

Supporting Information For

Post-Synthetic Modification of Tryptophan Containing Peptides via NIS Mediation

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General Conditions

All reactions were run under an inert atmosphere (Ar) with flame-dried glassware using standard techniques for manipulating air-sensitive compounds. 1,4-dioxane were obtained through distillation over Calciumhydride. Commercial reagents were used as supplied or purified by standard techniques where necessary. The dipeptides **1a-1g**, tripeptides **11a-11b** and triazoles **2a-2m** were prepared according to the reported procedures.²² The tetrapeptide **13** was bought from commercial source. Column chromatography was performed using 200-300 mesh silica with the proper solvent system according to TLC analysis using KMnO₄ stain and UV light to visualize the reaction components. Unless otherwise noted, nuclear magnetic resonance spectra were recorded on 400 MHz spectrometer. NMR data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet and bs = broad singlet), coupling constant in Hz and integration. Chemical shifts for ¹³C NMR spectra were recorded in parts per million from tetramethylsilane using the central peak of deuteriochloroform (77.0 ppm), hexadeuterodimethyl sulfoxide (39.5 ppm) as the internal standard. IR spectra were recorded on an FTIR spectrometer (KBr) and reported in reciprocal centimeters (cm⁻¹). HRMS data were obtained using ESI ionization. Mp data were measured with micro melting point apparatus. Electronic absorption spectra were obtained on a Shimadzu UV-3600 UV-visible spectrometer; Photoluminescent spectra were recorded with a Hitachi F-4600 luminescence spectrometer with the excitation and emission slit widths at 2.5 nm. Analytical as well as semi-preparative reversed-phase high-performance liquid chromatography (RP-HPLC) were performed on a LC3000 Binary chromatography system with a UV3000 UV-VIS Detector. The semi-preparative HPLC was performed with a Daisogel C18 10 μm 100 Å column (10 micron, 250 × 30 mm). The flow was 20 mL/min, with the mobile phase starting from 95% solvent A (0.1% TFA in water) and 5% solvent B (0.1% TFA in acetonitrile) (0–5 min) to 5% solvent A and 95% solvent B at 45 min. Analytical HPLC was performed using the same gradient system, but with a Gemini 5 μm C18 110A column (250 × 10 mm) and flow of 2 mL/min. Ultraviolet (UV) absorbance was monitored at 254 nm.

General procedure for NIS mediated coupling reaction of dipeptide **1a** with phenyl *NH*-1,2,3-triazole **2a**. (Condition A)

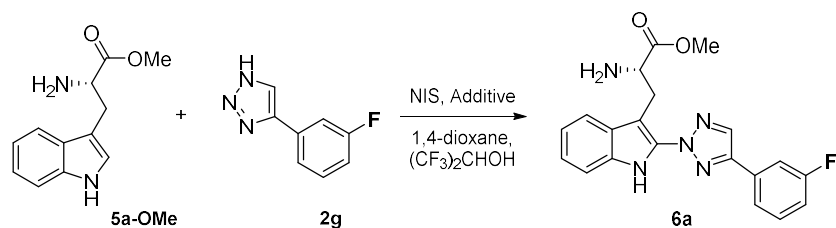
To a solution of peptide **1a** (20 mg, 0.05 mmol), 1,2,3-triazole **2a** (29 mg, 0.2 mmol) and (CF₃)₂CHOH (0.3 mL) in 1,4-dioxane (1 mL), was added dropwise a solution of NIS (*N*-iodosuccinimide, 4 mol equiv) in 1,4-dioxane (1 mL) in 2 hours. 1 hour later, the reaction mixture was quenched by the addition of saturated aqueous Na₂S₂O₃ solution (3 mL), then diluted with EtOAc (20 mL). The organic phase was washed with distilled water (10 mL) and brine (10 mL), and dried with Na₂SO₄.

Concentration of the reaction mixture in vacuum followed by flash column chromatography over SiO₂ (CH₂Cl₂/CH₃OH = 50/1 to 10/1) afforded 24 mg **3a** as a colorless oil in 86% yield.

General procedure for NIS mediated coupling reaction of the esterified tryptophan **5a-OMe with m-fluorophenyl *NH*-1,2,3-triazole **2g**. (Condition B)**

To a solution of peptide **2g** (20 mg, 0.05 mmol), 1,2,3-triazole **5a-OMe** (29 mg, 0.2 mmol), (CF₃)₂CHOH (0.3 mL) and BF₃·Et₂O (56.25 µL, 4.5 mol equiv) in 1,4-dioxane (1 mL), was added dropwise a solution of NIS (2.5 mol equiv) in 1,4-dioxane (0.5 mL) in 2 hours. 1.5 hour later, the reaction mixture was quenched by the addition of saturated aqueous Na₂S₂O₃ solution (1 mL). Concentration of the reaction mixture in vacuum followed by flash column chromatography over SiO₂ (CH₂Cl₂/CH₃OH = 100/1 to 30/1) afforded the crude product, which was then purified through semi-preparative HPLC. The collected fractions were combined and lyophilized to give a fluffy white powder **6a** (14.6 mg, yield 77%); {HPLC condition: Daisogel C-18 10 µm 100 Å column (10 micron, 250 × 30 mm), 30×250 mm, flow: 20 mL/min; linear gradient : 2.25 % CH₃CN (containing 1% CF₃COOH) increased per minute; wavelength: 300 nm}.

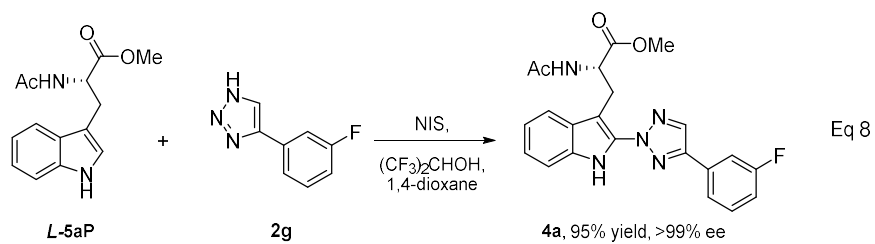
Stable1: Optimization studies of the NIS mediated Coupling reaction of peptide **5a-OMe** with triazole **2g**.^a



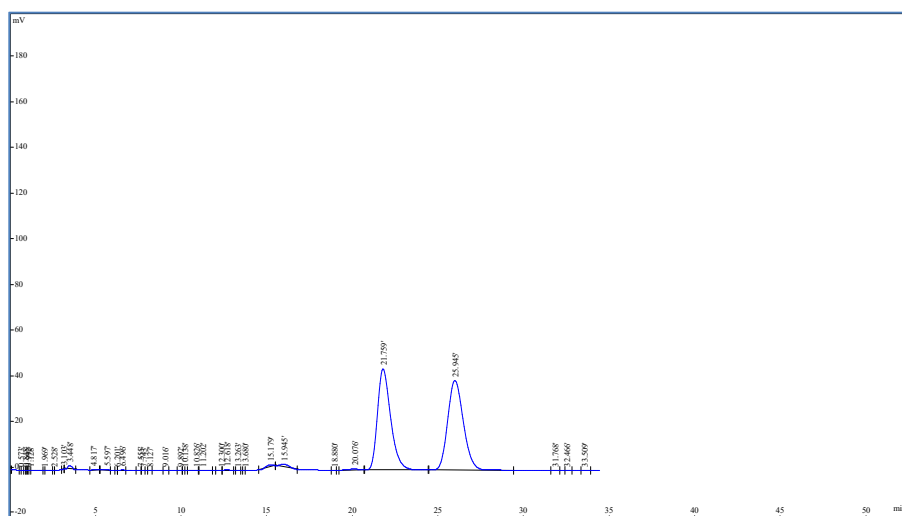
Entry	Additive	Volume [mL]	Time [h]	yield [%] ^b
1			1	trace
2	HCl(4M) ^c	0.25	1	<5%
3	CF_3COOH	0.25	1	trace
4	$\text{CF}_3\text{SO}_3\text{H}$	0.25	1	<5%
5	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	0.025	1	34
6	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	0.056	1	72
7	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	0.056	1.5	77
^a 8 ^d	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	0.056	1.5	trace

Unless noted, all reactions were carried out at 0.05 mmol scale in 2 mL 1,4-dioxane at rt with the addition of 2.5 mol equiv of NIS, 0.3 mL $(\text{CF}_3)_2\text{CHOH}$ (the ratio of **5a-OMe**/**2** = 1/4). ^b Unless noted, the reaction yields were determined by ^1H NMR spectral data of the crude products. ^c 4M HCl solution in 1,4-dioxane. ^d no $(\text{CF}_3)_2\text{CHOH}$ was added.

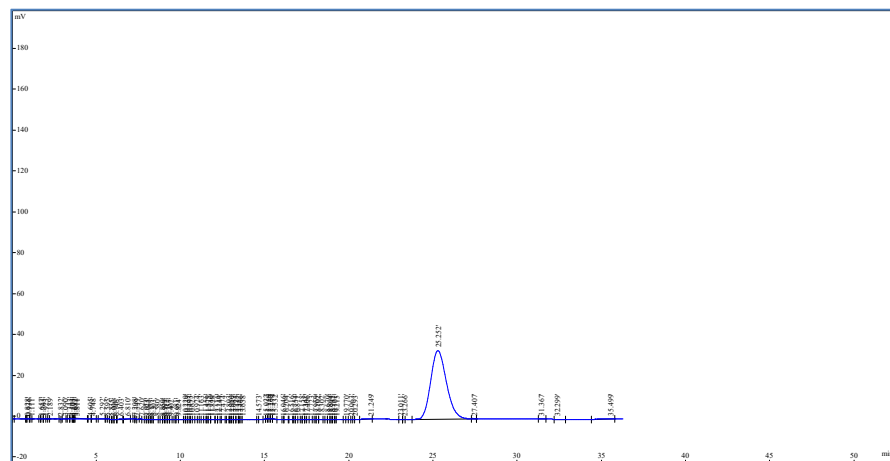
Racemization test experiment for the reaction of **L-5aP** with **2g**.



Racemic-4a's HPLC spectrum.



(*L*)-4a's HPLC spectrum.



HPLC condition: CHIRALPAK AD-H column; iPrOH/n-Hexane = 20/80; Flow = 1mL/min; Wavelength = 300 nm.

The absorption and emission spectra of products¹

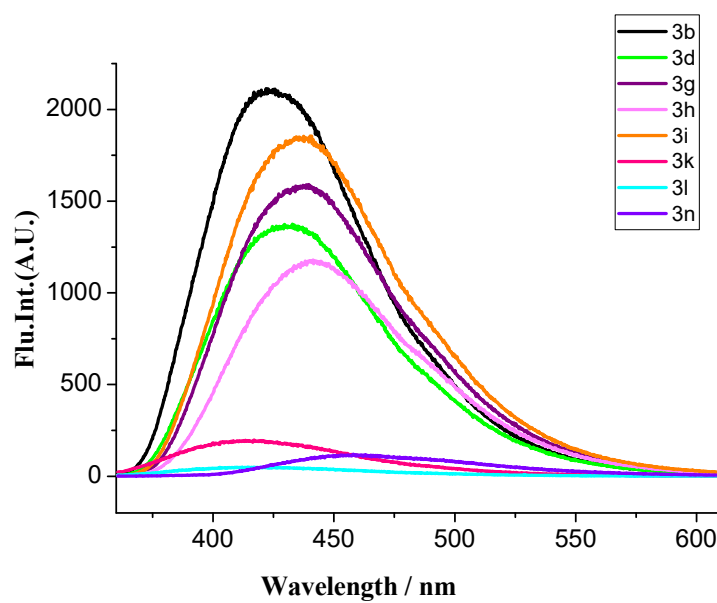
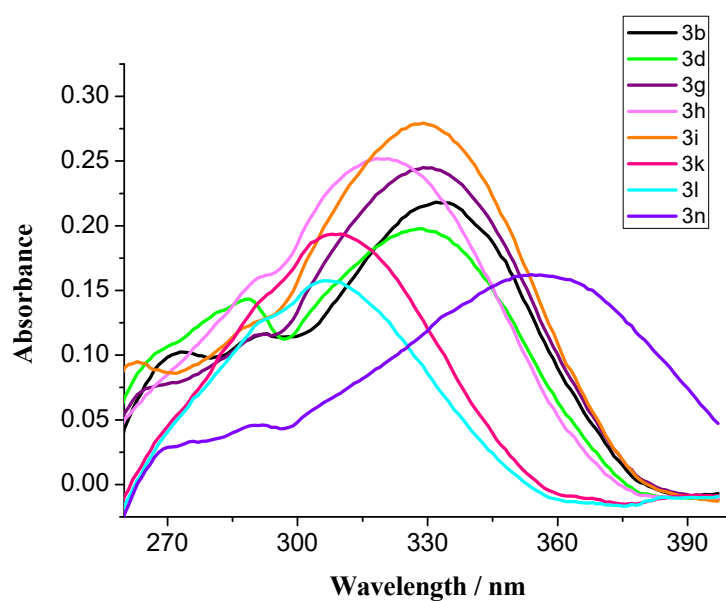
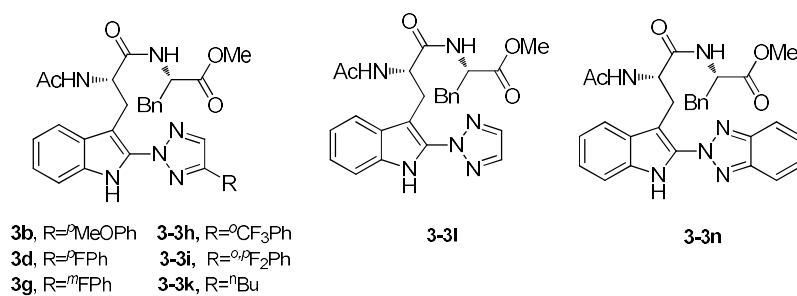
For the method to determine the fluorescence quantum yield:

Fluorescence quantum yield was determined in DMF using optically matching solutions of 9,10-Diphenylanthracene ($\Phi_f = 0.95$ in cyclohexane) as standard at an excitation wavelength of 350 nm and the quantum yield was calculated using the following equation:

$$\Phi_f = \Phi_r (A_r F_s / A_s F_r) (n_s^2 / n_r^2)$$

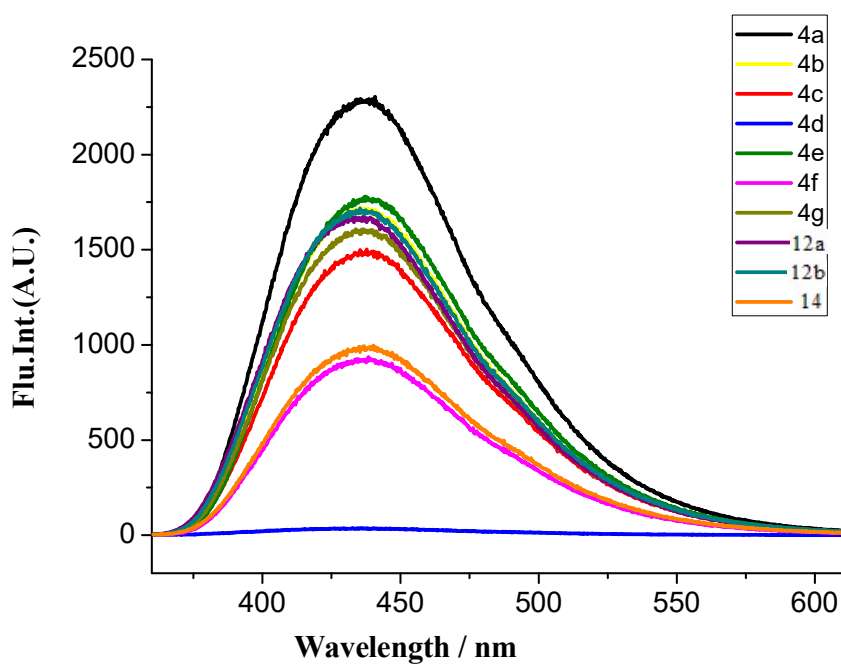
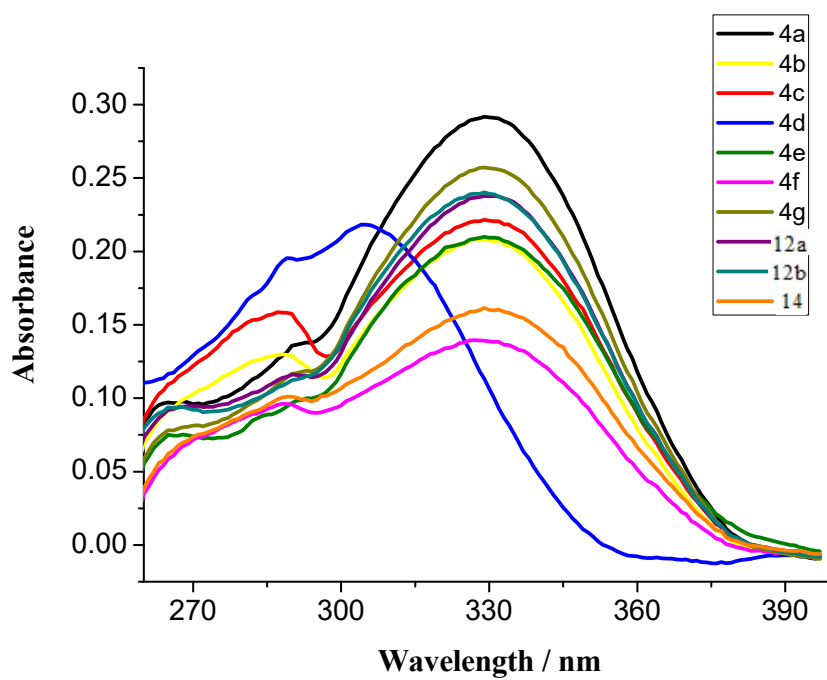
where, A_s and A_r are the absorbance of the sample and the reference, respectively, at the same excitation wavelength, F_s and F_r are the corresponding relative integrated fluorescence intensities, and n is the refractive index of the solvent.

The absorption and emission spectra of products **3(b, d, g, h, I, k, l, n)**:



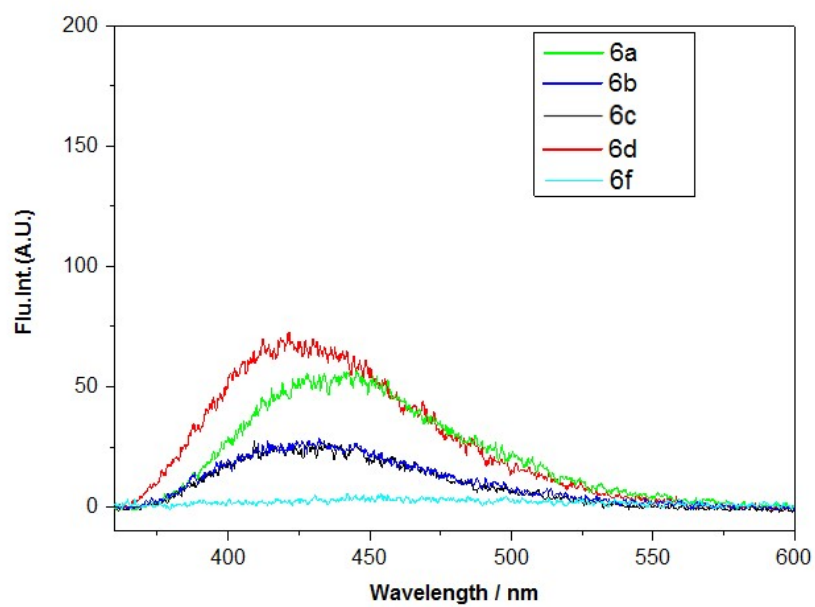
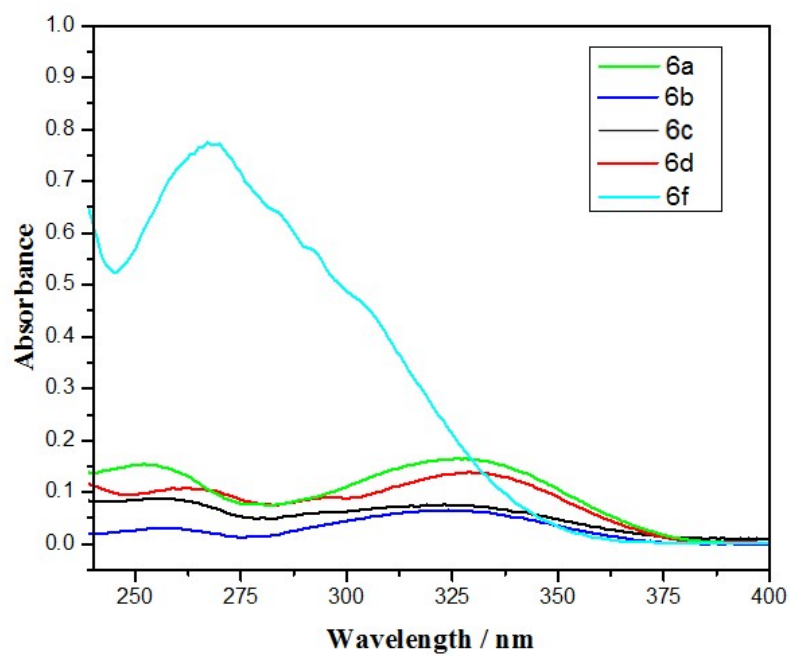
Sample preparation: 1.0×10^{-5} mol/L in CH₂Cl₂, with 2.5 nm slit.

The absorption and emission spectra of products **4(a-g)**、**12(a-b)**、**14**:



Sample preparation: 1.0×10^{-5} mol/L in CH_2Cl_2 , with 2.5 slit.

The absorption and emission spectra of products **6a**, **6b**, **6c**, **6d**, **6f**



Sample preparation: 1.0×10^{-5} mol/L in CH₃OH, with 2.5 slit.

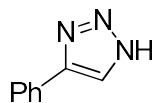
Stable 2. Fluorescence quantum yield of products (DMF as solvent)

Entry	Φ_f
3a	0.69
3b	0.78
3c	0.69
3d	0.63
3e	0.30
3f	0.47
3g	0.41
3h	0.44
3i	0.57
3j	0.58
3k	0.32
3l	0.13
3m	0.09
3n	0.03
4a	0.63
4b	0.57
4c	0.38
4d	0.10
4e	0.57
4f	0.39
4g	0.42
12a	0.57
12b	0.56
14	0.31

Stable 3. Fluorescence quantum yield of products 3b and 12a in different solvents.

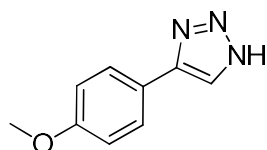
Solvent	Fluorescence quantum	Fluorescence quantum
	yield $\Phi_f(3b)$	yield $\Phi_f(12a)$
H ₂ O	0.01	0.18
HOCH ₂ CH ₂ OH	0.33	0.12
Petroleum ether	0.67	0.48
THF	0.55	0.21
CH ₃ CH ₂ OH	0.38	0.13
CH ₃ CN	0.32	0.25
EtOAc	0.56	0.45
CH ₂ Cl ₂	0.71	0.41
CH ₃ OH	0.22	0.05
ⁱ PrOH	0.29	0.07
Acetone	0.23	0.26
Toluene	0.60	0.22
1,4-Dioxane	0.53	0.41
Cyclohexanol	0.52	0.27
Cyclohexane	0.88	0.60
DMSO	0.47	0.37

Characterization Data:



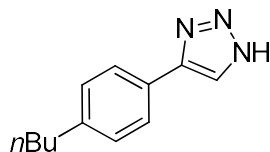
4-Phenyl-1*H*-1,2,3-triazole 2a:²

¹H NMR (400 MHz, (CD₃)₂SO): δ 8.34 (s, 1H), 7.89 (d, J = 7.5Hz, 2H), 7.44 (t, J = 7.5Hz, 2H), 7.34 (t, J = 7.3Hz, 1H); ¹³C NMR (100 MHz, (CD₃)₂SO): δ 146.5, 143.4, 131.1, 129.4, 128.6, 126.0.



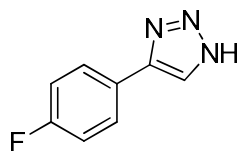
4-(4-Methoxyphenyl)-1*H*-1,2,3-triazole 2b: ²

¹H NMR (400 MHz, CD₃OD): δ 7.99 (s, 1H), 7.69 (d, J = 7.6Hz, 2H), 6.95 (d, J = 7.8Hz, 2H), 3.77 (s, 3H); ¹³C NMR (100 MHz, CD₃OD): δ 160.1, 145.1, 144.1, 126.9, 122.1, 114.0, 54.3.



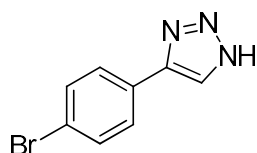
4-(4-Butylphenyl)-1*H*-1,2,3-triazole 2c: ²

¹H NMR (400 MHz, CD₃OD): δ 8.00 (s, 1H), 7.65 (d, J = 8.0Hz, 2H), 7.13 (d, J = 8.0Hz, 2H), 2.50 (t, J = 7.6Hz, 2H), 1.52-1.45 (m, 2H), 1.29-1.20 (m, 2H), 0.83 (t, J = 7.3Hz, 3H); ¹³C NMR (100 MHz, CD₃OD): δ 145.6, 143.2, 128.7, 128.4, 127.0, 125.6, 35.0, 33.3, 22.0, 13.0.



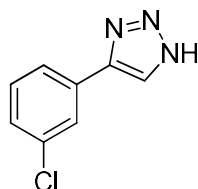
4-(4-Fluorophenyl)-1*H*-1,2,3-triazole 2d: ²

¹H NMR (400 MHz, (CD₃)₂SO): δ 8.33(s, 1H), 7.91 (dd, J = 8.4, 5.6Hz, 2H), 7.27 (t, J = 8.8Hz, 2H); ¹³C NMR (100 MHz, (CD₃)₂SO): δ 162.4 (d, J = 243.3Hz), 145.5, 130.3, 128.0 (d, J = 7.7Hz), 127.6, 116.3 (d, J = 21.5Hz).



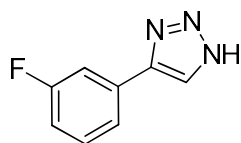
4-(4-bromophenyl)-1H-1,2,3-triazole 2e:²

¹H NMR (400 MHz, (CD₃)₂SO): δ 8.38(s, 1H), 7.82 (d, J = 8.3Hz, 2H), 7.62 (d, J = 8.3Hz, 2H); ¹³C NMR (100 MHz, (CD₃)₂SO): δ 144.9, 132.3, 130.2, 128.0, 121.6.



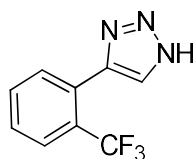
4-(3-Chlorophenyl)-1H-1,2,3-triazole 2f:²

¹H NMR (400 MHz, (CD₃)₂SO): δ 8.44(s, 1H), 7.91 (s, 1H), 7.82 (d, J = 7.7Hz, 1 H), 7.44 (t, J = 7.9Hz, 1H), 7.36 (d, J = 8.1Hz, 1H); ¹³C NMR (100 MHz, (CD₃)₂SO): δ 144.9, 134.2, 133.0, 131.3, 129.4, 128.3, 125.6, 124.5.



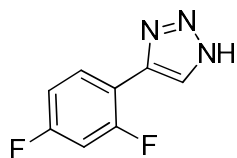
4-(3-Fluorophenyl)-1H-1,2,3-triazole 2g:²

¹H NMR (400 MHz, CD₃OD): δ 8.15(s, 1H), 7.61 (d, J = 7.6Hz, 1H), 7.55 (d, J = 8.8Hz, 1H), 7.42-7.37 (m, 1H), 7.05 -7.01 (m, 1H); ¹³C NMR (100 MHz, CD₃OD): δ 163.2 (d, J = 242.9Hz), 145.2, 132.4, 130.4 (d, J = 8.4Hz), 126.7, 121.3, 114.6 (d, J = 21.3Hz), 112.2 (d, J = 21.2Hz).



4-(2-(Trifluoromethyl)phenyl)-1H-1,2,3-triazole 2h:²

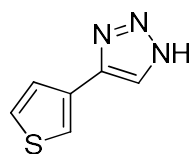
¹H NMR (400 MHz, CD₃OD): δ 7.92 (s, 1H), 7.78 (m, 1H), 7.66 (m, 2H), 7.56 (m, 1H); ¹³C NMR (100 MHz, CD₃OD): δ 143.1, 131.9, 129.1, 128.7, 128.3 (d, J = 30.4 Hz), 127.7 (d, J = 30.1Hz), 125.9 (dd, J = 10.7, 5.3Hz), 124.1(d, J = 271.1Hz), 120.0;



4-(2,4-Difluorophenyl)-1H-1,2,3-triazole 2i: ²

¹H NMR (400 MHz, CD₃OD): δ 8.00(s, 1H), 7.97-7.93 (m, 1H), 6.98-6.94 (m, 2H);

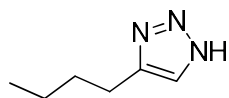
¹³C NMR (100 MHz, CD₃OD): δ 162.7 (dd, J = 247.9, 12.3Hz), 159.5 (dd, J = 249.1, 11.5Hz), 139.3, 128.9, 127.2, 114.5, 111.5 (d, J = 21.6Hz), 103.8 (t, J = 25.9Hz).



4-(Thiophen-3-yl)-1H-1,2,3-triazole 2j: ²

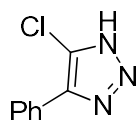
¹H NMR (400 MHz, CD₃OD): δ 8.01 (s, 1H), 7.75-7.74 (m, 1H), 7.48 (s, 1H), 7.47 (s,

1H); ¹³C NMR (100 MHz, CD₃OD): δ 141.7, 130.8, 126.3, 125.5, 121.4.



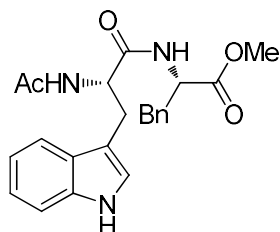
4-Butyl-1H-1,2,3-triazole 2k: ²

¹H NMR (400 MHz, CDCl₃): δ 7.51 (s, 1H), 2.75 (t, J = 7.6Hz, 2 H), 1.71-1.64 (m, 2H), 1.42-1.36 (m, 2H), 0.94 (t, J = 7.4Hz, 3H); ¹³C NMR (100 MHz, CD₃OD): δ 144.0, 128.0, 31.1, 23.6, 21.9, 12.9.



5-Chloro-4-phenyl-1H-1,2,3-triazole 2m: ³

¹H NMR (400 MHz, CD₃OD): δ 7.84 (d, J = 7.3Hz, 2H), 7.45(t, J = 7.1Hz, 2H), 7.40 (d, J = 7.2Hz, 1H); ¹³C NMR (100 MHz, CD₃OD): δ 139.5, 132.3 128.6, 128.4, 127.9, 126.6.

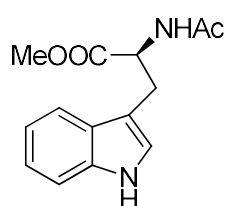


(S)-Methyl

2-((S)-2-acetamido-3-(1H-indol-3-yl)propanamido)-3-phenyl

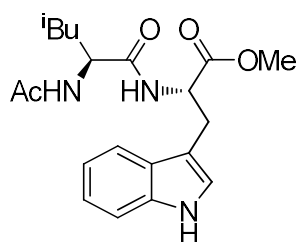
propanoate 1a:⁵

¹H NMR (400 MHz, CDCl₃): δ 8.58 (br, 1H), 7.64 (d, J = 7.8 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 7.17-7.14 (m, 4H), 7.08 (t, J = 7.6 Hz, 1H), 6.98 (s, 1H), 6.91-6.89 (m, 2H), 6.57 (d, J = 7.5 Hz, 1H), 6.52 (d, J = 7.5 Hz, 1H), 4.77 (q, J = 7.4 Hz, 1H), 4.69 (q, J = 6.4 Hz, 1H), 3.59 (s, 3H), 3.24 (dd, J = 14.6 Hz, 5.7 Hz, 1H), 3.13 (dd, J = 14.6 Hz, 7.6 Hz, 1H), 2.99 (dd, J = 13.8 Hz, 5.8 Hz, 1H), 2.90 (dd, J = 13.8 Hz, 6.5 Hz, 1H), 1.89 (s, 9H); ¹³C NMR (100 MHz, CDCl₃): δ 171.4, 171.2, 170.3, 136.2, 135.6, 129.2, 128.5, 127.5, 127.0, 123.5, 122.0, 119.6, 118.7, 111.4, 110.2, 53.8, 53.5, 52.3, 37.8, 28.2, 23.1.



(S)-Methyl 2-acetamido-3-(1H-indol-3-yl)propanoate 1b:⁴

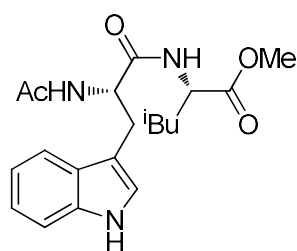
¹H NMR (400 MHz, (CD₃)₂SO): δ 10.90 (br, 1H), 8.36 (d, J = 7.5 Hz, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H), 7.18 (br, 1H), 7.09 (t, J = 7.2 Hz, 1H), 7.01 (t, J = 7.4 Hz, 1H), 4.57-4.51 (m, 1H), 3.59 (s, 3H), 3.18 (dd, J = 13.9 Hz, 5.2 Hz, 1H), 3.05 (dd, J = 14.5 Hz, 8.4 Hz, 1H), 1.84 (s, 3H); ¹³C NMR (100 MHz, (CD₃)₂SO): δ 173.0, 169.9, 136.5, 127.5, 124.1, 121.4, 118.9, 118.4, 111.9, 109.9, 53.6, 52.2, 27.6, 22.7.



(S)-Methyl 2-((S)-2-acetamido-4-methylpentanamido)-3-(1H-indol-3-yl)propanoate 1c:⁵

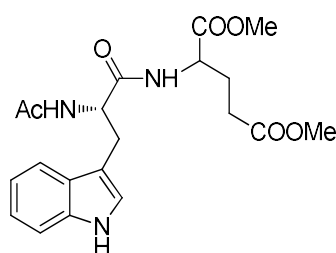
¹H NMR (400 MHz, CD₃OD): δ 7.51 (d, J = 7.8 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 7.08 (t, J = 7.4 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 4.75-4.71 (m, 1H), 4.23 (d, J = 8.0 Hz, 1H), 3.62 (s, 3H), 3.27 (d, J = 6.0 Hz, 1H), 3.17 (dd, J = 14.6 Hz, 7.7 Hz, 1H), 1.93 (s, 3H), 1.84-1.76 (m, 1H), 1.51-1.45 (m, 1H), 1.16-1.09 (m, 1H), 0.88 (t, J = 6.6 Hz, 6H); ¹³C NMR (100 MHz, CD₃OD): δ 172.4, 172.3, 171.7, 136.5, 127.2, 123.2, 121.0,

118.4, 117.7, 110.8, 109.1, 57.7, 53.4, 51.2, 36.6, 27.0, 24.4, 21.0, 14.3, 9.9.



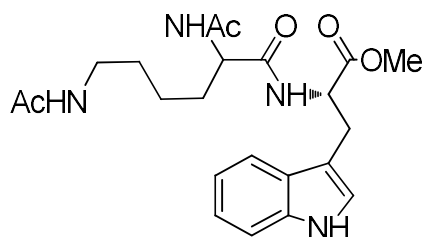
(S)-Methyl 2-((S)-2-acetamido-3-(1H-indol-3-yl)propanamido)-4-methylpentanoate 1d: ⁵

¹H NMR (400 MHz, CDCl₃): δ (major) 8.32 (br, 1H), 7.70 (d, J =7.8Hz, 1H), 7.34 (d, J =8Hz, 1H), 7.18 (t, J =7.16Hz, 1H), 7.13-7.04 (m, 2H), 6.45 (d, J =7.52Hz, 1H), 6.38-6.33 (m, 1H), 4.82-4.77 (m, 1H), 4.42-4.36 (m, 1H), 3.62 (s, 3H), 3.31-3.26 (m, 1H), 3.17-3.11 (m, 1H), 1.96 (s, 3H), 1.75 (br, 1H), 1.32-1.25 (m, 1H), 1.05-0.96 (m, 1H), 0.85-0.81 (m, 2H), 0.77 (s, 3H), 0.60 (d, J =6.88Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 172.1, 171.8, 170.4, 136.3, 127.6, 123.5, 121.9, 119.5, 118.7, 111.3, 110.3, 56.8, 54.0, 52.0, 37.6, 28.5, 25.1, 23.1, 15.3, 11.6.



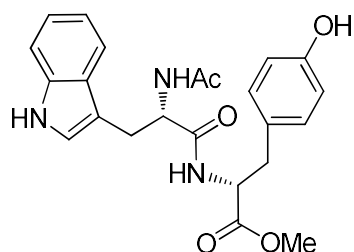
Dimethyl 2-((S)-2-acetamido-3-(1H-indol-3-yl)propanamido)pentanedioate 1e: ⁵

¹H NMR (400 MHz, CDCl₃): δ (major isomer) 8.56 (br, 1H), 7.60 (d, J =7.84Hz, 1H), 7.32-7.29 (m, 1H), 7.16-7.12 (m, 1H), 7.09-7.15 (m, 2H), 6.88 (d, J =4.76Hz, 1H), 6.64 (d, J =5.16Hz, 1H), 4.82-4.71 (m, 1H), 4.46-4.41 (m, 1H), 3.61 (s, 3H), 3.59 (s, 3H), 3.27-3.22 (m, 1H), 3.19-3.14 (m, 1H), 2.32-2.16 (m, 2H), 2.12-2.03 (m, 1H), 1.94 (s, 3H), 1.91-1.82 (m, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 173.2, 171.6, 170.5, 136.2, 127.7, 123.4, 122.0, 119.6, 118.5, 111.3, 110.1, 54.0, 52.4, 51.8, 29.7, 28.3, 27.0, 23.0.



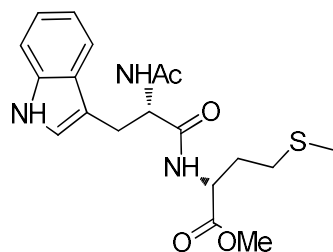
(2S)-Methyl 2-(2,6-diacetamidohexanamido)-3-(1H-indol-3-yl)propanoate 1f: ⁵

¹H NMR (400 MHz, CDCl₃): δ 9.55 (br, 1H), 7.55-7.49 (m, 2H), 7.21 (d, J = 7.72 Hz, 1H), 7.16-7.12 (m, 2H), 7.02 (d, J = 8.56 Hz, 2H), 6.12 (t, J = 5.52 Hz, 1H), 4.85-4.81 (m, 2H), 3.71 (s, 3H), 3.39-3.35 (m, 1H), 3.28-3.23 (m, 2H), 3.10-3.07 (m, 1H), 1.95 (s, 3H), 1.86 (s, 3H), 1.76-1.69 (m, 1H), 1.62-1.53 (m, 2H), 1.42-1.37 (m, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 172.5, 171.7, 170.8, 170.5, 136.4, 127.3, 123.5, 122.0, 119.4, 118.2, 111.6, 109.4, 52.9, 52.5, 39.2, 32.2, 29.0, 27.5, 23.2, 23.0, 22.1, 21.9.



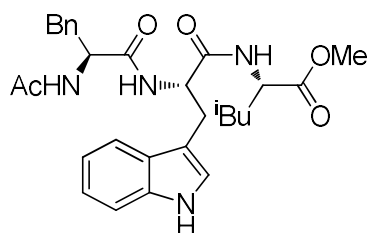
(R)-methyl 2-((S)-2-acetamido-3-(1H-indol-3-yl)propanamido)-3-(4-hydroxyphenyl)propanoate 1g: ⁵

¹H NMR (400 MHz, (CD₃)CO): δ 10.07 (br, 1H), 8.35 (s, 1H), 7.62-7.58 (m, 1H), 7.45-7.39 (m, 1H), 7.37-7.32 (m, 2H), 7.16 (d, J = 1.6 Hz, 1H), 7.09-7.05 (m, 1H), 7.03-6.98 (m, 1H), 6.96-6.89 (m, 2H), 4.79-4.73 (m, 1H), 4.64-4.59 (m, 1H), 3.61 (s, 3H), 3.26-3.21 (m, 1H), 3.10-3.04 (m, 1H), 3.00-2.95 (m, 1H), 2.89-2.84 (m, 1H), 1.85 (s, 3H); ¹³C NMR (100 MHz, (CD₃)CO): δ 171.6, 171.3, 169.6, 156.2, 136.6, 130.3, 127.8, 127.2, 123.5, 121.1, 118.6, 118.4, 115.1, 111.2, 110.4, 53.9, 53.6, 51.3, 36.6, 27.5, 22.0.



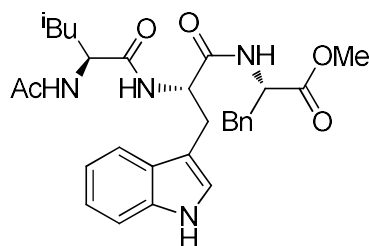
(R)-Methyl 2-((S)-2-acetamido-3-(1H-indol-3-yl)propanamido)-4-(methylthio)butanoate 1h: ⁵

¹H NMR (400 MHz, CDCl₃): δ 8.66 (br, 1H), 7.59 (d, J = 7.84 Hz, 1H), 7.30 (d, J = 8.08 Hz, 1H), 7.13 (t, J = 7.32 Hz, 1H), 7.07-7.03 (m, 2H), 6.98 (d, J = 7.52 Hz, 1H), 6.72 (d, J = 7.72 Hz, 1H), 4.82 (q, J = 6.96 Hz, 1H), 4.57-4.52 (m, 1H), 3.60 (s, 3H), 3.25-3.15 (m, 2H), 3.34 (t, J = 7.36 Hz, 2H), 2.05-2.00 (m, 1H), 1.97 (s, 3H), 1.91 (s, 3H), 1.87-1.80 (m, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 171.8, 171.7, 170.4, 136.2, 127.5, 123.5, 122.0, 119.5, 118.5, 111.3, 110.1, 54.0, 52.4, 51.6, 31.2, 29.7, 28.4, 23.1, 15.3.



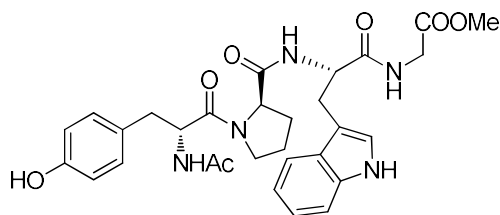
(S)-Methyl 2-((S)-2-((S)-2-acetamido-3-phenylpropanamido)-3-(1H-indol-3-yl)propanamido)-4-methylpentanoate 11a:

¹H NMR (400 MHz, CD₃OD): δ 7.52 (d, J = 7.9 Hz, 1H), 7.31 (d, J = 8.1 Hz, 1H), 7.25-7.16 (m, 5H), 7.09-7.06 (m, 2H), 6.99 (t, J = 7.1 Hz, 1H), 4.70 (t, J = 6.9 Hz, 1H), 4.58 (dd, J = 9.2 Hz, 5.2 Hz, 1H), 4.30 (d, J = 6.3 Hz, 1H), 3.62 (s, 3H), 3.22 (dd, J = 14.6 Hz, 6.5 Hz, 1H), 3.13 (dd, J = 14.6 Hz, 5.7 Hz, 1H), 3.13 (dd, J = 14.6 Hz, 7.2 Hz, 1H), 3.06 (dd, J = 14.0 Hz, 5.2 Hz, 1H), 2.79 (dd, J = 13.9 Hz, 9.2 Hz, 1H), 1.78 (s, 3H), 1.42-1.28 (m, 2H), 1.19-1.08 (m, 1H), 0.89-0.83 (m, 6H); ¹³C NMR (100 MHz, CD₃OD): δ 172.3, 171.9, 171.8, 137.0, 136.6, 128.8, 128.0, 127.4, 126.3, 123.4, 120.9, 118.4, 117.9, 110.8, 109.1, 56.9, 54.6, 53.9, 50.9, 37.1, 37.0, 27.4, 24.9, 20.8, 14.4, 10.3.



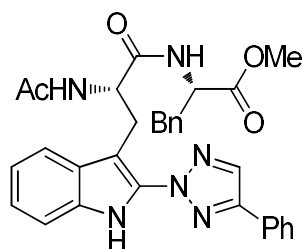
(S)-Methyl 2-((S)-2-((S)-2-acetamido-4-methylpentanamido)-3-(1H-indol-3-yl)propanamido)-3-phenylpropanoate 11b:

^1H NMR (400 MHz, CD_3OD): δ 7.56 (d, J = 7.84 Hz, 1H), 7.31 (d, J = 8.12 Hz, 1H), 7.23-7.14 (m, 3H), 7.09-7.05 (m, 4H), 7.01-6.97 (m, 1H), 4.68 (t, J = 7.04 Hz, 1H), 4.58 (dd, J = 7.8 Hz, 6 Hz, 1H), 4.14 (d, J = 7.84 Hz, 1H), 3.58 (s, 3H), 3.23-3.18 (m, 1H), 3.11-3.05 (m, 1H), 3.04-2.99 (m, 1H), 2.93-2.88 (m, 1H), 1.92 (s, 3H), 1.75-1.68 (m, 1H), 1.44-1.35 (m, 1H), 1.12-1.01 (m, 1H), 0.82 (t, J = 7.44 Hz, 3H), 0.76 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ 171.4, 171.3, 170.9, 135.9, 135.8, 128.2, 127.4, 126.7, 125.8, 122.7, 120.3, 117.8, 117.3, 110.2, 108.5, 57.4, 53.2, 53.1, 50.6, 36.4, 35.7, 26.9, 23.8, 20.4, 13.8, 9.3.



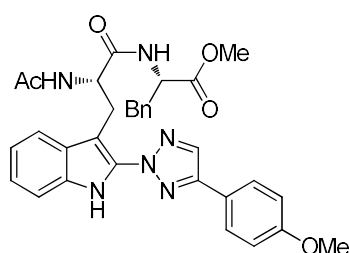
methyl 2-((S)-2-((R)-1-((R)-2-acetamido-3-(4-hydroxyphenyl)propanoyl)pyrrolidine-2-carboxamido)-3-(1H-indol-3-yl)propanamido)acetate 13:

^1H NMR (400 MHz, CD_3OD): δ 7.55 (d, J = 7.64 Hz, 1H), 7.23 (d, J = 7.88 Hz, 1H), 7.12 (s, 1H), 7.07 (d, J = 6.44 Hz, 1H), 7.02 (d, J = 8.2 Hz, 1H), 6.73 (d, J = 8.44 Hz, 1H), 4.73-4.69 (m, 1H), 4.66-4.62 (m, 1H), 4.33-4.30 (m, 1H), 3.95 (d, J = 3.68 Hz, 2H), 3.70 (s, 3H), 3.68-3.64 (m, 1H), 3.38-3.33 (m, 1H), 3.28-3.25 (m, 1H), 3.23-3.17 (m, 1H), 2.95-2.86 (m, 1H), 2.60-2.51 (m, 2H), 1.85 (s, 3H), 1.81-1.69 (m, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ 171.2, 170.8, 170.4, 170.0, 168.5, 155.0, 154.4, 135.0, 128.6, 126.0, 124.6, 122.0, 121.8, 119.6, 117.0, 116.3, 113.6, 109.6, 108.3, 107.4, 59.3, 53.5, 52.4, 49.7, 44.6, 39.0, 35.6, 34.2, 28.8, 27.0, 25.0. HRMS (ESI) Calcd for $\text{C}_{30}\text{H}_{35}\text{N}_5\text{O}_7$ $[\text{M}+\text{H}]^+$: 578.261; Found: 578.273.



(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-phenyl-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3a:

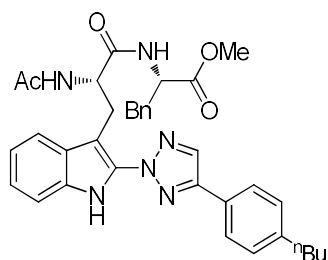
Obtained as a white solid in 87% yield (Condition A), $[\alpha]_{\text{D}}^{20} = -7.0$ ($c = 0.25$, CH_3OH); M.p. 233-235 °C; ^1H NMR (400 MHz, $(\text{CD}_3)_2\text{SO}$): δ 11.99 (br, 1H), 8.69 (s, 1H), 8.17 (d, $J = 7.6\text{Hz}$, 1H), 8.07-8.03 (m, 3H), 7.75 (d, $J = 7.9\text{Hz}$, 1H), 7.53 (t, $J = 7.3\text{Hz}$, 2H), 7.46 (d, $J = 7.3\text{Hz}$, 1H), 7.40 (d, $J = 8.1\text{Hz}$, 1H), 7.24-7.13 (m, 6H), 7.07 (t, $J = 7.3\text{Hz}$, 1H), 4.73-4.67 (m, 1H), 4.47-4.41 (m, 1H), 3.47 (s, 3H), 3.35 (s, 1H), 3.19 (dd, $J = 14.1\text{Hz}$, 8.8Hz, 1H), 2.96 (dd, $J = 13.7\text{Hz}$, 6.1Hz, 1H), 2.87 (dd, $J = 13.7\text{Hz}$, 8.1Hz, 1H), 1.64 (s, 3H); ^{13}C NMR (100 MHz, $(\text{CD}_3)_2\text{SO}$): δ 171.9, 171.8, 169.2, 148.7, 137.4, 133.6, 131.8, 129.6, 129.5, 128.6, 128.2, 126.9, 126.5, 122.8, 120.0, 119.9, 111.9, 100.8, 53.9, 53.8, 52.2, 37.2, 26.9, 22.9; IR (KBr): ν (cm^{-1}) 3055, 2922, 1734, 1653, 1533, 1456, 1265, 975, 740 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{31}\text{H}_{31}\text{N}_6\text{O}_4$ $[\text{M}+\text{H}]^+$: 551.2407; Found: 551.2401.



(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-(4-methoxyphenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3b:

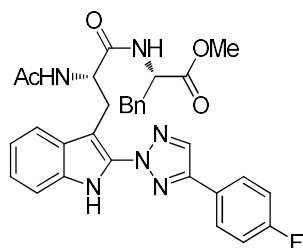
Obtained as a white solid in 69% yield (Condition A), $[\alpha]_{\text{D}}^{20} = 30.5$ ($c = 0.2$, CH_3OH); M.p. 105-107 °C; ^1H NMR (400 MHz, CDCl_3): δ 9.42 (br, 1H), 8.09 (s, 1H), 7.69-7.64 (m, 3H), 7.49 (d, $J = 6.76\text{Hz}$, 1H), 7.34 (d, $J = 8\text{Hz}$, 1H), 7.22 (t, $J = 7.32\text{Hz}$, 1H), 7.15-7.12 (m, 3H), 7.10-7.05 (m, 2H), 7.02 (d, $J = 7.08\text{Hz}$, 2H), 6.89 (d, J

=8.52Hz, 2H), 4.89-4.84 (m, 1H), 4.82-4.79 (m, 1H), 3.84 (s, 3H), 3.63-3.61 (m, 1H), 3.57 (s, 3H), 3.54-3.47 (m, 1H), 3.08-2.94 (m, 2H), 1.91 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 171.9, 171.7, 170.4, 160.1, 148.8, 135.6, 132.9, 132.2, 131.3, 129.3, 128.3, 127.4, 126.8, 122.8, 121.5, 120.5, 118.8, 114.3, 111.5, 55.2, 54.5, 53.1, 52.3, 38.3, 27.0, 22.9; IR (KBr): ν (cm^{-1}) 3223, 3086, 2926, 1737, 1662, 1537, 1406, 1292, 1178, 974, 831, 742 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{32}\text{H}_{33}\text{N}_6\text{O}_5$ $[\text{M}+\text{H}]^+$: 581.2507; Found: 581.2516.



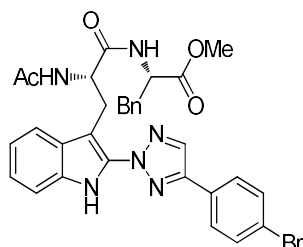
(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-(4-butylphenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3c:

Obtained as a white solid in 72% yield, $[\alpha]_{\text{D}}^{20} = 40.0$ ($c = 0.2$, CH_3OH); M.p. 244-246 $^{\circ}\text{C}$; ^1H NMR (400 MHz, $(\text{CD}_3)_2\text{SO}$): δ 11.97 (br, 1H), 8.63 (s, 1H), 8.16 (d, $J = 7.56\text{Hz}$, 1H), 8.03 (d, $J = 8.36\text{Hz}$, 1H), 7.95 (d, $J = 8.04\text{Hz}$, 2H), 7.75 (d, $J = 7.92\text{Hz}$, 1H), 7.40 (d, $J = 8.08\text{Hz}$, 1H), 7.34 (d, $J = 8\text{Hz}$, 2H), 7.24-7.13 (m, 6H), 7.07 (t, $J = 7.6\text{Hz}$, 1H), 4.72-4.67 (m, 1H), 4.48-4.42 (m, 1H), 3.47 (s, 3H), 3.45-3.43 (m, 1H), 3.21-3.16 (m, 1H), 2.99-2.94 (m, 1H), 2.91-2.85 (m, 1H), 2.64 (t, $J = 7.56\text{Hz}$, 2H), 1.64 (s, 3H), 1.61-1.55 (m, 2H), 1.37-1.28 (m, 2H), 0.90 (t, $J = 7.32\text{Hz}$, 3H); ^{13}C NMR (100 MHz, $(\text{CD}_3)_2\text{SO}$): δ 171.9, 171.8, 169.2, 148.7, 143.9, 137.4, 133.6, 133.4, 131.8, 129.5, 129.4, 128.6, 128.1, 127.1, 126.9, 126.5, 122.7, 119.9, 111.9, 100.6, 53.9, 53.8, 52.1, 37.2, 35.1, 33.4, 26.8, 22.9, 22.2, 14.2; IR (KBr): ν (cm^{-1}) 3232, 3059, 2927, 1730, 1637, 1541, 1381, 1128, 975, 734, 617 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{35}\text{H}_{39}\text{N}_6\text{O}_4$ $[\text{M}+\text{H}]^+$: 607.3027; Found: 607.3021.



(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-(4-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3d:

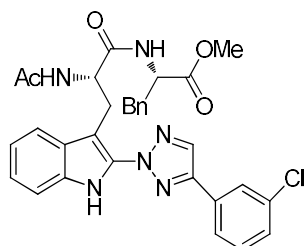
Obtained as a white solid in 54% yield (Condition A), $[\alpha]_D^{20} = 28.5$ ($c = 0.2$, CH_3OH); M.p. 250-252 °C; ^1H NMR (400 MHz, CDCl_3): δ 9.50 (br, 1H), 8.20 (br, 1H), 7.72-7.68 (m, 2H), 7.62 (d, $J = 7.84\text{Hz}$, 1H), 7.35-7.31 (m, 2H), 7.25-7.21 (m, 1H), 7.14-7.08 (m, 3H), 7.05-6.98 (m, 6H), 4.89-4.81 (m, 2H), 3.63-3.59 (m, 1H), 3.56 (s, 3H), 3.52-3.47 (m, 1H), 3.05-2.94 (m, 2H), 1.98 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 172.2, 171.8, 170.3, 163.0 (d, $J = 246.86\text{Hz}$), 147.9, 135.4, 132.9, 132.5, 130.9, 129.3, 128.3, 127.8 (d, $J = 8\text{Hz}$), 126.8, 125.0, 122.6, 120.4, 118.6, 115.8 (d, $J = 21.58\text{Hz}$), 111.7, 99.0, 54.3, 53.0, 52.4, 38.5, 27.6, 23.0; IR (KBr): ν (cm^{-1}) 3250, 3070, 1737, 1654, 1539, 1413, 1386, 1220, 1157, 979, 742 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{31}\text{H}_{30}\text{FN}_6\text{O}_4$ $[\text{M}+\text{H}]^+$: 569.2307; Found: 569.2316.



(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-(4-bromophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3e:

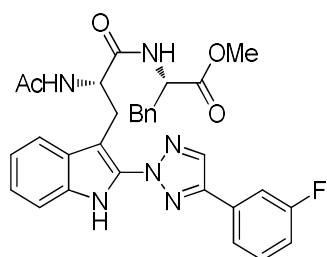
Obtained as a white solid in 81% yield (Condition A), $[\alpha]_D^{20} = 29.5$ ($c = 0.2$, CH_3OH); M.p. 244-246 °C; ^1H NMR (400 MHz, CDCl_3): δ 9.71 (br, 1H), 8.36 (s, 1H), 7.58-7.52 (m, 3H), 7.45-7.40 (m, 3H), 7.32 (d, $J = 8.04\text{Hz}$, 1H), 7.21 (t, $J = 7.28\text{Hz}$, 1H), 7.15 (d, $J = 8.28\text{Hz}$, 1H), 7.11-7.05 (m, 3H), 7.01-6.97 (m, 3H), 4.94-4.86 (m, 2H), 3.68-3.63 (m, 1H), 3.53 (s, 3H), 3.51-3.45 (m, 1H), 3.03-2.92 (m, 2H), 2.05 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 172.2, 171.8, 170.2, 147.8, 135.4, 132.9, 132.6,

132.6, 131.9, 130.8, 129.3, 128.3, 127.6, 127.3, 126.8, 123.1, 122.6, 120.4, 118.6, 111.8, 99.0, 54.1, 52.9, 52.4, 38.8, 27.8, 23.1; IR (KBr): ν (cm^{-1}) 3230, 3080, 3053, 1735, 1654, 1539, 1390, 1215, 975, 748 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{31}\text{H}_{30}\text{BrN}_6\text{O}_4$ $[\text{M}+\text{H}]^+$: 629.1506; Found: 629.1514.



(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-(3-chlorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3f:

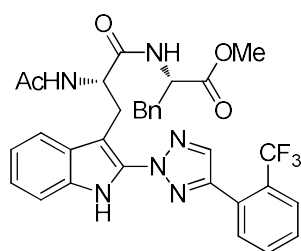
Obtained as a white solid in 73% yield (Condition A), $[\alpha]_{\text{D}}^{20} = 46.5$ ($c = 0.2$, CH_3OH); M.p. 223-224 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3): δ 8.41 (br, 1H), 7.67 (s, 1H), 7.57 (d, $J = 7.56\text{Hz}$, 2H), 7.32 (d, $J = 8.04\text{Hz}$, 1H), 7.24 (s, 1H), 7.22-7.20 (m, 2H), 7.11 (d, $J = 7.6\text{Hz}$, 1H), 7.08-7.04 (m, 2H), 6.98 (d, $J = 7.12\text{Hz}$, 3H), 4.91-4.88 (m, 1H), 4.86-4.82 (m, 1H), 3.64-3.59 (m, 1H), 3.54 (s, 3H), 3.50-3.44 (m, 1H), 3.04-2.94 (m, 2H), 2.08 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 172.7, 171.9, 170.6, 147.6, 135.4, 134.7, 133.2, 133.0, 130.7, 130.5, 130.0, 129.4, 128.8, 128.6, 128.4, 126.8, 125.6, 124.2, 122.5, 120.4, 118.6, 111.9, 99.0, 54.4, 53.0, 52.5, 38.8, 28.0, 23.1; IR (KBr): ν (cm^{-1}) 3236, 3051, 2991, 1735, 1651, 1537, 1456, 1396, 1274, 1012, 744 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{31}\text{H}_{30}\text{ClN}_6\text{O}_4$ $[\text{M}+\text{H}]^+$: 585.2012; Found: 585.2013.



(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3g:

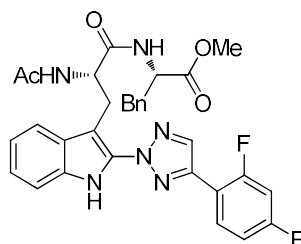
Obtained as a white solid in 90% yield (Condition A), $[\alpha]_{\text{D}}^{20} = 44.5$ ($c = 0.2$, CH_3OH); M.p. 247-249 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3): δ 9.58 (br, 1H), 8.35 (br, 1H), 7.59 (d,

$J = 7.72\text{Hz}$, 1H), 7.47-7.41 (m, 2H), 7.33 (d, $J = 8.04\text{Hz}$, 1H), 7.24-7.21 (m, 3H), 7.13-7.06 (m, 4H), 7.02-6.96 (m, 4H), 4.90-4.83 (m, 2H), 3.64-3.59 (m, 1H), 3.54 (s, 3H), 3.50-3.46 (m, 1H), 3.05-2.94 (m, 2H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 172.0, 171.7, 170.3, 162.9 (d, $J = 244.29\text{Hz}$), 147.7, 135.4, 132.9, 130.7 (d, $J = 6.74\text{Hz}$), 130.3 (d, $J = 8.12\text{Hz}$), 129.3, 128.2, 126.7, 122.7, 121.6, 120.4, 115.7 (d, $J = 20.85\text{Hz}$), 112.7 (d, $J = 23.33\text{Hz}$), 111.7, 99.2, 54.2, 52.9, 52.3, 38.5, 27.5, 22.9; IR (KBr): ν (cm^{-1}) 3217, 3084, 2924, 1737, 1654, 1539, 1454, 1409, 1269, 972, 742 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{31}\text{H}_{30}\text{FN}_6\text{O}_4$ $[\text{M}+\text{H}]^+$: 569.2307; Found: 569.2324.



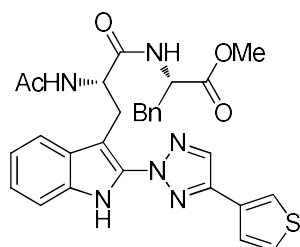
(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-(2-(trifluoromethyl)phenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3h:

Obtained as a white solid in 78% yield (Condition A), $[\alpha]_{\text{D}}^{20} = 24.5$ ($c = 0.2$, CH_3OH); M.p. 215-216 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3): δ 9.51 (br, 1H), 8.05 (br, 1H), 7.79 (d, $J = 7.56\text{Hz}$, 1H), 7.72-7.67 (m, 2H), 7.58-7.46 (m, 3H), 7.34 (d, $J = 8.04\text{Hz}$, 1H), 7.22 (t, $J = 7.32\text{Hz}$, 1H), 7.15-7.10 (m, 4H), 7.02-6.96 (m, 3H), 4.85-4.81 (m, 1H), 4.81-4.78 (m, 1H), 3.60 (s, 3H), 3.55 (d, $J = 7.32\text{Hz}$, 1H), 3.08-3.04 (m, 1H), 3.00-2.95 (m, 1H), 1.78 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 171.5, 170.7, 146.4, 135.7, 135.3, 133.0, 132.1, 131.8, 131.0, 129.3, 128.3, 127.9 (d, $J = 4.35\text{Hz}$), 126.9, 126.5 (d, $J = 4.35\text{Hz}$), 122.1 (d, $J = 271.36\text{Hz}$), 119.3, 111.4, 100.4, 54.6, 53.3, 52.2, 38.0, 26.3, 22.7; IR (KBr): ν (cm^{-1}) 3244, 3070, 1739, 1637, 1525, 1415, 1386, 1267, 977, 744 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{32}\text{H}_{30}\text{F}_3\text{N}_6\text{O}_4$ $[\text{M}+\text{H}]^+$: 619.2275; Found: 619.2271.



(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-(2,4-difluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3i:

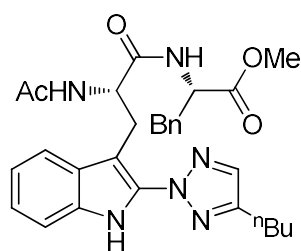
Obtained as a white solid in 75% yield (Condition A), $[\alpha]_D^{20} = 15.0$ ($c = 0.2$, CH₃OH); M.p. 281-282 °C; ¹H NMR (400 MHz, (CD₃)₂SO): δ 12.04 (br, 1H), 8.45 (d, $J = 3.44$ Hz, 1H), 8.26-8.20 (m, 1H), 8.17 (d, $J = 7.64$ Hz, 1H), 8.02 (d, $J = 8.48$ Hz, 1H), 7.76 (d, $J = 7.92$ Hz, 1H), 7.54-7.48 (m, 1H), 7.40 (d, $J = 8.08$ Hz, 1H), 7.31-7.27 (m, 1H), 7.24-7.15 (m, 4H), 7.12 (d, $J = 7$ Hz, 2H), 7.07 (t, $J = 7.6$ Hz, 1H), 4.73-4.67 (m, 1H), 4.45-4.40 (m, 1H), 3.49-3.48 (m, 1H), 3.45 (s, 3H), 3.22-3.16 (m, 1H), 2.97-2.92 (m, 1H), 2.88-2.83 (m, 1H), 1.64 (s, 3H); ¹³C NMR (100 MHz, (CD₃)₂SO): δ 171.9, 171.7, 162.9 (d, $J = 248.32$ Hz), 160.1 (d, $J = 250.41$ Hz), 142.5, 137.4, 135.0 (d, $J = 9.96$ Hz), 133.6, 131.5, 130.6 (d, $J = 3.89$ Hz), 130.5 (d, $J = 4.39$ Hz), 129.5, 128.6, 128.1, 126.9, 122.9, 120.0, 114.3 (d, $J = 12.91$ Hz), 113.1, 112.9, 112.0, 105.5, 105.3, 105.0, 101.1, 53.9, 53.7, 52.1, 37.2, 26.9, 22.9; IR (KBr): ν (cm⁻¹) 3228, 3082, 1757, 1645, 1544, 1411, 1388, 1267, 1082, 985, 740 cm⁻¹; HRMS (ESI) Calcd for C₃₁H₂₉F₂N₆O₄ [M+H]⁺: 587.2213; Found: 587.2227.



(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-(thiophen-3-yl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3j:

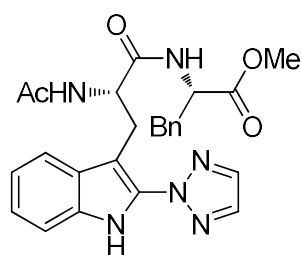
Obtained as a white solid in 87% yield (Condition A), $[\alpha]_D^{20} = 32.0$ ($c = 0.2$, CH₃OH); M.p. 251-253 °C; ¹H NMR (400 MHz, CDCl₃): δ 9.49 (br, 1H), 8.05 (br, 1H), 7.67-7.63 (m, 2H), 7.46-7.41 (m, 2H), 7.35-7.33 (m, 2H), 7.22 (t, $J = 7.36$ Hz, 1H), 7.15-7.08 (m, 4H), 7.04-7.00 (m, 3H), 4.88-4.83 (m, 2H), 3.61-3.59 (m, 1H), 3.56 (s, 3H), 3.52-3.47 (m, 1H), 3.07-3.02 (m, 1H), 3.00-2.95 (m, 1H), 1.93 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 171.7, 171.6, 170.4, 145.0, 135.6, 132.9, 132.8, 131.2, 130.2, 129.3, 128.3, 128.2, 126.8, 126.7, 125.7, 122.9, 120.6, 119.0, 111.4, 99.4, 54.3, 53.1, 52.3, 38.3, 26.9, 23.0; IR (KBr): ν (cm⁻¹) 3221, 3086, 1739, 1653, 1521, 1411, 1390,

1215, 970, 742 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{29}\text{H}_{29}\text{N}_6\text{O}_4\text{S}$ $[\text{M}+\text{H}]^+$: 557.1966; Found: 557.1969.



(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-butyl-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3k:

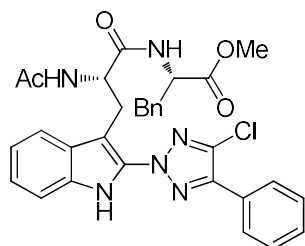
Obtained as a white solid in 46% yield (Condition A), $[\alpha]_{\text{D}}^{20} = 24.0$ ($c = 0.2$, CH_3OH); M.p. 74-77 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3): δ 8.98 (br, 1H), 7.68-7.64 (m, 2H), 7.57 (s, 1H), 7.33 (d, $J = 8\text{Hz}$, 1H), 7.24-7.19 (m, 4H), 7.18-7.14 (m, 1H), 7.06-7.02 (m, 3H), 4.84-4.79 (m, 1H), 4.71-4.66 (m, 1H), 3.66 (s, 3H), 3.49-3.41 (m, 2H), 3.12-3.07 (m, 1H), 3.04-2.99 (m, 1H), 2.76 (t, $J = 7.6\text{Hz}$, 2H), 1.80 (s, 3H), 1.74-1.67 (m, 2H), 1.47-1.38 (m, 2H), 0.97 (t, $J = 7.32\text{Hz}$, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 171.5, 171.3, 170.8, 150.3, 135.9, 134.4, 132.7, 131.6, 129.3, 128.4, 127.9, 126.9, 123.4, 120.8, 119.2, 111.0, 99.8, 54.5, 53.3, 52.2, 38.0, 31.0, 25.6, 25.0, 22.8, 22.3, 13.8; IR (KBr): ν (cm^{-1}) 3209, 3089, 2922, 1734, 1647, 1521, 1456, 1274, 970, 750 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{29}\text{H}_{35}\text{N}_6\text{O}_4$ $[\text{M}+\text{H}]^+$: 531.2714; Found: 531.2721.



(S)-Methyl 2-((S)-3-(2-(2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)-2-acetamidopropanamido)-3-phenylpropanoate 3m:

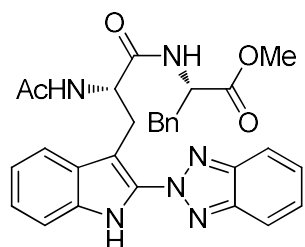
Obtained as a white solid in 76% yield (Condition A), $[\alpha]_{\text{D}}^{20} = 23.0$ ($c = 0.2$, CH_3OH); M.p. 104-106 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3): δ 9.27 (br, 1H), 7.79 (s, 2H), 7.65 (d, $J = 7.92\text{Hz}$, 1H), 7.40 (d, $J = 7.28\text{Hz}$, 1H), 7.33 (d, $J = 8.08\text{Hz}$, 1H), 7.23-7.19 (m, 2H), 7.17-7.13 (m, 3H), 7.05-7.01 (m, 3H), 4.86-4.81 (m, 1H), 4.77-4.72 (m, 1H), 3.63 (s,

3H), 3.47 (d, $J=7.28\text{Hz}$, 2H), 3.09-3.04 (m, 1H), 3.03-2.99 (m, 1H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 171.6, 171.4, 170.7, 135.7, 135.5, 132.8, 131.3, 129.3, 128.4, 127.9, 126.9, 123.4, 120.7, 119.2, 111.3, 100.2, 54.4, 53.3, 52.3, 38.1, 26.4, 22.9; IR (KBr): ν (cm^{-1}) 3215, 3086, 3005, 1739, 1653, 1521, 1415, 1386, 1259, 952, 748 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{25}\text{H}_{26}\text{N}_6\text{O}_4\text{Na}$ $[\text{M}+\text{Na}]^+$: 497.1908; Found: 497.1912.



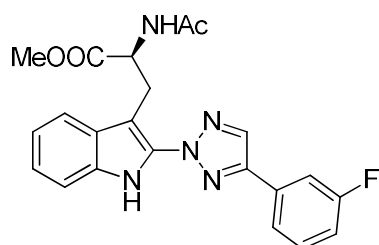
(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-chloro-5-phenyl-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 3n:

Obtained as a white solid in 88% yield (Condition A), $[\alpha]_{\text{D}}^{20} = 74.0$ ($c = 0.2$, CH_3OH); M.p. 205-207 °C; ^1H NMR (400 MHz, CDCl_3): δ 9.04 (br, 1H), 7.99 (d, $J=6.96\text{Hz}$, 2H), 7.75 (d, $J=7.8\text{Hz}$, 1H), 7.53-7.47 (m, 3H), 7.35 (d, $J=8\text{Hz}$, 1H), 7.27-7.23 (m, 2H), 7.20-7.15 (m, 4H), 6.99 (d, $J=6.72\text{Hz}$, 2H), 6.63 (d, $J=7.48\text{Hz}$, 1H), 4.77-4.74 (m, 2H), 3.58 (s, 3H), 3.57-3.55 (m, 1H), 3.50-3.44 (m, 1H), 3.09-3.04 (m, 1H), 2.98-2.94 (m, 1H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 171.3, 170.9, 170.6, 144.2, 135.7, 132.8, 130.8, 129.7, 129.2, 129.0, 128.4, 127.8, 127.5, 127.1, 127.0, 123.9, 121.1, 119.6, 111.2, 100.6, 54.2, 53.3, 52.2, 38.0, 26.4, 23.0; IR (KBr): ν (cm^{-1}) 3203, 3095, 2926, 1726, 1649, 1539, 1454, 1409, 1392, 1273, 948, 738 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{31}\text{H}_{29}\text{N}_6\text{O}_4\text{NaCl}$ $[\text{M}+\text{Na}]^+$: 607.1837; Found: 607.1841.



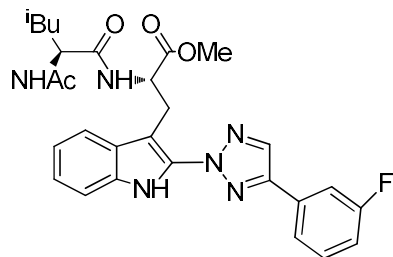
(S)-Methyl 2-((S)-3-(2-(2H-benzo[d][1,2,3]triazol-2-yl)-1H-indol-3-yl)-2-acetamidopropanamido)-3-phenylpropanoate 3o:

Obtained as a light-green solid in 77% yield (Condition A), $[\alpha]_{\text{D}}^{20} = -45.0$ ($c = 0.2$, CH₃OH); M.p. 169-171 °C; ¹H NMR (400 MHz, CDCl₃): δ 9.50 (br, 1H), 7.83-7.81 (m, 2H), 7.76 (d, $J = 7.92$ Hz, 1H), 7.65 (d, $J = 6.6$ Hz, 1H), 7.46-7.43 (m, 2H), 7.38 (d, $J = 8.08$ Hz, 1H), 7.29-7.24 (m, 1H), 7.22-7.17 (m, 4H), 7.07-7.03 (m, 3H), 4.89-4.81 (m, 2H), 3.66-3.61 (m, 2H), 3.58 (s, 3H), 3.11-3.07 (m, 1H), 3.04-2.99 (m, 1H), 1.80 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 171.5, 171.2, 170.7, 144.4, 135.8, 133.4, 131.5, 129.3, 128.4, 128.0, 127.8, 127.0, 124.4, 121.1, 119.7, 117.8, 111.4, 103.3, 54.5, 53.3, 52.2, 38.1, 26.6, 22.9; IR (KBr): ν (cm⁻¹) 3223, 3084, 2926, 1743, 1651, 1546, 1411, 1390, 1180, 946, 746 cm⁻¹; HRMS (ESI) Calcd for C₂₉H₂₈N₆O₄Na [M+Na]⁺: 547.2070; Found: 547.2072.



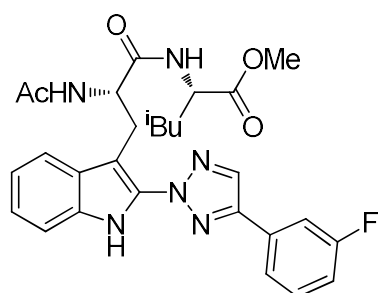
(S)-Methyl 2-acetamido-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanoate 4a:

Obtained as a white solid in 98% yield (Condition A), $[\alpha]_{\text{D}}^{20} = 42.5$ ($c = 0.2$, CH₃OH); M.p. 212-214 °C; ¹H NMR (400 MHz, (CD₃)₂SO): δ 12.09 (br, 1H), 8.78 (s, 1H), 8.45 (d, $J = 7.76$ Hz, 1H), 7.90-7.86 (m, 2H), 7.63-7.57 (m, 2H), 7.41 (d, $J = 8.04$ Hz, 1H), 7.33-7.28 (m, 1H), 7.18 (t, $J = 7.32$ Hz, 1H), 7.09 (t, $J = 7.44$ Hz, 1H), 4.69-4.63 (m, 1H), 3.60 (dd, $J = 13.92$ Hz, 7.28 Hz, 1H), 3.42 (s, 3H), 3.32 (dd, $J = 13.92$ Hz, 7.48 Hz, 1H), 1.72 (s, 3H); ¹³C NMR (100 MHz, (CD₃)₂SO): δ 172.2, 169.1, 162.6 (d, $J = 242.26$ Hz), 147.2, 133.5, 133.1, 131.4 (d, $J = 8.74$ Hz), 131.1 (d, $J = 9.62$ Hz), 128.6, 127.6, 122.5, 122.0, 119.7, 118.8, 115.8 (d, $J = 20.89$ Hz), 112.6 (d, $J = 23.01$ Hz), 111.6, 99.8, 52.7, 51.5, 26.1, 22.2; IR (KBr): ν (cm⁻¹) 3217, 3080, 1718, 1658, 1552, 1411, 1388, 1292, 1176, 972, 862, 738 cm⁻¹; HRMS (ESI) Calcd for C₂₂H₂₀N₅O₃FN_a [M+Na]⁺: 444.1448; Found: 444.1443.



(S)-Methyl 2-((S)-2-acetamido-4-methylpentanamido)-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanoate 4b:

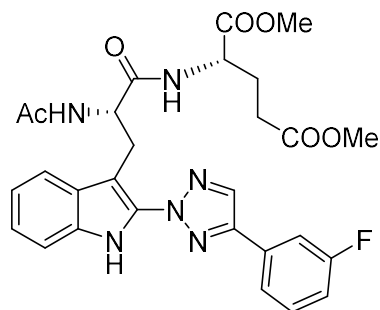
Obtained as a white solid in 91% yield (Condition A), $[\alpha]_D^{20} = -38.5$ ($c = 0.2$, CH₃OH); M.p. 108-112 °C; ¹H NMR (400 MHz, (CD₃)₂SO): δ 12.10 (br, 1H), 8.79 (s, 1H), 8.55 (d, $J = 6.84$ Hz, 1H), 7.87 (d, $J = 8.12$ Hz, 2H), 7.76 (d, $J = 8.96$ Hz, 1H), 7.62-7.56 (m, 2H), 7.41 (d, $J = 8$ Hz, 1H), 7.31 (t, $J = 7.92$ Hz, 1H), 7.18 (t, $J = 7.36$ Hz, 1H), 7.08 (t, $J = 7.48$ Hz, 1H), 4.67-4.61 (m, 1H), 4.22-4.17 (m, 1H), 3.60-3.54 (m, 1H), 3.40-3.35 (m, 1H), 3.33 (s, 3H), 1.79 (s, 3H), 1.66-1.59 (m, 1H), 1.34-1.30 (m, 1H), 1.03-0.95 (m, 1H), 0.77-0.74 (m, 6H); ¹³C NMR (100 MHz, (CD₃)₂SO): δ 172.4, 171.7, 169.4, 163.0 (d, $J = 242.12$ Hz), 147.7, 134.1, 133.6, 131.8 (d, $J = 9.44$ Hz), 131.7 (d, $J = 9.59$ Hz), 127.8, 123.0, 122.5, 120.3, 119.2, 116.3 (d, $J = 21.3$ Hz), 113.1 (d, $J = 22.53$ Hz), 112.1, 99.7, 56.9, 53.3, 51.9, 37.2, 26.4, 24.6, 22.9, 15.5, 11.4; IR (KBr): ν (cm⁻¹) 3223, 3103, 2929, 1728, 1641, 1541, 1454, 1286, 1122, 977, 740 cm⁻¹; HRMS (ESI) Calcd for C₂₈H₃₁N₆O₄NaF [M+Na]⁺: 557.2289; Found: 557.2288.



(S)-Methyl 2-((S)-2-acetamido-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-4-methylpentanoate 4c:

Obtained as a white solid in 82% yield (Condition A) (mixture of conformational isomers, Major/Minor=66/34), $[\alpha]_D^{20} = -18.5$ ($c = 0.2$, CH₃OH); M.p. 197-199 °C; ¹H NMR (400 MHz, (CD₃)₂SO): δ (major isomer) 11.99 (br, 1H), 8.76 (s, 1H), 8.10 (t, $J = 8.6$ Hz, 2H), 7.91 (d, $J = 8.28$ Hz, 3H), 7.60-7.55 (m, 1H), 7.41-7.37 (m, 1H),

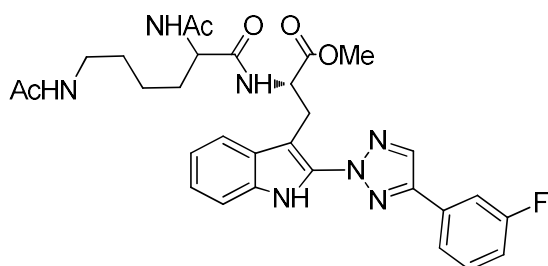
7.31-7.26 (m, 1H), 7.19-7.13 (m, 1H), 7.08-7.05 (m, 1H), 4.75-4.70 (m, 1H), 4.23-4.17 (m, 1H), 3.54-3.49 (m, 1H), 3.45 (s, 3H), 3.28-3.23 (m, 1H), 1.69 (s, 3H), 1.66-1.63 (m, 1H), 1.39-1.30 (m, 1H), 1.11-1.04 (m, 1H), 0.79-0.73 (m, 6H); (minor isomer) 11.97 (br, 1H), 8.75 (s, 1H), 7.95 (t, $J=8.24\text{Hz}$, 2H), 7.78-7.66 (m, 3H), 7.60-7.55 (m, 1H), 7.41-7.37 (m, 1H), 7.31-7.26 (m, 1H), 7.19-7.13 (m, 1H), 7.08-7.05 (m, 1H), 4.84-4.78 (m, 1H), 4.23-4.17 (m, 1H), 3.56 (s, 3H), 3.41-3.39 (m, 1H), 3.28-3.23 (m, 1H), 1.76 (s, 3H), 1.66-1.63 (m, 1H), 1.39-1.30 (m, 1H), 0.99-0.95 (m, 1H), 0.62-0.58 (m, 3H), 0.51 (d, $J=6.72\text{Hz}$, 3H); ^{13}C NMR (100 MHz, $(\text{CD}_3)_2\text{SO}$): δ 172.3, 172.0, 171.8, 169.3, 169.1, 163.1 (d, $J=242.04\text{Hz}$), 147.6, 133.8, 133.7, 133.6, 132.1, 132.0 (d, $J=11.21\text{Hz}$), 131.7, 131.6 (d, $J=8.65\text{Hz}$), 129.1, 128.2, 123.0, 122.8, 122.6, 119.9, 116.2 (d, $J=20.96\text{Hz}$), 113.2 (d, $J=23.09\text{Hz}$), 111.9, 100.7, 100.3, 65.4, 56.9, 56.5, 53.8, 53.3, 51.9, 37.1, 36.4, 30.4, 27.1, 25.2, 22.9, 19.1, 15.6, 15.2, 14.0, 11.5, 11.4; IR (KBr): ν (cm^{-1}) 3172, 3055, 2960, 1732, 1658, 1539, 1456, 1406, 1269, 975, 862, 740 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{28}\text{H}_{31}\text{N}_6\text{O}_4\text{FNa}$ $[\text{M}+\text{Na}]^+$: 557.2289; Found: 557.2287.



Dimethyl 2-((*S*)-2-acetamido-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)pentanedioate **4d:**

Obtained as a white solid in 73% yield (Condition A) (mixture of conformational isomers, Major/Minor=78/22), $[\alpha]_{\text{D}}^{20} = -26.0$ ($c = 0.2$, CH_3OH); M.p. 116-118 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3): δ (major isomer) 10.12 (br, 1H), 8.66 (br, 1H), 7.88 (s, 1H), 7.50 (d, $J=7.84\text{Hz}$, 1H), 7.42-7.30 (m, 5H), 7.21-7.13 (m, 3H), 4.93-4.90 (m, 1H), 4.76-4.75 (m, 1H), 3.66 (s, 2H), 3.54-3.53 (m, 6H), 2.40-2.3 (m, 2H), 2.15 (s, 3H), 1.89-1.85 (m, 2H); (minor isomer) 9.71 (br, 1H), 8.10 (br, 1H), 7.67 (d, $J=7.72\text{Hz}$, 1H), 7.50 (d, $J=7.84\text{Hz}$, 1H), 7.05-7.01 (m, 5H), 6.86-6.83 (m, 3H), 4.93-4.90 (m,

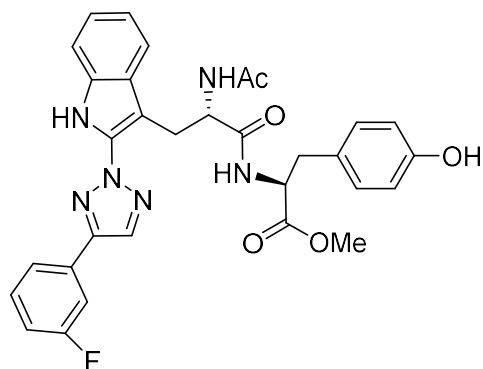
1H), 4.54-4.52 (m, 1H), 3.61 (s, 2H), 3.54-3.49 (m, 6H), 2.26-2.21 (m, 2H), 2.10-2.07 (m, 3H), 1.89-1.85 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 173.2, 172.9, 172.3, 171.9, 171.7, 170.8, 162.8 (d, *J*=244.52Hz), 148.0, 147.8, 133.0, 132.8, 131.2, 130.7 (d, *J*=8.44Hz), 130.6, 130.2 (d, *J*=7.78Hz), 128.4, 123.6, 122.6, 121.6, 120.8, 120.4, 119.3, 118.4, 115.6 (d, *J*=21.14Hz), 112.6 (d, *J*=24.4Hz), 111.9, 111.3, 100.5, 99.1, 54.7, 54.6, 52.6, 52.4, 51.7, 51.6, 50.9, 29.7, 29.5, 28.2, 27.7, 26.9, 26.4, 22.9, 22.8; IR (KBr): ν (cm⁻¹) 3228, 3082, 2924, 1732, 1645, 1537, 1413, 1386, 1267, 1209, 972, 862, 746 cm⁻¹; HRMS (ESI) Calcd for C₂₈H₂₉N₆O₆FNa [M+Na]⁺: 587.2030; Found: 587.2034.



(2S)-Methyl 2-(2,6-diacetamidohexanamido)-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanoate 4e:

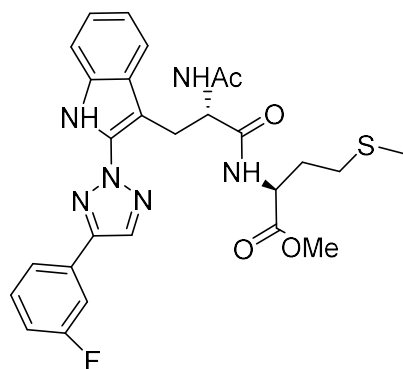
Obtained as a white solid in 87% yield (Condition A) (mixture of conformational isomers, ratio = 50/50), [α]_D²⁰ = -6.2 (*c* = 0.2, CH₃OH); M.p. 240-242 °C; ¹H NMR (400 MHz, (CD₃)₂SO): δ (one isomer) 12.09 (br, 1H), 8.78 (s, 1H), 8.45 (d, *J*=7.68Hz, 1H), 7.90-7.84 (m, 2H), 7.82-7.73 (m, 2H), 7.68-7.59 (m, 2H), 7.41 (t, *J*=7.32Hz, 1H), 7.30 (t, *J*=8.4Hz, 1H), 7.20-7.15 (m, 1H), 7.10-7.07 (m, 1H), 4.84-4.79 (m, 1H), 4.23-4.16 (m, 1H), 3.64-3.55 (m, 1H), 3.52 (s, 3H), 2.97-2.92 (m, 2H), 1.77 (s, 6H), 1.61-1.49 (m, 1H), 1.38-1.28 (m, 2H), 1.16-1.07 (m, 3H), 0.97-0.95 (m, 1H); (another isomer) 12.08 (br, 1H), 8.78 (s, 1H), 8.45 (d, *J*=7.68Hz, 1H), 7.90-7.84 (m, 2H), 7.82-7.73 (m, 2H), 7.68-7.59 (m, 2H), 7.41 (t, *J*=7.32Hz, 1H), 7.30 (t, *J*=8.4Hz, 1H), 7.20-7.15 (m, 1H), 7.10-7.07 (m, 1H), 4.68-4.63 (m, 1H), 4.23-4.16 (m, 1H), 3.64-3.55 (m, 1H), 3.36 (s, 3H), 2.87-2.84 (m, 2H), 1.77 (s, 3H), 1.73 (s, 3H), 1.61-1.49 (m, 1H), 1.38-1.28 (m, 2H), 1.16-1.07 (m, 3H), 0.97-0.95 (m, 1H); ¹³C NMR (100 MHz, (CD₃)₂SO): δ 172.6, 172.5, 172.3, 172.2, 169.5, 169.4, 163.1 (d, *J*=242.37Hz), 147.7, 134.1, 134.0, 133.6 (d, *J*=5.99Hz), 131.9, 131.7 (d, *J*=7.12Hz),

131.5, 128.2, 127.9, 123.0, 122.5, 120.3, 120.2, 119.4, 119.2, 116.3 (d, $J = 21\text{Hz}$), 113.1 (d, $J = 22.43\text{Hz}$), 113.0, 112.1, 112.0, 99.9, 99.7, 53.2, 52.8, 52.6, 52.4, 52.2, 52.0, 38.8, 32.2, 32.1, 29.3, 29.2, 26.7, 26.5, 23.1, 23.0, 22.9, 22.8; IR (KBr): ν (cm^{-1}) 3267, 3053, 1749, 1662, 1541, 1425, 1398, 1373, 974, 862, 736 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{30}\text{H}_{35}\text{FN}_7\text{O}_5$ $[\text{M}+\text{H}]^+$: 592.2678; Found: 592.2676.



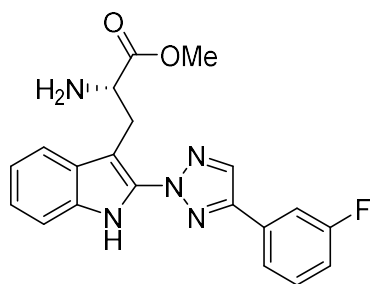
(*R*)-Methyl 2-((*S*)-2-acetamido-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-(4-hydroxyphenyl)propanoate 4f:

Obtained as a white solid in 59% yield (Condition A), $[\alpha]_{\text{D}}^{20} = -7.5$ ($c = 0.2$, CH_3OH); M.p. 271-273 $^{\circ}\text{C}$; ^1H NMR (400 MHz, $(\text{CD}_3)_2\text{SO}$): δ 11.99 (br, 1H), 9.36 (s, 1H), 8.74 (s, 1H), 8.22 (d, $J = 7.56\text{Hz}$, 1H), 8.00 (d, $J = 8.52\text{Hz}$, 1H), 7.91 (d, $J = 8.32\text{Hz}$, 2H), 7.76 (d, $J = 7.84\text{Hz}$, 1H), 7.34-7.67 (m, 1H), 7.60-7.56 (m, 1H), 7.53 (s, 2H), 7.39 (d, $J = 8.08\text{Hz}$, 1H), 7.30-7.26 (m, 1H), 7.18-7.16 (m, 1H), 7.09-7.05 (m, 1H), 4.71-4.66 (m, 1H), 4.38-4.33 (m, 1H), 3.51-3.49 (m, 1H), 3.46 (s, 3H), 3.22-3.16 (m, 1H), 2.86-2.81 (m, 1H), 2.74-2.69 (m, 1H), 1.65 (s, 3H); ^{13}C NMR (100 MHz, $(\text{CD}_3)_2\text{SO}$): δ 179.8, 171.8, 169.2, 163.1 (d, $J = 273.48\text{Hz}$), 154.4, 147.6, 140.0, 133.9, 133.6, 132.0 (d, $J = 7.71\text{Hz}$), 131.6 (d, $J = 7.45\text{Hz}$), 129.1, 128.2, 122.9, 122.6, 119.9, 116.2 (d, $J = 22.24\text{Hz}$), 113.3 (d, $J = 17.84\text{Hz}$), 111.9, 100.9, 87.3, 53.9, 52.1, 35.1, 29.9, 27.3, 23.1; IR (KBr): ν (cm^{-1}) 3259, 3089, 2929, 1728, 1643, 1541, 1431, 1409, 1392, 1286, 1120, 948, 864, 744 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{31}\text{H}_{28}\text{FN}_6\text{O}_4$ $[\text{M}-\text{H}]^-$: 583.2111; Found: 583.2115.



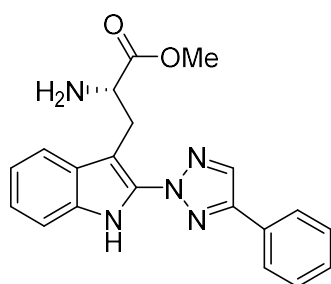
(R)-Methyl 2-((S)-2-acetamido-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-4-(methylthio)butanoate 4g:

Obtained as a white solid in 80% yield (Condition A) (mixture of conformational isomers, ratio = 50/50), $[\alpha]_D^{20} = -73.0$ ($c = 0.2$, CH_3OH); M.p. 233-234 °C; ^1H NMR (400 MHz, CDCl_3): δ (one isomer) 9.81 (br, 1H), 8.41 (br, 1H), 7.57 (t, $J = 6.84\text{Hz}$, 1H), 7.43 (t, $J = 7.08\text{Hz}$, 1H), 7.39-7.34 (m, 2H), 7.28-7.27 (m, 1H), 7.24-7.22 (m, 3H), 7.12 (t, $J = 7.56\text{Hz}$, 1H), 6.94-6.91 (m, 1H), 4.79-4.66 (m, 2H), 3.59 (s, 3H), 3.56-3.55 (m, 1H), 3.49-3.41 (m, 1H), 2.84-2.75 (m, 1H), 2.70-2.66 (m, 1H), 2.51 (s, 3H), 2.34-2.26 (m, 1H), 2.06 (s, 3H), 2.01-1.92 (m, 1H); (another isomer) 9.77 (br, 1H), 8.39 (br, 1H), 7.57 (t, $J = 6.84\text{Hz}$, 1H), 7.43 (t, $J = 7.08\text{Hz}$, 1H), 7.39-7.34 (m, 2H), 7.28-7.27 (m, 1H), 7.24-7.22 (m, 3H), 7.12 (t, $J = 7.56\text{Hz}$, 1H), 6.94-6.91 (m, 1H), 4.79-4.66 (m, 2H), 3.59 (s, 3H), 3.56-3.55 (m, 1H), 3.49-3.41 (m, 1H), 2.70-2.66 (m, 1H), 2.63-2.56 (m, 1H), 2.51 (s, 3H), 2.34-2.26 (m, 1H), 2.06 (s, 3H), 2.01-1.92 (m, 1H); ^{13}C NMR (100 MHz, CD_3OD): δ 173.0, 172.9, 171.8, 171.7, 170.8, 163.2 (d, $J = 243.25\text{Hz}$), 147.7, 133.6, 133.5, 132.6, 131.7 (d, $J = 8.59\text{Hz}$), 131.5, 130.6 (d, $J = 8.33\text{Hz}$), 127.9, 122.5, 121.7, 119.7, 118.6, 115.3 (d, $J = 21.27\text{Hz}$), 112.4 (d, $J = 23.42\text{Hz}$), 111.1, 99.1, 54.8, 54.7, 51.5, 51.3, 50.7, 49.3, 36.7, 36.6, 26.0, 25.0, 24.8, 21.1; IR (KBr): ν (cm^{-1}) 3190, 3097, 2926, 1747, 1633, 1539, 1456, 1409, 1392, 1369, 1004, 970, 864, 742 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{27}\text{H}_{29}\text{FN}_6\text{O}_4\text{SK}$ $[\text{M}+\text{K}]^+$: 591.1587; Found: 591.1795.



Methyl (*S*)-2-amino-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanoate 6a:

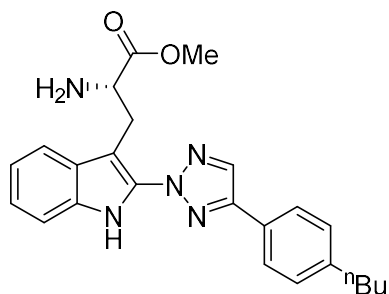
Obtained as a fluffy white powder in 77% yield (Condition B), $[\alpha]_D^{20} = -50$ ($c = 0.2$, CH₃OH); M.p. 107–127 °C; ¹H NMR (400 MHz, CD₃OD): δ 8.46 (s, 1H), 7.81–7.86 (m, 2H), 7.73 (d, $J = 6.5$ Hz, 1H), 7.63 (d, $J = 7.9$ Hz, 1H), 7.53–7.56 (m, 1H), 7.49 (d, $J = 8.2$ Hz, 1H), 7.26 (t, $J = 7.6$ Hz, 1H), 7.19–7.21 (m, 1H), 4.50 (t, $J = 7.4$ Hz, 1H), 3.89–3.94 (m, 1H), 3.65 (s, 3H), 3.60–3.63 (m, 1H); ¹³C NMR (150 MHz, CD₃OD): δ 171.1, 164.2 (d, $J = 237$ Hz), 138.4, 134.7, 134.4, 133.1, 132.2, 130.9, 124.4, 123.3, 121.7, 119.2, 117.0 (d, $J = 21$ Hz), 113.9 (d, $J = 24$ Hz), 112.8, 54.6, 53.5, 26.7. ¹⁹F NMR (565 MHz, CD₃OD, CF₃COOH as external standard): -114.5. IR (KBr): ν (cm⁻¹) 3363, 3192, 2922, 2851, 1739, 1650, 1620, 1589, 1423, 1207, 1135, 863, 722, 686, 523 cm⁻¹; HRMS (ESI) Calcd for C₂₀H₁₈FN₅O₂Na [M+ Na]⁺: 402.1337; Found: 402.1322.



Methyl (*S*)-2-amino-3-(2-(4-phenyl-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanoate 6b:

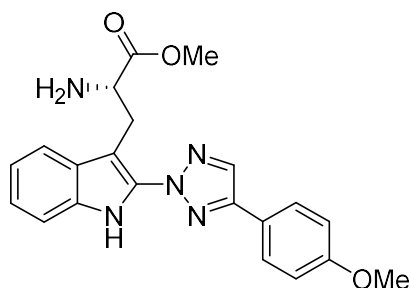
Obtained as a fluffy white powder in 71% yield (Condition B), $[\alpha]_D^{20} = 25$ ($c = 0.2$, CH₃OH); M.p. 130–150 °C; ¹H NMR (400 MHz, CD₃OD): δ 8.42 (s, 1H), 8.04 (d, $J = 8.6$ Hz, 2H), 7.62 (d, $J = 8.2$ Hz, 1H), 7.42–7.56 (m, 4H), 7.26 (t, $J = 7.4$ Hz, 1H), 7.18 (t, $J = 7.4$ Hz, 1H), 4.51 (t, $J = 7.1$ Hz, 1H), 3.88–3.94 (m, 1H), 3.63 (s, 3H), 3.59–3.62 (m, 1H); ¹³C NMR (150 MHz, CD₃OD): δ 169.5, 148.5, 146.6, 138.6, 132.9, 129.5,

129.3, 129.0, 128.8, 126.0, 122.9, 120.3, 117.8, 111.4, 53.2, 52.2, 29.3. IR (KBr): ν (cm^{-1}) 3355, 3187, 2922, 2852, 1749, 1689, 1660, 1634, 1469, 1251, 1073, 978, 721, 528 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{20}\text{H}_{19}\text{N}_5\text{O}_2\text{Na}$ $[\text{M}+\text{Na}]^+$: 384.1431; Found: 384.1425.



Methyl (*S*)-2-amino-3-(2-(4-(4-butylphenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanoate 6c:

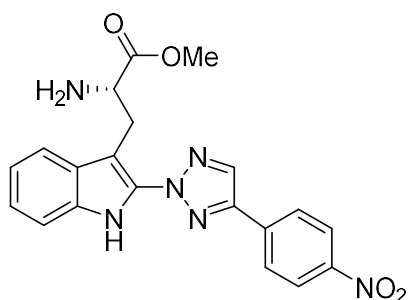
Obtained as a white solid in 42% yield (Condition B), $[\alpha]_{\text{D}}^{20} = 125.5$ ($c = 0.2$, CH_3OH); M.p. 109-112 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CD_3OD): δ 8.38 (s, 1H), 7.93 (d, $J = 8.1\text{Hz}$, 2H), 7.61 (d, $J = 8.0\text{Hz}$, 1H), 7.48 (d, $J = 8.0\text{Hz}$, 1H), 7.34 (d, $J = 8.1\text{Hz}$, 2H), 7.25 (t, $J = 7.5\text{Hz}$, 1H), 7.18 (t, $J = 7.5\text{Hz}$, 1H), 4.50 (t, $J = 7.2\text{Hz}$, 1H), 3.86-3.94 (m, 2H), 3.63 (s, 3H), 2.67-2.72 (m, 2H), 1.63-1.70 (m, 2H), 1.38-1.44 (m, 2H), 0.97 (t, $J = 7.3\text{Hz}$, 3H); ^{13}C NMR (150 MHz, CD_3OD): δ 169.5, 167.9, 164.4, 133.6, 132.4, 130.8, 130.2, 129.8, 127.4, 119.7, 118.1, 117.6, 117.2, 69.3, 49.9, 40.3, 31.7, 30.7, 28.1, 25.1. IR (KBr): ν (cm^{-1}) 3441, 3381, 3253, 2991, 2881, 2777, 1792, 1732, 1624, 1436, 1087, 844, 766, 612, 569 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{24}\text{H}_{27}\text{N}_5\text{O}_2\text{Na}$ $[\text{M}+\text{Na}]^+$: 440.2057; Found: 440.2045.



Methyl (*S*)-2-amino-3-(2-(4-(4-methoxyphenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanoate 6d:

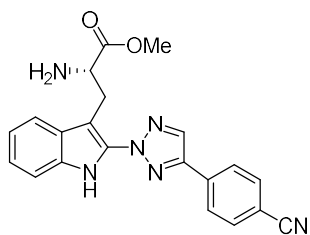
Obtained as a fluffy white powder in 55% yield (Condition B), $[\alpha]_{\text{D}}^{20} = 200$ ($c = 0.2$, CH_3OH); M.p. 138.0-140.5 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CD_3OD): δ 8.33 (s, 1H), 7.96 (d,

$J = 8.7\text{Hz}$, 2H), 7.61 (d, $J = 8.1\text{Hz}$, 1H), 7.48 (d, $J = 8.1\text{Hz}$, 1H), 7.25 (t, $J = 7.5\text{Hz}$, 1H), 7.17 (t, $J = 7.5\text{Hz}$, 1H), 7.07 (d, $J = 8.7\text{Hz}$, 2H), 4.49 (t, $J = 7.4\text{Hz}$, 1H), 3.87 (s, 3H), 3.63 (s, 3H), 3.46-3.52 (m, 2H); ^{13}C NMR (150 MHz, CD_3OD): δ 169.7, 160.7, 149.3, 140.8, 133.5, 132.4, 129.4, 127.5, 122.7, 125.4, 120.2, 117.7, 114.3, 111.3, 65.5, 54.5, 53.4, 26.7. IR (KBr): ν (cm^{-1}) 3357, 3188, 3004, 2021, 2851, 1742, 1704, 1661, 1634, 1504, 1488, 1209, 1140, 695, 634 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{21}\text{H}_{21}\text{N}_5\text{O}_3\text{Na}$ $[\text{M}+\text{Na}]^+$: 414.1537; Found: 414.1538.



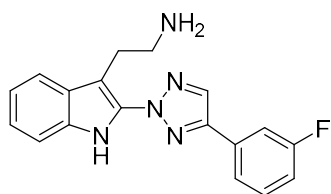
Methyl (S)-2-amino-3-(2-(4-(4-nitrophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanoate 6c:

Obtained as a fluffy white powder in 83% yield (Condition B), $[\alpha]_{\text{D}}^{20} = -40$ ($c = 0.2$, CH_3OH); M.p. 128.4-130.3 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CD_3OD): δ 8.99 (s, 1H), 8.37 (d, $J = 9.0\text{Hz}$, 2H), 8.21 (d, $J = 9.0\text{Hz}$, 2H), 7.65 (d, $J = 8.1\text{Hz}$, 1H), 7.49 (d, $J = 8.1\text{Hz}$, 1H), 7.32 (t, $J = 7.7\text{Hz}$, 1H), 7.22 (t, $J = 7.7\text{Hz}$, 1H), 4.42 (t, $J = 7.2\text{Hz}$, 1H), 3.63 (s, 3H), 3.58-3.61 (m, 1H), 3.47-3.53 (m, 1H); ^{13}C NMR (100 MHz, CD_3OD): δ 179.0, 145.7, 143.3, 142.6, 139.5, 134.2, 126.5, 124.0, 123.7, 122.7, 120.6, 118.4, 111.9, 53.4, 52.3, 25.0. IR (KBr): ν (cm^{-1}) 3351, 3183, 3004, 1827, 1691, 1659, 1648, 1521, 1470, 1027, 934, 721 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{20}\text{H}_{18}\text{N}_6\text{O}_4\text{Na}$ $[\text{M}+\text{Na}]^+$: 429.1282; Found: 429.1285.



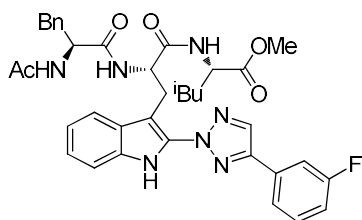
Methyl (S)-2-amino-3-(2-(4-(4-cyanophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanoate 6f:

Obtained a fluffy white powder in 82% yield (Condition B), $[\alpha]_D^{20} = 125.5$ ($c = 0.2$, CH₃OH); M.p. 127.6-135 °C; ¹H NMR (400 MHz, CD₃OD): δ 8.96 (s, 1H), 8.16 (d, $J = 8.5$ Hz, 2H), 8.02 (d, $J = 8.5$ Hz, 1H), 7.88 (d, $J = 8.5$ Hz, 2H), 7.50 (d, $J = 8.5$ Hz, 1H), 7.33 (t, $J = 7.6$ Hz, 1H), 7.24 (t, $J = 7.6$ Hz, 1H), 4.43 (t, $J = 7.2$ Hz, 1H), 3.64 (s, 3H), 3.58-3.62 (m, 1H), 3.47-3.52 (m, 1H); ¹³C NMR (150 MHz, CD₃OD): δ 169.1, 146.0, 134.4, 134.2, 132.7, 132.5, 129.4, 126.8, 126.1, 123.7, 122.3, 120.6, 118.3, 118.1, 111.8, 111.7, 54.6, 53.7, 28.1. IR (KBr): ν (cm⁻¹) 3305, 3187, 2921, 2850, 1747, 1704, 1648, 1634, 1470, 1422, 1245, 1024, 803, 721, 551 cm⁻¹; HRMS (ESI) Calcd for C₂₁H₁₈N₆O₂Na [M+Na]⁺: 409.1383; Found: 409.1383.



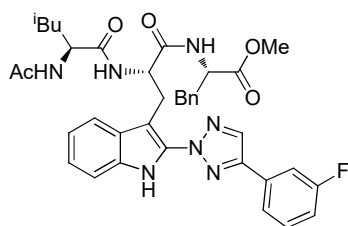
2-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)ethan-1-amine 8:

Obtained as a fluffy white powder in 87% yield (Condition B), M.p. 110 –120°C; ¹H NMR (400 MHz, CD₃OD): δ 8.38 (s, 1H), 7.82 (d, $J = 7.8$ Hz, 1H), 7.73-7.78 (m, 1H), 7.64 (d, $J = 7.8$ Hz, 1H), 7.48-7.55 (m, 1H), 7.42 (d, $J = 8.1$ Hz, 1H), 7.09-7.23 (m, 3H), 3.56 (t, $J = 7.0$ Hz, 2H), 3.34 (t, $J = 7.0$ Hz, 2H); ¹³C NMR (150 MHz, CD₃OD): δ 163.0 (d, $J = 245$ Hz), 133.6, 132.6, 132.0, 131.1, 130.7, 128.0, 122.5, 121.7, 119.6, 118.6, 115.3 (d, $J = 21$ Hz), 112.6 (d, $J = 22$ Hz), 111.0, 101.9, 39.7, 23.2. ¹⁹F NMR (565 MHz, CD₃OD, CF₃COOH as external standard): -114.5. IR (KBr): ν (cm⁻¹) 3698, 3669, 2921, 2851, 2526, 2355, 2071, 1681, 1632, 1589, 1207, 1063, 804, 786, 647, 534 cm⁻¹; HRMS (ESI) Calcd. for C₁₈H₁₆FN₅Na [M+ Na]⁺: 344.1282; Found: 344.1280.



(S)-Methyl 2-((S)-2-((S)-2-acetamido-3-phenylpropanamido)-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-4-methylpentanoate 12a:

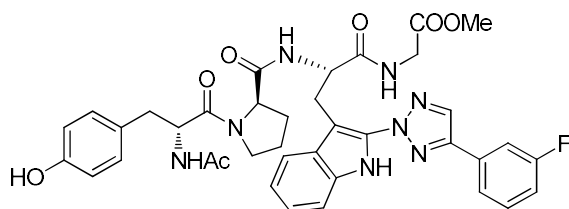
Obtained as a white solid in 71% yield (Condition A) (mixture of conformational isomers, ratio = 50/50), $[\alpha]_D^{20} = -7.5$ ($c = 0.2$, CH₃OH); M.p. 217-218 °C; ¹H NMR (400 MHz, (CD₃)₂SO): δ (one isomer) 12.01 (br, 1H), 8.75 (s, 1H), 8.20 (dd, $J = 15.32\text{Hz}$, 7.72Hz, 1H), 8.06 (d, $J = 7.56\text{Hz}$, 1H), 7.99 (d, $J = 7.96\text{Hz}$, 1H), 7.94-7.90 (m, 2H), 7.80-7.76 (m, 1H), 7.57-7.50 (m, 3H), 7.17-7.10 (m, 4H), 7.09-7.02 (m, 3H), 4.76-4.70 (m, 1H), 4.37-4.32 (m, 1H), 4.22-4.18 (m, 1H), 3.60-3.36 (m, 2H), 3.44 (s, 3H), 2.82-2.75 (m, 1H), 2.60-2.54 (m, 1H), 1.69-1.64 (m, 1H), 1.62 (s, 3H), 1.34-1.31 (m, 1H), 1.15-1.11 (m, 1H), 0.83-0.75 (m, 6H); (another isomer) 12.00 (br, 1H), 8.69 (s, 1H), 8.20 (dd, $J = 15.32\text{Hz}$, 7.72Hz, 1H), 8.06 (d, $J = 7.56\text{Hz}$, 1H), 7.99 (d, $J = 7.96\text{Hz}$, 1H), 7.94-7.90 (m, 2H), 7.80-7.76 (m, 1H), 7.46-7.40 (m, 3H), 7.17-7.10 (m, 4H), 7.09-7.02 (m, 3H), 4.76-4.70 (m, 1H), 4.37-4.32 (m, 1H), 4.22-4.18 (m, 1H), 3.60-3.36 (m, 2H), 3.43 (s, 3H), 2.82-2.75 (m, 1H), 2.60-2.54 (m, 1H), 1.69-1.64 (m, 1H), 1.62 (s, 3H), 1.34-1.31 (m, 1H), 1.15-1.11 (m, 1H), 0.83-0.75 (m, 6H); ¹³C NMR (100 MHz, (CD₃)₂SO): δ 171.7, 171.6, 171.4, 169.5, 163.1 (d, $J = 242.88\text{Hz}$), 148.6, 147.6, 138.3, 133.9, 133.7, 133.5, 132.1 (d, $J = 6.84\text{Hz}$), 132.0, 131.8, 131.6 (d, $J = 8.77\text{Hz}$), 129.6, 129.5, 129.4, 129.1, 128.3, 128.2, 126.5, 122.8, 122.7, 122.6, 120.0, 116.2 (d, $J = 23.22\text{Hz}$), 113.3 (d, $J = 22.73\text{Hz}$), 111.9, 100.2, 100.0, 56.6, 54.4, 54.0, 51.9, 37.6, 37.1, 30.4, 25.2, 22.7, 15.6, 11.5; IR (KBr): ν (cm⁻¹) 3221, 3086, 2927, 1741, 1639, 1541, 1454, 1409, 1269, 970, 864, 740 cm⁻¹; HRMS (ESI) Calcd for C₃₇H₄₁FN₇O₅ [M+H]⁺: 682.3148; Found: 682.3164.



(S)-Methyl 2-((S)-2-((S)-2-acetamido-4-methylpentanamido)-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)-3-phenylpropanoate 12b:

Obtained as a white solid in 65% yield (Condition A) (mixture of conformational isomers, Major/Minor=72/28), $[\alpha]_D^{20} = -1.2$ ($c = 0.2$, CH₃OH); M.p. 276-278 °C; ¹H NMR (400 MHz, (CD₃)₂SO): δ (major isomer) 11.99 (br, 1H), 8.75 (s, 1H), 8.16-8.13

(m, 1H), 8.06 (d, $J=7\text{Hz}$, 1H), 7.93-7.91 (m, 2H), 7.75 (d, $J=7.2\text{Hz}$, 2H), 7.61-7.51 (m, 2H), 7.39 (d, $J=7.96\text{Hz}$, 1H), 7.24-7.21 (m, 3H), 7.18-7.12 (m, 4H), 4.75-4.71 (m, 1H), 4.44-4.41 (m, 1H), 4.23-4.20 (m, 1H), 3.99-3.95 (m, 1H), 3.50 (d, $J=5.2\text{Hz}$, 1H), 3.41 (s, 3H), 3.30-3.20 (m, 1H), 2.96-2.87 (m, 2H), 2.02-1.98 (m, 1H), 1.74 (s, 3H), 1.65-1.61 (m, 1H), 0.67-0.63 (m, 3H), 0.69 (d, $J=6.28\text{Hz}$, 3H); (minor isomer) 11.99 (br, 1H), 8.69 (s, 1H), 8.37-8.36 (m, 1H), 8.27-8.22 (m, 1H), 8.01-7.97 (m, 2H), 7.72 (d, $J=7.2\text{Hz}$, 2H), 7.67-7.65 (m, 2H), 7.46 (d, $J=7.96\text{Hz}$, 1H), 7.31-7.27 (m, 3H), 7.08-7.05 (m, 4H), 5.40-5.31 (m, 1H), 4.82-4.78 (m, 1H), 4.50-4.48 (m, 1H), 4.06-4.01 (m, 1H), 3.50 (d, $J=5.2\text{Hz}$, 1H), 3.41 (s, 3H), 3.30-3.20 (m, 1H), 3.02-3.01 (m, 2H), 2.02-1.98 (m, 1H), 1.74 (s, 3H), 1.65-1.61 (m, 1H), 1.52-1.45 (m, 3H), 1.41-1.34 (m, 3H); ^{13}C NMR (100 MHz, $(\text{CD}_3)_2\text{SO}$): δ 171.3, 171.2, 171.0, 169.1, 162.6 (d, $J=240.81\text{Hz}$), 148.2, 147.1, 137.9, 133.4, 133.2, 133.1, 131.5, 131.4, 131.2 (d, $J=9.12\text{Hz}$), 129.2, 129.0, 128.6, 127.9, 127.8, 126.1, 122.3, 119.5, 112.8 (d, $J=22.74\text{Hz}$), 111.5, 99.8, 99.6, 56.2, 54.0, 53.5, 51.4, 37.1, 36.7, 30.0, 24.7, 22.3, 15.2, 13.5, 11.1; IR (KBr): ν (cm^{-1}) 3244, 3062, 2924, 1732, 1635, 1473, 1456, 1363, 1338, 972, 862, 744 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{37}\text{H}_{41}\text{FN}_7\text{O}_5$ $[\text{M}+\text{H}]^+$: 682.3148; Found: 682.3164.



Methyl 2-((S)-2-((R)-1-((R)-2-acetamido-3-(4-hydroxyphenyl)propanoyl)pyrrolidine-2-carboxamido)-3-(2-(4-(3-fluorophenyl)-2H-1,2,3-triazol-2-yl)-1H-indol-3-yl)propanamido)acetate 14:

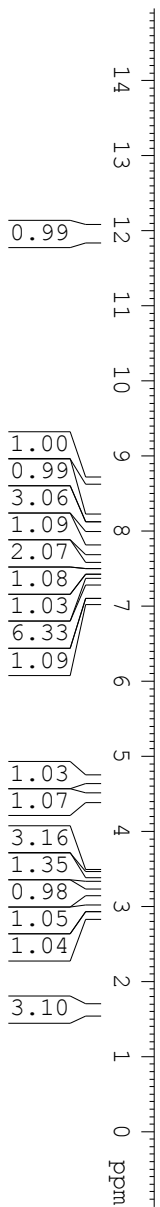
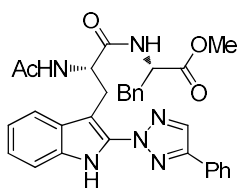
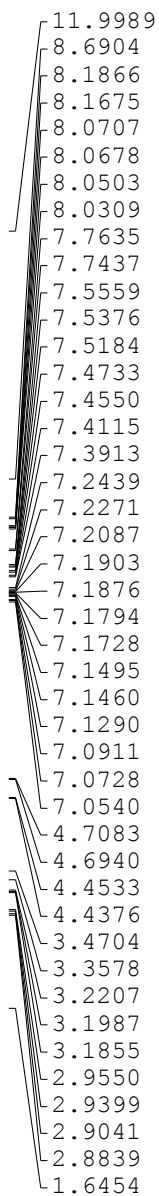
Obtained as a white solid in 79% yield (Condition A) (mixture of conformational isomers, Major/Minor=75/25), $[\alpha]_{\text{D}}^{20} = -10.0$ ($c = 0.2$, CH_3OH); M.p. 170-172 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3): δ (major isomer) 9.21 (br, 1H), 8.07 (s, 1H), 7.66-7.57 (m, 3H), 7.47-7.42 (m, 2H), 7.38 (s, 2H), 7.26-7.24 (m, 3H), 7.17-7.09 (m, 3H), 6.41 (s, 1H), 5.77 (s, 1H), 4.94-4.90 (m, 1H), 4.78-4.72 (m, 1H), 4.30-4.28 (m, 1H), 4.15 (d, $J=5.96\text{Hz}$, 1H), 3.89-3.84 (m, 1H), 3.71-3.69 (m, 2H), 3.67 (s, 3H), 3.58-3.56 (m, 1H),

3.14-3.12 (m, 1H), 2.53-2.50 (m, 1H), 2.44-2.39 (m, 1H), 1.85-1.81 (m, 6H); (minor isomer) 9.15 (br, 1H), 8.17 (s, 1H), 7.75-7.68 (m, 3H), 7.47-7.42 (m, 2H), 7.34 (s, 2H), 7.26-7.24 (m, 3H), 7.01-6.98 (m, 3H), 6.76 (s, 1H), 5.86 (s, 1H), 4.94-4.85 (m, 1H), 4.47-4.45 (m, 1H), 4.19 (d, $J = 5.96\text{Hz}$, 1H), 4.07-4.01 (m, 1H), 3.73 (s, 3H), 3.71-3.69 (m, 2H), 3.58-3.56 (m, 1H), 3.23-3.20 (m, 1H), 2.94-2.89 (m, 1H), 2.73-2.67 (m, 1H), 2.01-1.90 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 171.6, 171.2, 170.8, 170.3, 169.9, 163.1 (d, $J = 246.25\text{Hz}$), 152.6, 147.9, 147.7, 140.2, 132.9, 132.7 (d, $J = 8.72\text{Hz}$), 132.0, 131.4, 130.8 (d, $J = 7.62\text{Hz}$), 128.0, 123.7, 121.8, 120.8, 119.5, 116.3 (d, $J = 19.97\text{Hz}$), 115.9, 113.1 (d, $J = 23.05\text{Hz}$), 111.5, 100.0, 82.3, 60.7, 54.3, 52.3, 51.6, 47.4, 41.2, 35.5, 28.7, 25.9, 25.0, 22.8; IR (KBr): ν (cm^{-1}) 3257, 3045, 2924, 1747, 1635, 1591, 1417, 1384, 1228, 1047, 879, 748 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{39}\text{H}_{40}\text{FN}_8\text{O}_9$ $[\text{M}+\text{FORMATE}]^-$: 783.2908; Found: 783.2912.

References:

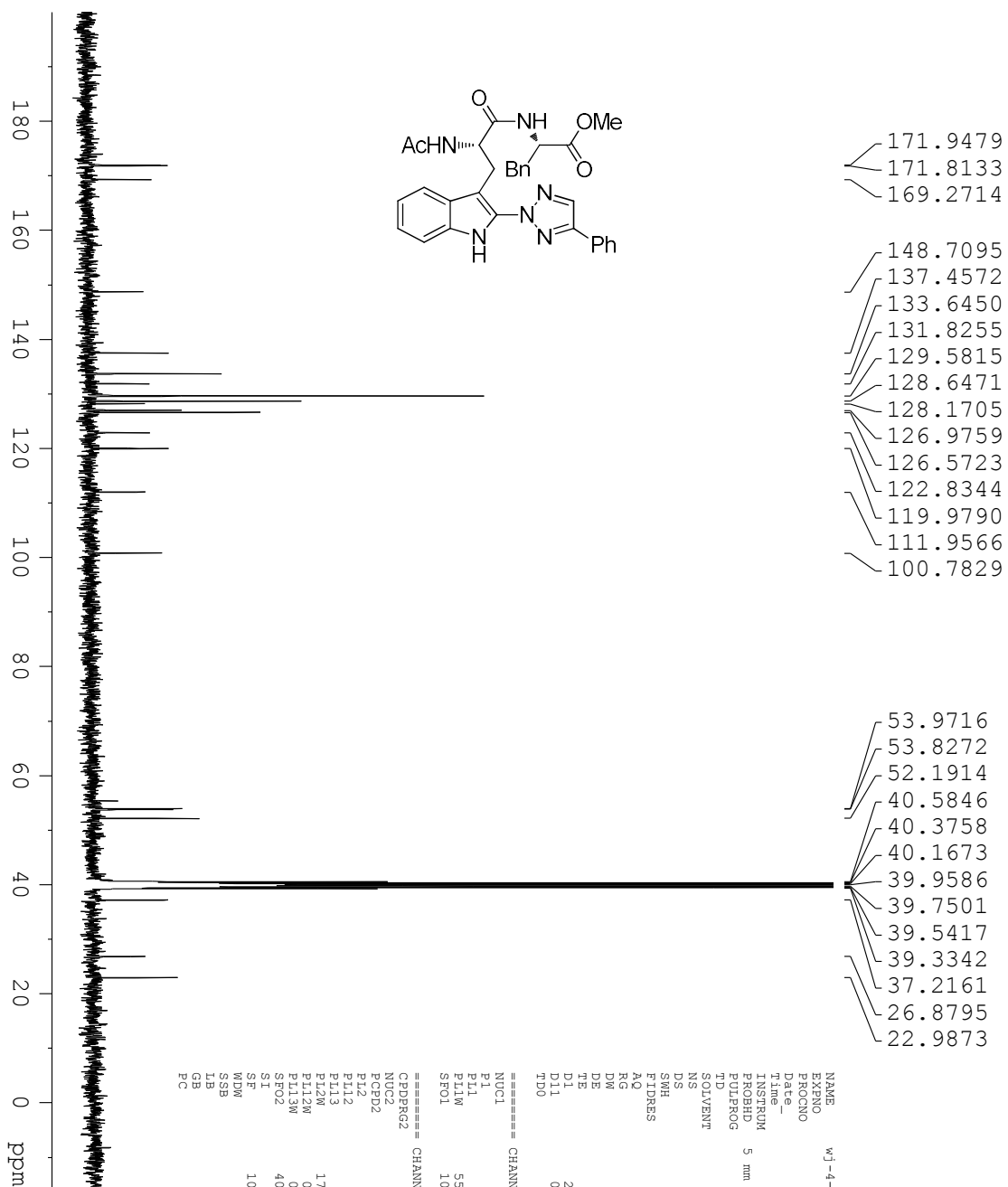
- 1, (a) Parker, C. A.; Rees, W. T. *Analyst*, **1960**, 85, 587. (b) Forgues, S. F.; Lavabre, D. *J. Chem. Educ.* **1999**, 76, 1260. (c) Berlman, I. B. Handbook of fluorescence spectra of aromatic molecules, Academic Press, New York, **1971**. (d) Ajayaghosh, A.; Carol, P.; Sreejith, S. *J. Am. Chem. Soc.* **2005**, 127, 14962. (e) Lin, W.; Yuan, L.; Feng, J.; Cao, X. *Eur. J. Org. Chem.* **2008**, 2689.
- 2, Jin, T.; Kamijo, S.; Yamamoto, Y. *Eur. J. Org. Chem.* **2004**, 3789.
- 3, Huang, Q.; Zheng, M.; Yang, S.; Kuang, C.; Yu, C.; Yang, Q. *Eur. J. Med. Chem.* **2011**, 46, 5680.

^1H NMR and ^{13}C NMR spectra



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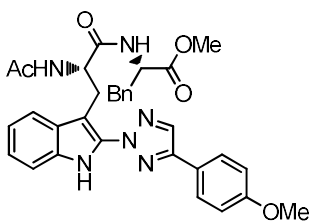
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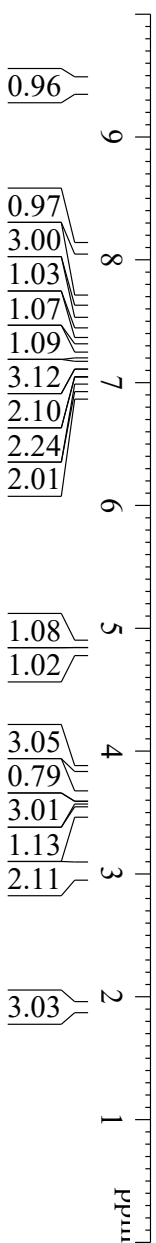


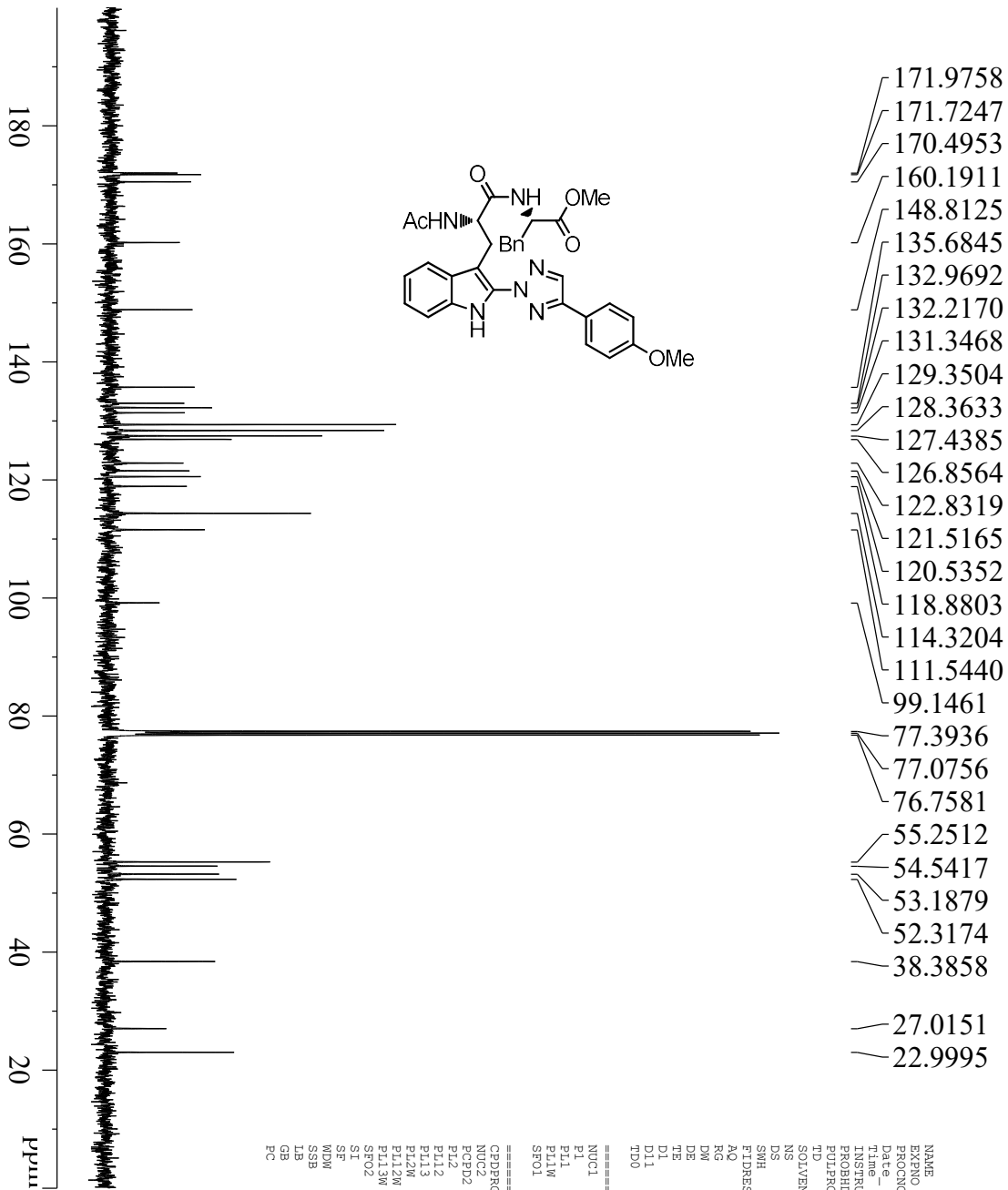
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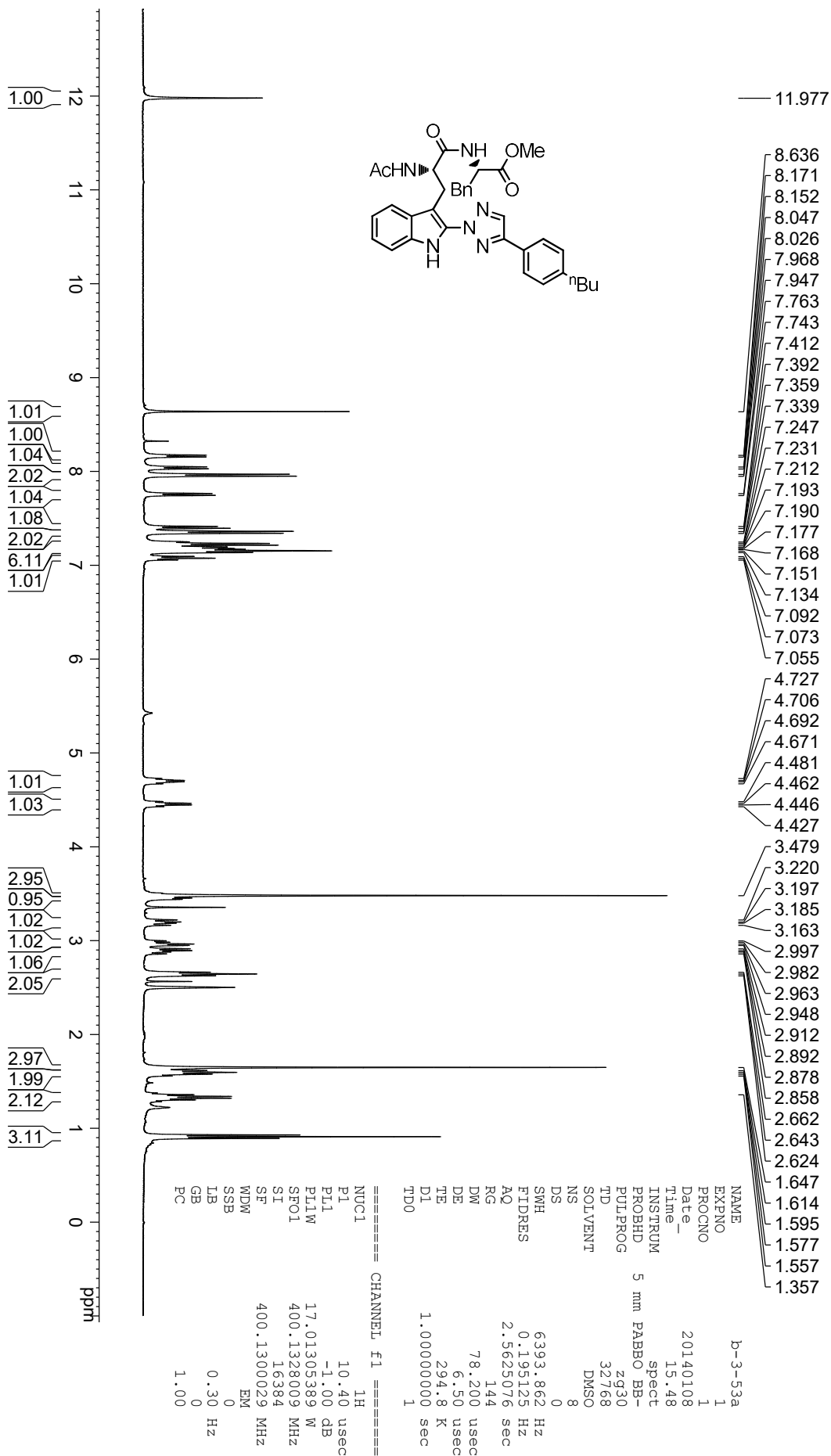
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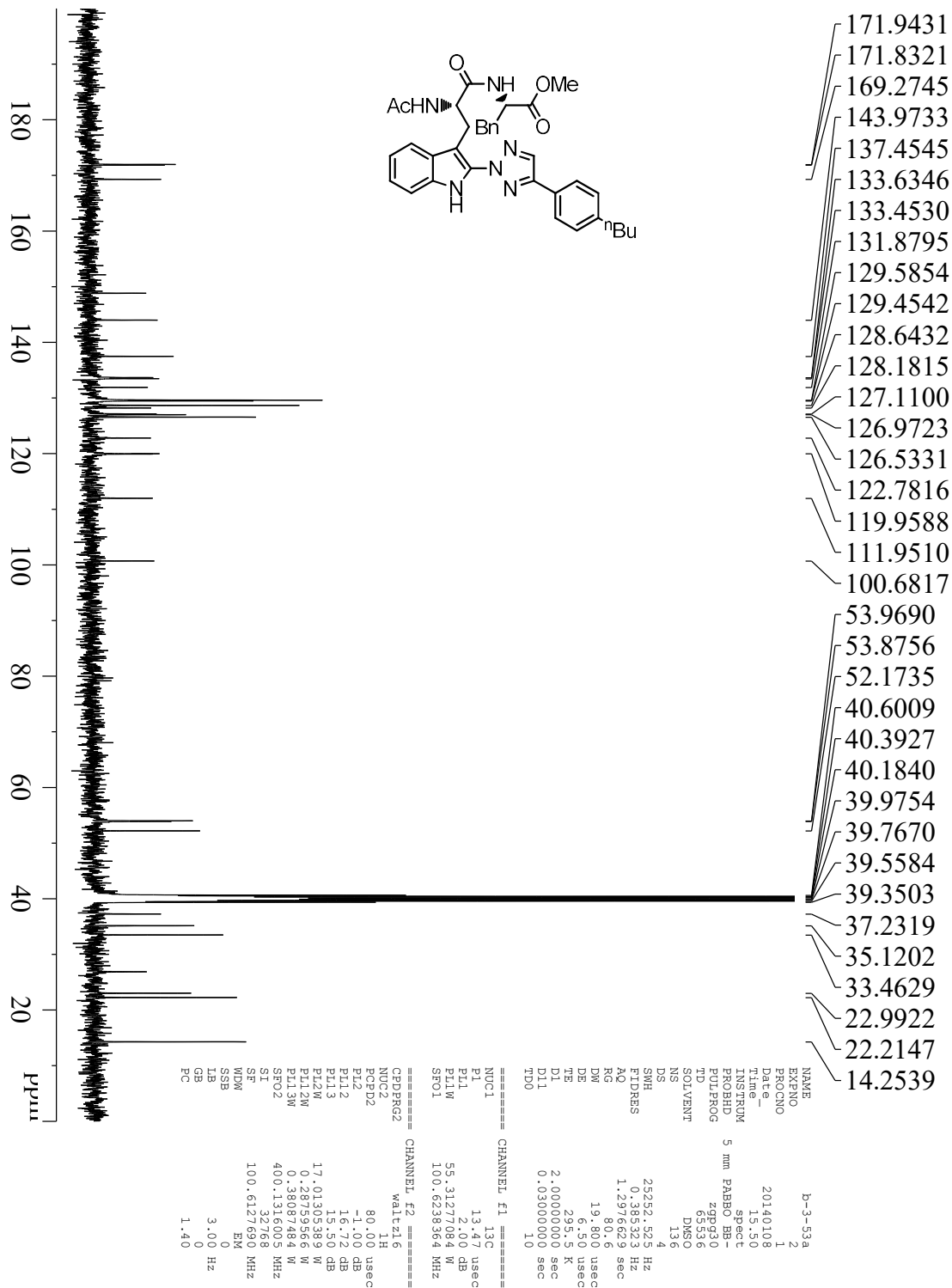
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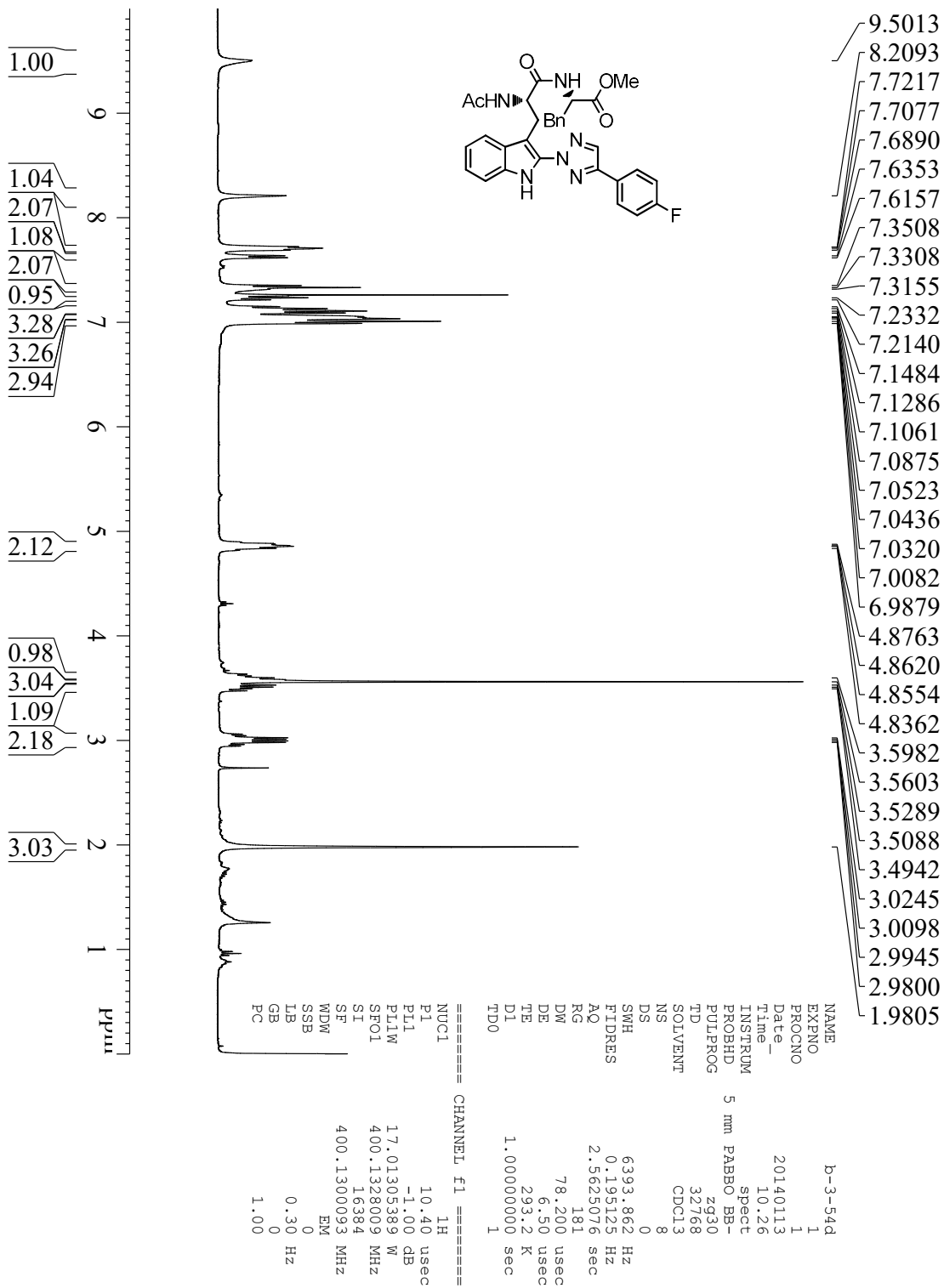
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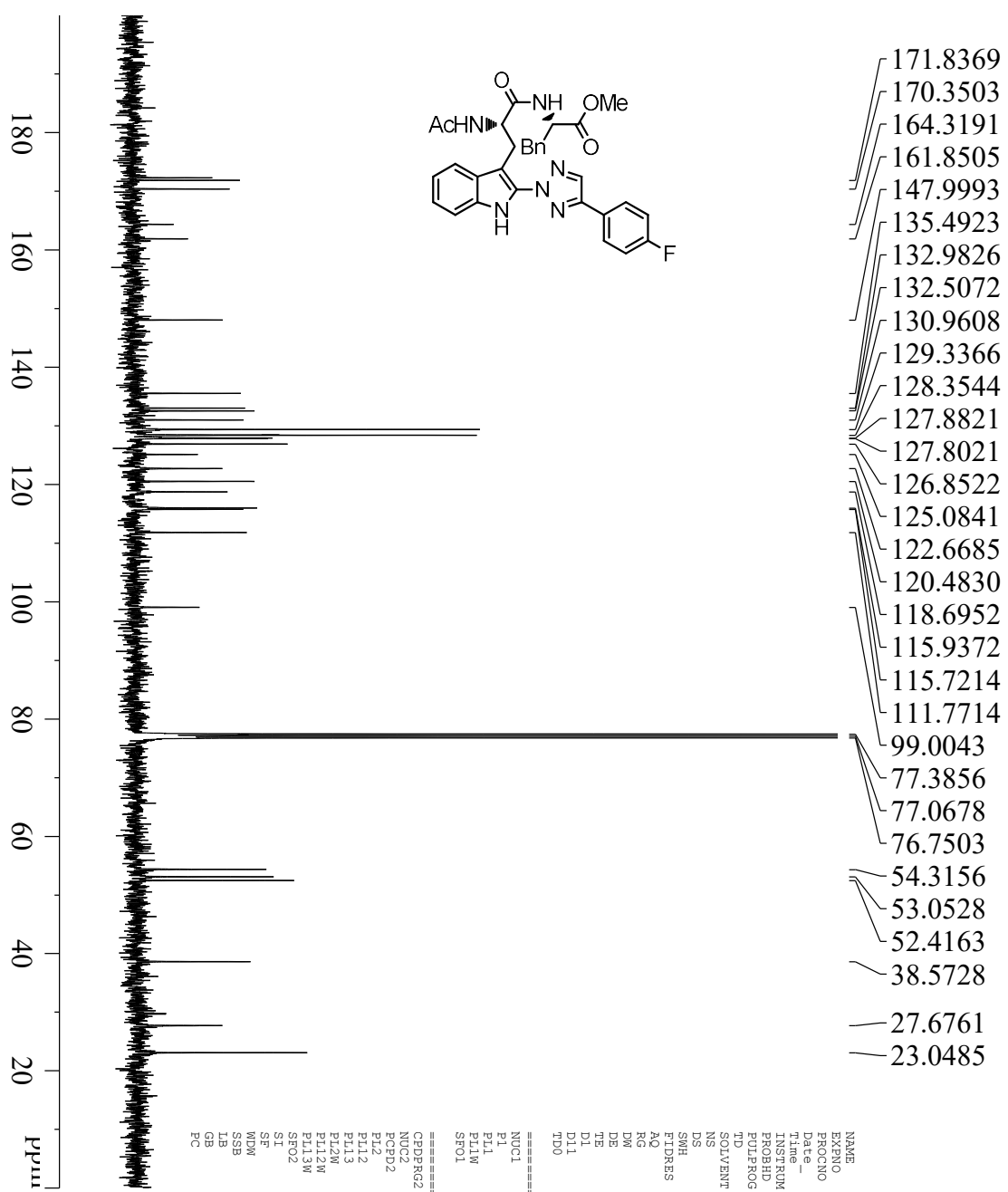
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PL12W 0.28759566 W
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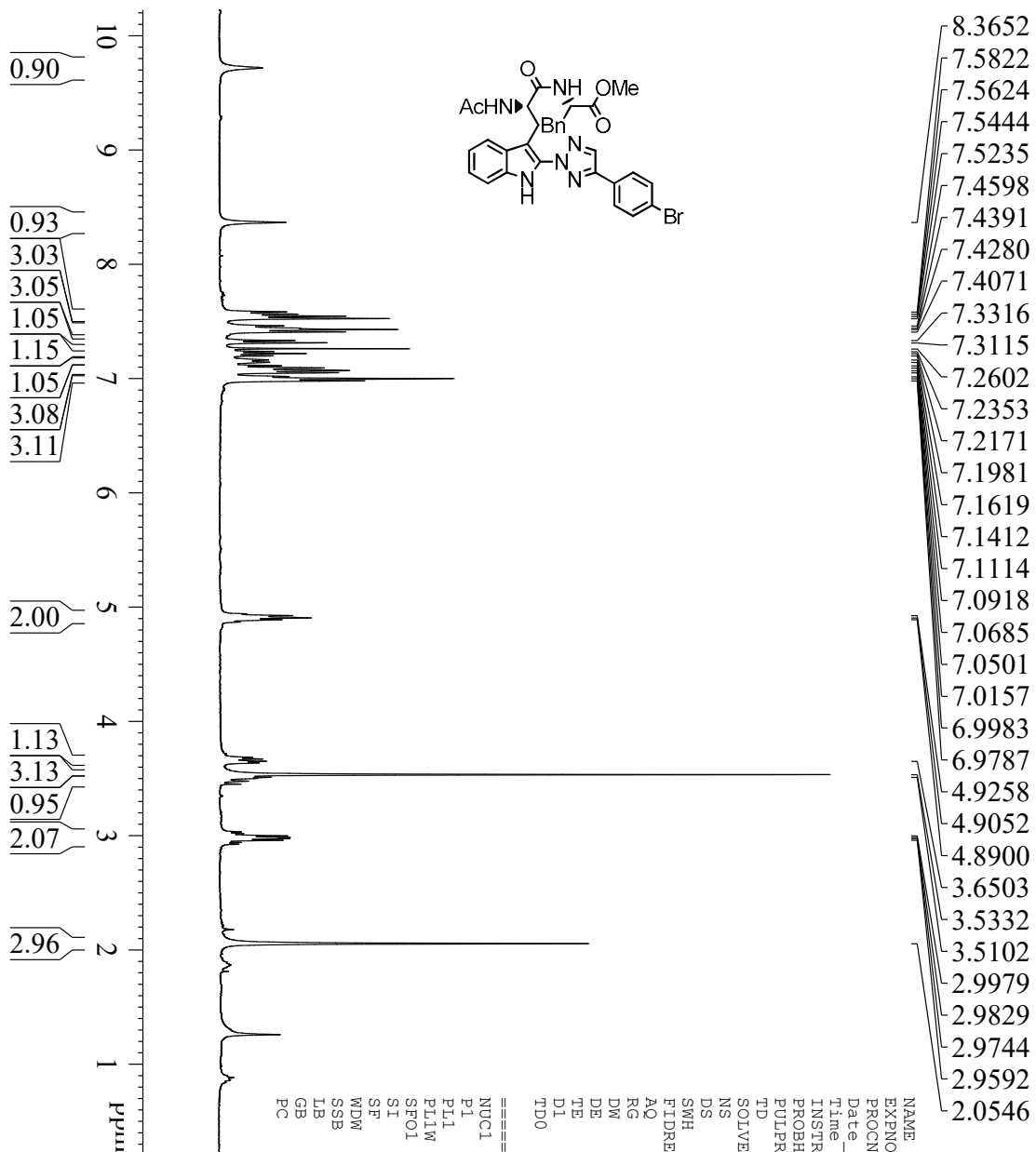


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D11 0.03000000 sec
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PL2 16.72 dB
PL3 15.50 dB
PL2W 17.01305389 W
PL3W 0.28759566 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

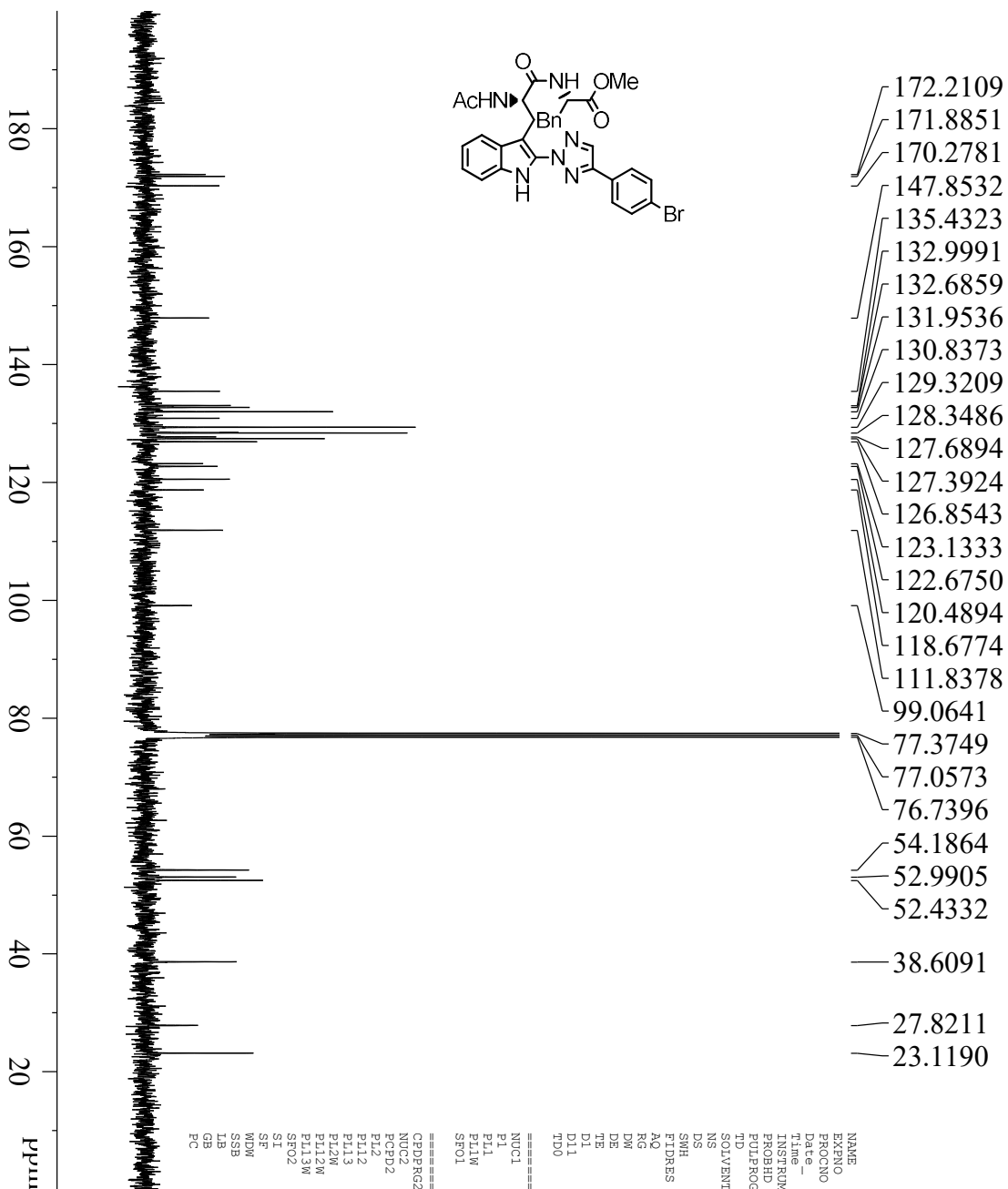
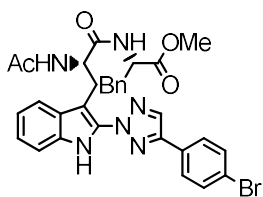


```

NAME b-3-52a
EXPNO 1
PROCNO 1
Date_ 20140106
Time_ 16.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 90.5
DW 78.200 usec
DE 6.50 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.40 usec
PL1 -1.00 dB
PLI1 17.01305389 W
SFO1 400.1328009 MHz
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```

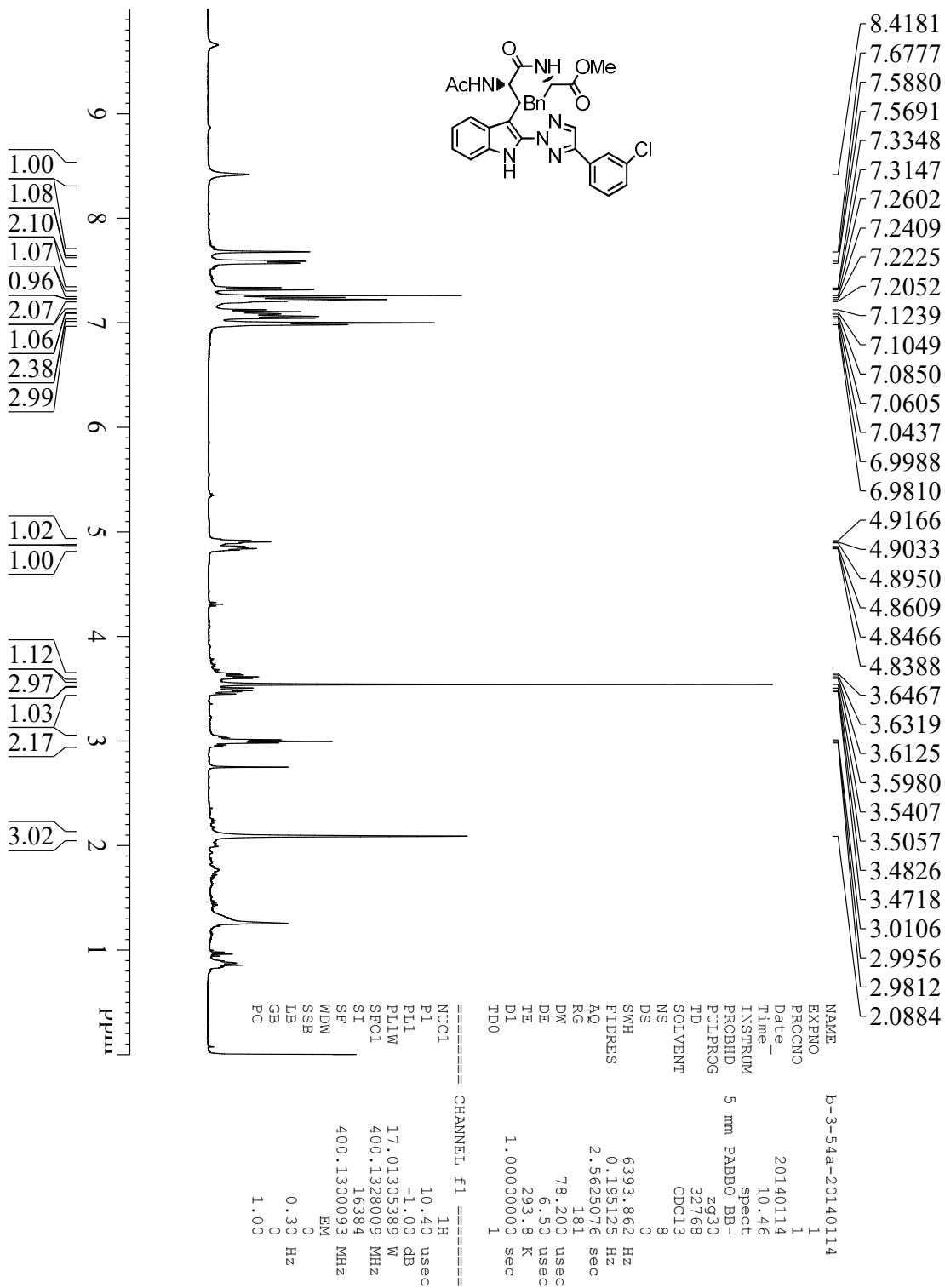
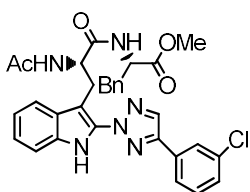


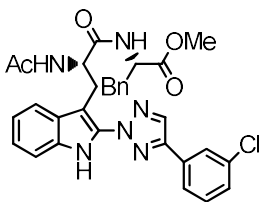
```

NAME          b-3-52a
EXPNO         2
PROCNO        1
Date_         20140106
Time-         16.07
INSTRUM       spect
PROBHD        5 mm PAEBQ BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            104
DS            4
SWH           25252.525 Hz
FIDRES        0.385323 Hz
AQ            1.297629 sec
RG            80.6
DW            19.800 usec
DE            6.50 usec
TE            295.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           10

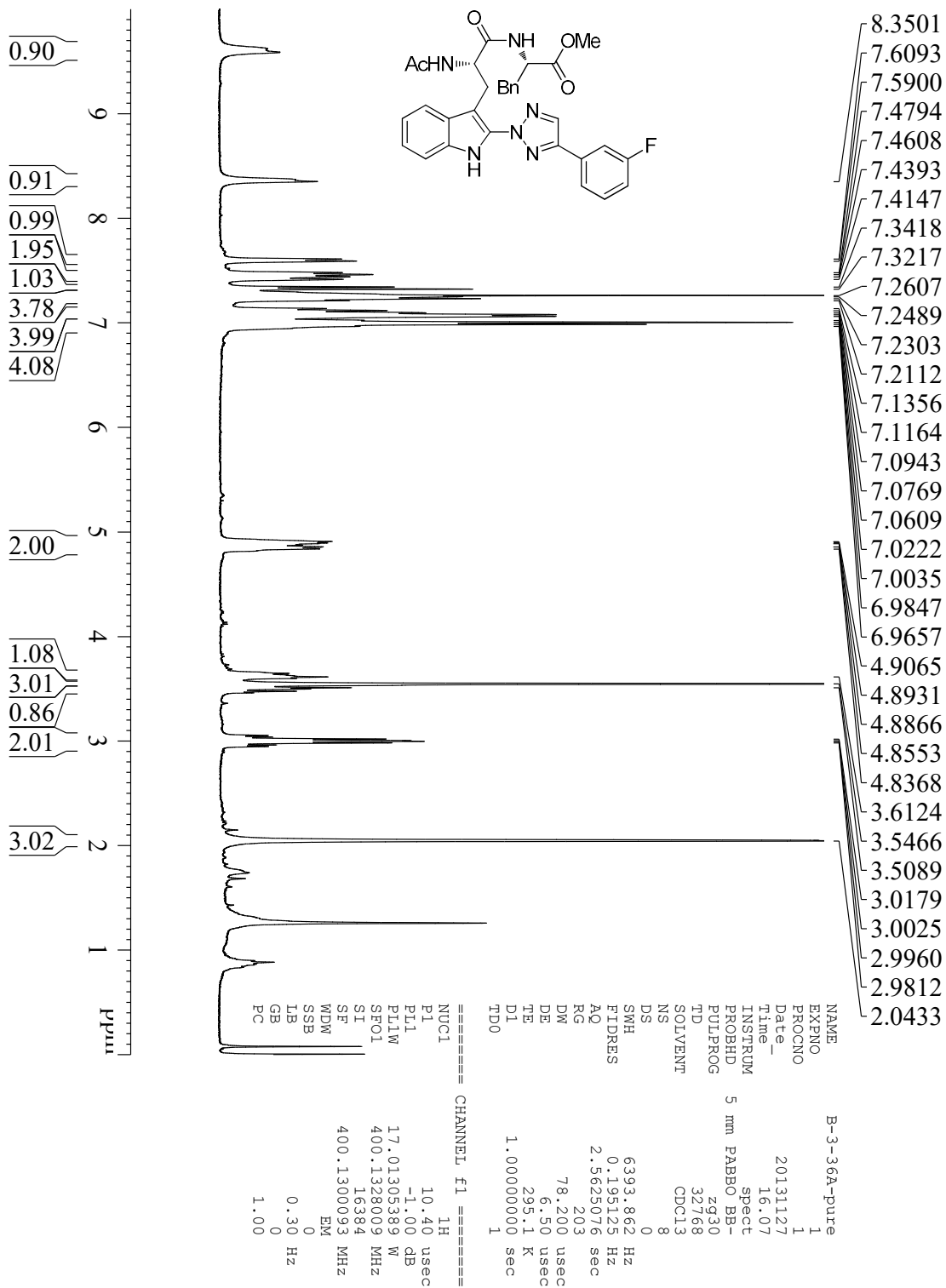
===== CHANNEL f1 =====
NUC1          13C
P1            13.47 usec
PL1           2.00 dB
PL1W          55.31271084 W
SFO1          100.6236364 MHz

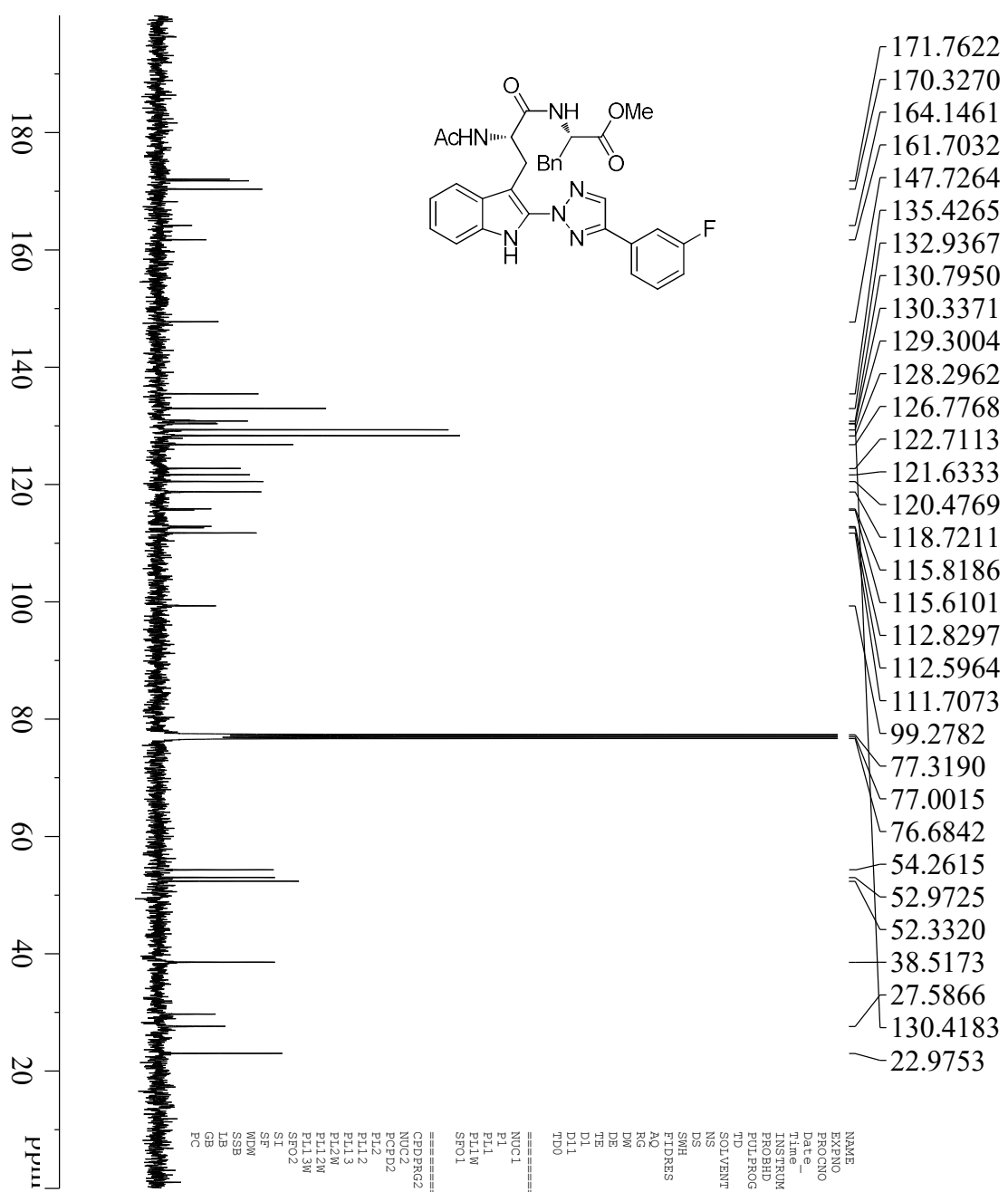
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PT2           -1.00 dB
PL12          16.72 dB
PL13          15.50 dB
PL1W          17.01305389 W
PL12W         0.28759566 W
PL13W         0.38087484 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.40
  
```





NAME	b-3-54a1	
EXPNO	2	
PROCNO	1	
Date_	20140110	
Time	15.45	
INSTRUM	5 mm PABBO BBO	
PROBHD	zpg3030	
PULPROG	65536	
TD	65536	
SOLVENT	CDCl3	
NS	64	
DS	4	
SWH	25252.525 Hz	
FIDRES	0.385323 Hz	
AQ	1.2976229 sec	
RG	80.6	
DW	19.800 usec	
DE	6.50 usec	
TE	294.4 K	
D1	2.00000000 sec	
D11	0.03000000 sec	
TD0	10	
=====		
NUC1	13C	
P1	13.47 usec	
P11	2.00 dB	
P1M	55.31277054 W	
SFO1	100.628364 MHz	
=====		
CHANNEL f2		
CEDRG2	waltz16	
NUC2	1H	
PCPD2	80.00 usec	
P12	-1.00 dB	
P112	16.72 dB	
P113	13.50 dB	
P12W	17.0130389 W	
P112M	0.28579556 W	
P113M	0.38087484 W	
SFO2	400.1316005 MHz	
SI	32768	
WDW	100.6127605 MHz	
SSB	EM	
ZB	0	
GB	3.00 Hz	
PC	0	
FC	1.40	

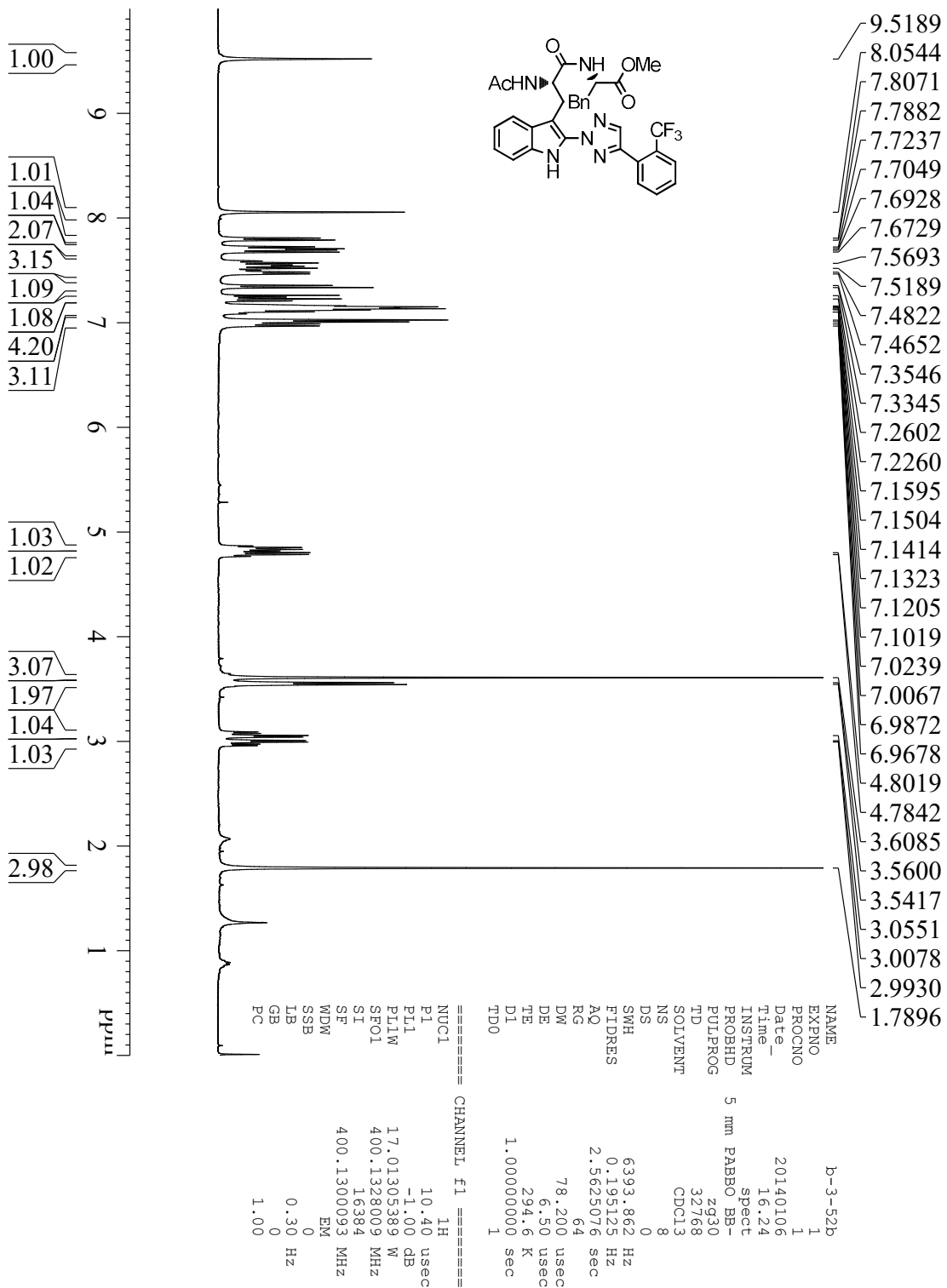
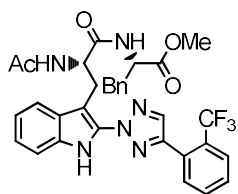


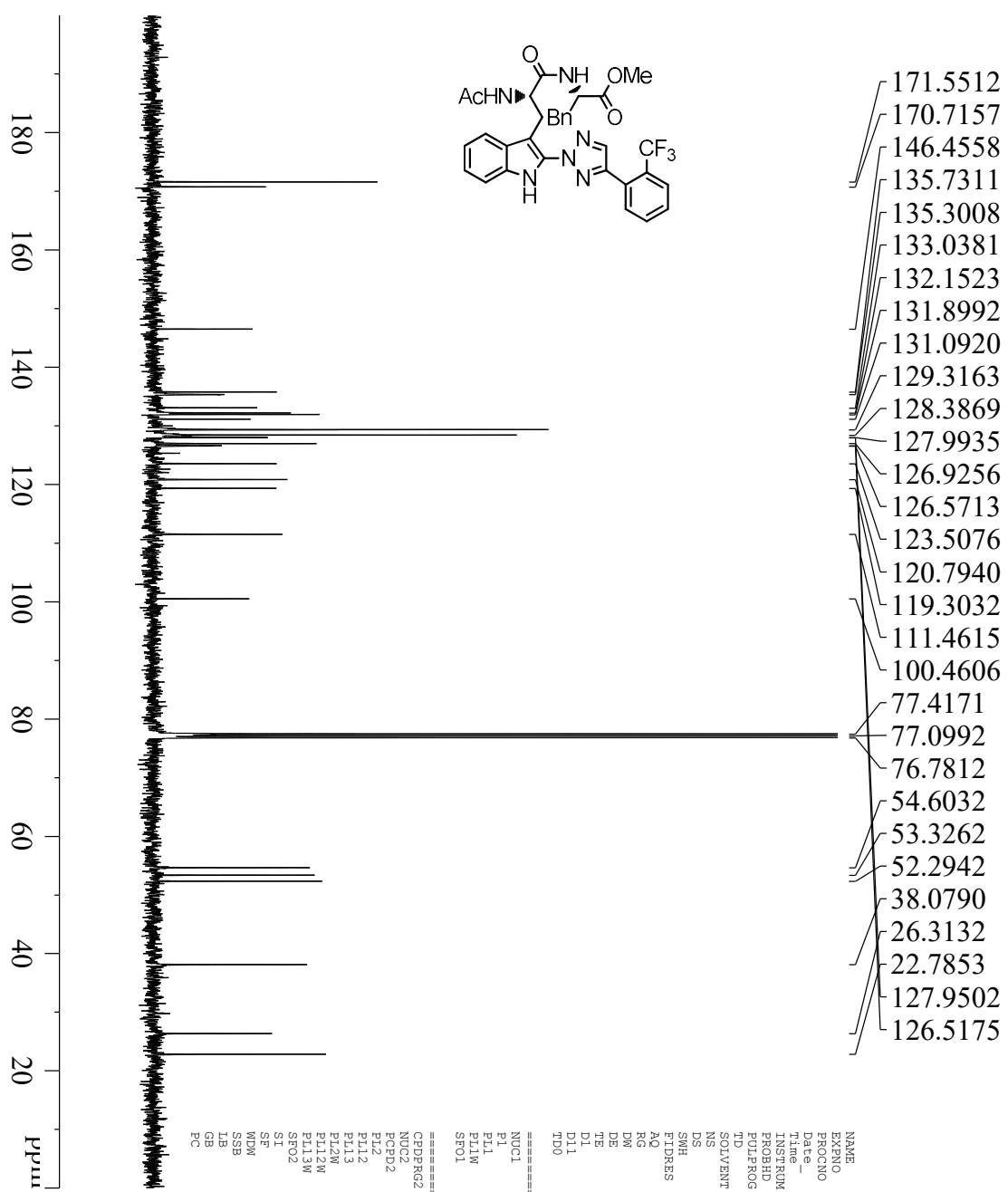


NAME B-3-36A-20131212
EXPNO 2
PROCNO 1
Date_ 20131212
Time_ 15.36
INSTRUM spect
PROBHD 5 mm PA6B0 BB-
PULPROG zgpg30
TD 65536
FIDRES 0.385323 Hz
AQ 1.297629 sec
RG 181
DW 19.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 13.47 usec
PL 2.00 dB
PL1W 55.31271084 W
SFO1 100.6238364 MHz

===== CHANNEL f2 =====
CDEPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PT2 -1.00 dB
PL12 16.72 dB
PL13 15.50 dB
PL12W 17.01305389 W
PL13W 0.28759566 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127734 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



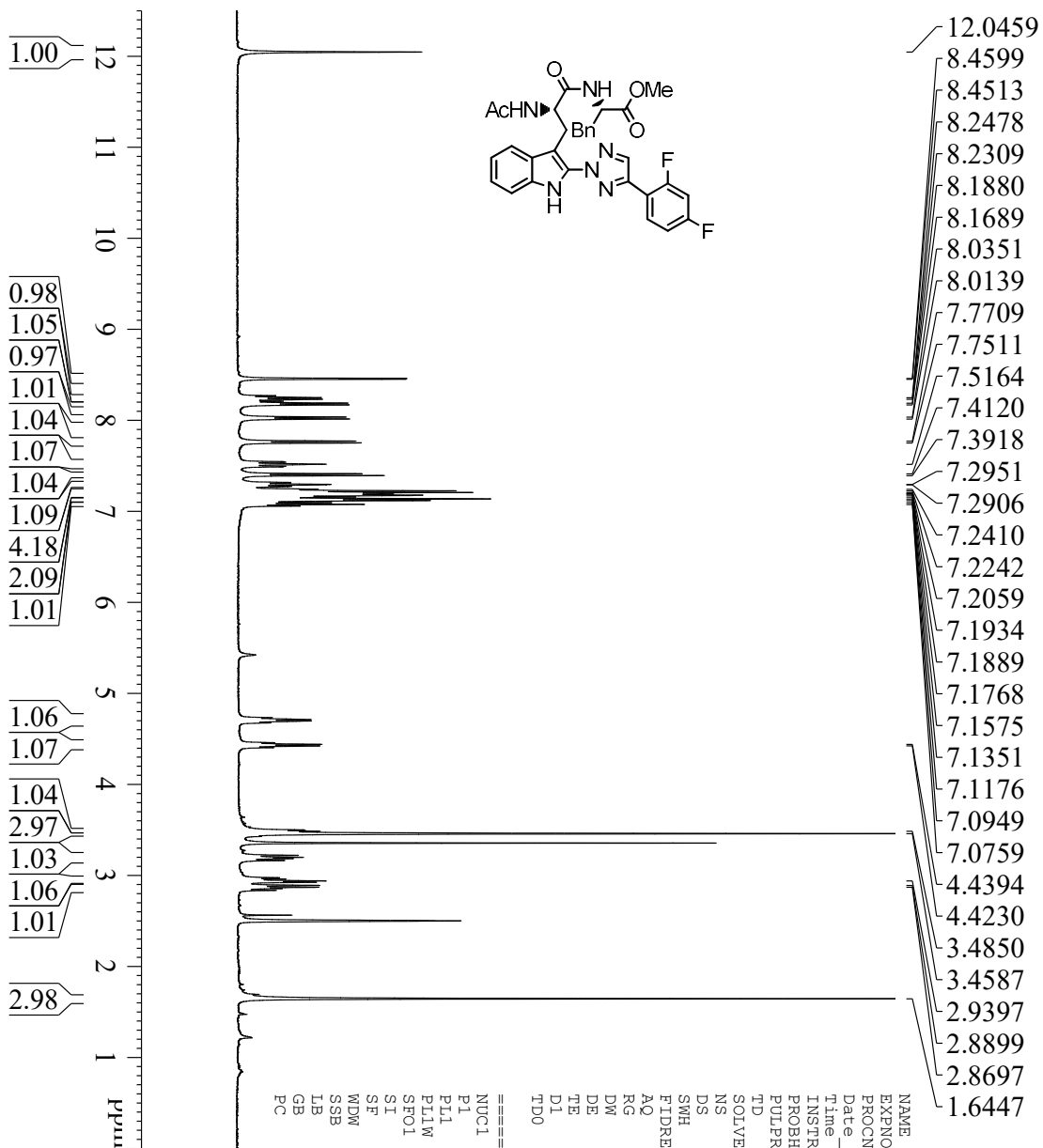
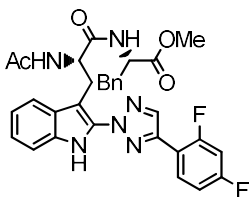


- 171.5512
- 170.7157
- 146.4558
- 135.7311
- 135.3008
- 133.0381
- 132.1523
- 131.8992
- 131.0920
- 129.3163
- 128.3869
- 127.9935
- 126.9256
- 126.5713
- 123.5076
- 120.7940
- 119.3032
- 111.4615
- 100.4606
- 77.4171
- 77.0992
- 76.7812
- 54.6032
- 53.3262
- 52.2942
- 38.0790
- 26.3132
- 22.7853
- 127.9502
- 126.5175

NAME b-3-52b2
EXPNO 2
PROCNO 1
Date_ 20140107
Time_ 10.47
INSTRUM spect
PROBHD 5 mm PAEB0 BB-
PULPROG zgpg30
TD 65536
FIDRES 1.297629 sec
SOLVENT CDCl3
NS 80
DS 4
SWH 2522.525 Hz
FIDRES 0.385323 Hz
AQ 1.297629 sec
RG 80.6
DE 19.800 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 13.47 usec
PL1 2.00 dB
PL1W 55.31277084 W
SFO1 100.6236364 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PT2 -1.00 dB
PL2 16.72 dB
PL3 15.50 dB
PL2W 17.01305389 W
PL3W 0.28759566 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

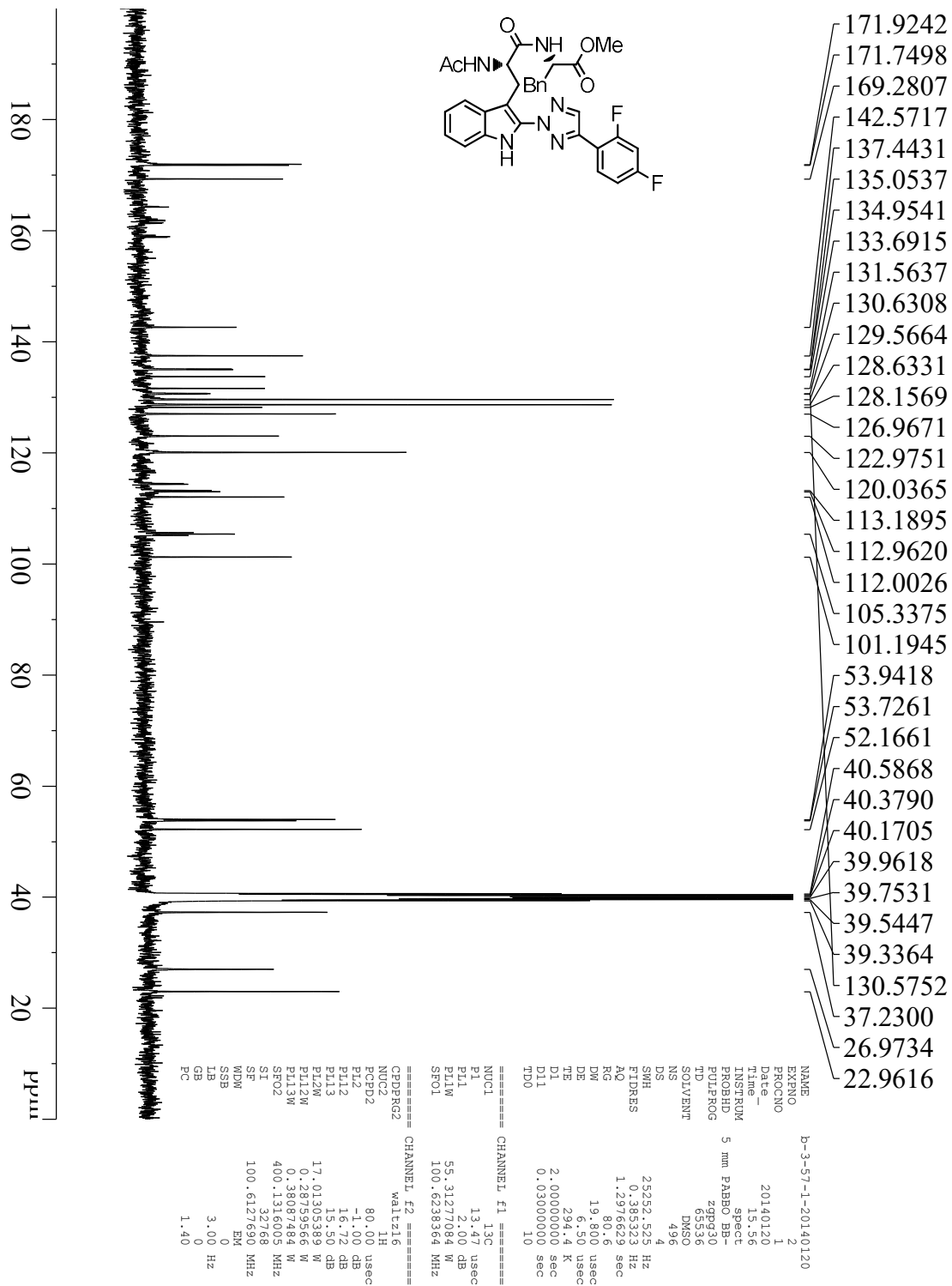


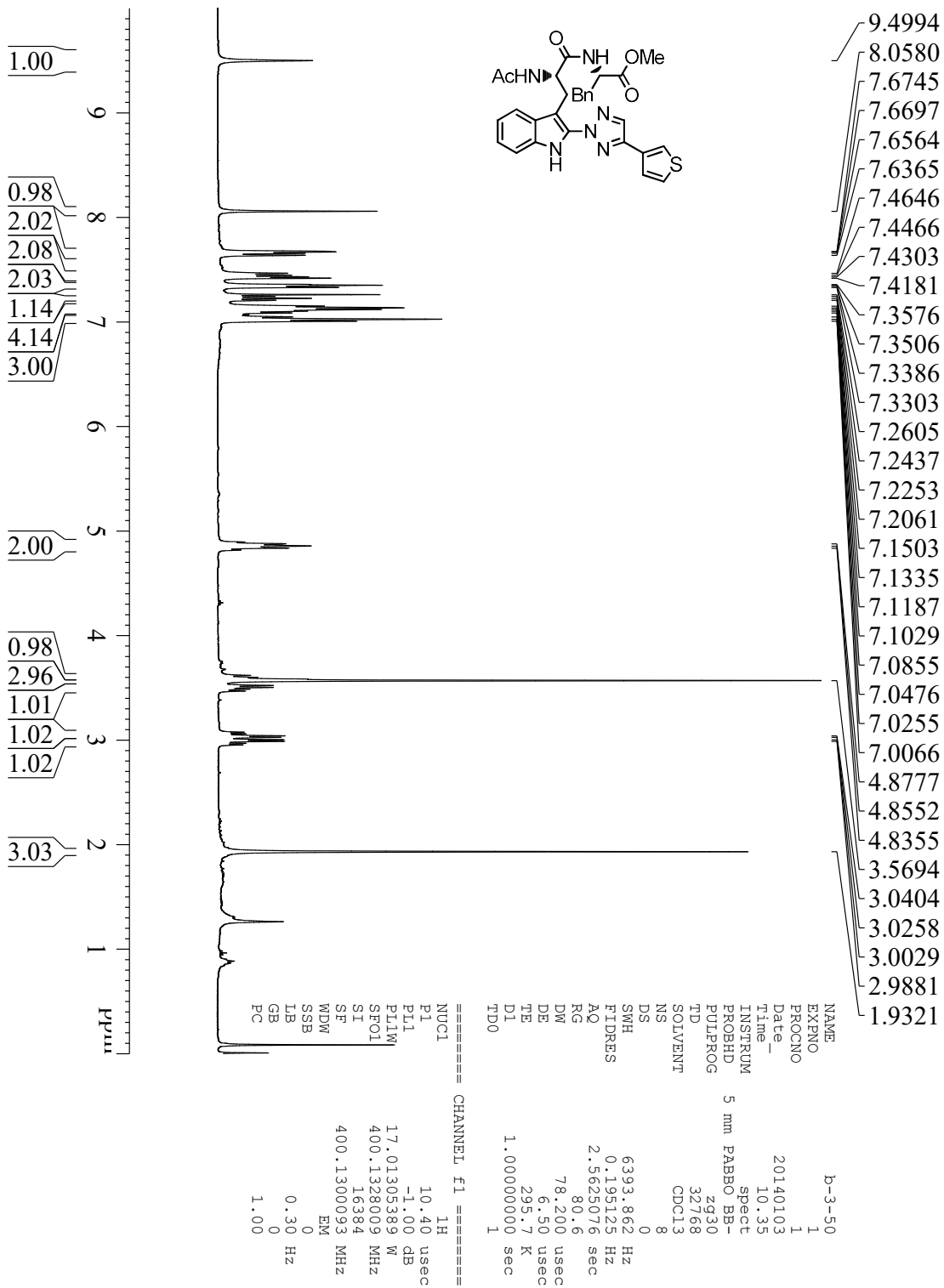
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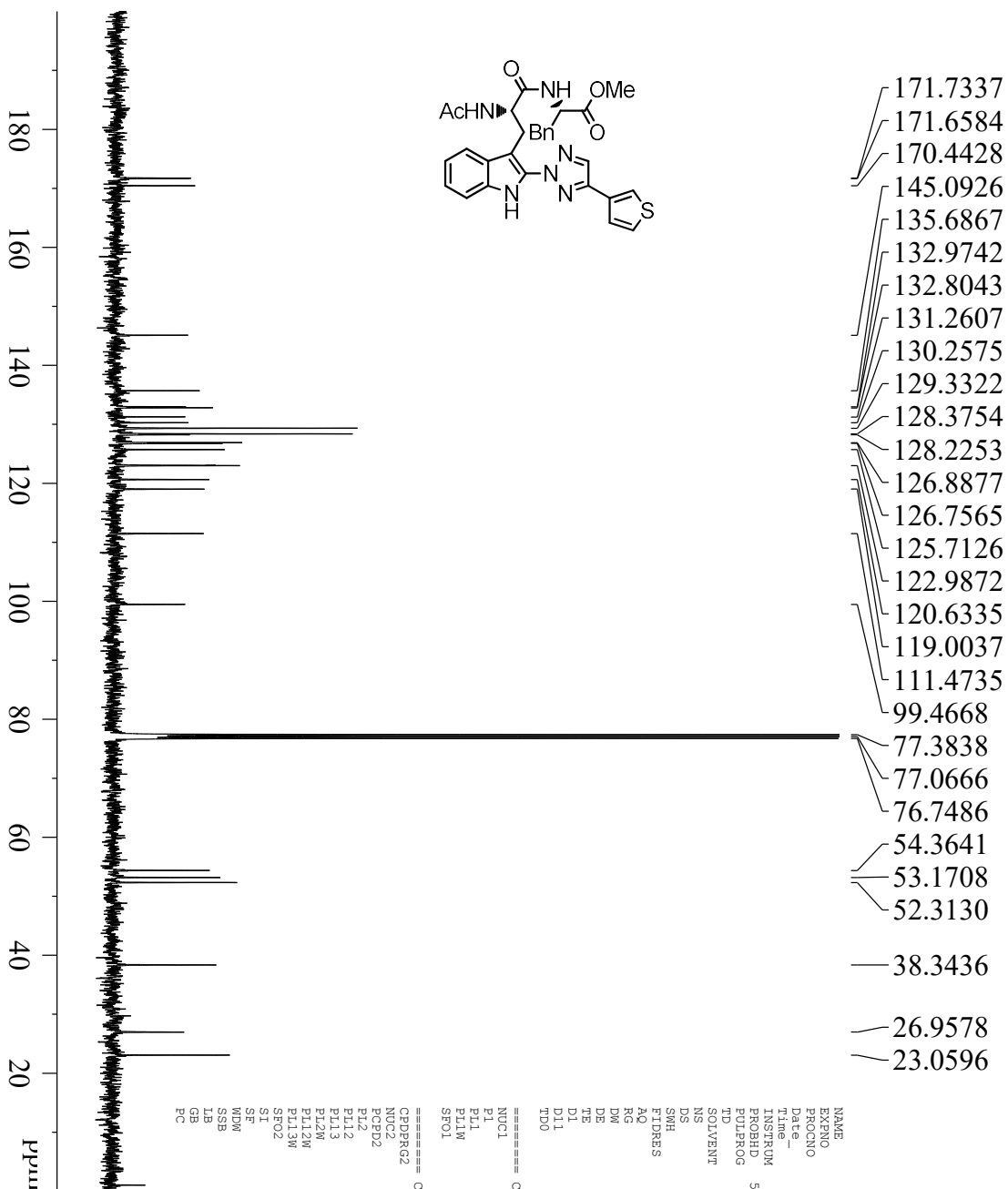
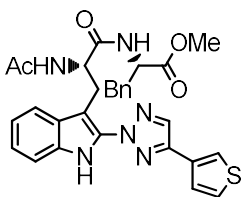
NAME b-3-57-1
EXPNO 1
PROCNO 1
Date_ 20140117
Time_ 16.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 203
DW 78.200 usec
DE 6.50 usec
TE 293.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.40 usec
PL1 -1.00 dB
PL1W 17.01305389 W
SFO1 400.1328009 MHz
SI 16384
SF 400.1300027 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```





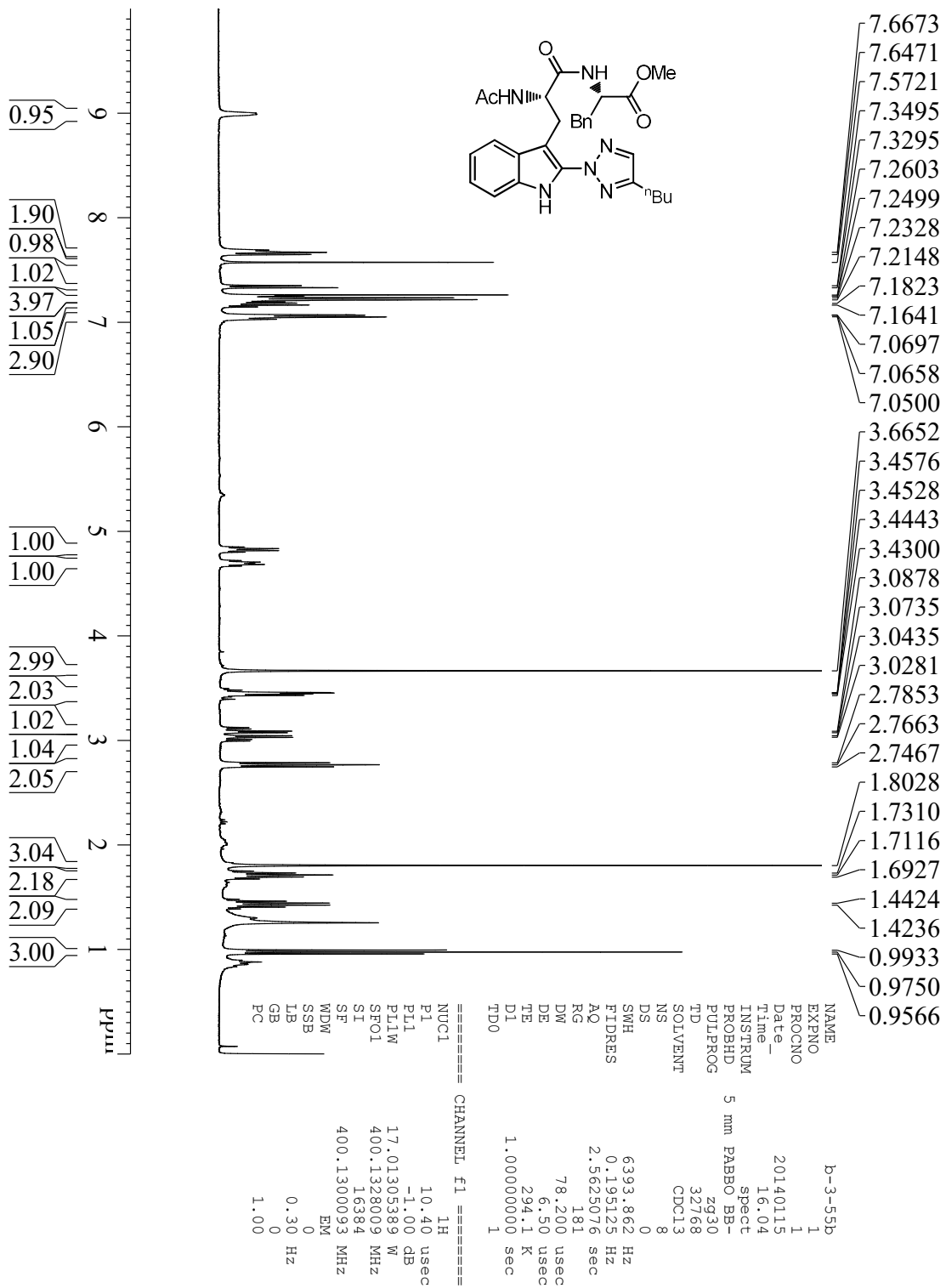


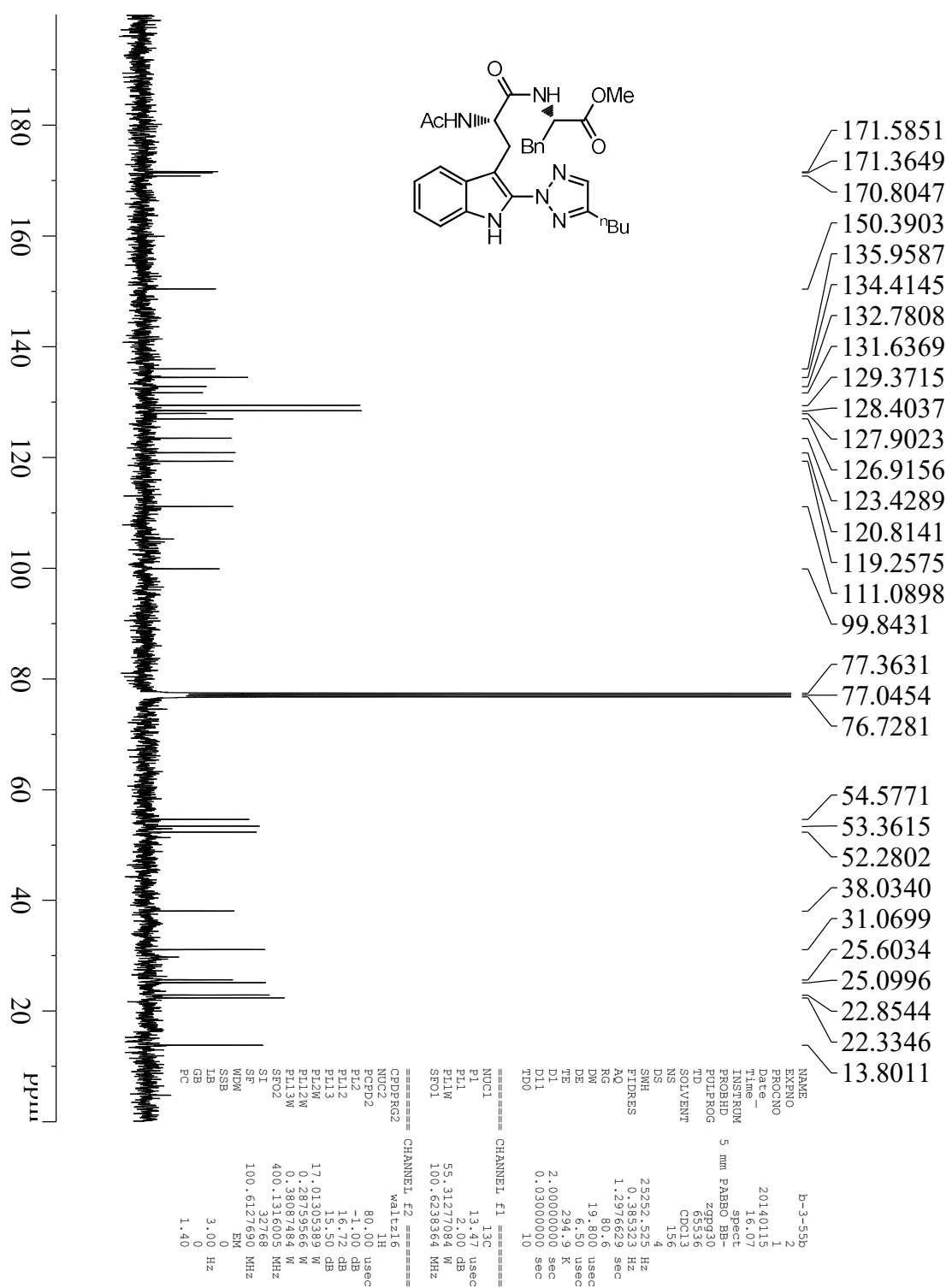
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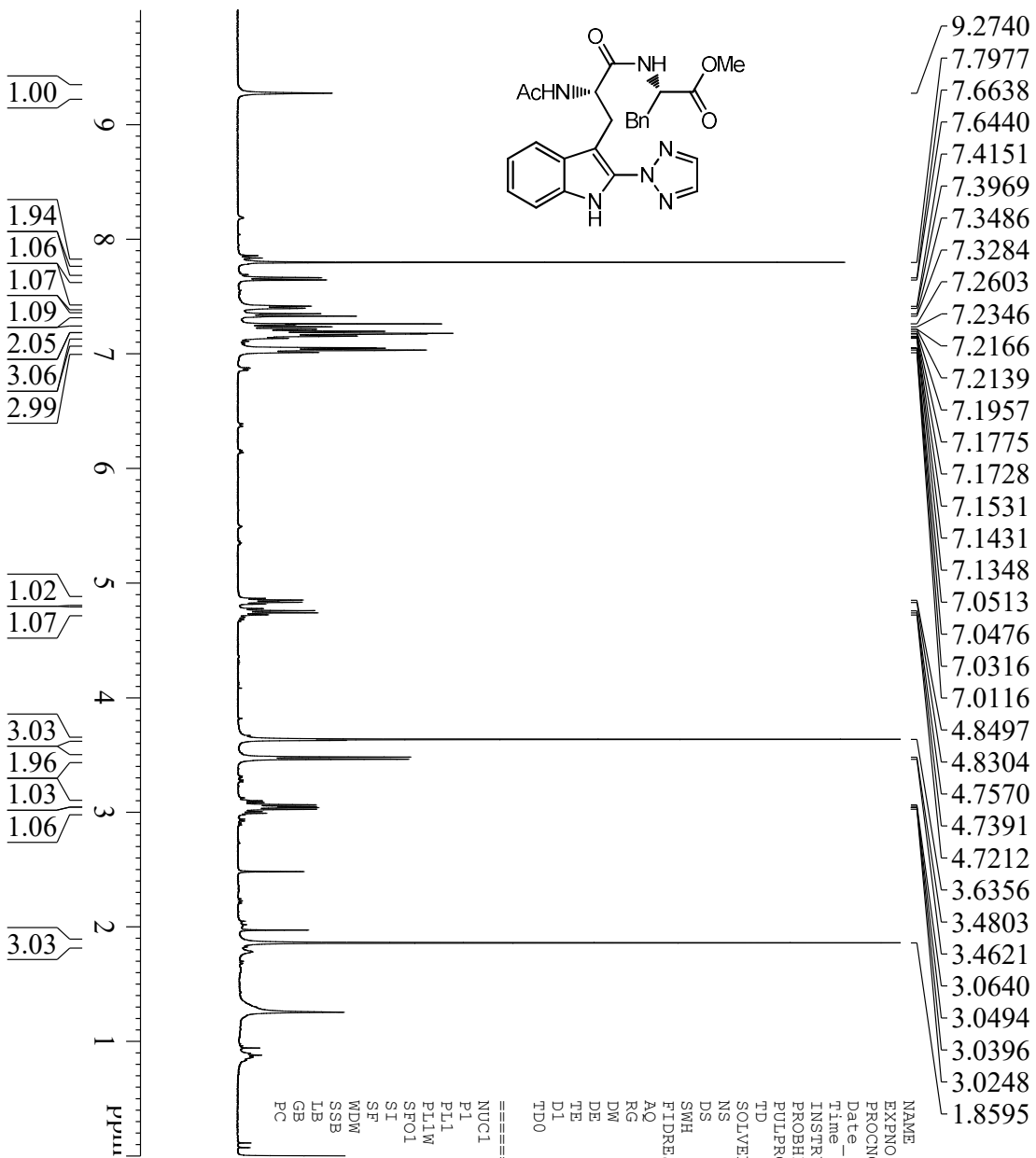
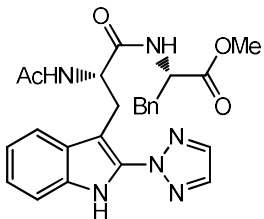
NAME b-3-50-2
EXPNO 2
PROCNO 1
Date_ 20140103
Time 15:43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 144
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 80.6
DE 19.800 usec
TE 297.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 13.47 usec
PL1 2.00 dB
FLLW 55.3127084 W
SFO1 100.6236364 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.72 dB
PL13 15.50 dB
PL12W 17.01305389 W
PL13W 0.28759566 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
MDM EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
  
```

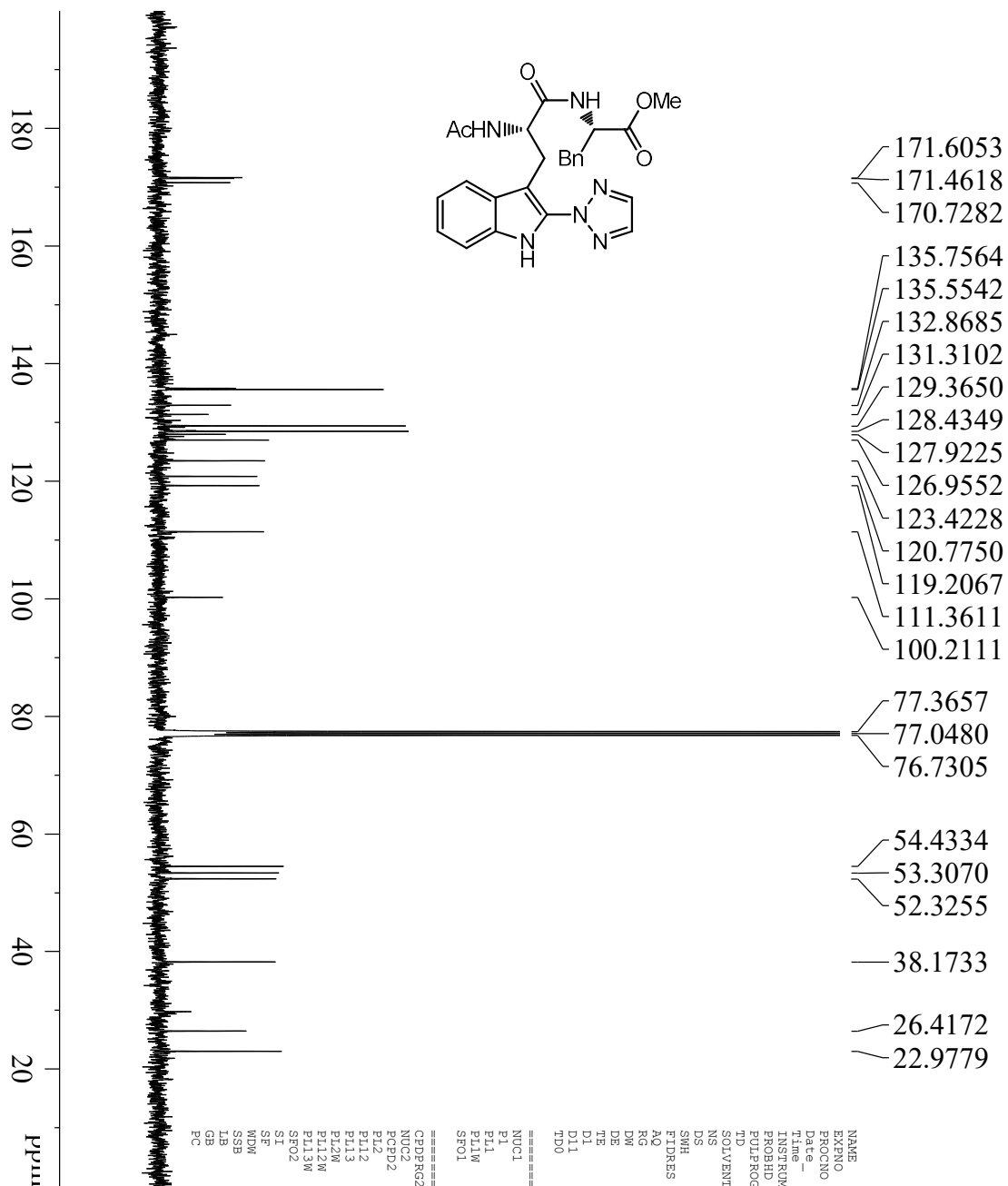


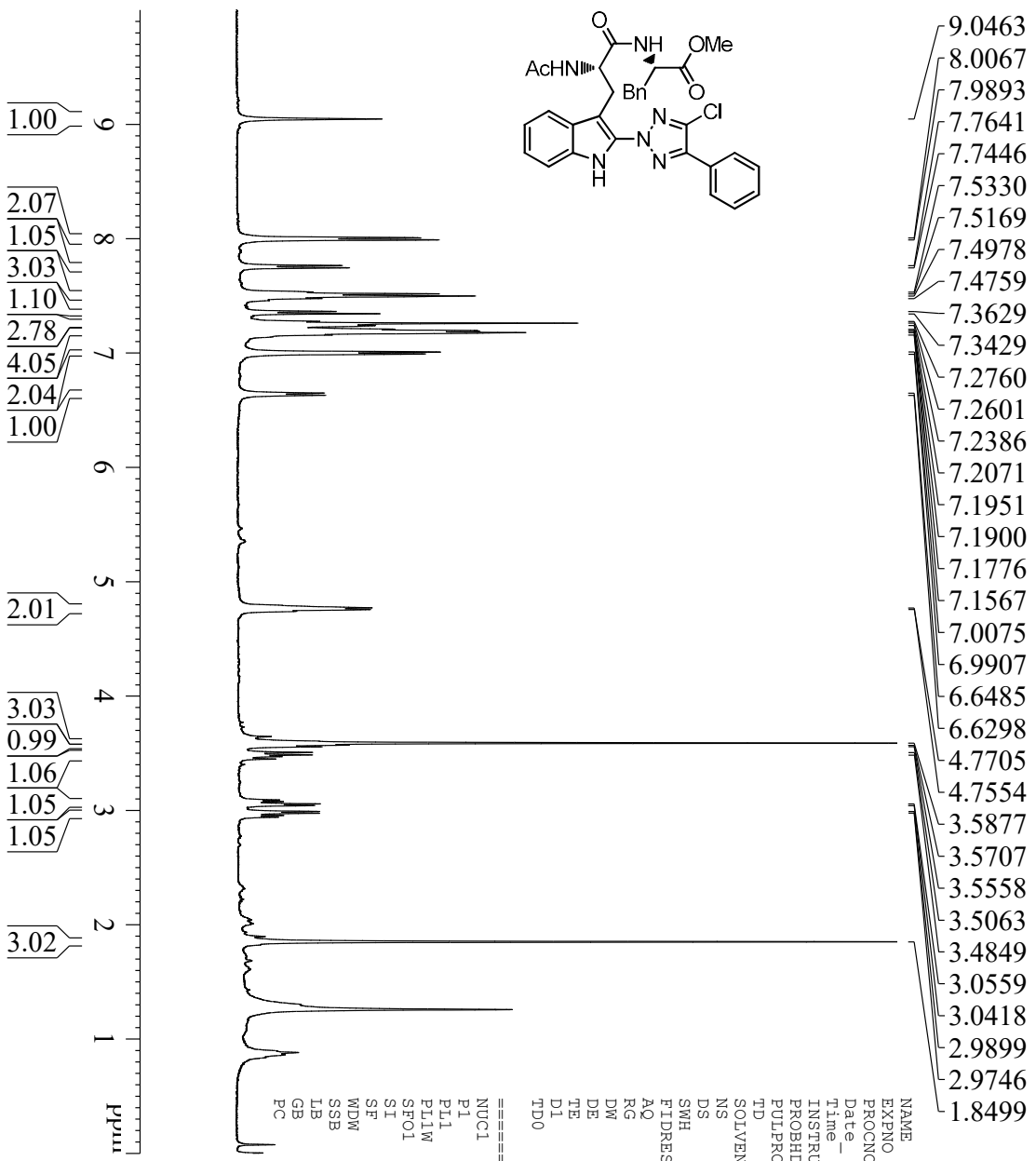
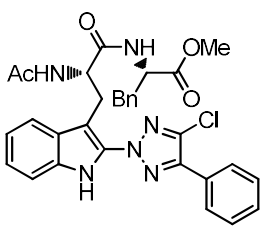


```

NAME b-3-55a
EXPNO 1
PROCNO 1
Date_ 20140116
Time_ 16.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 203
DW 78.200 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.40 usec
PL1 -1.00 dB
PLI1 17.01305389 W
SF01 400.1328009 MHz
SI 16384
SF 400.130093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
  
```

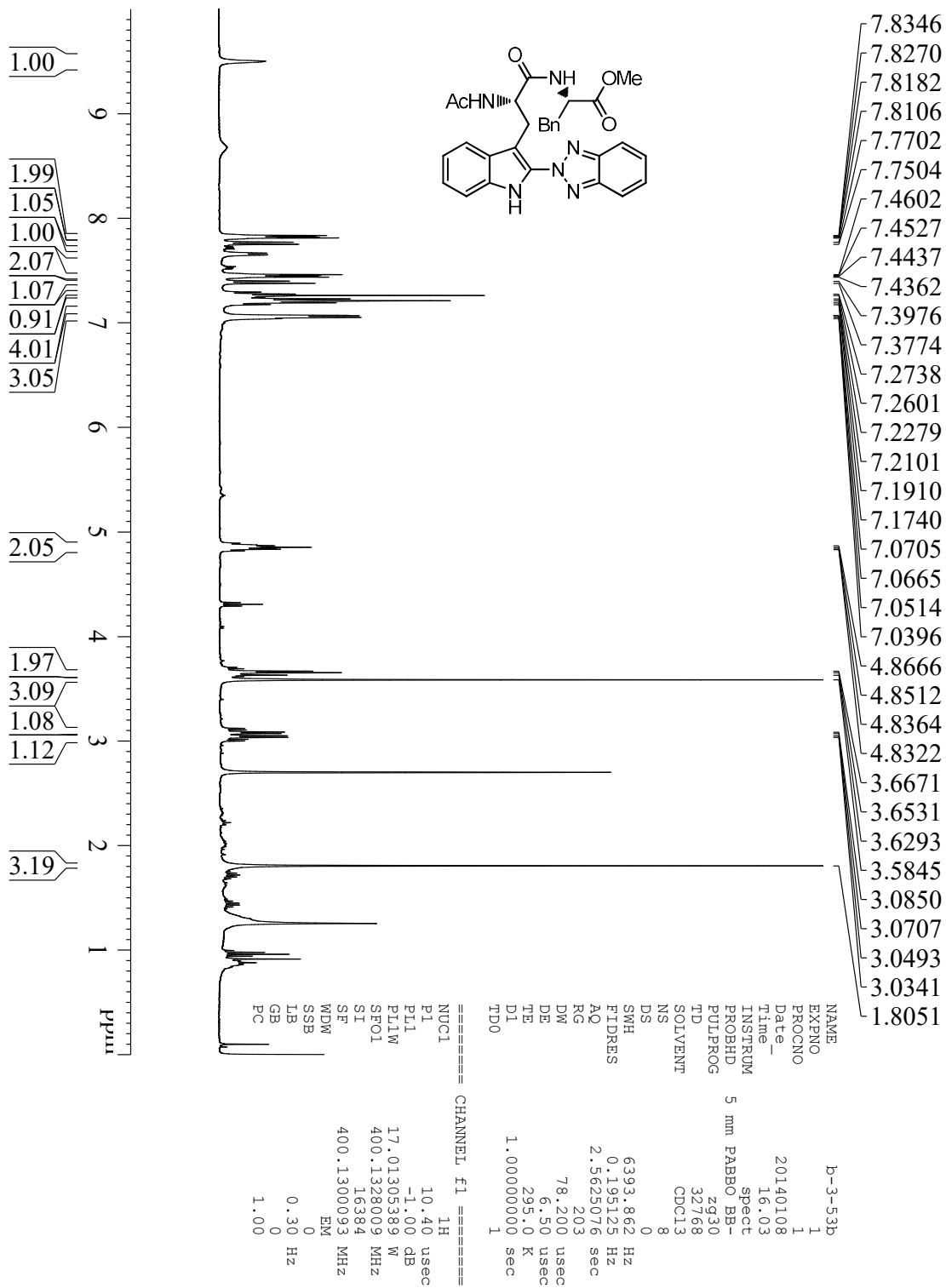


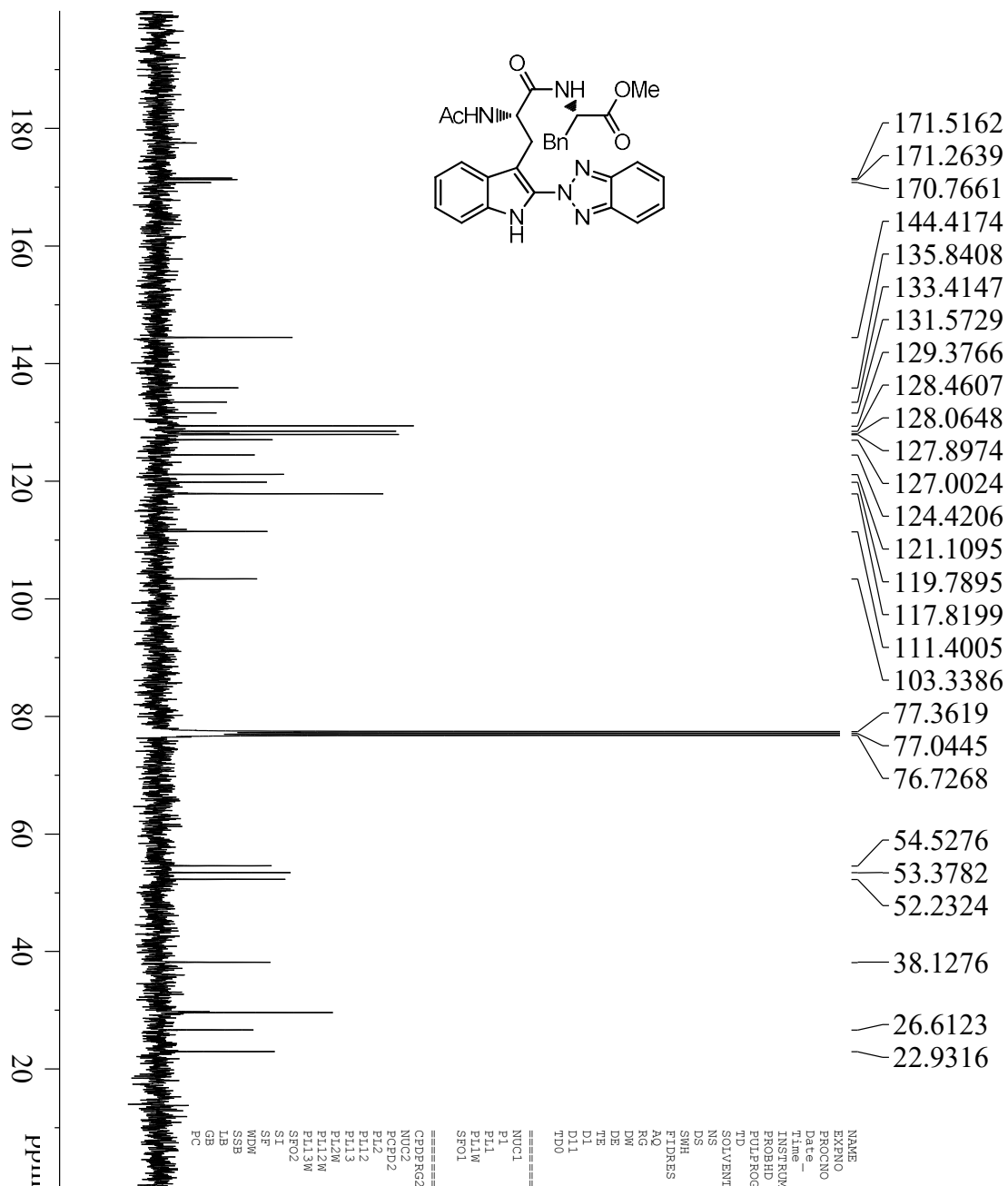


```

NAME b-3-7014
EXPNO 1
PROCNO 1
Date_ 20140114
Time_ 15.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 181
DW 78.200 usec
DE 6.50 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.40 usec
PL1 -1.00 dB
PLI1 17.01305389 W
SFO1 400.1328009 MHz
SI 16384
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
  
```



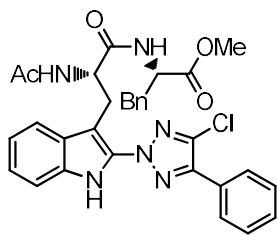


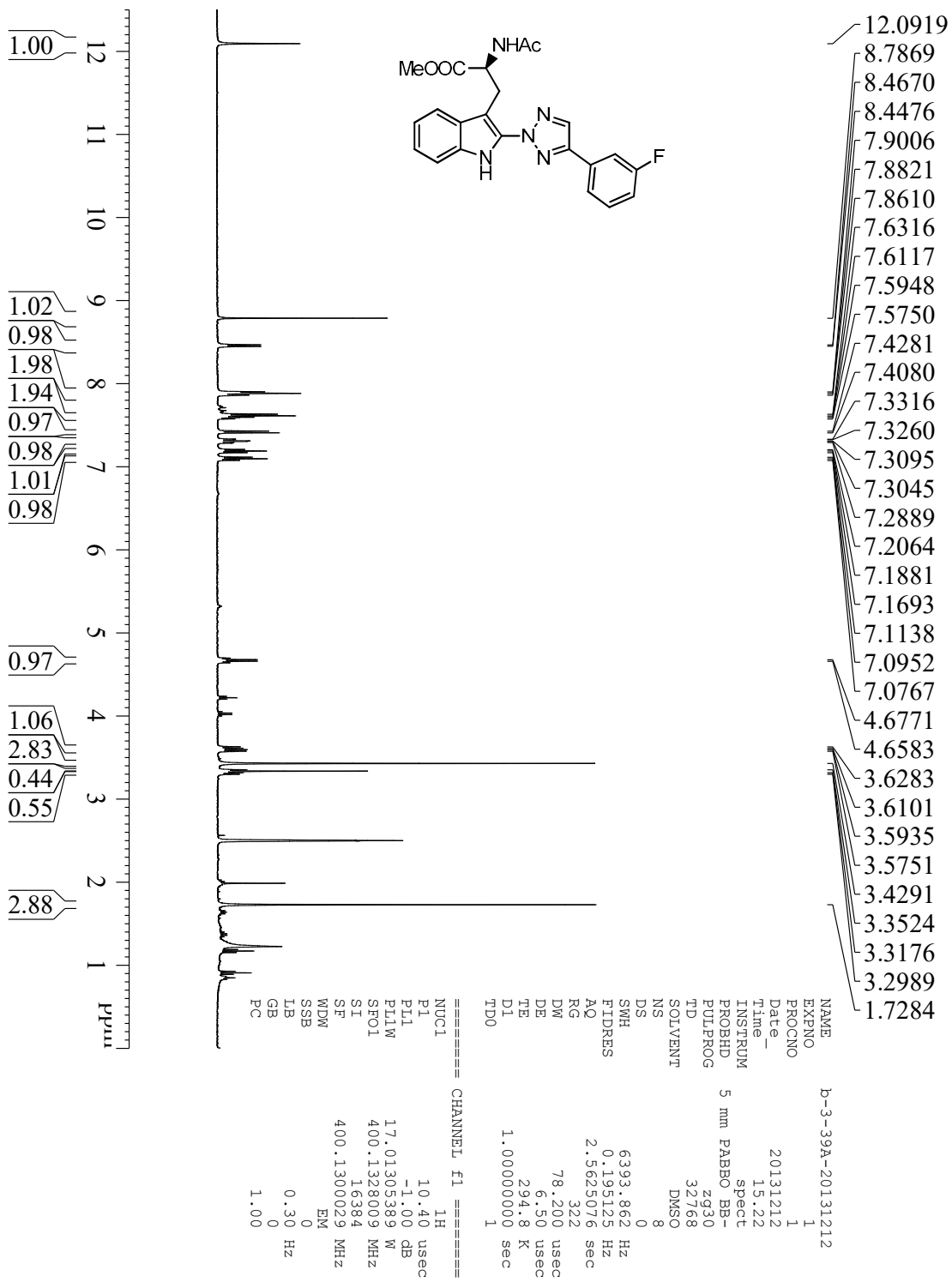
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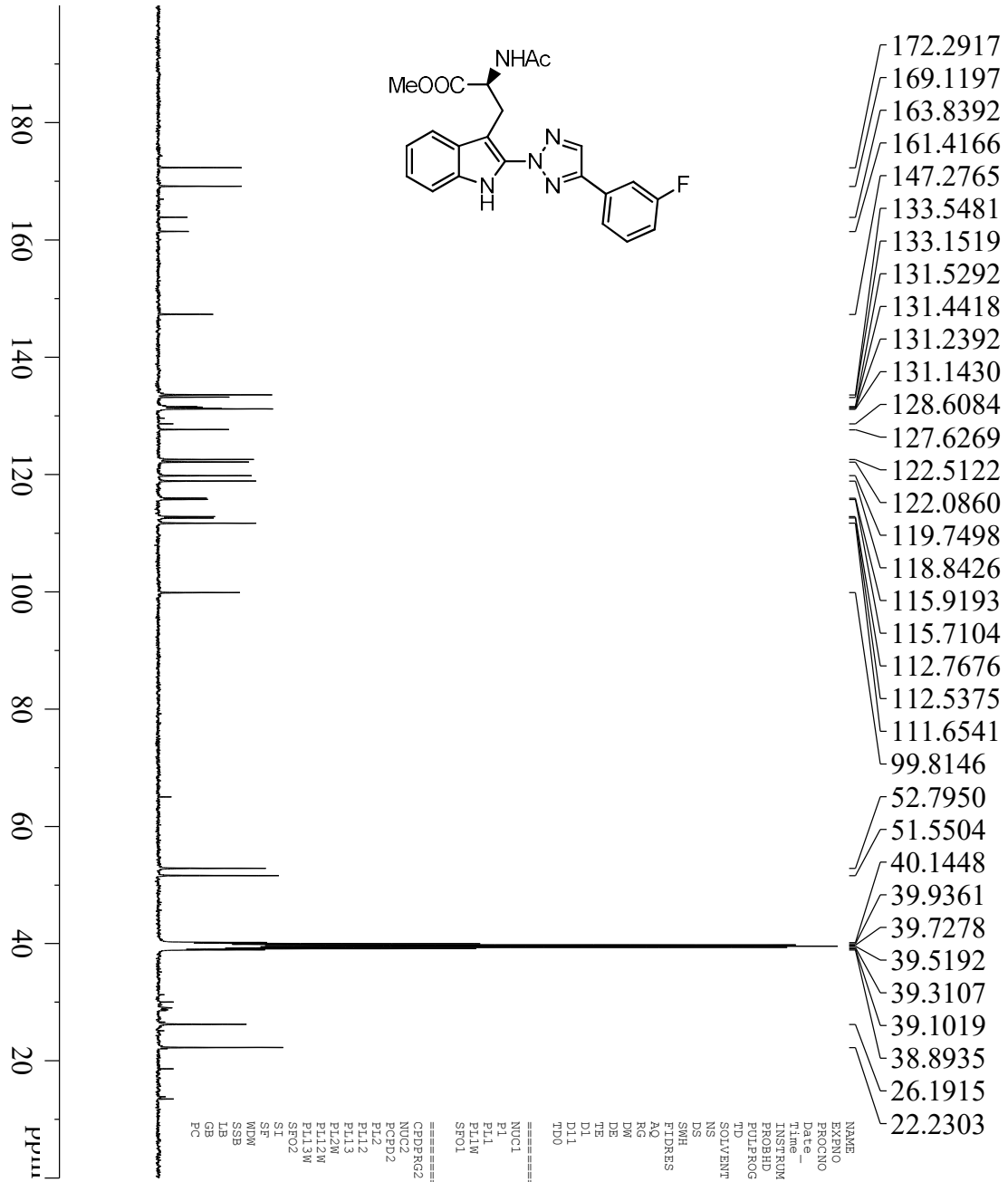
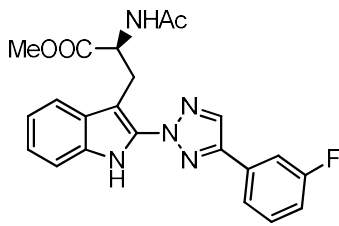
NAME          b-3-53b
EXPNO         2
PROCNO        1
Date_         20140108
Time-         16.05
INSTRUM       spect
PROBHD        5 mm PAEBQ BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            168
DS            4
SWH           25252.525 Hz
FIDRES       0.385323 Hz
AQ           1.297629 sec
RG            80.6
DW           19.800 usec
DE           6.50 usec
TE           295.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0          10

===== CHANNEL f1 =====
NUC1          13C
P1            13.47 usec
PL1           2.00 dB
PIL1         55.31271084 W
SFO1         100.6236364 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
P12           -1.00 dB
PIL2         16.72 dB
PIL3         15.50 dB
PIL2W        17.01305389 W
PIL3W        0.28759566 W
SFO2         400.1316005 MHz
SI           32768
SF           100.6127690 MHz
WDW           EM
SSB           0
LB           3.00 Hz
GB           0
PC           1.40
  
```







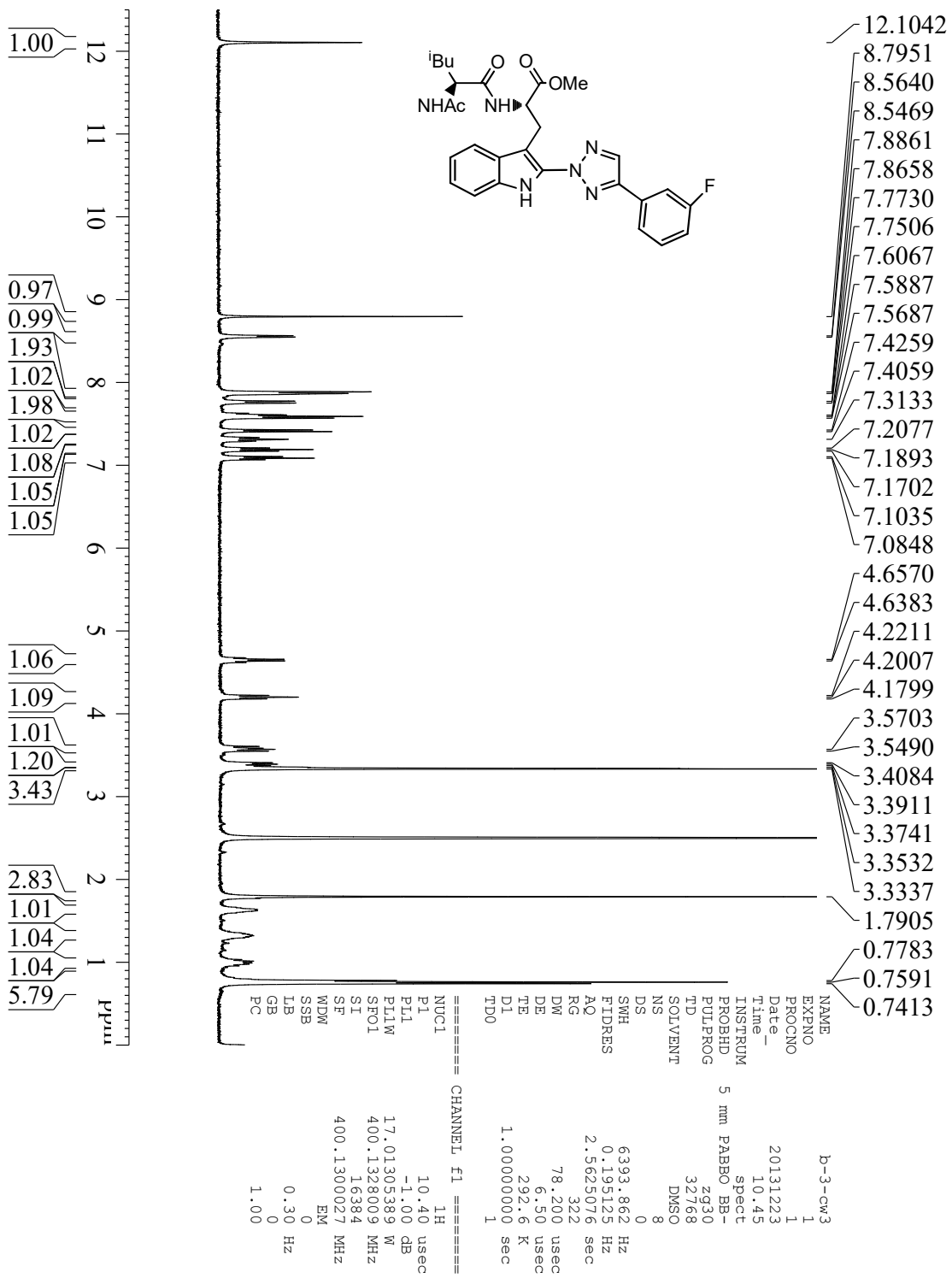
- 172.2917
- 169.1197
- 163.8392
- 161.4166
- 147.2765
- 133.5481
- 133.1519
- 131.5292
- 131.4418
- 131.2392
- 131.1430
- 128.6084
- 127.6269
- 122.5122
- 122.0860
- 119.7498
- 118.8426
- 115.9193
- 115.7104
- 112.7676
- 112.5375
- 111.6541
- 99.8146
- 52.7950
- 51.5504
- 40.1448
- 39.9361
- 39.7278
- 39.5192
- 39.3107
- 39.1019
- 38.8935
- 26.1915
- 22.2303

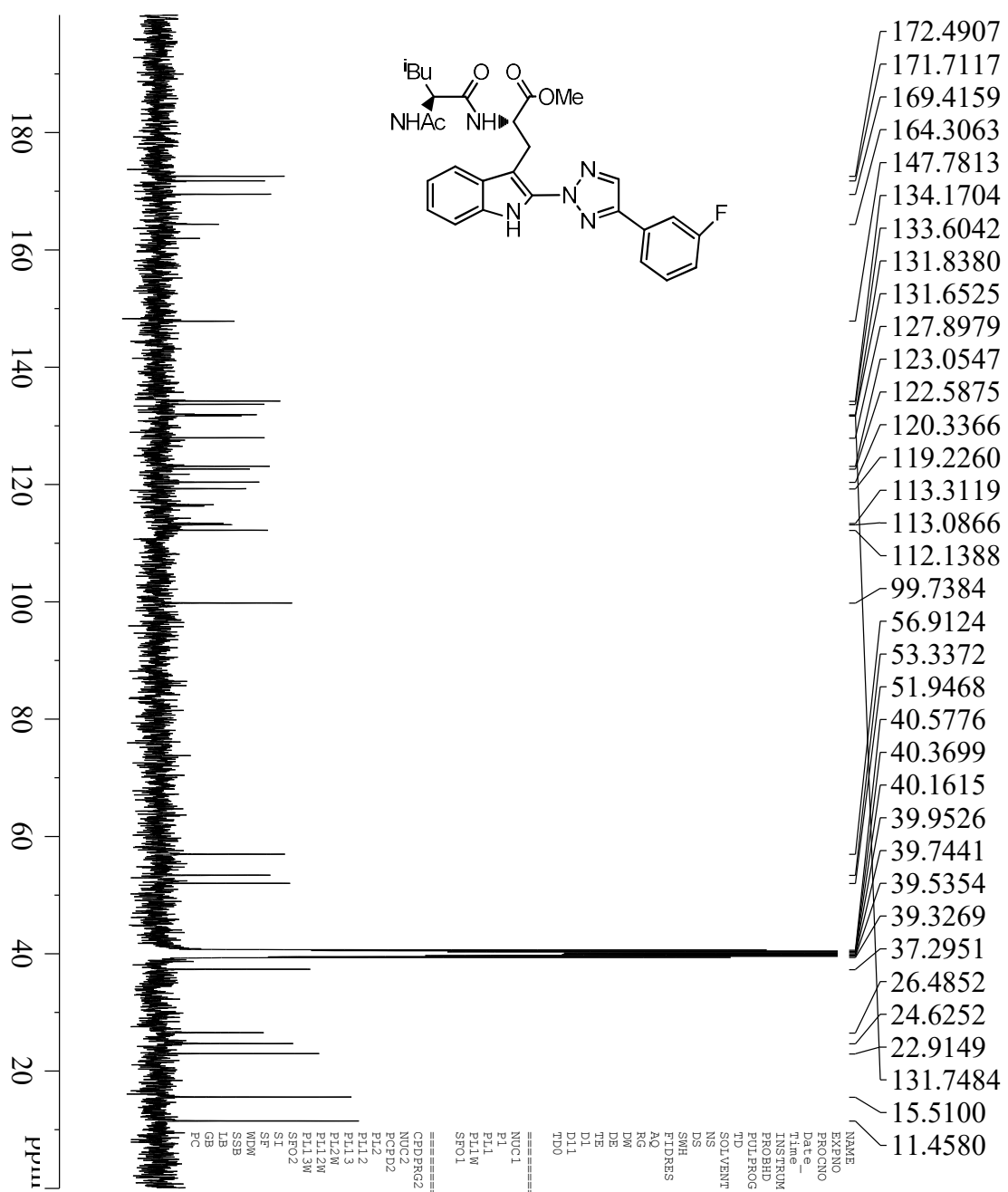
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NAME b-3-39a-20131213
EXPNO 2
PROCNO 1
Date_ 20131213
Time 12.09
INSTRUM spect
PROBHD 5 mm PAEBQ BB-
PULPROG zgpg30
TD 65536
FIDRES 0.385323 Hz
AQ 1.297629 sec
RG 181
DE 19.800 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 13.47 usec
PL1 2.00 dB
PILW 55.31271084 W
SFO1 100.6236364 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
P12 -1.00 dB
PIL2 16.72 dB
PIL3 15.50 dB
PIL2W 17.01305389 W
PIL3W 0.28759566 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128191 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
  
```



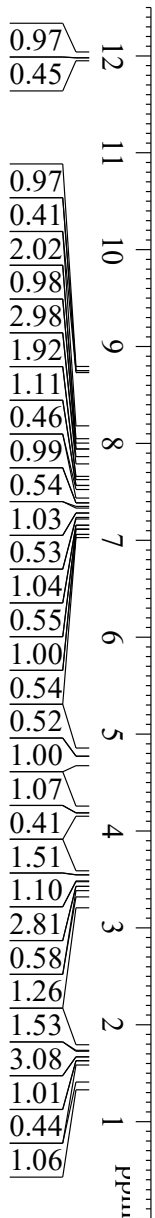
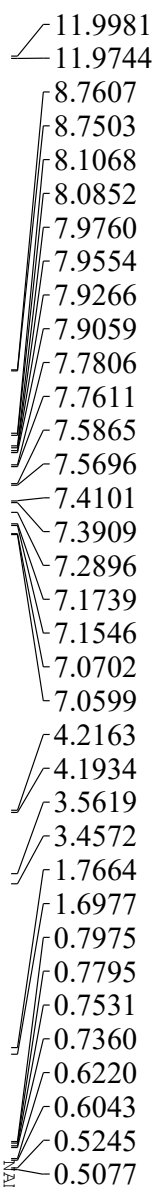
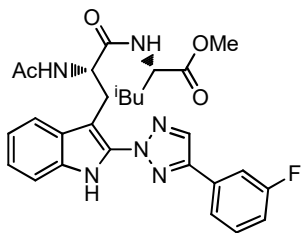


- 172.4907
- 171.7117
- 169.4159
- 164.3063
- 147.7813
- 134.1704
- 133.6042
- 131.8380
- 131.6525
- 127.8979
- 123.0547
- 122.5875
- 120.3366
- 119.2260
- 113.3119
- 113.0866
- 112.1388
- 99.7384
- 56.9124
- 53.3372
- 51.9468
- 40.5776
- 40.3699
- 40.1615
- 39.9526
- 39.7441
- 39.5354
- 39.3269
- 37.2951
- 26.4852
- 24.6252
- 22.9149
- 131.7484
- 15.5100
- 11.4580

NAME b-3-cw3-20131224
EXPNO 2
PROCNO 1
Date_ 20131224
Time_ 10.31
INSTRUM spect
PROBHD 5 mm PAEBB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 288
DS 4
SWH 2522.525 Hz
FIDRES 0.385323 Hz
AQ 1.297629 sec
RG 80.6
DE 19.800 usec
TE 293.3 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 13.47 usec
PL1 2.00 dB
PI1W 55.3127084 W
SFO1 100.6238364 MHz

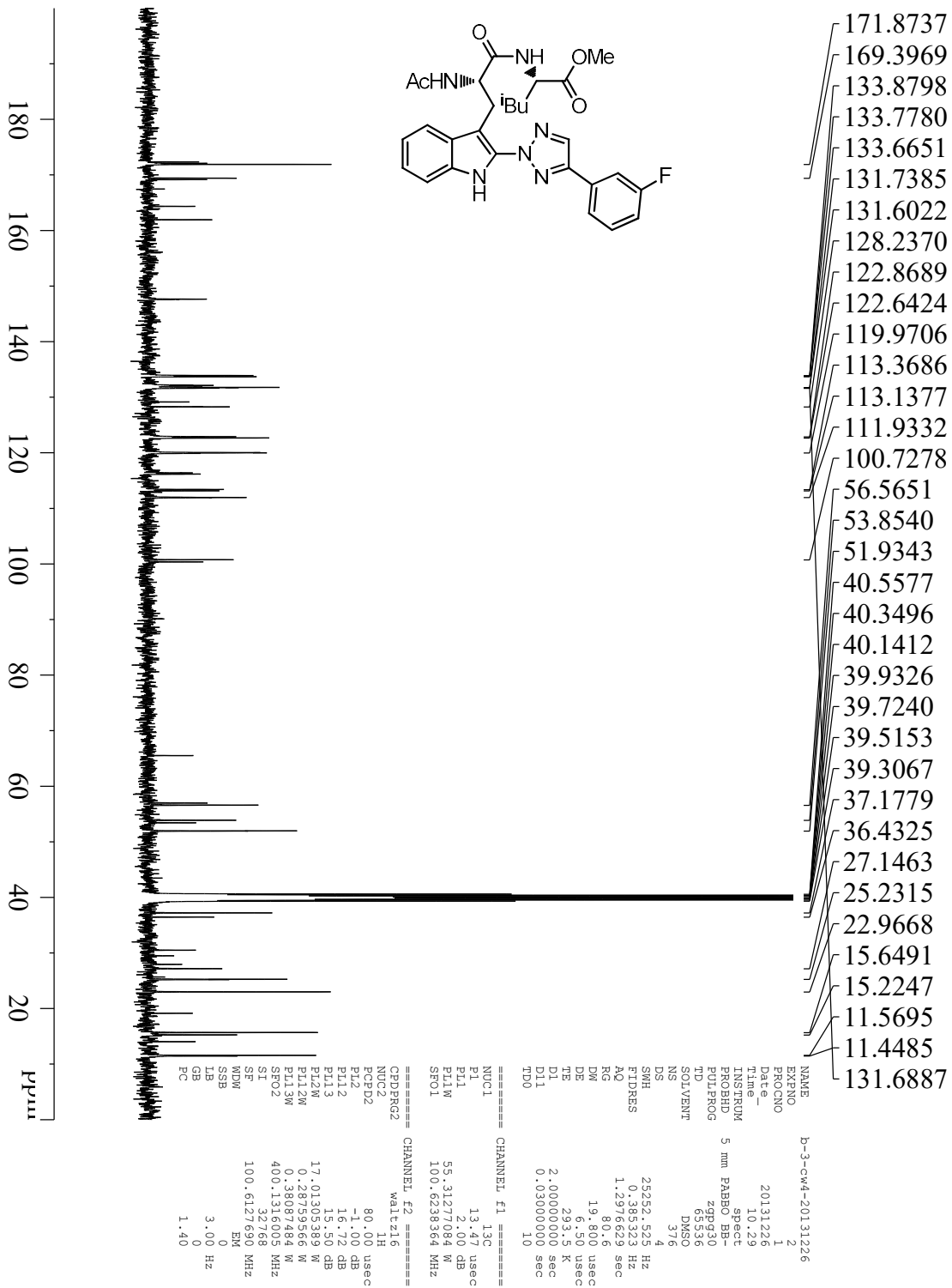
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PT2 -1.00 dB
PI12 16.72 dB
PI13 15.50 dB
PI12W 17.01305389 W
PI13W 0.28759566 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

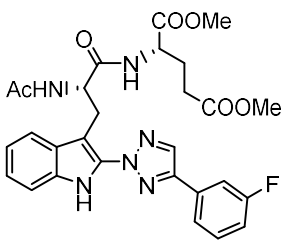


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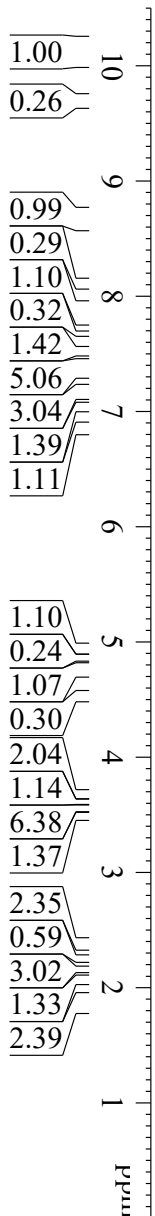
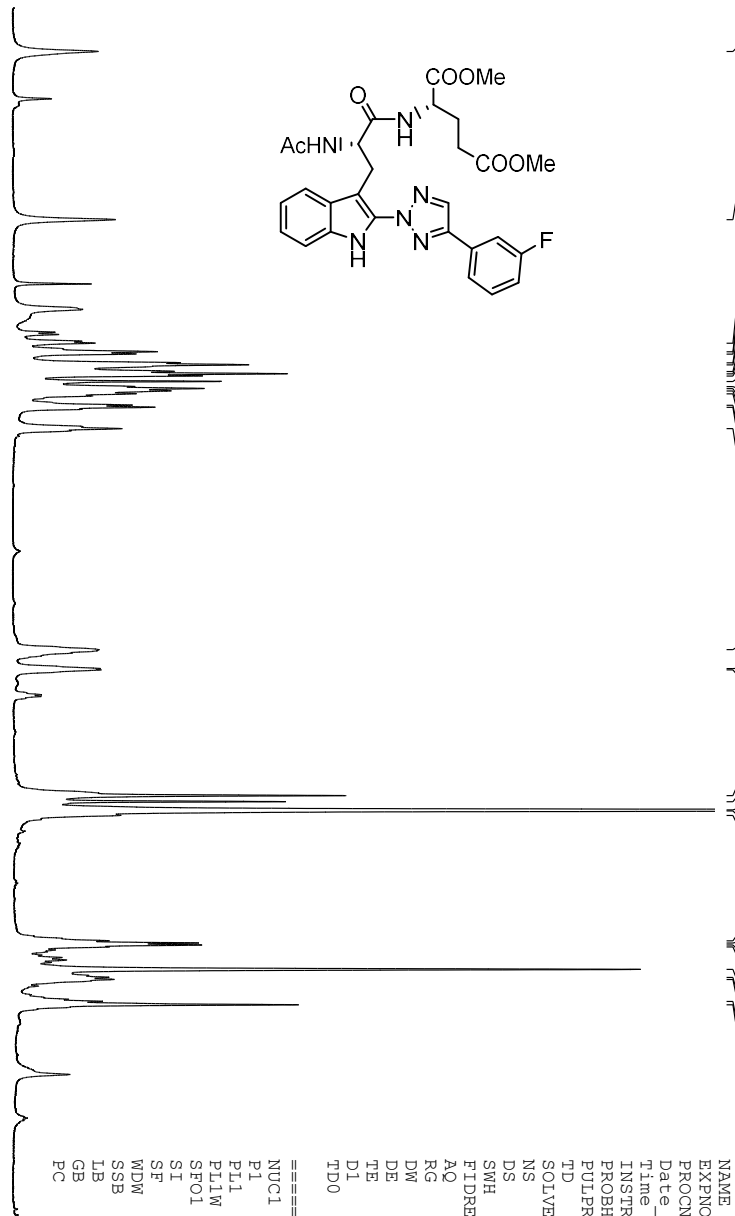
===== CHANNEL f1 =====
NAME      b-3-cw4
EXPNO     1
PROCNO    1
Date_     20131223
Time      10.32
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         32768
SOLVENT   DMSO
NS         8
DS         0
SWH        6393.862 Hz
FIDRES     0.195125 Hz
AQ         2.5625076 sec
RG         181
DW         78.200 usec
DE         6.50 usec
TE         292.7 K
D1         1.0000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         10.40 usec
PL1        -1.00 dB
PL1W       17.01305389 W
SF01       400.1328009 MHz
SI         16384
SE         400.1300028 MHz
WDW        EM
SSB        0
GB         0
PC         0.30 Hz
RB         0
GC         1.00
  
```





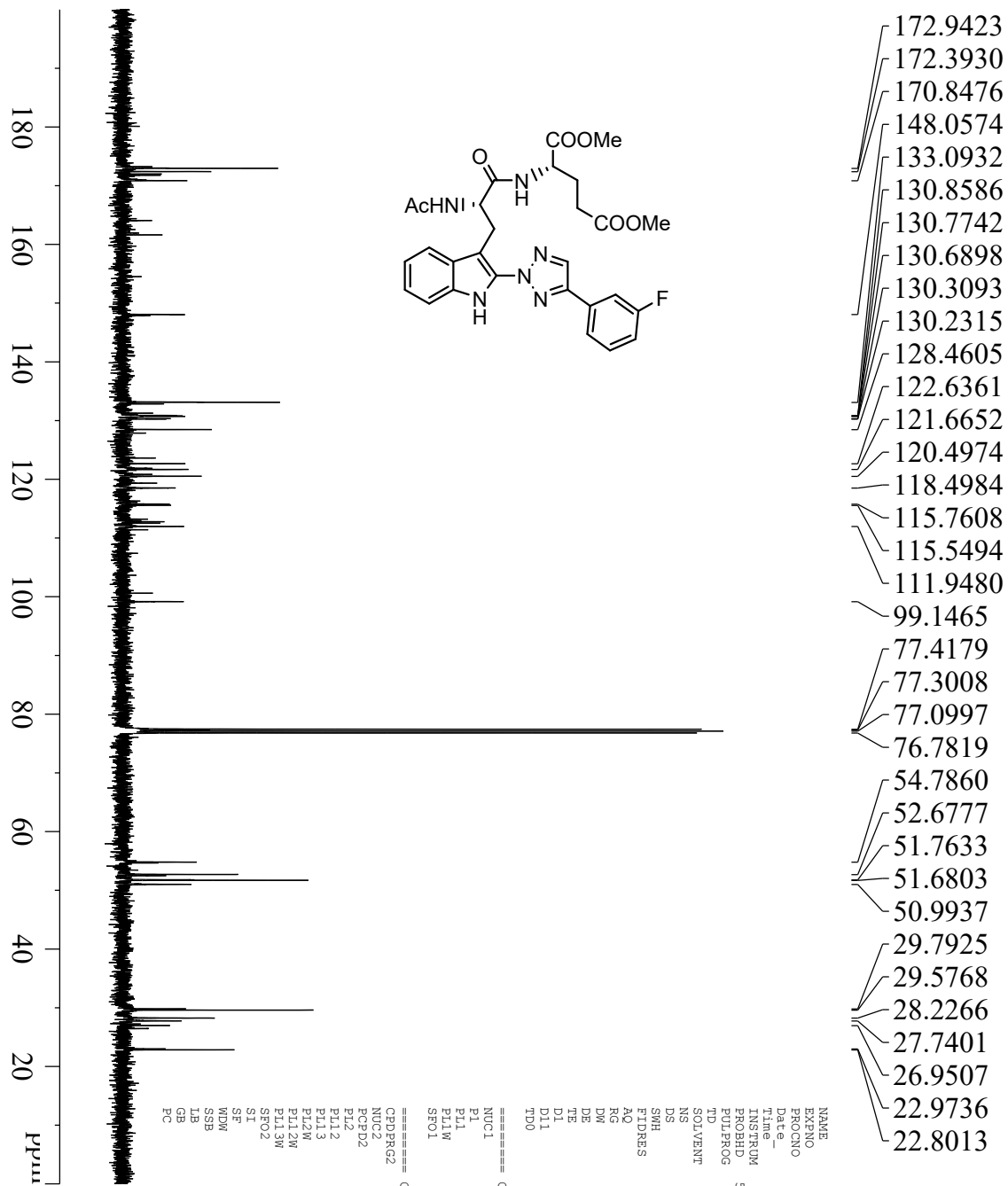
- 10.1232
- 8.6635
- 7.5916
- 7.5174
- 7.4978
- 7.4213
- 7.4039
- 7.3466
- 7.3259
- 7.3074
- 7.2597
- 7.2152
- 7.1980
- 7.1776
- 7.1528
- 7.0536
- 7.0353
- 6.8507
- 4.9326
- 4.7682
- 4.7571
- 3.6658
- 3.6136
- 3.5418
- 3.5337
- 3.4941
- 2.4064
- 2.3870
- 2.3696
- 2.3527
- 2.1578
- 2.0890
- 2.0705
- 1.8802
- 1.8507



```

NAME          bqw
EXPNO         3
PROCNO        1
Date_         20140222
Time_         15.22
INSTRUM       Spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            40.3
DW            60.800 usec
DE            6.50 usec
TE            294.4 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            13.70 usec
PL1           -2.00 dB
PL1W          15.24750423 W
SFO1          400.1324710 MHz
SI            SF
SF            400.1300095 MHz
WDW            EM
SSB            0
GB            0
PC            1.00
  
```

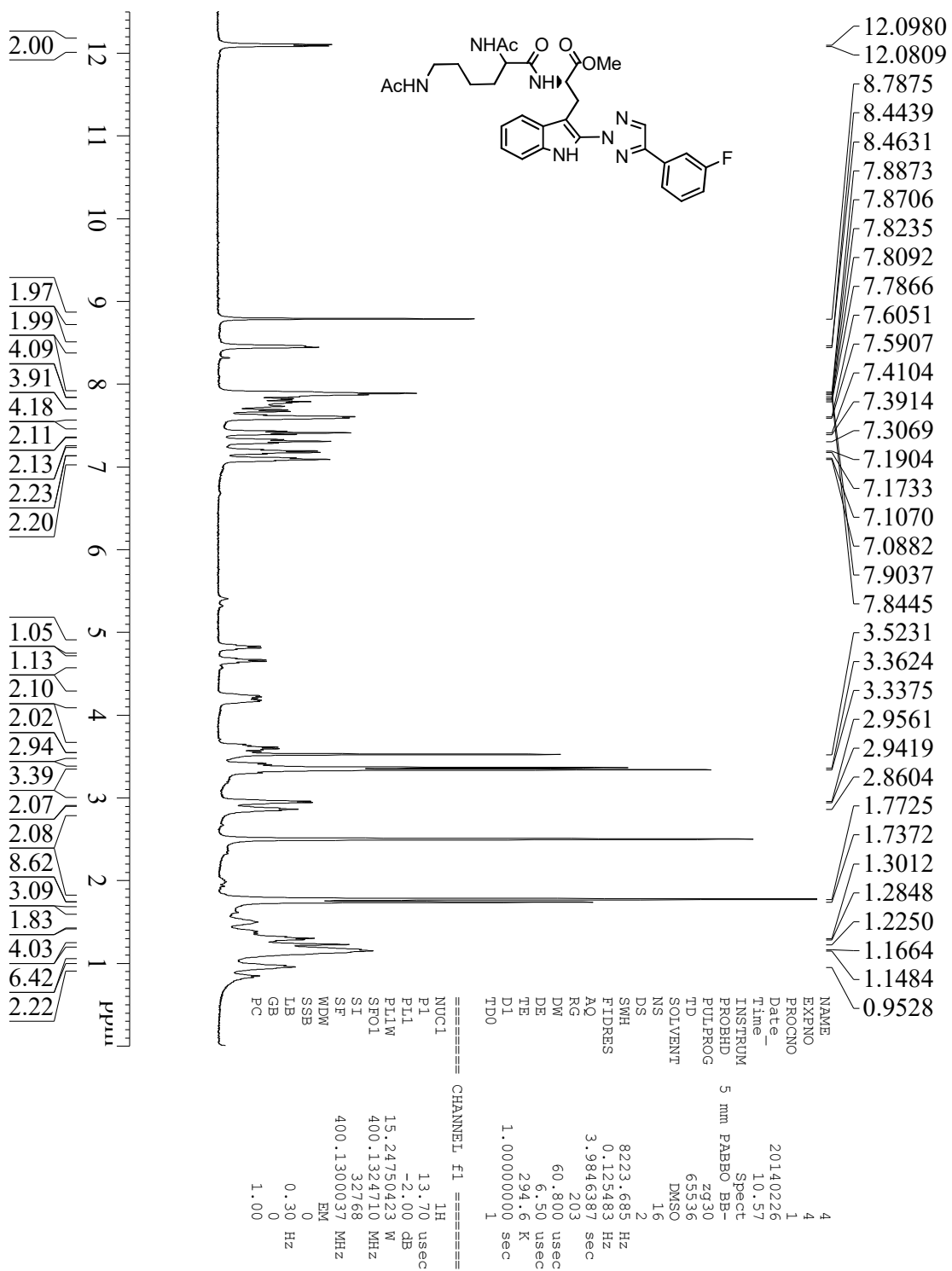


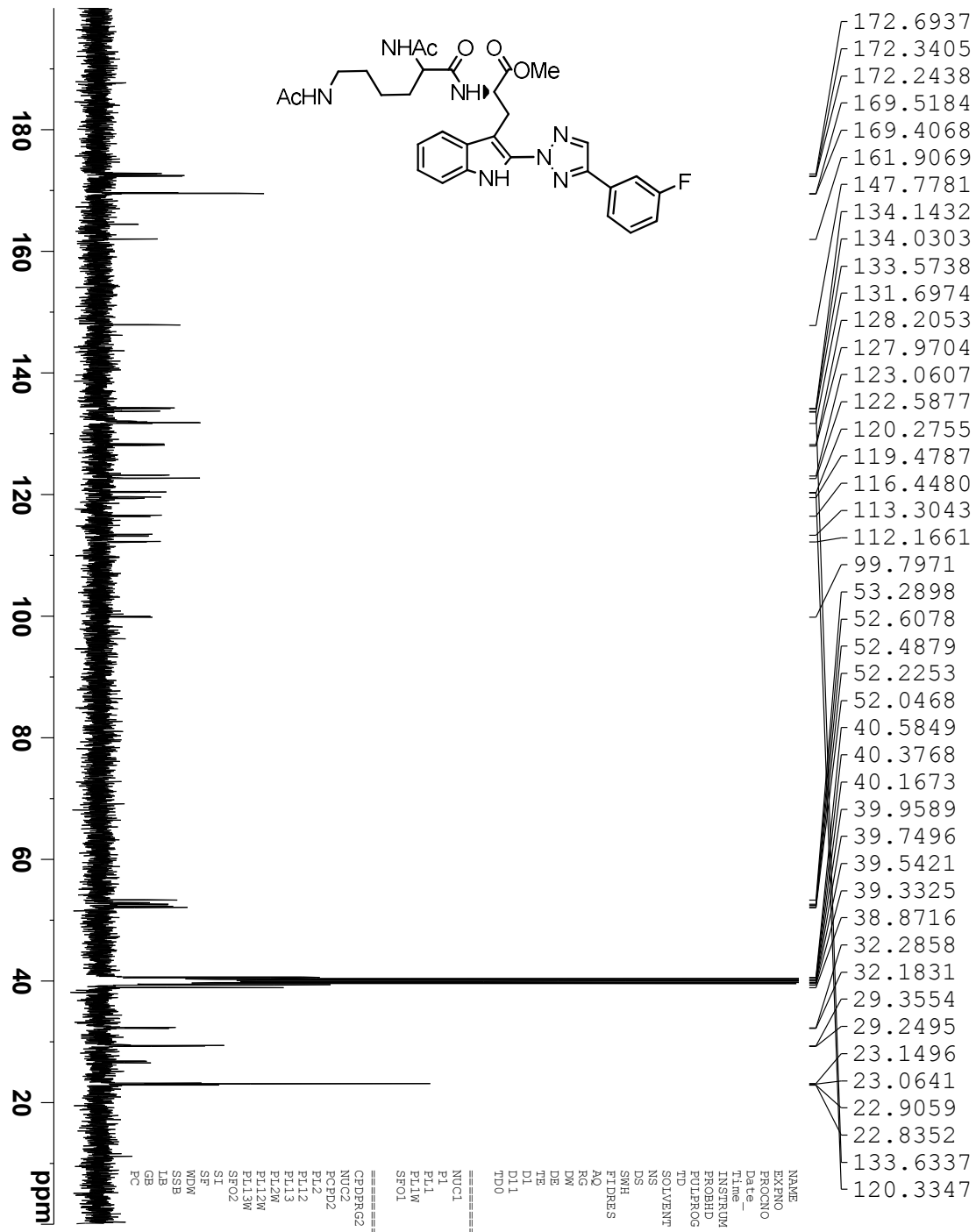
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NAME                               8
EXNO                               8
PROCNO                             1
Date_                             20140222
Time_                             16.04
INSTRUM                           5 mm PABBO BB-
PROBHD                            zgpg30
PULPROG                           65536
TD                                120
SOLVENT                           CDCl3
NS                                 120
DS                                 4
SWH                               24038.461 Hz
FIDRES                            0.366798 Hz
AQ                                1.3631988 sec
RG                                 203
DW                               20.800 usec
DE                               6.50 usec
TE                               295.0 K
D1                               2.00000000 sec
D11                              0.03000000 sec
TD0                               1

===== CHANNEL f1 =====
NUC1                               13C
P1                               10.69 usec
P1L                              -2.00 dB
P1LW                             48.56907654 W
SFO1                             100.628298 MHz

===== CHANNEL f2 =====
CPDPRG2                          waltz16
NUC2                               1H
PCPD2                             80.00 usec
P12                              -2.00 dB
P1L2                             13.33 dB
P1L3                             13.33 dB
P1LW                             15.24750423 W
P12W                             0.44688809 W
P1L3W                             0.44688809 W
SFO2                             400.131605 MHz
SI                               32768
SF                               100.6127690 MHz
WDW                               EM
SSB                               0
LB                               1.00 Hz
GB                               0
PC                               1.40
  
```

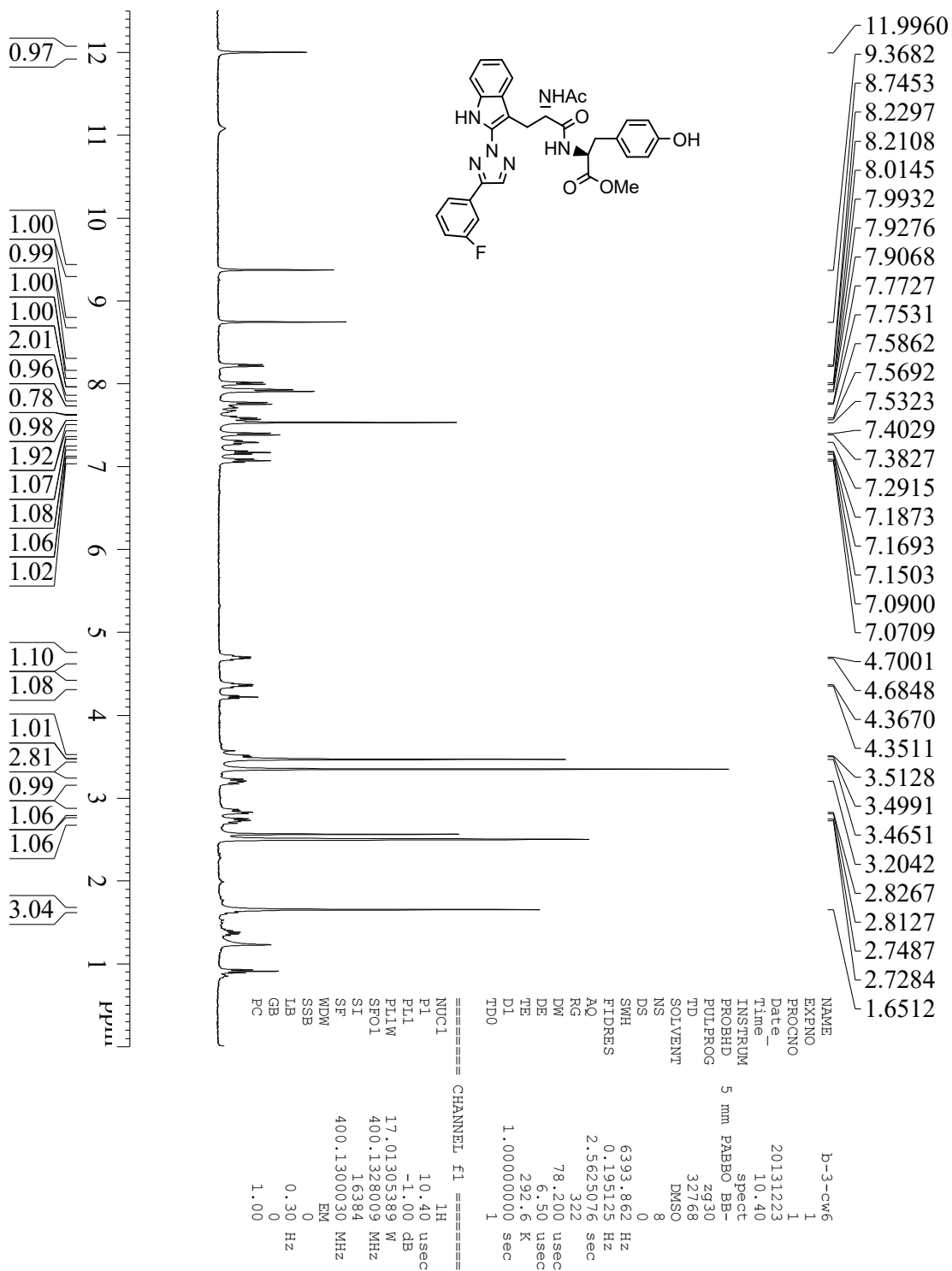


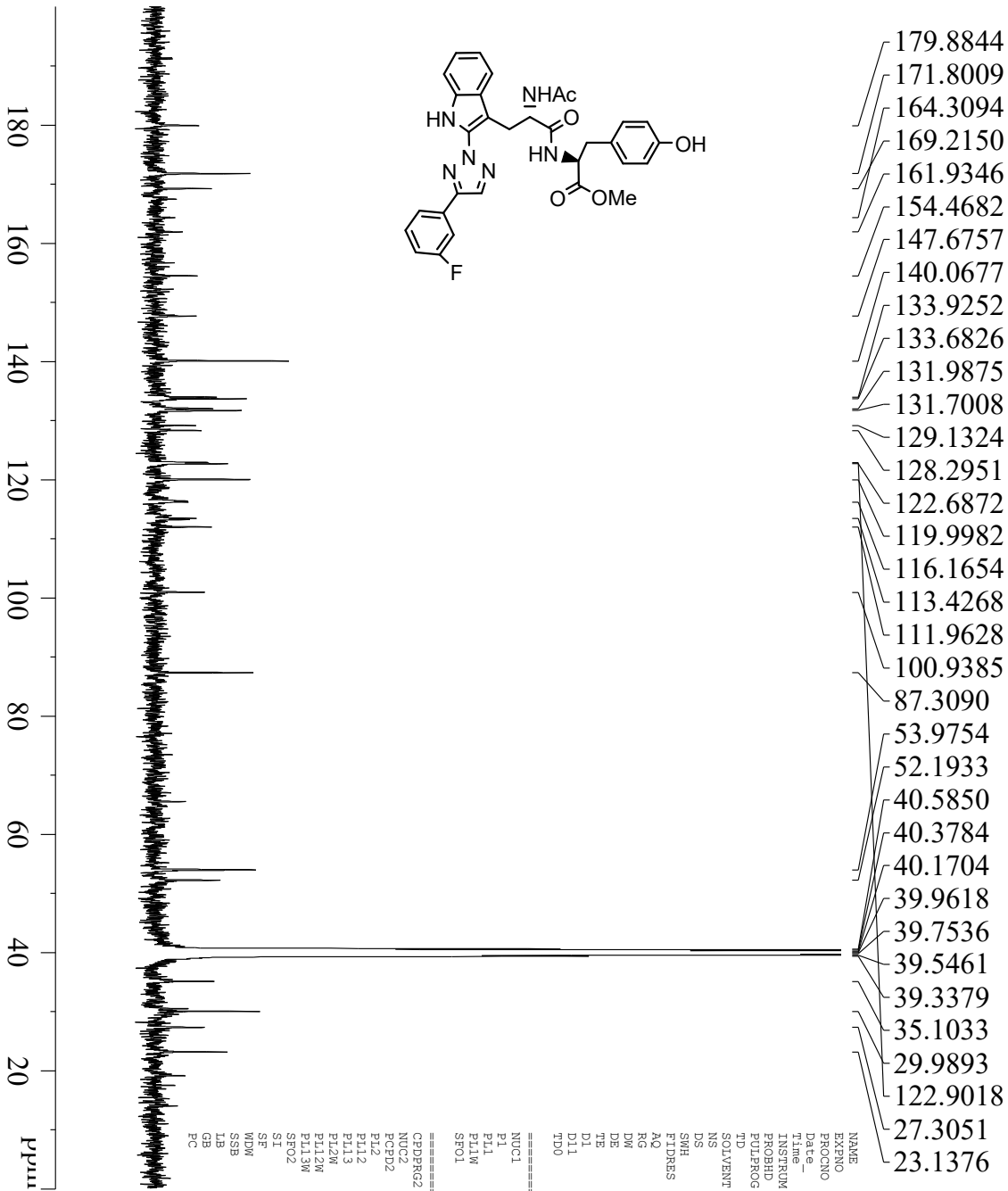
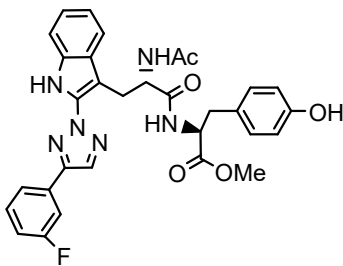
- 172.6937
- 172.3405
- 172.2438
- 169.5184
- 169.4068
- 161.9069
- 147.7781
- 134.1432
- 134.0303
- 133.5738
- 131.6974
- 128.2053
- 127.9704
- 123.0607
- 122.5877
- 120.2755
- 119.4787
- 116.4480
- 113.3043
- 112.1661
- 99.7971
- 53.2898
- 52.6078
- 52.4879
- 52.2253
- 52.0468
- 40.5849
- 40.3768
- 40.1673
- 39.9589
- 39.7496
- 39.5421
- 39.3325
- 38.8716
- 32.2858
- 32.1831
- 29.3554
- 29.2495
- 23.1496
- 23.0641
- 22.9059
- 22.8352
- 133.6337
- 120.3347

NAME 7-1
EXPNO 7
PROCNO 1
Date_ 20140226
Time 11.18
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 96
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.69 usec
PL1 -2.00 dB
PL1W 48.56907654 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.33 dB
PL13 13.33 dB
PL12W 15.24750423 W
PL12W 0.44688809 W
PL13W 0.44688809 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





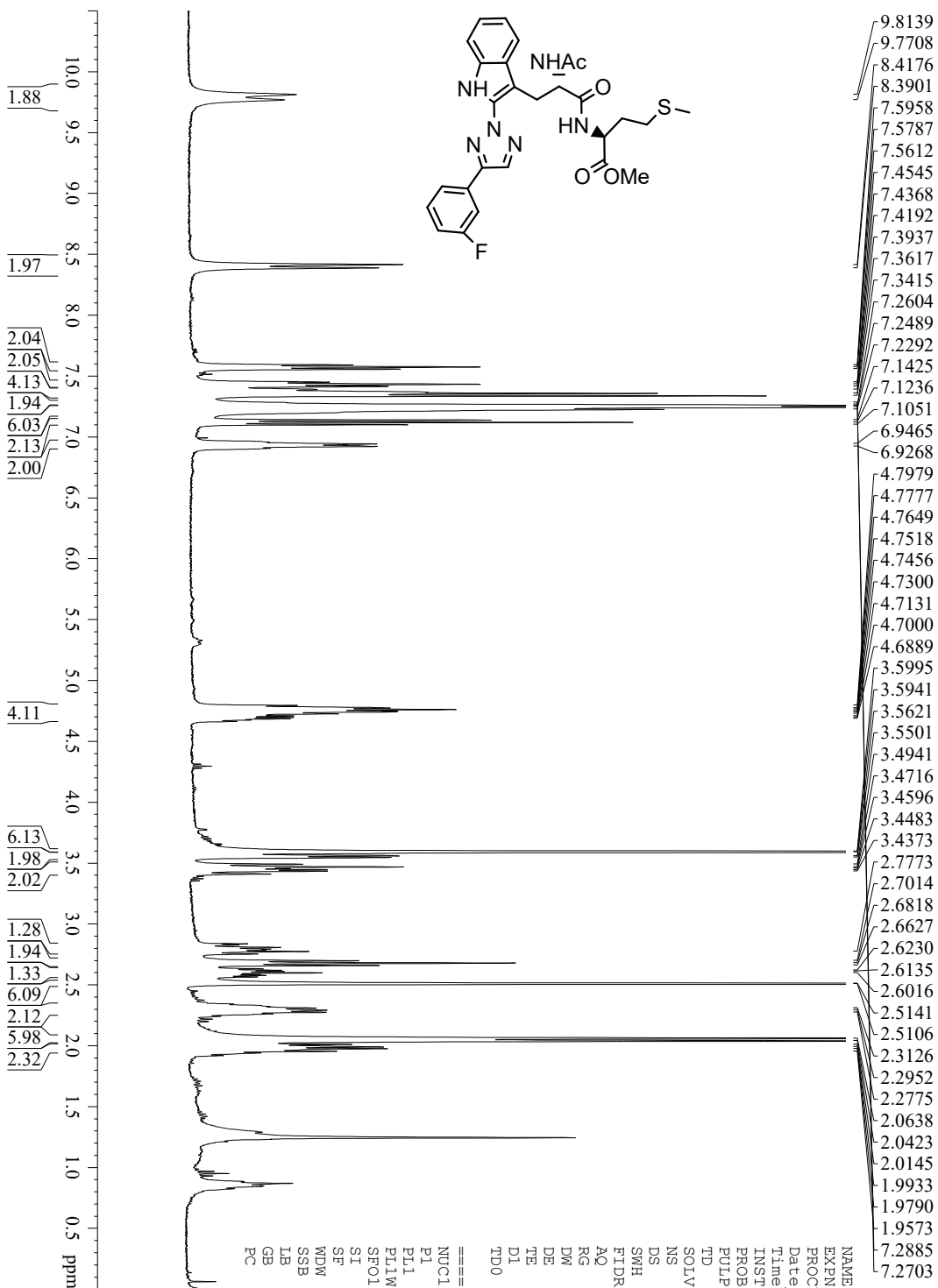
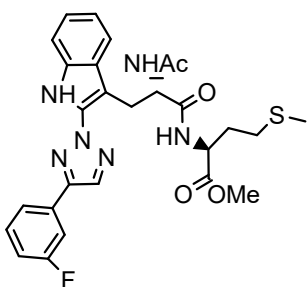
```

NAME b-3-cw6-20131224
EXENO 2
PROCNO 1
Date 20131224
Time 15.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 632
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 80.6
DE 19.800 usec
TE 294.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 13.47 usec
PL1 2.00 dB
PL1W 55.31277084 W
SF01 100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.72 dB
PL13 15.50 dB
PL1W 17.01305389 W
PL2W 0.28795566 W
PL13W 0.38087484 W
SF02 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

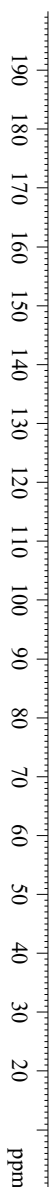
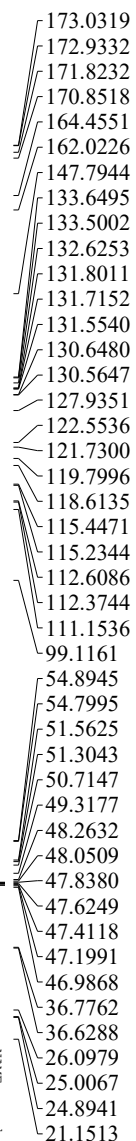
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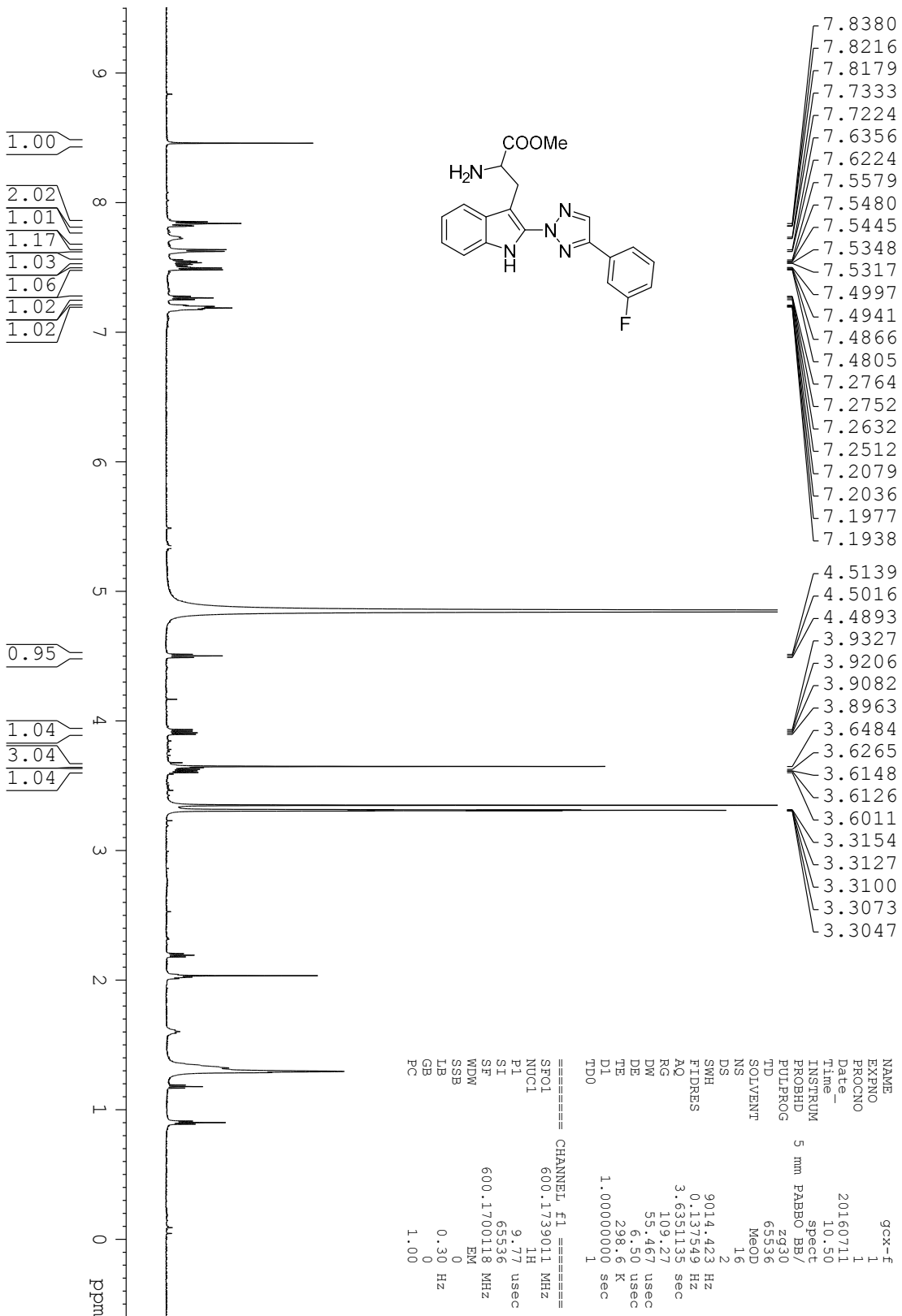
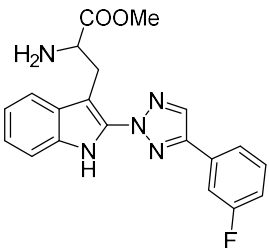


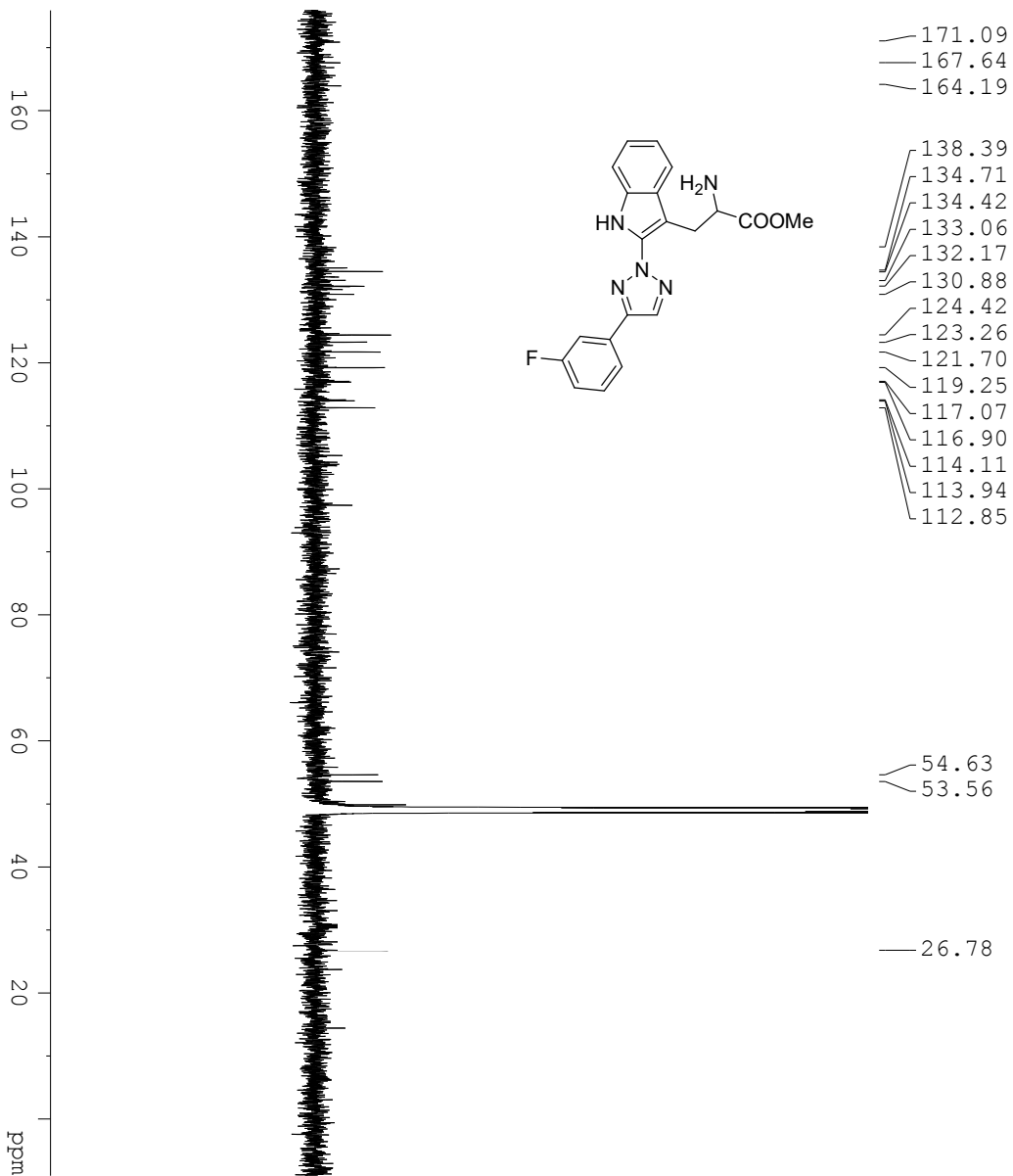
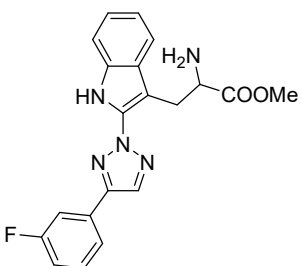
```

NAME b-3-cws
EXPNO 1
PROCNO 1
Date_ 20131223
Time 10.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 181
DW 78.200 usec
DE 6.50 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.40 usec
PL1 -1.00 dB
PL1W 17.01305389 W
SFO1 400.1328009 MHz
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
  
```

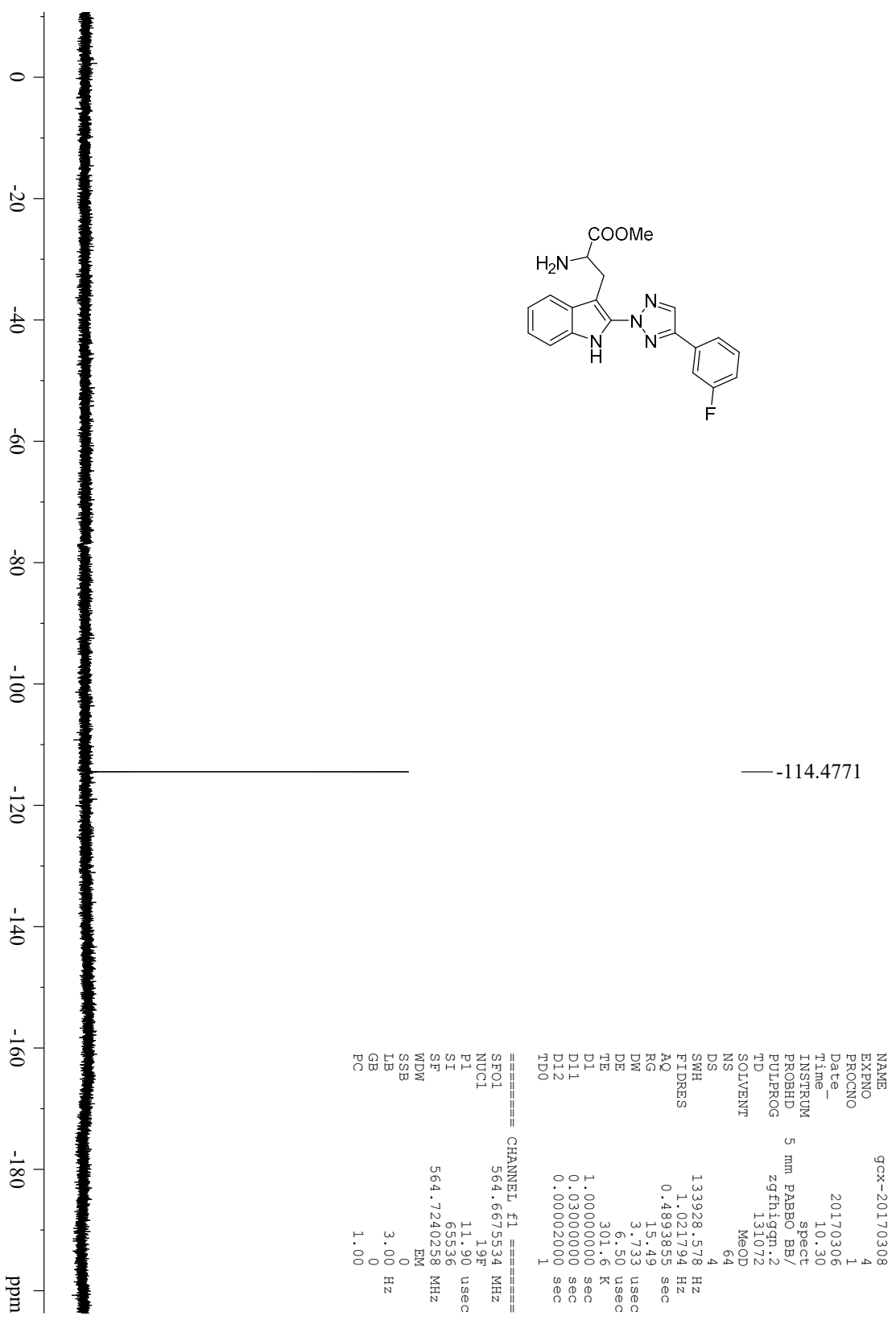
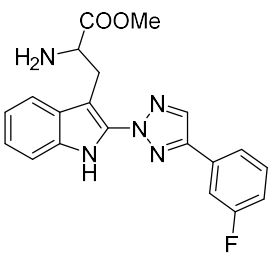






NAME f
EXNO 2
PROCNO 1
Date_ 20160712
Time_ 10.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 1024
DS 4
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8651252 sec
RG 190.02
DW 13.200 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 20

===== CHANNEL f1 =====
SFO1 150.929469 MHz
NUC1 13C
P1 11.90 usec
SI 32768
SF 150.912653 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

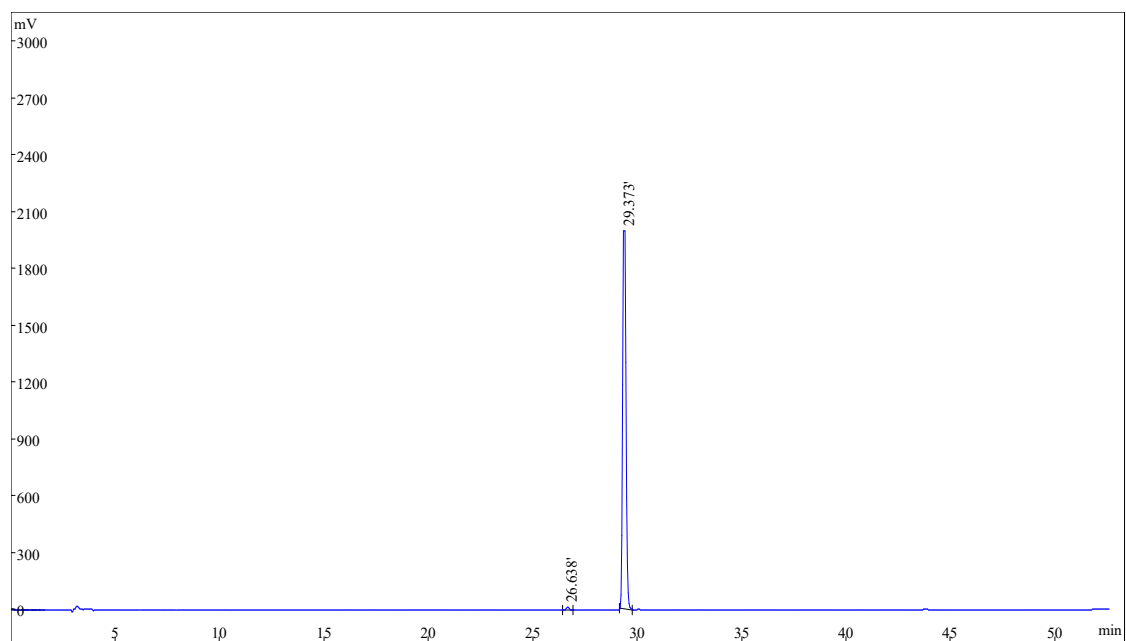


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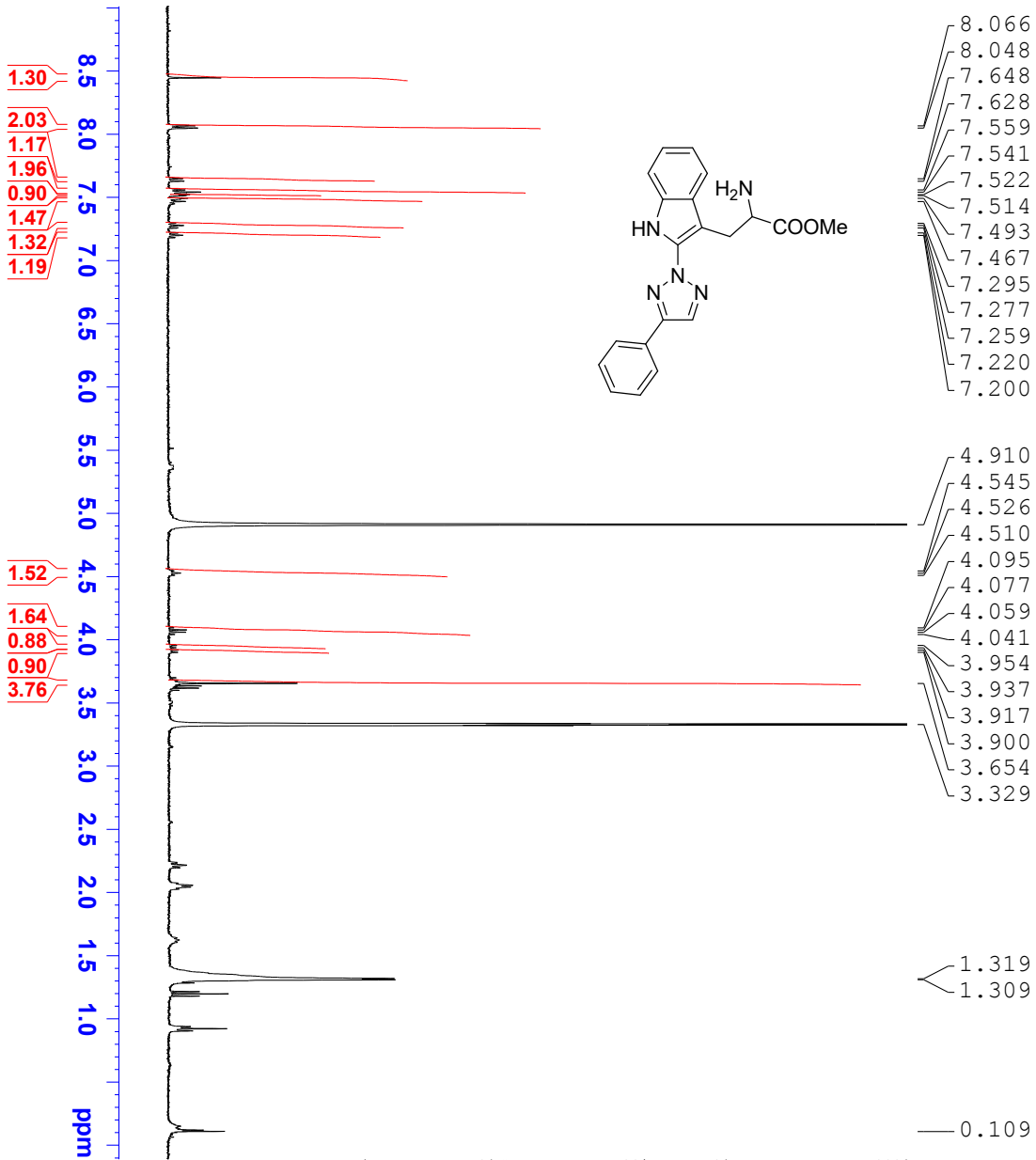
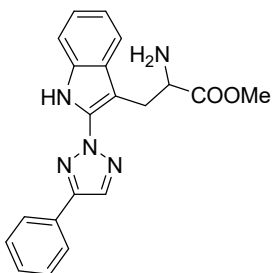
NAME gcx-20170308
EXPNO 4
PROCNO 1
Date_ 20170306
Time_ 10.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT MeOD
NS 64
DS 4
SWH 133928.578 Hz
FIDRES 1.021794 Hz
AQ 0.4893855 sec
RG 15.49
DW 3.733 usec
DE 6.50 usec
TE 301.6 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
SF01 564.6675534 MHz
NUC1 19F
P1 11.90 usec
SI 65536
SF 564.7240258 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

```



No	Retention Time	Content	Peak Area	Peak Separation
1	26.638	0.6207	114100	12.07
2	29.373	99.38	181896545	4.65
Total		100	18382857	



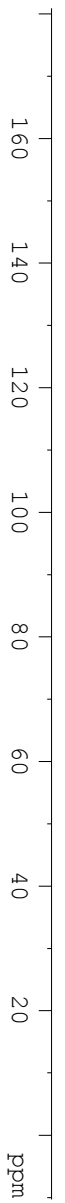
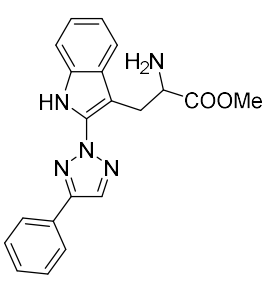
NAME ph
EXPNO 1
PROCNO 1
Date_ 20161201
Time_ 16.22
INSTRUM spect
PROBHD 5 mm PADUL13C
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4526453 sec
RG 575
DW 83.200 usec
DE 8.00 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

169.46
148.57
146.64
138.61
132.90
129.46
129.34
128.99
128.75
126.01
122.88
120.24
117.79
111.43

53.23
52.17

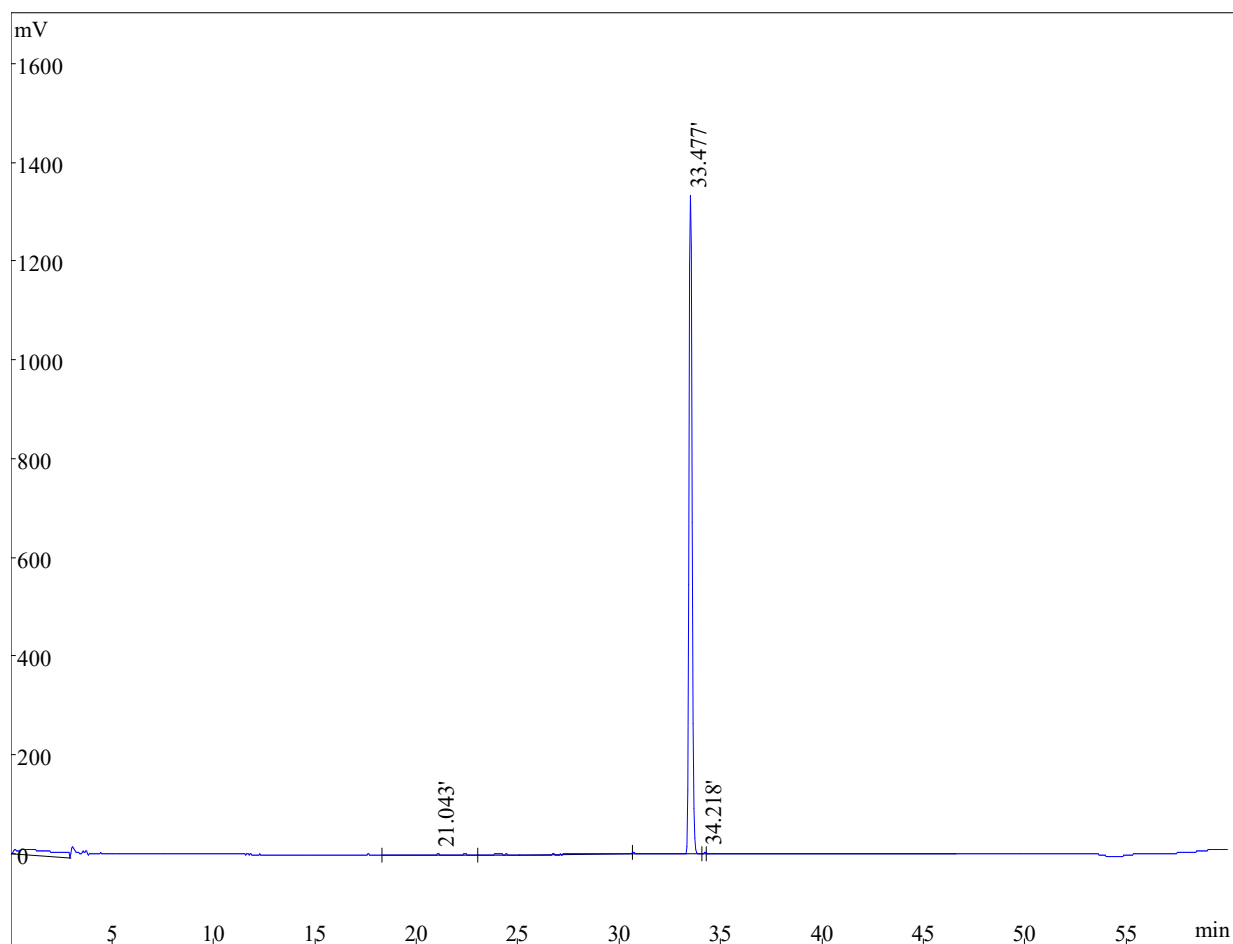
29.28



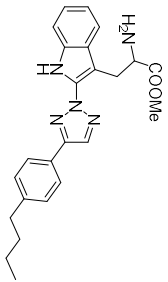
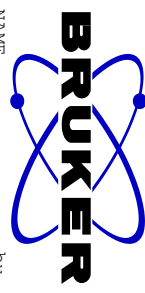
```

NAME                               ph
EXPNO                               2
PROCNO                              1
Date_                               20161212
Time_                               10.07
INSTRUM                             spect
PROBHD                               5 mm PABBO BB/
PULPROG                             zgpg30
TD                                   65536
SOLVENT                             MeOD
NS                                   10240
DS                                   4
SWH                                   37878.789 Hz
FIDRES                               0.577984 Hz
AQ                                   0.8651252 sec
RG                                   190.02
DW                                   13.200 usec
DE                                   6.50 usec
TE                                   298.9 K
D1                                   2.00000000 sec
D11                                  0.03000000 sec
TD0                                  10

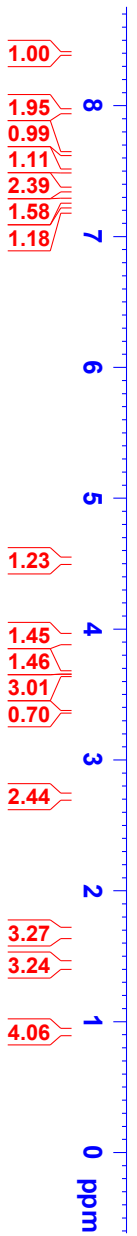
===== CHANNEL f1 =====
SF01                                150.929469 MHz
NUC1                                 13C
P1                                   11.90 usec
SI                                   32768
SF                                   150.912865 MHz
WDW                                  EM
SSB                                  0
LB                                   3.00 Hz
GB                                   0
PC                                   1.40
  
```



No	Retention Time	Content	Peak Area	Peak Separation
1	30.642	0.1823	20337	19.43
2	33.477	99.29	11075029	3.40
3	34.218	0.5316	59296	0.00
Total		100	11154662	



- 8.396
- 7.963
- 7.943
- 7.641
- 7.621
- 7.509
- 7.489
- 7.370
- 7.350
- 7.290
- 7.270
- 7.250
- 7.215
- 7.195
- 4.918
- 4.521
- 3.908
- 3.890
- 3.676
- 3.658
- 3.649
- 3.333
- 3.329
- 3.325
- 2.731
- 2.712
- 2.693
- 1.694
- 1.675
- 1.656
- 1.637
- 1.625
- 1.447
- 1.429
- 1.410
- 1.391
- 1.305
- 1.006
- 0.988
- 0.969
- 0.958
- 0.936
- 0.919
- 0.902



NAME bu
EXPNO 1
PROCNO 1
Date_ 20161010
Time_ 16.05
INSTRUM spect
PROBHD 5 mm PADUL13C
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4526453 sec
RG 256
DW 83.200 usec
DE 8.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

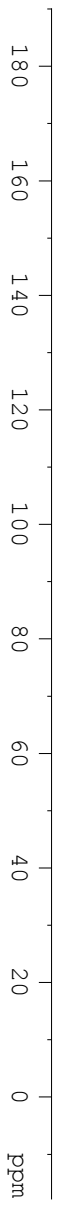
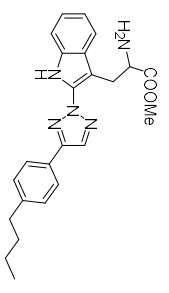
169.48
167.87
164.42

133.60
132.44
130.84
130.22
129.85
127.38
119.74
118.13
117.57
117.21

69.31

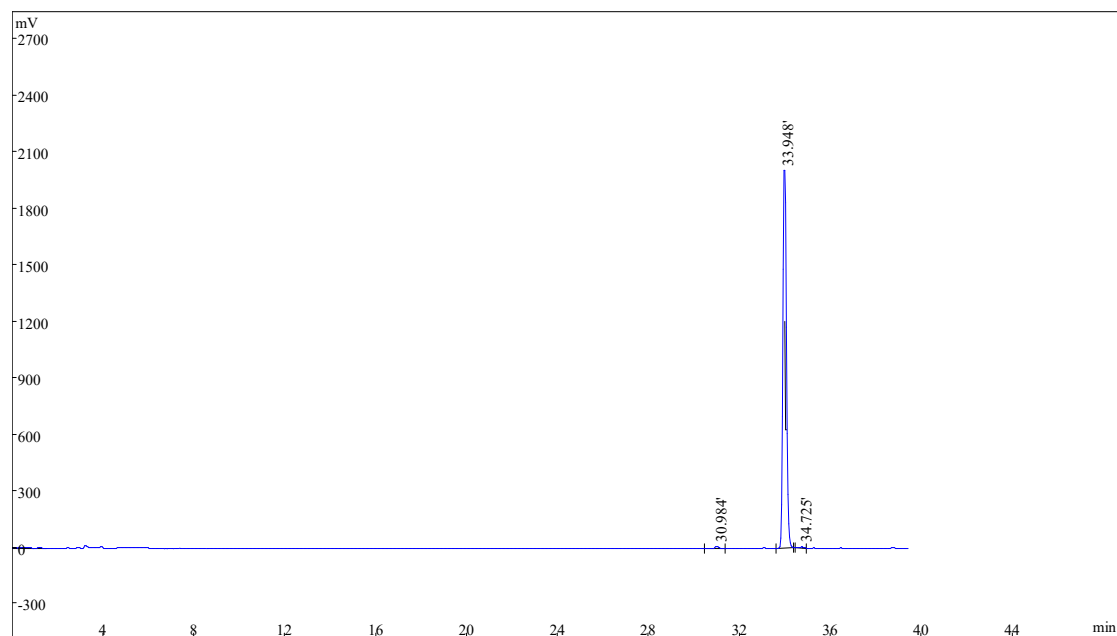
49.90

40.28
31.70
30.72
28.10
25.08



NAME gcx-20160914
EXPNO 2
PROCNO 1
Date_ 20160914
Time 10.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 2048
DS 4
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8651252 sec
RG 190.02
DW 13.200 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 2

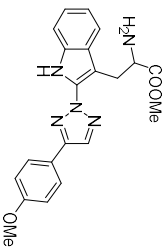
===== CHANNEL f1 =====
SFO1 150.929469 MHz
NUC1 13C
P1 11.90 usec
SI 32768
SF 150.9126587 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



No	Retention Time	Content	Peak Area	Peak Separation
1	30.984	0.6038	110649	12.16
2	33.948	99.18	18176365	3.65
3	34.725	0.213	39041	0.00
Total		100	18326055	

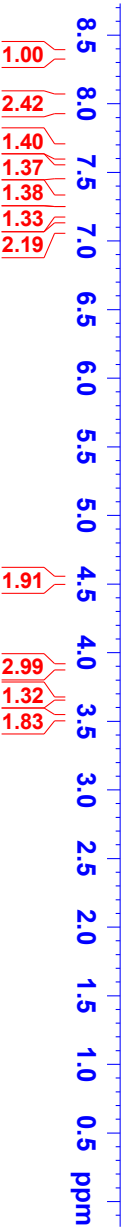


7.999
7.978
7.648
7.628
7.515
7.495
7.277
7.258
7.221
7.202
7.183
7.110
7.088



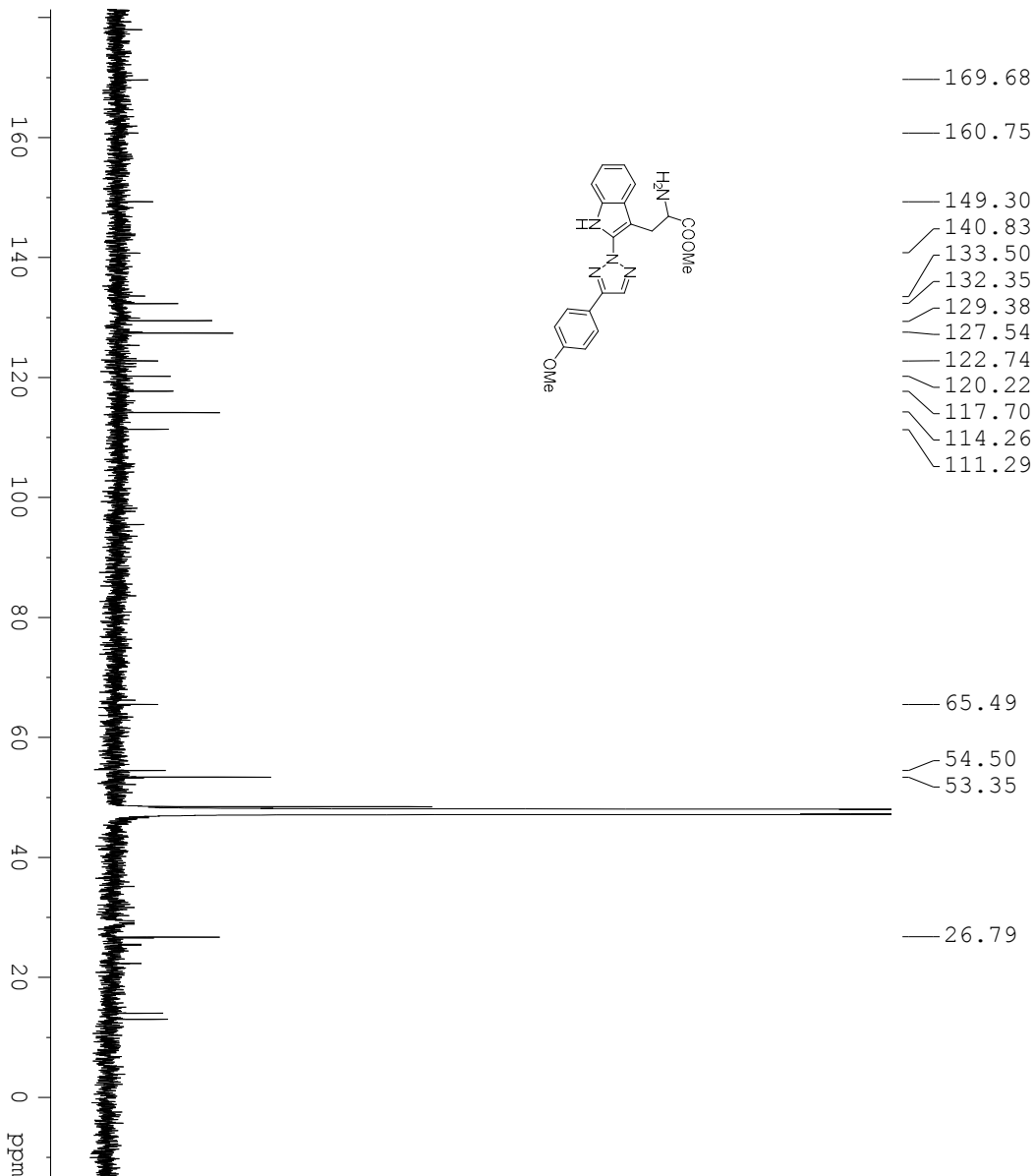
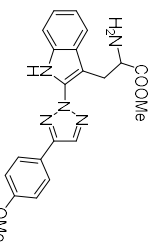
5.520
4.909
3.901
3.663
3.530
3.379
3.340
3.336

1.326



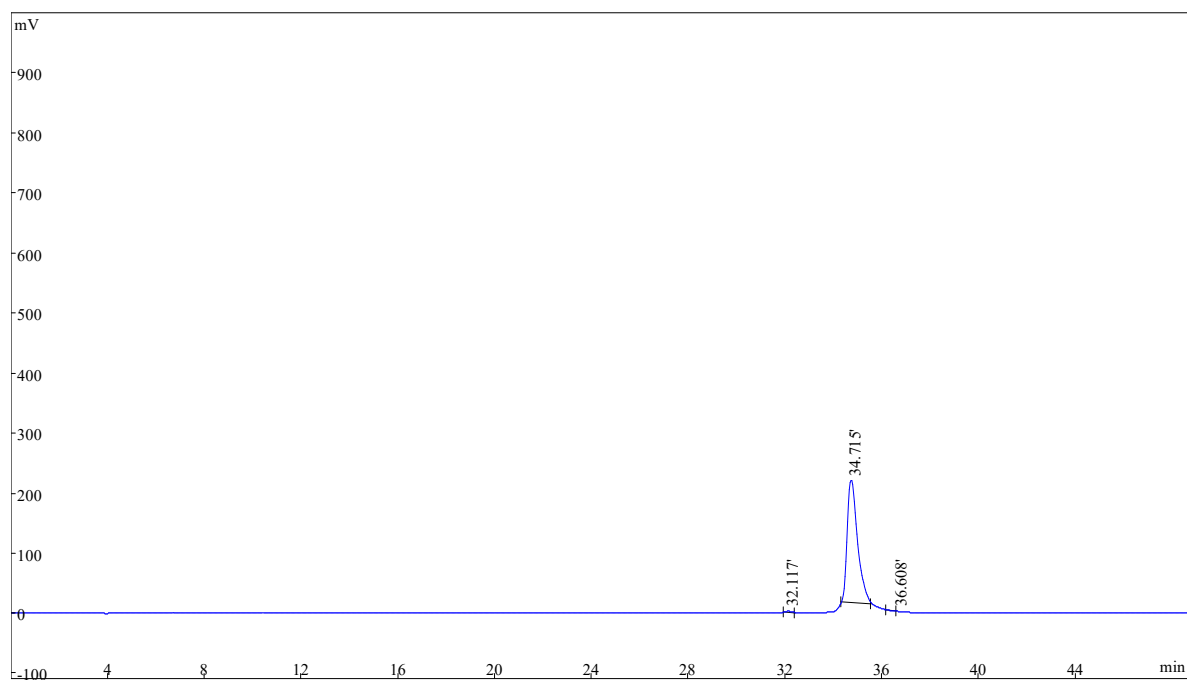
NAME ome
EXPNO 1
PROCNO 1
Date_ 20160913
Time_ 15.58
INSTRUM spect
PROBHD 5 mm PABUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4526453 sec
RG 287
DW 83.200 usec
DE 8.00 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1315723 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

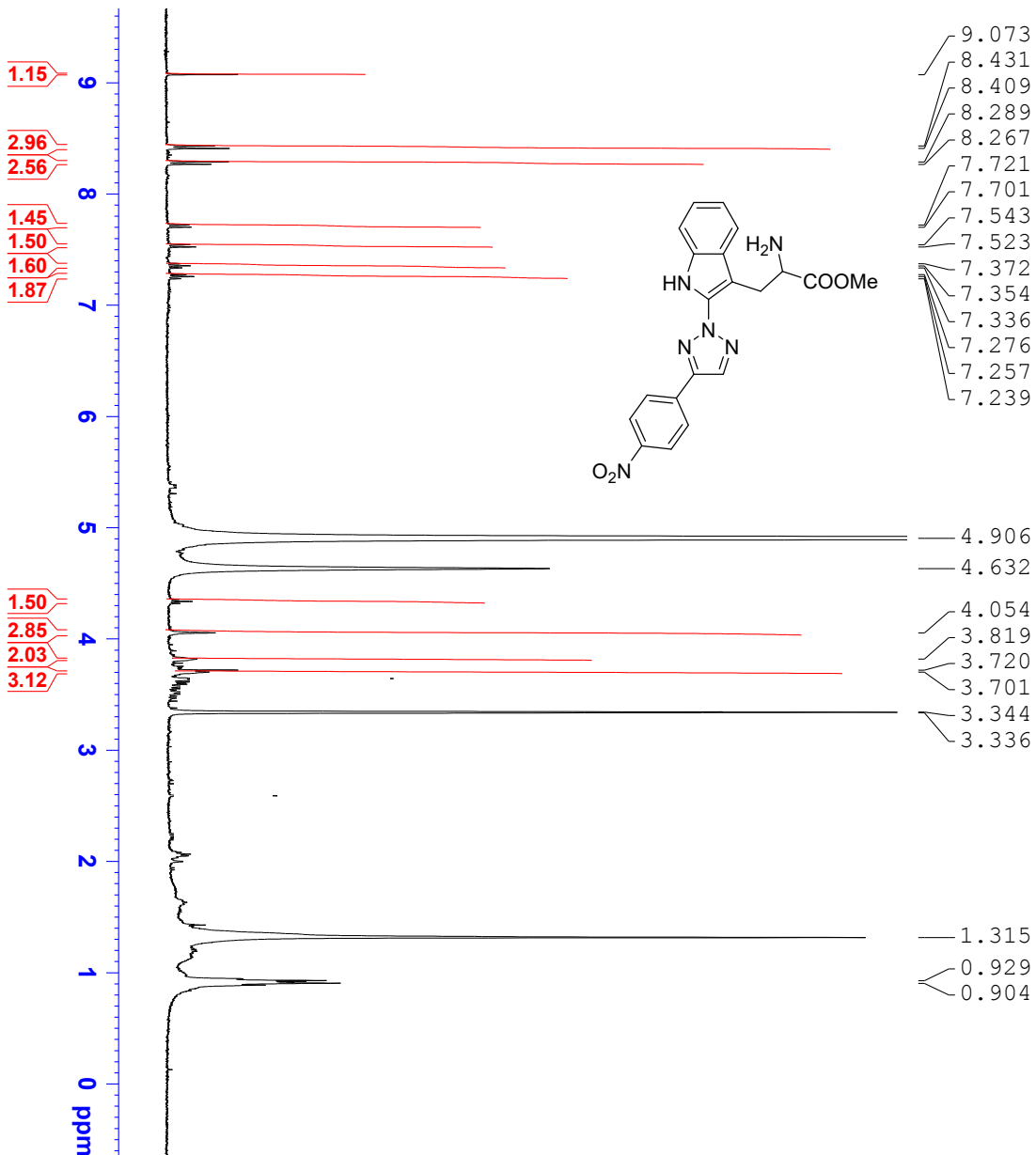
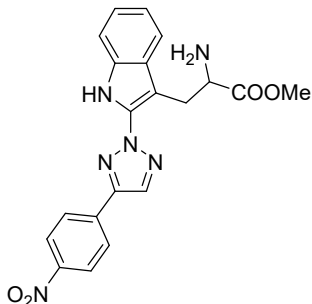


NAME ome
EXPNO 2
PROCNO 1
Date_ 20160919
Time 9.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 8000
DS 4
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8651252 sec
RG 190.02
DW 13.200 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10

===== CHANNEL f1 =====
SF01 150.9294669 MHz
NUC1 13C
P1 11.90 usec
SI 32768
SF 150.9128665 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



No	Retention Time	Content	Peak Area
1	32.117	0.4096	23120
2	34.715	99.59	5622034
3	36.608	0	-3508
Total		100	5641646



NAME no2
EXPNO 1
PROCNO 1
Date_ 20160929
Time_ 15.40
INSTRUM spect
PROBHD 5 mm PABUL 13C
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4526453 sec
RG 256
DW 83.200 usec
DE 8.00 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

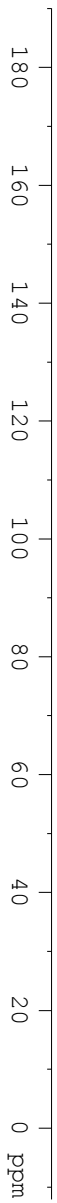
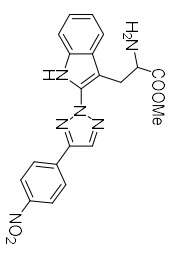
===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFOL 400.1326008 MHz
SI 32768
SF 400.1299356 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

179.03

145.70
143.33
142.58
139.58
134.21
131.47
126.47
123.98
123.71
122.73
120.73
118.48
111.86

53.42
52.27

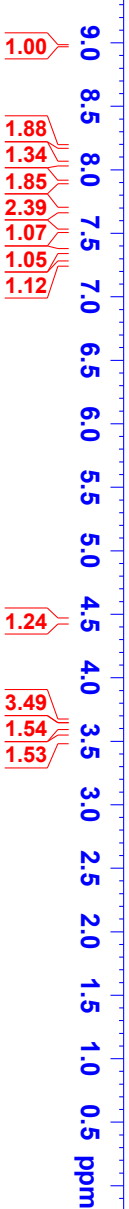
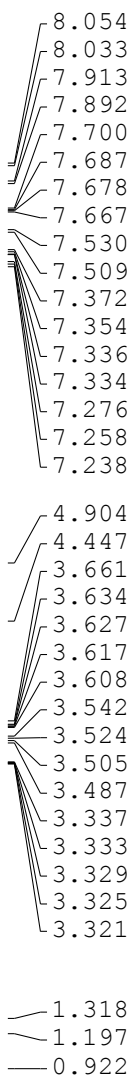
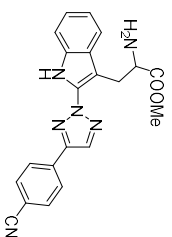
24.96



NAME no2
EXPNO 2
PROCNO 1
Date_ 20160603
Time 16.01
INSTRUM spect
PROBHD 5 mm PABUL 13C
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 216
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.297629 sec
RG 181
DW 19.800 usec
DE 8.00 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

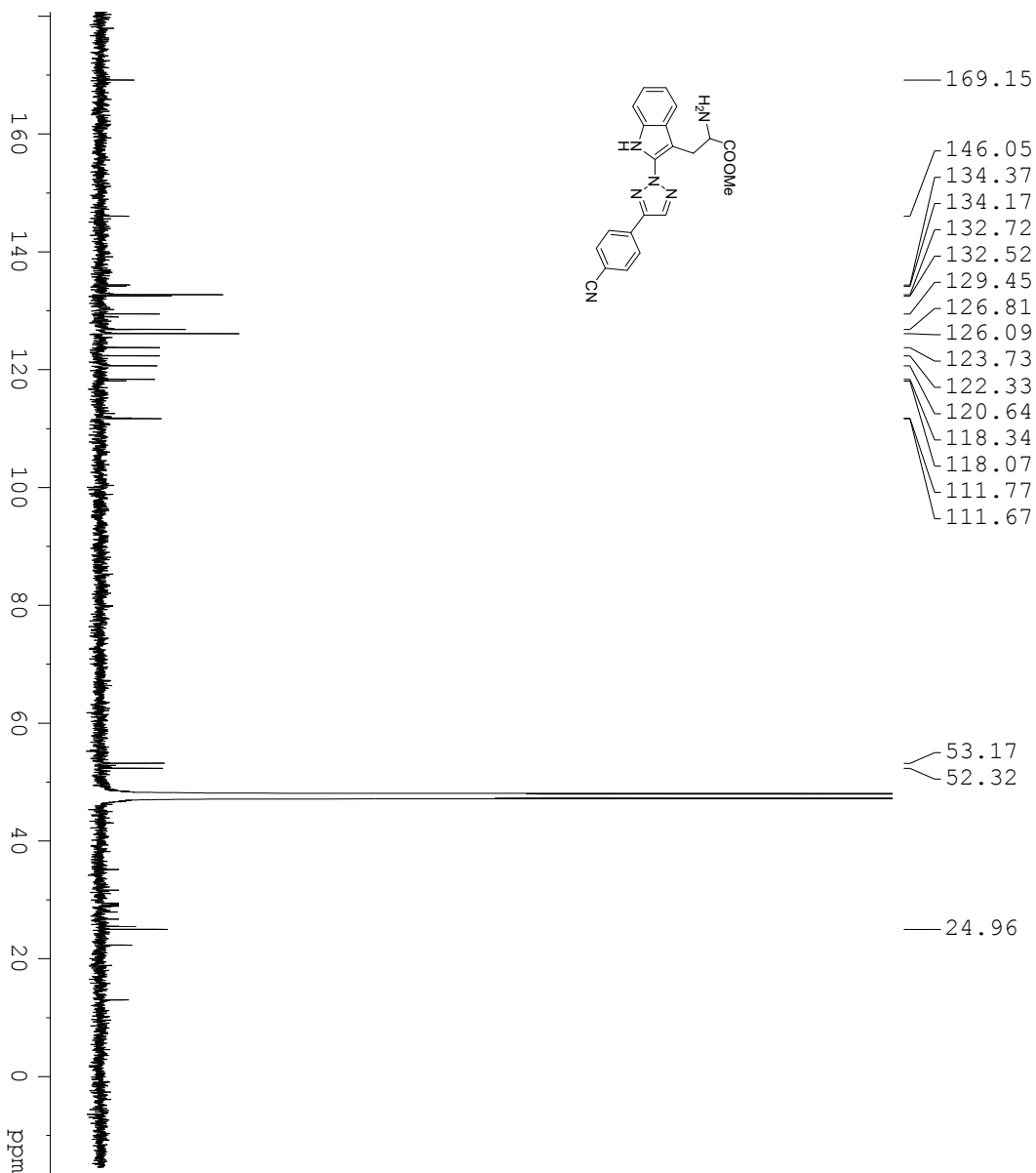
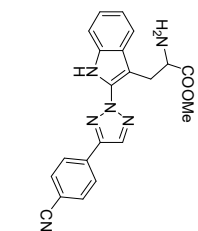
===== CHANNEL f1 =====
NUC1 13C
P1 13.50 usec
PL1 3.00 dB
PL1W 43.93649673 W
SFO1 100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.80 dB
PL12 17.19 dB
PL13 18.46 dB
PL1W 8.92857742 W
PL12W 0.25809658 W
PL13W 0.19265592 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



NAME cn
EXPNO 1
PROCNO 1
Date_ 20161202
Time_ 16.12
INSTRUM spect
PROBHD 5 mm PADUL13C
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4526453 sec
RG 362
DW 83.200 usec
DE 8.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



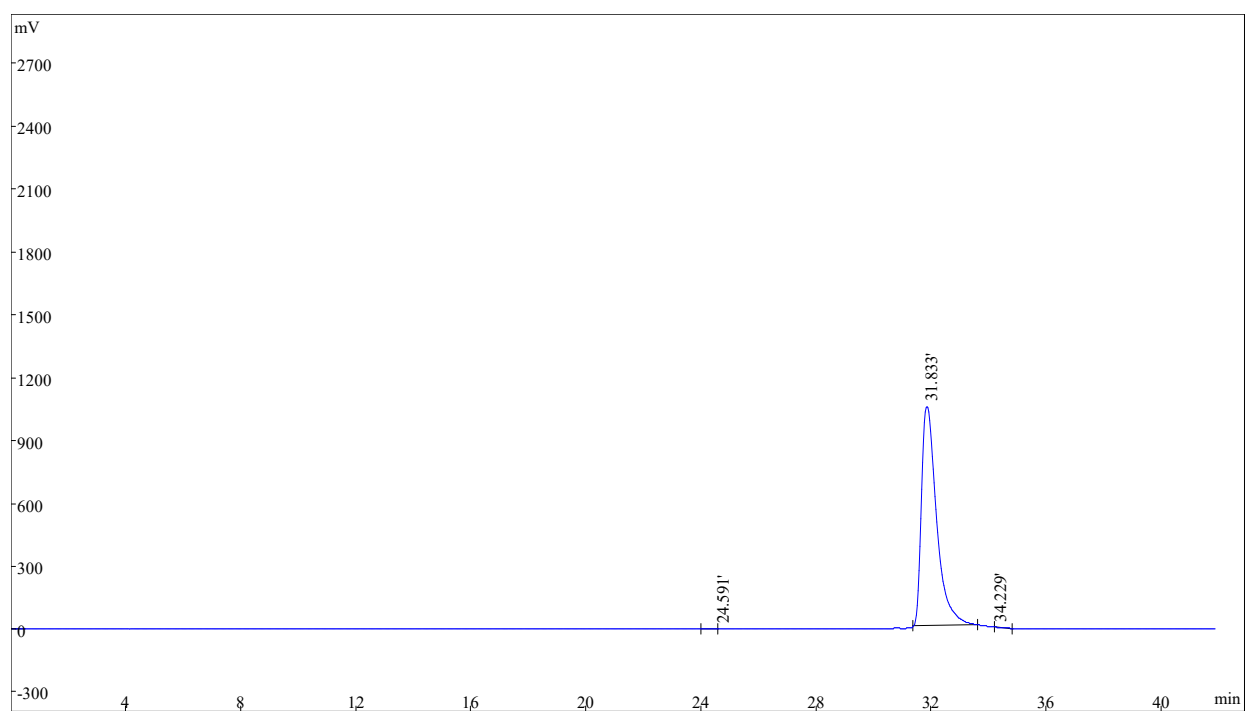
169.15
146.05
134.37
134.17
132.72
132.52
129.45
126.81
126.09
123.73
122.33
120.64
118.34
118.07
111.77
111.67

53.17
52.32

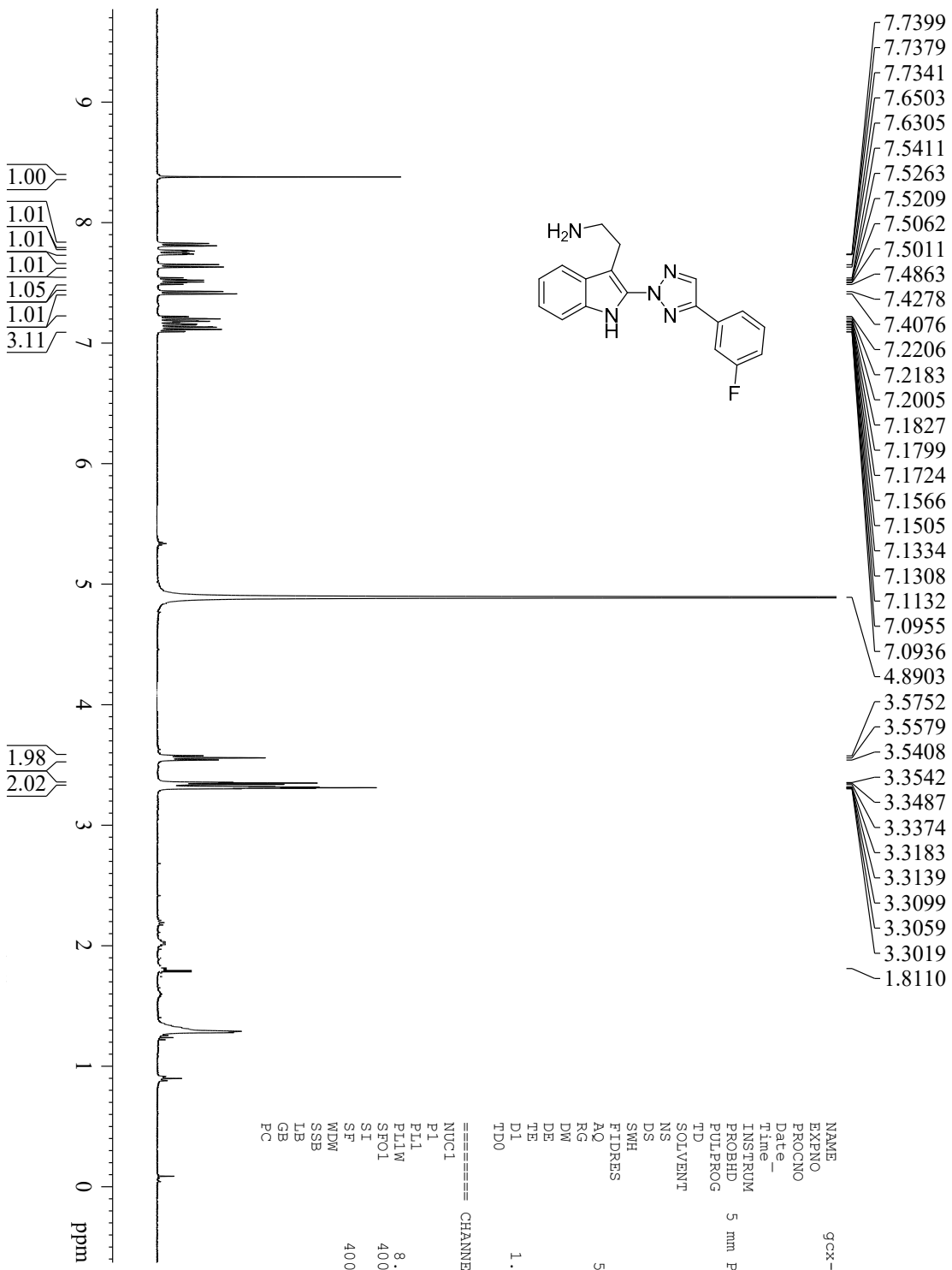
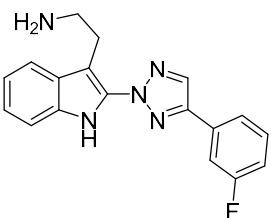
24.96

NAME cn
EXPNO 2
PROCNO 1
Date_ 20161212
Time 19.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 10240
DS 4
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8651252 sec
RG 190.02
DW 13.200 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10

===== CHANNEL f1 =====
SFO1 150.9294669 MHz
NUC1 13C
P1 11.90 usec
SI 32768
SF 150.9128665 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



No	Retention Time	Content	Peak Area
1	24.591	0	-364
2	31.833	100	36568595
3	34.229	0	-14991
Total		100	36553240

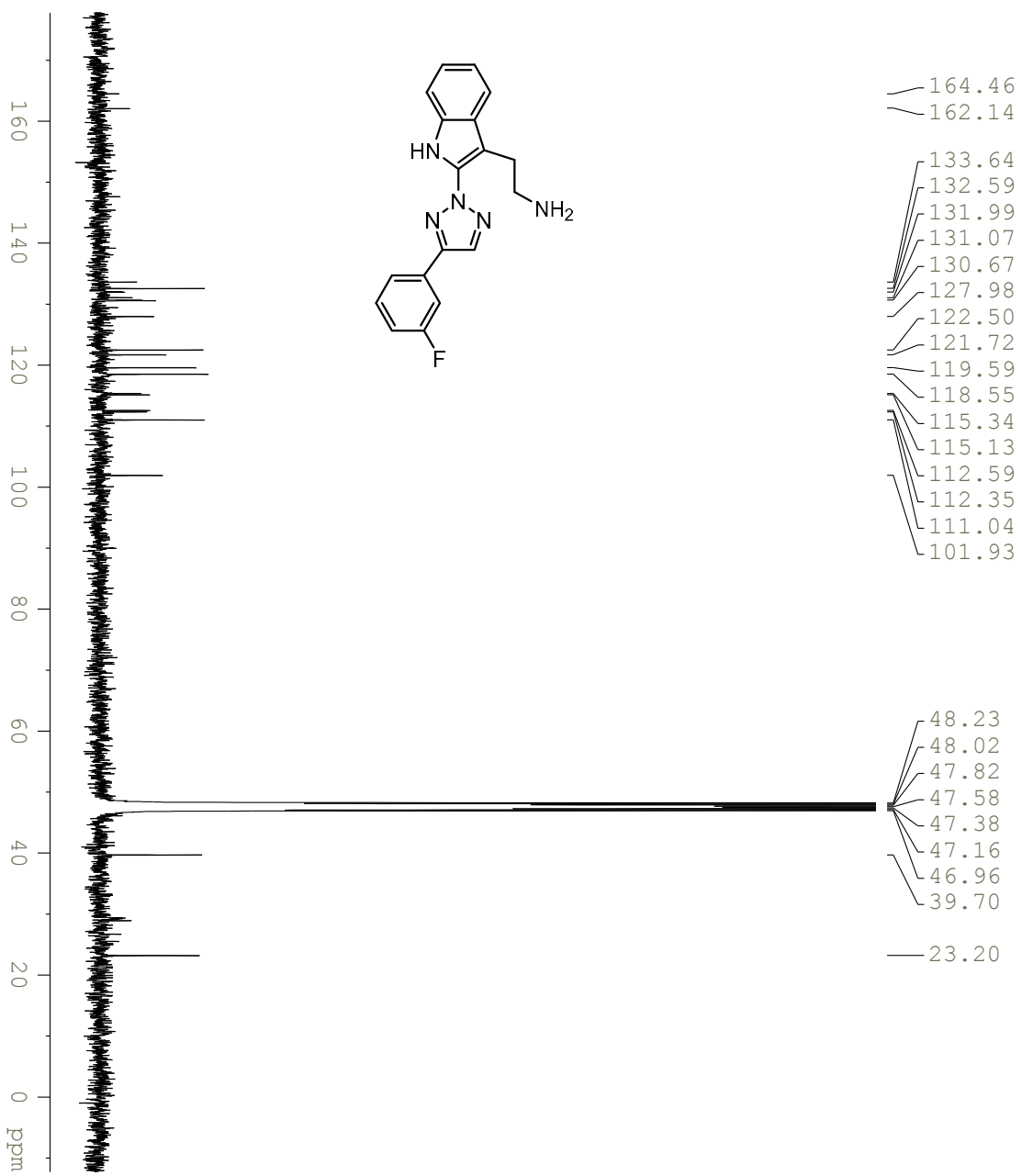


- 7.7399
- 7.7379
- 7.7341
- 7.6503
- 7.6305
- 7.5411
- 7.5263
- 7.5209
- 7.5062
- 7.5011
- 7.4863
- 7.4278
- 7.4076
- 7.2206
- 7.2183
- 7.2005
- 7.1827
- 7.1799
- 7.1724
- 7.1566
- 7.1505
- 7.1334
- 7.1308
- 7.1132
- 7.0955
- 7.0936
- 4.8903
- 3.5752
- 3.5579
- 3.5408
- 3.3542
- 3.3487
- 3.3374
- 3.3183
- 3.3139
- 3.3099
- 3.3059
- 3.3019
- 1.8110

```

NAME          gcx-20170308
EXPNO         1
PROCNO        1
Date_         20170306
Time_         16.13
INSTRUM       5 mm PABUL
PROBHD        zg30
PULPROG       65536
TD            8
SOLVENT       MeOD
NS            8
DS            0
SWH           6009.615 Hz
FIDRES        0.091699 Hz
AQ           5.4526453 sec
RG           322
DW           83.200 usec
DE           8.00 usec
TE           294.6 K
D1           1.00000000 sec
TD0          1

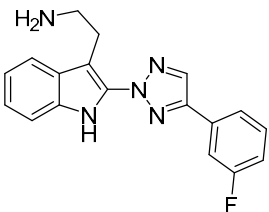
===== CHANNEL f1 =====
NUC1          1H
P1           13.10 usec
PL1          1.80 dB
PL1W         8.92857742 W
SFO1         400.1326008 MHz
SI           32768
SF           400.1300074 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```



NAME gcx-20170310
EXPNO 2
PROCNO 1
Date_ 20170310
Time 11.00
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 3128
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.297629 sec
RG 181
DM 19.800 usec
DE 8.00 usec
TE 295.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 13.50 usec
PL1 3.00 dB
PL1W 43.93649673 W
SFO1 100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.80 dB
PL12 17.19 dB
PL13 18.46 dB
PL12W 8.92857742 W
PL12W 0.25809658 W
PL13W 0.19265592 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



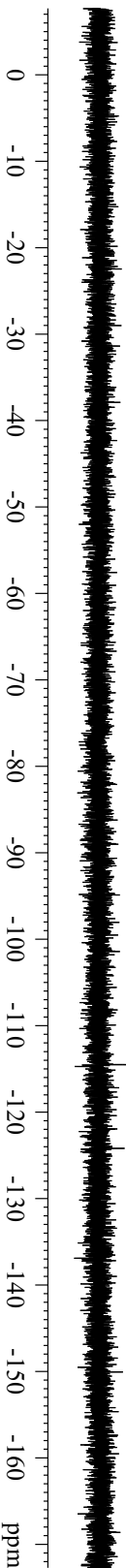
— -114.5213

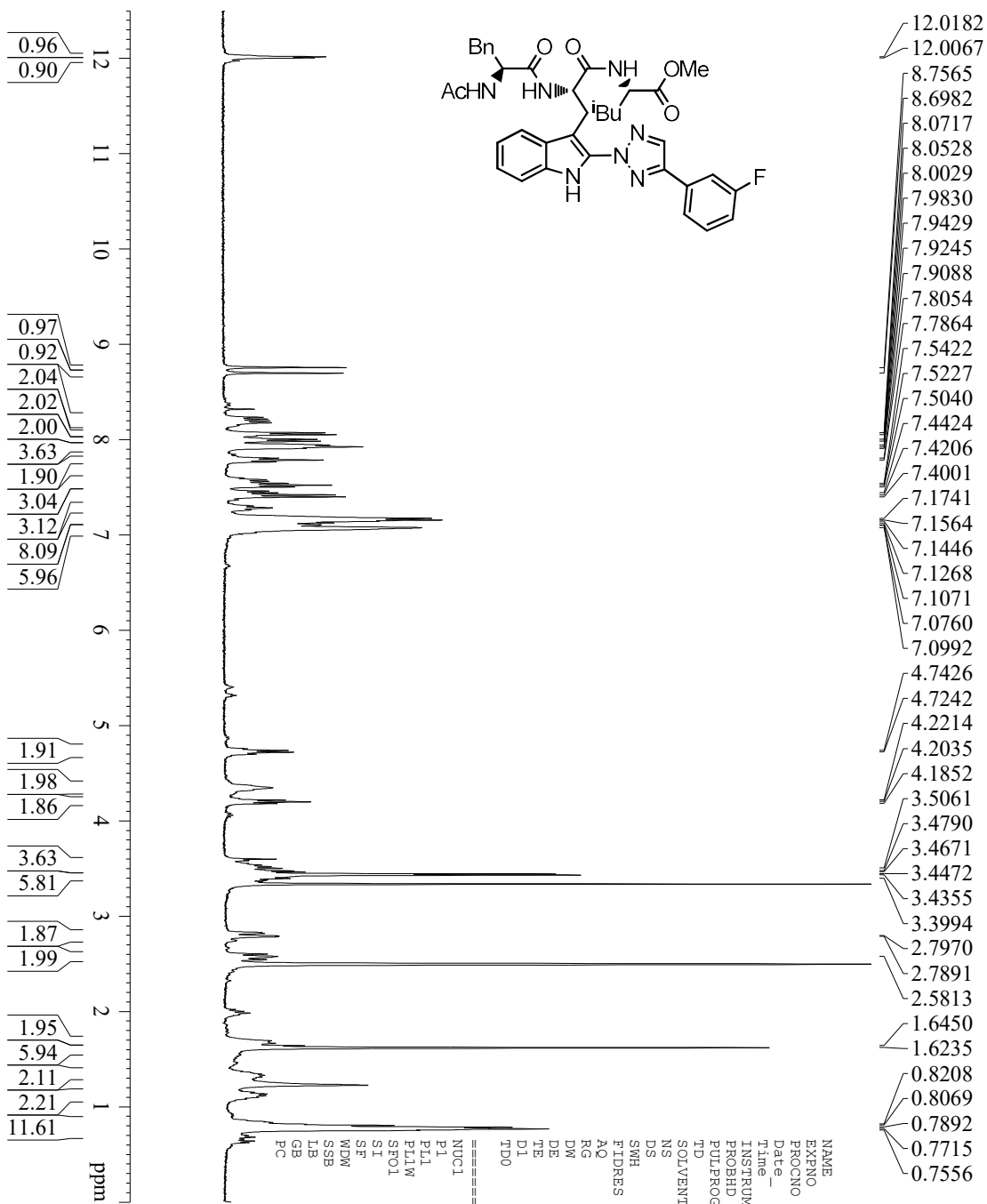
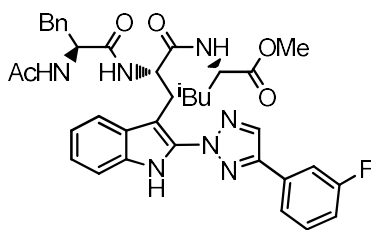
```

NAME          gcx-20170308
EXPNO         3
PROCNO        1
Date_         20170306
Time_         10.42
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgfh1q9n.2
TD            131072
SOLVENT       MeOD
NS            16
DS            4
SMH           133928.578 Hz
FIDRES        1.021794 Hz
AQ            0.4893855 sec
RG            15.49
DW            3.733 usec
DE            6.50 usec
TE            301.5 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0           1

===== CHANNEL f1 =====
SF01          564.6675534 MHz
NUC1          19F
P1            11.90 usec
SI            65536
SF            564.7240258 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.00

```





NAME b-3b-staw-20130122
 EXPNO 1
 PROCNO 1
 Date_ 20140122
 Time 15:50
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 6393.862 Hz
 FIDRES 0.195125 Hz
 AQ 2.5625076 sec
 RG 322
 DW 78.200 usec
 DE 6.50 usec
 TE 293.5 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.40 usec
 PL1 -1.00 dB
 PL1W 17.01303389 W
 SF01 400.1328009 MHz
 SI 16384
 SF 400.1300027 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

