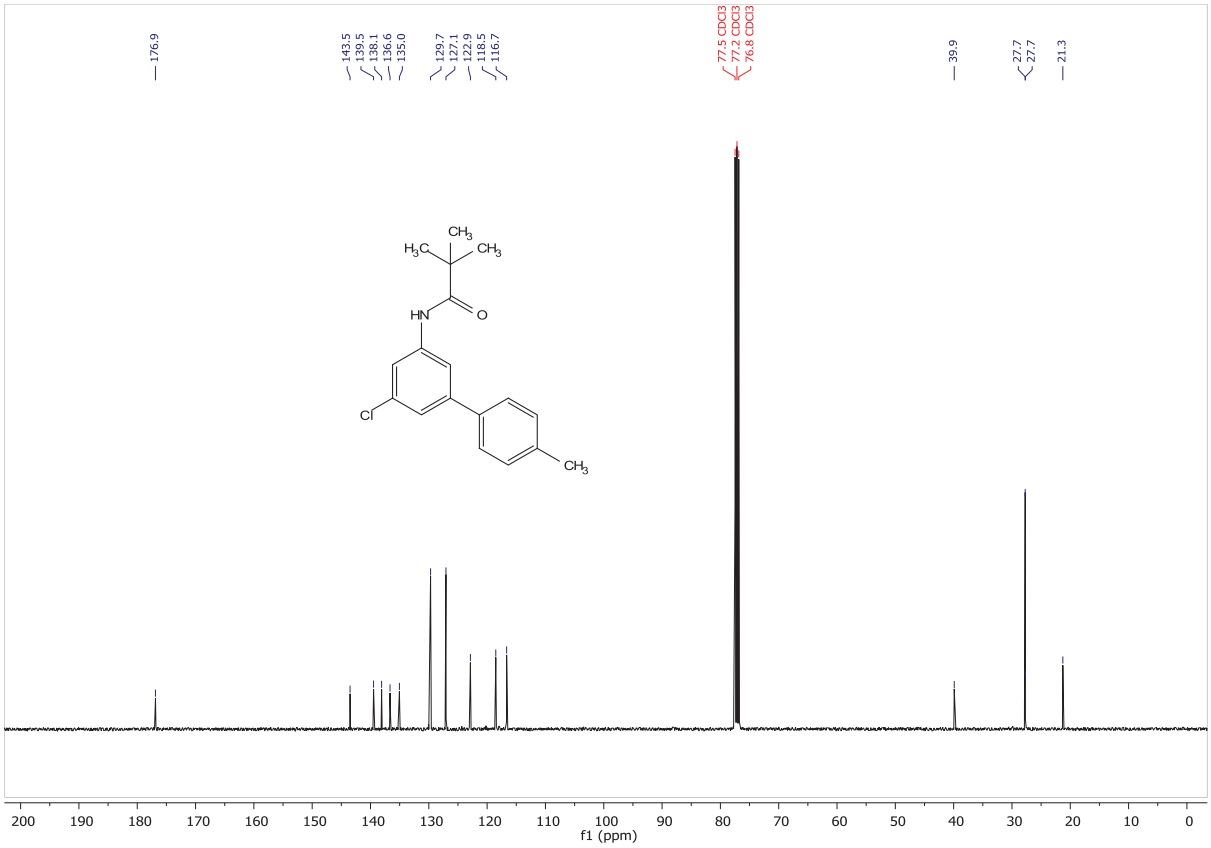
7.45
7.44
7.38
7.30
7.30
7.29
7.26 CDCl3
7.24
7.24
7.24
7.22
7.22
7.22
2.39
1.33
CH3
H3C
CH3
HN
O
Cl
CH3
2.00
2.01
1.00
1.01
2.05
3.00
9.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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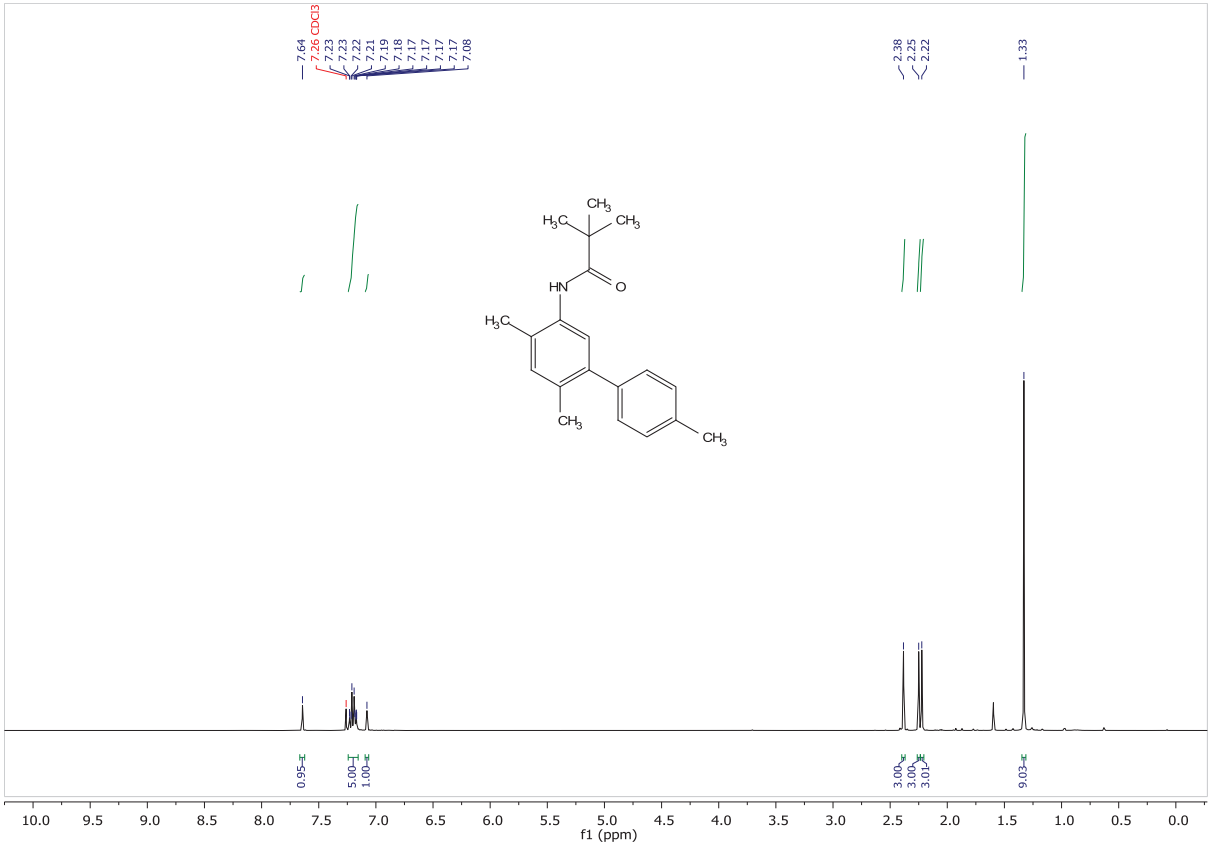
135.0
129.7
127.1
122.9
118.5
116.7
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
39.9
27.7
27.7
21.3
CH3
H3C
CH3
HN
O
Cl
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.26 CDCl3
7.23
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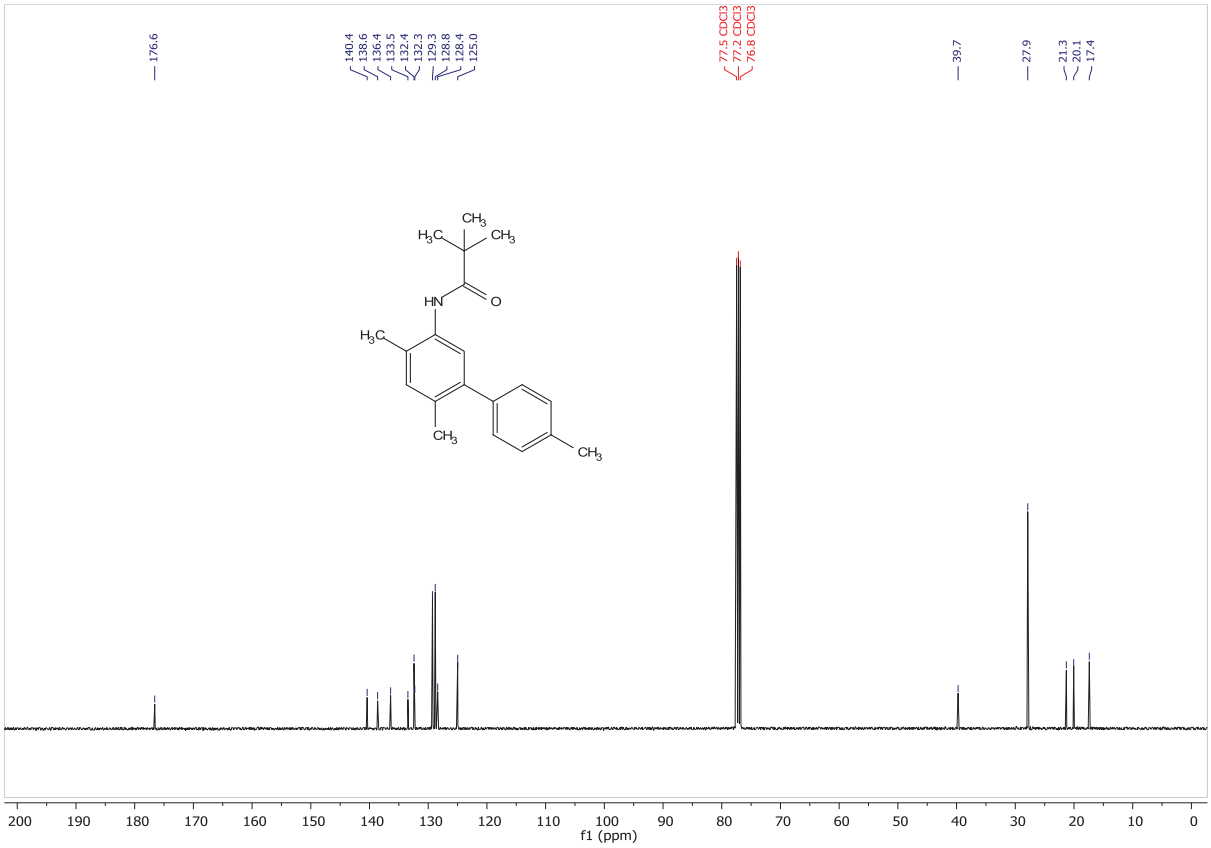
7.22
7.21
7.19
7.18
7.17
7.17
7.17
7.17
7.08
2.38
2.25
2.22
1.33
0.95
5.00
1.00
3.00
3.00
3.01
9.03
f1 (ppm)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132.4
132.3
129.3
128.8
128.4
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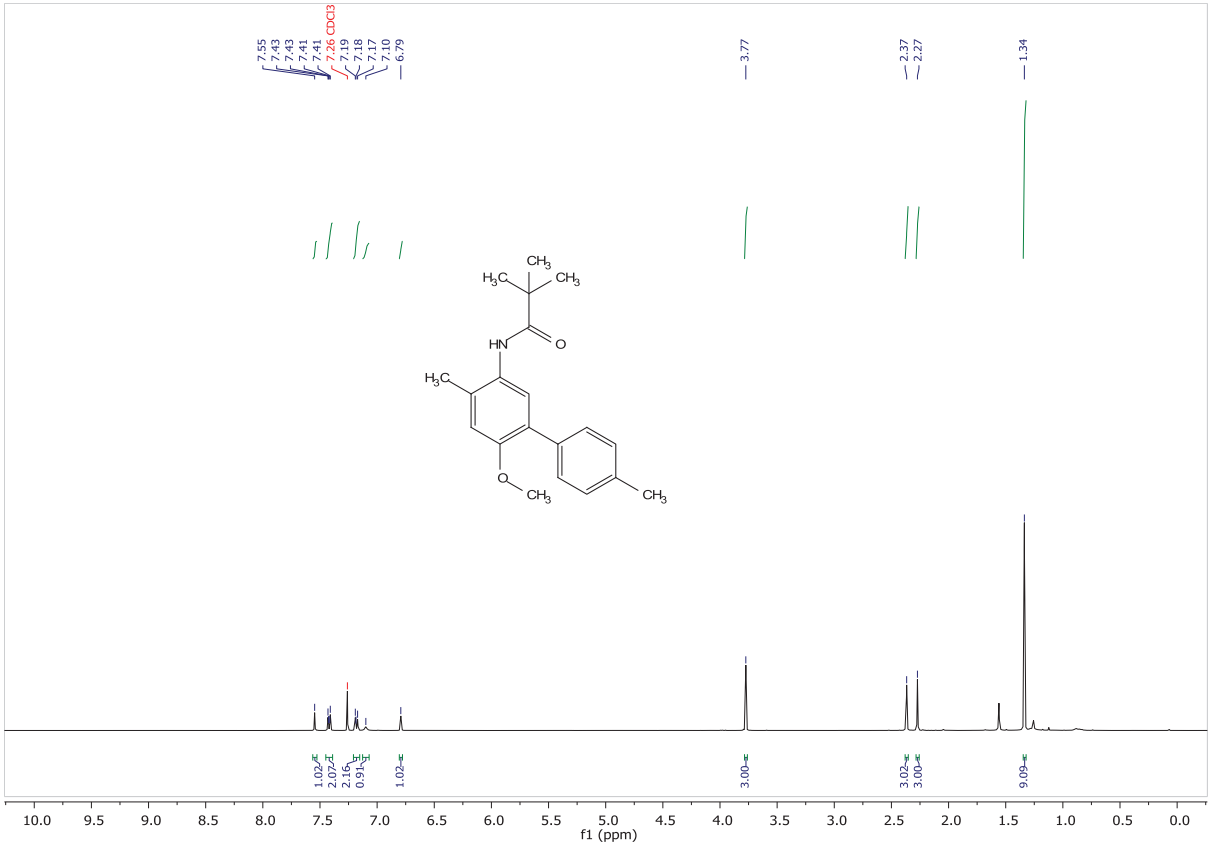
77.2 CDCl3
76.8 CDCl3
39.7
27.9
21.3
20.1
17.4
f1 (ppm)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7.43
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7.41
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7.18
7.17
7.10
6.79
3.77
2.37
2.27
1.34
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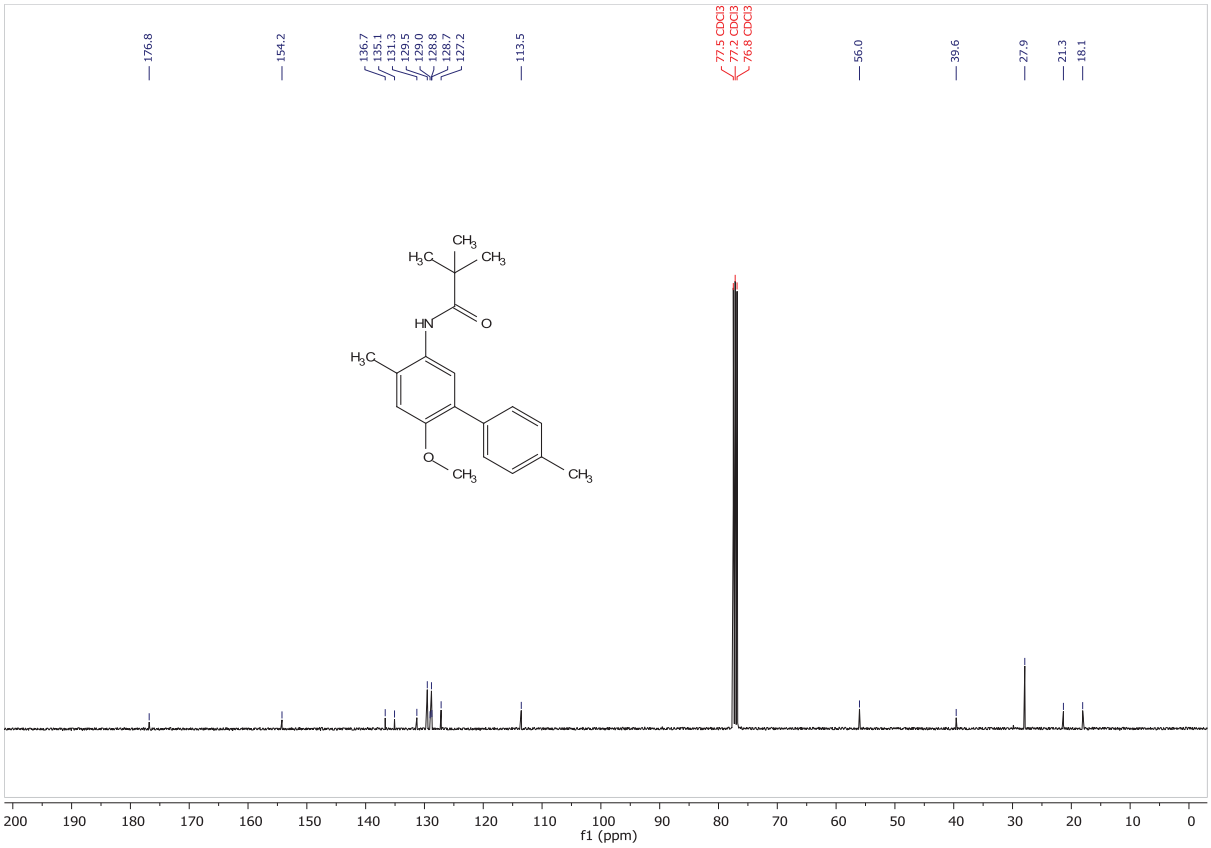
2.07
2.16
0.91
1.02
3.00
3.02
3.00
9.09
f1 (ppm)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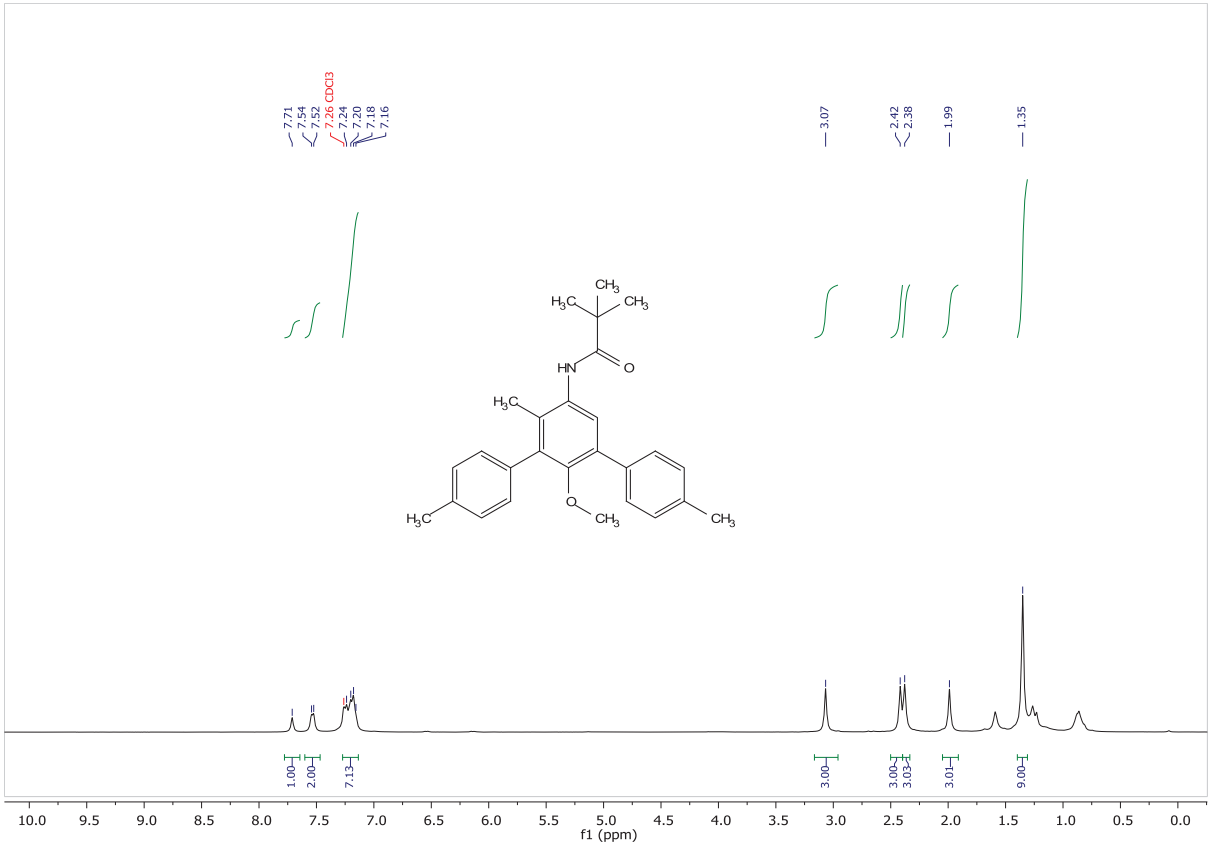
136.7
135.1
133.3
129.5
129.0
128.8
128.7
127.2
113.5
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
56.0
39.6
27.9
21.3
18.1
f1 (ppm)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7.20
7.18
7.16
3.07
2.42
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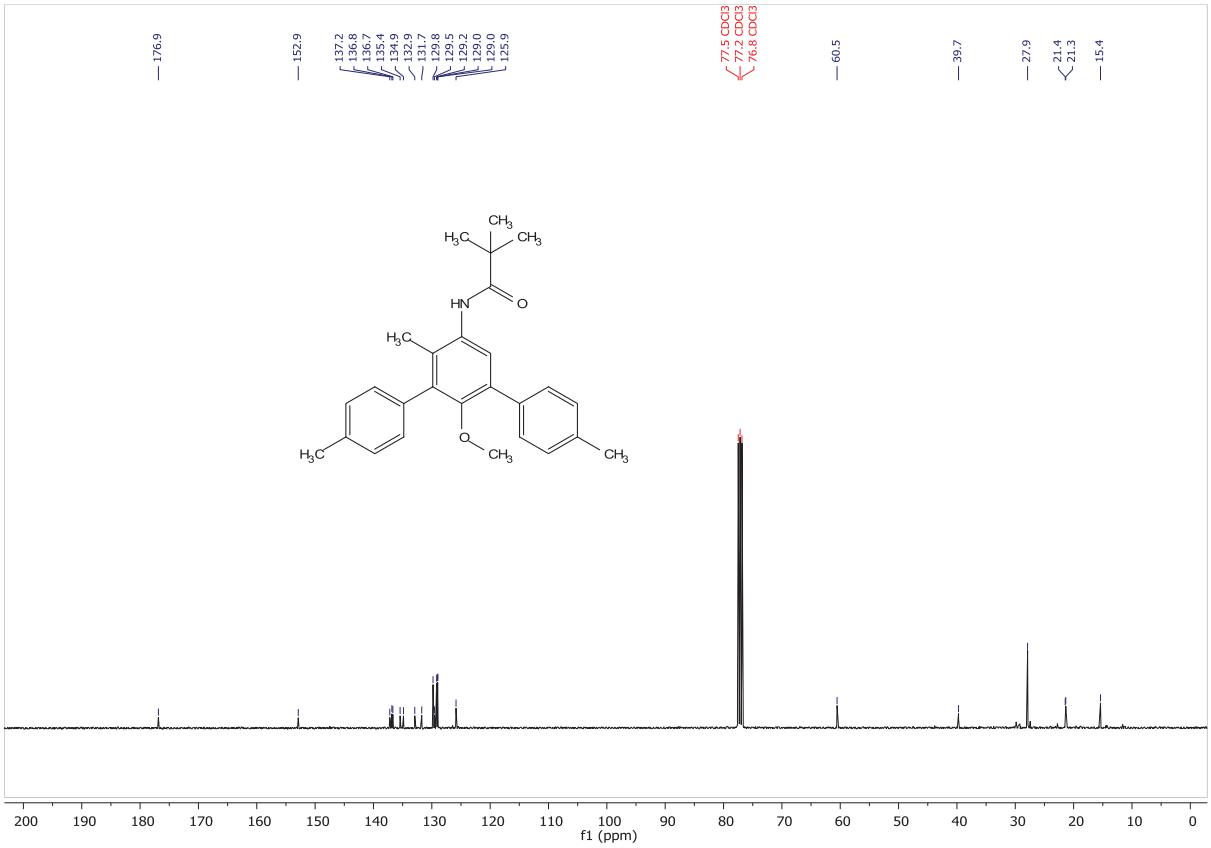
3.00
3.03
3.01
9.00
f1 (ppm)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136.8
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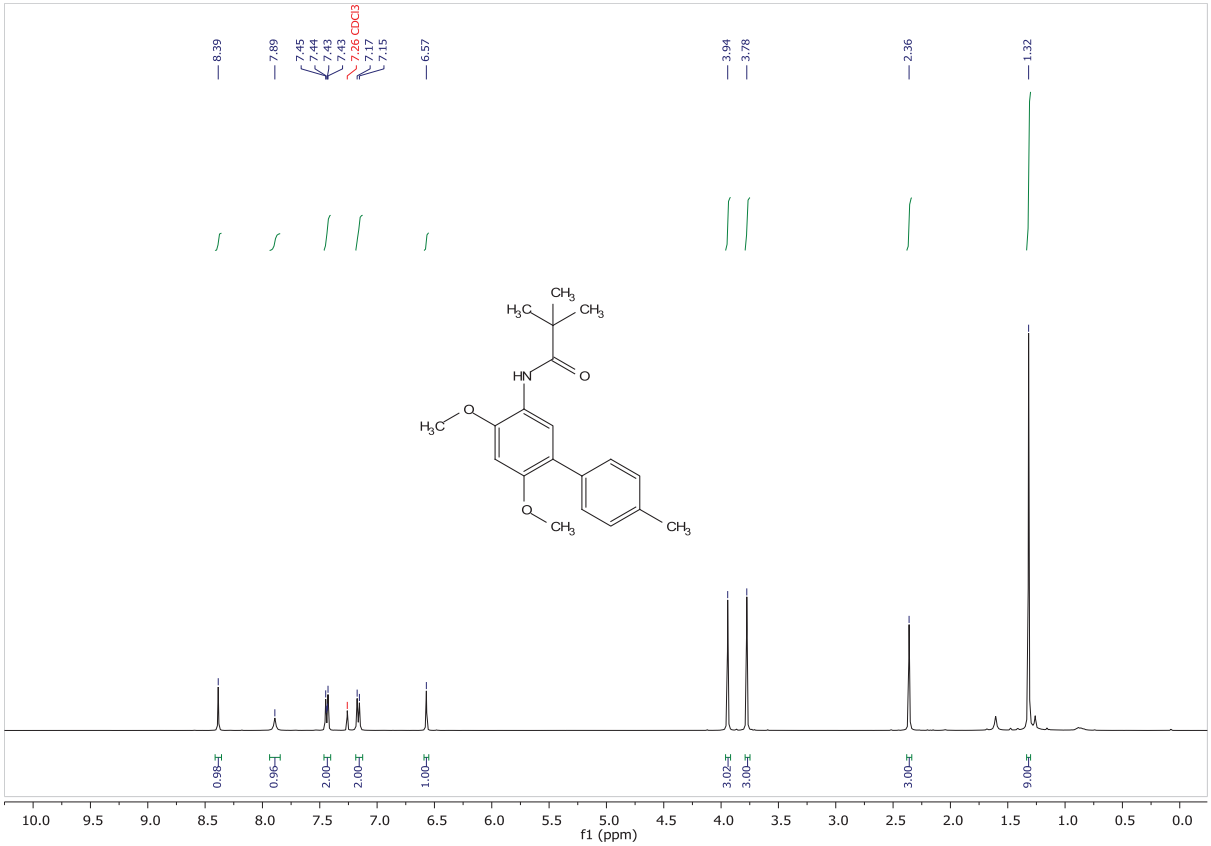
135.4
134.9
132.9
131.7
129.8
129.5
129.2
129.0
129.0
125.9
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
60.5
39.7
27.9
21.4
21.3
15.4
f1 (ppm)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7.43
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7.17
7.15
6.57
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3.78
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1.32
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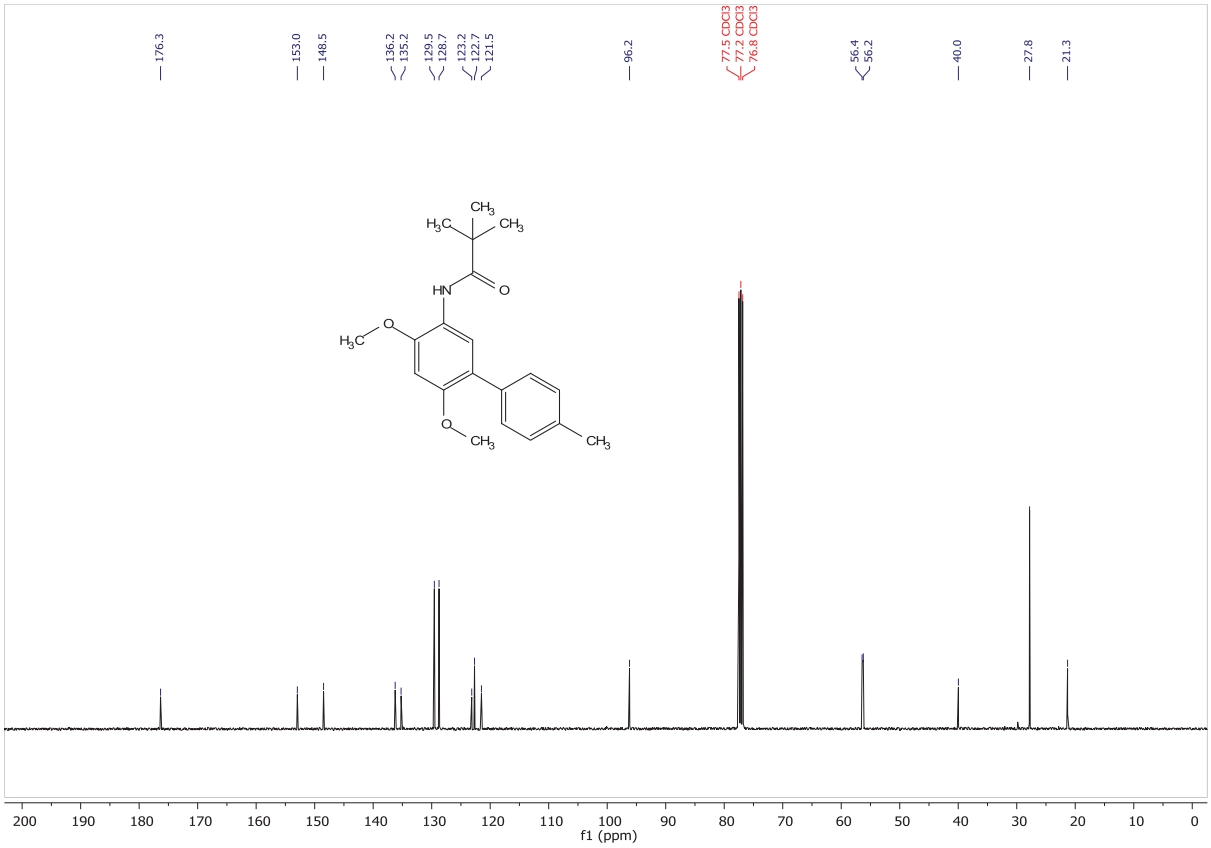
0.96
2.00
2.00
1.00
3.02
3.00
3.00
9.00
f1 (ppm)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135.2
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128.7
123.2
122.7
121.5
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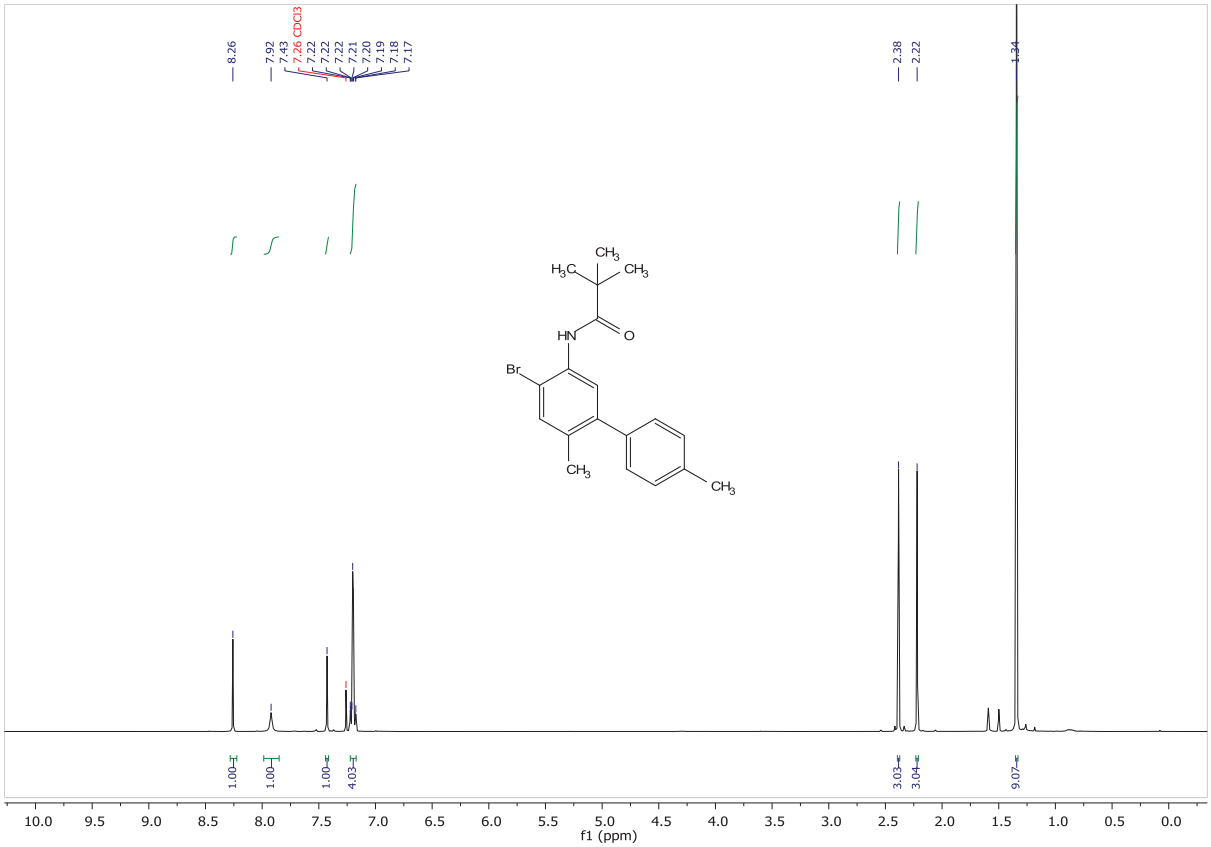
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
56.4
56.2
40.0
27.8
21.3
f1 (ppm)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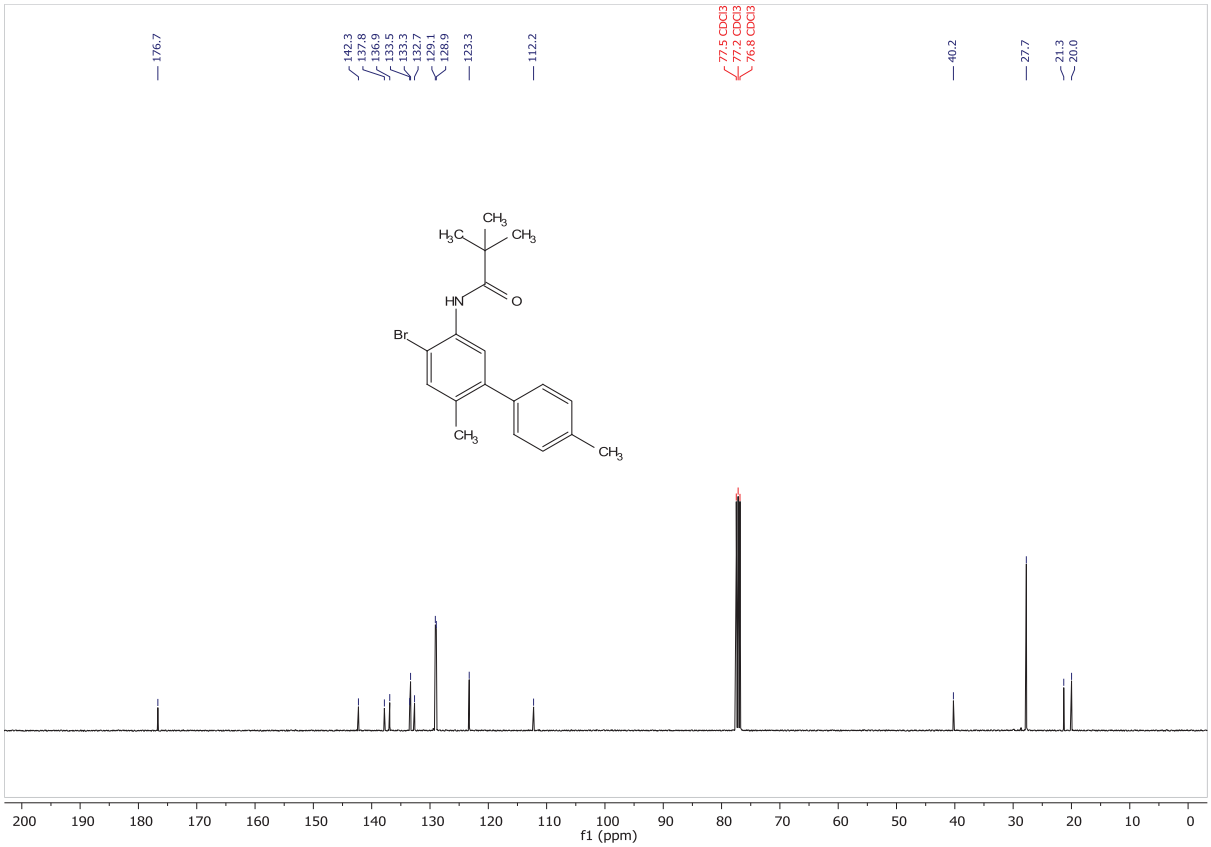
7.20
7.19
7.18
7.17
2.38
2.22
1.34
CH3
H3C
CH3
HN
O
Br
CH3
CH3
1.00
1.00
1.00
4.03
3.03
3.04
9.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.3
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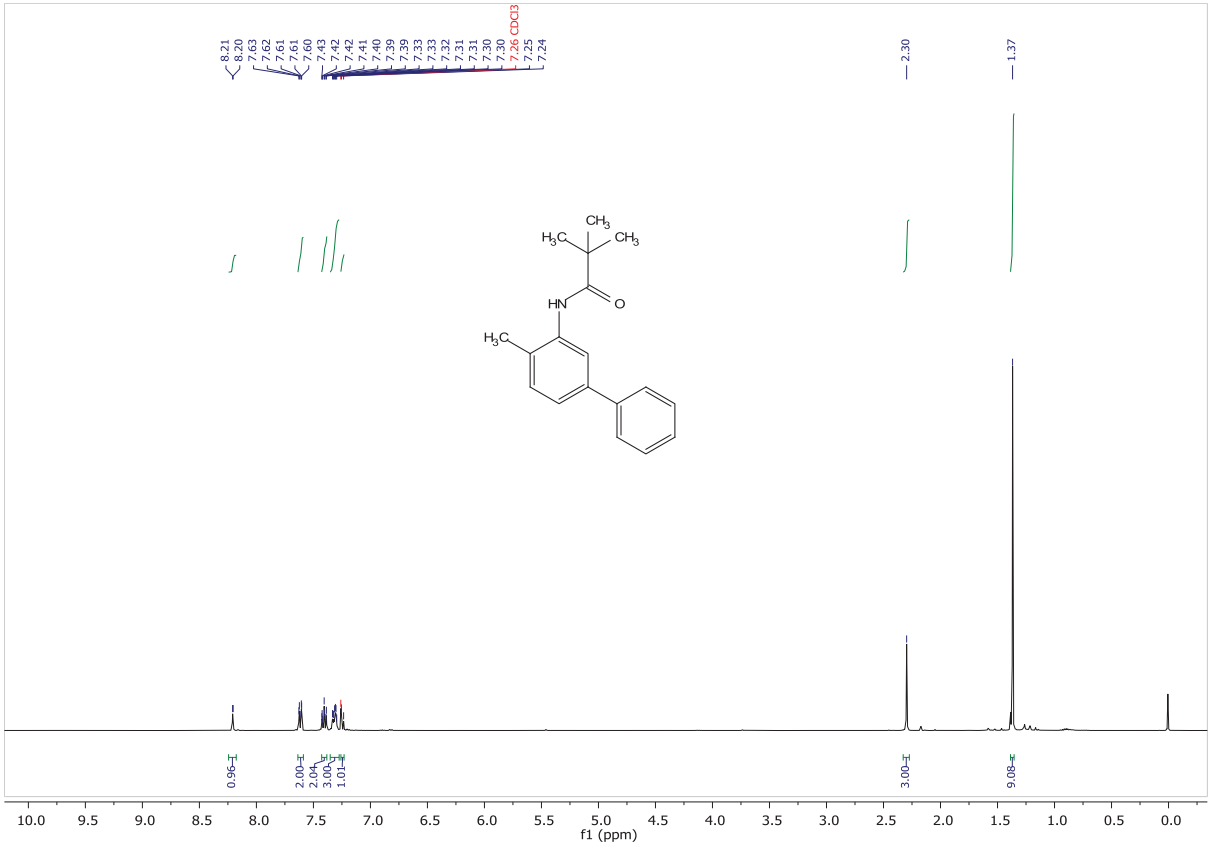
128.9
123.3
112.2
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
40.2
27.7
21.3
20.0
CH3
H3C
CH3
HN
O
Br
CH3
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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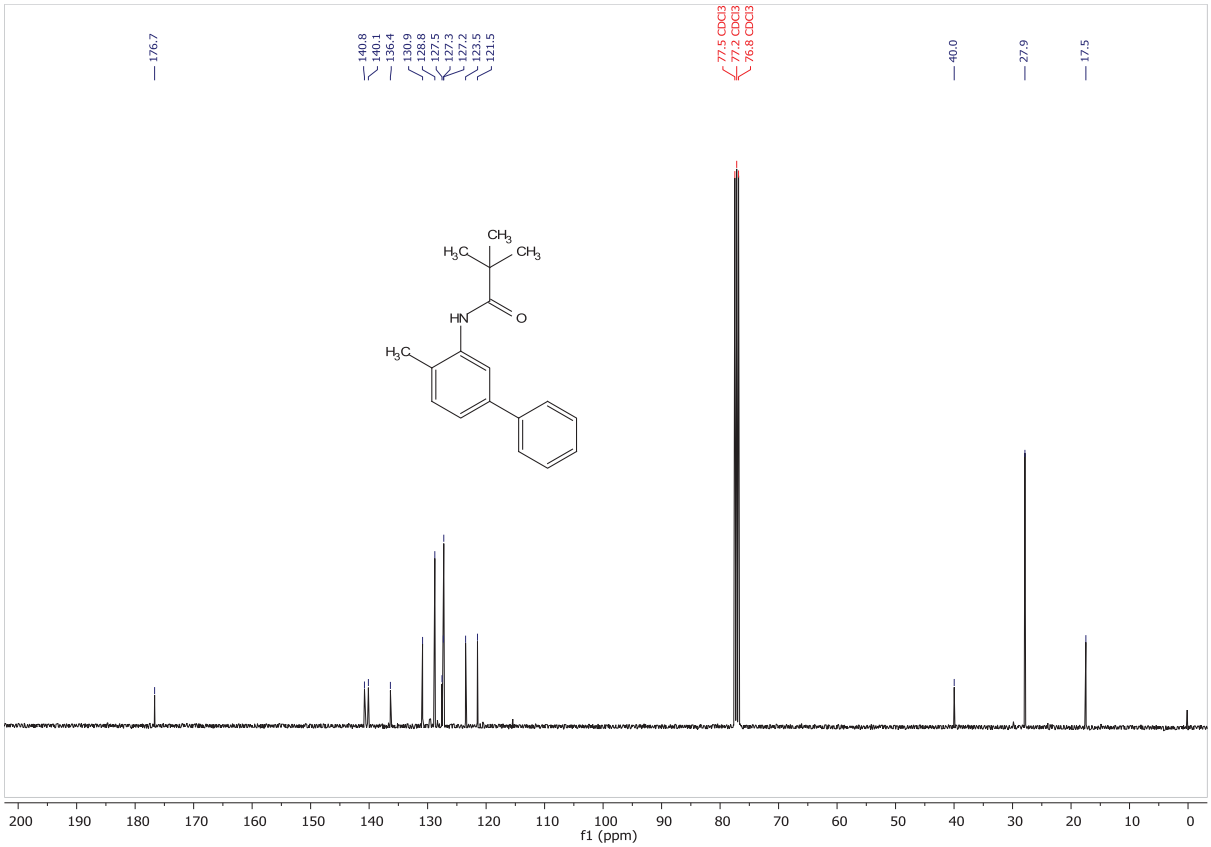
7.39
7.33
7.32
7.31
7.31
7.30
7.30
7.26 CDCl3
7.25
7.24
2.30
1.37
0.96
2.00
2.04
3.00
1.01
3.00
9.08
f1 (ppm)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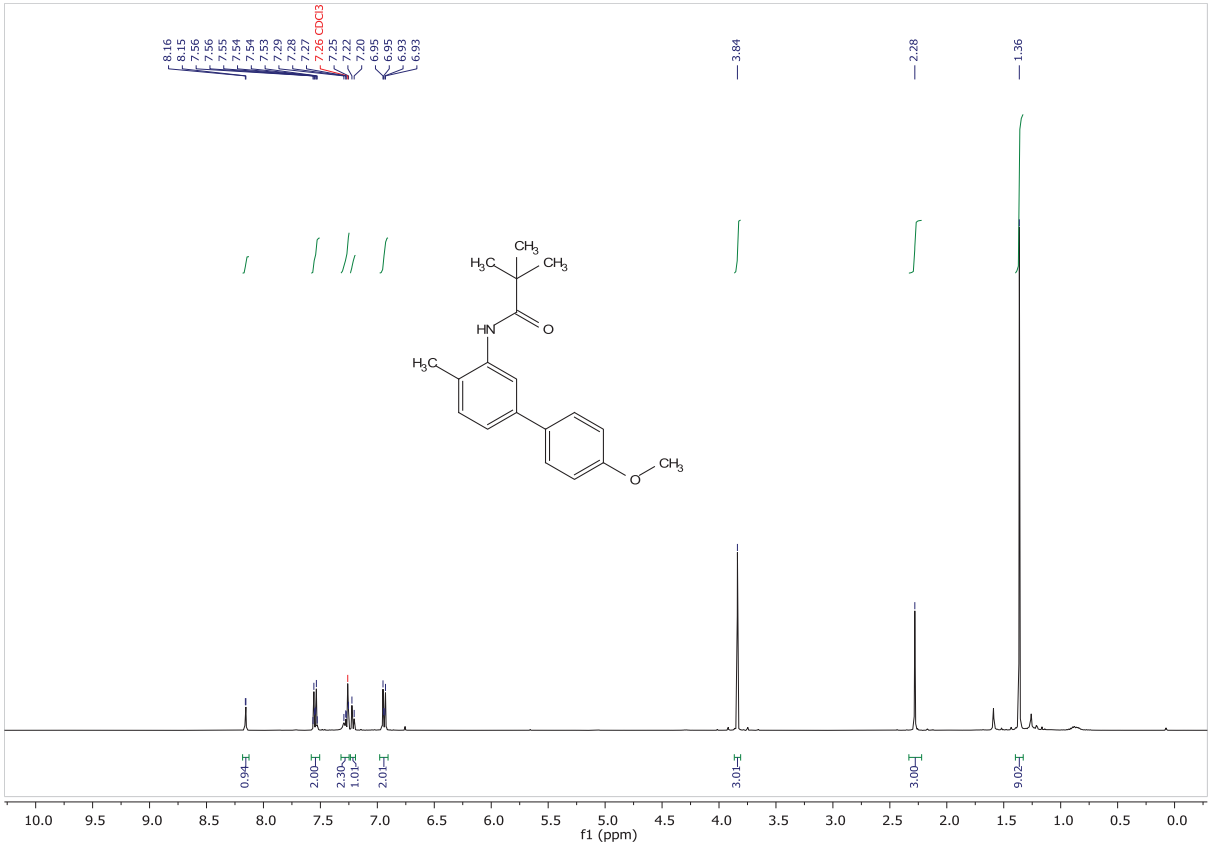
130.9
128.8
127.5
127.3
127.2
123.5
121.5
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
40.0
27.9
17.5
f1 (ppm)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7.27
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7.25
7.22
7.20
6.95
6.95
6.93
6.93
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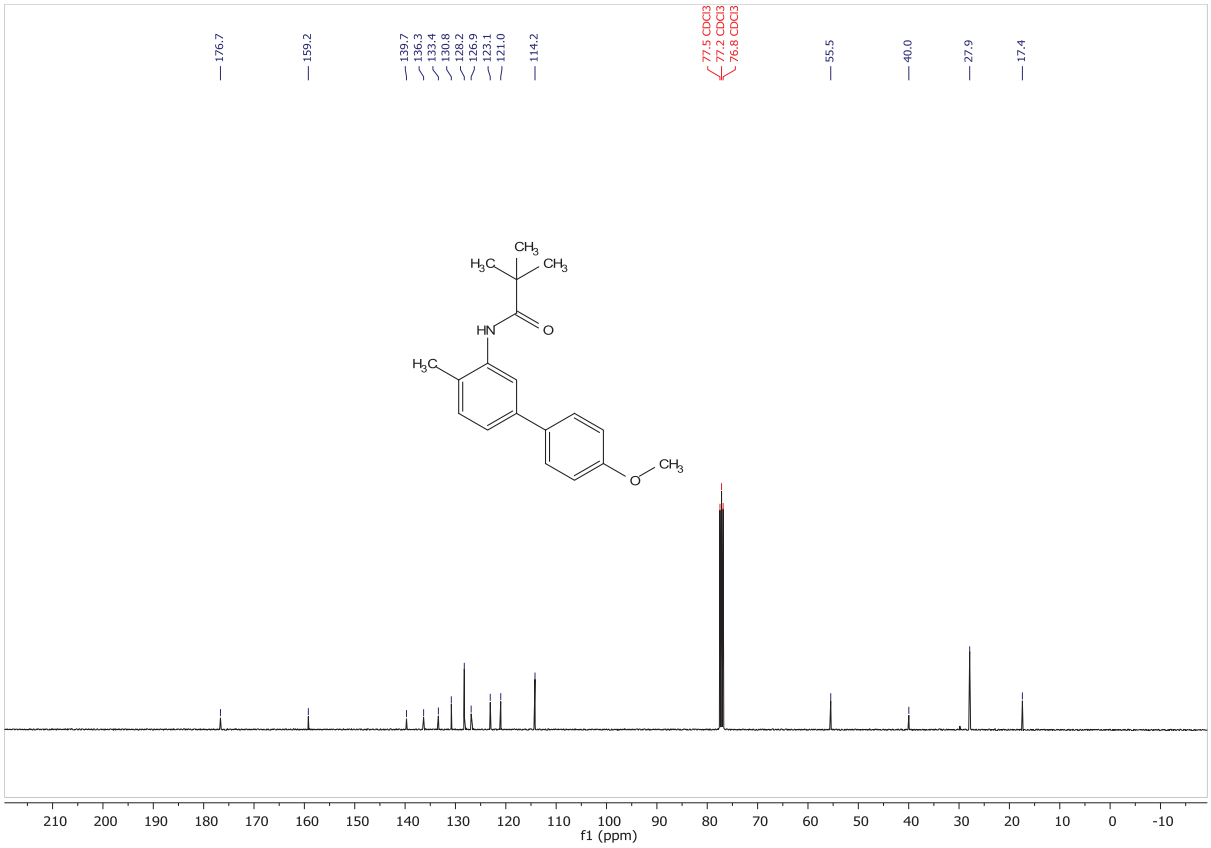
0.94
2.00
2.30
1.01
2.01
3.01
3.00
9.02
f1 (ppm)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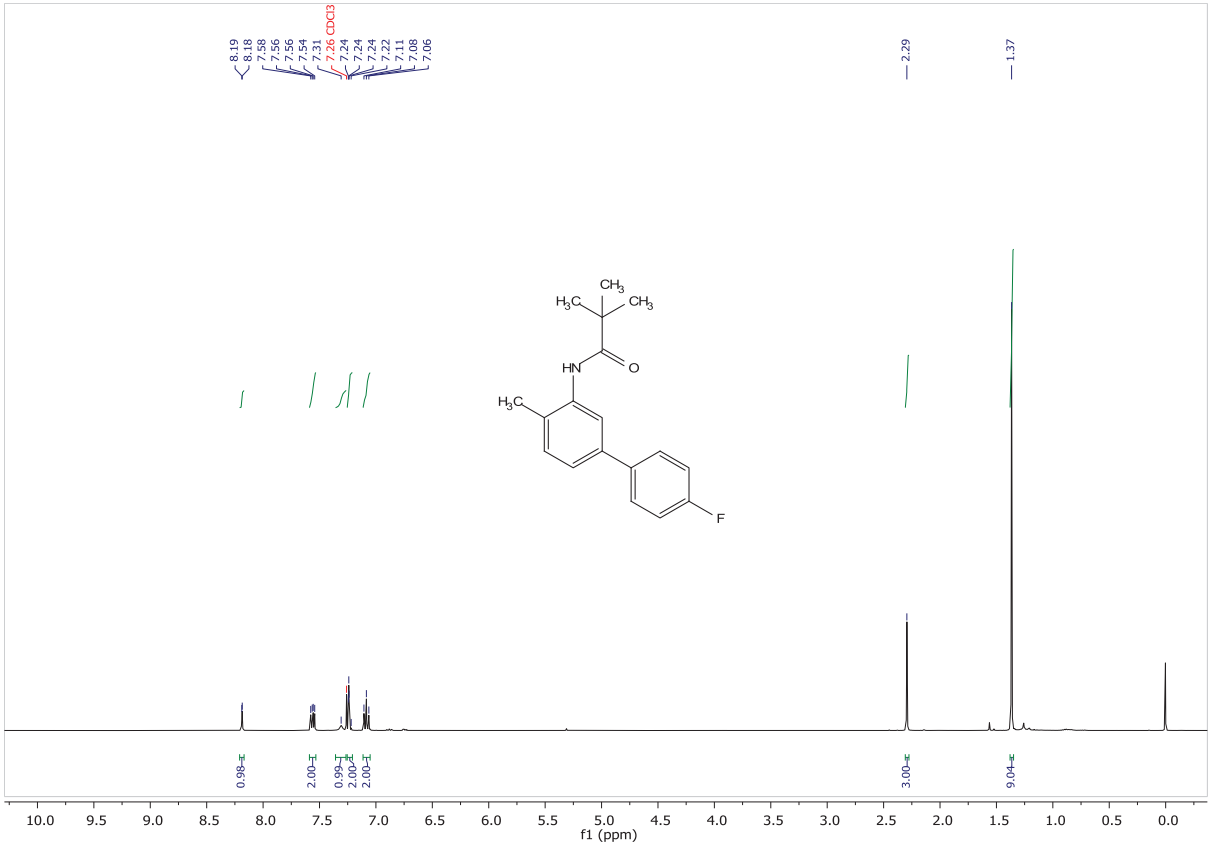
139.7
136.3
133.4
130.8
128.2
126.9
123.1
121.0
114.2
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
55.5
40.0
27.9
17.4
f1 (ppm)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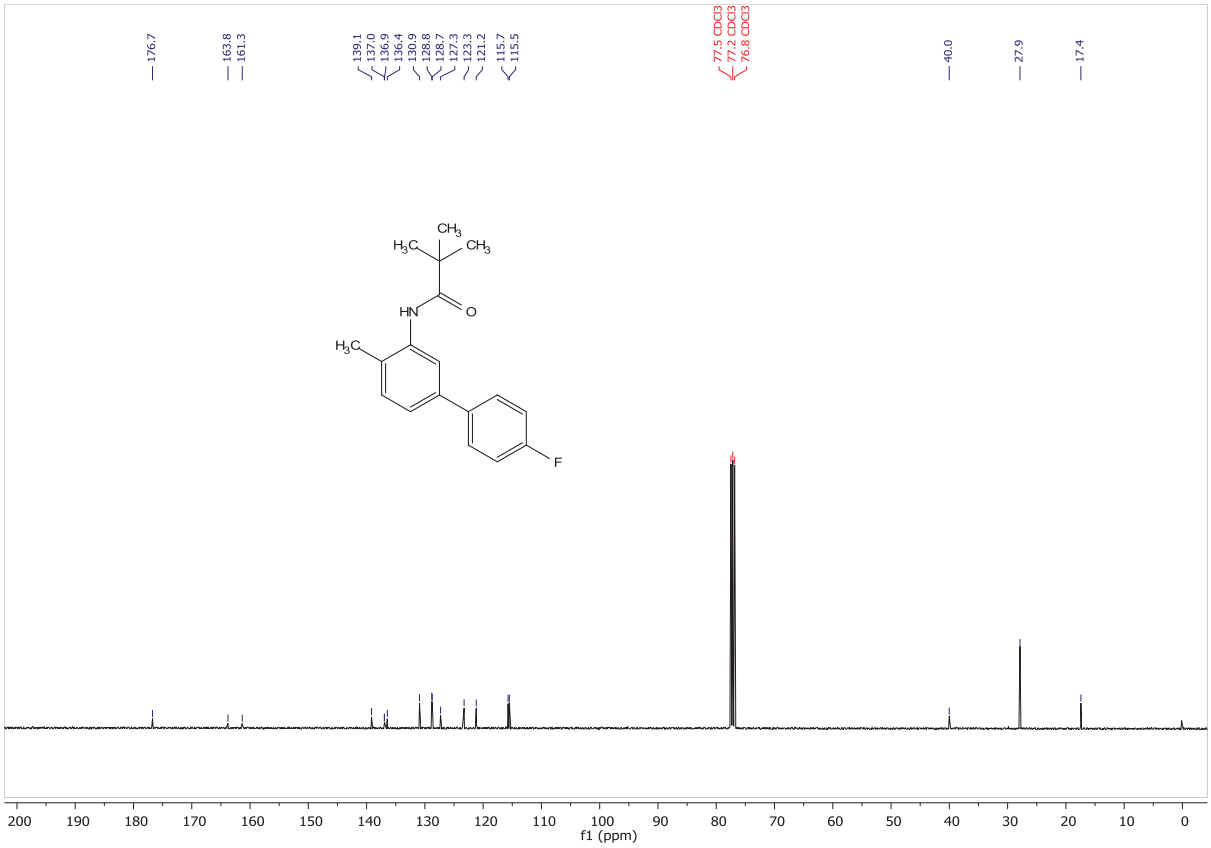
7.24
7.22
7.11
7.08
7.06
2.29
1.37
CH3
H3C
CH3
HN
O
H3C
F
0.98
2.00
0.99
2.00
2.00
3.00
9.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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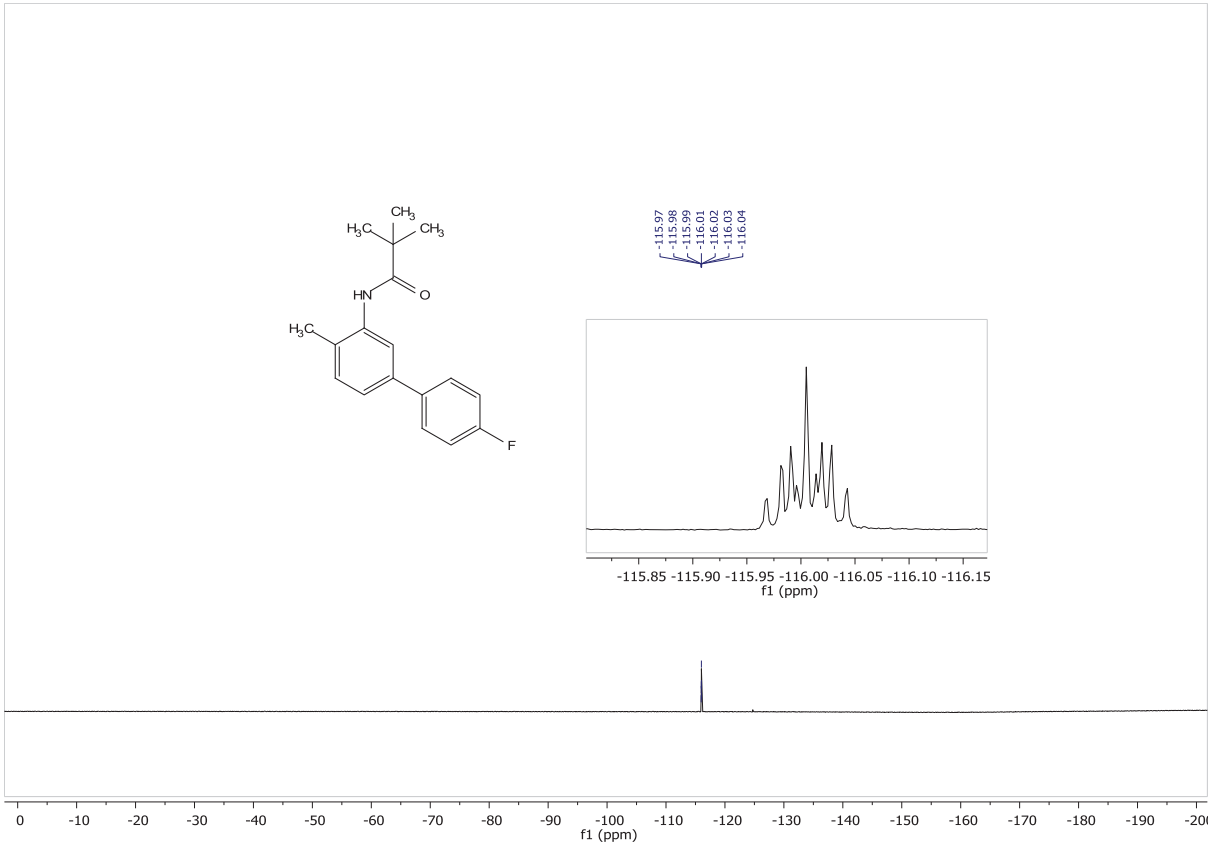
161.3
139.1
137.0
136.9
136.4
130.9
128.8
128.7
127.3
123.3
121.2
115.7
115.5
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
40.0
27.9
17.4
CH3
H3C
CH3
HN
O
H3C
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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CH3
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O
H3C
F
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-115.98
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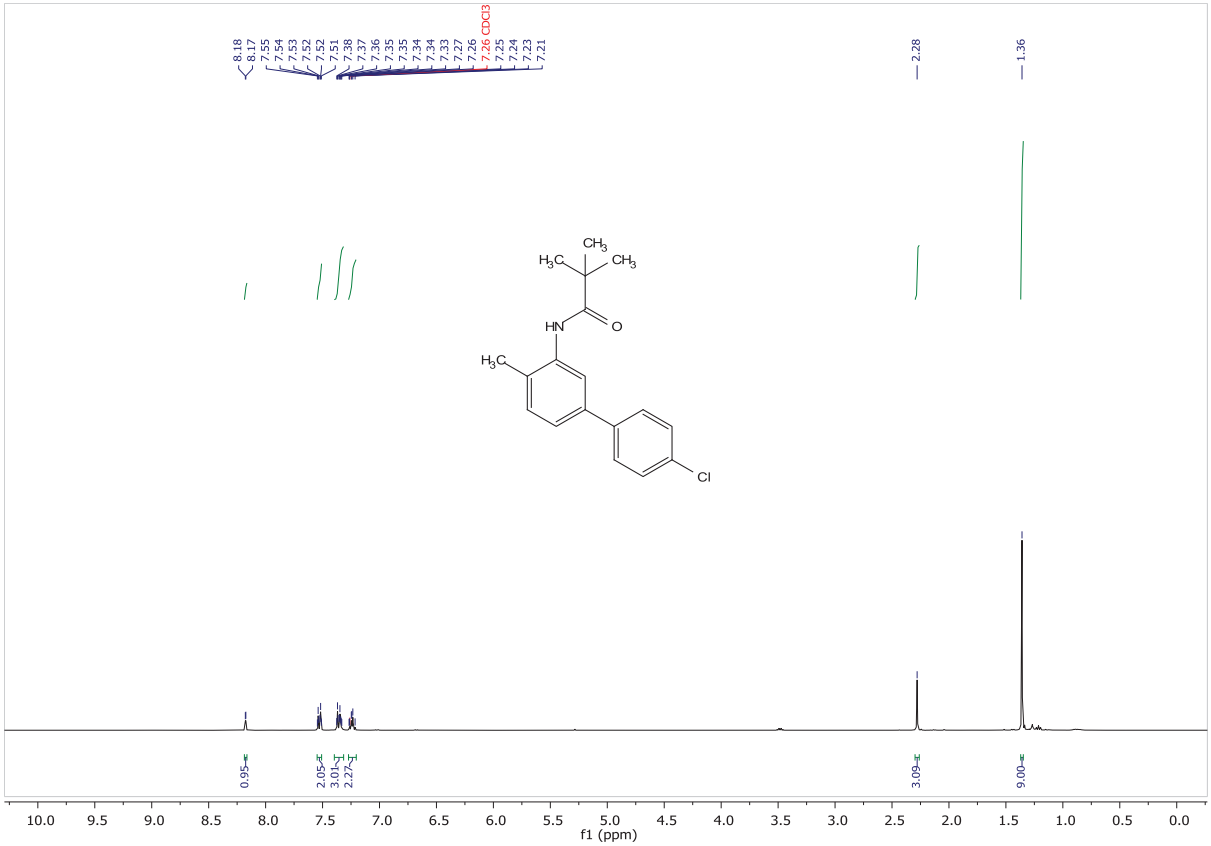
-116.01
-116.02
-116.03
-116.04
-115.85 -115.90 -115.95 -116.00 -116.05 -116.10 -116.15
f1 (ppm)
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -20
f1 (ppm)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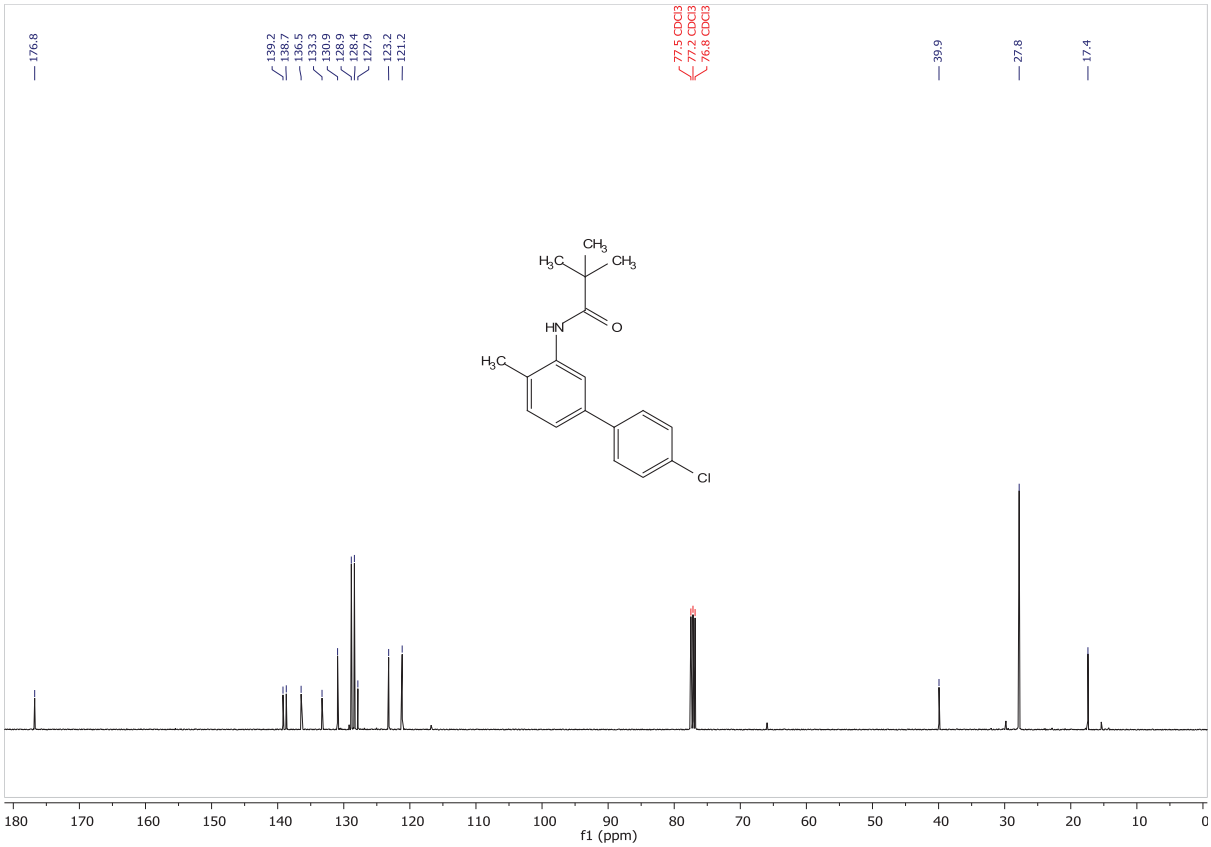
7.25
7.24
7.23
7.21
2.28
1.36
CH3
H3C
CH3
HN
O
H3C
Cl
0.95
2.05
3.01
2.27
3.09
9.00
f1 (ppm)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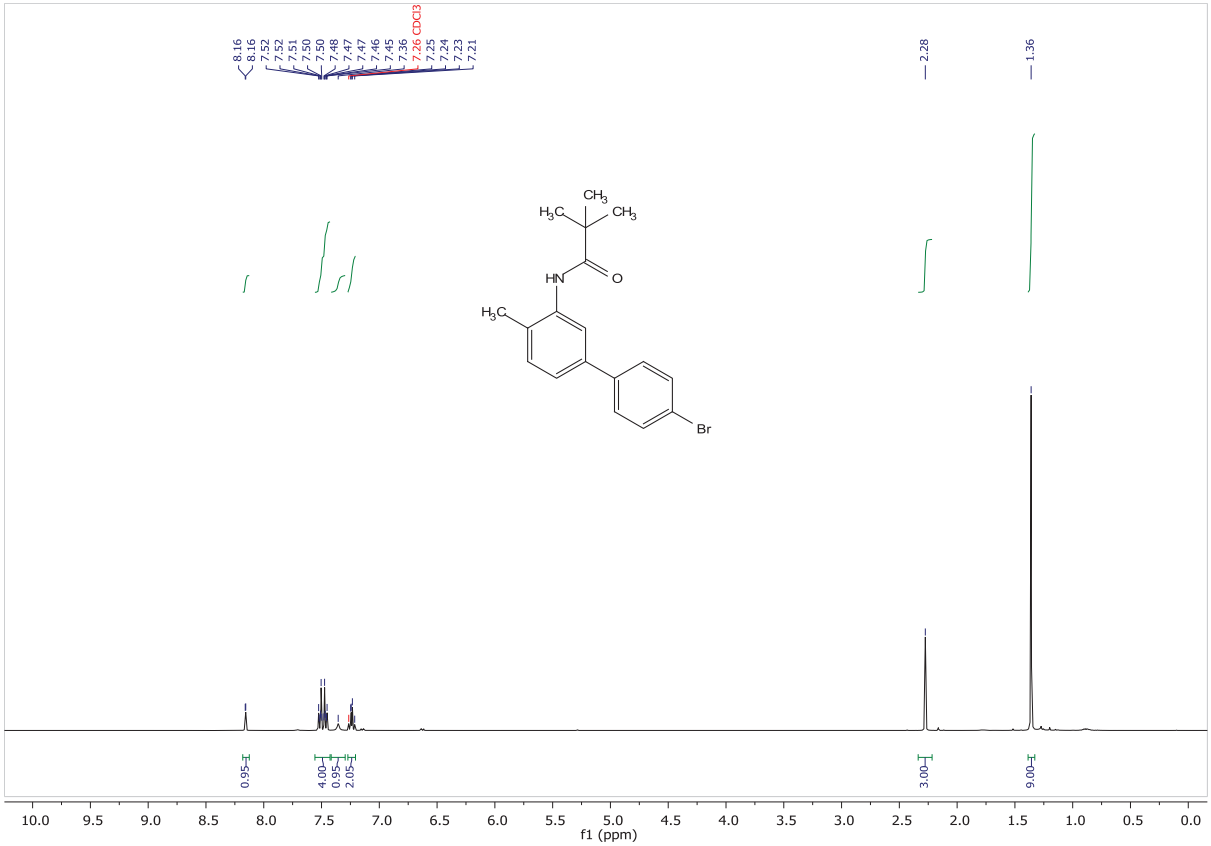
128.4
127.9
123.2
121.2
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
39.9
27.8
17.4
CH3
H3C
CH3
HN
O
H3C
Cl
f1 (ppm)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7.47
7.46
7.45
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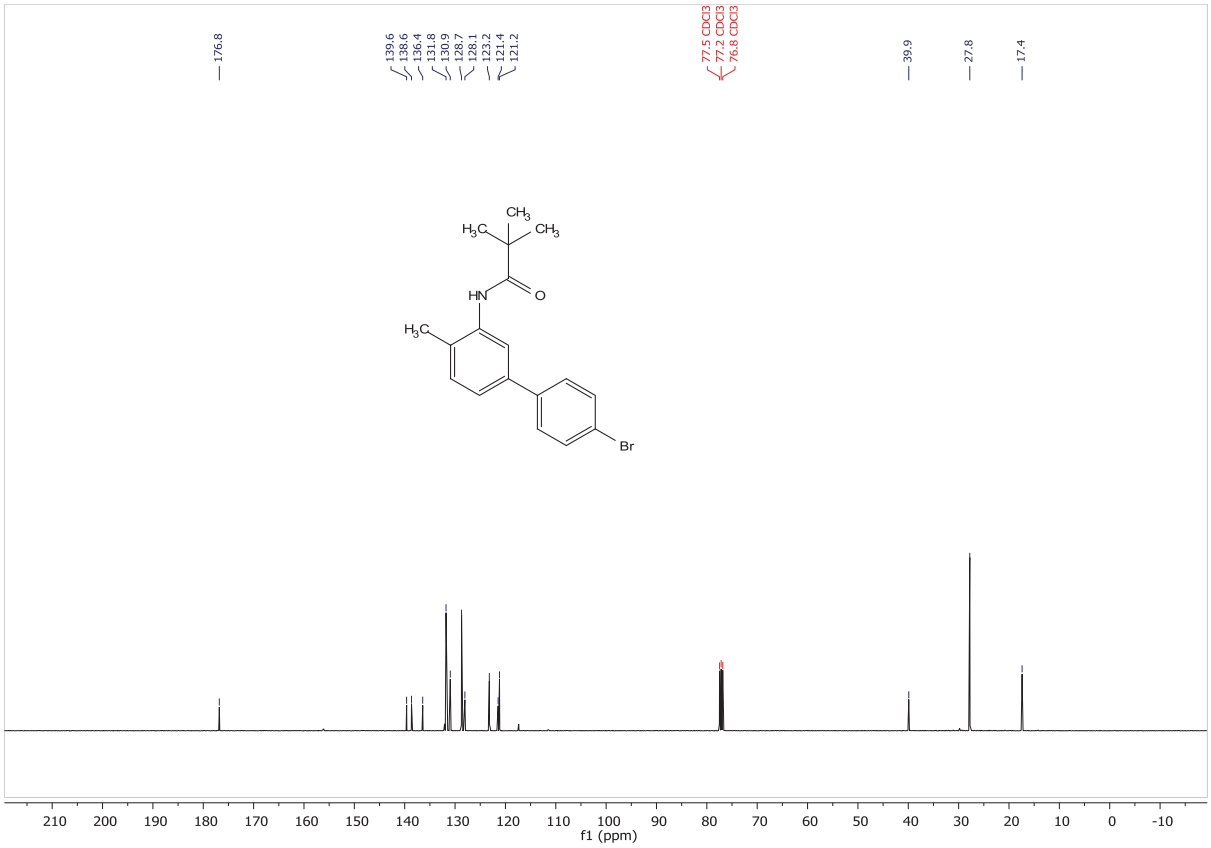
7.25
7.24
7.23
7.21
2.28
1.36
CH3
H3C
CH3
HN
O
H3C
Br
0.95
4.00
0.95
2.05
3.00
9.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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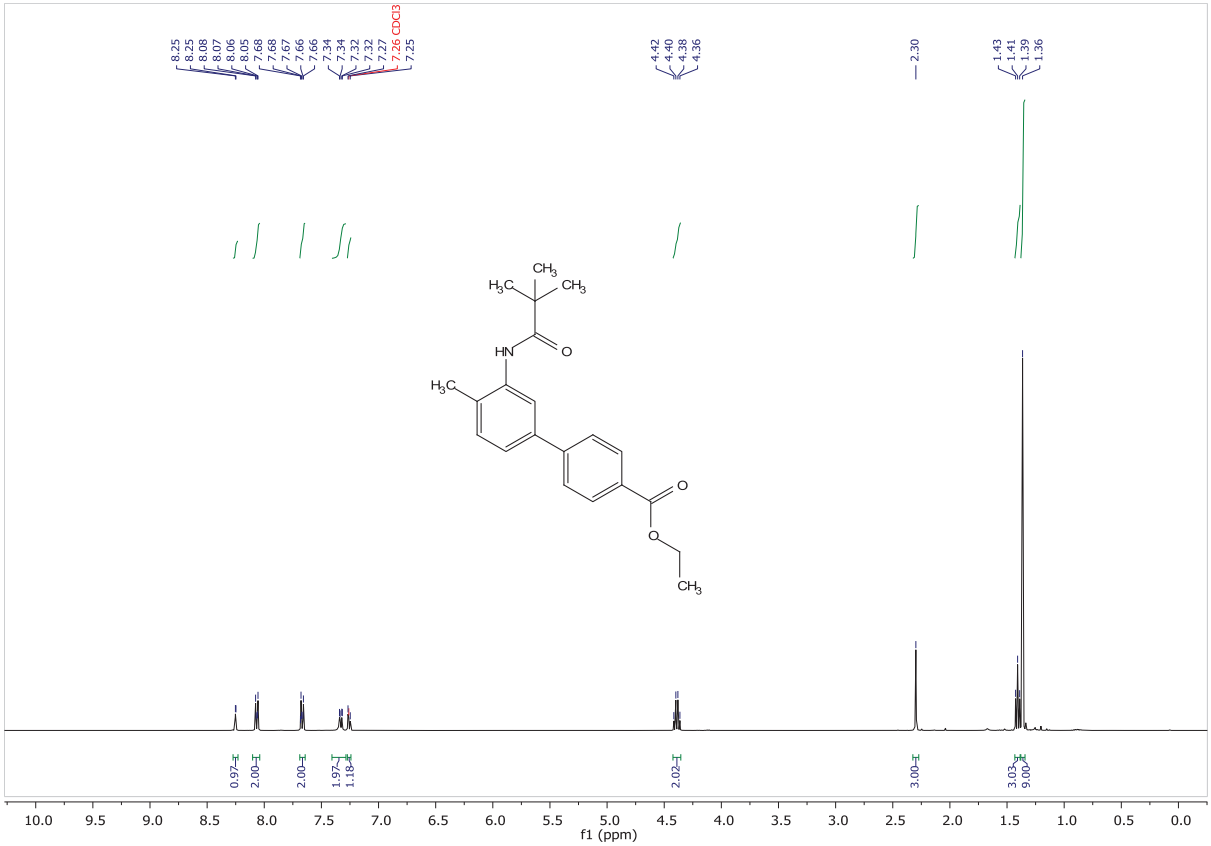
136.4
131.8
130.9
128.7
128.1
123.2
121.4
121.2
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
39.9
27.8
17.4
CH3
H3C
CH3
HN
O
H3C
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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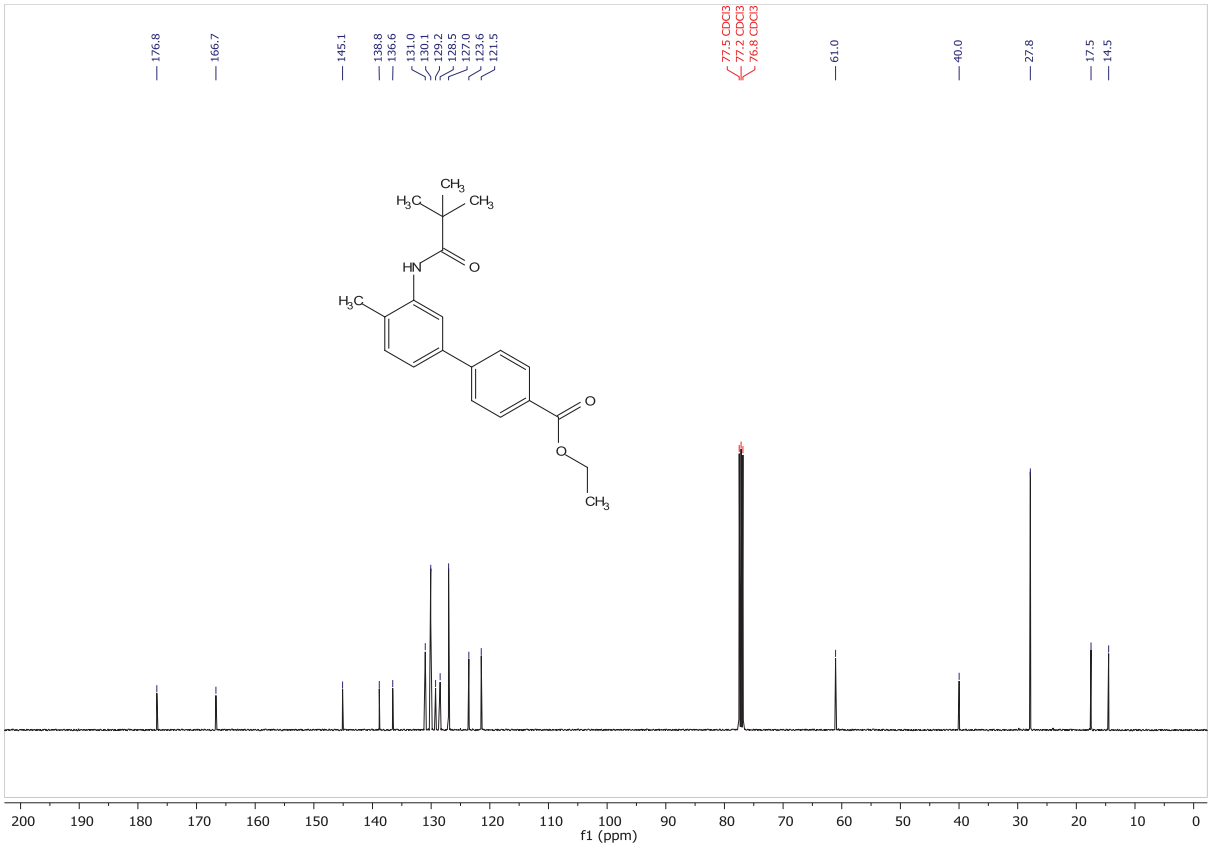
7.34
7.32
7.32
7.27
7.26 CDCl3
7.25
4.42
4.40
4.38
4.36
2.30
1.43
1.41
1.39
1.36
CH3
H3C
CH3
HN
O
H3C
O
O
CH3
0.97
2.00
2.00
1.97
1.18
2.02
3.00
3.03
9.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.2
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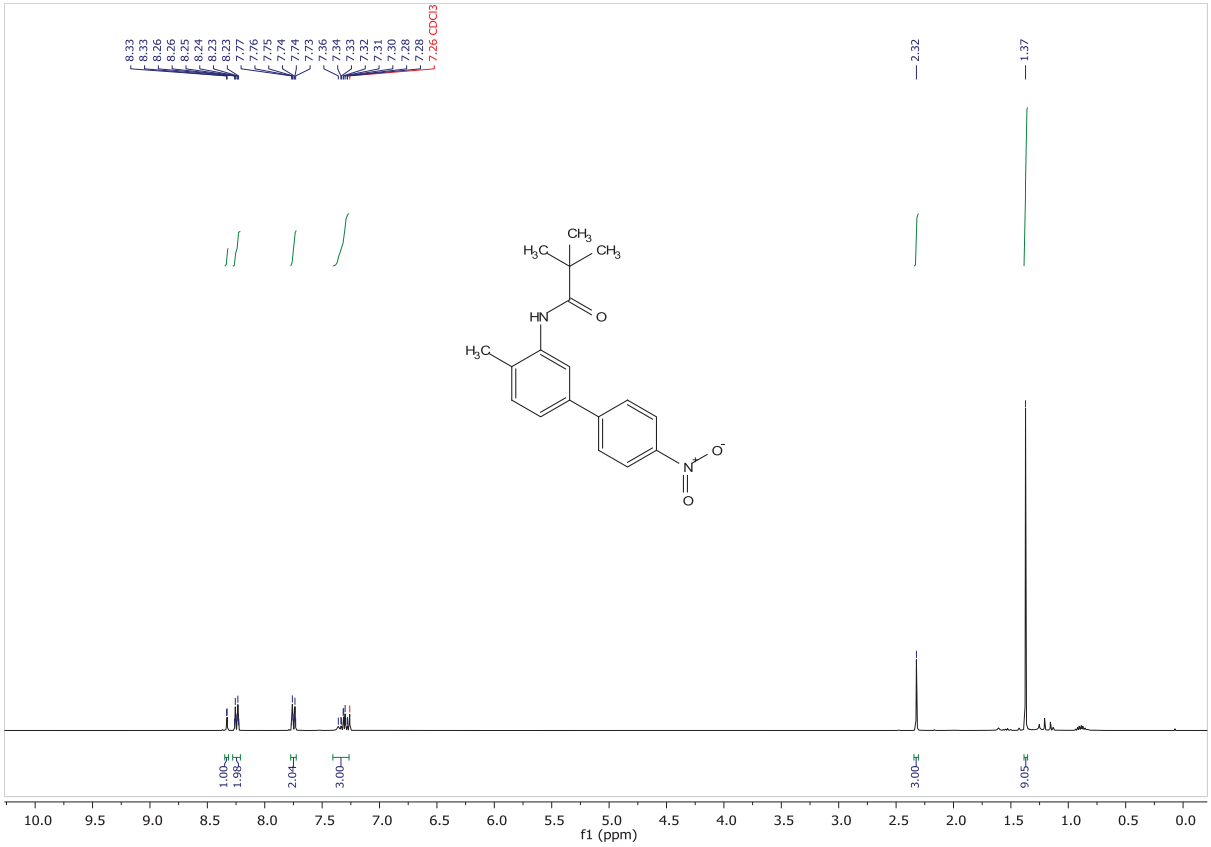
123.6
121.5
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
61.0
40.0
27.8
17.5
14.5
CH3
H3C
CH3
HN
O
H3C
O
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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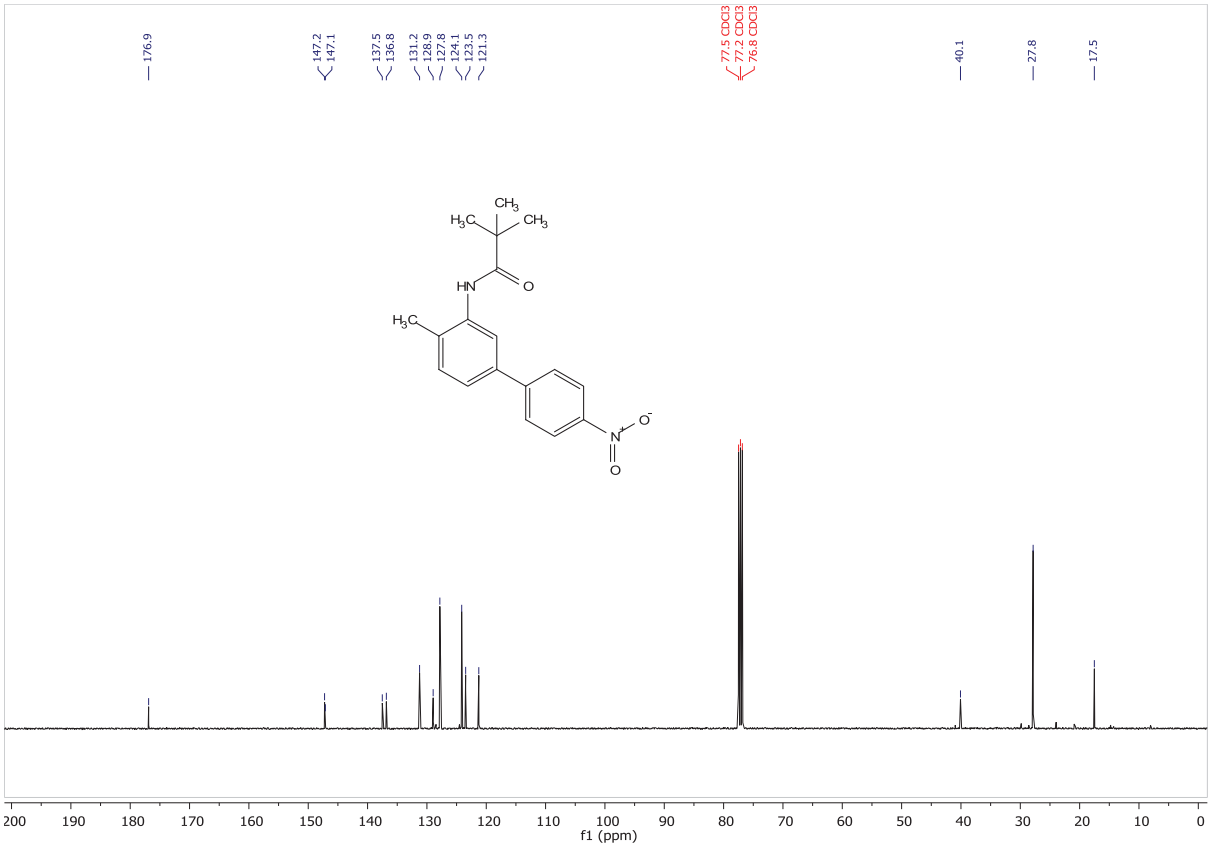
8.33
8.26
8.26
8.25
8.24
8.23
8.23
7.77
7.76
7.75
7.74
7.74
7.73
7.36
7.34
7.33
7.32
7.31
7.30
7.28
7.26 CDCl3
2.32
1.37
1.00
1.98
2.04
3.00
3.00
9.05
f1 (ppm)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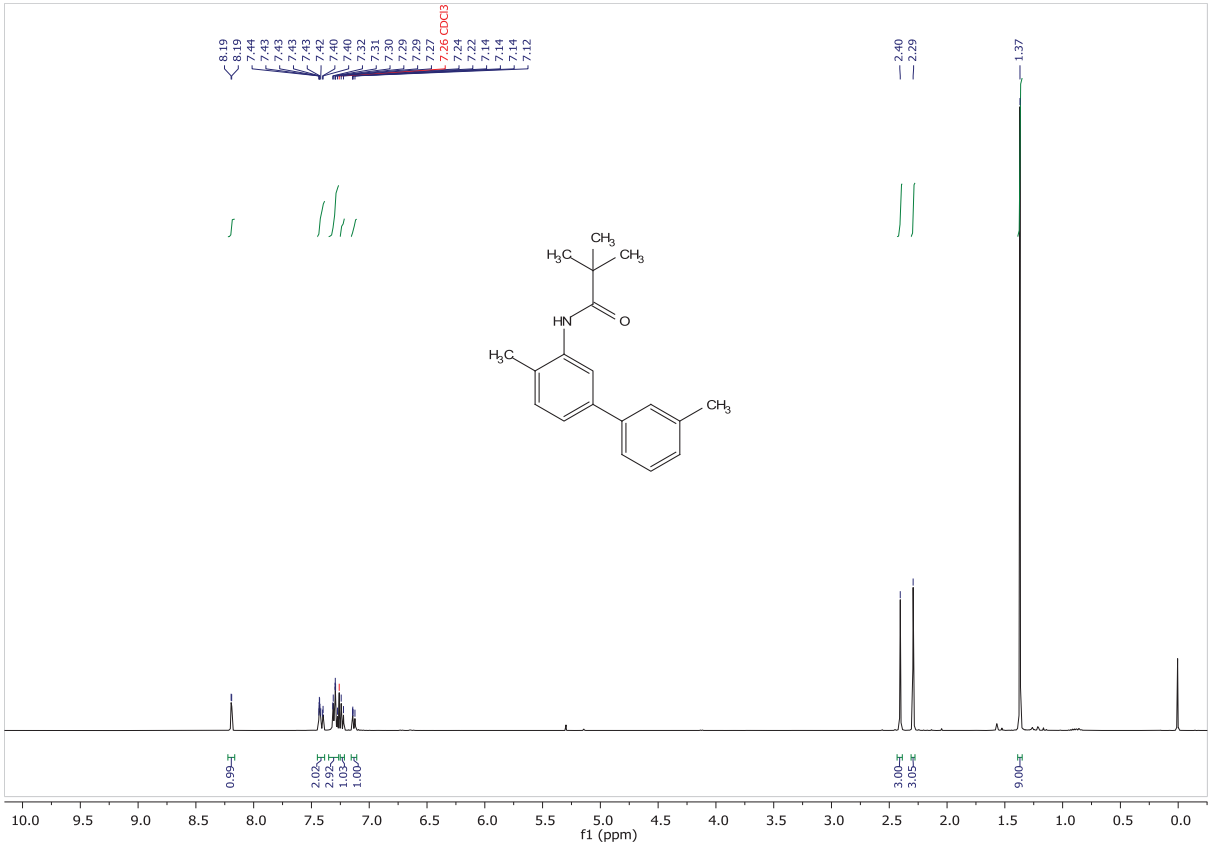
147.1
137.5
136.8
131.2
128.9
127.8
124.1
123.5
121.3
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
40.1
27.8
17.5
f1 (ppm)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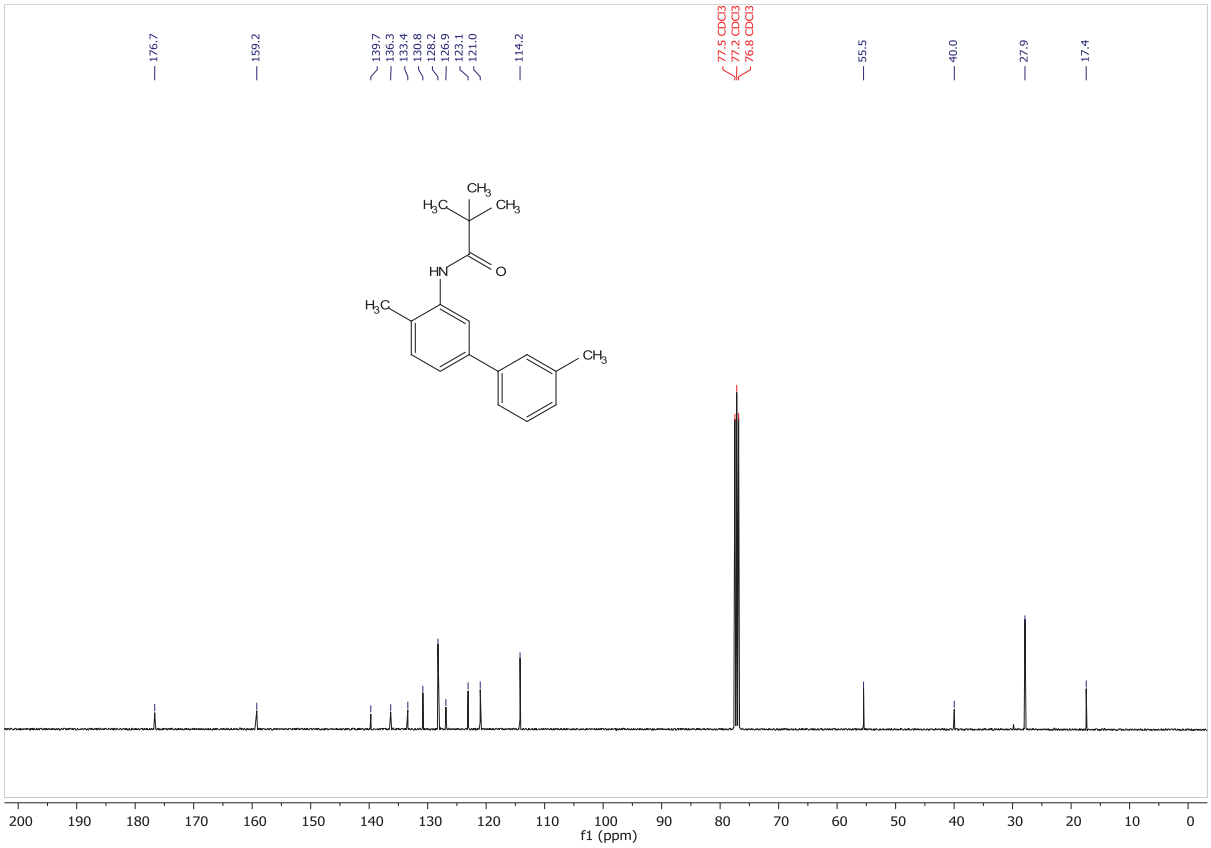
8.19
7.44
7.43
7.43
7.43
7.43
7.42
7.40
7.40
7.32
7.31
7.30
7.29
7.29
7.27
7.26 CDCl3
7.24
7.22
7.14
7.14
7.14
7.12
2.40
2.29
1.37
CH3
H3C
CH3
HN
O
H3C
CH3
0.99
2.02
2.92
1.03
1.00
3.00
3.05
9.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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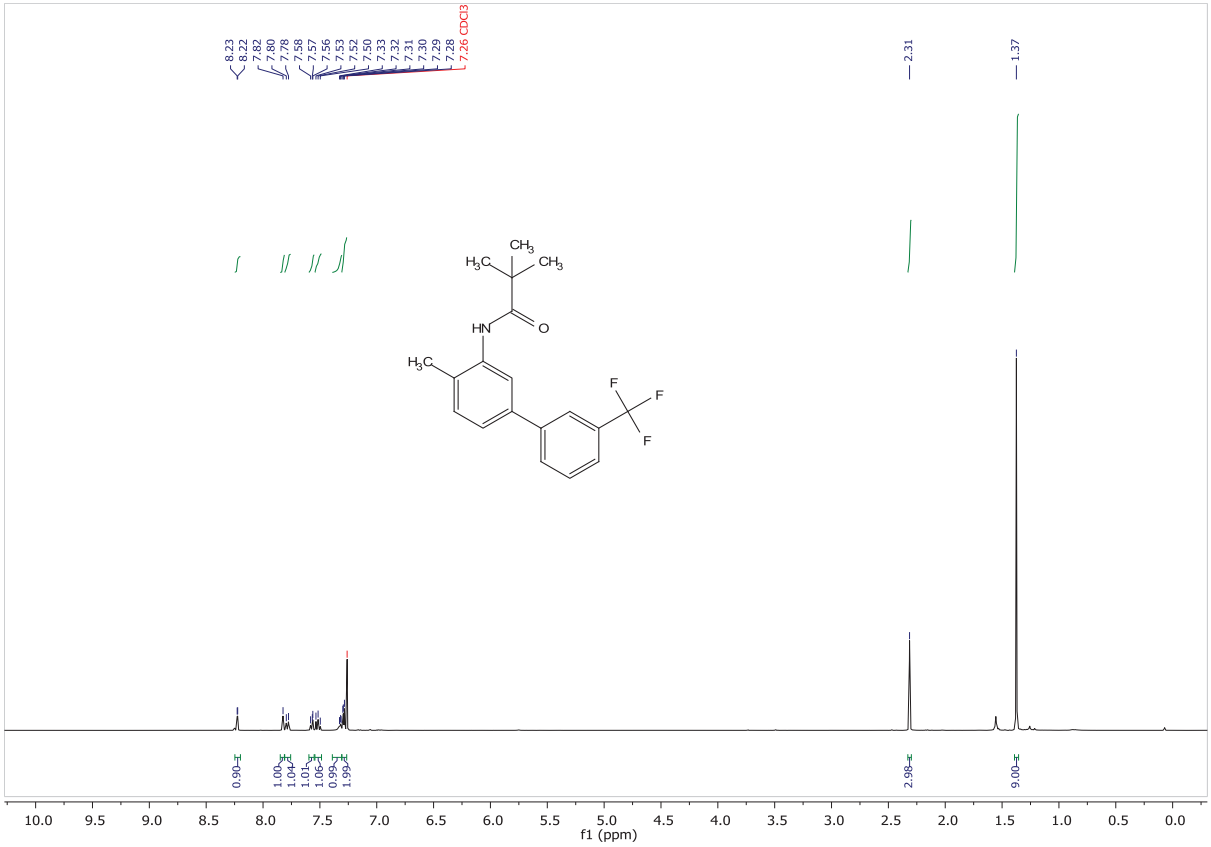
159.2
139.7
136.3
133.4
130.8
128.2
126.9
123.1
121.0
114.2
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
55.5
40.0
27.9
17.4
CH3
H3C
CH3
HN
O
H3C
CH3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.23
8.22
7.82
7.80
7.78
7.58
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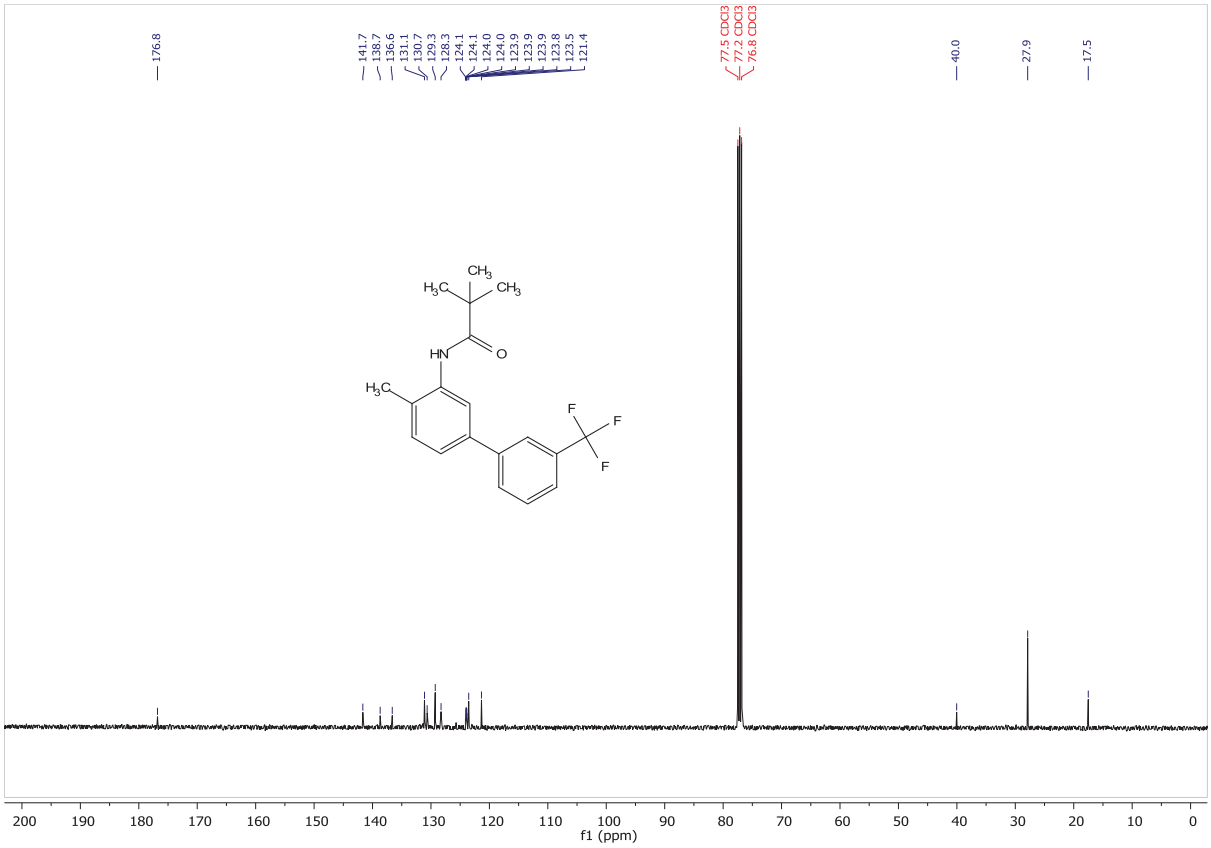
7.56
7.53
7.52
7.50
7.33
7.32
7.31
7.30
7.29
7.28
7.26 CDCl3
2.31
1.37
0.90
1.00
1.04
1.01
1.06
0.99
1.99
2.98
9.00
f1 (ppm)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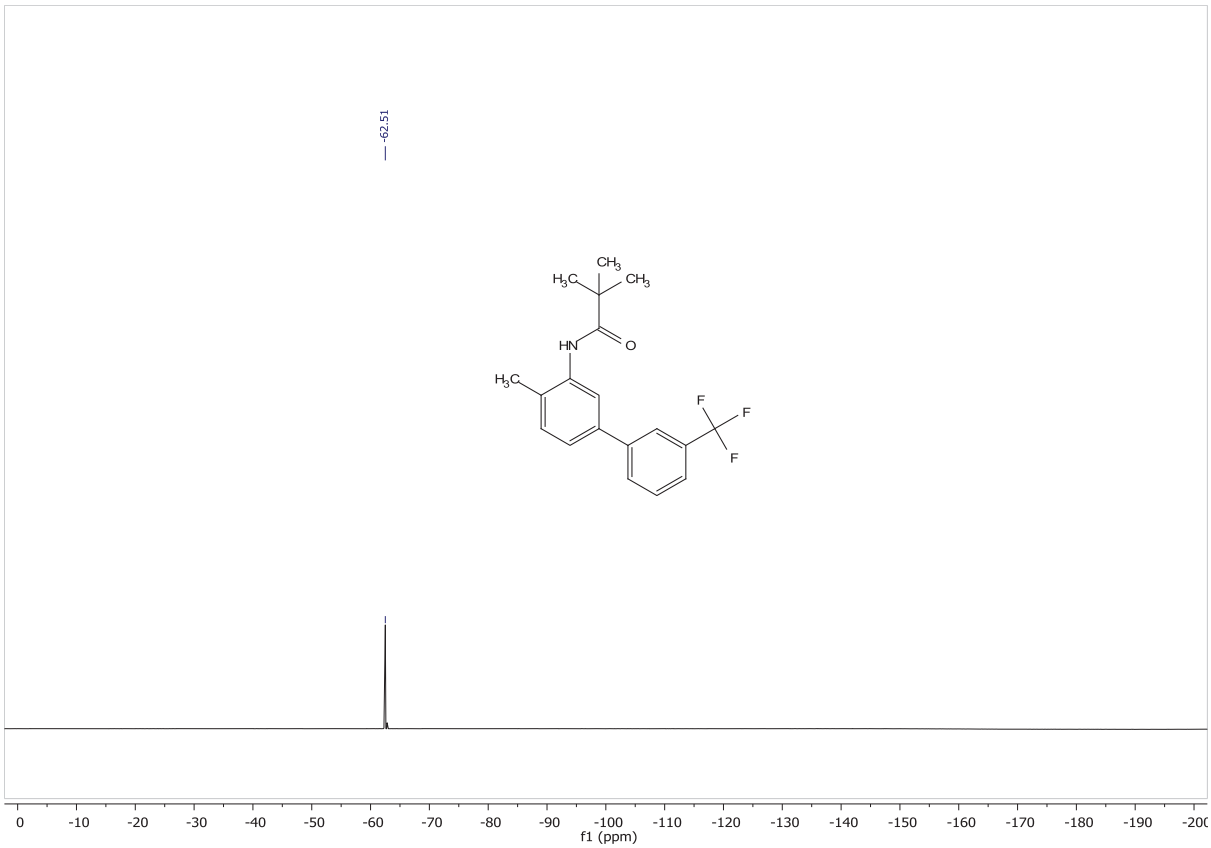
138.7
136.6
131.1
130.7
129.3
128.3
124.1
124.1
124.0
124.0
123.9
123.9
123.9
123.8
123.5
121.4
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
40.0
27.9
17.5
f1 (ppm)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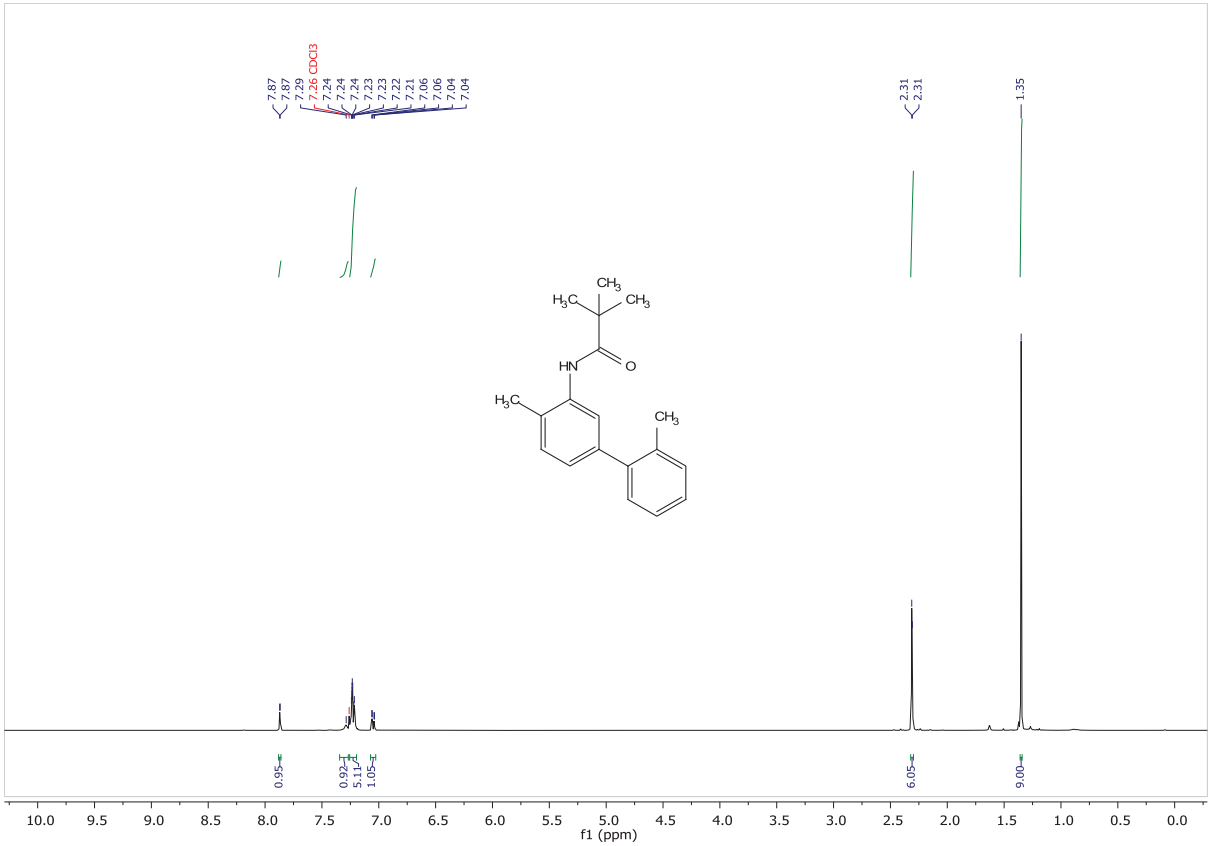
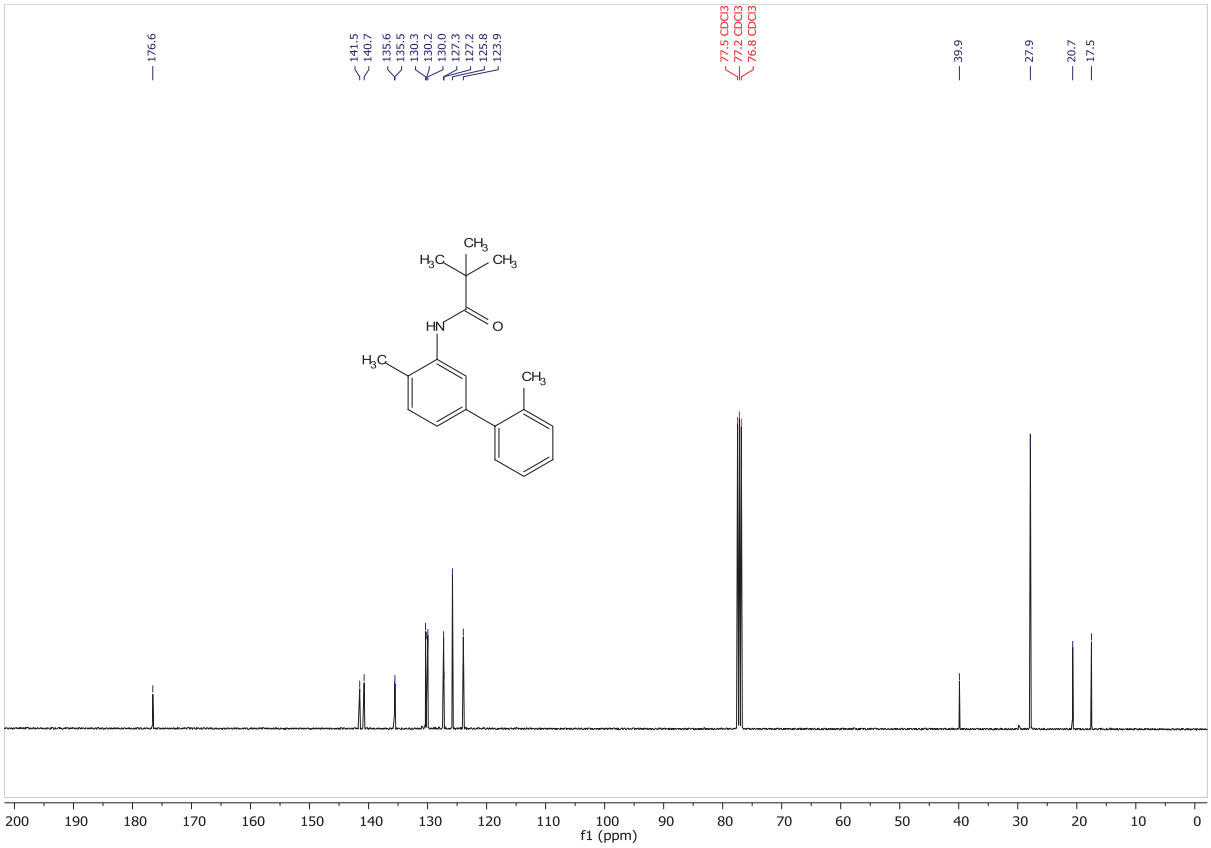
CH3
H3C
CH3
HN
O
H3C
F
F
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


7.87
7.87
7.29
7.26 CDCl3
7.24
7.24
7.24
7.23
7.23
7.22
7.21
7.06
7.06
7.04
7.04
2.31
2.31
1.35
CH3
H3C
CH3
HN
O
H3C
CH3
0.95
0.92
5.11
1.05
6.05
9.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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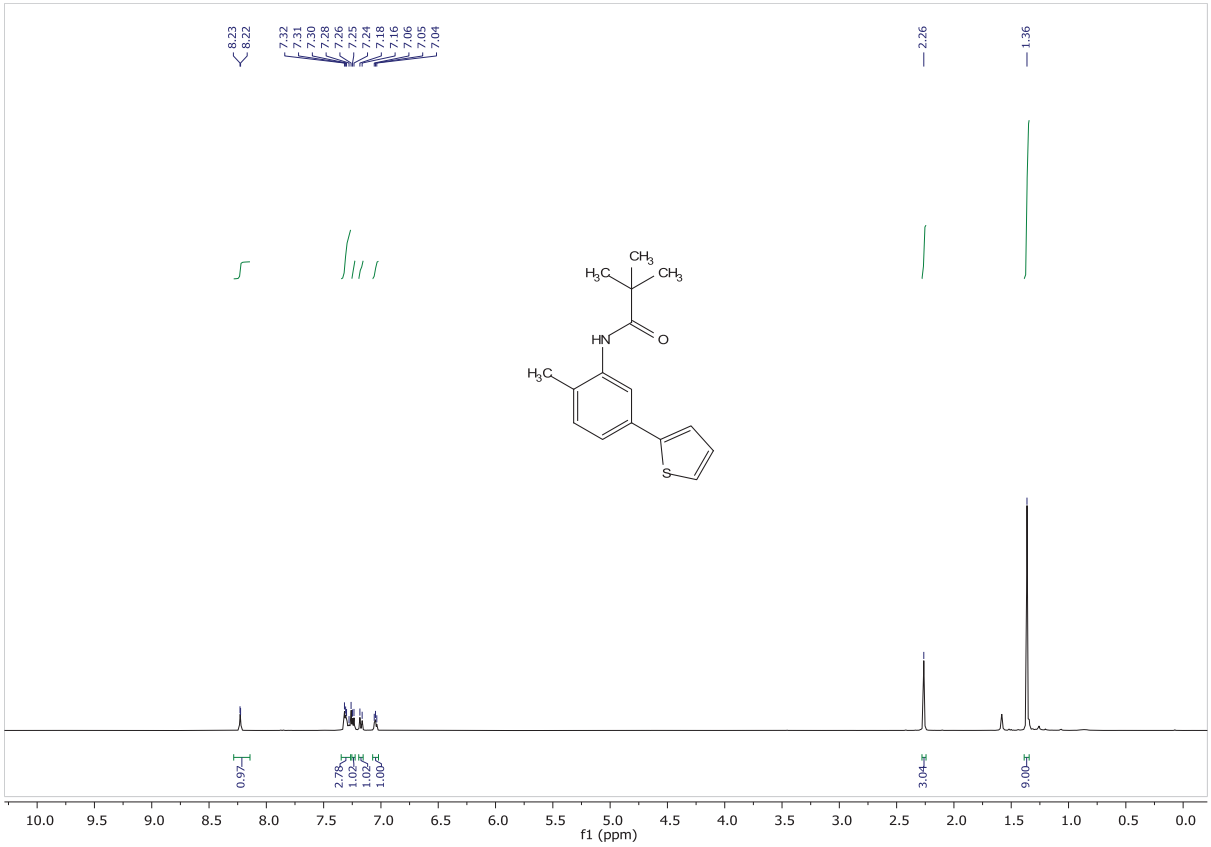
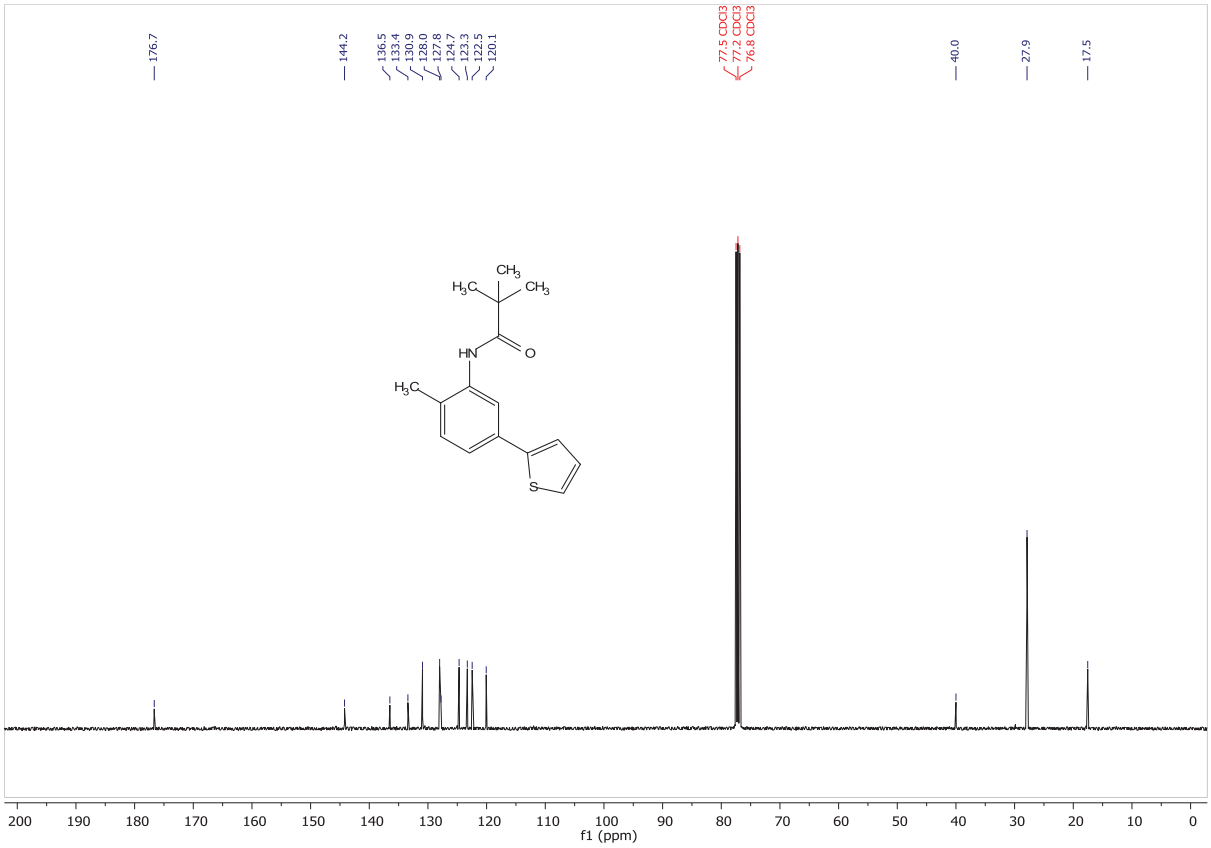
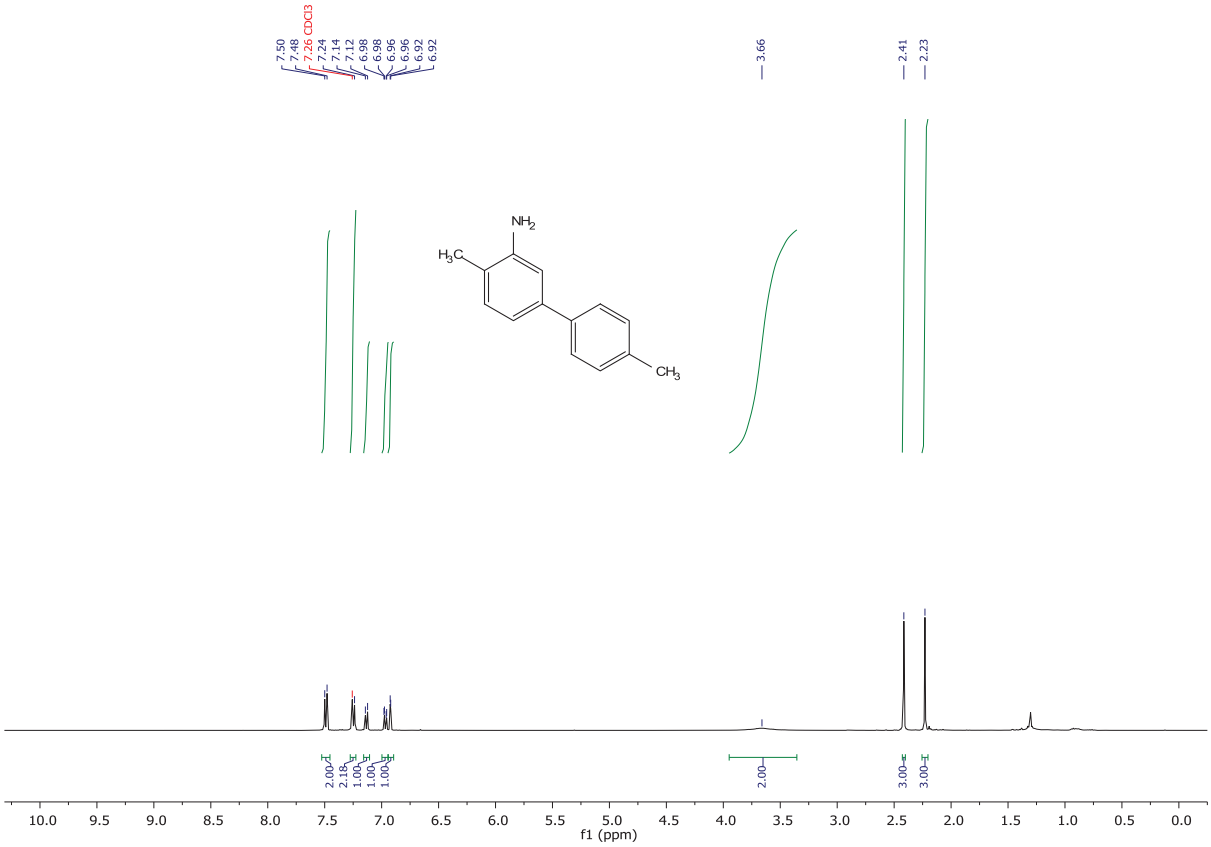
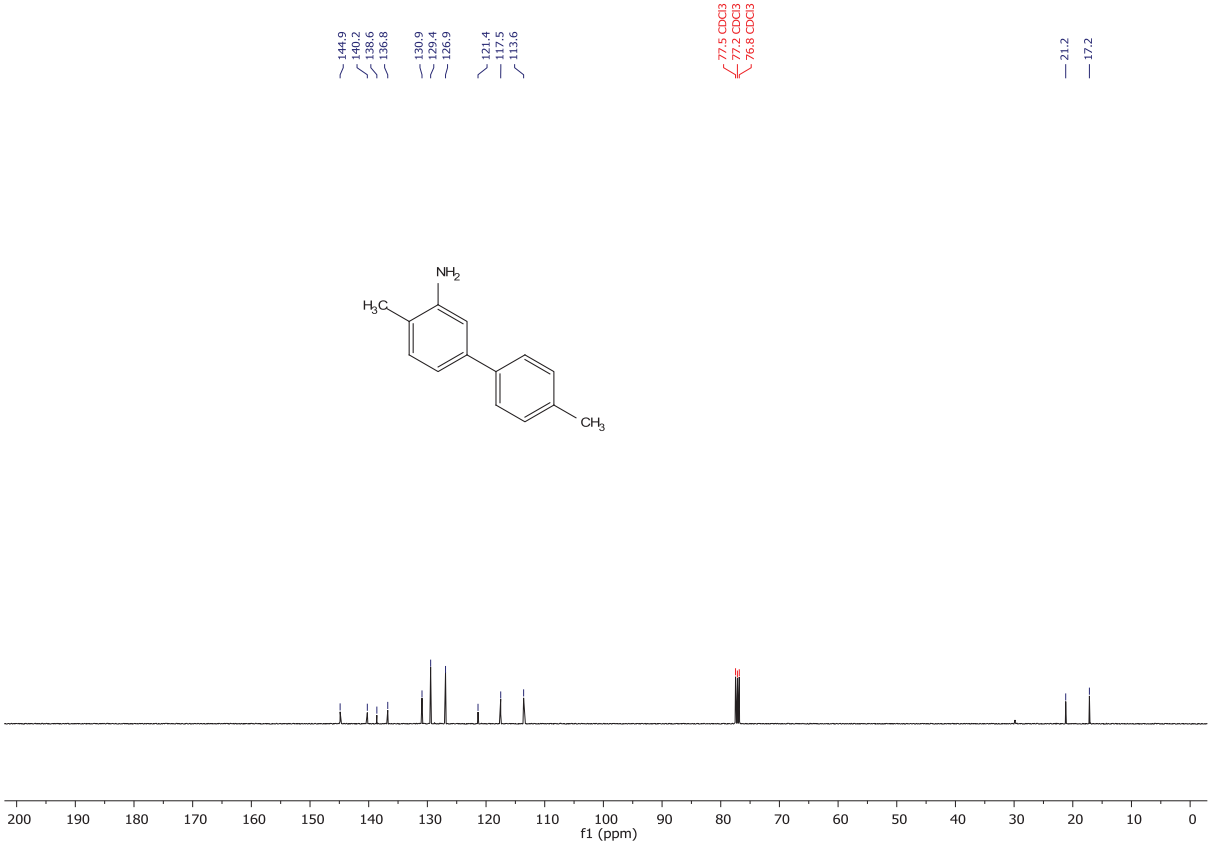
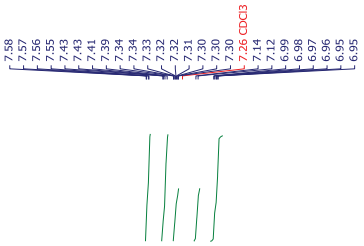
141.5
140.7
135.6
135.5
130.3
130.2
130.0
127.3
127.2
125.8
123.9
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
39.9
27.9
20.7
17.5
CH3
H3C
CH3
HN
O
H3C
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.23
8.22
7.32
7.31
7.30
7.28
7.26
7.25
7.24
7.18
7.16
7.06
7.05
7.04
2.26
1.36
CH3
H3C
CH3
HN
O
H3C
S
0.97
2.78
1.02
1.02
1.00
3.04
9.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


176.7
144.2
136.5
133.4
130.9
128.0
127.8
124.7
123.3
122.5
120.1
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
40.0
27.9
17.5
CH3
H3C
CH3
HN
O
H3C
S
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.50
7.48
7.26 CDCl3
7.24
7.14
7.12
6.98
6.98
6.96
6.96
6.92
6.92
3.66
2.41
2.23
NH2
H3C
CH3
2.00
2.18
1.00
1.00
1.00
2.00
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


144.9
140.2
138.6
136.8
130.9
129.4
126.9
121.4
117.5
113.6
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
21.2
17.2
NH2
H3C
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.58
7.57
7.56
7.55
7.43
7.42
7.41
7.38
7.34
7.34
7.33
7.32
7.32
7.31
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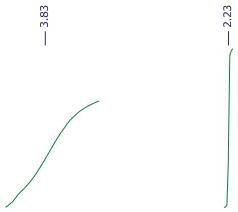
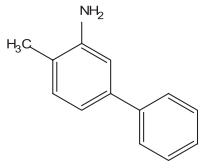
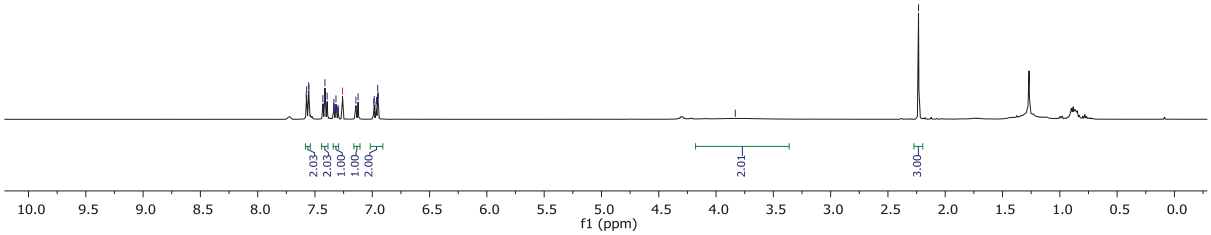
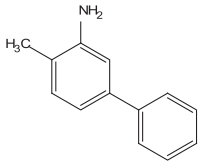
6.99
6.98
6.97
6.96
6.95
6.95

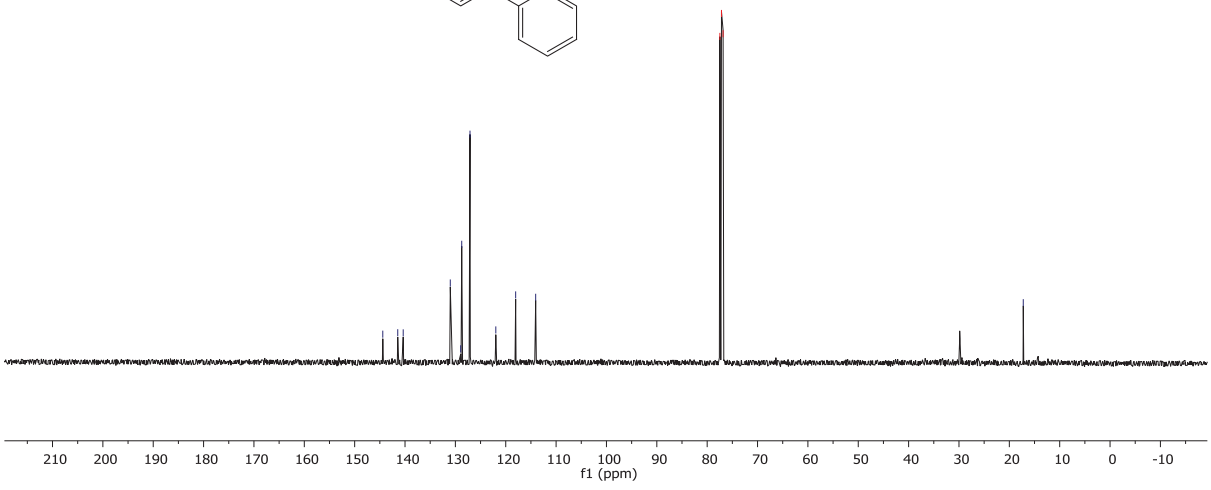

3.83
2.23

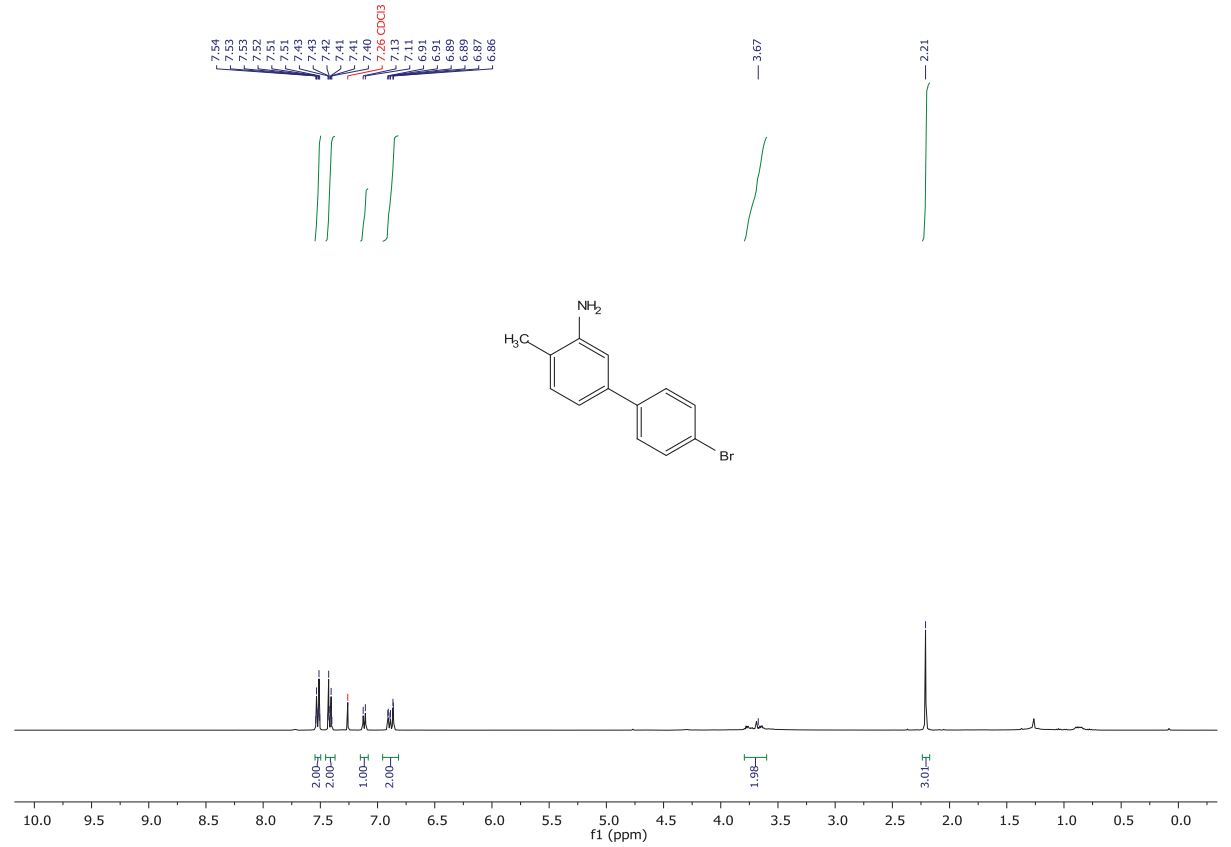

NH2
H3C


2.03
2.03
1.00
1.00
2.00
2.01
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


144.4
141.4
140.4
131.0
128.9
128.7
127.1
122.0
118.0
114.1
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
17.2


NH2
H3C


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


7.54
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7.53
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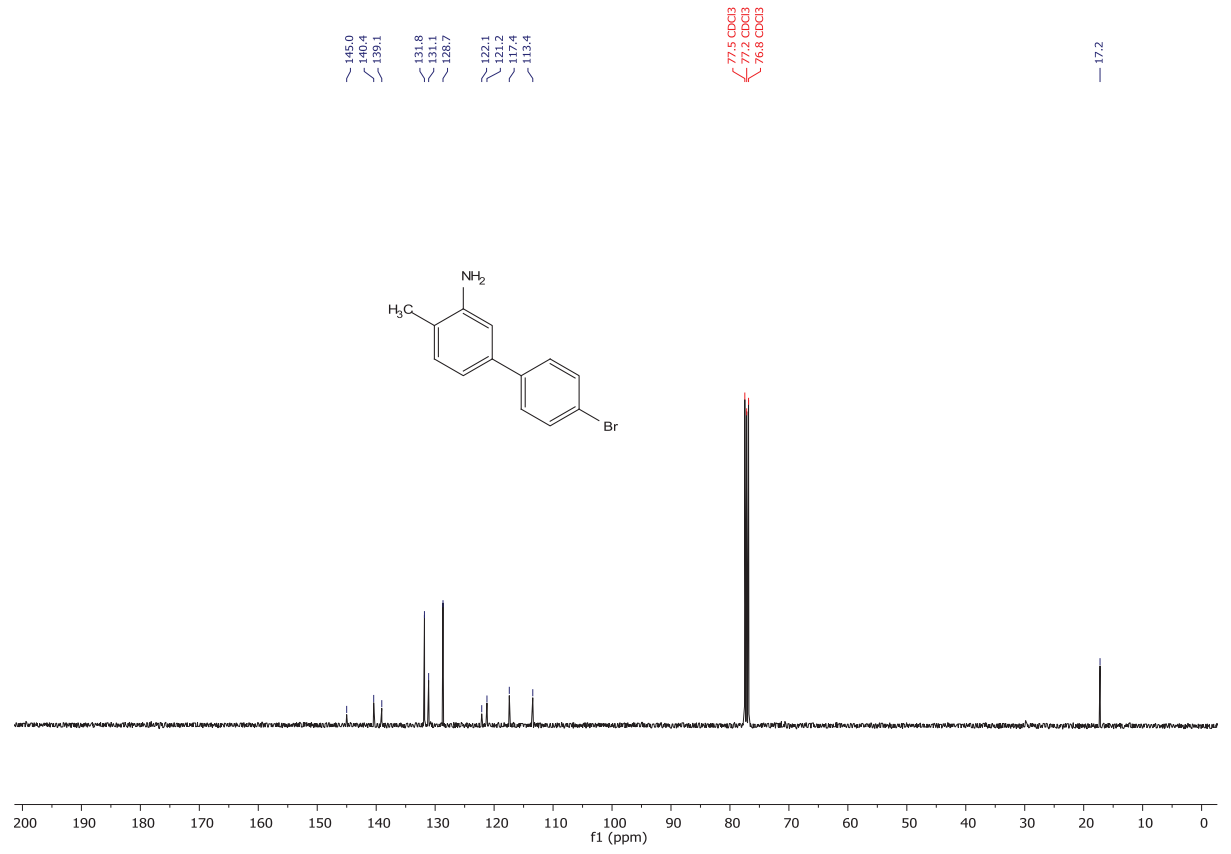
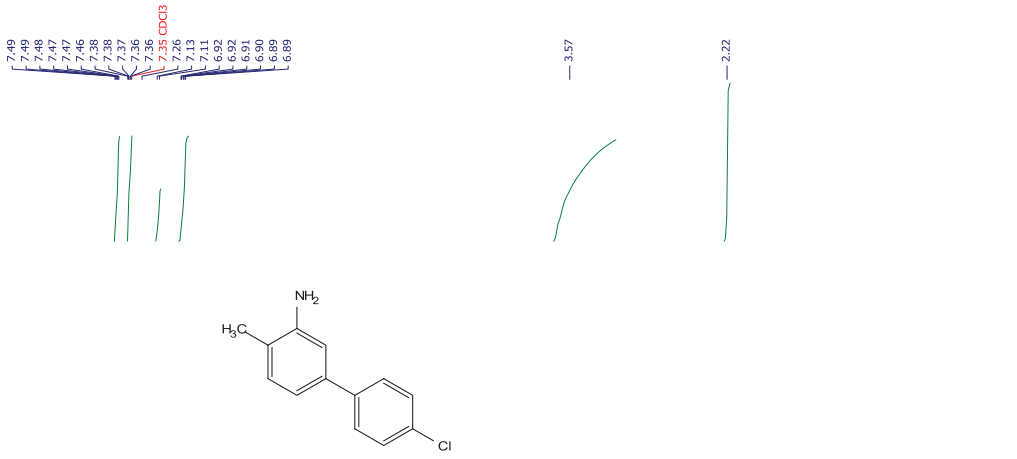
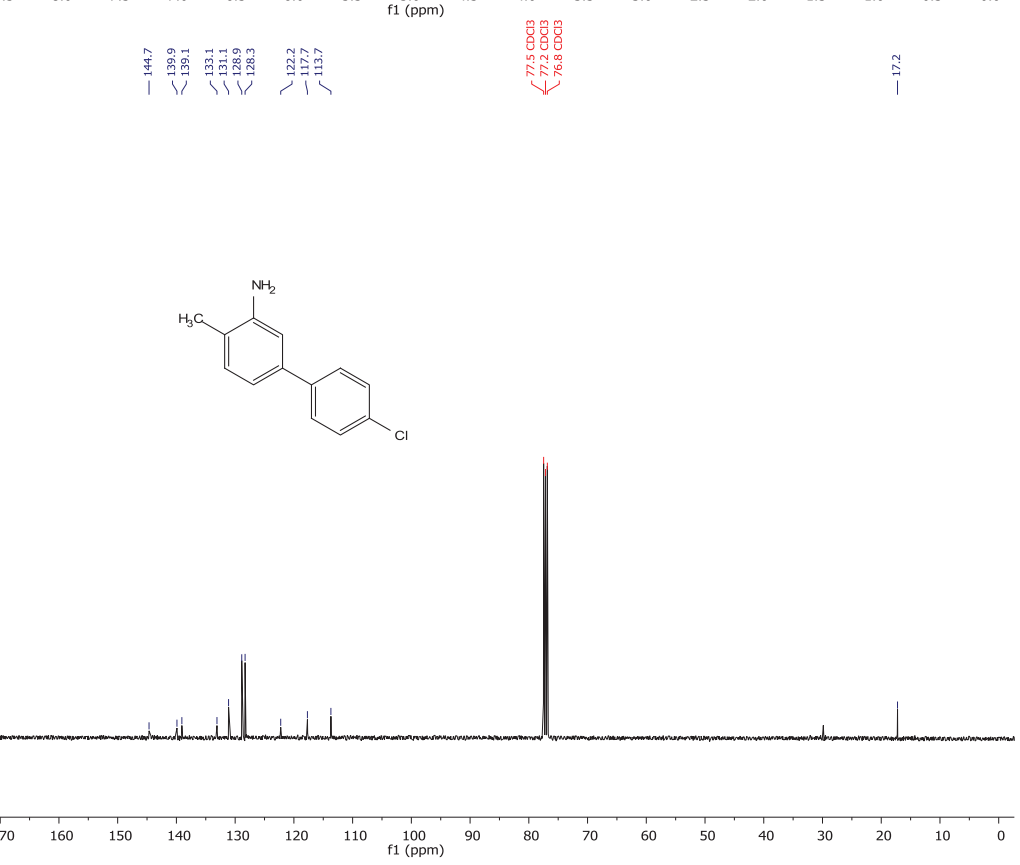
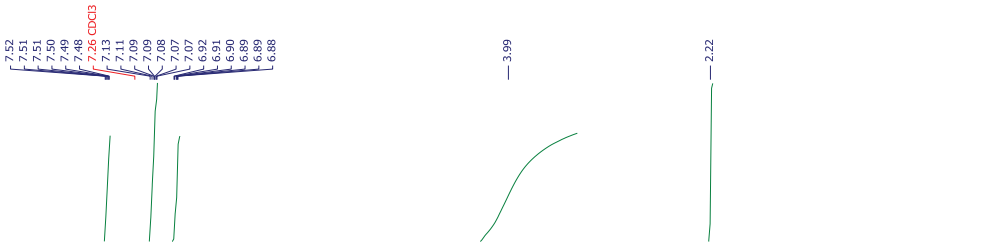
7.51
7.51
7.43
7.42
7.41
7.41
7.40
7.26 CDCl3
7.13
7.11
6.91
6.91
6.89
6.89
6.87
6.86
3.67
2.21
NH2
H3C
Br
2.00
2.00
1.00
2.00
1.98
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


145.0
140.4
139.1
131.8
131.1
128.7
122.1
121.2
117.4
113.4
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
17.2
NH2
H3C
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.49
7.49
7.48
7.47
7.47
7.46
7.38
7.38
7.37
7.36
7.36
7.35 CDCl3
7.26
7.13
7.11
6.92
6.92
6.91
6.90
6.89
6.89
3.57
2.22
NH2
H3C
Cl
2.00
2.00
1.00
2.00
1.93
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


144.7
139.9
139.1
133.1
131.1
128.9
128.3
122.2
117.7
113.7
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
17.2
NH2
H3C
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.52
7.51
7.51
7.50
7.49
7.48
7.26 CDCl3
7.13
7.11
7.09
7.09
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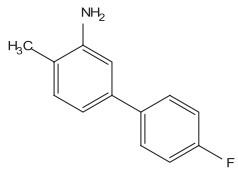
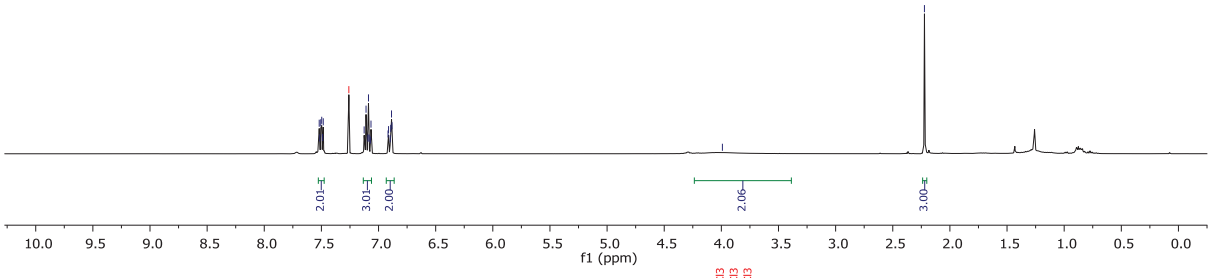
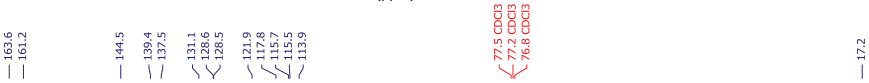
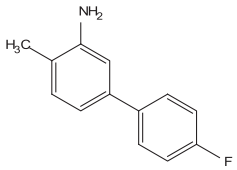
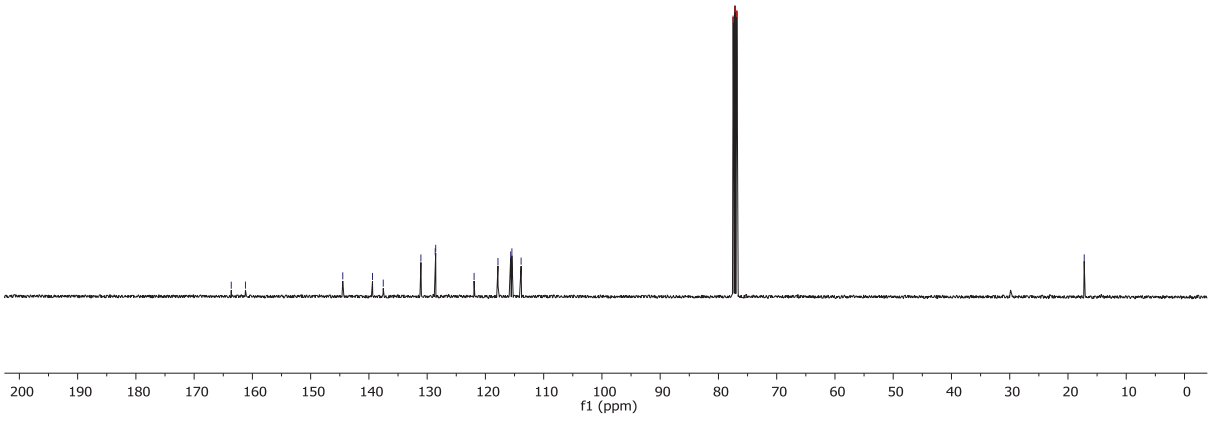
6.90
6.89
6.89
6.88
3.99
2.22


NH2
H3C
F

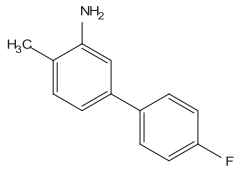

2.01
3.01
2.00
2.06
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

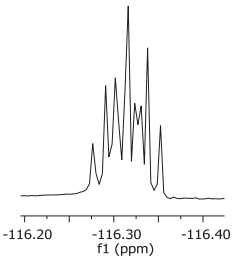

163.6
161.2
144.5
139.4
137.5
131.1
128.6
128.5
121.9
117.8
115.7
115.5
113.9
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
17.2

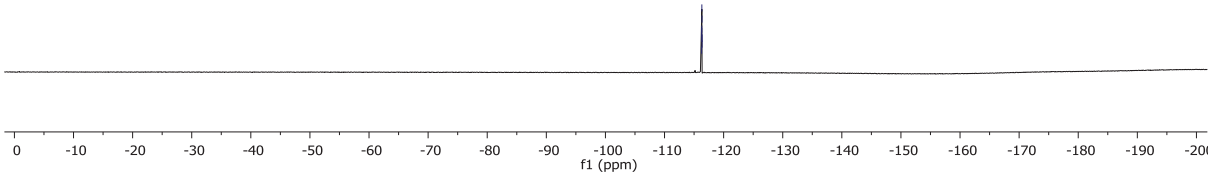

NH2
H3C
F

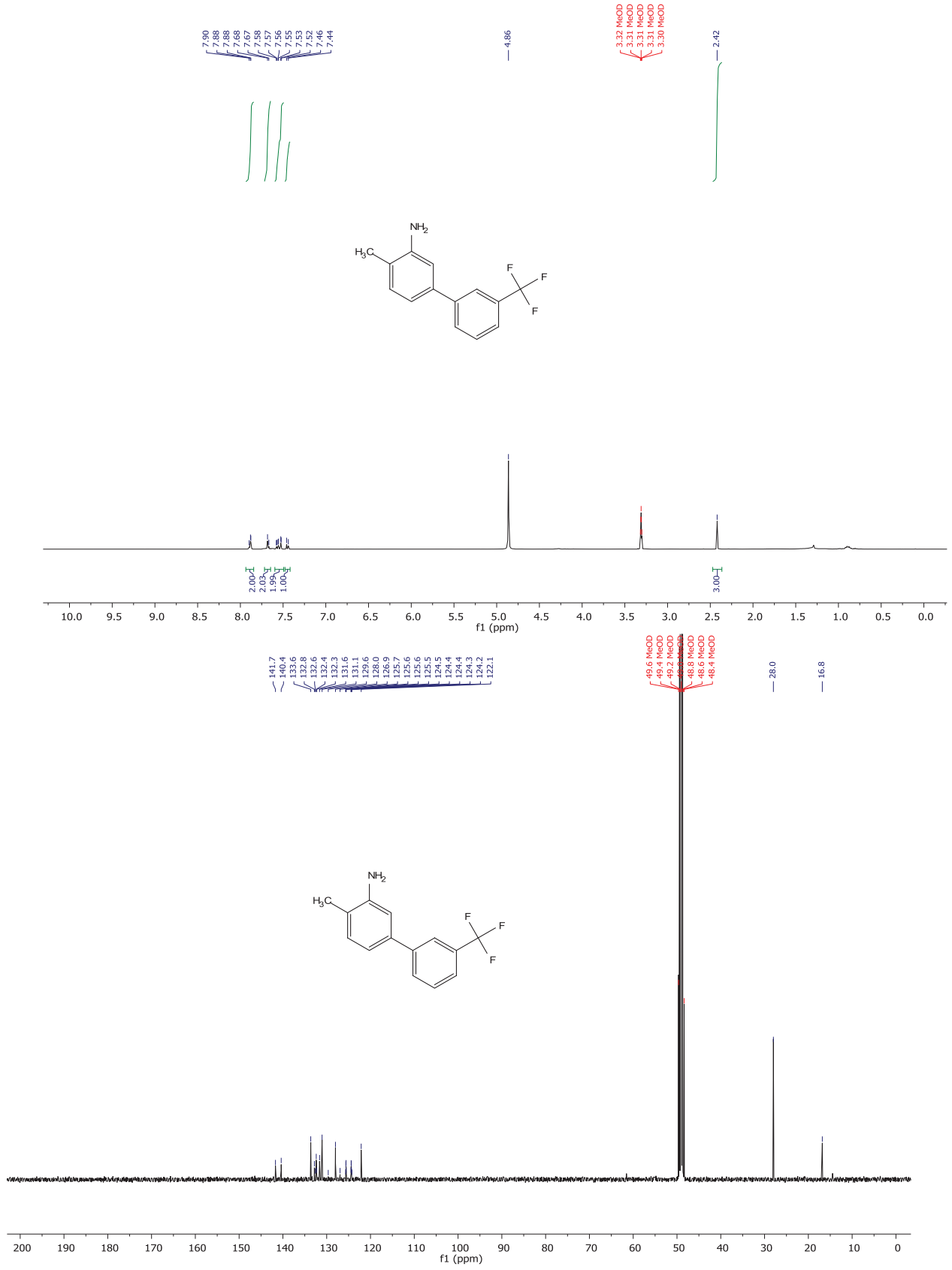

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

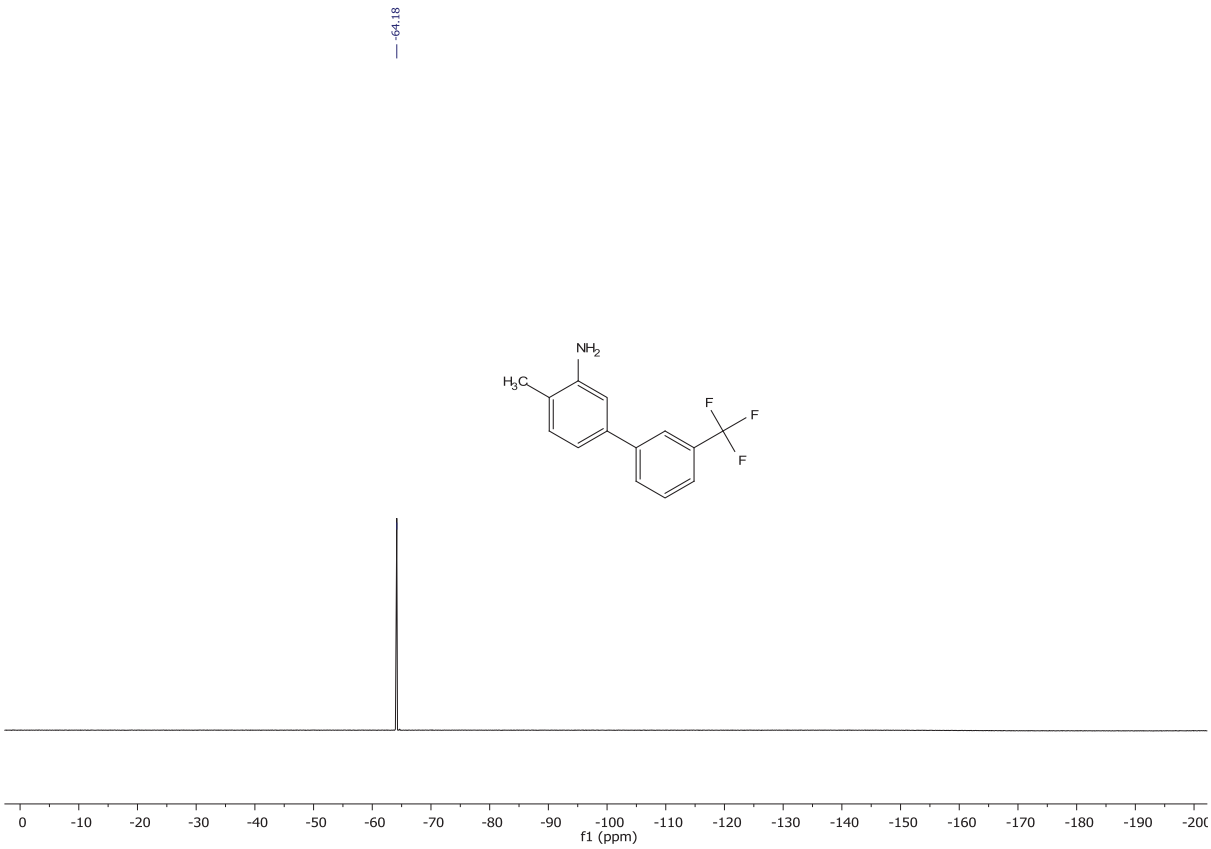

-116.3
-116.3
-116.3
-116.3
-116.3
-116.3
-116.3
-116.4


NH2
H3C
F

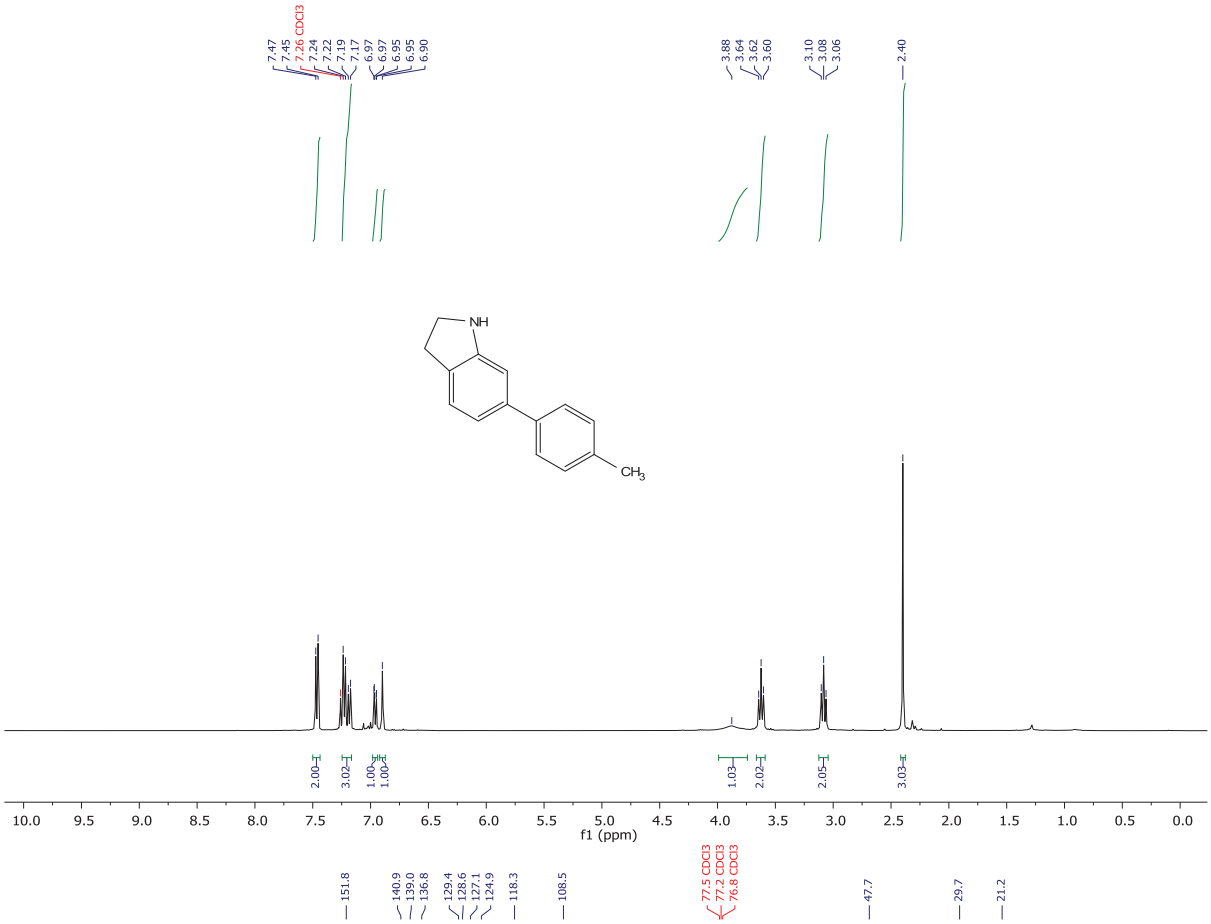

-116.20
-116.30
-116.40
f1 (ppm)

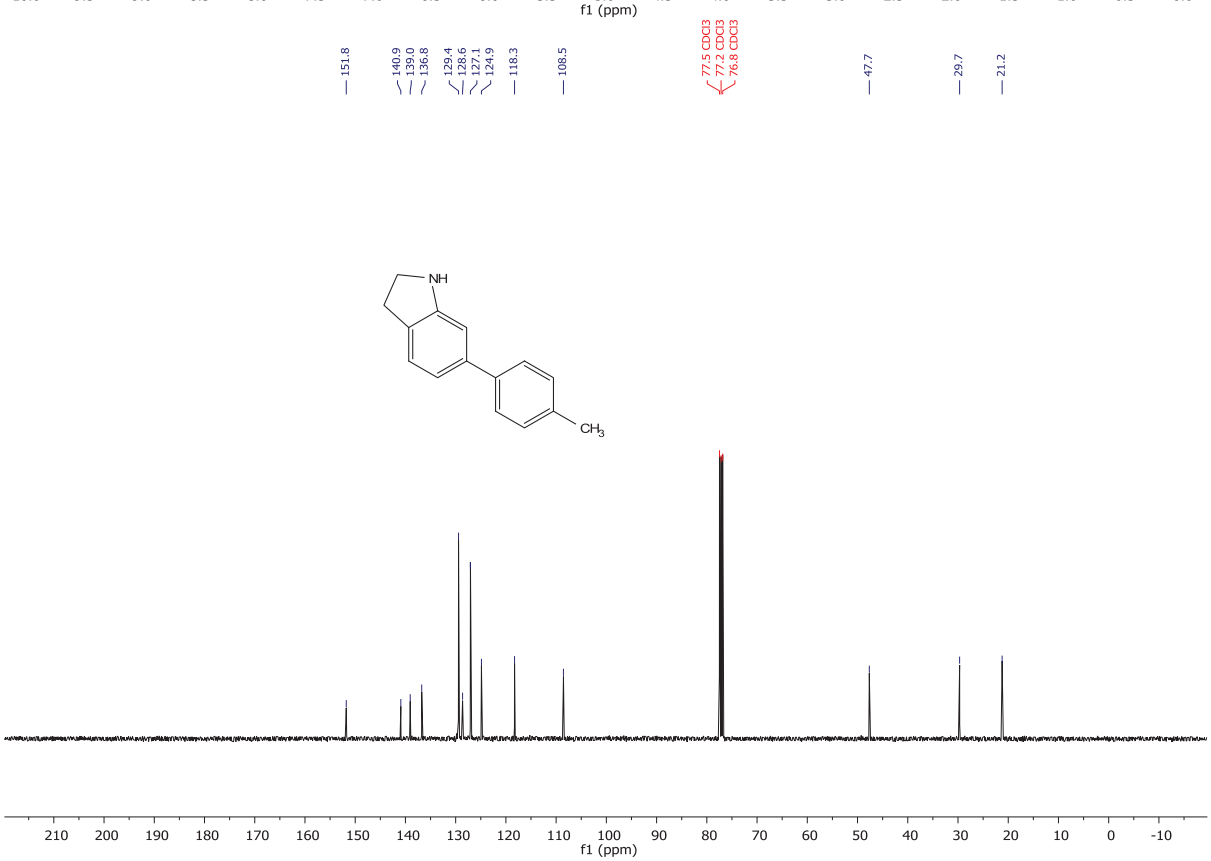

0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


7.90
7.88
7.88
7.68
7.67
7.58
7.57
7.56
7.55
7.53
7.52
7.46
7.44
4.86
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
2.42
NH2
H3C
F
F
F
2.00
2.03
1.99
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
141.7
140.4
133.6
132.8
132.6
132.4
132.3
131.6
131.1
129.6
128.0
126.9
125.7
125.6
125.6
125.5
124.5
124.4
124.4
124.3
124.2
122.1
49.6 MeOD
49.4 MeOD
49.2 MeOD
48.8 MeOD
48.6 MeOD
48.4 MeOD
28.0
16.8
NH2
H3C
F
F
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-64.18
NH2
H3C
F
F
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


7.44
7.44
7.43
7.42
7.26 CDCl3
7.22
7.20
6.96
6.95
6.94
6.94
6.86
6.83
3.89
3.79
2.38
NH2
O
H3C
CH3
2.00
2.03
2.00
1.02
3.00
1.64
3.01
f1 (ppm)
146.9
138.5
137.0
136.4
134.4
129.4
126.8
117.2
113.8
110.8
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
55.8
21.2
f1 (ppm)


7.47
7.45
7.26 CDCl3
7.24
7.22
7.19
7.17
6.97
6.97
6.95
6.95
6.90
3.88
3.64
3.62
3.60
3.10
3.08
3.06
2.40
NH
CH3
2.00
3.02
1.00
1.00
1.03
2.02
2.05
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


151.8
140.9
139.0
136.8
129.4
129.6
127.1
124.9
118.3
108.5
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
47.7
29.7
21.2
NH
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)