

Supporting Information

Novel Peptoid Building Blocks: Synthesis of Functionalized Aromatic Helix-Inducing Submonomers

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1. General Methods.

Biotage SPITM purification system and flash cartridges were used for flash column chromatography. Thin-layer chromatography was carried out on precoated aluminum-backed TLC sheets (silica gel 60 F₂₅₄, EMD chemicals, San Diego, CA). Compounds were visualized with a ninhydrin spray reagent or a UV/vis lamp. ¹H and ¹³C NMR spectra were recorded on a Bruker 500 MHz NMR spectrometer. Chemical shifts were reported as δ values in parts per million downfield from TMS (δ 0.0) as the internal standard in CDCl₃. All reagents were purchased from Sigmaaldrich, Fisher and Novabiochem. They were used without further purification unless stated otherwise. (*R*)-(+)-*tert*-Butanesulfinamide was purchased from Advanced Asymmetrics, Inc., IL, USA. (*S*)- α -Methyl-4-nitrobenzylamine hydrochloride was purchased from TCI America, OR, USA. *N,N'*-Diisopropylcarbodiimide was purchased from Advanced ChemTech, KY, USA.

The peptoid oligomers were synthesized by solid-phase submonomer method on solid support using an automated synthesis (Aapptec Apex 396 parallel synthesizer, Louisville, KY, USA) or a manual synthesis. Rink amide resin (0.60 mmol/g, Novabiochem, San Diego, CA, USA) was used to generate C-terminal amide peptoids. After Fmoc deprotection, each monomer was added by a series of bromoacetylation and displacement by a primary amine. These two steps were iterated with appropriate primary amines until desired peptoid sequence was obtained. Typically, 0.06 mmol reaction scale was used (0.1 g of the resin). For bromoacetylation, the addition of bromoacetic acid (1 mL, 1.2 M in DMF, 1.2 mmol) followed by *N,N'*-diisopropylcarbodiimide (0.15 mL, neat, 1.0 mmol), and then agitation at room temperature for 20 min were performed. For the displacement reaction, primary amine (1 mL, 1.2 M in NMP or *N*-methylpyrrolidone) was added, and the reactor was agitated at room temperature for 1 h. The resin was washed with DMF (6 mL \times 5) between each step. *N*-Terminal acetylation was performed manually by adding acetic anhydride (0.12 mL, 1.3 mmol) and pyridine (0.13 mL, 1.6 mmol) to the resin-bound peptoid in DMF (1 mL). The reaction was continued at room temperature for 2 hours. Peptoid **20** was cleaved from the resin with 42.5:50:5:2.5 TFA/CH₂Cl₂/water/triisopropylsilane (v/v/v/v) for 5 minutes at room temperature. Other peptoids

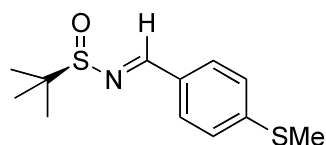
were cleaved with 95:2.5:2.5 TFA/water/triisopropylsilane (v/v/v) for 10 - 20 minutes at room temperature (i.e. longer TFA treatment was applied for *tert*-butyl ester deprotection). The cleavage solution was filtered by solid-phase extraction (SPE) cartridges (Applied Separations, Allentown, PA, USA) and the volatiles were removed by a stream of nitrogen. The crude peptoid was dissolved in acetonitrile and analyzed by ESI, MALDI-TOF, and analytical HPLC.

LC-MS data were obtained using an Agilent Technologies 1100 Series and LC/MSD Trap XCT system (Agilent Technologies, Santa Clara, CA, USA). Vydac C4 column was used with mobile phase of water (0.1% TFA) and acetonitrile (0.1% TFA). The MALDI-TOF mass spectra were obtained by an Applied Biosystems 4800 MALDI TOF/TOF Analyzer system (Applied Biosystems, Foster City, CA, USA). α -Cyano-4-hydroxycinnamic acid (5 mg/mL in CH₃CN/H₂O = 1:1 with 0.1% TFA) was used as the matrix. Analytical HPLC was performed on a Varian modular HPLC system (ProStar 210 solvent delivery system, ProStar 325 UV-Vis dual wavelength detector, autosampler model 430, and column oven model 510). Sample purity was monitored by absorbance at 220 nm. Grace Vydac protein & peptide C18 column (cat #: 218TP5415) was used for the analytical HPLC. The peptoids were purified by preparative HPLC system (Varian ProStar 210 solvent delivery system, ProStar 345 UV-Vis detector, fraction collector model 210) using a C18 column [Varian Dynamax, 250×21.4 mm, Omnispher 5] at a flow rate of 10 mL/min. Sample elution was detected by absorbance at 220 nm. The mobile phase was used as follows: (A, water + 0.1% TFA; B, CH₃CN + 0.1% TFA) 5 min using 5% B, then a gradient to 99% B over 35 min, 5 min using 99% B, and then a gradient to 5% B over 5 min. For peptoid **20 - 22**, acetonitrile and water were degassed and TFA was added. The purity of the product fractions were confirmed by analytical HPLC, and fractions containing pure product were collected, lyophilized, and stored at -80 °C.

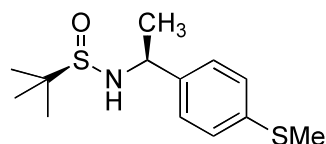
Circular dichroism measurements were carried out at 25 °C with a Jasco J-815 circular dichroism spectrometer (Jasco, Inc., Easton, MD, USA). CD spectra were obtained in a 1 mm pathlength quartz cell and recorded from 190 to 260 nm in 1 nm increments with a scanning speed of 20 nm/min and a response time of 4 second. Three scans for each sample were averaged. Stock

solutions of peptoids (1 - 5 mM in acetonitrile) were used, and appropriate dilutions were made immediately before the measurements. Sample concentrations were in the range of 46 - 50 μ M. Data are expressed in terms of per-residue molar ellipticity ($\text{deg cm}^2/\text{dmol}$) calculated per number of amides in a molecule.

2. Synthesis of Submonomers 6, 11, and 12.

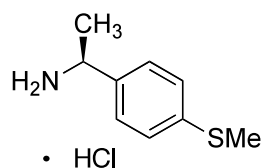


(*R, E*)-*N*-[4-(methylthio)benzylidene]-*tert*-butanesulfonamide (2). To a mixture of (*R*)-(+)-*tert*-butanesulfonamide (**1**, 500 mg, 4.12 mmol) and 4-(methylthio)benzaldehyde (691 mg, 4.54 mmol) in dry THF (10 mL) under nitrogen was added $\text{Ti}(\text{OEt})_4$ (2.07 g, 9.07 mmol) dropwise. After stirring for overnight, the reaction mixture was poured into brine (10 mL). The resulting white suspension was filtered through Celite, and the filter cake was washed twice with EtOAc (10 mL). The filtrate was transferred to a separatory funnel where the organic layer was washed with brine. The aqueous solution was extracted twice with EtOAc (20 mL), and the combined organic solution was dried over Na_2SO_4 , filtered, and concentrated in vacuo. The residue was recrystallized in EtOAc/hexane to afford **2** (989 mg, 94%) as a white solid. $R_f = 0.2$ (hexane/EtOAc = 10 : 1); ^1H NMR (500 MHz, CDCl_3) δ 8.52 (s, 1H), 7.75 (d, $J = 8.5$ Hz, 2H), 7.28 (d, $J = 8.5$ Hz, 2H), 2.52 (s, 3H), 1.25 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ 161.9, 145.0, 130.7, 129.6, 125.6, 57.8, 22.6, 14.9.

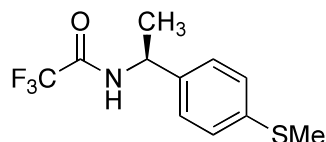


(*R,S*)-*N*-{1-[4-(methylthio)phenyl]ethyl}-*tert*-butanesulfonamide (3). To a solution of **2** (0.32 g, 1.25 mmol) in dry CH_2Cl_2 (7 mL) was slowly added methylmagnesium bromide (3.0 M in ether, 0.83 mL) at -78 $^\circ\text{C}$. The mixture was stirred at -78 $^\circ\text{C}$ for 1 h under nitrogen and then allowed to warm to room temperature and stirred for additional 1 h. The reaction was quenched by slowly adding saturated NH_4Cl aqueous solution (3 mL) at 0 $^\circ\text{C}$, and the aqueous layer was extracted twice with

EtOAc (10 mL). The combined organic solution was dried over Na₂SO₄, filtered, and concentrated in vacuo. The residue was recrystallized in EtOAc/hexane to afford **3** (323 mg, 95%) as a white needle-shaped solid. *R_f* = 0.1 (hexane/EtOAc = 3 : 1); ¹H NMR (500 MHz, CDCl₃) δ 7.24 (m, 4H), 4.53 (q, *J* = 3.5 Hz, 1H), 3.29 (d, *J* = 3.0 Hz, 1H), 2.48 (s, 3H), 1.51 (d, *J* = 7.0 Hz, 3H), 1.19 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 140.3, 137.6, 127.5, 126.6, 55.5, 54.2, 25.1, 22.6, 15.8; MS (ESI, CH₃CN) [M+H⁺] = 271.5.

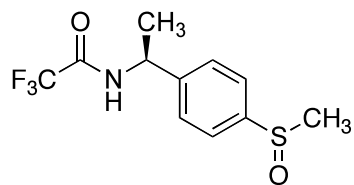


(S)-1-[4-(methylthio)phenyl]ethan-1-amine hydrochloride (3-S1). To a solution of **3** (1.03 g, 3.79 mmol) in MeOH (1 mL) was slowly added 4 M HCl in 1,4-dioxane solution (7 mL) at 0 °C. The mixture was stirred at room temperature for 45 min. The volume of the reaction mixture was reduced by evaporation, and diethyl ether was added to precipitate the product. The white precipitate was then filtered and washed with ether (10 mL) three times to provide **3-S1** (770 mg, 99%) as a white crystalline solid. *R_f* = 0.2 (EtOAc/MeOH = 1 : 1); ¹H NMR (500 MHz, D₂O) δ 7.37 (m, 4H), 4.49 (q, *J* = 7.0 Hz, 1H), 2.47 (s, 3H), 1.60 (d, *J* = 7.0 Hz, 3H).

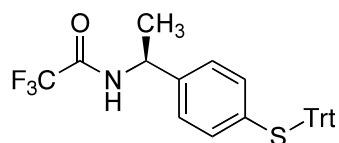


(S)-N-[1-[4-(methylthio)phenyl]ethyl]trifluoroacetamide (4). To a solution of **3-S1** (0.57 g, 3.41 mmol) in anhydrous CH₂Cl₂ (20 mL) was added ethyl trifluoroacetate (1.45 g, 10.2 mmol) followed by triethylamine (1.03 g, 10.2 mmol). The reaction mixture was stirred for 16 h under nitrogen and concentrated under reduced pressure. The residue was dissolved in EtOAc (30 mL), washed three times with brine (15 mL), and dried over Na₂SO₄. After evaporation of the organic solvent, the residue was recrystallized in hot hexane/CH₂Cl₂ solution to provide **4** (0.77 g, 86%) as a white needle-shaped solid. *R_f* = 0.3 (hexane/EtOAc = 10 : 1); ¹H NMR (500 MHz, CDCl₃) δ 7.23 (m, 4H), 6.35 (s, 1H), 5.09 (m, 1H), 2.46 (s, 3H), 1.56 (d, *J* = 6.5 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 156.4, 138.8,

137.6, 127.0, 126.7, 116.9, 49.4, 20.9, 15.7.

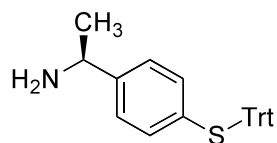


(S)-N-{1-[4-(methylsulfinyl)phenyl]ethyl}trifluoroacetamide (4-S1). Compound **4** (5.15 g, 19.6 mmol) was dissolved in CH₃CN (99.8% anhydrous, Aldrich, 20 mL) and THF (99.9% anhydrous, Aldrich, 40 mL), and to this solution was added Selectfluor (F-TEDA•BF₄, 7.62 g, 21.5 mmol) in CH₃CN (99.8% anhydrous, Aldrich, 10 mL) and H₂O (miliQ, 6 mL) dropwise at 0 °C. After a stirring time of 30 minutes at room temperature, the mixture was concentrated and redissolved in a mixture of EtOAc (50 mL) and 5% aqueous NaHCO₃ (50 mL). The organic phase was washed with brine, dried over Na₂SO₄, filtered and concentrated. The residue was dried under high vacuum pump overnight, and the resulting white solid was recrystallized in hot hexane/EtOAc solution to provide **4-S1** (5.18 g, 95%). **Caution.** This reaction was successful only when the highly pure solvents were used. *R_f* = 0.4 (EtOAc); ¹H NMR (500 MHz, CDCl₃) δ 8.15 and 8.16 (2 × s, 1H), 7.41 – 7.50 (m, 4H), 5.13 (m, 1H), 2.64 and 2.65 (2 × s, 3H), 1.53 – 1.55 (m, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 156.6, 145.1, 145.0, 144.7, 127.4, 127.3, 124.1, 124.0, 117.1, 49.2, 49.2, 43.7, 21.1, 20.9; MS (ESI, CH₃CN) [M+H⁺] = 279.5. The NMR data showed the presence of sulfoxide diastereomers.

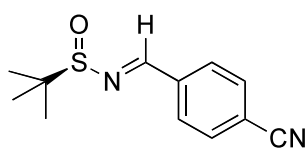


(S)-N-{1-[4-(tritylthio)phenyl]ethyl}trifluoroacetamide (5). A solution of sulfoxide **4-S1** (4.33 g, 15.5 mmol) and 2,6-lutidine (5.15 g, 48.1 mmol) in freshly distilled THF (150 mL) was cooled to -78 °C. To this solution was added trifluoroacetic anhydride (9.77 g, 46.5 mmol) dropwise, and the stirring continued for 1.5 h at -78 °C under nitrogen. After evaporation of volatile components in the reaction mixture, a precooled mixture (0 °C) of triethylamine (25 mL) and methanol (25 mL) was added to the residue. The solution was allowed to warm to room temperature, stirred for 40 min, and then concentrated under reduced pressure. The residue was dissolved in CH₂Cl₂ (100 mL) and

extracted with saturated NH_4Cl (100 mL). The organic layer was separated, dried under Na_2SO_4 , and concentrated to dryness giving an oily residue. Thin layer chromatography showed the free thiol spot as $R_f = 0.3$ (hexane/EtOAc = 3 : 1). Without purification, the aromatic thiol was dissolved in freshly distilled CH_2Cl_2 (150 mL), and to this solution was added trityl chloride (8.64 g, 31.0 mmol) and pyridine (2.45 g, 31.0 mmol). The reaction mixture was stirred for 2 days at room temperature under nitrogen, and washed successively with water (100 mL), 5% NaHCO_3 (100 mL), and brine (2 x 100 mL), and dried over Na_2SO_4 . The solution was concentrated in vacuo until white solid precipitated out, and the precipitate was filtered. The crude solid product was recrystallized in hot CH_2Cl_2 three times to provide **5** (5.64 g, 74%) as a white solid. $R_f = 0.6$ (hexane/EtOAc = 3 : 1); ^1H NMR (500 MHz, CDCl_3) δ 7.42 – 7.44 (m, 6H), 7.21 – 7.27 (m, 9H), 6.96 – 6.97 (m, 4H), 6.33 (d, $J = 5.5$ Hz, 1H), 5.04 (m, 1H), 1.50 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 156.0, 144.4, 140.2, 134.9, 134.7, 130.0, 127.7, 126.8, 125.8, 116.9, 71.0, 49.3, 20.9; MS (ESI, CH_3CN) $[\text{M}+\text{Na}^+] = 513.7$.

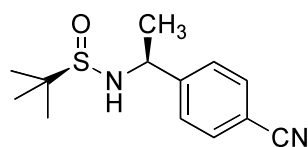


(S)-1-[4-(tritylthio)phenyl]ethylamine (6). To a stirred ice-cold solution of **5** (3.68 g, 7.49 mmol) in MeOH (20 mL) and THF (30 mL) under nitrogen was added 2.0 M aq. LiOH (30 mL) dropwise, and the mixture was stirred at room temperature for 3 h. After evaporation of organic solvents under reduced pressure, the aqueous solution was extracted three times with EtOAc (70 mL). The organic extract was washed with brine, dried over Na_2SO_4 , filtered, and evaporated. A yellowish solid was obtained (2.94 g, 99%). $R_f = 0.25$ (EtOAc/MeOH = 1 : 1); ^1H NMR (500 MHz, CDCl_3) δ 7.45 – 7.50 (m, 6H), 7.21 – 7.35 (m, 9H), 7.01 – 7.02 (m, 2H), 6.95 – 6.98 (m, 2H), 3.98 – 4.02 (m, 1H), 1.73 (br s, 2H), 1.31 (d, $J = 6.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 147.6, 144.6, 135.0, 132.4, 130.1, 127.7, 126.7, 125.5, 70.8, 50.9, 25.6; MS (ESI, CH_3CN) $[\text{M}+\text{Na}^+] = 417.9$.

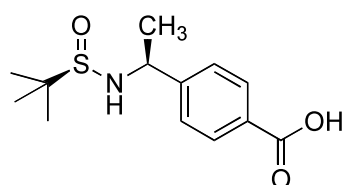


(R, E)-N-(4-cyanobenzylidene)-tert-butanesulfinamide (7). To a mixture of (*R*)-(+)-tert-

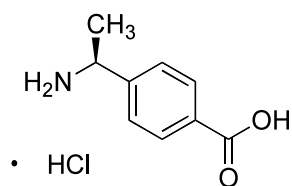
butanesulfonamide (**1**, 20 g, 165 mmol) and 4-cyanobenzaldehyde (22 g, 167 mmol) in freshly distilled THF (500 mL) under nitrogen was slowly added titanium ethoxide (50 g, 219 mmol). After stirring for overnight, the reaction mixture was poured into brine (500 mL). The resulting white suspension was filtered through Celite, and the filter cake was washed twice with EtOAc (100 mL). The filtrate was transferred to a separatory funnel where the organic layer was washed with brine. The aqueous solution was extracted twice with EtOAc (100 mL), and the combined organic solution was dried over Na₂SO₄, filtered, and concentrated in vacuo. The residue was recrystallized in EtOAc/hexane to afford **7** (35 g, 91%) as a white solid. $R_f = 0.35$ (hexane/EtOAc = 3 : 1); ¹H NMR (500 MHz, CDCl₃) δ 8.60 (s, 1H), 7.93 – 7.95 (m, 2H), 7.75 – 7.77 (m, 2H), 1.26 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 161.1, 137.4, 132.8, 129.6, 118.1, 115.5, 58.4, 22.7.



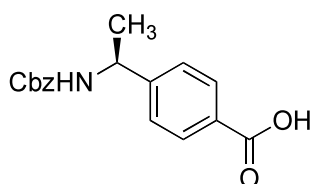
(*R,S*)-*N*-[1-(4-cyanophenyl)ethyl]-*tert*-butanesulfonamide (8**)**. To a solution of **7** (19.8 g, 85 mmol) in dry CH₂Cl₂ (500 mL) was added methylmagnesium bromide (3.0 M in ether, 35 mL) at -78 °C. The mixture was stirred at -78 °C for 1 h under nitrogen and then allowed to warm to room temperature and stirred for additional 1 h. The reaction was quenched by slow addition of saturated NH₄Cl aqueous solution at 0 °C, and the aqueous layer was extracted twice with EtOAc (350 mL). The combined organic solution was dried over Na₂SO₄, filtered, and concentrated in vacuo. Compound **8** was obtained as an oily residue (18.0 g, 85%) and used for the next reaction without further purification. $R_f = 0.25$ (100% EtOAc); ¹H NMR (500 MHz, CDCl₃) δ 7.62 – 7.64 (m, 2H), 7.44 – 7.46 (m, 2H), 4.61 – 4.65 (m, 1H), 3.45 (d, $J = 2.5$ Hz, 1H), 1.53 (d, $J = 7.0$ Hz, 3H), 1.21 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 149.1, 132.4, 127.8, 118.7, 111.4, 55.8, 54.3, 24.9, 22.5; MS (ESI, CH₃CN) [M+H⁺] = 250.6.



4-[(S)-1-((R)-tert-butylsulfonamido)ethyl]benzoic acid (9). Compound **8** (5.4 g, 21.5 mmol) was stirred in a mixture of ethylene glycol (70 mL), water (30 mL), and KOH (12.1 g, 215 mmol) for 20 h at 110 °C. The reaction mixture was poured on crushed ice and washed with diethyl ether to remove some impurities. The pH of the aqueous solution was adjusted to 5 by dropwise addition of concentrated aqueous HCl, and the precipitate was filtered. The filtrate was acidified further to pH 4, and the precipitate was filtered. The crude product was collected and recrystallized in hot MeOH/DMSO mixture to provide **9** (4.29 g, 74%) as a yellowish solid. $R_f = 0.35$ (EtOAc/MeOH = 19 : 1); $^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 12.85 (s, 1H), 7.90 (d, $J = 7.0$ Hz, 2H), 7.46 (d, $J = 8.5$ Hz, 2H), 5.45 (d, $J = 5.0$ Hz, 1H), 4.47 (m, 1H), 1.46 (d, $J = 7.0$ Hz, 3H), 1.11 (s, 9H); $^{13}\text{C NMR}$ (125 MHz, DMSO- d_6) δ 167.6, 150.4, 129.9, 129.8, 127.3, 55.5, 55.2, 25.1, 23.1; MS (ESI, CH_3CN) $[\text{M}+\text{H}^+] = 269.8$.

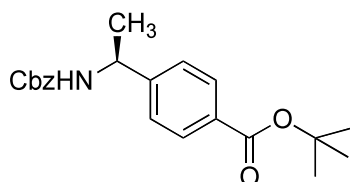


(S)-4-(1-aminoethyl)benzoic acid hydrochloride (10). To an ice-cold solution of **9** (2.0 g, 7.42 mmol) in MeOH (15 mL) was slowly added 4 M HCl in 1,4-dioxane solution (40 mL). The mixture was stirred at room temperature for 40 min. The volume of the reaction mixture was reduced by evaporation, and diethyl ether was added to precipitate the product. The white precipitate was then filtered and washed thoroughly with ether (50 mL) three times to provide **10** (1.48 g, 99%) as a white solid. $R_f = 0.15$ (EtOAc/MeOH = 1 : 1); $^1\text{H NMR}$ (500 MHz, D_2O) δ 8.10 (d, $J = 7.0$ Hz, 2H), 7.60 (d, $J = 7.0$ Hz, 2H), 4.65 (q, $J = 7.0$ Hz, 1H), 1.69 (d, $J = 6.5$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, D_2O) δ 168.7, 143.0, 130.4, 130.2, 126.8, 50.7, 19.2.

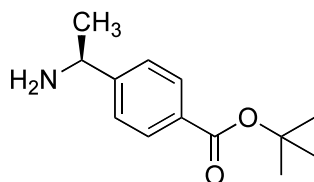


(S)-4-[1-(benzyloxycarbonylamino)ethyl]benzoic acid (10-S1). To a solution of **10** (2.47 g, 12.2

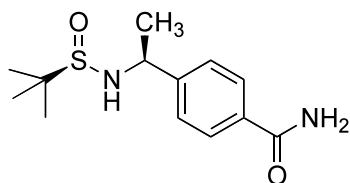
mmol) in THF (80 mL) and 1.0 M aq. NaOH (35 mL) was added benzylchloroformate (2.51 g, 14.7 mmol) dropwise at 0 °C. After being stirred for 1 h at room temperature, the volatile part was removed in vacuo. The aqueous solution was washed with EtOAc, acidified to pH 4, and the precipitate was filtered. The solid was washed twice with 0.5 N aq. HCl solution (20 mL) and dried under high vacuum for overnight. Purity of the product was confirmed by TLC analysis and ¹H NMR, and the product was used for the next reaction without further purification. White solid was obtained (2.63 g, 72%). *R_f* = 0.45 (100% EtOAc); ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.79 (br s, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.88 – 7.90 (m, 2H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.31 – 7.37 (m, 4H), 5.00 (q, *J* = 12.5 Hz, 2H), 4.74 (m, 1H), 1.35 (d, *J* = 7.0 Hz, 3H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 167.6, 155.9, 150.6, 137.5, 129.9, 129.7, 128.8, 128.3, 126.4, 65.8, 50.5, 23.0 (two aromatic peaks are overlapped).



(*S*)-tert-butyl 4-[1-(benzyloxycarbonylamino)ethyl]benzoate (10-S2). To a solution of **10-S1** (2.35 g, 7.85 mmol) in anhydrous CH₂Cl₂ (50 mL) was added concentrated sulfuric acid (0.3 mL). The solution was saturated with isobutylene at -78 °C, causing a volume increase of 30 mL. After stirring in a pressure tube for 7 days at room temperature, the suspension was changed to a clear solution, and the reaction was stopped. To this solution was added 5% aq. NaHCO₃ (50 mL), and the aqueous phase was extracted twice with CH₂Cl₂ (50 mL). The combined organic phase was washed with brine, dried over Na₂SO₄, filtered, and concentrated. The residue was purified by short silica gel plug to afford **10-S2** (2.46 g, 88%) as a transparent oil. *R_f* = 0.5 (hexane/EtOAc = 3 : 1); ¹H NMR (500 MHz, CDCl₃) δ 7.93 (d, *J* = 8.0 Hz, 2H), 7.32 (br s, 7H), 5.01 – 5.10 (m, 3H), 4.87 (s, 1H), 1.57 (s, 9H), 1.44 (d, *J* = 8.5 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 165.6, 155.8, 148.7, 136.6, 130.9, 129.8, 129.8, 128.5, 128.1, 125.8, 80.9, 66.7, 60.4, 50.6, 28.2, 22.4; MS (ESI, CH₃CN) [2M+Na⁺] = 734.2.

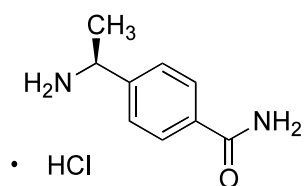


(S)-tert-butyl 4-(1-aminoethyl)benzoate (11). Compound **10-S2** (0.65 g, 1.84 mmol) was dissolved in a mixture of MeOH/H₂O/AcOH (7:2:1, 20 mL) and subjected to catalytic hydrogenation on 5% Pd/C (50 mg) at 1 atm. After stirring for 1.5 h, the reaction mixture was filtered through Celite, and the filtrate was concentrated under reduced pressure. Acetic acid was removed by an extraction with a 5% aq. NaHCO₃ solution to provide free amine **11** as a white powder (0.40 g, 99%). $R_f = 0.2$ (EtOAc/MeOH = 1 : 1); ¹H NMR (500 MHz, CD₃OD) δ 7.92 (d, $J = 8.0$ Hz, 2H), 7.45 (d, $J = 8.0$ Hz, 2H), 4.38 (q, $J = 6.0$ Hz, 1H), 1.50 – 1.52 (m, 12H); ¹³C NMR (125 MHz, CDCl₃) δ 165.1, 143.3, 132.1, 129.9, 126.5, 81.2, 50.7, 28.1, 20.7; MS (ESI, CH₃CN) $[M+H^+] = 221.9$

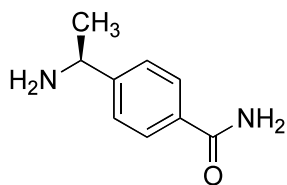


4-[(S)-1-((R)-tert-butylsulfinamido)ethyl]benzamide (9-S1). Compound **9** (6.63 g, 24.6 mmol) was dissolved in THF (100 mL) at ambient temperature and the solution was cooled down to -10 °C. To this solution, *N*-methylmorpholine (2.98 g, 29.5 mmol) and *iso*-butyl chloroformate (4.03 g, 29.5 mmol) were added successively, and stirring continued for 30 min at -10 °C, and then 29% aqueous ammonia (14 mL) was added. The mixture was stirred at -10 °C for 30 min and at room temperature for overnight. The solution was concentrated to a reduced volume (~30 mL) and partitioned to EtOAc/water (100 mL : 100 mL). Aqueous phase was extracted four times with EtOAc (80 mL), and the combined organic solution was washed with brine, dried over Na₂SO₄, filtered, and evaporated. The residue was recrystallized in EtOH/ether or in MeOH/DMF/ether to afford **9-S1** (6.23 g, 94%) as a yellowish solid. $R_f = 0.15$ (100% EtOAc); ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.92 (s, 1H), 7.83 (d, $J = 8.0$ Hz, 2H), 7.42 (d, $J = 8.5$ Hz, 2H), 7.31 (s, 1H), 5.42 (d, $J = 5.0$ Hz, 1H), 4.46 (m, 1H), 1.47 (d, $J = 7.0$ Hz, 3H), 1.11 (s, 9H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 168.2, 148.6, 133.4, 127.9, 126.9,

55.5, 55.1, 25.2, 23.1; MS (ESI, CH₃CN) [M+H⁺] = 269.5.



(S)-4-(1-aminoethyl)benzamide hydrochloride (12·HCl). To an ice-cold solution of **9-S1** (3.96 g, 14.7 mmol) in MeOH (30 mL) was slowly added 4 M HCl in 1,4-dioxane solution (60 mL). The mixture was stirred at room temperature for 2.5 h. The volume of the reaction mixture was reduced by evaporation, and diethyl ether was added to precipitate the product. The white precipitate was then filtered and washed thoroughly with ether (50 mL) three times to provide **12·HCl** (2.93 g, 99%) as a white solid.

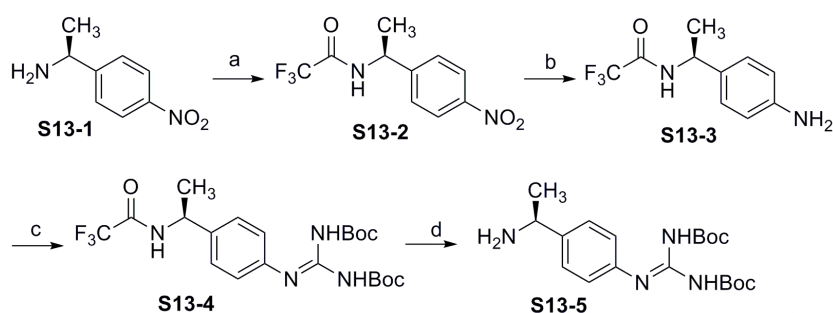


(S)-4-(1-aminoethyl)benzamide (12). To an ice-cold solution of **9-S1** (3.96 g, 14.7 mmol) in MeOH (30 mL) was slowly added 4 M HCl in 1,4-dioxane solution (60 mL). The mixture was stirred at room temperature for 2.5 h. The volume of the reaction mixture was reduced by evaporation, and diethyl ether was added to precipitate the product. The white precipitate was then filtered and washed thoroughly with ether (50 mL) three times to provide an HCl salt form of **12** (2.93 g, 99%) as a white solid. HCl salt form of **12**: ¹H NMR (500 MHz, D₂O) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.5 Hz, 2H), 4.58 (q, *J* = 7.0 Hz, 1H), 1.62 (d, *J* = 7.0 Hz, 3H); ¹³C NMR (125 MHz, D₂O) δ 171.6, 141.8, 132.9, 128.3, 126.9, 50.7, 19.4. Free amine **12** was obtained after dissolving the salt in small amount of 5% aq. NaHCO₃ solution and extraction with EtOAc several times. The organic solution was dried over Na₂SO₄ and concentrated in vacuo to provide a yellowish solid. ¹H NMR (500 MHz, D₂O) δ 7.67 – 7.70 (m, 2H), 7.37 – 7.40 (m, 2H), 4.02 (q, *J* = 7.0 Hz, 1H), 1.27 (d, *J* = 7.0 Hz, 3H); ¹³C NMR (125 MHz, D₂O) δ 172.7, 151.5, 131.0, 127.8, 126.1, 50.0, 23.8 ; MS (ESI, CH₃OH) [2M+H⁺] = 329.1, [3M+H⁺] = 493.2.

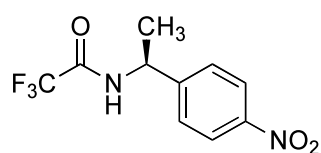
3. Synthesis of Guanidine-Functionalized Nspe Derivative.

S13-5 (*N*spe-guanidine) was synthesized starting from commercially available (*S*)- α -methyl-4-nitrobenzylamine hydrochloride (Scheme S1). The amino group was protected by the treatment of ethyl trifluoroacetate under basic conditions. Reduction of nitro group employing a catalytic hydrogenation provided aromatic amine **S13-3**. Guanidination of **S13-3** using 1,3-bis(*tert*-butoxycarbonyl)-2-methyl-2-thiopseudourea in the presence of mercury (II) chloride provided **S13-4** in a 90% yield. Deprotection of trifluoroacetamide afforded **S13-5**.

Scheme S1. Synthesis of **S13-5** (*N*spe-guanidine).

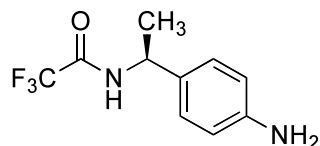


Reagents and conditions: (a) Ethyl trifluoroacetate, Et₃N, CH₂Cl₂, 89%; (b) H₂, Pd/C, MeOH, quant.; (c) 1,3-Bis(*tert*-butoxycarbonyl)-2-methylthiopseudourea, HgCl₂, Et₃N, DMF, 90%; (d) LiOH (aq.), MeOH, 74%.

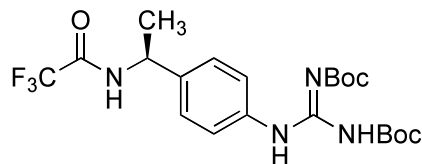


(*S*)-*N*-[1-(4-nitrophenyl)ethyl]trifluoroacetamide (S13-2**).** To a stirred ice-cold solution of (*S*)- α -methyl-4-nitrobenzylamine hydrochloride (**S13-1**, 10.3 g, 50.8 mmol) in anhydrous CH₂Cl₂ (250 mL) was added ethyl trifluoroacetate (21.7 g, 152.5 mmol) followed by triethylamine (15.3 g, 152.5 mmol). The reaction mixture was stirred under nitrogen at room temperature for 5 days, and the solution was concentrated in vacuo. The residue was dissolved in EtOAc (250 mL), washed with 1.0N HCl (2 \times 50 mL), 5% NaHCO₃ (2 \times 50 mL), and brine (100 mL), and dried over Na₂SO₄. After evaporation of the organic solvent, the purity of the product was confirmed by ¹H NMR, and the compound was used for

next reaction without further purification. A white crystalline solid was obtained (11.8 g, 89%). $R_f = 0.3$ (hexane/EtOAc = 3 : 1); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.19 – 8.21 (m, 2H), 7.45 – 7.48 (m, 2H), 6.75 (s, 1H), 5.18 (m, 1H), 1.60 (d, $J = 7.0$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 148.3, 147.6, 127.1, 124.2, 116.8, 114.5, 49.4, 21.3.

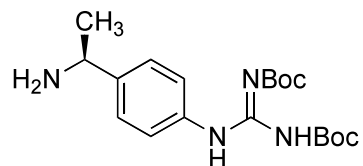


(S)-N-[1-(4-aminophenyl)ethyl]trifluoroacetamide (S13-3). Compound **S13-2** (13.0 g, 49.6 mmol) was dissolved in MeOH (100 mL) and subjected to catalytic hydrogenation on Pd/C (5 wt.%, 200 mg) at 1 atm. After the 2 days stirring at room temperature, the reaction was completed according to the TLC. The reaction mixture was filtered through Celite, and the filtrate was concentrated in vacuo. The residue was purified by short silica gel plug to afford **S13-3** (11.4 g, 99%) as a reddish solid. $R_f = 0.1$ (hexane/EtOAc = 3 : 1); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.07 – 7.10 (m, 2H), 6.63 – 6.65 (m, 2H), 6.54 (s, 1H), 5.02 (m, 1H), 3.70 (br s, 2H), 1.52 (d, $J = 7.0$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 146.4, 130.6, 127.5, 117.0, 115.3, 114.7, 49.4, 20.7; MS (ESI, CH_3CN) $[\text{M}+\text{H}^+] = 233.0$.



(S)-N-{1-[4-(N,N'-bis(*tert*-butoxycarbonyl)guanidino)phenyl]ethyl}trifluoroacetamide (S13-4). To a solution of **S13-3** (5.91 g, 25.5 mmol) in anhydrous DMF (150 mL) was added 1,3-bis(*tert*-butylcarbonyl)-2-methylthiopseudourea (11.09 g, 38.2 mmol), triethylamine (10.3 g, 101.8 mmol), and mercury(II) chloride (10 g, 36.8 mmol). The suspension was kept stirring at room temperature for overnight. The reaction mixture was diluted with CH_2Cl_2 , washed with Na_2CO_3 solution, and filtered through a pad of Celite. The organic layer was washed with water and brine, dried over Na_2SO_4 , and then concentrated in vacuo. The residue was purified by flash column chromatography (hexane/EtOAc = 10 : 1, $R_f = 0.3$), to give **S13-4** (10.8 g, 90%) as a white foamy solid. $R_f = 0.65$

(hexane/EtOAc = 3 : 1); ^1H NMR (500 MHz, CDCl_3) δ 11.57 (s, 1H), 10.28 (s, 1H), 7.52 (d, $J = 8.5$ Hz, 2H), 7.22 (d, $J = 8.5$ Hz, 2H), 6.91 (br s, 1H), 5.03 (m, 1H), 1.43 - 1.50 (m, 21 H); ^{13}C NMR (125 MHz, CDCl_3) δ 163.4, 156.5, 153.6, 153.3, 137.3, 136.5, 126.8, 122.8, 117.0, 83.9, 79.8, 49.3, 28.1, 28.0, 20.7; MS (ESI, CH_3CN) $[\text{M}+\text{H}^+] = 474.9$.



(S)-1-(4-([N,N'-bis(*tert*-butoxycarbonyl)guanidino]phenyl)ethylamine (S13-5). To a stirred ice-cold solution of **S13-4** (5.34 g, 11.3 mmol) in MeOH (80 mL) and THF (100 mL) under nitrogen was added 2.0 M aq. LiOH (50 mL) dropwise, and the mixture was stirred at room temperature for 3 h. After evaporation of organic solvents under reduced pressure, the aqueous solution was extracted three times with EtOAc (100 mL). The combined organic extract was washed with brine, dried over Na_2SO_4 , filtered, and concentrated. The residue was purified by flash column chromatography ($\text{CH}_2\text{Cl}_2/\text{MeOH}/\text{Et}_3\text{N} = 15 : 1 : 0.1$, $R_f = 0.35$), to give **S13-5** (3.16 g, 74%) as a white foamy solid. ^1H NMR (500 MHz, CDCl_3) δ 11.61 (s, 1H), 10.26 (s, 1H), 7.48 – 7.52 (m, 2H), 7.26 – 7.28 (m, 2H), 4.07 (q, $J = 6.5$ Hz, 1H), 2.25 (br s, 2H), 1.51 (s, 9H), 1.47 (s, 9H), 1.35 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 163.6, 153.7, 153.3, 143.4, 135.5, 126.3, 122.6, 83.7, 79.6, 50.9, 28.2, 28.1, 25.1; MS (ESI, CH_3CN) $[\text{M}+\text{H}^+] = 378.9$.

4. Sidechain cleavage in strong acidic conditions:

A (*S*)-*N*-(1-Phenylethyl)glycine (*N*spe) derivative with electron-donating substituent at the *para*-position can undergo sidechain cleavage in strong acidic conditions (i.e. cleavage from resin using 95% TFA for 10 minutes). Proposed cleavage mechanism is shown in Scheme S2. Model peptoid containing *N*spe-guanidine underwent the sidechain cleavage (Figure S1).

Scheme S2. Proposed cleavage mechanism.

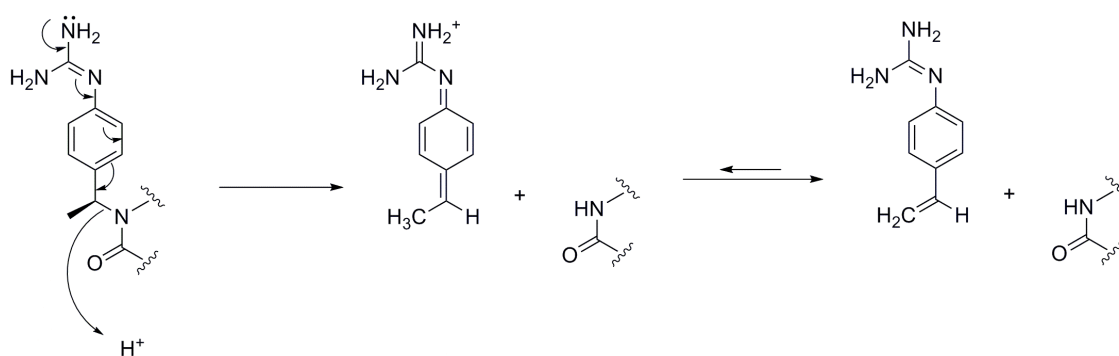
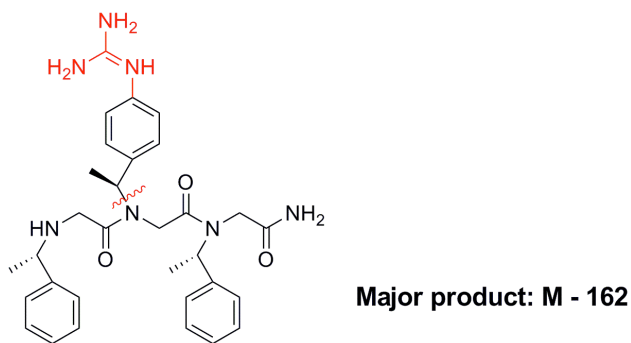
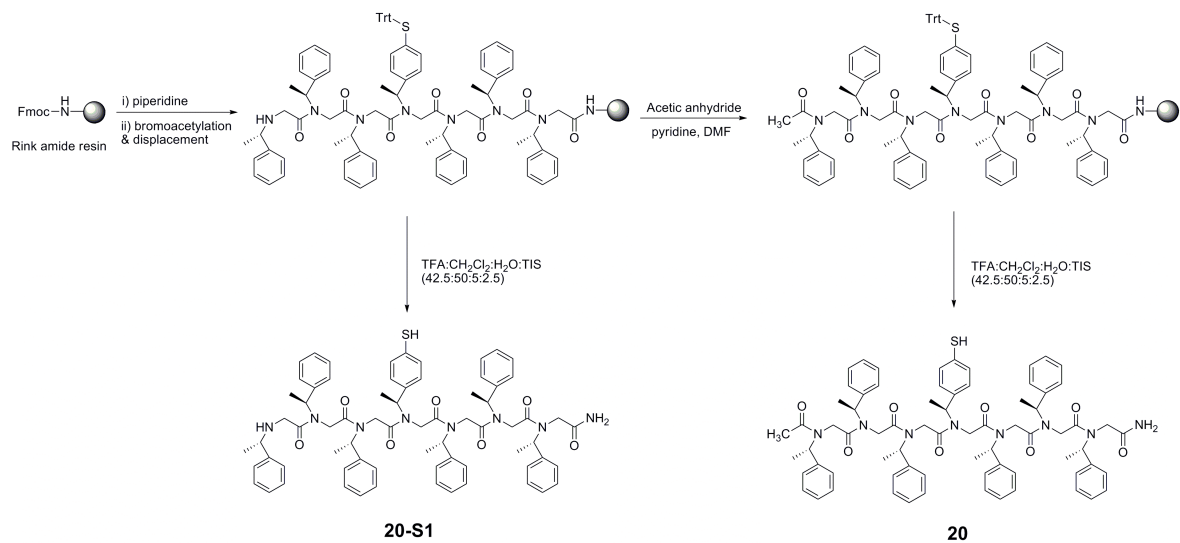


Figure S1. Observed example of the sidechain cleavage.



5. Synthesis of peptoid 20.



Scheme S3. Synthesis of **20**.

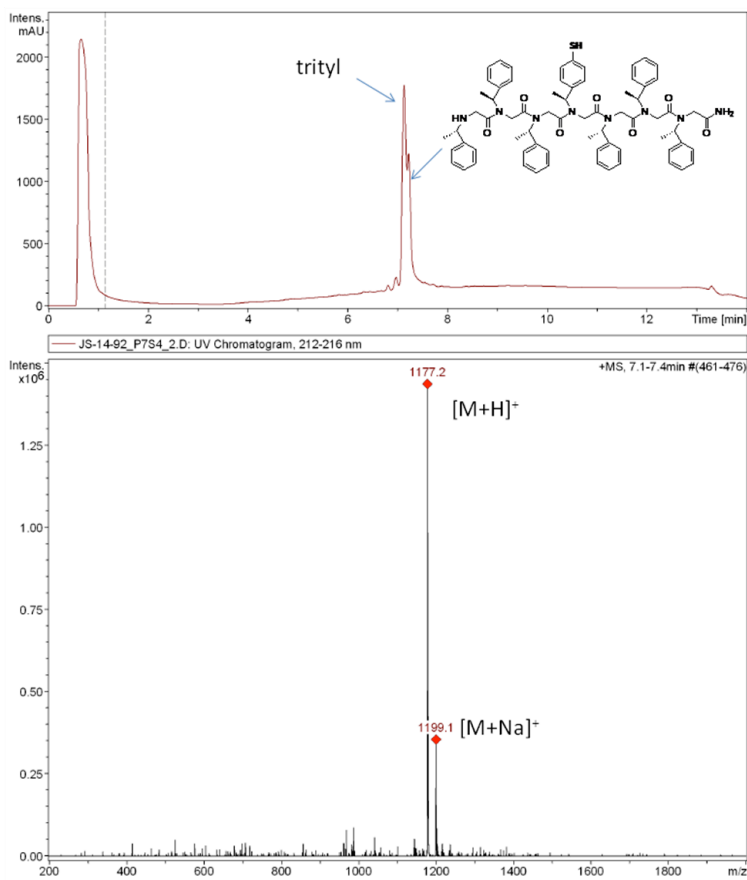


Figure S2. LC-MS data of crude **20-S1**.

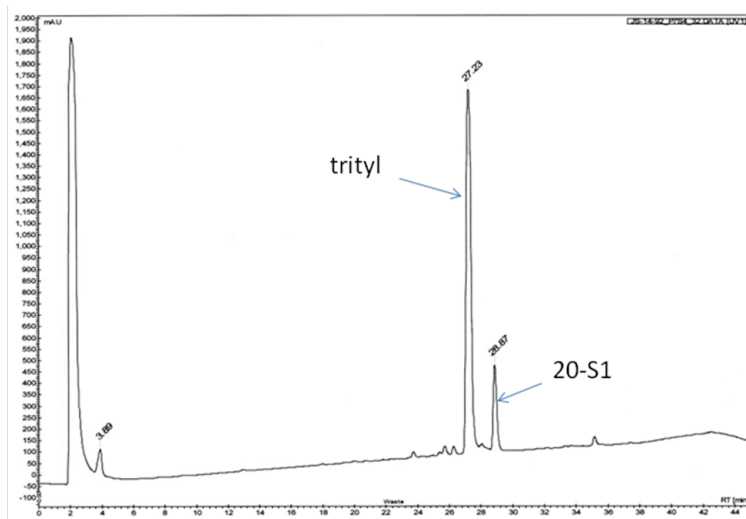


Figure S3. Analytical HPLC spectrum of crude **20-S1**. Vydac C18 column was used at a flow rate of 1 mL/min at 60 °C. The mobile phase was used as follows: (A, water + 0.1% TFA; B, CH₃CN + 0.1% TFA) a gradient starting with 20% B to 70% B over 35 min, a gradient to 95% B over 5 min, and then a gradient to 20% B over 5 min. UV detection was at 220 nm.

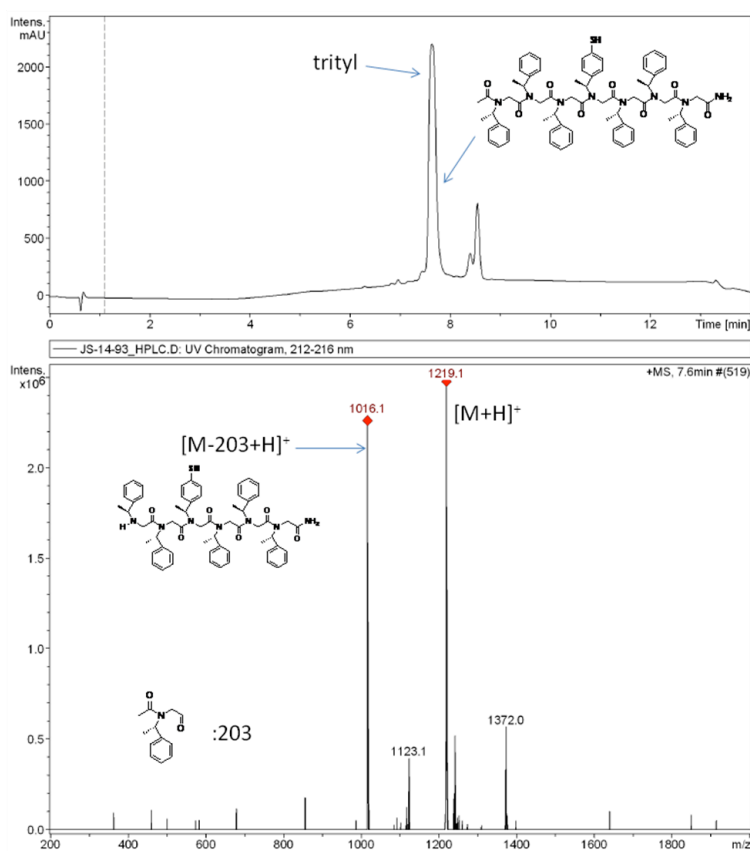


Figure S4. LC-MS data of crude **20**. Trityl and peptoid peaks are overlapped.

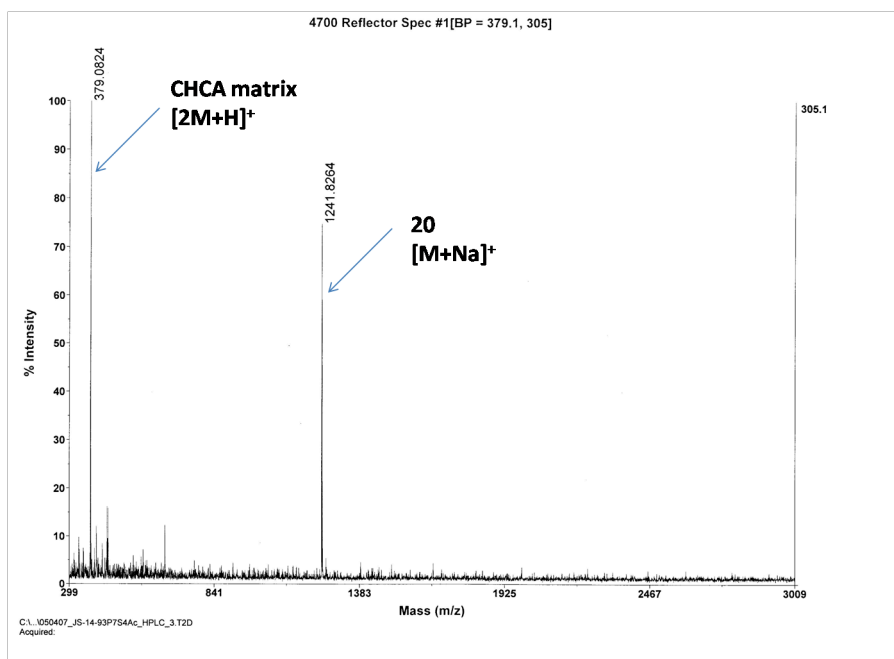
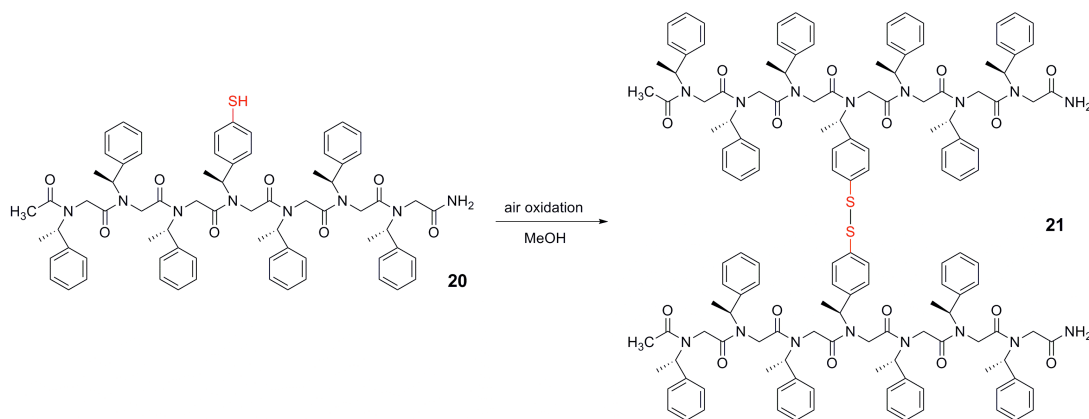


Figure S5. MALDI-TOF mass spectrometry data of purified **20**.

6. Synthesis of homodimeric peptoid helix bundle **21**.

Peptoid **20** (13 mg, 11 μmol) was dissolved in MeOH (1 mL). The reaction flask containing the solution was open to air, and the stirring continued for 2 days at room temperature. The reaction mixture was directly used for MS and analytical HPLC analyses, and purified by preparative HPLC.



Scheme S4. Synthesis of **21**.

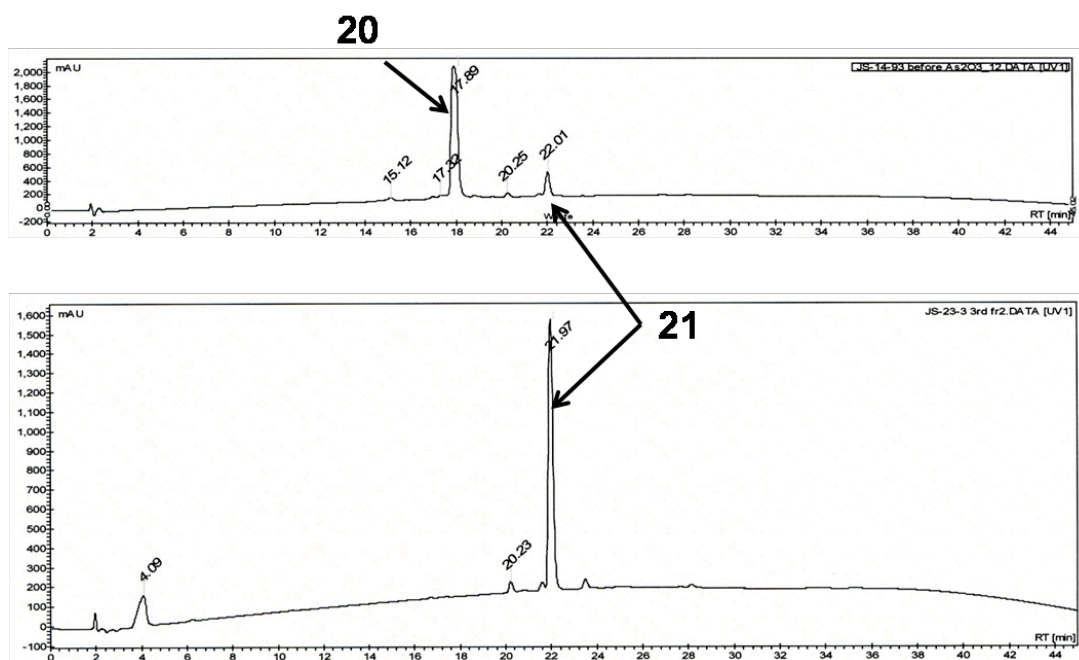


Figure S6. Analytical HPLC chromatogram of thiol peptoid **20** and peptoid disulfide **21**. Vydac C18 column was used at a flow rate of 1 mL/min at 60 °C. The mobile phase was used as follows: (A, water + 0.1% TFA; B, CH₃CN + 0.1% TFA) a gradient starting with 20% B to 100% B over 25 min, 5 min using 100% B, and then a gradient to 20% B over 15 min. UV detection was at 220 nm.

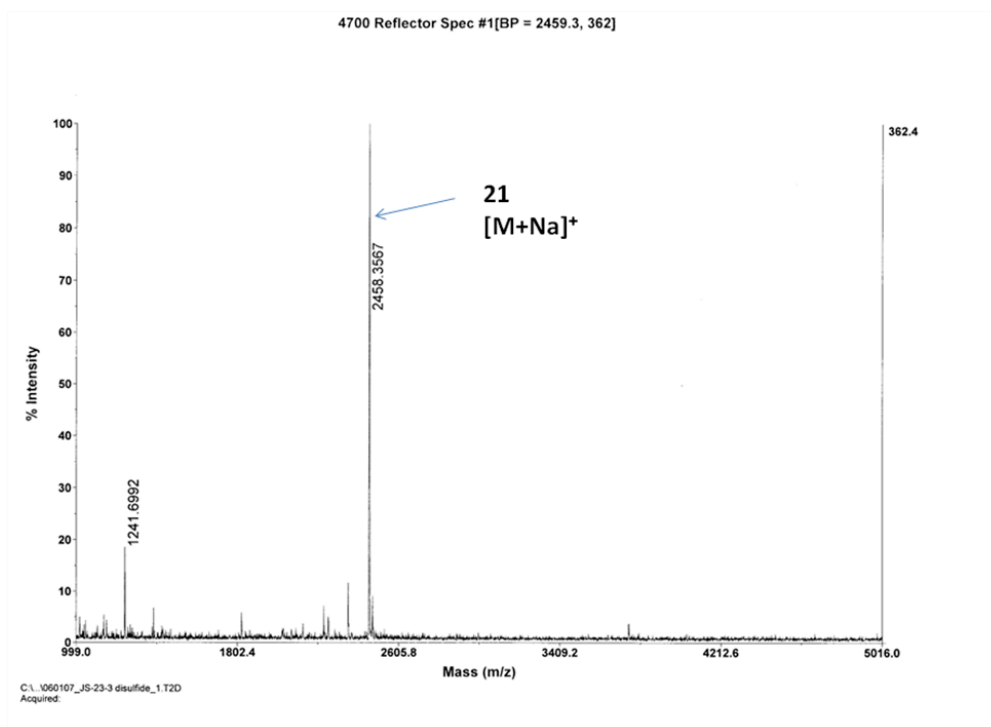
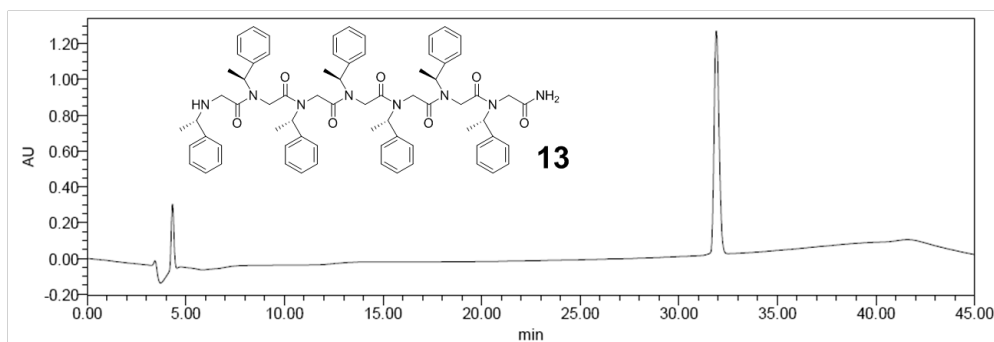


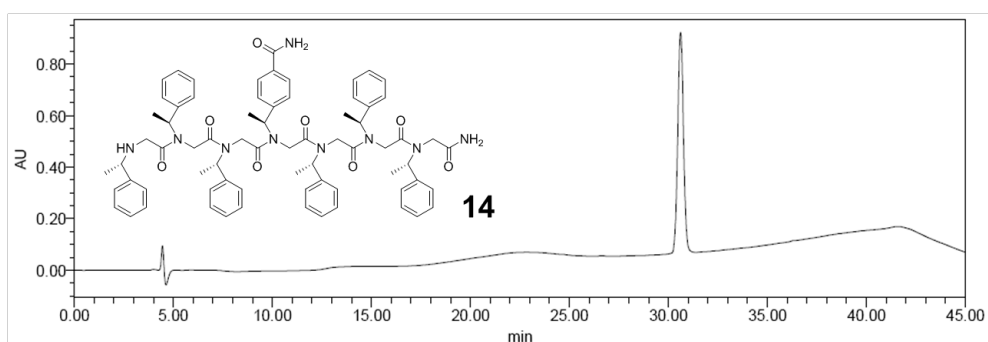
Figure S7. MALDI-TOF mass spectrometry data of purified **21**.

7. HPLC and ESI-mass data of peptoids 13-19.

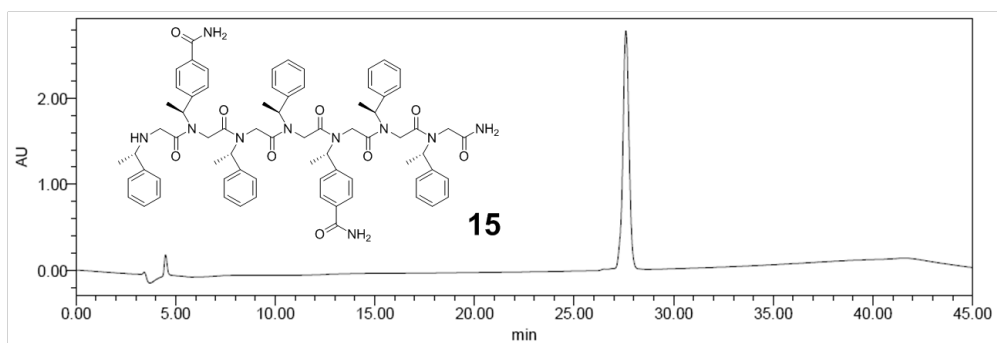
13:



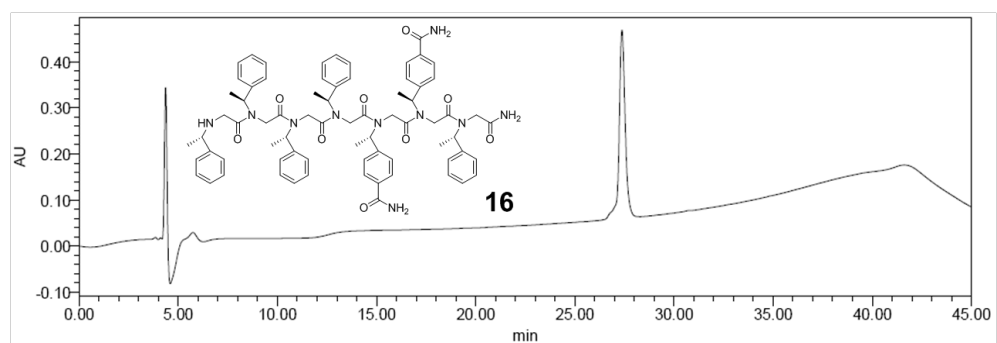
14:



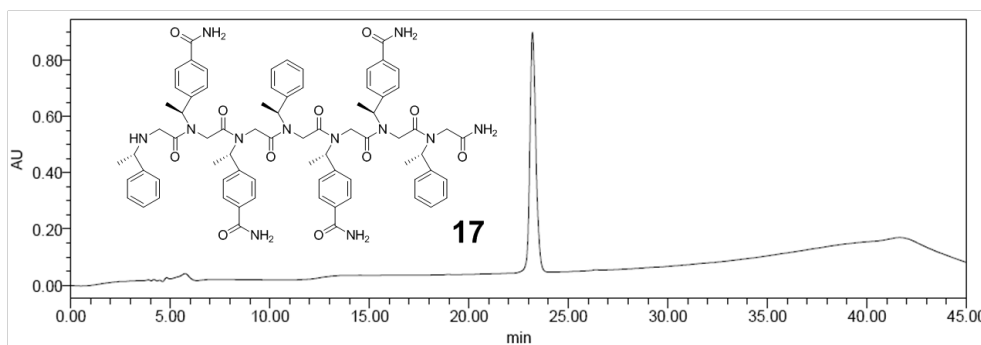
15:



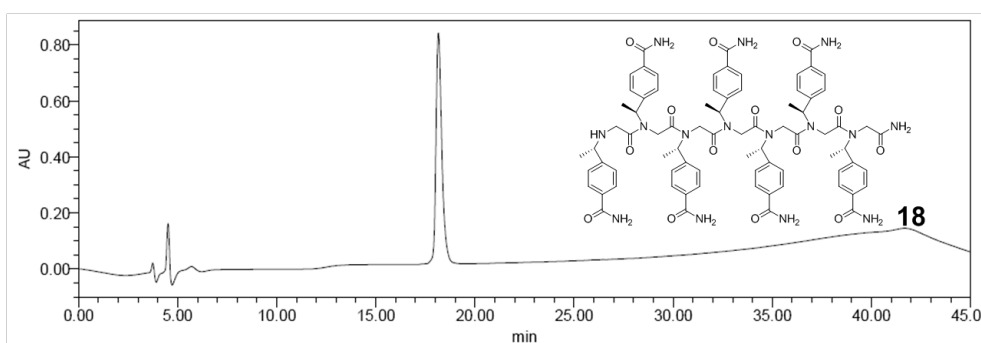
16:



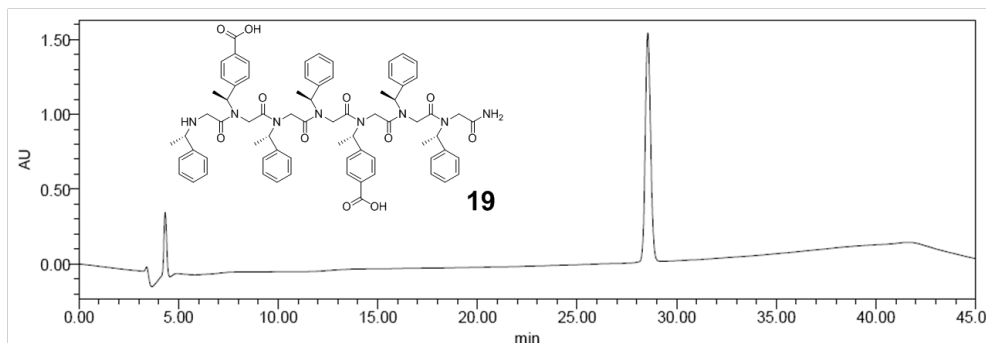
17:



18:



19:



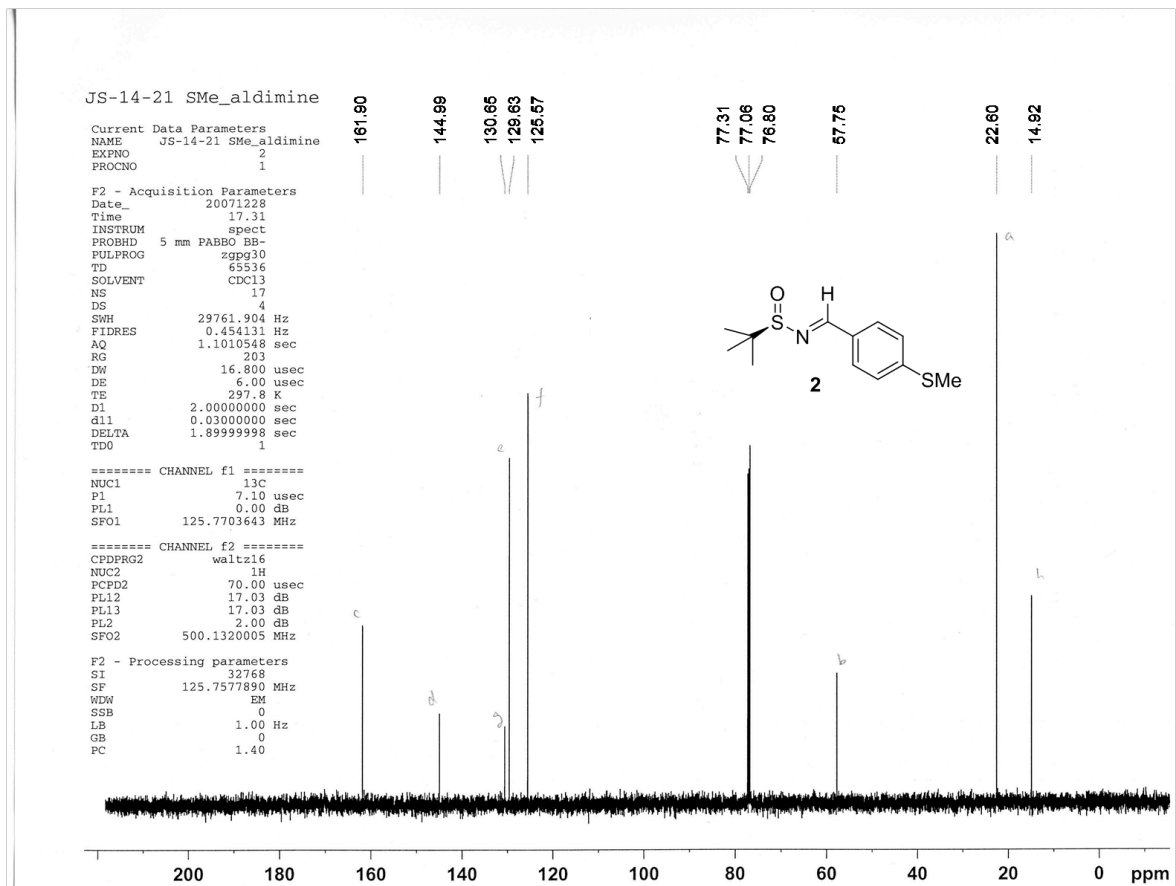
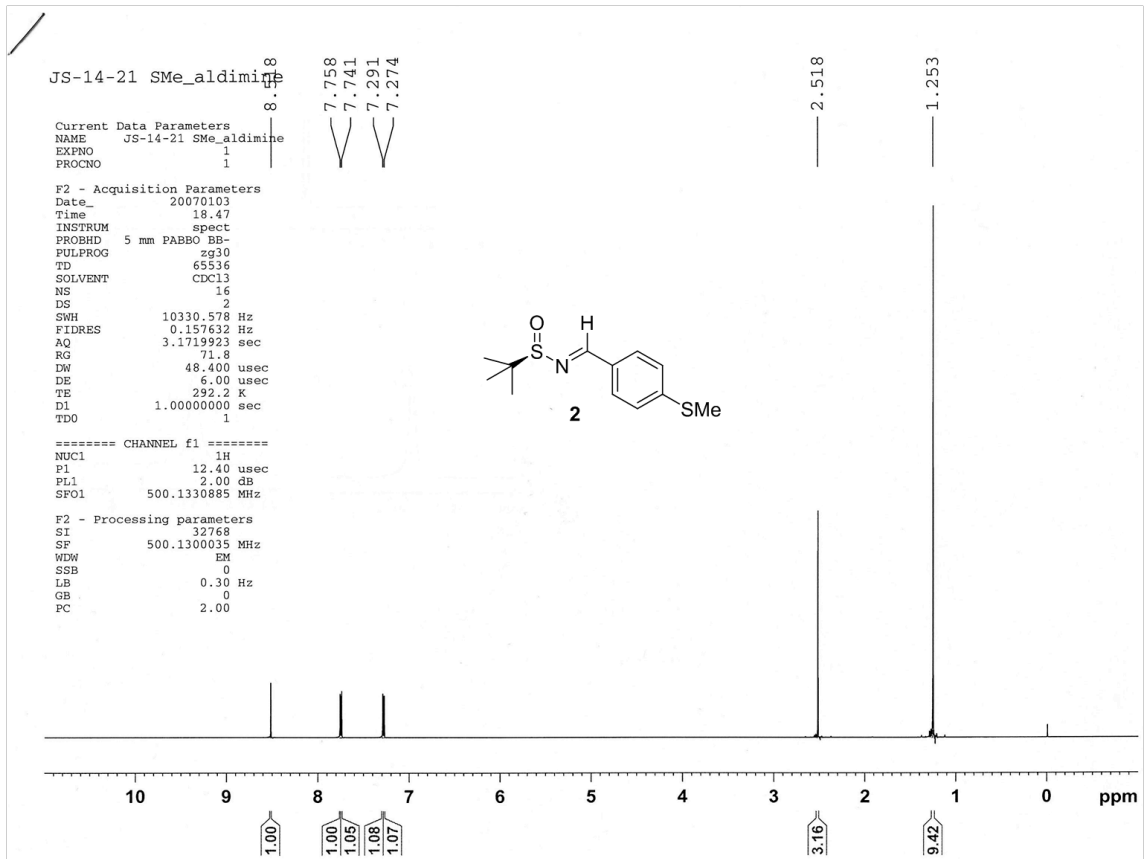
HPLC conditions for peptoid **13-19**:

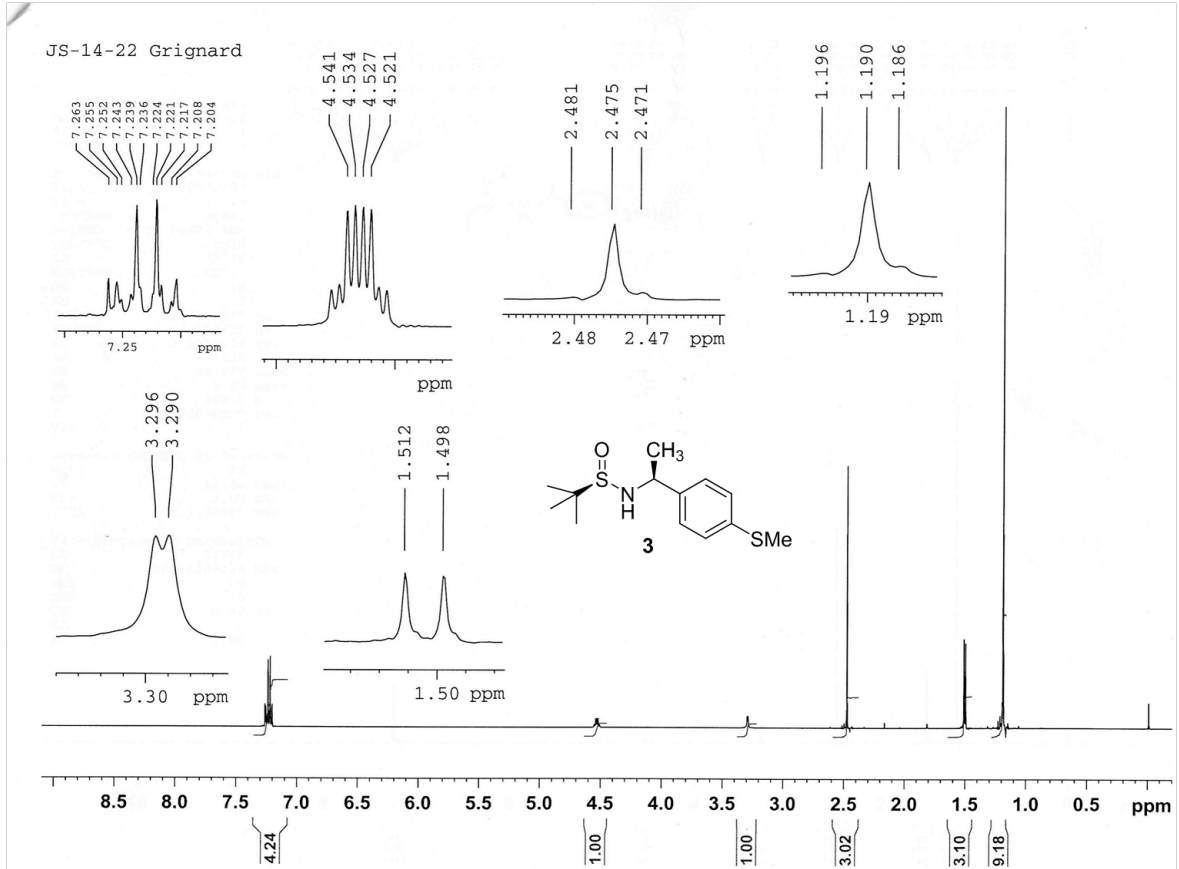
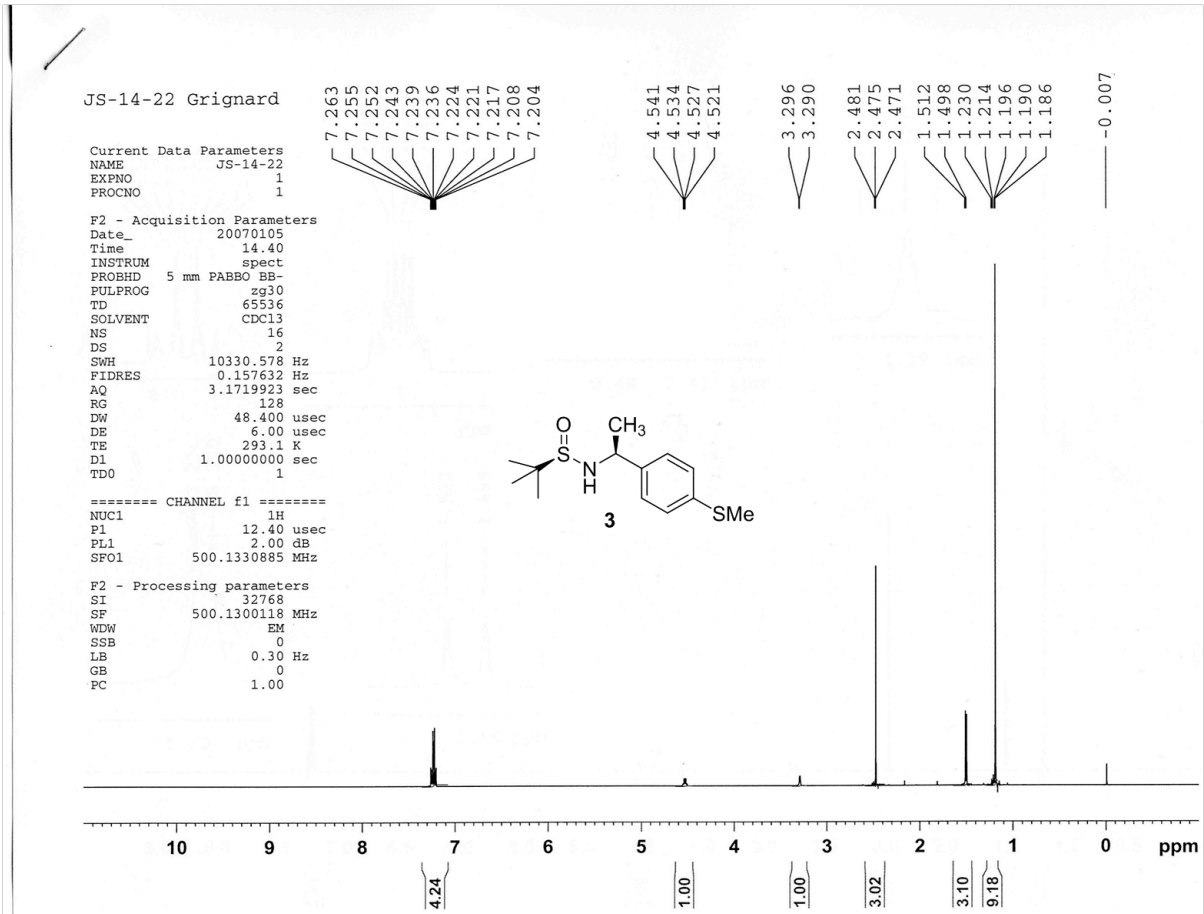
Waters analytical HPLC system (2695 Separations Module, 2998 detector) was used. Phenomenex Jupiter C18 column (250 x 2.00 mm) was used at a flow rate of 0.2 mL/min at 55 °C. The mobile phase was used as follows: (A, water + 0.1% TFA; B, CH₃CN + 0.1% TFA) a gradient starting with 1% B to 99% B over 40 min and a gradient to 1% B over 5 min. UV detection was at 220 nm.

peptoids	mass calculated	mass observed
13	1144.61	1146.65 (H ⁺)
14	1187.62	1189.90 (H ⁺)
15	1230.63	1231.70 (H ⁺)
16	1230.63	1232.18 (H ⁺)
17	1316.64	1317.92 (H ⁺)
18	1445.66	1447.36 (H ⁺)
19	1232.59	1233.50 (H ⁺)

Table S1. ESI-MS data of peptoids **13 - 19**.

8. ¹H and ¹³C NMR spectra.





JS-14-22 Grignard

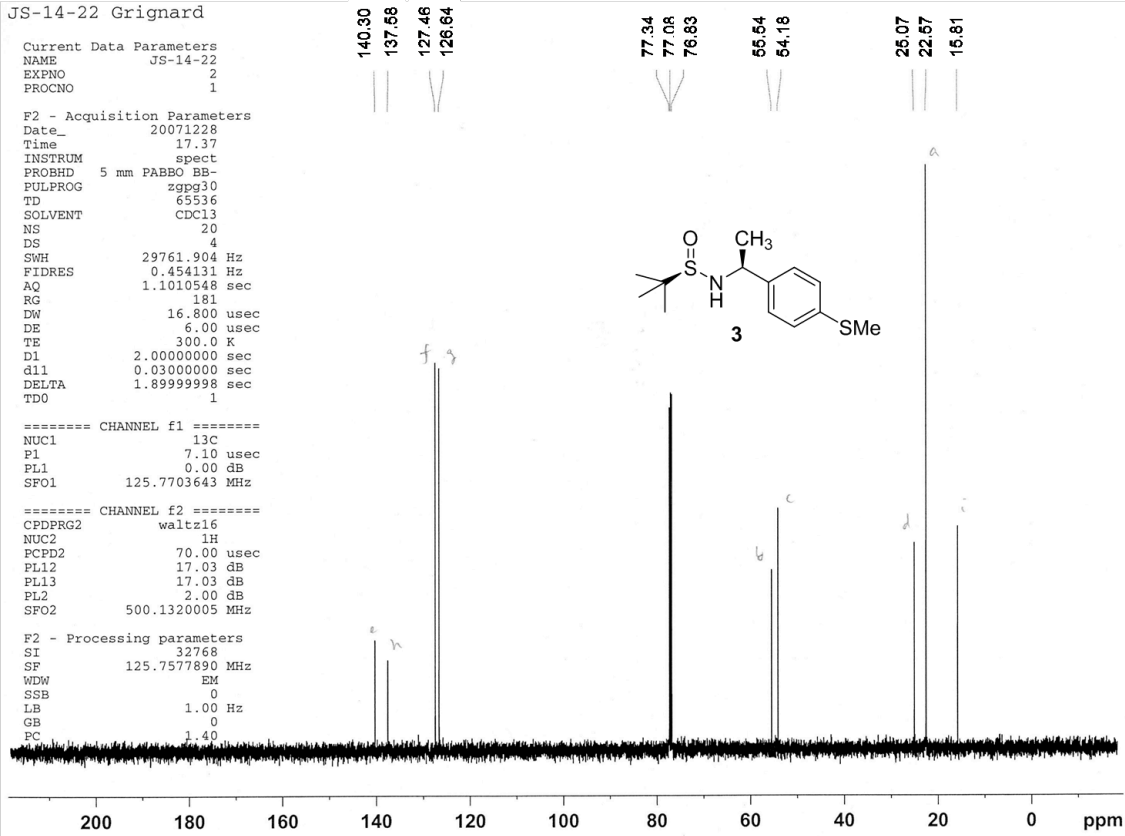
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 PL1 0.00 dB
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
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 PCPD2 70.00 usec
 PL12 17.03 dB
 PL13 17.03 dB
 PL2 2.00 dB
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F2 - Processing parameters
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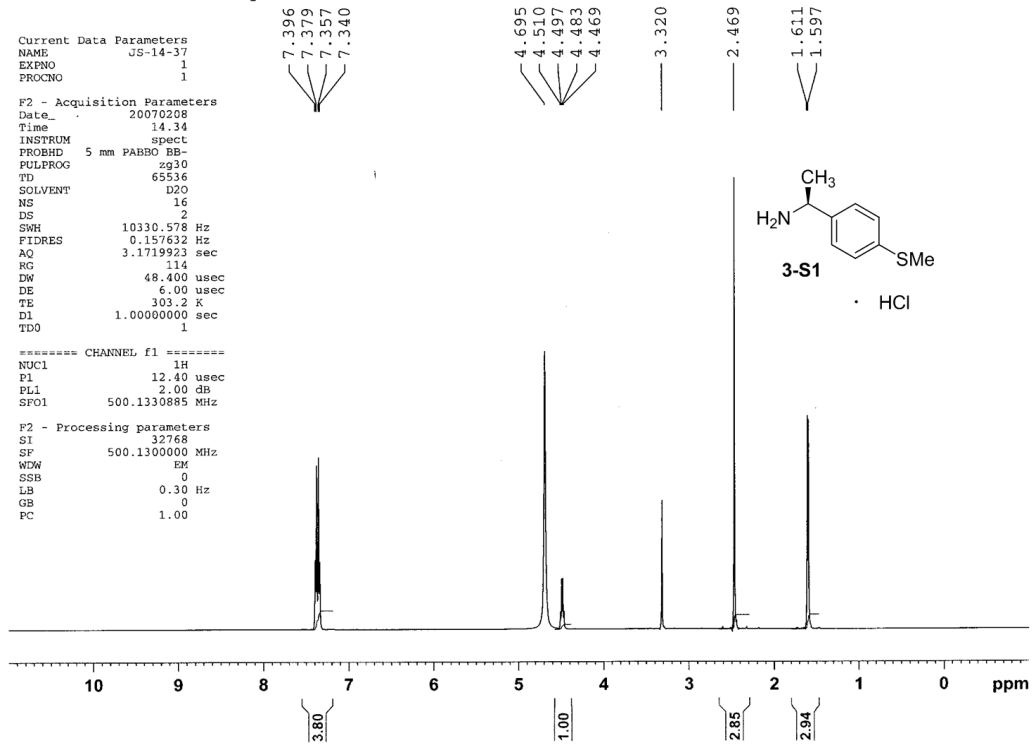
JS-14-37 sulfonamide deprotection

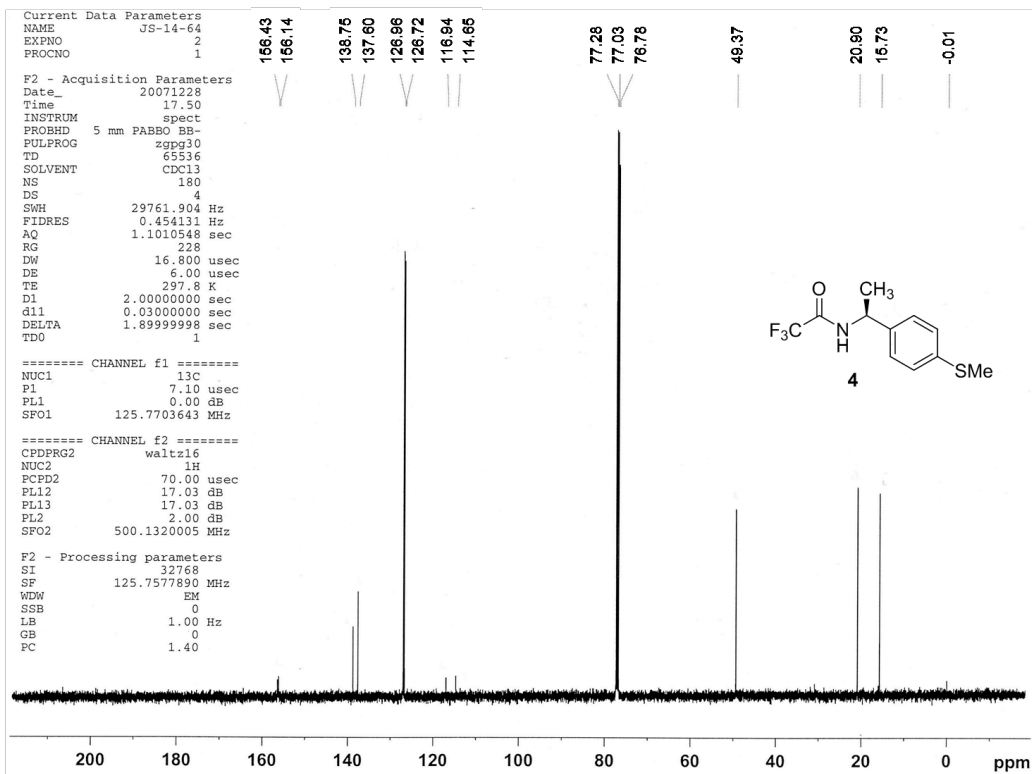
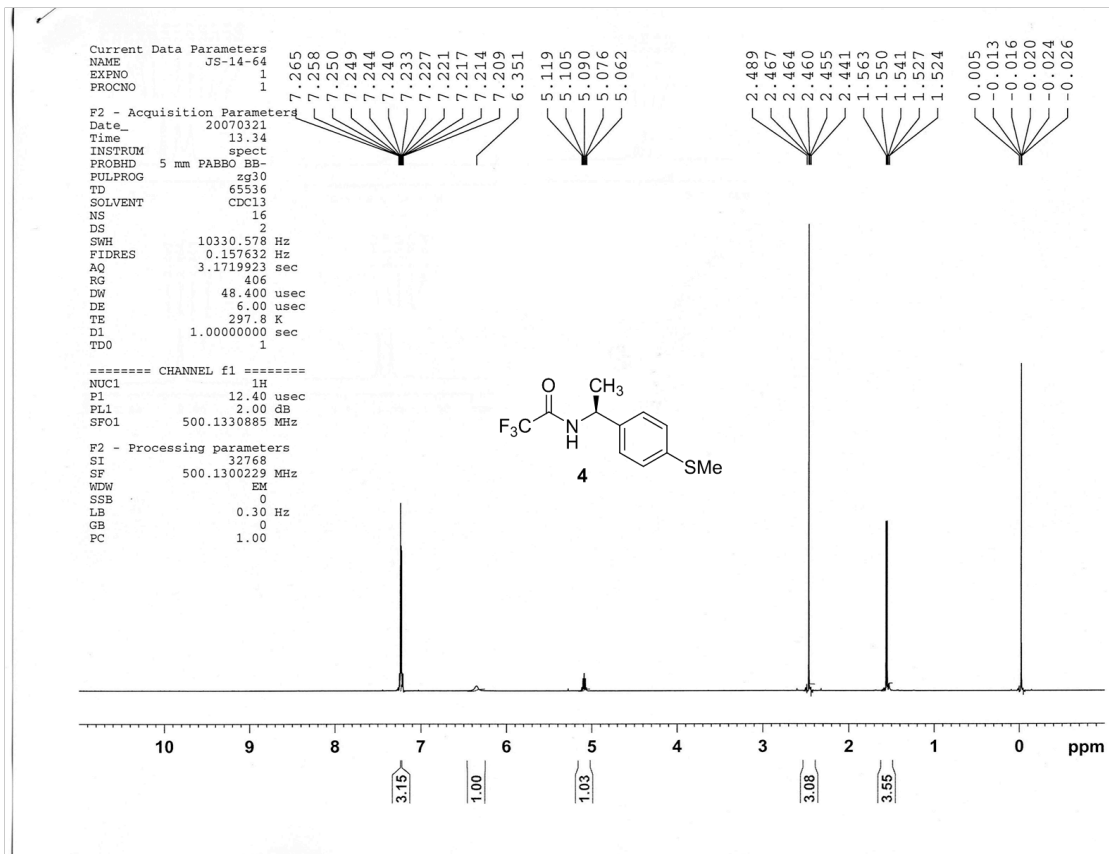
Current Data Parameters
 NAME JS-14-37
 EXPNO 1
 PROCNO 1

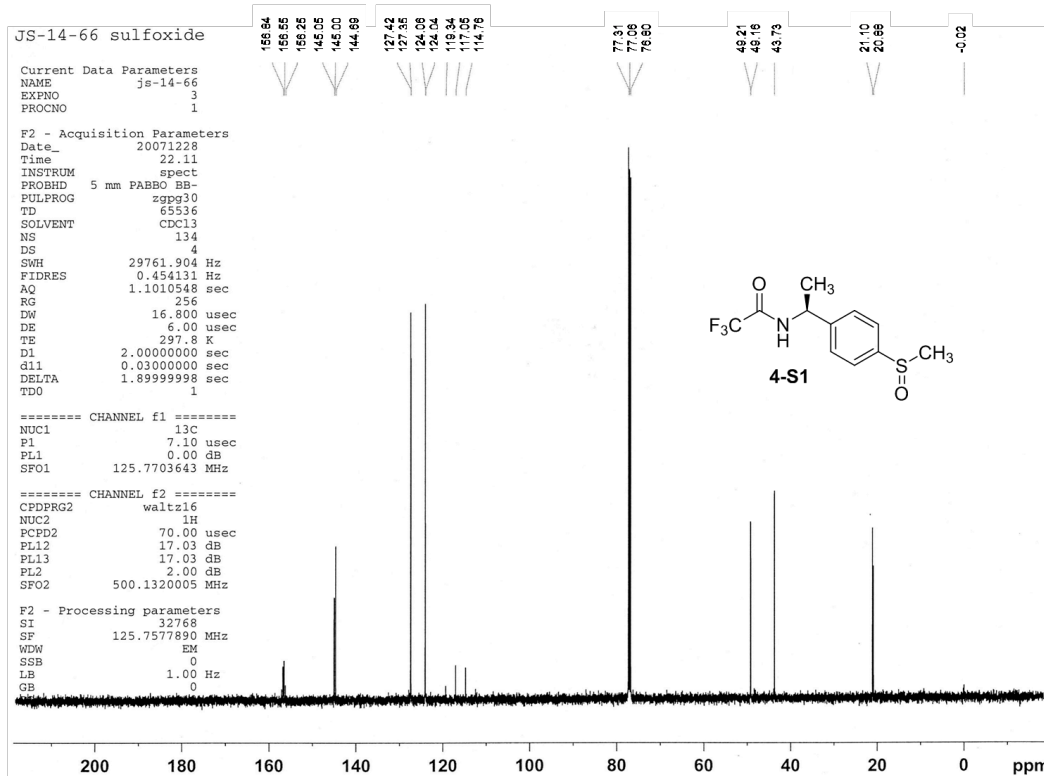
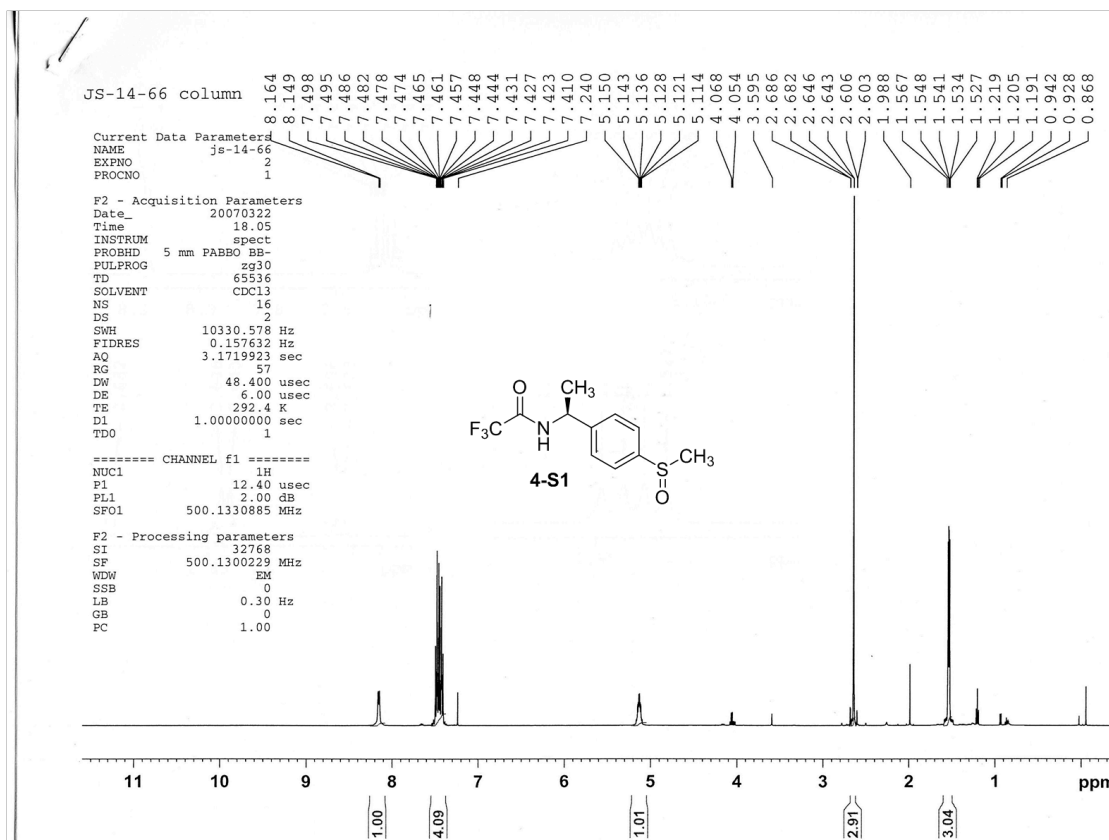
F2 - Acquisition Parameters
 Date_ 20070208
 Time 14.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 114
 DW 48.400 usec
 DE 6.00 usec
 TE 303.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.40 usec
 PL1 2.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00







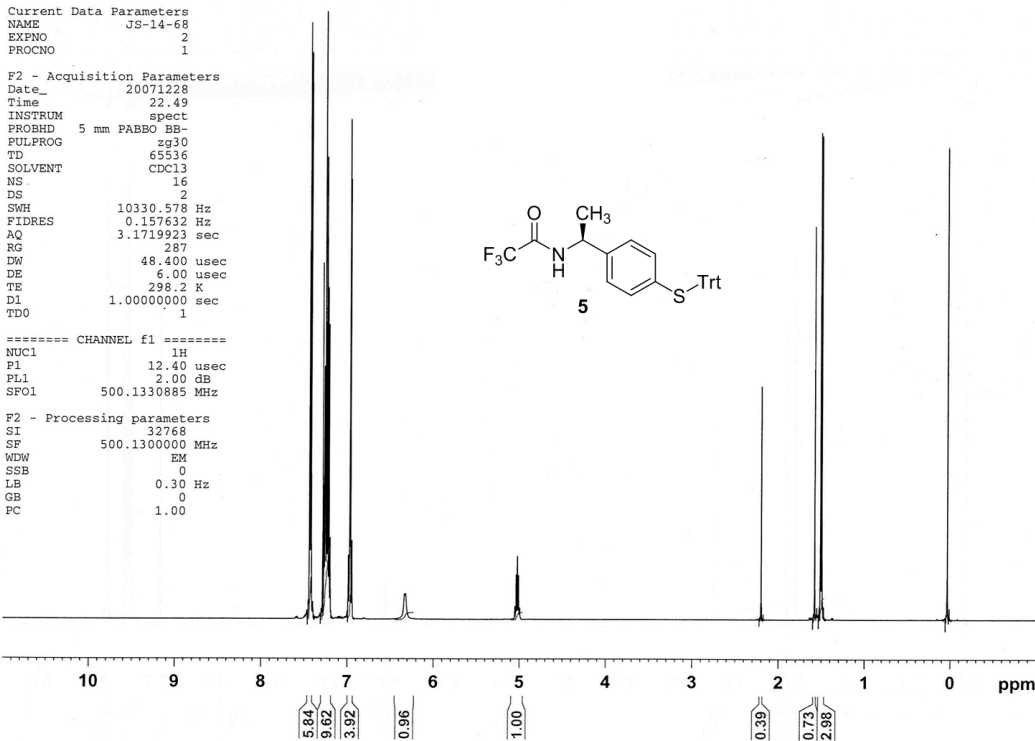
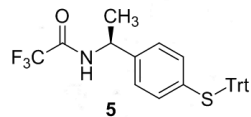
JS-14-68 trityl

Current Data Parameters
NAME JS-14-68
EXPNO 2
PROCNO 1

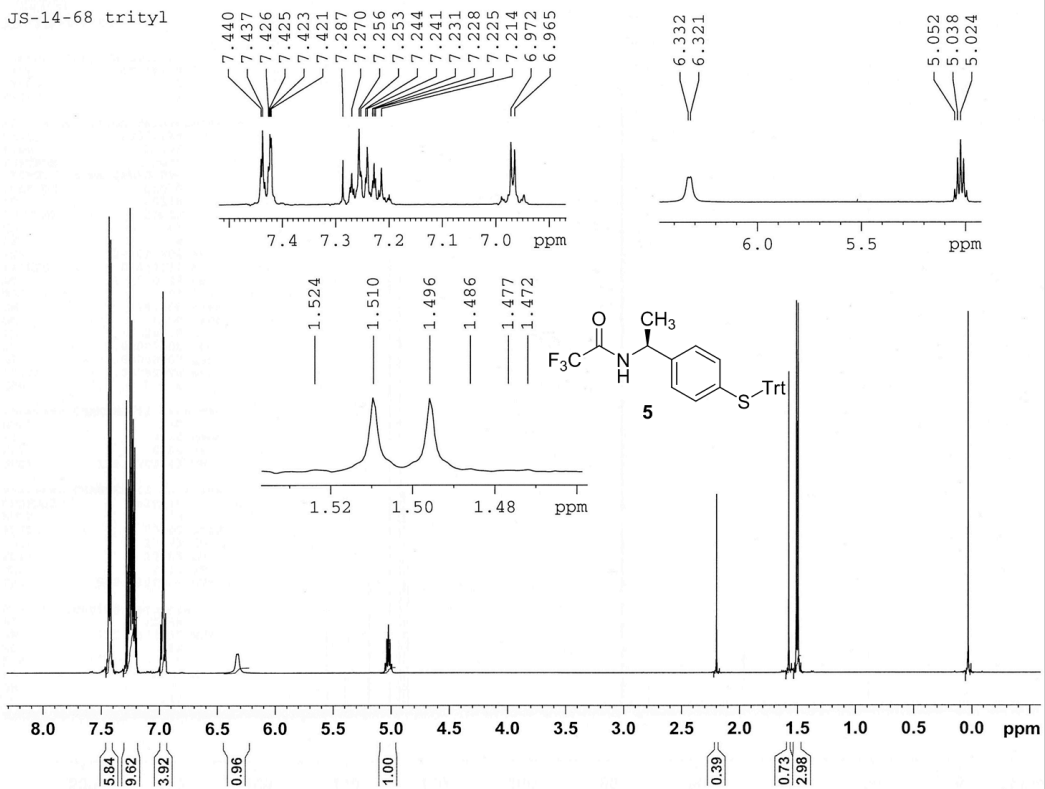
F2 - Acquisition Parameters
Date_ 20071228
Time 22.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 287
DW 48.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.0000000 sec
TDO 1

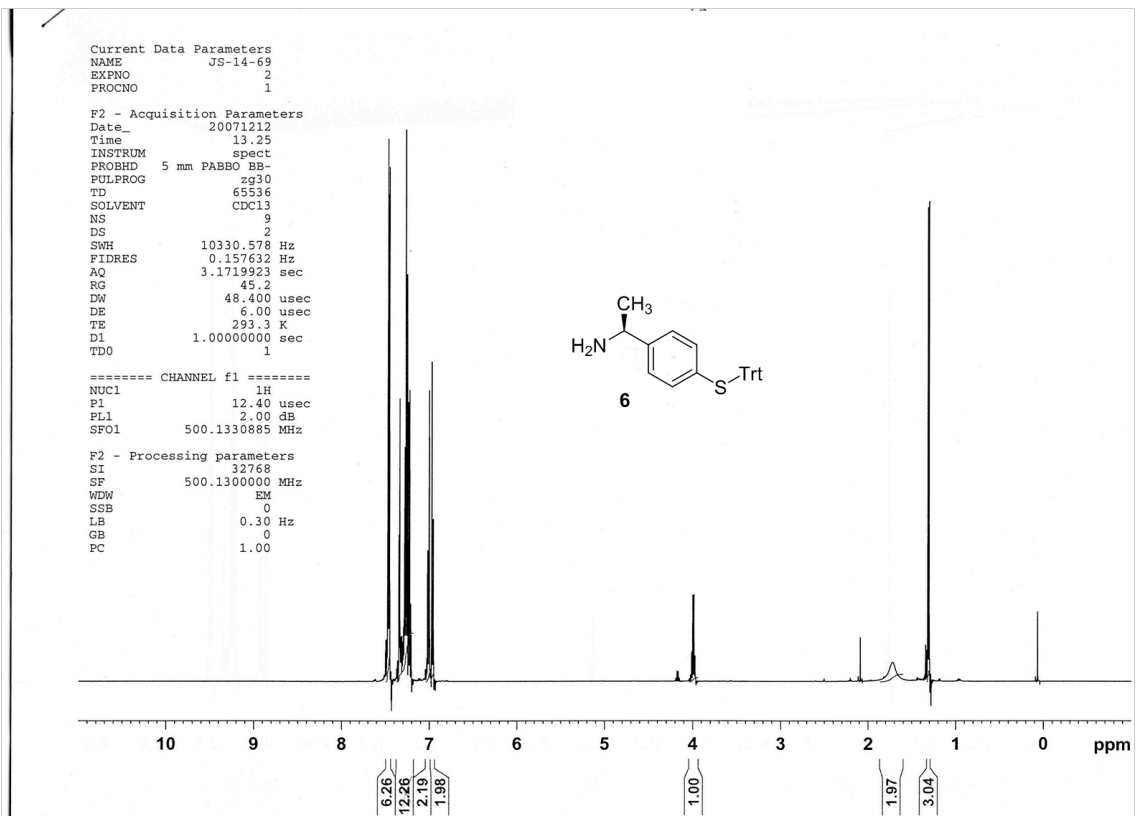
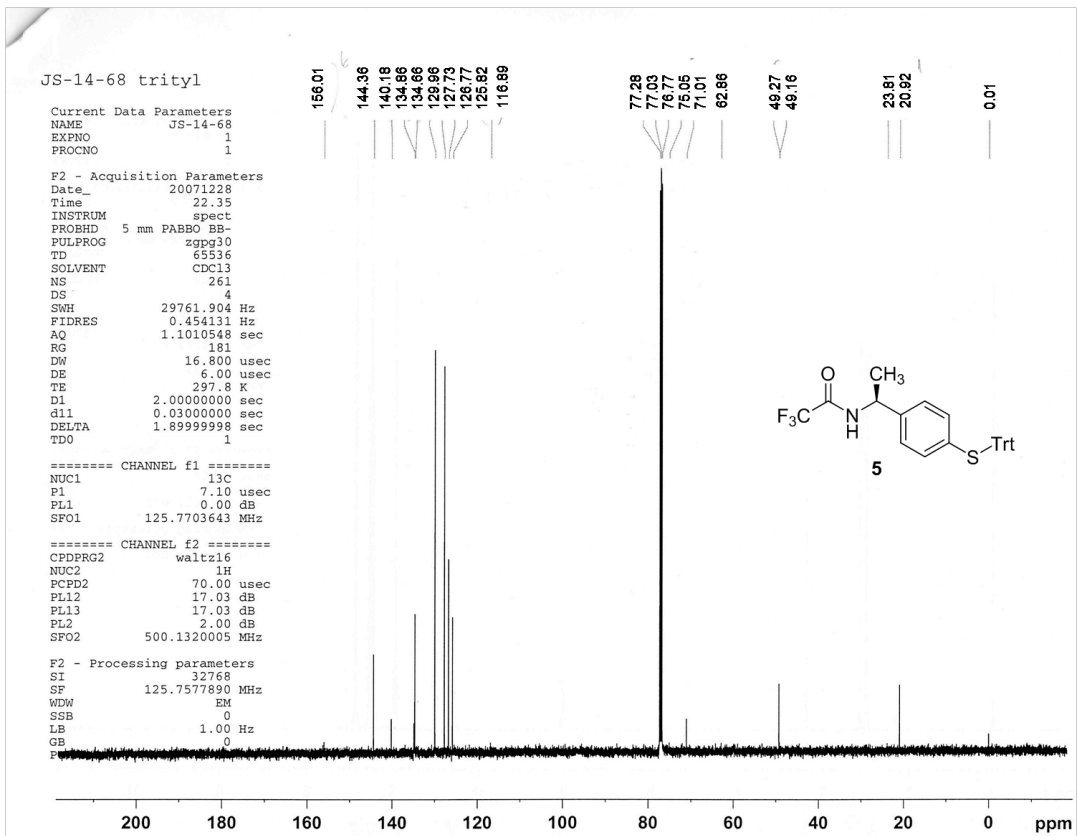
===== CHANNEL f1 =====
NUC1 1H
P1 12.40 usec
PL1 2.00 dB
SFO1 500.1330885 MHz

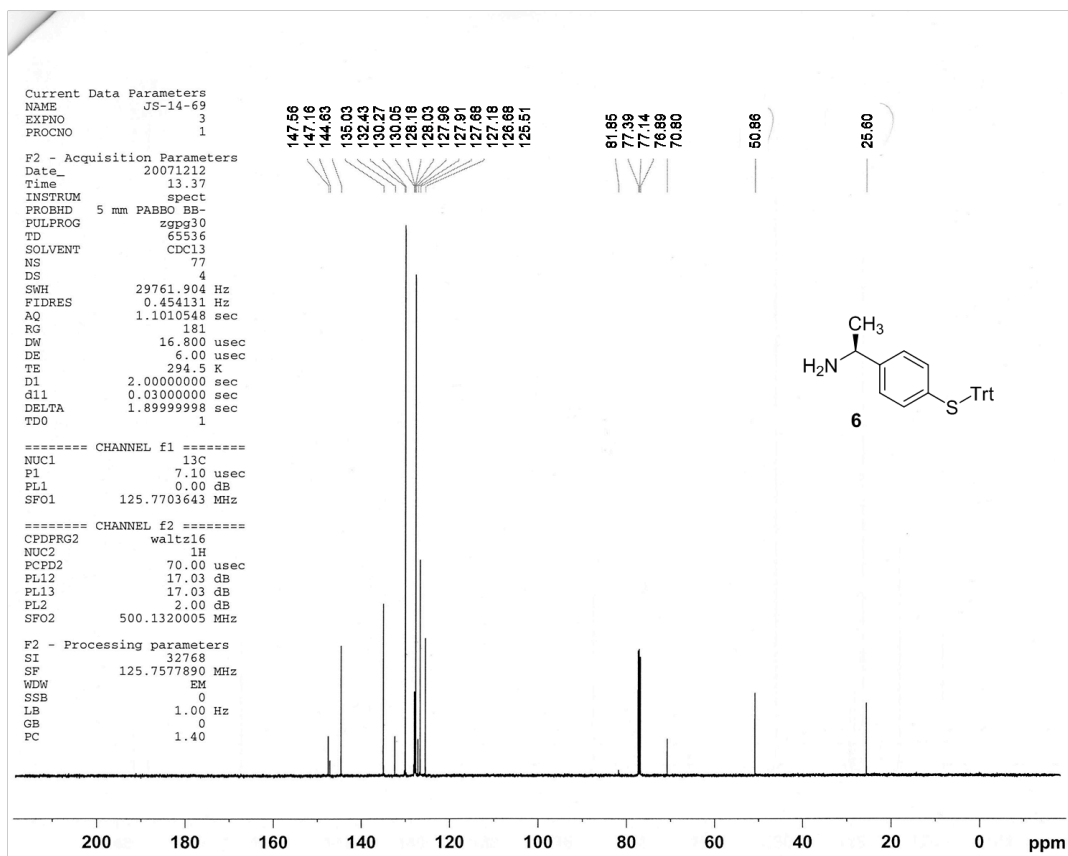
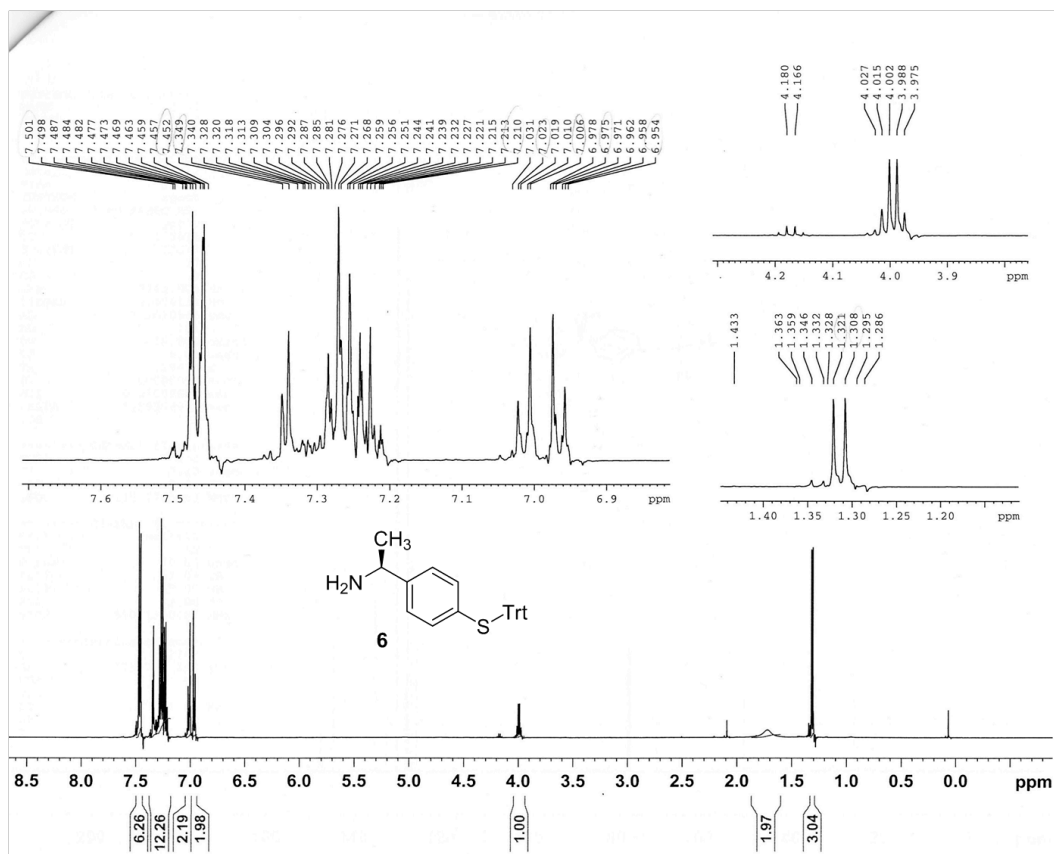
F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



JS-14-68 trityl







```

Current Data Parameters
NAME JS-14-69
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071212
Time 13.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 77
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 181
DW 16.800 usec
DE 6.00 usec
TE 294.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.10 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 17.03 dB
PL13 17.03 dB
PL2 2.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```


JS-14-1 Ti(OEt)4

Current Data Parameters
 NAME JS-14-1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20071018
 Time 15.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 128
 DW 48.400 usec
 DE 6.00 usec
 TE 298.1 K
 D1 1.0000000 sec
 TD0 1

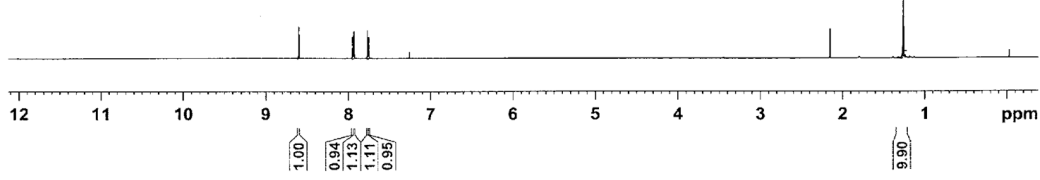
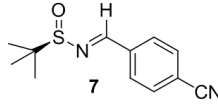
===== CHANNEL f1 =====
 NUC1 1H
 P1 12.40 usec
 PL1 2.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300129 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.601
7.951
7.948
7.944
7.939
7.935
7.931
7.768
7.764
7.760
7.754
7.751
7.260

2.149
1.275
1.264
1.260
1.252
1.236

-0.026



JS-14-1 Ti(OEt)4

Current Data Parameters
 NAME JS-14-1
 EXPNO 3
 PROCNO 1

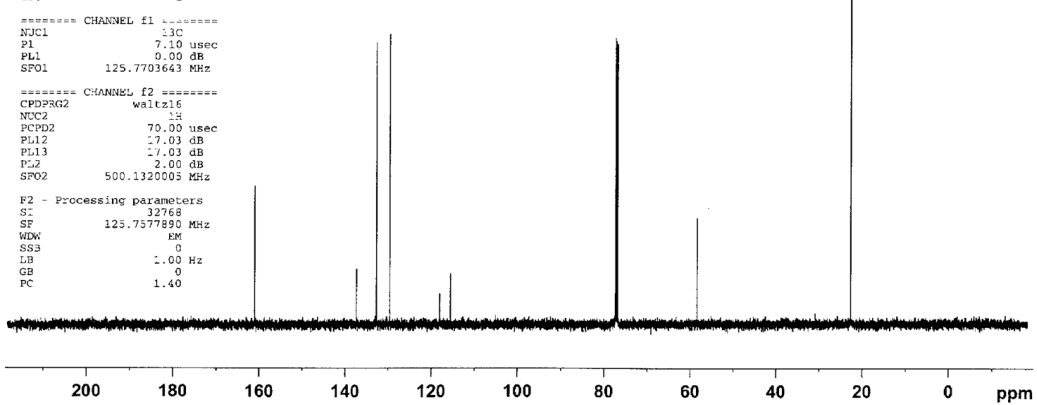
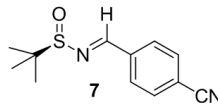
F2 - Acquisition Parameters
 Date_ 20071018
 Time 15.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 43
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 228
 DW 16.800 usec
 DE 6.00 usec
 TE 299.2 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.10 usec
 PL1 0.00 dB
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NDC2 15
 PCPD2 70.00 usec
 PL12 -7.03 dB
 PL13 -7.03 dB
 PL2 2.00 dB
 SFO2 500.1320003 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

161.07
137.39
132.75
129.62
118.06
115.53
77.31
77.06
76.80
58.38
30.90
22.67



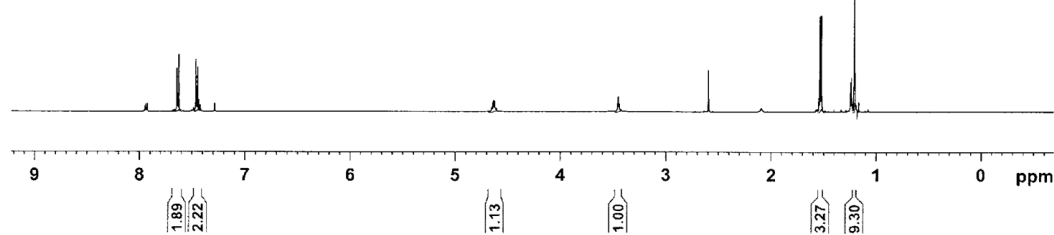
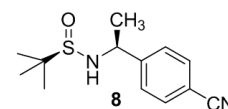
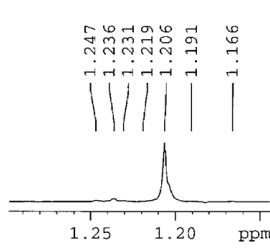
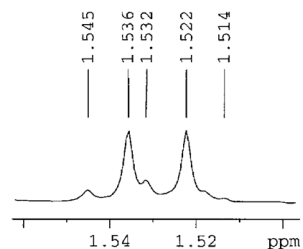
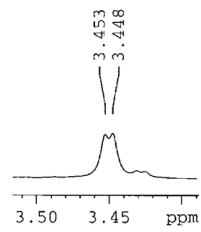
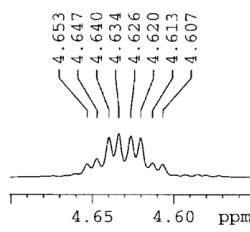
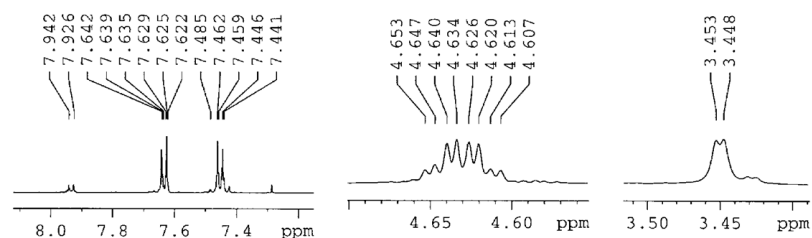
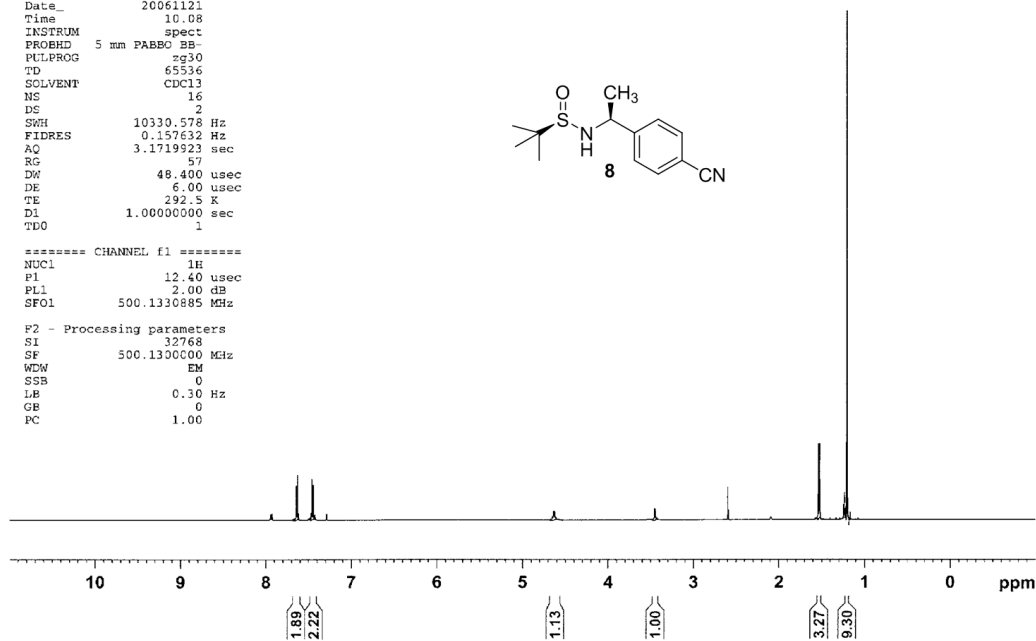
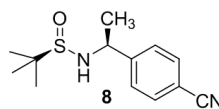
JS-14-2

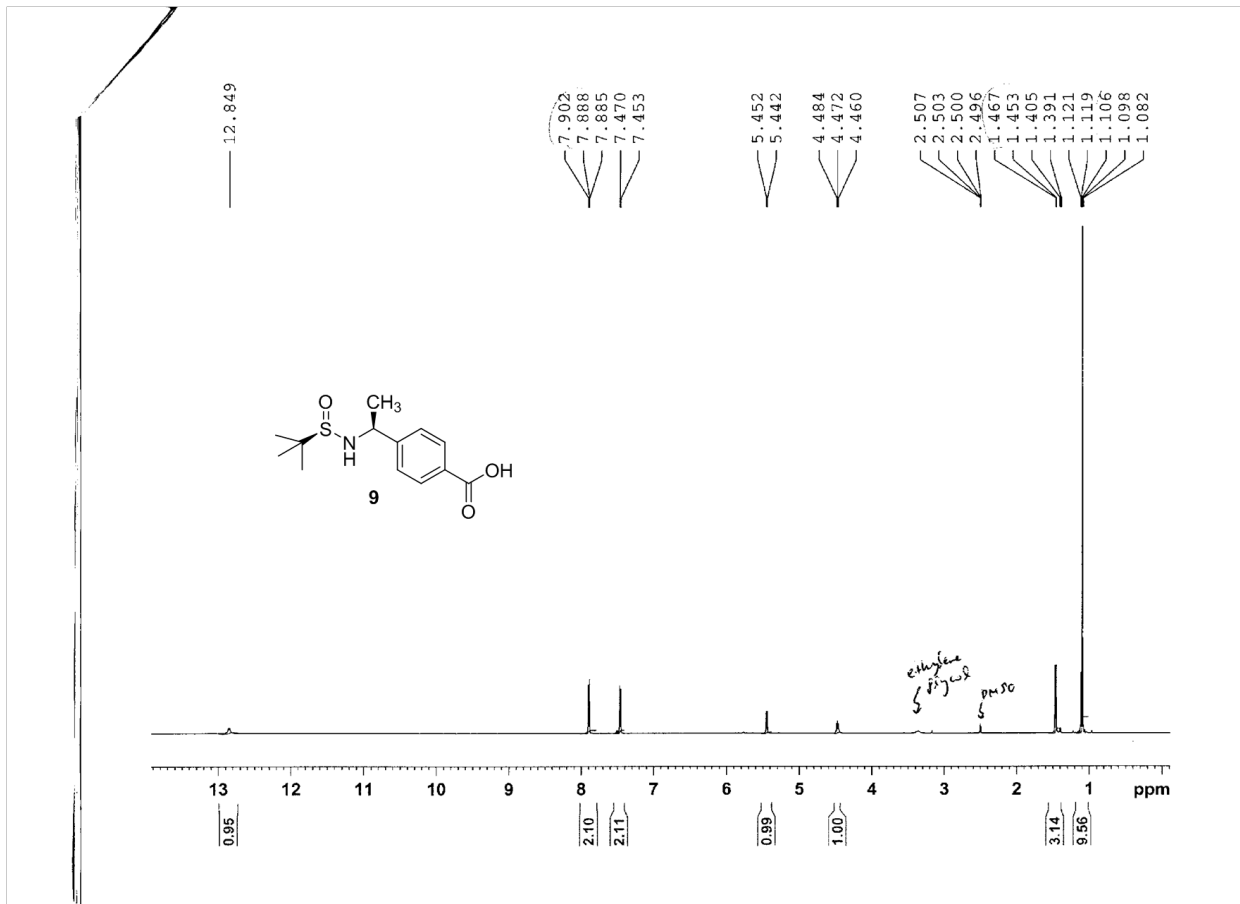
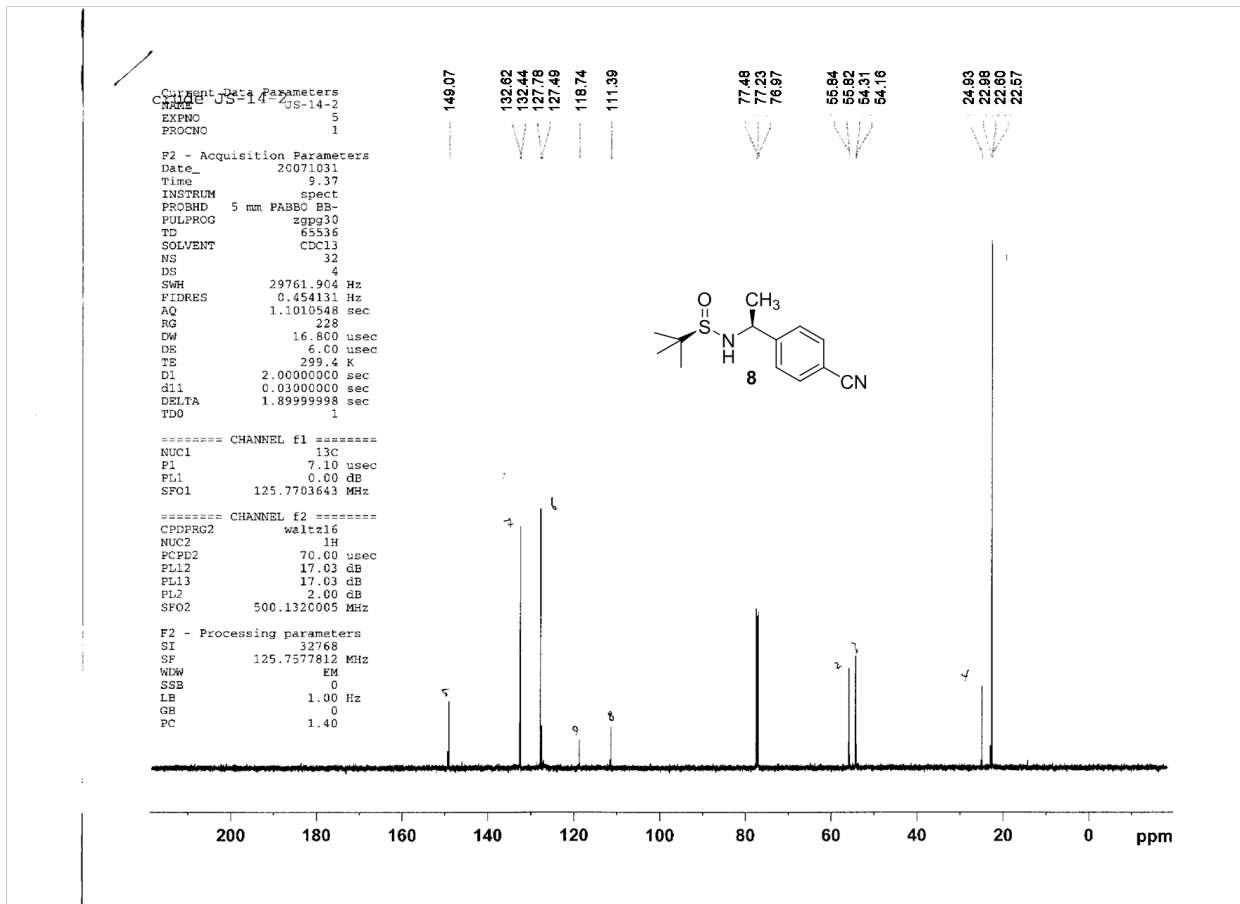
Current Data Parameters
NAME JS-14-2
EXPRO 51
PROCNO 1

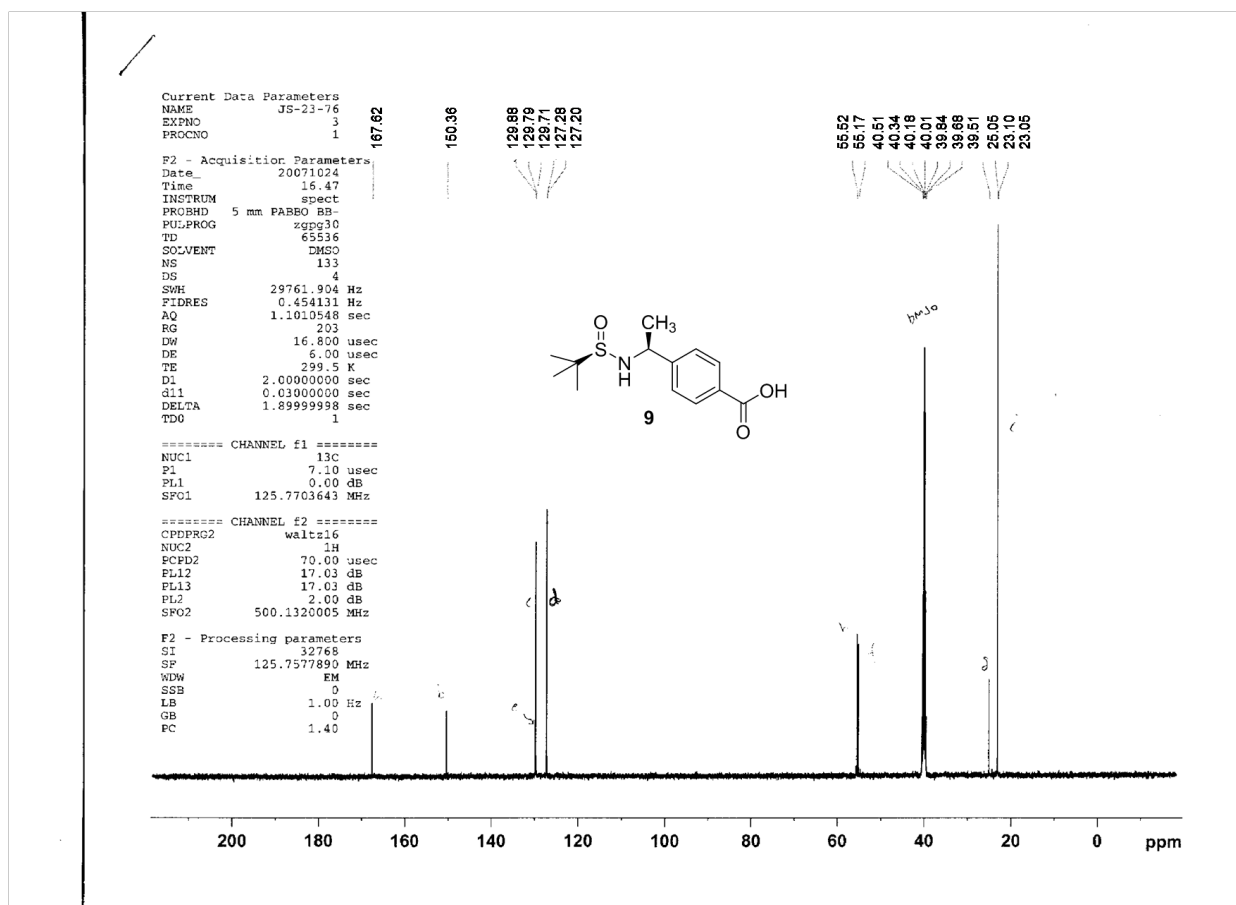
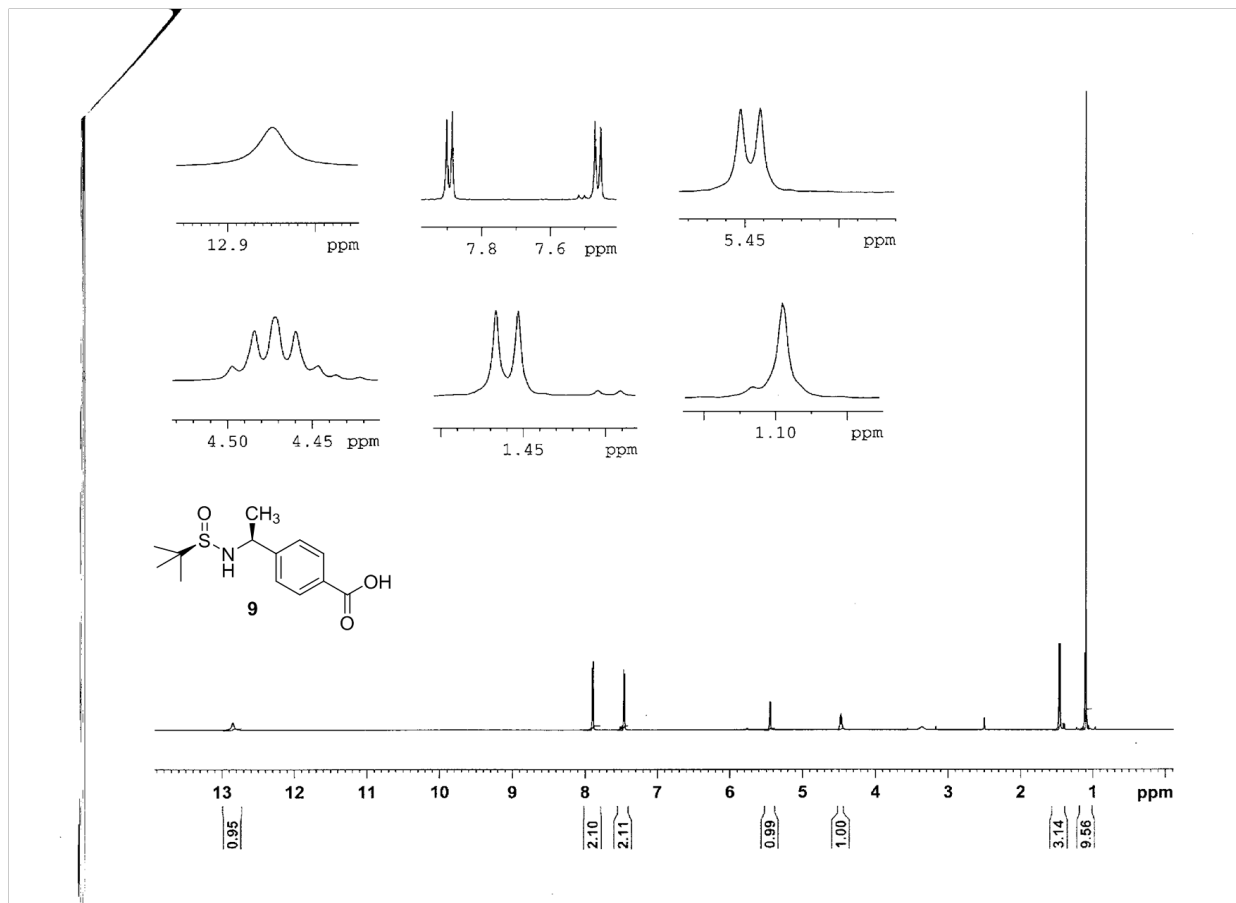
F2 - Acquisition Parameters
Date_ 20061121
Time 10.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 57
DW 48.400 usec
DE 6.00 usec
TE 292.5 K
DS 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
PI 12.40 usec
PL1 2.00 dB
SFO1 500.1300885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







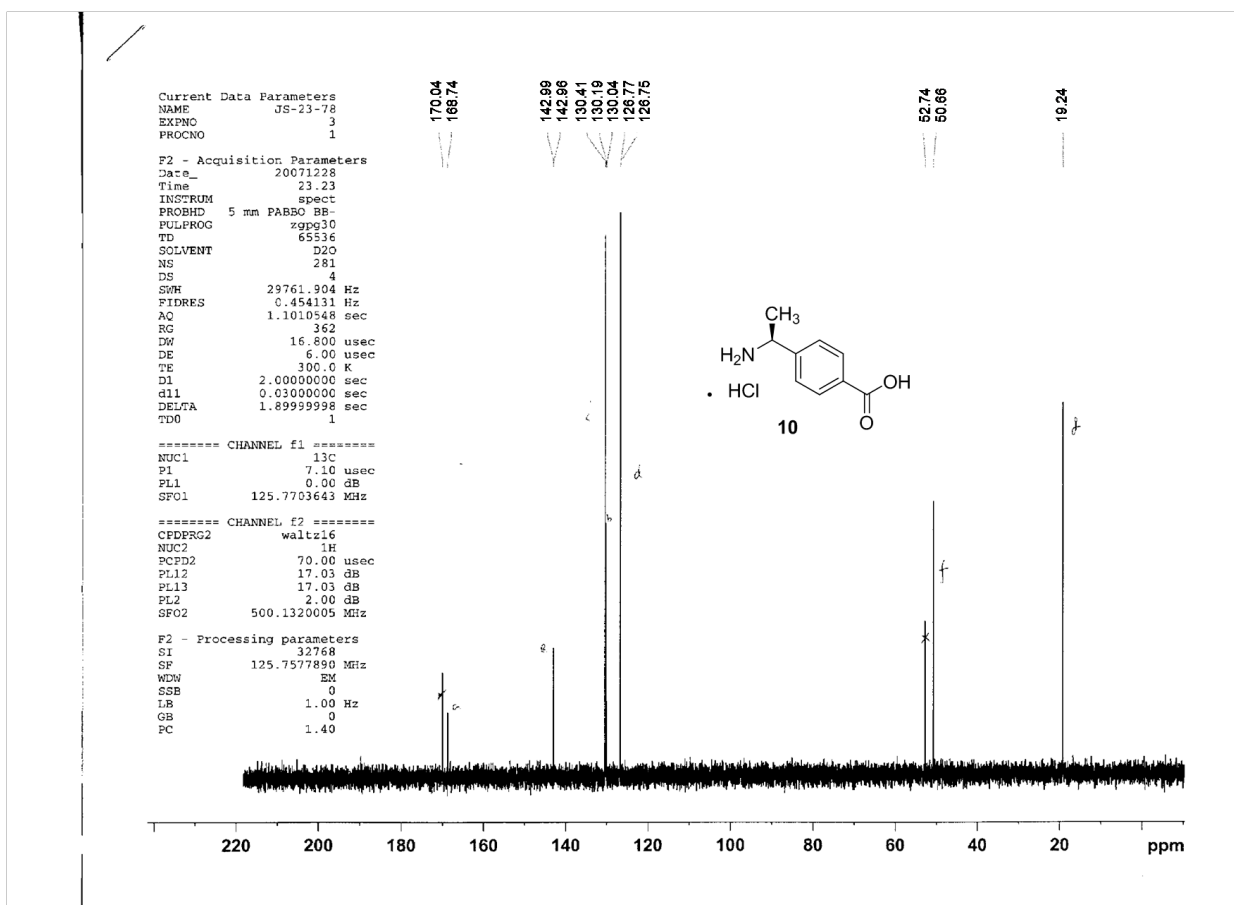
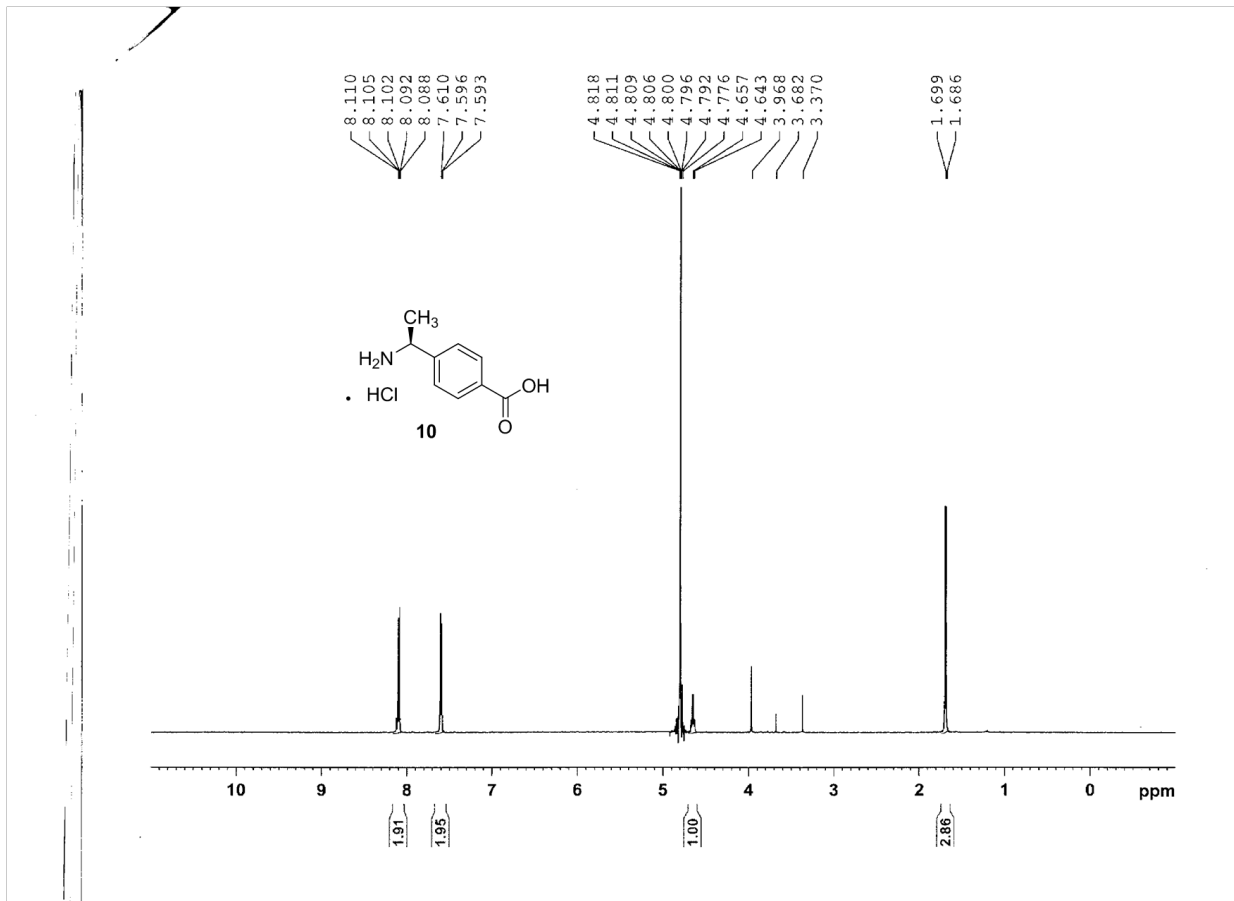
Current Data Parameters
 NAME JS-23-76
 EXPNO 3
 PROCNO 1

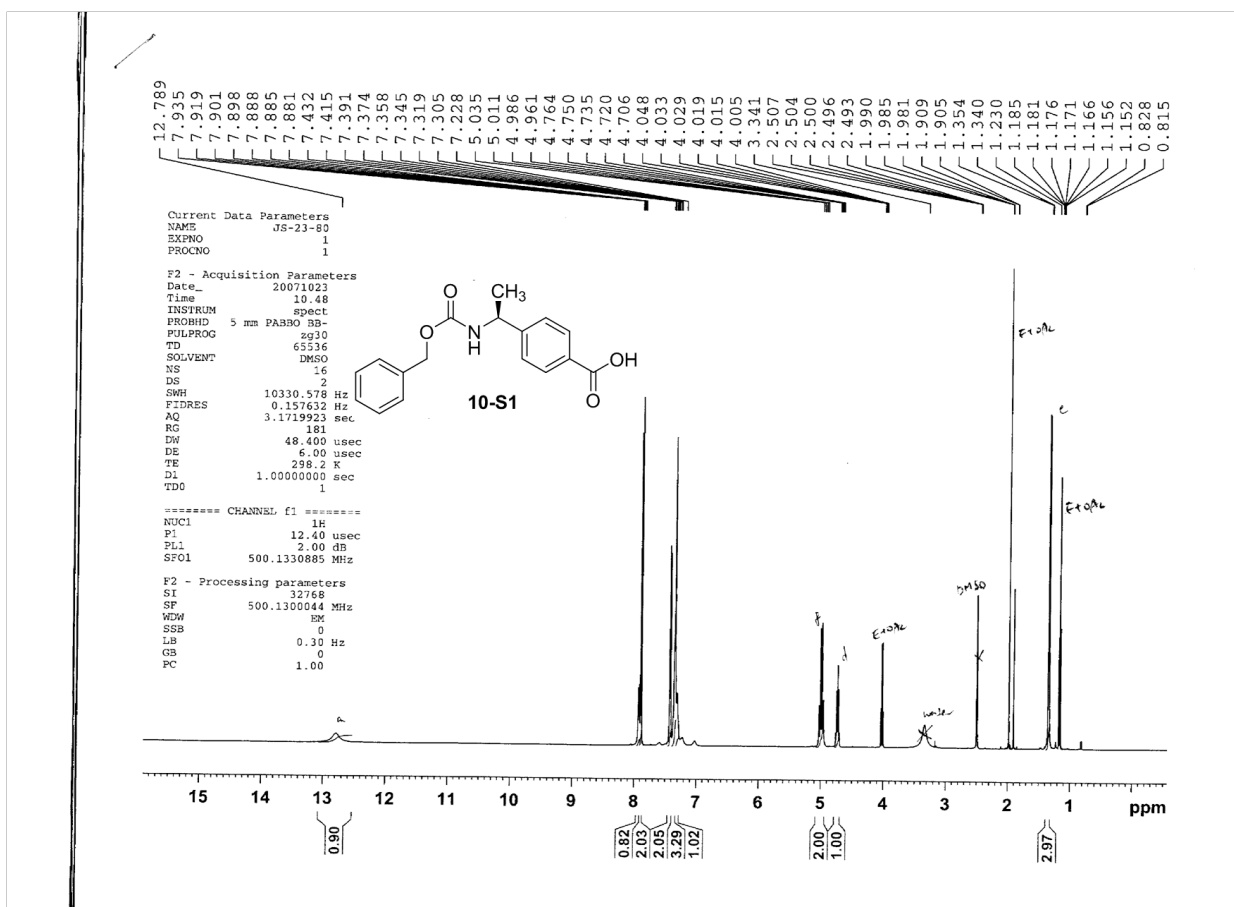
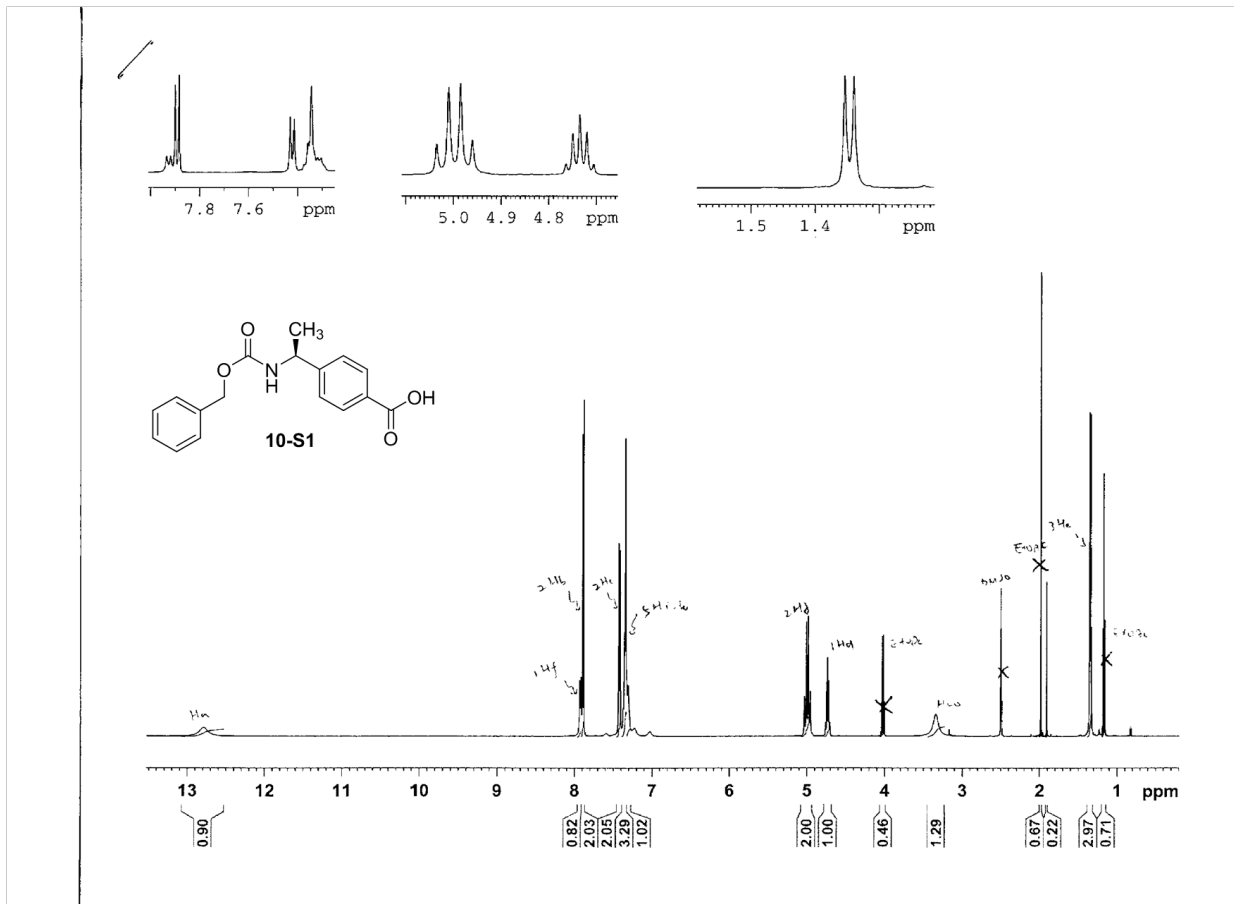
F2 - Acquisition Parameters
 Date_ 20071024
 Time 15.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 133
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 203
 DW 16.800 usec
 DE 6.00 usec
 TE 299.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.10 usec
 PL1 0.00 dB
 SFO1 125.7703643 MHz

===== CHANNEL #2 =====
 CPDPRG2 waltz16
 NUC2 1H
 ECFD2 70.00 usec
 FL12 17.03 dB
 FL13 17.03 dB
 PL2 2.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40





JS-23-80 Chz protection

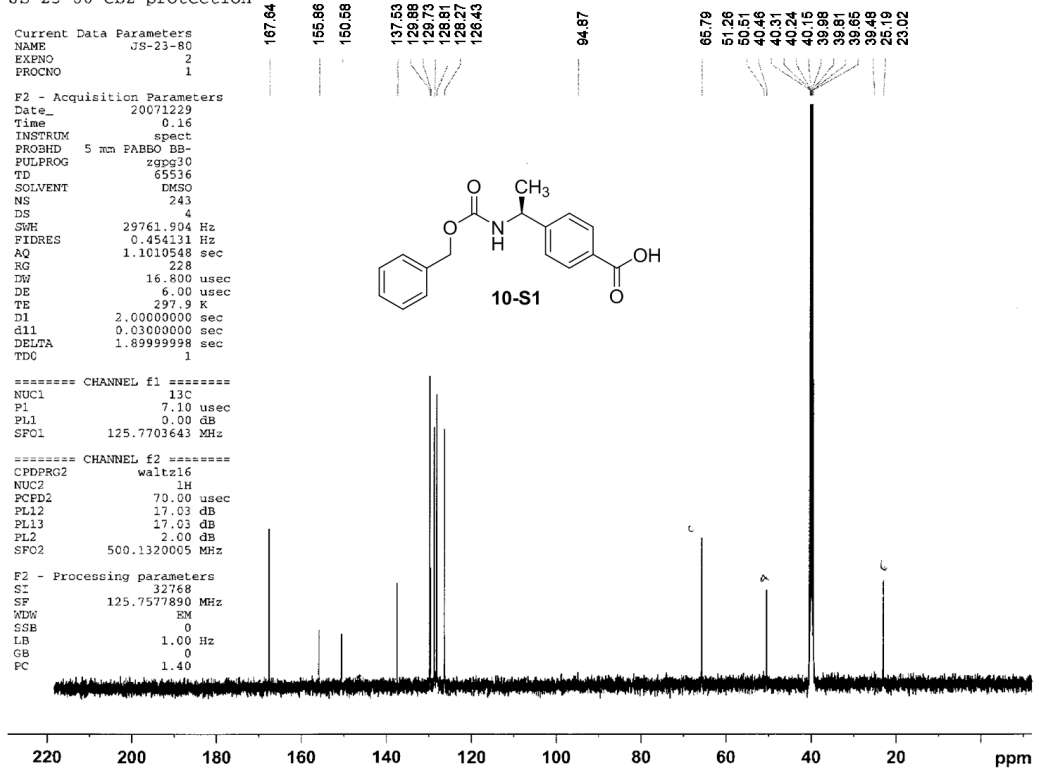
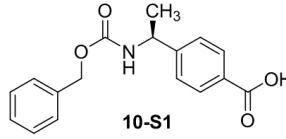
Current Data Parameters
 NAME JS-23-80
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20071229
 Time 0.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 243
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 228
 DW 16.800 usec
 DE 6.00 usec
 TE 297.9 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDC 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 7.10 usec
 PL1 0.00 dB
 SFO1 125.7703643 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL12 17.03 dB
 PL13 17.03 dB
 PL2 2.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

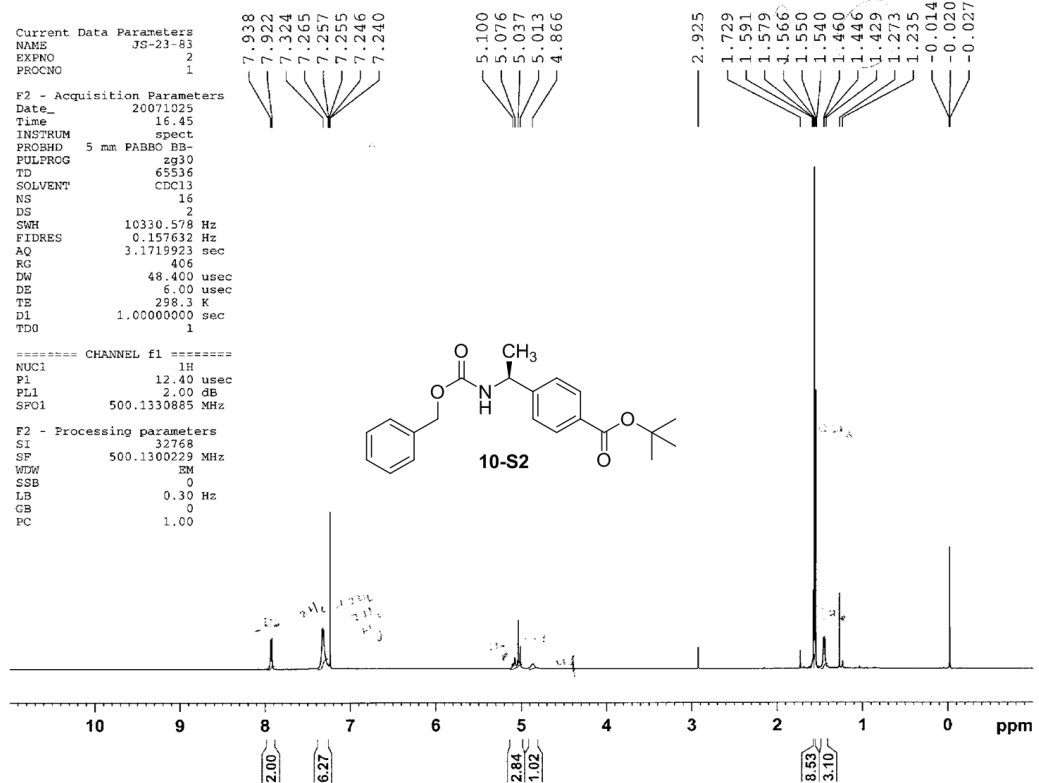
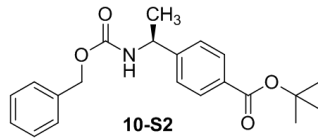


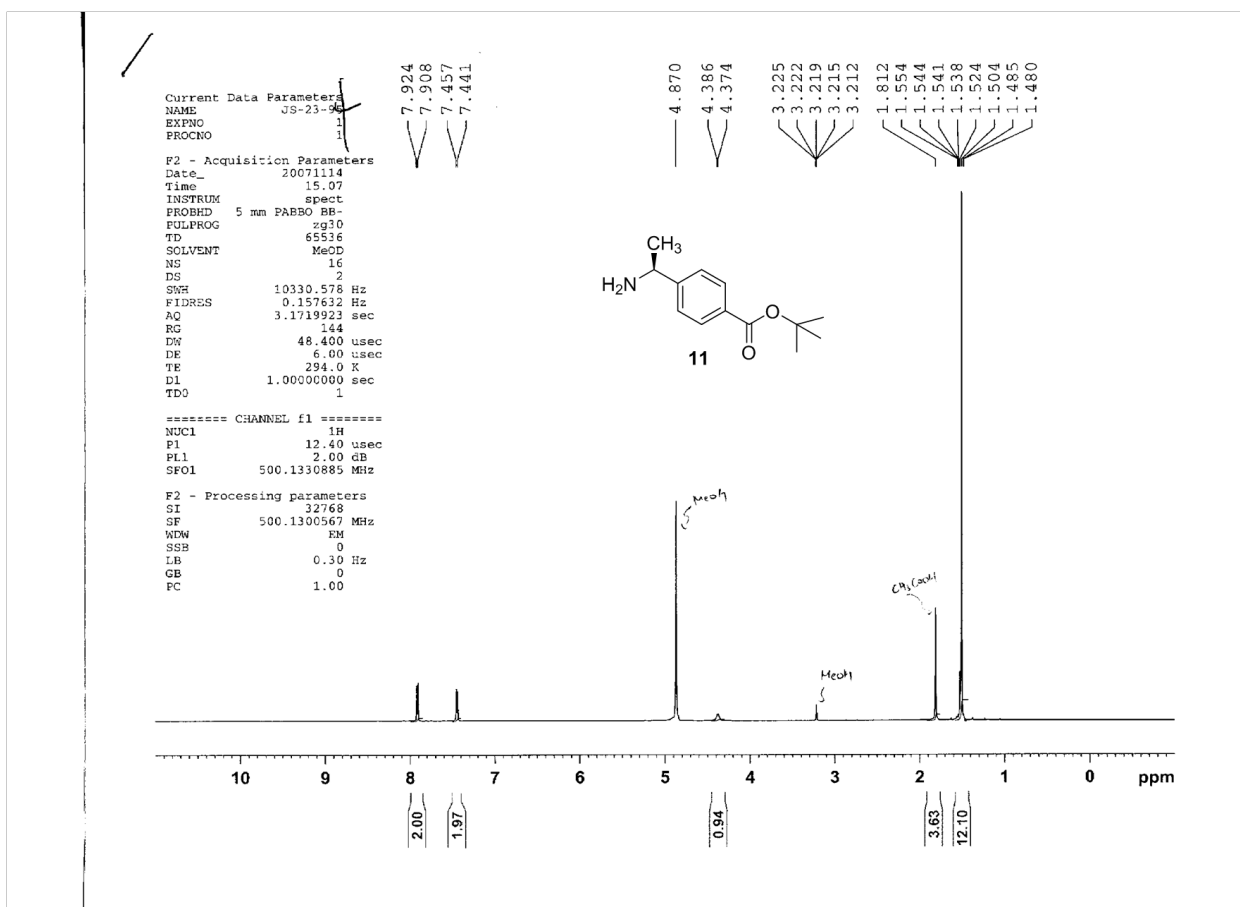
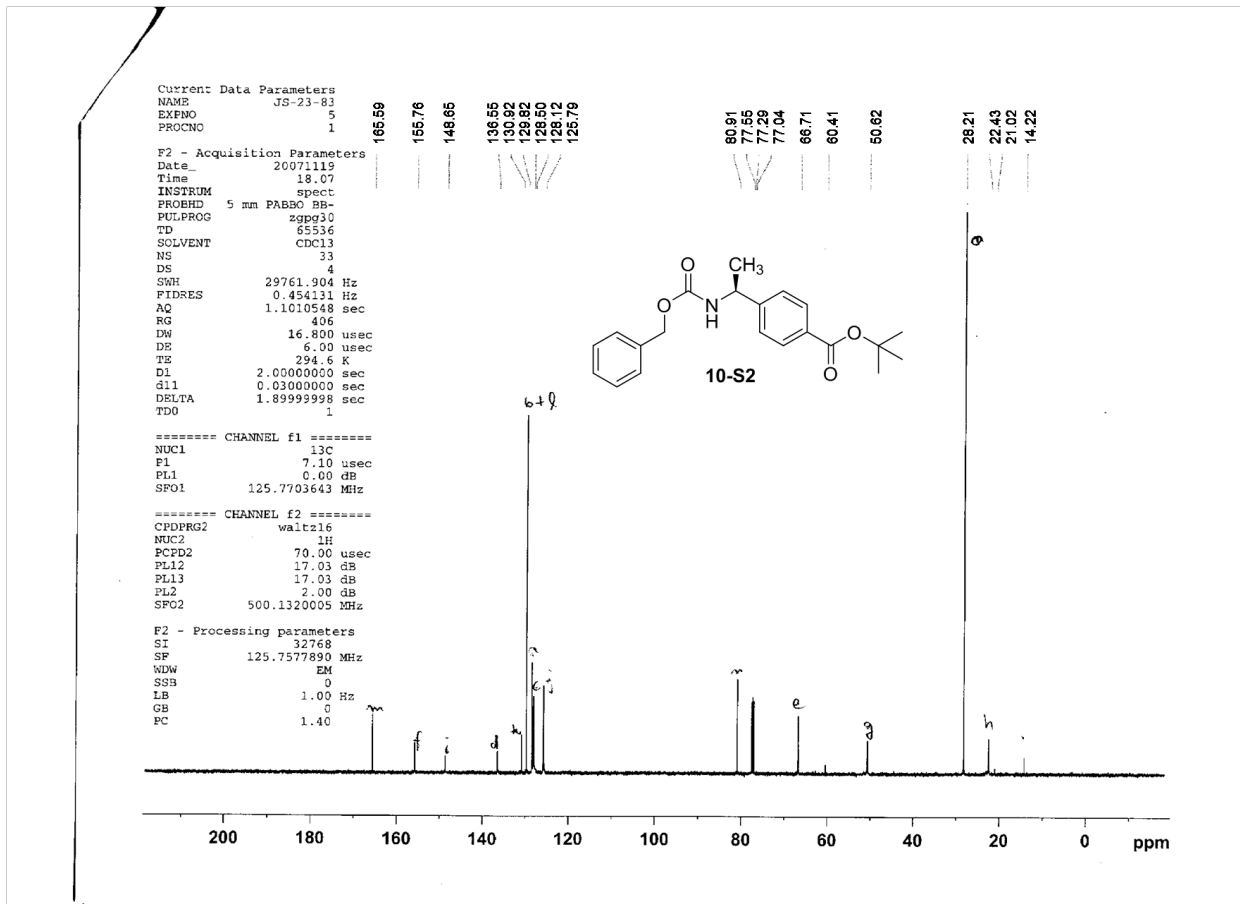
Current Data Parameters
 NAME JS-23-83
 EXPNO 2
 PROCNO 1

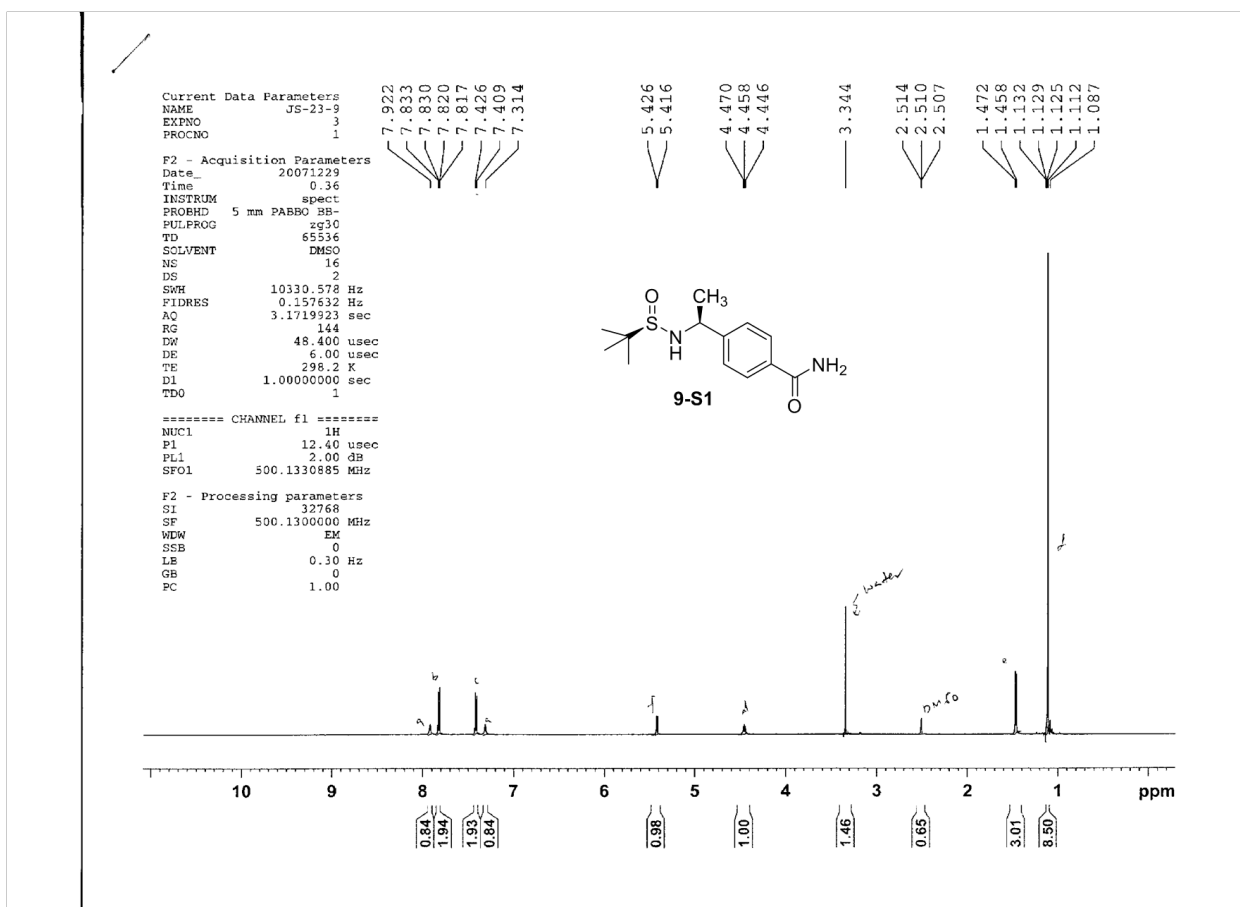
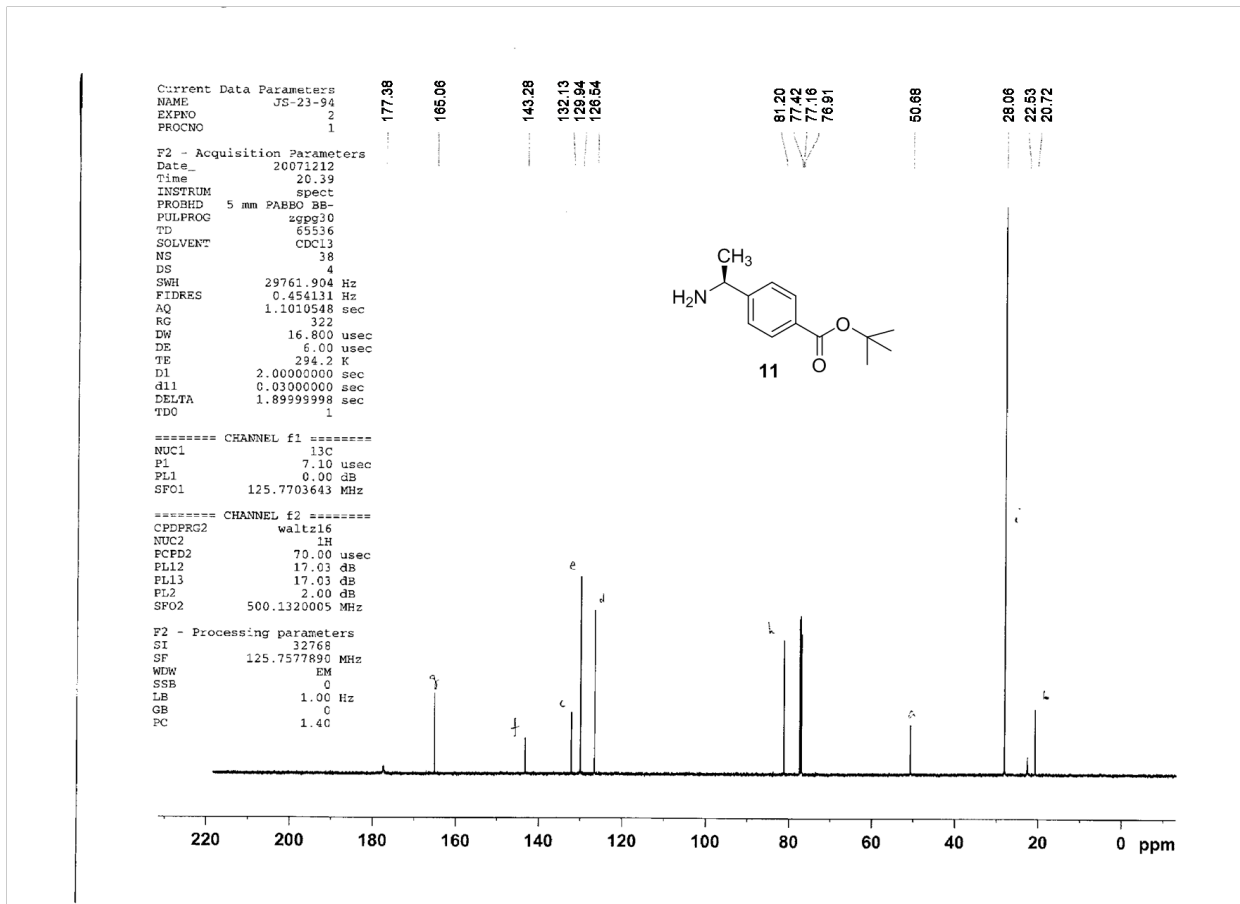
F2 - Acquisition Parameters
 Date_ 20071025
 Time 16.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 406
 DW 48.400 usec
 DE 6.00 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1

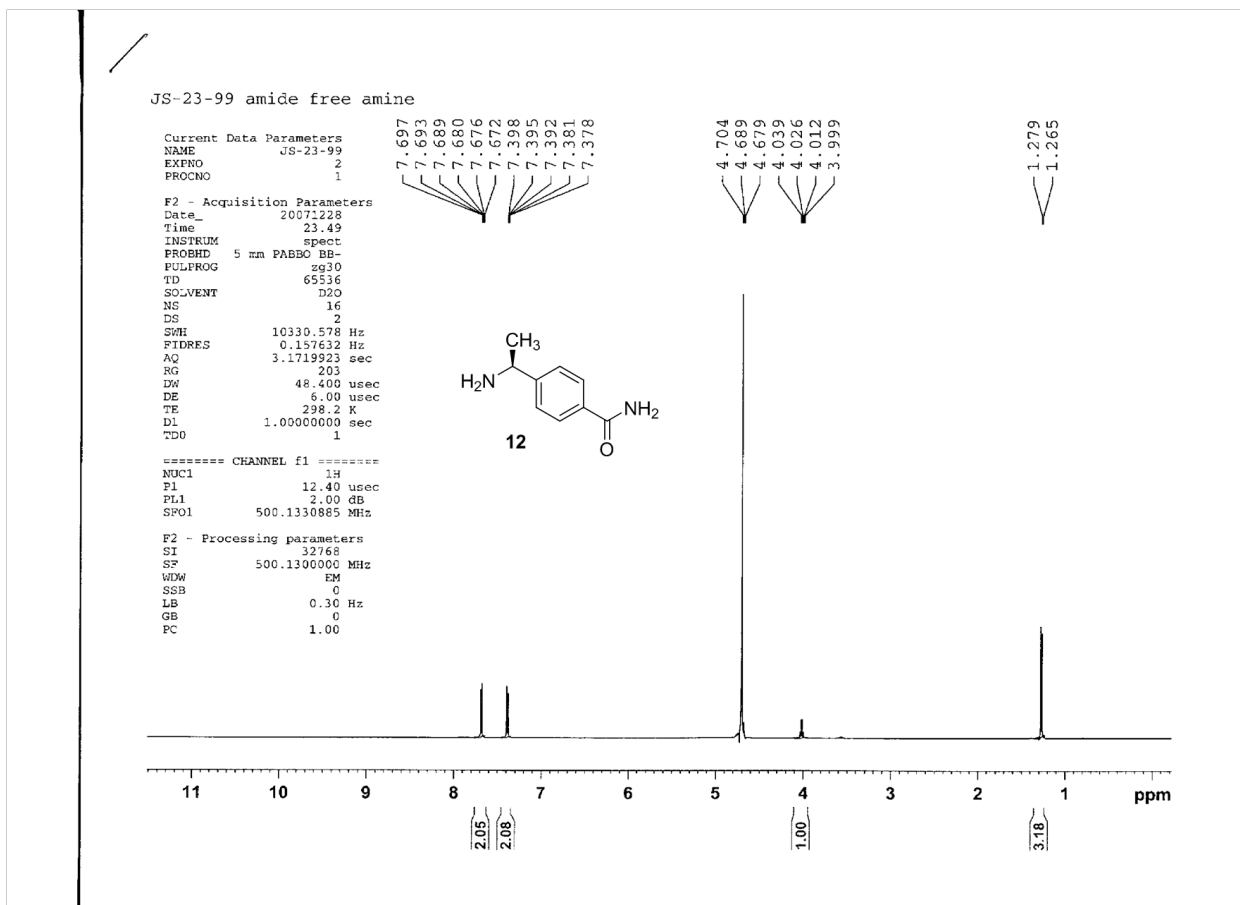
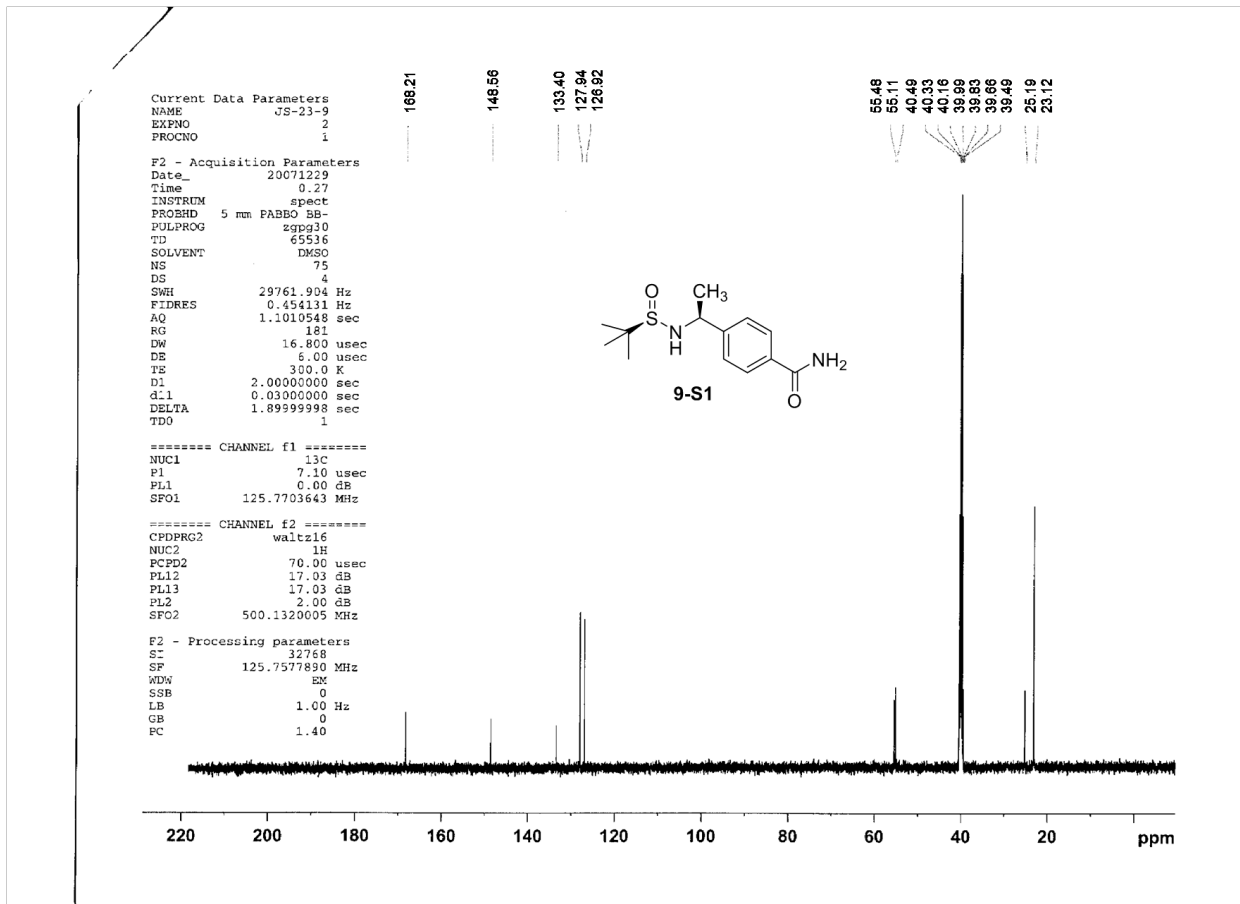
==== CHANNEL f1 =====
 NUC1 1H
 P1 12.40 usec
 PL1 2.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300229 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00









JS-23-99 amide free amine

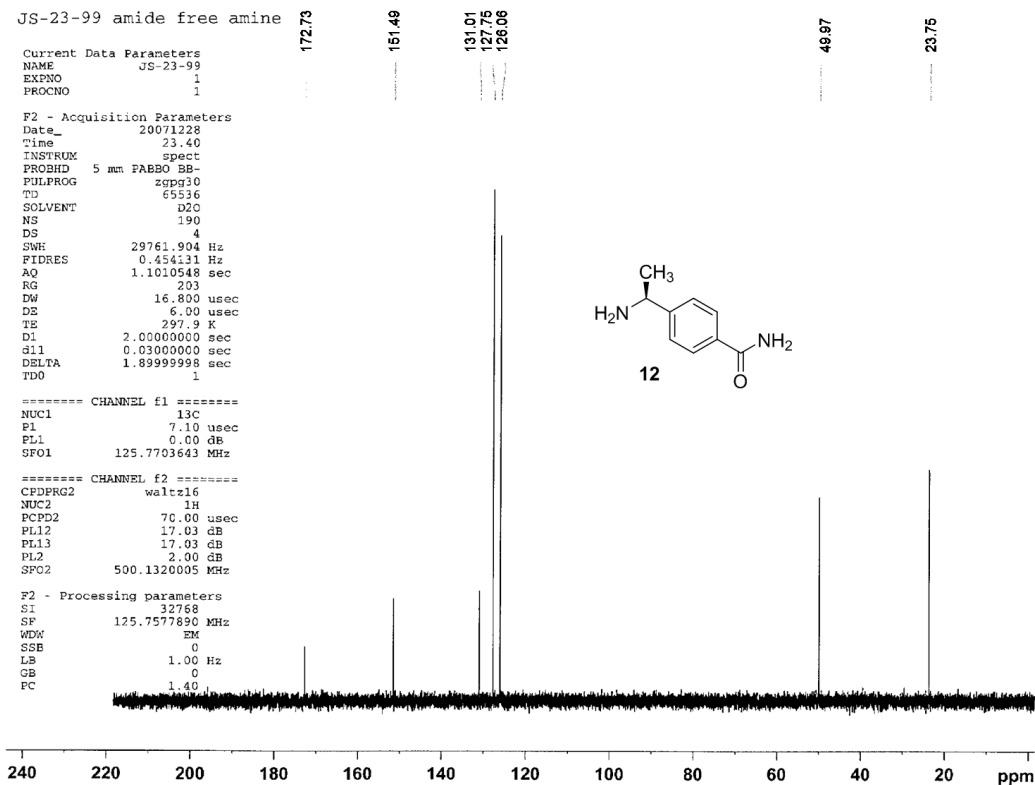
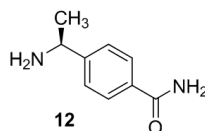
Current Data Parameters
 NAME JS-23-99
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20071228
 Time 23.40
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 190
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454211 Hz
 AQ 1.1010548 sec
 RG 203
 DW 16.800 usec
 DE 6.00 usec
 TE 297.9 K
 DI 2.0000000 sec
 S11 0.0300000 sec
 DELTA 1.8999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 7.10 usec
 PL1 0.00 dB
 SFO1 125.7703643 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 ECPD2 70.00 usec
 PL12 17.03 dB
 PL13 17.03 dB
 PL2 2.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40



Current Data Parameters
 NAME JS-14-77
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20071211
 Time 20.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 228
 DW 48.400 usec
 DE 6.00 usec
 TE 293.3 K
 DI 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 12.40 usec
 PL1 2.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300233 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 FC 1.00

