Electronic Supporting Information

Upgrading the ferribactin pre-chromophore – synthesis, modification and polymerization

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1. Materials and experimental methods

Materials

All chemicals were used as purchased from commercial suppliers, unless otherwise specified. Water and oxygen sensitive reactions were performed with Schlenk technique under nitrogen atmosphere (dried via absorption tower with Sicapent®) in dry solvents. Low temperatures were achieved with ice/water mixtures (0 °C). Ethyl acetate (EtOAc), petrol ether (PE) and dichloromethane (CH_2Cl_2) were distilled prior to use.

NMR spectroscopy

NMR spectroscopy was performed in deuterated solvents ($CDCl_3$, CD_3OD or DMSO-d_6 at room temperature (rt) (if not indicated otherwise) using the spectrometers Avance 300, Avance III HD 400 NanoBay, Avance 500 or Avance III HD 700 by Bruker.
^1H NMR spectra were measured at 300, 400, 500 or 700 MHz. ^{13}C NMR spectra were measured at 75, 101, 126 or 176 MHz. The abbreviations for the NMR signal multiplicities are: s (singlet), d (doublet), t (triplet), q (quartet) und m (multiplet). Combined abbreviations are indicated as dt (doublet of triplets). The numbering of atoms does not comply with IUPAC rules.

IR spectroscopy

IR spectroscopy was performed on the Alpha Platinum ATR spectrometer by Bruker. The absorption bands are indicated in wavenumbers (cm^{-1}). The intensities are distinguished as: w = weak, m = middle, s = strong, vs = very strong, br = broad.

UV-VIS spectroscopy

UV-VIS measurements were performed on the UV-2600 UV-VIS spectrometer by Shimadzu.

Mass spectrometry

Mass spectrometry was performed on the micro-TOF-Q (ESI) by Bruker, the Exactive GC Orbitrap MS by Thermo Fisher Scientific or the Exactive Plus Orbitrap MS by Thermo Fisher Scientific. MALDI measurements were performed on the Bruker

Microflex MS in the linear positive mode with a N_2 laser (337 nm). 2,5-dihydroxybenzoic acid (DHB) was used as matrix.

Chromatography

Column chromatography was performed with silica gel by Fluka (type 60, grain size 40-70 µm or by SiliCycle (SiliaFlash F60, grain size 40-63 µm). The solvent mixtures used are specified in the synthesis chapter.

Thin layer chromatography (TLC) was performed with 60 F 254 TLC plates on aluminum by Macherey-Nagel (layer thickness 0.20 mm). The UV lamp used emitted light at 254 nm and 366 nm. Some TLC plates were colored with staining solution (heating included). The staining solutions used are anisaldehyde solution, Seebach solution, potassium permanganate solution and ninhydrin solution.

Anisaldehyde solution was prepared by mixing concentrated sulfuric acid (10 mL), acetic acid (3.0 mL) and 4-anisaldehyde (4.0 mL) in ethanol (200 mL).

Seebach solution was prepared by mixing phosphomolybdic acid (5.0 g), concentrated sulfuric acid (16 mL) and cerium (IV)sulfate (2.0 g) in water (200 mL).

Potassium permanganate solution was prepared by mixing 1% aqueous potassium permanganate solution and 2% aqueous sodium carbonate solution (vol 1 : 1).

Ninhydrin solution was prepared by dissolving 0.3 g ninhydrin in 95 mL acetone.

Optical rotation

Optical rotation measurements were performed on the P8000-T80 by KRÜSS with the Na-D line (λ = 289 nm). The specific optical rotation is calculated using the formula:

$$[\alpha]_D^{20} = \frac{\alpha_m \cdot 100}{c \cdot l}$$

With α_m as measured optical rotation, c (in g/100 mL) as mass concentration and l as path length through the sample (l = 0.5 dm).

2. Synthesis

2.1 General procedures (GP)

General procedure to synthesize the carboxamides (GP 1)

Using the example of **15b-D**.

The acid **20b-D** (10.4 g, 19.7 mmol) was dissolved in CH_2Cl_2 (72 mL) and cooled to 0 °C. *N*-Methylmorpholine (5.00 mL, 4.55 g, 45.0 mmol) was added, then isopropyl chloroformate (5.60 mL, 5.88 g, 43.1 mmol) was added in milliliter portions. The reaction was stirred for 30 min at 0 °C, then concentrated ammonia solution (25%, 18.0 mL, 239.4 mmol) was added and the flask closed with a septum. The reaction was stirred slowly for 21 h at rt. Then water (60 mL) was added, the phases separated, and the water phase extracted with CH_2Cl_2 (3 x 100 mL). The combined organic phases were dried over Na_2SO_4, filtered and dried under reduced pressure. The resulting orange crude product was purified by column chromatography (PE / EtOAc 1 : 1) and obtained as colorless solid.

General procedure for the synthesis of ferribactin pre-chromophore derivatives (GP 2)

Using the example of **14a-T**.

The amid **15a-T** (2.16 g, 4.16 mmol) was dissolved with CH_2Cl_2 (45 mL) in a dried Schlenk flask under N_2. MeOTf (0.71 mL, 1.03 g, 6.27 mmol) was added and the mixture was refluxed for 3 h. Then the reaction was stirred at rt for 21.5 h. The solvent was evaporated under reduced pressure and the remaining compound was dissolved in dried EtOH (28 mL). L-2,4-Diaminobutyric acid dihydrochloride (DABA **16·2HCl**; 0.80 mg, 4.18 mmol) was added and the mixture was stirred for 10 min at rt. Then *N*,*N*-Diisopropylethylamine (*i*Pr_2EtN; 2.60 mL, 1.93 mg, 14.9 mmol) was added and the mixture refluxed for 19.5 h. After cooling, the solvent was evaporated under reduced pressure and the crude product was purified by column chromatography (CH_2Cl_2 / MeOH 7 : 1, 5 : 1). The product **14a-T** (2.34 g, 3.89 mmol, 93%) was obtained as colorless solid.

Purification by column chromatography left traces of byproducts in the derivatives **14a-T**, **14b-D**, **14c-T**, **14d-D** and **S1a-T**. For some NMR measurements, a fraction of the derivatives was recrystallized.

It should be noted that the yields of products **14a-T**, **14b-D**, **14c-T**, **14d-D** and **S1a-T** were not affected whether synthesized or commercially available DABA **16** was used.

General procedure for the deprotection and coupling of the ferribactin pre-chromophore derivatives (GP 3)

Using the example of **23a-T**.

Boc-β-alanine **S2** (126 mg, 665 µmol), EDC·HCl (128 mg, 668 µmol) and HOBt·H_2O (104 mg, 679 µmol) were dissolved in CH_2Cl_2 (3.4 mL) and stirred at rt for 1.5 h. Then *N*-methylmorpholine (1.10 ml, 1.00 g, 9.90 mmol) was added.

The derivative **14a-T** (401 mg, 666 µmol) was suspended in CH_2Cl_2 (5.0 mL), mixed with TFA (0.52 mL, 770 mg, 6.75 mmol) and stirred for 4 h at rt. After evaporation of the solvent under reduced pressure, the deprotected derivative was dissolved in CH_2Cl_2 (3.6 mL) and added dropwise to the prepared alanine mixture. The reaction was stirred for another 16 h at rt, then mixed with water (30 mL). After extraction with CH_2Cl_2 (3 x 50 mL), the combined organic phases were dried over Na_2SO_4, filtered and the solvent removed under reduced pressure. The crude product was purified by column chromatography (Silicycle F60 silica gel, CH_2Cl_2 / MeOH 10 : 1 to CH_2Cl_2 / MeOH 3 : 1). The product **23a-T** (370 mg, 550 µmol, 83%) was obtained as colorless solid.

General procedure for the polymerization (GP 4)

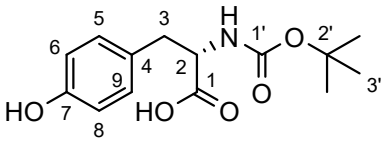
Using the example of **11c-T**.

The monomer **13c-T** (9.98 mg, 24.0 µmol), RAFT-agent **25** (0.83 mg, 3.98 µmol), *N*-vinylpyrrolidone (NVP) **9** (19.3 µL, 20.0 mg, 180 µmol) and TMEDA (2.6 µL, 2.03 mg, 17.5 µmol) were dissolved in water (150 µL) in a GC vial. The mixture was degassed for 5 min with N_2 while stirring vigorously. Then *tert*-Butyl hydroperoxide (TBHP; 70% in water, 2.4 µL, 2.23 mg, 17.3µmol) was added and the reaction stirred for 19 h at 40 °C (under N_2). Afterwards the mixture was diluted with 20 mL MeOH, filtered and the solvent removed under reduced pressure. MeOH (1 mL) was added and mixed with 60 mL MTBE while stirring. A colorless solid precipitated. After filtration and drying under reduced pressure the polymer **11c-T** (20 mg, 65%) was obtained.

2.2 Tyrosine derivatives

(tert-Butoxycarbonyl)-L-tyrosine (19a-T)

L-Tyrosine **18a** (3.15 g, 17.4 mmol) was dissolved in water (40 mL) and THF (80 mL) and mixed with 1 M sodium hydroxide solution (35.0 mL, 35.0 mmol). Boc_2O (4.19 g, 19.2 mmol) was added and the mixture stirred for 22 h at rt. Then the pH value was adjusted to pH = 2 with 1 M hydrochloric acid. The mixture was extracted with CH_2Cl_2 (3 x 60 mL) and the combined organic phases were dried over Na_2SO_4 and filtered. After evaporation of the solvent under reduced pressure, **19a-T** (4.89 g, 17.4 mmol, quant.) was obtained as colorless foam.



$C_{14}H_{19}NO_5$
281.31

19a-T

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.42 (s, 9H, 3‘-H), 3.04 (t, *J* = 7.1 Hz, 2H, 3-H), 4.56 (s, 1H, 2-H), 5.11 (s, 1H, 7-O*H*), 6.70 (d, *J* = 7.7 Hz, 2H, 5-H, 9-H), 6.97 (d, *J* = 7.7 Hz, 2H, 6-H, 8-H), 9.00 (s, 1H, COO*H*) ppm.

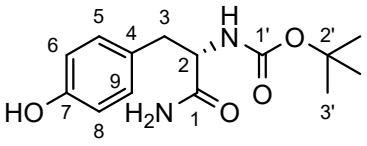
^{13}C-NMR (101 MHz, $CDCl_3$): δ = 28.4 (C-3‘), 37.2 (C-3), 54.6 (C-2), 84.0 (C-2‘),121.5 (C-5, C-9), 130.5 (C-6, C-8), 134.3 (C-4), 155.1 (C-7), 155.8 (C-1‘), 176.2 (C-1) ppm.

The spectroscopic data match the literature data.[1]

tert-Butyl-(*S*)-(1-amino-3-(4-hydroxyphenyl)-1-oxopropan-2-yl)carbamate (S3-T)

Boc-tyrosine **19a-T** (1.01 g, 3.60 mmol) was dried in vacuo and dissolved in dried THF (12 mL). *N*-Methylmorpholine (0.88 mL, 0.80 g 7.92 mmol) was added and the mixture cooled to 0 °C. Then isopropyl chloroformate (1.03 mL, 1.08 g, 7.92 mmol) was added slowly and the resulting mixture stirred for 30 min. Afterwards, concentrated ammonia solution (25%, 3.40 mL, 45.2 mmol) was added and, the flask closed with a septum and the reaction stirred for 18 h at rt. The solvent was evaporated under reduced pressure and the remaining substance was mixed with THF (36 mL) and 1 M sodium hydroxide solution (36 mL, 36,0 mmol). The mixture was stirred for 3 h at rt. Then the THF was removed under reduced pressure and the pH value of the remaining solution was adjusted to pH = 2. After extraction with EtOAc (3 x 20 mL), the combined organic phases were dried over Na_2SO_4 and the solvent was removed under reduced pressure.

The crude product was purified by column chromatography (PE / EtOAc 1 : 4) and **S3-T** (545 mg, 1.94 mmol, 54%) was obtained as colorless solid.



$C_{14}H_{20}N_2O_4$
280.32

S3-T

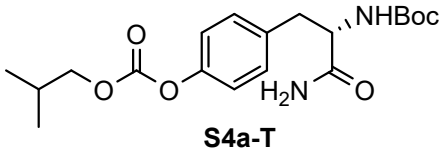
^{1}H-NMR (500 MHz, $CDCl_3$): δ = 1.39 (s, 9H, 3'-H), 2.88–3.12 (m, 2H, 3-H), 4.42 (s, 1H, 2-H), 5.33 (s, 1H, 2-NH), 6.04 (s, 1H, 1-NH_aH), 6.31 (s, 1H, 1-NH_bH), 7.09 (d, *J* = 8.0 Hz, 2H, 5-H, 9-H), 7.22 (d, *J* = 8.0 Hz, 2H, 6-H, 8-H) ppm.

^{13}C-NMR (126 MHz, $CDCl_3$): δ = 28.4 (C-3'), 37.9 (C-3), 55.3 (C-2), 83.7 (C-2'), 121.4 (C-5, C-9), 130.5 (C-6, C-8), 134.4 (C-4), 150.1 (C-7), 155.6 (C-1'), 174.1 (C-1) ppm.

R_f = 0.44 (PE / EtOAc = 1 : 4, UV).

The spectroscopic data match the literature data (DMSO-d_6, 200 MHz), small deviations are caused by the solvent.[2]

The additional stirring with 1 M NaOH reduced the formation of the carbonate side product **S4a-T**.

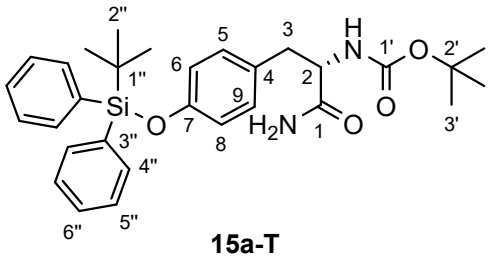


S4a-T

It should be noted, that compound **S3-T** showed gelling abilities with $CHCl_3$ or CH_2Cl_2. The ability of tyrosine derivatives containing hydrophobic protection groups, including silyl groups, or short tyrosine peptides to gel chlorinated solvents is literature known.[3,4]

tert-Butyl-(*S*)-(1-amino-3-(4-((tert-butyldiphenylsilyl)oxy)phenyl)-1-oxopropan-2-yl)carbamate (15a-T)

Imidazole (0.78 g, 11.5 mmol) and **S3-T** (2.15 g, 7.68 mmol) were dissolved in CH_2Cl_2 (77 mL). TBDPSCl (3.00 mL, 3.17 g, 11.5 mmol) was added dropwise and the mixture was stirred for 25 h at rt (up to 30 °C). Then water (60 mL) was added and the reaction was extracted with CH_2Cl_2 (3 x 80 mL). After drying over Na_2SO_4 and filtration, the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (PE / EtOAc 1 : 1) and **15a-T** (1.51 g, 2.91 mmol, 38%) was obtained as colorless solid.



$C_{30}H_{38}N_2O_4Si$
518.73

15a-T

^{1}H-NMR (700 MHz, $CDCl_3$): δ = 1.10 (s, 9H, 2''-H), 1.39 (s, 9H, 3'-H), 2.81–2.98 (m, 2H, 3-H), 4.26 (s, 1H, 2-H), 5.13 (d, J = 7.9 Hz, 1H, 2-NH), 5.69 (s, 1H, 1-NH_aH), 5.82 (s, 1H, 1-NH_bH), 6.65–6.73 (m, 2H, 5-H, 9-H), 6.88–6.97 (m, 2H, 6-H, 8-H), 7.33–7.37 (m, 4H, 5''-H), 7.39–7.43 (m, 2H, 6''-H), 7.68–7.72 (m, 4H, 4''-H) ppm.

^{13}C-NMR (176 MHz, $CDCl_3$): δ = 19.5 (C-1''), 26.6 (C-2''), 28.4 (C-3'), 37.8 (C-3), 55.6 (C-2), 80.2 (C-2'), 120.0 (C-5, C-9), 127.9 (C-5''), 129.1 (C-4), 130.0 (C-6''), 130.2 (C-6, C-8), 133.0 (C-3''), 135.6 (C-4''), 154.7 (C-7), 155.6 (C-1'), 174.1 (C-1) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3305 (w), 2961 (w), 2931 (w), 2858 (w), 1671 (vs), 1609 (m), 1509 (vs), 1473 (m), 1428 (m), 1391 (m), 1366 (m), 1251 (vs), 1166 (s), 1107 (s), 1051 (w), 1018 (w), 908 (vs), 822 (m), 730 (vs), 699 (vs), 647 (m), 636 (m), 611 (s), 560 (m), 499 (vs) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{30}H_{38}N_2O_4Si$: 519.2674; found: 519.2672.

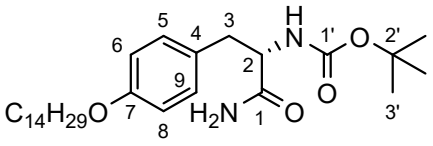
$[\alpha]_D^{20}$ = + 15.2°·mL·dm^{-1}·g^{-1} (c = 0.145, MeOH).

R_f = 0.29 (PE / EtOAc = 1 : 1, UV).

Mp. 164 °C.

tert-Butyl (*S*)-(1-amino-1-oxo-3-(4-(tetradecyloxy)phenyl)propan-2-yl)carbamate (S4b-T)

Potassium carbonate (3.78 g, 27.4 mmol), **S3-T** (2.52 g, 8.98 mmol) and potassium iodide (213 mg, 1.28 mmol) were suspended in acetonitrile (100 mL) and degassed for 20 min with N_2. 1-Bromotetradecane (3.00 mL, 2.80 g, 10.1 mmol) was added and the reaction was refluxed for 21 h under N_2. Then water (300 mL) was added and the mixture extracted with EtOAc (3 x 100 mL). The combined organic phases were dried over Na_2SO_4, filtered and the solvent was evaporated under reduced pressure. The crude product was purified by recrystallization in EtOH (40 mL) and the amide **S4b-T** (117 g, 2.45 mmol, 27%) was obtained as colorless solid.



$C_{28}H_{48}N_2O_4$
476.70

S4b-T

^{1}H-NMR (700 MHz, $CDCl_3$): δ = 0.88 (t, *J* = 6.8 Hz, 3H, Alkyl-H), 1.22–1.37 (m, 20H, Alkyl-H), 1.41 (s, 12H, 3‘-H, Alkyl-H), 1.76 (p, *J* = 6.8 Hz, 2H, Alkyl-H), 2.93–2.99 (m, 1H, 3-H_a), 3.00–3.06 (m, 1H, 3-H_b), 3.91 (t, *J* = 6.8 Hz, 2H, Alkyl-H), 4.27–4.36 (m, 1H, 2-H), 5.09 (s, 1H, 2-NH), 5.55 (s, 1H, 1-N*H*$_a$H,), 5.83 (s, 1H, 1-N*H*$_b$H), 6.82 (d, *J* = 8.2 Hz, 2H, 5-H, 9-H), 7.12 (d, *J* = 8.2 Hz, 2H, 6-H, 8-H) ppm.

^{13}C-NMR (176 MHz, $CDCl_3$): δ = 14.3, 22.8, 26.2 (Alkyl-C), 28.4 (C-3‘), 29.4, 29.5, 29.5, 29.7, 29.7, 29.8, 29.8, 29.8, 29.8, 32.1 (Alkyl-C), 37.7 (C-3), 55.7 (C-2), 68.1 (Alkyl-C), 80.3 (C-2‘), 114.8 (C-5, C-9), 128.4 (C-4), 130.4 (C-6, C-8), 155.6 (C-7), 158.4 (C-1‘), 173.9 (C-1) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3388 (w), 3348 (m), 3192 (w), 2919 (s), 2851 (m), 1684 (m), 1658 (vs), 1613 (w), 1511 (vs), 1468 (m), 1445 (m), 1423 (w), 1391 (m), 1367 (m), 1328 (m), 1291 (m), 1244 (vs), 1167 (s), 1047 (m), 1023 (m), 827 (m), 812 (w), 779 (w), 721 (w), 629 (m), 562 (w), 538 (w) cm^{-1}.

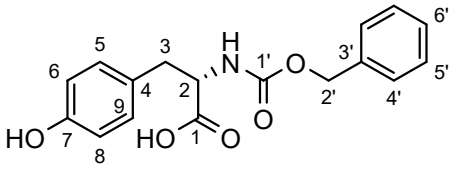
HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{28}H_{48}N_2O_4$: 477.3687; found: 477.3674.

$[\alpha]_D^{20}$ = + 8.3°·mL·dm^{-1}·g^{-1} (c = 0.145, $CHCl_3$).

Mp. 124 °C.

(Benzyloxy)carbonyl)-L-tyrosine (19c-T)

L-Tyrosine **18a** (5.03 g, 27.8 mmol) was suspended in THF (51 mL) and mixed with 1 M sodium hydroxide solution (56.0 mL, 56.0 mmol). Then CbzCl (4.60 mL, 5.61 g, 32.9 mmol) was added dropwise and the mixture was stirred for 26 h at rt. The mixture was washed with PE (3 x 30 mL) and the pH value of the water phase was adjusted to pH = 2 with 1 M hydrochloric acid. Then the water phase was extracted with EtOAc (3 x 100 mL) and the combined organic phases were dried over Na_2SO_4. After filtration, the solvent was evaporated under reduced pressure. The product **19c-T** (4.68 g, 14.8 mmol, 53%) was obtained as orange foam.



$C_{17}H_{17}NO_5$
315.33

19c-T

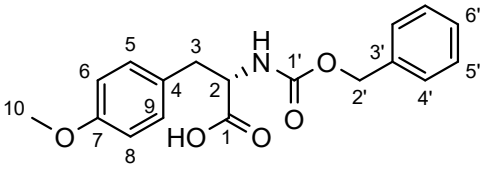
^{1}H-NMR (400 MHz, CD_3OD): δ = 2.84 (dd, *J* = 14.0 Hz, 9.0 Hz, 1H, 3-H_a), 3.09 (dd, *J* = 14.0 Hz, 5.0 Hz, 1H, 3-H_b), 4.36 (dd, *J* = 9.0 Hz, 5.0 Hz, 1H, 2-H), 5.03 (q, *J* = 12.6 Hz, 2H, 2‘-H), 6.65–6.73 (m, 2H, 6-H, 8-H), 6.99–7.05 (m, 2H, 5-H, 9-H), 7.18–7.48 (m, 5H, 4‘-H, 5‘-H, 6‘-H) ppm.

^{13}C-NMR (101 MHz, CD_3OD): δ = 36.5 (C-3), 55.6 (C-2), 66.1 (C-2‘), 114.8 (C-6, C-8), 127.2, 127.5, 127.8, 128.0 (C-4, C-4‘, C-5‘, C-6‘), 129.9 (C-5, C-9), 136.9 (C-3‘), 155.9 (C-7), 157.0 (C-1‘), 173.9 (C-1) ppm.

The spectroscopic data match the literature data (DMSO-d_6, 600 MHz), small deviations are caused by the solvent.[5]

(*S*)-2-(((Benzyloxy)carbonyl)amino)-3-(4-methoxyphenyl)propanoic acid (20c-T)

Cbz-tyrosine **19c-T** (2.90 g, 9.21 mmol) was dissolved in DMF (38 mL), then mixed with K_2CO_3 (5.10 g, 36.9 mmol) and iodomethane (1.80 mL, 4.10 g, 28.9 mmol). The reaction was stirred for 26 h at rt, then 2 M sodium hydroxide solution (47 mL, 94.0 mmol) was added and the mixture stirred for an additional 19 h at rt. Afterwards the pH value was adjusted to pH = 2 and the solution extracted with EtOAc (3 x 100 mL). The DMF was washed out with water (6 x 100 mL). The combined organic phases were dried over Na_2SO_4 and filtered. After evaporation of the solvent under reduced pressure, the product **20c-T** (2.43 g, 7.38 mmol, 80%) was obtained as yellow solid.



$C_{18}H_{19}NO_5$
329.35

20c-T

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 3.06 (dd, *J* = 14.1 Hz, 6.1 Hz, 1H, 3-H_a), 3.15 (dd, *J* = 14.1 Hz, 6.2 Hz, 1H, 3-H_b), 3.77 (s, 3H, 10-H), 4.65 (q, *J* = 6.2 Hz, 1H, 2-H), 5.04–5.15 (m, 2H, 2‘-H), 5.21 (d, J = 8.1 Hz, 1H, 2-NH), 6.81 (d, *J* = 8.5 Hz, 2H, 6-H, 8-H), 7.06 (d, *J* = 8.5 Hz, 2H, 5-H, 9-H), 7.28–7.42 (m, 5H, 4‘-H, 5‘-H, 6‘-H), 7.98 (s, 1H, COOH) ppm.

^{13}C-NMR (101 MHz, $CDCl_3$): δ = 37.0 (C-3), 54.9 (C-10), 55.3 (C-2), 67.3 (C-2‘), 114.2 (C-6, C-8), 127.5, 128.2, 128.4, 128.7 (C-4, C-4‘, C-5‘, C-6‘), 130.5 (C-5, C-9), 136.3 (C-3‘), 156.0 (C-7), 158.9 (C-1‘), 176.1 (C-1) ppm.

The spectroscopic data match the literature data.[6]

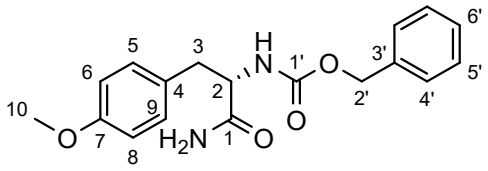
Benzyl-(*S*)-(1-amino-3-(4-methoxyphenyl)-1-oxopropan-2-yl)carbamate (15c-T)

Synthesis according to **GP 1**:

Acid **20c-T** (2.43 g, 7.38 mmol), CH_2Cl_2 (25 mL), *N*-methylmorpholine (1.00 mL, 0.91 g, 9.00 mmol), isopropyl chloroformate (1.10 mL, 1.16 g, 8.46 mmol), concentrated ammonia solution (25%, 7.00 mL, 93.1 mmol), 24 h rt.

Extraction: Water (50 mL), then CH_2Cl_2 (3 x 50 mL)

Purification: Recrystallization in $CHCl_3$ (80 mL), solid washed with $CHCl_3$ (10 mL). product **15c-T** (1.33 g, 4.05 mmol, 55%) obtained as colorless solid.



$C_{18}H_{20}N_2O_4$
328.37

15c-T

^{1}H-NMR (500 MHz, $CDCl_3$): δ = 2.90–3.15 (m, 2H, 3-H), 3.77 (s, 3H, 10-H), 4.40 (s, 1H, 2-H), 5.08 (s, 2H, 2‘-H), 5.45 (s, 1H, 2-NH), 5.64 (s, 1H, 1-NH_aH), 5.83 (s, 1H, 1-NH_bH), 6.82 (d, *J* = 8.1 Hz, 2H, 6-H, 8-H), 7.12 (d, *J* = 8.1 Hz, 2H, 5-H, 9-H), 7.28–7.46 (m, 5H, 4‘-H, 5‘-H, 6‘-H) ppm.

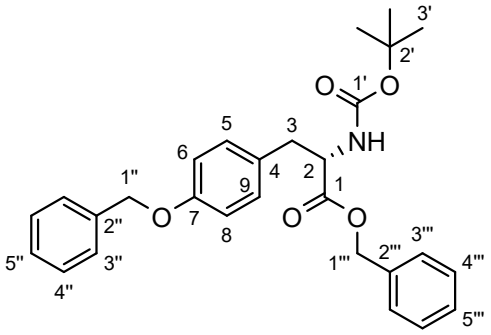
^{13}C-NMR (126 MHz, $CDCl_3$): δ = 37.7 (C-3), 55.3 (C-10), 56.1 (C-2), 67.2 (C-2‘), 114.3 (C-6, C-8), 127.6, 128.2, 128.4, 128.7 (C-4, C-4‘, C-5‘, C-6‘), 130.5 (C-5, C-9), 136.2 (C-3‘), 156.1 (C-7), 158.8 (C-1‘), 173.4 (C-1) ppm.

The spectroscopic data match the literature data.[7] Small deviations are caused by the solvent (Lit: CD_3OD).

Benzyl-(*S*)-3-(4-(benzyloxy)phenyl)-2-((*tert*-butoxycarbonyl)amino)propanoate (S5-T)

Boc-tyrosine **19a-T** (4.38 g, 15.6 mmol) was), K_2CO_3 (10.8 g, 78.0 mmol) and KI (1.30 g, 7.81 mmol) were suspended in acetonitrile (26 mL). BnBr (3.80 mL, 5.47 g, 32.0 mmol) was added dropwise and the reaction stirred at reflux for 27 h. The reaction was cooled to rt, then H_2O (100 mL) was added and the mixture extracted

with EtOAc (3 x 50 mL). The combined organic phases were washed with saturated NaCl solution (1 x 90 mL). The solvent was evaporated under reduced pressure and yielded an orange oil as crude product. Purification via recrystallization (PE / Et_2O 1 : 1, 4 mL) and washing with PE (200 mL) yielded **S5-T** (6.04 g, 13.1 mmol, 84%) as pale yellow solid.



$C_{28}H_{31}NO_5$
461.56

S5-T

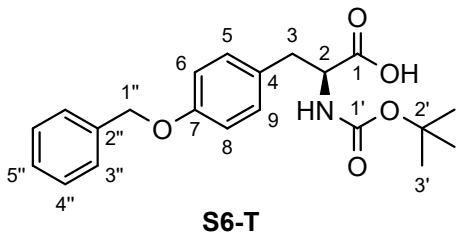
^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.43 (s, 9H, 3‘-H), 3.03 (d, *J* = 6.0 Hz, 2H, 3-H), 4.59 (q, *J* = 6.0 Hz, 1H, 2-H), 4.97 (d, *J* = 8.3 Hz, 1H, 2-NH), 5.02 (s, 2H, 1‘‘-H), 5.07–5.22 (m, 2H, 1‘‘‘-H), 6.91 (d, *J* = 8.4 Hz, 2H, 6-H, 8-H), 7.10 (d, *J* = 8.4 Hz, 2H, 5-H, 9-H), 7.27–7.47 (m, 10H, 3‘‘-H bis 5‘‘-H und 3‘‘‘-H bis 5‘‘‘-H) ppm.

^{13}C-NMR (101 MHz, $CDCl_3$): δ = 28.4 (C-3‘), 37.6 (C-3), 54.7 (C-2), 67.2 (C-1‘‘), 70.1 (C-1‘‘‘), 80.0 (C-2‘), 115.0, 127.6, 128.1, 128.3, 128.6, 128.7, 128.7, 130.5, 135.4, 137.2 (Ar-C’s), 155.2 (C-7), 158.0 (C-1’), 171.9 (C-1) ppm.

The spectroscopic data match the literature data.[8]

(*S*)-3-(4-(Benzyloxy)phenyl)-2-((*tert*-butoxycarbonyl)amino)propanoic acid (S6-T)

The benzyl ester **S5-T** (6.04 g, 13.1 mmol) was dissolved in THF (33 mL) and treated with 2 M sodium hydroxide solution. The reaction was stirred at rt for 19 h, then the pH value was adjusted to pH = 2 with 1 M HCl. After extraction with Et_2O (3 x 40 mL) the combined organic phases were dried over Na_2SO_4, filtered and the solvent was evaporated under reduced pressure. After filtration over silica gel and Celite® (PE / EtOAc 10 : 1 ,then EtOAc) **S6-T** (3.05 g, 8.21 mmol, 63%) was obtained as colorless solid. Due to the free carboxylic acid, not all byproducts could be separated.



$C_{21}H_{25}NO_5$
371.43

S6-T

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.42 (s, 9H, 3‘-H), 2.95–3.18 (m, 2H, 3-H), 4.47–4.62 (m, 1H, 2-H), 4.95 (d, *J* = 7.8 Hz, 1H, 2-NH), 5.03 (s, 2H, 1‘‘-H), 6.92 (d, *J* = 8.4 Hz, 2H, 6-H, 8-H), 7.10 (d, *J* = 8.4 Hz, 2H, 5-H, 9-H), 7.28–7.44 (m, 5H, 3‘‘-H bis 5‘‘-H), 8.91 (s broad, 1H, COOH) ppm.

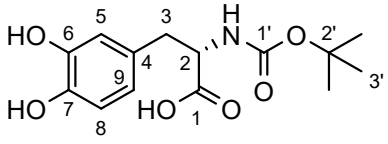
^{13}C-NMR (101 MHz, $CDCl_3$): δ = 28.4 (C-3‘), 37.1 (C-3), 54.6 (C-2), 70.2 (C-1‘‘), 80.5 (C-2‘), 115.1, 127.2, 127.6, 128.1, 128.7, 130.6, 137.1 (Ar-C’s), 155.6 (C-7), 158.1 (C-1‘), 176.5 (C-1) ppm.

The spectroscopic data match the literature data (DMSO-d_6,) small deviations are caused by the solvent.[9]

2.3 DOPA derivatives

(*S*)-2-((*tert*-Butoxycarbonyl)amino)-3-(3,4-dihydroxyphenyl)propanoic acid (19b-D)

Water (60 mL) und THF (120 mL) were degassed with N_2 for 10 min. Then $NaHCO_3$ (8.56 g, 101.9 mmol) and L-DOPA **18b** (10.0 g, 50.9 mmol) were suspended in the mixture. Afterwards, Boc_2O (12.2 g, 55.7 mmol) was added and the flask closed with a septum. The reaction was stirred for 25 h at rt. Then the pH value was adjusted to pH = 2 with concentrated hydrochloric acid and the mixture was extracted with EtOAc (3 x 200 mL). The combined organic phases were dried over Na_2SO_4, filtered and the solvent evaporated under reduced pressure. The product **19b-D** (15.2 g, 50.5 mmol, quant) was obtained as slightly yellow foam.



$C_{14}H_{19}NO_6$
297.31

19b-D

^{1}H-NMR (400 MHz, CD_3OD): δ = 1.40 (s, 9H, 3'-H), 2.77 (dd, J = 13.9 Hz, 8.4 Hz, 1H, 3-H_a), 2.98 (dd, J = 13.9 Hz, 5.2 Hz, 1H, 3-H_b), 4.27 (dd, J = 8.4 Hz, 5.2 Hz, 1H, 2-H), 6.54 (dd, J = 8.0 Hz, 2.1 Hz, 1H, 8-H), 6.63–6.71 (m, 2H, 5-H, 9-H) ppm.

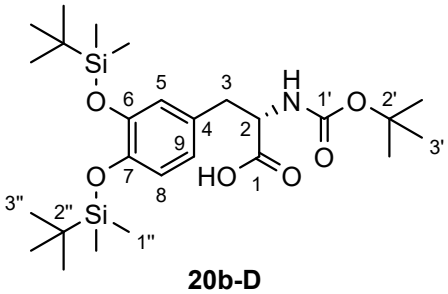
^{13}C-NMR (101 MHz, CD_3OD): δ = 27.6 (C-3'), 38.2 (C-3), 56.5 (C-2), 80.5 (C-2'), 116.3 (C-8), 117.4, 121.7 (C-5, C-9), 129.9 (C-4), 145.2, 146.2 (C-6, C-7), 157.8 (C-1'), 175.6 (C-1) ppm.

The spectroscopic data match the literature data (DMSO-d_6), small deviations are caused by the solvent.[10]

(*S*)-3-(3,4-Bis((*tert*-butyldimethylsilyl)oxy)phenyl)-2-((*tert*-butoxycarbonyl)-amino)propanoic acid (20b-D)

Boc-DOPA **19b-D** (5.32 g, 17.9 mmol) was dissolved in acetonitrile (91 mL) and degassed with N_2 for 10 min. Then imidazole (3.67 g, 53.9 mmol) and TBDMSCl (8,08 g, 53.6 mmol) were added, the flask closed with a septum and the reaction stirred for 42 h at rt. Afterwards, water (500 mL) was added and the pH value adjusted to pH = 3 with 1 M hydrochloric acid. The mixture was extracted with $CHCl_3$ (3 x 100 mL) and the combined organic phases were washed with saturated NaCl solution (1 x 100 mL). Then the organic phase was dried over Na_2SO_4, filtered and the solvent was removed under reduced pressure. The crude product was purified by column

chromatography (CH_2Cl_2 / MeOH 40 : 1, 10 : 1) and the product **20b-D** (4.03 g, 7.67 mmol, 43%) obtained as colorless oil. The silyl byproducts could not be separated fully by column chromatography.



$C_{26}H_{47}NO_6Si_2$
525.83

20b-D

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 0.14–0.30 (m, 12H, 1‘‘-H), 0.99 (dd, J = 10.8 Hz, 2.1 Hz, 18H, 3‘‘-H), 1.42 (s, 9H, 3‘-H), 2.72–3.17 (m, 2H, 3-H), 4.54 (s, 1H, 2-H), 4.90 (d, J = 8.3 Hz, 1H, 2-NH), 6.52–6.79 (m, 3H, 5-H, 8-H, 9-H) ppm.

^{13}C-NMR (101 MHz, $CDCl_3$): δ = -4.0, -3.9, -3.9 (C-1‘‘), 18.3, 18.6 (C-2‘‘), 26.1, 26.1 (C-3‘‘), 28.4 (C-3‘), 37.1 (C-3), 54.4 (C-2), 80.4 (C-2‘), 121.3 (C-8), 122.3, 122.4 (C-5, C-9), 128.9 (C-4), 146.2, 146.9 (C-6, C-7), 155.6 (C-1‘), 176.4 (C-1) ppm.

HRMS (ESI): m/z $[M-H]^-$ calculated for $C_{26}H_{47}NO_6Si_2$: 524.2869; found: 524.2870.

R_f = 0.5 (CH_2Cl_2 / MeOH 10 : 1, UV).

The spectroscopic data match the literature data.[11] The product was also confirmed via mass spectrometry.

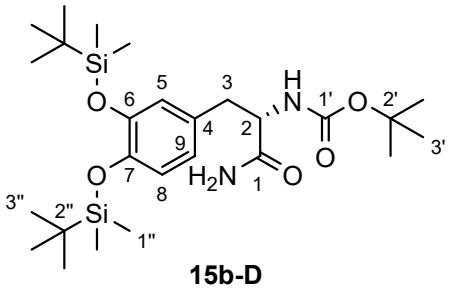
tert-Butyl-(*S*)-(1-amino-3-(3,4-bis((*tert*-butyldimethylsilyl)oxy)phenyl)-1-oxopropan-2-yl)carbamate (15b-D)

Synthesis according to **GP 1**:

Acid **20b-D** (10.4 g, 19.7 mmol), CH_2Cl_2 (72 mL), *N*-methylmorpholine (5.00 mL, 4.55 g, 45.0 mmol), isopropyl chloroformate (5.60 mL, 5.88 g, 43.1 mmol), concentrated ammonia solution (25%, 18.0 mL, 239.4 mmol), 21 h rt.

Extraction: Water (60 mL), then CH_2Cl_2 (3 x 100 mL)

Purification: Column chromatography (PE / EtOAc 1 : 1). Product **15b-D** (6.03 g, 11.5 mmol, 58%) obtained as colorless solid.



$C_{26}H_{48}N_2O_5Si_2$
524.85

15b-D

^{1}H-NMR (500 MHz, $CDCl_3$): δ = 0.16–0.20 (m, 12H, 1''-H), 0.97 (d, *J* = 4.3 Hz, 18H, 3''-H), 1.41 (s, 9H, 3'-H), 2.81–3.03 (m, 2H, 3-H), 4.29 (s, 1H, 2-H), 5.00 (s, 1H, 2-NH), 5.57 (s, 1H, 1-NH_aH), 5.89 (s, 1H, 1-NH_bH), 6.63–6.70 (m, 2H, 5-H, 9-H), 6.75 (d, *J* = 8.0 Hz, 1H, 8-H) ppm.

^{13}C-NMR (126 MHz, $CDCl_3$): δ = -4.0, -4.0, -3.9, -3.9 (C-1''), 18.5, 18.6 (C-2''), 26.1 (C-3''), 28.4 (C-3'), 37.6 (C-3), 55.5 (C-2), 80.3 (C-2'), 121.3 (C-8), 122.3, 122.4 (C-5, C-9), 129.6 (C-4), 146.1, 147.0 (C-6, C-7), 155.6 (C-1'), 174.0 (C-1) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 2956 (m), 2929 (m), 2897 (w), 2858 (m), 1673 (s), 1607 (w), 1577 (w), 1509 (vs), 1473 (m), 1463 (m), 1442 (w), 1420 (m), 1391 (m), 1367 (m), 1332 (w), 1293 (s), 1252 (vs), 1163 (s), 1128 (m), 1053 (w), 1020 (w), 983 (m), 908 (s), 836 (vs), 804 (m), 779 (vs), 734 (m), 696 (m), 667 (w), 647 (w), 620 (w), 561 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{26}H_{48}N_2O_5Si_2$: 525.3175; found: 525.3167.

$[\alpha]_D^{20}$ = + 7.7°·mL·dm^{-1}·g^{-1} (c = 0.287, $CHCl_3$).

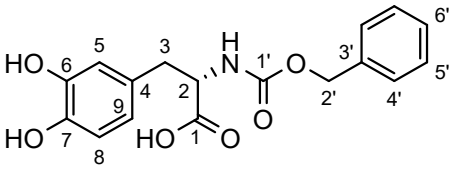
R_f = 0.42 (PE / EtOAc = 1 : 1, UV).

Mp. 140 °C.

(*S*)-2-(((Benzyloxy)carbonyl)amino)-3-(3,4-dihydroxyphenyl)propanoicacid (19d-D)

Potassium carbonate (7.05 g, 51.0 mmol) was added to a degassed (10 min, N_2) mixture of water (30 mL) and THF (60 mL). The mixture was degassed for another 10 min, then L-DOPA **18b** (5.00 g, 25.4 mmol) was added. After the fast dropwise addition of CbzCl (4.40 mL, 5.37 g, 31.5 mmol), the reaction was stirred for 23 h under N_2 at rt. Then the pH value was adjusted to pH = 2 with concentrated hydrochloric acid and the mixture was extracted with EtOAc (3 x 100 mL). The combined organic phases were dried over Na_2SO_4 and filtered. After evaporation of the solvent under reduced pressure, a brown oil was obtained as crude product. After purification by Kugelrohr distillation (high vacuum 10^{-2} mbar, up to 90 °C, roughly 6 h, interrupted by freezing with liquid N_2) the product **19d-D** (4.00 g, 12.1 mmol, 48%) was obtained as brown

glass. Due to its high oxygen sensitivity the product could not be synthesized completely pure.



$C_{17}H_{17}NO_6$
331.32

19d-D

^{1}H-NMR (700 MHz, $CDCl_3$): δ = 2.79 (dd, *J* = 14.0 Hz, 9.1 Hz, 1H, 3-H_a), 3.04 (dd, *J* = 14.0 Hz, 5.0 Hz, 1H, 3-H_b), 4.36 (dd, *J* = 9.1 Hz, 5.0 Hz, 1H, 2-H), 4.97–5.10 (m, 2H, 2‘-H), 6.54 (dd, *J* = 8.1 Hz, 2.2 Hz, 1H, 9-H), 6.62–6.71 (m, 2H, 5-H, 8-H), 7.22–7.38 (m, 5H, 4‘-H, 5‘-H, 6‘-H) ppm.

^{13}C-NMR (176 MHz, $CDCl_3$): δ = 38.1 (C-3), 57.0 (C-2), 67.5 (C-2‘), 116.3, 117.3 (C-5, C-8), 121.7 (C-9), 128.6, 128.9, 129.4 (C-4‘, C-5‘, C-6‘), 129.9 (C-4), 138.2 (C-3‘), 145.2, 146.2 (C-6, C-7), 158.4 (C-1‘), 175.4 (C-1) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3323 (m, br), 3064 (m), 3033 (m), 2958 (m), 2513 (w), 1693 (vs), 1607 (m), 1520 (s), 1442 (vs), 1348 (s), 1285 (vs), 1214 (s), 1116 (m), 1059 (m), 1026 (m), 973 (w), 814 (w), 775 (w), 738 (m), 698 (m) cm^{-1}.

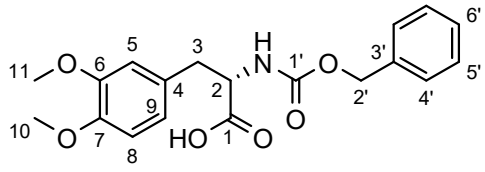
HRMS (ESI): m/z $[M-H]^-$ calculated for $C_{17}H_{17}NO_6$: 330.0983; found: 330.0969.

$[\alpha]_D^{20}$ = + 6.9°·mL·dm^{-1}·g^{-1} (c = 0.144, MeOH).

Mp. 172 °C.

(*S*)-2-(((Benzyloxy)carbonyl)amino)-3-(3,4-dimethoxyphenyl)propanoic acid (20d-D)

Cbz-DOPA **19d-D** (4.00 g, 12.1 mmol) was dissolved in DMF (49 mL) and degassed for 20 min. Potassium carbonate (6.68 g, 48.4 mmol) and iodomethane (3.20 mL, 7.30 g, 51.4 mmol) was added. The reaction was stirred for 18 h under N_2 at rt. Then 2 M sodium hydroxide solution (60 mL, 120 mmol) was added and the mixture stirred for an additional 6 h at rt. Afterwards, the pH value was adjusted to pH = 1 with concentrated hydrochloric acid and the mixture extracted with (3 x 150 mL). The combined organic phases were washed with water (6 x 100 mL) and dried over Na_2SO_4. After filtration and evaporation of the solvent under reduced pressure, the product **20d-D** (3.41 g, 9.48 mmol, 78%) was obtained as black oil.



$C_{19}H_{21}NO_6$
359.38

20d-D

^{1}H-NMR (700 MHz, $CDCl_3$): δ = 3.05 (dd, J = 14.3 Hz, 6.5 Hz, 1H, 3-H_a), 3.15 (dd, J = 14.3 Hz, 5.5 Hz, 1H, 3-H_b), 3.77 (s, 3H, 10-H/11-H), 3.84 (s, 3H, 10-H/11-H), 4.66 (q, J = 6.5 Hz, 1H, 2-H), 5.04–5.15 (m, 2H, 2‘-H), 5.20 (d, J = 8.1 Hz, 1H, 2-NH), 6.63–6.71 (m, 2H, 5-H, 9-H), 6.72–6.80 (m, 1H, 8-H), 7.29–7.37 (m, 5H, 4‘-H, 5‘-H, 6‘-H) ppm.

^{13}C-NMR (176 MHz, $CDCl_3$): δ = 37.5 (C-3), 54.8 (C-2), 55.9, 55.9 (C-10, C-11), 67.3 (C-2‘), 111.4, 112.4 (C-5, C-8), 121.5 (C-9), 127.9 (C-4), 128.3, 128.4, 128.7 (C-4‘, C-5‘, C-6‘), 136.2 (C-3‘), 148.3, 149.1 (C-6, C-7), 156.0 (C-1‘), 176.4 (C-1) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3323 (w), 3064 (w), 3033 (w), 2935 (m), 2837 (w), 1716 (vs), 1591 (w), 1516 (vs), 1454 (m), 1420 (m), 1344 (m), 1263 (vs), 1236 (vs), 1159 (m), 1142 (s), 1057 (m), 1028 (s), 912 (w), 734 (m), 698 (m) cm^{-1}.

HRMS (ESI): m/z $[M-H]^-$ calculated for $C_{19}H_{21}NO_6$: 358.1296; found: 358.1295.

$[\alpha]_D^{20}$ = + 20.6°·mL·dm^{-1}·g^{-1} (c = 0.243, $CHCl_3$).

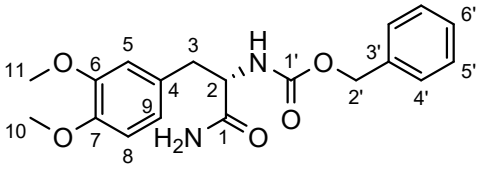
Benzyl (*S*)-(1-amino-3-(3,4-dimethoxyphenyl)-1-oxopropan-2-yl)carbamate (15d-D)

Synthesis according to **GP 1**:

Acid **20d-D** (3.45 g, 9.59 mmol), CH_2Cl_2 (35 mL), *N*-methylmorpholine (1.30 mL, 1.18 g, 11.7 mmol), isopropyl chloroformate (1.50 mL, 1.58 g, 11.5 mmol), concentrated ammonia solution (25%, 9.0 mL, 119.7 mmol), 23 h rt.

Extraction: Water (100 mL), then CH_2Cl_2 (3 x 100 mL)

Purification: Recrystallization in $CHCl_3$ (230 ml), residue recrystallized in MeOH (60 mL), product **15d-D** (1.67 g, 4.67 mmol, 49%) obtained as colorless solid.



$C_{19}H_{22}N_2O_5$
358.39

15d-D

^{1}H-NMR (500 MHz, $CDCl_3$): δ = 2.97 (dd, *J* = 14.1 Hz, 7.4 Hz, 1H, 3-H_a), 3.09 (dd, *J* = 14.1 Hz, 6.3 Hz, 1H, 3-H_b), 3.82 (s, 3H, 10-H/11-H), 3.85 (s, 3H, 10-H/11-H), 4.36–

4.46 (m, 1H, 2-H), 5.09 (d, *J* = 1.6 Hz, 2H, 2‘-H), 5.39 (s, 1H, 2-NH), 5.51 (s, 1H, 1-N*H*$_a$H), 5.74 (s, 1H, 1-N*H*$_b$H), 6.71–6.81 (m, 3H, 5-H, 8-H, 9-H), 7.27–7.39 (m, 5H, 4‘-H, 5‘-H, 6‘-H) ppm.

^{13}C-NMR (126 MHz, $CDCl_3$): δ = 38.2 (C-3), 56.0 (C-2, C-10, C-11), 67.3 (C-2‘), 111.4, 112.4 (C-5, C-8), 121.5 (C-9), 128.2, 128.4, 128.7 (C-4‘, C-5‘, C-6‘), 128.8 (C-4), 136.2 (C3‘), 148.3, 149.2 (C-6, C-7), 156.1 (C-1‘), 173.3 (C-1) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3394 (w), 3317 (m), 3201 (w), 1687 (s), 1660 (vs), 1624 (w), 1591 (w), 1536 (m), 1518 (s), 1465 (w), 1454 (m), 1440 (m), 1420 (m), 1320 (w), 1265 (s), 1238 (s), 1159 (m), 1140 (m), 1028 (m), 734 (m), 698 (m), 663 (w), 624 (w) cm^{-1}.

HRMS (ESI): m/z $[M+Na]^+$ calculated for $C_{19}H_{22}N_2O_5$: 381.1421; found: 381.1420.

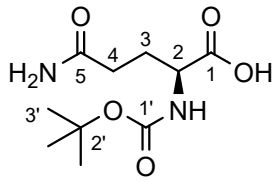
$[\alpha]_D^{20}$ = - 40.7°·mL·dm^{-1}·g^{-1} (c = 0.054, $CHCl_3$ / MeOH 1 : 1).

Mp. 205 °C

2.4 Diaminobutyric acid derivatives

(*tert*-Butoxycarbonyl)-L-glutamine (21)

L-Glutamine **17** (2.01 g, 13.7 mmol) was dissolved in water (30 mL) and THF (60 mL) and mixed with 1 M sodium hydroxide solution (29.0 mL, 29.0 mmol). Boc_2O (3.30 g, 15.1 mmol) was added and the reaction was stirred for 22 h at rt. Afterwards, the pH value was adjusted to pH = 2 with 1 M hydrochloric acid and the mixture extracted with EtOAc (3 x 20 mL). The combined organic phases were washed with saturated NaCl solution (1 x 25 mL), dried over Na_2SO_4 and filtered. After evaporation of the solvent under reduced pressure, **21** (2.26 g, 9.17 mmol, 67%) was obtained as colorless foam.



$C_{10}H_{18}N_2O_5$
246.26

21

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.44 (s, 9H, 3'-H), 2.00–2.27 (m, 2H, 3-H), 2.42 (s, 2H, 4-H), 4.18–4.37 (m, 1H, 2-H), 5.61 (d, J = 7.3 Hz, 1H, 2-NH), 6.40 (s, 1H, 5-NH_aH), 6.60 (s, 1H, 5-NH_bH) ppm.

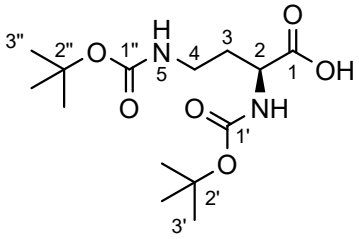
^{13}C-NMR (101 MHz, $CDCl_3$): δ = 28.4 (C-3'), 28.5 (C-3), 31.8 (C-4), 53.1 (C-2), 80.1 (C-2'), 156.2 (C-1'), 175.3 (C-1), 177.2 (C-5) ppm.

The spectroscopic data match the literature data[12]. Small deviations in the carbon NMR are caused by the solvent used in literature (DMSO-d_6).[13]

(*S*)-2,4-Bis((*tert*-butoxycarbonyl)amino)butanoic acid (22)

Sodium hydroxide (2.97 g, 74.3 mmol) was dissolved in water (30 mL) and cooled to 0 °C. Then bromine (0.68 mL, 2.12 g, 13.3 mmol) as added dropwise and the resulting mixture was stirred for 10 min at 0 °C. Boc-glutamine **21** (2.50 g, 10.2 mmol) was dissolved in 10% sodium hydroxide solution (16 mL, 40 mmol) and afterwards added to the bromine solution. The reaction was then stirred for another 20 min at 0 °C and then heated to 80 °C for 2 h. After cooling to 0 °C, the mixture was neutralized with 1 M hydrochloric acid. Then the pH value was adjusted to pH = 10 with 1 M sodium hydroxide solution, warmed to rt and Boc_2O (2.50 g, 11.5 mmol) dissolved in 1,4-dioxane (15 mL) was added. The reaction was stirred for 24 h at rt, then the pH value was adjusted to pH = 2 with concentrated hydrochloric acid. The mixture was extracted with EtOAc (3 x 20 mL) and the combined organic phases were washed with saturated

NaCl solution (1 x 30 mL). Afterwards, the organic phase was dried over Na_2SO_4, filtered and the solvent evaporated under reduced pressure. The crude product was purified by column chromatography (PE / EtOAc = 3 : 1, anisaldehyde staining solution for TLC). Product **22** (1.43 g, 4.48 mmol, 44%) was obtained as colorless foam.



$C_{14}H_{26}N_2O_6$
318.37

22

^{1}H-NMR (700 MHz, $CDCl_3$): δ = 1.34–1.57 (m, 18H, 3'-H, 3''-H), 1.75–2.35 (m, 2H, 3-H), 2.93–3.53 (m, 2H, 4-H), 4.28–4.40 (m, 1H, 2-H), 5.16–5.55 (m, 1H, NH), 6.68 (s, 1H, NH) ppm.

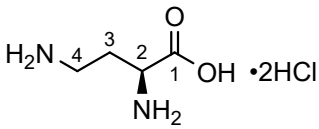
^{13}C-NMR (176 MHz, $CDCl_3$): δ = 28.4 (C-3''), 28.5 (C-3'), 31.5, 33.7 (C-3), 36.9 (C-4), 51.0, 51.2 (C-2), 80.1, 81.6 (C-2'', C-2'), 155.4, 156.0 (C-1''), 157.0, 158.1 (C-1'), 175.4 (C-1) ppm.

HRMS (ESI): m/z $[M+Na]^+$ calculated for $C_{14}H_{26}N_2O_6$: 341.1683; found: 341.1681.

The ^{1}H NMR shows complex signal splitting due to rotamers. The spectroscopic data match the literature data and were confirmed via mass spectrometry.[14]

(*S*)-2,4-Diaminobutyric acid dihydrochloride (16·2HCl)

Concentrated hydrochloric acid (5.0 mL, 60.4 mmol) was added dropwise to **22** (1.95 g, 6.11 mmol) and the resulting mixture was stirred for 2 h at rt. After evaporation of the hydrochloric acid via water jet pump, the remaining solvent was evaporated under reduced pressure. The yellow crude product was treated with refluxing EtOH (10 mL), filtered and dried under reduced pressure. Product **16·2HCl** (983 mg, 5.15 mmol, 84%) was obtained as colorless platelets.



$C_4H_{12}Cl_2N_2O_2$
191.05

16•2HCl

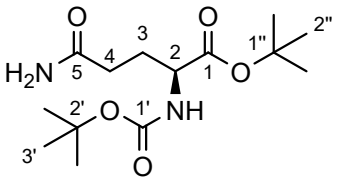
^{1}H-NMR (700 MHz, D_2O): δ = 2.20–2.27 (m, 1H, 3-H_a), 2.29–2.36 (m, 1H, 3-H_b), 3.16–3.23 (m, 1H, 4-H_a), 3.23–3.29 (m, 1H, 4-H_b), 4.14 (dd, *J* = 7.9 Hz, 5.7 Hz, 1H, 2-H) ppm.

^{13}C-NMR (176 MHz, D_2O): δ = 27.5 (t, C-3), 36.1 (t, C-4), 50.6 (d, C-2), 170.9 (C-1) ppm.

The spectroscopic data match the literature data.[15]

tert-Butyl (*tert*-butoxycarbonyl)-L-glutaminate (S7)

Boc-glutamine **21** (3.25 g, 13.2 mmol) was dissolved in acetonitrile (44 mL) and mixed with potassium carbonate (9.13 g, 66.1 mmol) and benzyltriethylammonium chloride (2.26 g, 9.93 mmol). The mixture was stirred for 2 h at rt, then *tert*-butyl bromide (8.90 mL, 10.9 g, 79.3 mmol) was added. The reaction was stirred at 50 °C for 21 h, then diluted with water (200 mL). The mixture was extracted with EtOAc (3 x 150 mL) and the combined organic phases were washed with water (1 x 100 mL). Afterwards the organic phase was dried over Na_2SO_4, filtered and the solvent was evaporated under reduced pressure. After recrystallization in PE / EtOAc (1.5 mL : 1.5 mL), the product **S7** (2.13 g, 7.05 mmol, 53%) was obtained as colorless solid.



$C_{14}H_{26}N_2O_5$
302.37

S7

^{1}H-NMR (500 MHz, $CDCl_3$): δ = 1.45 (s, 9H, 3'-H), 1.47 (s, 9H, 2''-H), 1.82–1.93 (m, 1H, 3-H_a), 2.11–2.21 (m, 1H, 3-H_b), 2.24–2.39 (m, 2H, 4-H), 4.19 (s, 1H, 2-H), 5.33 (d, J = 8.0 Hz, 1H, 2-NH), 5.69–5.86 (m, 1H, 5-NH_aH), 6.39 (s, 1H, 5-NH_bH) ppm.

^{13}C-NMR (126 MHz, $CDCl_3$): δ = 28.1 (C-2''), 28.4 (C-3'), 29.6 (C-3), 32.2 (C-4), 53.5 (C-2), 80.1 (C-2'), 82.5 (C-1''), 156.1 (C-1'), 171.5 (C-1), 174.9 (C-5) ppm.

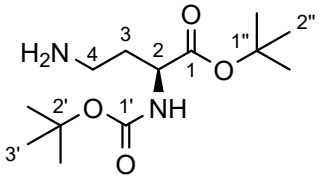
The spectroscopic data match the literature data.[16]

tert-Butyl (*S*)-4-amino-2-((*tert*-butoxycarbonyl)amino)butanoate (S8)

Phenyliodine(III) diacetate (PIDA) was synthesized according to literature and used without recrystallization.[17]

Amino acid **S7** (3.16 g, 10.5 mmol) was dissolved in water (7 mL) and THF (29 mL; THF : H_2O 4 : 1) and cooled to 0 °C. PIDA (4.05 g, 12.6 mmol) was added and the reaction was stirred for 6 h at 0 °C. Afterwards, the solvent was evaporated under reduced pressure and the remaining oily mixture was diluted with water (20 mL). The pH value was adjusted to pH = 1 with 1 M hydrochloric acid and the mix washed with

EtOAc (2 x 20 mL). Then the pH value was adjusted to pH = 11 with 1 M sodium hydroxide solution and the mixture was extracted with EtOAc (3 x 45 mL). The combined organic phases were washed with saturated NaCl solution (1 x 90 mL), dried over Na_2SO_4, filtered and the solvent was evaporated under reduced pressure. The product **S8** (1.23 g, 4.47 mmol, 43%) was obtained as colorless oil and was used without further purification.



$C_{13}H_{26}N_2O_4$
274.36

S8

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.44 (s, 9H, 3‘-H), 1.47 (s, 9H, 2‘‘-H), 1.68–1.81 (m, 1H, 3-H_a), 1.86–2.01 (m, 1H, 3-H_b), 2.83 (s, 2H, 4-H), 4.25 (s, 1H, 2-H), 5.54 (s, 1H, 2-NH) ppm.

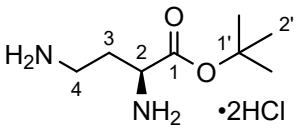
^{13}C-NMR (101 MHz, $CDCl_3$): δ = 27.9 (C-2’’), 28.3 (C-3’), 35.8 (C-3), 38.1 (C-4), 52.1 (C-2), 79.6 (C-2’), 81.8 (C-1’’), 155.7 (C-1’), 171.9 (C-1) ppm.

The spectroscopic data match the literature data.[18]

tert-Butyl (*S*)-2,4-diaminobutanoate dihydrochloride (S9·2HCl)

The used HCl in EtOAc was freshly prepared by adding concentrated sulfuric acid (10 mL) dropwise to NaCl (12 g) and bubbling the resulting gas through EtOAc (40 mL).

The boc protected amino acid **S8** (853 mg, 3.11 mmol) was mixed with freshly prepared HCl in EtOAc (40 mL) and stirred for 3 h at rt. Then the HCl and solvent were evaporated via water jet pump. The crude product was dissolved in refluxing EtOH (4 mL) and crystallized by adding diethyl ether (8 mL). After decanting of the solvent and washing with additional diethyl ether, product **S9·2HCl** (359 mg, 1.45 mmol, 47%) was obtained as a slightly yellow solid.



$C_8H_{20}Cl_2N_2O_2$
247.16

S9•2HCl

^{1}H-NMR (500 MHz, D_2O): δ = 1.54 (s, 9H, 2‘-H), 2.20–2.32 (m, 1H, 3-H_a), 2.32–2.42 (m, 1H, 3-H_b), 3.18–3.33 (m, 2H, 4-H), 4.17 (dd, J = 8.2 Hz, 5.5 Hz, 1H, 2-H) ppm.

^{13}C-NMR (126 MHz, D_2O): δ = 27.0 (C-2‘), 27.6 (C-3), 36.0 (C-4), 50.8 (C-2), 86.5 (C-1‘), 167.6 (C-1) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 2978 (vs, br), 2925 (vs), 1738 (vs), 1599 (m), 1499 (m), 1395 (m), 1371 (s), 1287 (m), 1250 (m), 1157 (vs), 840 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_8H_{18}N_2O_2$: 175.1441; found: 175.1438.

$[\alpha]_D^{20}$ = 10.1°·mL·dm^{-1}·g^{-1} (c = 1.007, H_2O).

Mp. 142 °C.

2.5 Ferribactin pre-chromophore derivatives

(*S*)-2-((*S*)-1-((*tert*-butoxycarbonyl)amino)-2-(4-((*tert*-butyldiphenylsilyl)oxy)phenyl)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (14a-T)

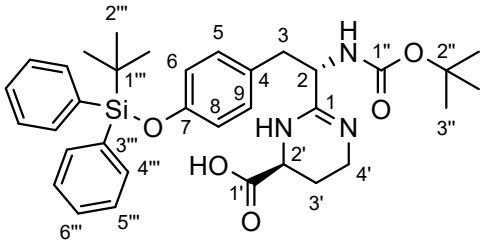
Synthesis according to **GP 2**:

Amide **15a-T** (2.16 g, 4.16 mmol), MeOTf (0.71 mL, 1.03 g, 6.27 mmol) in CH_2Cl_2 (45 mL), 3 h reflux, 21.5 h rt.

EtOH (28 mL), DABA **16·2HCl** (0.80 mg, 4.18 mmol), 10 min rt, *i*Pr_2EtN (2.60 mL, 1.93 mg, 14.9 mmol), 19.5 h reflux.

Purification: Column chromatography (CH_2Cl_2 / MeOH 7 : 1, 5 : 1). Slightly impure product **14a-T** (2.34 g, 3.89 mmol, 93%) obtained as colorless solid.

For NMR measurements and additional biological testing, the product was recrystallized several times (20 mL EtOAc, then 40 mL EtOAc / MeOH 1 : 1, then 5 mL EtOAc / MeOH 1 : 1), so 35 mg (1.4%) completely pure product were obtained.



$C_{34}H_{43}N_3O_5Si$
601.82

14a-T

^{1}H-NMR (700 MHz, CD_3OD): δ = 1.07 (s, 9H, 2‘‘‘-H), 1.37 (s, 9H, 3‘‘-H), 1.88 (s, 1H, 3‘-H_a), 2.05 (s, 1H, 3‘-H_b), 2.94 (d, *J* = 8.2 Hz, 2H, 3-H), 3.15 (s, 1H, 4‘-H_a), 3.86 (s, 1H, 2‘-H), 4.38 (s, 1H, 2-H), 6.71 (d, *J* = 8.1 Hz, 2H, 5-H, 9-H), 7.05 (d, *J* = 8.1 Hz, 2H, 6-H, 8-H), 7.35–7.41 (m, 4H, 5‘‘‘-H), 7.41–7.48 (m, 2H, 6‘‘‘-H), 7.65–7.75 (m, 4H, 4‘‘‘-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 13.1, 17.3, 18.7, 20.1 (C-1‘‘‘), 22.8 (C-3‘), 26.9 (C-2‘‘‘), 28.5 (C-3‘‘), 38.6 (C-3), 38.9, 43.7, 54.4 (C-2‘), 55.8 (C-2), 81.4, 120.9 (C-5, C-9), 128.9, 128.9 (C-5‘‘‘), 129.3 (C-4), 131.2 (C-6‘‘‘), 131.4 (C-6, C-8), 133.9, 133.9 (C-3‘‘‘), 136.6, 136.6 (C-4‘‘‘), 156.2 (C-7), 157.2, 164.5 (C-1), 174.9 (C-1‘) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3239 (m, br), 3072 (w), 2960 (m), 2931 (m), 2893 (m), 2858 (m), 1689 (m), 1654 (s), 1607 (vs), 1509 (vs), 1473 (m), 1442 (m), 1428 (s), 1389 (vs), 1367 (s), 1306 (s), 1252 (vs), 1167 (s), 1112 (s), 1048 (w), 1016 (w), 918 (s), 822 (s), 779 (w), 743 (m), 700 (vs), 636 (m), 610 (s), 502 (s) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{34}H_{43}N_3O_5Si$: 602.3045; found: 602.3069.

$[\alpha]_D^{20}$ = + 36.7°·mL·dm^{-1}·g^{-1} (c = 0.109, MeOH).

R_f = 0.18 (CH_2Cl_2 / MeOH 7 : 1, UV).

Mp. 208 °C (decomposition).

(*S*)-2-((*S*)-1-(3-((*tert*-Butoxycarbonyl)amino)propanamido)-2-(4-((*tert*-butyldiphenylsilyl)oxy)phenyl)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (23a-T)

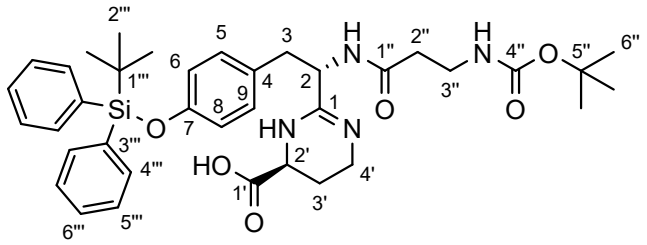
Synthesis according to **GP 3**.

Activation of the acid: Boc-β-alanine **S2** (126 mg, 665 µmol), EDC·HCl (128 mg, 668 µmol), HOBt·H_2O (104 mg, 679 µmol) in CH_2Cl_2 (3.4 mL) 1.5 h RT. Then *N*-methylmorphine (1.10 ml, 1.00 g, 9.90 mmol).

Deprotection: Ferribactin pre-chromophore derivative **14a-T** (401 mg, 666 µmol) in CH_2Cl_2 (5.0 mL), TFA (0.52 mL, 770 mg, 6.75 mmol) 4 h rt.

Coupling: Deprotected derivative dissolved and added in CH_2Cl_2 (3.6 mL), 16 h rt.

Purification: Column chromatography (Silicycle F60 silica gel, CH_2Cl_2 / MeOH 10 : 1 to CH_2Cl_2 / MeOH 3 : 1). Product **23a-T** (370 mg, 550 µmol, 83%) obtained as colorless solid.



$C_{37}H_{48}N_4O_6Si$
672.90

23a-T

^{1}H-NMR (700 MHz, CD_3OD): δ = 1.07 (d, *J* = 2.6 Hz, 9H, 2‘‘‘-H), 1.41 (s, 9H, 6‘‘-H), 1.86–1.98 (m, 1H, 3‘-H_a), 1.99–2.08 (m, 1H, 3‘-H_b), 2.31–2.43 (m, 2H, 2‘‘-H), 2.99 (dd, *J* = 14.3 Hz, 9.4 Hz, 0.4H, 3-H minor), 3.03 (d, *J* = 8.0 Hz, 1H, 3-H, major), 3.08 (dd, *J* = 14.3 Hz, 6.0 Hz, 0.4H, 3-H minor), 3.13 (m, 1H, 4‘-H_a), 3.22 (q, *J* = 7.1 Hz, 2H, 3‘‘-H), 3.26–3.30 (m, 1H, 4‘-H_b), 3.86 (t, *J* = 5.5 Hz, 0.6H, 2‘-H major), 3.94 (t, *J* = 5.5 Hz, 0.4H, 2‘-H minor), 4.59 (t, *J* = 8.0 Hz, 0.6H, 2-H major), 4.67 (dd, *J* = 9.0 Hz, 6.0 Hz, 0.4H, 2-H minor), 6.67–6.75 (m, 2H, 5-H, 9-H), 7.05 (m, 2H, 6-H, 8-H), 7.38 (m, 4H, 5‘‘‘-H), 7.44 (m, 2H, 6‘‘‘-H), 7.64–7.73 (m, 4H, 4‘‘‘-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 20.1 (C-1‘‘‘), 22.7, 22.8 (C-3‘), 26.9 (C-2‘‘‘), 28.8 (C-6‘‘), 36.9, 37.0 (C-3‘‘), 37.6 (C-2‘‘), 37.7, 37.8 (C-3), 38.0, 38.8 (C-4‘), 54.5 (C-2), 54.7 (C-2‘), 80.2 (C-5‘‘), 120.9, 121.0 (C-5, C-9), 128.9 (C-5‘‘‘), 129.2 (C-4), 131.2, 131.2

(C-6‘‘‘), 131.4 (C-6, C-8), 133.8, 133.9 (C-3‘‘‘), 136.6, 136.6 (C-4‘‘‘), 156.2 (C-7), 158.3 (C-4‘‘), 163.8, 163.9 (C-1), 174.5, 174.6 (C-1‘‘), 175.0 (C-1‘) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3400 (s, br), 3072 (w), 2960 (m), 2931 (m), 2858 (m), 2503 (s), 1652 (vs), 1607 (vs), 1510 (vs), 1428 (vs), 1393 (vs), 1365 (s), 1310 (s), 1255 (vs), 1171 (s), 1114 (vs), 1067 (w), 973 (m), 918 (s), 822 (m), 743 (w), 700 (vs), 636 (w), 610 (m), 500 (vs) cm−1.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{37}H_{48}N_4O_6Si$: 673.3416; found: 673.3415.

$[\alpha]_D^{20}$ = + 37.5°·mL·dm^{-1}·g^{-1} (c = 0.096, MeOH).

R_f = 0.81 (CH_2Cl_2 / MeOH 3 : 1, UV).

Mp. 160 °C (decomposition).

(*S*)-2-((*S*)-2-(4-((*tert*-Butyldiphenylsilyl)oxy)phenyl)-1-(3-methacrylamidopropanamido)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (13a-T)

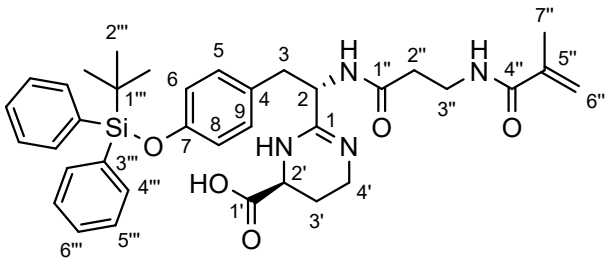
Synthesis according to **GP 3**.

Activation of the acid: Methacrylic acid (0.05 mL, 51 mg, 592 µmol), EDC·HCl (101 mg, 527 µmol), HOBt·H_2O (87 mg, 568 µmol) in CH_2Cl_2 (2.8 mL) 2 h rt. Then *N*-methylmorpholine (0.88 ml, 801 mg, 7.92 mmol).

Deprotection: Ferribactin pre-chromophore derivative **23a-T** (353 mg, 525 µmol) in CH_2Cl_2 (4.0 mL), TFA (0.41 mL, 606 mg, 5.32 mmol) 4 h rt.

Coupling: Deprotected derivative dissolved and added in CH_2Cl_2 (2.8 mL), 19 h rt.

Purification: Column chromatography (Silicycle F60 silica gel, CH_2Cl_2 / MeOH 5 : 1 to CH_2Cl_2 / MeOH 3 : 1). Product **13a-T** (315 mg, 492 µmol, 80%) obtained as colorless solid.



$C_{36}H_{44}N_4O_5Si$
640.86

13a-T

^{1}H-NMR (700 MHz, CD_3OD, $CDCl_3$): δ = 1.05 (s, 9H, 2‘‘‘-H), 1.85–1.91 (m, 5H, 3‘-H, 7‘‘-H), 2.39–2.46 (m, 1H, 2‘‘-H_a), 2.48–2.55 (m, 1H, 2‘‘-H_b), 2.94–3.04 (m, 2H, 3-H), 3.07 (dt, *J* = 13.2 Hz, 6.3 Hz, 1H, 4‘-H_a), 3.21–3.30 (m, 1H, 4‘-H_b), 3.40 (ddt, J = 20.0

Hz, 13.2 Hz, 6.8 Hz, 1H, 3‘‘-H_a), 3.56 (dt, J = 13.2 Hz, 6.8 Hz, 1H, 3‘‘-H_b), 3.76 (t, *J* = 5.4 Hz, 1H, 2‘-H), 4.57 (t, *J* = 8.1 Hz, 1H, 2-H), 5.32 (s, 1H, 6‘‘-H_a), 5.71 (s, 1H, 6‘‘-H_b), 6.66–6.72 (m, 2H, 5-H, 9-H), 6.94–7.01 (m, 2H, 6-H, 8-H), 7.32–7.36 (m, 4H, 5‘‘‘-H), 7.36–7.43 (m, 2H, 6‘‘‘-H), 7.64–7.69 (m, 4H, 4‘‘‘-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD, $CDCl_3$): δ =18.6 (C-7‘‘), 19.5, 19.9 (C-1‘‘‘), 22.1 (C-3‘), 26.8 (C-2‘‘‘), 36.0 (C-2‘‘), 36.2 (C-3‘‘), 37.5 (C-3), 38.2 (C-4‘), 53.9 (C-2‘), 54.5 (C-2), 120.6 (C-5, C-9), 121.4 (C-6‘‘), 128.1 (C-4), 128.5 (C-5‘‘‘), 130.7 (C-6‘‘‘), 130.7, 130.8 (C-6, C-8), 133.3, 133.3 (C-3‘‘‘), 136.1, 136.2 (C-4‘‘‘), 139.9 (C-5‘‘), 155.8 (C-7), 163.3 (C-1), 170.5 (C-4‘‘), 174.3 (C-1‘‘), 174.4 (C-1‘) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3270 (m, br), 3070 (m), 3048 (m), 3029 (m), 2999 (m), 2956 (m), 2931 (m), 2905 (m), 2893 (m), 2858 (m), 1652 (vs), 1605 (vs), 1542 (s), 1509 (vs), 1428 (s), 1391 (s), 1308 (s), 1255 (vs), 1222 (m), 1204 (m), 1136 (w), 1112 (s), 916 (s), 822 (m), 743 (m), 700 (vs), 636 (m), 610 (s), 543 (m), 502 (vs) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{36}H_{44}N_4O_5Si$: 641.3154; found: 641.3141.

$[\alpha]_D^{20}$ = + 28.6°·mL·dm^{-1}·g^{-1} (c = 0.133, MeOH).

R_f = 0.45 (CH_2Cl_2 / MeOH 5 : 1, UV).

Mp. 145 °C (decomposition).

(*S*)-2-((*S*)-2-(3,4-Bis((*tert*-butyldimethylsilyl)oxy)phenyl)-1-((*tert*-butoxycarbonyl)amino)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (14b-D)

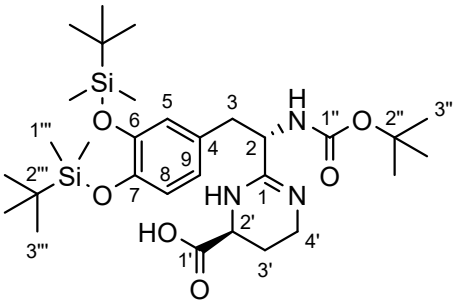
Synthesis according to **GP 2**:

Amide **15b-D** (3.66 g, 6.98 mmol), MeOTf (1.20 mL, 1.74 g, 10.6 mmol) in CH_2Cl_2 (70 mL), 1 h reflux, 26 h rt.

EtOH (47 mL), DABA **16·2HCl** (1.33 g, 6.98 mmol), 10 min rt, *i*Pr_2EtN (4.40 mL, 3.26 g, 25.3 mmol), 22 h reflux.

Purification: Column chromatography (CH_2Cl_2 / MeOH 7 : 1, 3 : 1). Slightly impure product **14b-D** (2.51 g, 4.13 mmol, 59%) obtained as colorless solid.

For NMR measurements and additional biological testing the product was recrystallized in $CHCl_3$ / MeOH 1 : 1 (400 mL), so 1.15 g completely pure product (27%) were obtained.



$C_{30}H_{53}N_3O_6Si_2$
607.94

14b-D

^{1}H-NMR (700 MHz, CD_3OD, $CDCl_3$): δ = 0.17 (dd, *J* = 9.7 Hz, 6.4 Hz, 12H, 1'''-H), 0.96 (d, *J* = 14.0 Hz, 18H, 3'''-H), 1.36 (s, 9H, 3''-H), 1.94–2.05 (m, 1H, 3'-H_a), 2.16–2.24 (m, 1H, 3'-H_b), 2.84 (dd, *J* = 14.0 Hz, 10.2 Hz, 1H, 3-H_a), 2.99 (dd, *J* = 14.0 Hz, 5.7 Hz, 1H, 3-H_b), 3.32–3.35 (m, 1H, 4'-H_a), 3.36–3.41 (m, 1H, 4'-H_b), 3.91 (t, *J* = 5.9 Hz, 1H, 2'-H), 4.45 (dd, *J* = 9.9 Hz, 5.8 Hz, 1H, 2-H), 6.69–6.75 (m, 2H, 5-H, 9-H), 6.78 (d, *J* = 8.1 Hz, 1H, 8-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD, $CDCl_3$): δ = -3.9, -3.9, -3.8, -3.8 (C-1'''), 18.9, 19.0 (C-2'''), 22.4, (C-3') 26.3, 26.3 (C-3'''), 28.5 (C-3''), 38.4 (C-3), 38.8 (C-4'), 53.9 (C-2'), 54.7 (C-2), 81.3 (C-2''), 121.9 (C-8), 122.8, 123.0 (C-5, C-9), 129.2 (C-4), 147.0, 147.5 (C-6, C-7), 156.5 (C-1''), 164.1 (C-1), 173.8 (C-1') ppm.

FT-IR (ATR): $\tilde{\nu}$ = 2929 (m), 2858 (w), 2374 (w), 2136 (w), 1962 (w), 1665 (vs), 1634 (m), 1609 (s), 1510 (s), 1487 (w), 1473 (m), 1450 (w), 1389 (s), 1332 (w), 1301 (s), 1283 (m), 1271 (s), 1263 (m), 1252 (s), 1193 (w), 1163 (s), 987 (m), 906 (s), 885 (w), 840 (vs), 814 (w), 779 (s), 671 (m), 545 (w), 455 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{30}H_{53}N_3O_6Si_2$: 608.3546; found: 608.3528.

$[\alpha]_D^{20}$ = + 40.8°·mL·dm^{-1}·g^{-1} (c = 0.103, $CHCl_3$ / MeOH 1 : 1 + 3% concentrated hydrochloric acid).

R_f = 0.53 (CH_2Cl_2 / MeOH 7 : 1, UV).

Mp. 210 °C (decomposition).

(*S*)-2-((*S*)-2-(3,4-Bis((*tert*-butyldimethylsilyl)oxy)phenyl)-1-(3-((*tert*-butoxycarbonyl)amino)propanamido)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (23b-D)

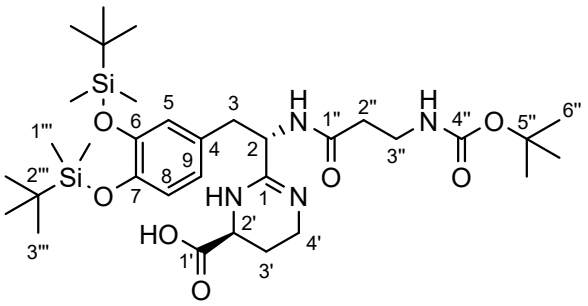
Synthesis according to **GP 3**.

Activation of the acid: Boc-β-alanine **S2** (233 mg, 1.23 mmol), EDC·HCl (235 mg, 1.23 mmol), HOBt·H_2O (190 mg, 1.24 mmol) in CH_2Cl_2 (6 mL) 3.5 h rt. Then *N*-methylmorphine (0.44 ml, 400 mg, 3.96 mmol).

Deprotection: Ferribactin pre-chromophore derivative **14b-D** (746 mg, 1.23 mmol) in CH_2Cl_2 (5 mL), TFA (0.95 mL, 1.41 g, 12.3 mmol) 4 h rt.

Coupling: Deprotected derivative dissolved and added in CH_2Cl_2 (6 mL), 18.5 h rt.

Purification: Column chromatography (Silicycle F60 silica gel, CH_2Cl_2 / MeOH 10 : 1 to CH_2Cl_2 / MeOH 3 : 1). Product **23b-D** (352 mg, 518 µmol, 42%) obtained as colorless solid.



$C_{33}H_{58}N_4O_7Si_2$
679.02

23b-D

^{1}H-NMR (700 MHz, CD_3OD, $CDCl_3$): δ = 0.17–0.23 (m, 12H, 1'''-H), 0.99 (dd, *J* = 12.6 Hz, 2.3 Hz, 12H, 3'''-H), 1.42 (s, 9H, 6''-H), 2.04 (dq, *J* = 14.1 Hz, 4.4 Hz, 3.0 Hz, 1H, 3'-H_a), 2.13 (tt, *J* = 9.1 Hz, 4.4 Hz, 1H, 3'-H_b), 2.32–2.43 (m, 2H, 2''-H), 2.99 (dd, *J* = 14.1 Hz, 9.4 Hz, 1H, 3-H_a), 3.10 (dd, *J* = 14.1 Hz, 6.5 Hz, 1H, 3-H_b), 3.18–3.28 (m, 2H, 3''-H), 3.34–3.39 (m, 1H, 4'-H_a), 3.39–3.45 (m, 1H, 4'-H_b), 3.96 (t, *J* = 4.4 Hz, 1H, 2'-H), 4.72 (dd, *J* = 9.4 Hz, 6.5 Hz, 1H, 2-H), 6.58–6.90 (m, 3H, 5-H, 8-H, 9-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD, $CDCl_3$): δ = -3.8, -3.8, -3.7, -3.7 (C-1'''), 19.3, 19.4 (C-2'''), 22.8 (C-3'), 26.5, 26.5 (C-3'''), 28.8 (C-6''), 37.1 (C-2''), 37.6 (C-3''), 38.0 (C-3), 39.0 (C-4'), 54.2 (C-2), 54.6 (C-2'), 80.3 (C-5''), 122.4, 123.1, 123.7 (C-5, C-8, C-9), 130.1 (C-4), 147.6, 148.2 (C-6, C-7), 158.4 (C-4''), 164.0 (C-1), 174.5 (C-1''), 174.9 (C-1') ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3382 (s, br), 2929 (m), 2856 (m), 2489 (vs, br), 2248 (m), 2075 (m), 1654 (m), 1609 (m), 1509 (m), 1424 (s), 1367 (m), 1299 (m), 1252 (m), 1220 (m), 1161 (m), 1118 (s), 971 (vs), 904 (w), 838 (m), 781 (m), 496 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{33}H_{58}N_4O_7Si_2$: 679.3917; found: 679.3918.

$[\alpha]_D^{20}$ = + 29.2°·mL·dm^{-1}·g^{-1} (c = 0.137, $CHCl_3$ / MeOH 1 : 1).

R_f = 0.45 (CH_2Cl_2 / MeOH 3 : 1, UV).

Mp. 135 °C (decomposition).

(*S*)-2-((*S*)-2-(3,4-bis((*tert*-butyldimethylsilyl)oxy)phenyl)-1-(3-methacrylamidopropanamido)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (13b-D)

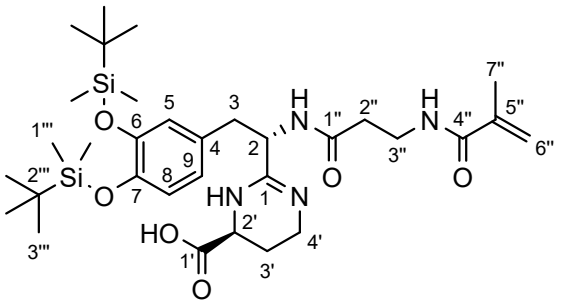
Synthesis according to **GP 3**.

Activation of the acid: Methacrylic acid (0.04 mL, 40.8 mg, 474 µmol), EDC·HCl (82.3 mg, 429 µmol), HOBt·H_2O (66.3 mg, 433 µmol) in CH_2Cl_2 (2.2 mL) 2 h rt. Then *N*-methylmorphine (0.72 ml, 655 mg, 6.48 mmol).

Deprotection: Ferribactin pre-chromophore derivative **23b-D** (291 mg, 429 µmol) in CH_2Cl_2 (1.6 mL), TFA (0.33 mL, 488 mg, 4.28 mmol) 2 h rt.

Coupling: Deprotected derivative dissolved and added in CH_2Cl_2 (2.2 mL), 16 h rt.

Purification: Column chromatography (Silicycle F60 silica gel, CH_2Cl_2 / MeOH 5 : 1 to CH_2Cl_2 / MeOH 3 : 1). Product **13b-D** (137 mg, 212 µmol, 49%) obtained as colorless solid.



$C_{32}H_{54}N_4O_6Si_2$
646.98

13b-D

^{1}H-NMR (700 MHz, CD_3OD): δ = 0.20 (dd, *J* = 6.8 Hz, 5.5 Hz, 12H, 1'''-H), 0.99 (dd, *J* = 11.3 Hz, 1.6 Hz, 18H, 3'''-H), 1.89–1.92 (m, 3H, 7''-H), 1.98–2.08 (m, 1H, 3'-H_a), 2.10–2.20 (m, 1H, 3'-H_b), 2.37–2.50 (m, 2H, 2''-H), 2.97 (ddd, *J* = 22.6 Hz, 14.2 Hz, 9.8 Hz, 1H, 3-H_a), 3.13 (ddd, *J* = 33.5 Hz, 14.2 Hz, 5.8 Hz, 1H, 3-H_b), 3.37 (td, *J* = 7.3 Hz, 5.0 Hz, 2H, 4'-H), 3.39–3.48 (m, 2H, 3''-H), 3.92–4.01 (m, 1H, 2'-H), 4.73 (ddd, *J* = 14.2 Hz, 9.8 Hz, 5.8 Hz, 1H, 2-H), 5.33–5.39 (m, 1H, 6''-H_a), 5.65–5.71 (m, 1H, 6''-H_b), 6.61–6.97 (m, 3H, 5-H, 8-H, 9-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = -3.8, -3.8, -3.8, -3.7 (C-1'''), 18.8 (C-7''), 19.3, 19.4 (C-2'''), 22.9 (C-3'), 26.5, 26.5 (C3'''), 36.4 (C-2''), 37.1 (C-3''), 37.8 (C-3), 39.2 (C-4'), 54.1 (C-2), 54.7 (C-2'), 120.8 (C-6''), 122.4, 123.0, 123.5 (C-5, C-8, C-9), 130.2 (C-4), 141.0 (C-5''), 147.5, 148.2 (C-6, C-7), 164.0 (C-1), 171.1 (C-4''), 174.6 (C-1''), 174.9 (C-1') ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3366 (vs, br), 2954 (m), 2929 (s), 2858 (m), 2480 (vs, br), 2238 (m), 2217 (m), 2181 (w), 2170 (w), 2148 (w), 2111 (w), 2075 (m), 1652 (vs), 1607 (vs), 1509

(s), 1461 (vs), 1391 (s), 1301 (s), 1255 (s), 1220 (m), 1161 (m), 1118 (s), 973 (vs), 908 (m), 838 (s), 802 (m), 779 (s), 694 (m), 575 (m), 524 (m), 463 (w), 447 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{32}H_{54}N_4O_6Si_2$: 647.3655; found: 647.3643.

$[\alpha]_D^{20}$ = + 42.2°·mL·dm^{-1}·g^{-1} (c = 0.109, MeOH).

R_f = 0.68 (CH_2Cl_2 / MeOH 3 : 1, UV, $KMnO_4$ staining solution).

Mp. 132 °C (decomposition).

(*S*)-2-((*S*)-1-(((Benzyloxy)carbonyl)amino)-2-(4-methoxyphenyl)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (14c-T)

Synthesis according to **GP 2**:

Amide **15c-T** (1.91 g, 5.80 mmol), MeOTf (0.80 mL, 1.16 g, 7.07 mmol) in $CHCl_3$ (58 mL), 3 h reflux, 19 h rt.

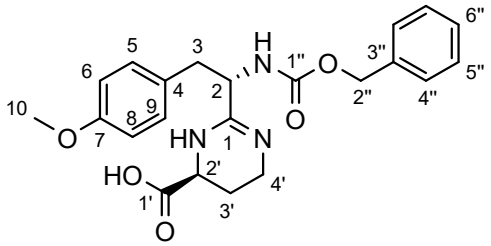
EtOH (40 mL), DABA **16·2HCl** (1.11 g, 5.82 mmol), 10 min RT, *i*Pr_2EtN (3.60 mL, 2.67 g, 20.7 mmol), 21 h reflux.

Purification: Column chromatography (CH_2Cl_2 / MeOH 5 : 1). Slightly impure product **14c-T** (1.75 g, 4.25 mmol, 73%) obtained as colorless solid.

Alternative Synthesis:

The amide **15c-T** (172 mg, 532 nmol) was dissolved in dry CH_2Cl_2 (3 mL) under N_2 and freshly opened Et_3OBF_4 (1 M in CH_2Cl_2; 0.78 mL, 785 nmol) was added. The reaction was stirred at reflux for 2 h, then the solvent was evaporated under reduced pressure. The residue was dissolved in dry MeOH (5 mL) and DABA **16·2HCl** (100 mg, 523 nmol) and distilled and dried *i*Pr_2EtN (0.22 mL, 169 mg, 1.31 mmol) was added. The reaction was stirred at reflux for 18 h. The crude product was purified by column chromatography (CH_2Cl_2 / MeOH 5 : 1) with dry loading on silica. Product **14c-T** (32 mg, 77.8 nmol, 15%) was obtained as yellow oil.

All material data for **14c-T** were obtained by product synthesized according to **GP 2**.



$C_{22}H_{25}N_3O_5$
411.46

14c-T

^{1}H-NMR (700 MHz, CD_3OD): δ = 1.96–2.05 (m, 1H, 3‘-H_a), 2.06–2.15 (m, 1H, 3‘-H_b), 3.02 (dd, *J* = 14.0 Hz, 8.2 Hz, 1H, 3-H_a), 3.10 (dd, *J* = 14.0 Hz, 7.0 Hz, 1H, 3-H_b), 3.23–3.29 (m, 1H, 4‘-H_a), 3.34–3.41 (m, 1H, 4‘-H_b), 3.89–3.96 (m, 1H, 2‘-H), 4.53 (t, *J* = 8.2 Hz, 1H, 2-H), 5.02 (d, *J* = 12.5 Hz, 1H, 2‘‘-H_a), 5.08 (d, *J* = 12.5 Hz, 1H, 2‘‘-H_b), 6.85 (d, *J* = 8.3 Hz 2H, 6-H, 8-H), 7.23 (d, *J* = 8.3 Hz, 2H, 5-H, 9-H), 7.25–7.36 (m, 5H, 4‘‘-H, 5‘‘-H, 6‘‘-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 22.8 (C-3‘), 38.4 (C-3), 38.9 (C-4‘), 54.6 (C-2‘), 55.6 (C-10), 56.4 (C-2), 68.0 (C-2‘‘), 115.1 (C-6, C-8), 128.5 (C-4), 128.9, 129.2, 129.5 (C-4‘‘, C-5‘‘, C-6‘‘), 131.6 (C-5, C-9), 137.8 (C-3‘‘), 158.0 (C-1‘‘), 160.5 (C-7), 164.3 (C-1), 175.1 (C-1‘) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3360 (m, br), 2468 (s, br), 2244 (m), 2221 (m), 2073 (s), 1611 (w), 1514 (w), 1120 (s), 1089 (m), 971 (vs), 824 (w), 483 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{22}H_{25}N_3O_5$: 412.1867; found: 412.1872.

$[\alpha]_D^{20}$ = + 77.7°·mL·dm^{-1}·g^{-1} (c = 0.103, MeOH + 3% concentrated hydrochloric acid).

R_f = 0.35 (CH_2Cl_2 / MeOH 5 : 1, UV).

Mp. 206 °C (decomposition).

(*S*)-2-((*S*)-1-(3-((*tert*-butoxycarbonyl)amino)propanamido)-2-(4-methoxyphenyl)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (23c-T)

Synthesis according to **GP 3** (under N_2).

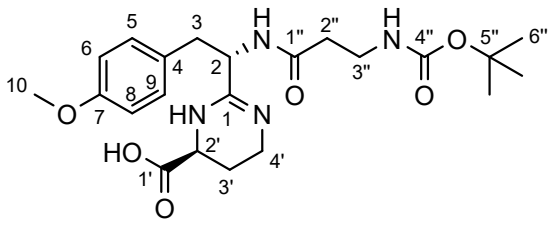
Activation of the acid: Boc-β-alanine **S2** (442 mg, 2.34 mmol), EDC·HCl (446 mg, 2.33 mmol), HOBt·H_2O (356 mg, 2.32 mmol) in dry DMF (12 mL) 2.5 h RT. Then *N*-methylmorphine (6.6 ml, 6.01 g, 59.4 mmol).

Deprotection: Ferribactin pre-chromophore derivative **14c-T** (958 mg, 2.33 mmol) in 6 M hydrochloric acid (16.0 mL, 3.50 g, 96.0 mmol) 6 h 100 °C.

Coupling: Deprotected derivative dissolved and added in dry DMF (12 mL), 16 h rt.

Purification: Washed with CH_2Cl_2, product remains in water phase. Multiple column chromatographies (Silicycle F60 silica gel, CH_2Cl_2 / MeOH 5 : 1, CH_2Cl_2 / MeOH 3 : 1).

Product **23c-T** (51 mg, 113 µmol, 5%) obtained as slightly yellow solid.



$C_{22}H_{32}N_4O_6$
448.52

23c-T

^{1}H-NMR (700 MHz, CD_3OD): δ = 1.43 (s, 9H, 6‘‘-H), 1.91–1.98 (m, 1H, 3‘-H_a), 2.10–2.17 (m, 1H, 3‘-H_b), 2.45–2.56 (m, 2H, 2‘‘-H), 3.09 (dd, *J* = 13.9 Hz, 8.1 Hz, 1H, 3-H_a), 3.18 (dd, *J* = 13.9 Hz, 8.1 Hz, 1H, 3-H_b), 3.22 (td, *J* = 9.5 Hz, 4.8 Hz, 1H, 4‘-H_a), 3.27 (dt, *J* = 13.6 Hz, 6.5 Hz, 1H, 3‘‘-H_a), 3.34–3.40 (m, 1H, 3‘‘-H_b), 3.44 (dtd, *J* = 13.7 Hz, 4.8 Hz, 1.4 Hz, 1H, 4‘-H_b), 3.76 (s, 3H, 10-H), 3.88–3.94 (m, 1H, 2‘-H), 4.65 (t, *J* = 8.1 Hz, 1H, 2-H), 6.88 (d, *J* = 8.6 Hz, 2H, 6-H, 8-H), 7.26 (d, *J* = 8.6 Hz, 2H, 5-H, 9-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 22.5 (C-3‘), 28.8 (C-6‘‘), 37.0 (C-3‘‘), 37.3 (C-2‘‘), 37.8 (C-3), 38.4 (C-4‘), 54.3 (C-2‘), 55.6 (C-2), 55.7 (C-10), 80.7 (C-5‘‘), 115.1 (C-6, C-8), 128.0 (C-4), 131.6 (C-5, C-9), 158.7 (C-4‘‘), 160.5 (C-7), 164.0 (C-1), 175.4 (C-1‘‘), 176.0 (C-1‘) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3345 (w), 2472 (m), 2244 (w), 2221 (w), 2070 (m), 1120 (s), 1091 (m), 971 (vs) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{22}H_{32}N_4O_6$: 449.2395; found: 449.2385.

$[\alpha]_D^{20}$ = + 52.1°·mL·dm^{-1}·g^{-1} (c = 0.119, MeOH).

R_f = 0.40 (CH_2Cl_2 / MeOH 3 : 1, UV, $KMnO_4$ staining solution).

Mp. 100 °C (decomposition).

(*S*)-2-((*S*)-1-(3-methacrylamidopropanamido)-2-(4-methoxyphenyl)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (13c-T)

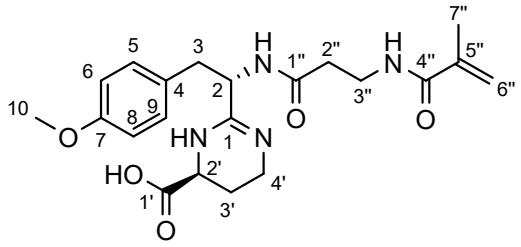
Synthesis according to **GP 3** (under N_2).

Activation of the acid: Methacrylic acid (0.04 mL, 40.8 mg, 474 µmol), EDC·HCl (84.3 mg, 439 µmol), HOBt·H_2O (65.3 mg, 426 µmol) in CH_2Cl_2 (2.2 mL) 2 h rt. Then *N*-Methylmorpholin (0.72 ml, 655 mg, 6.48 mmol).

Deprotection: Ferribactin pre-chromophore derivative **23c-T** (193 mg, 430 µmol) in CH_2Cl_2 (1.0 mL), TFA (1.0 mL, 1.48 g, 13.0 mmol) 2 h rt.

Coupling: Deprotected derivative dissolved and added in CH_2Cl_2 (2.2 mL) and DMF (1.0 mL), 23 h rt.

Purification: Washed with CH_2Cl_2, product remains in water phase. Column chromatography (Silicycle F60 silica gel, CH_2Cl_2 / MeOH 3 : 1), washed with CH_2Cl_2 (25 mL). Product **13c-T** (122 mg, 292 µmol, 68 %) obtained as colorless solid.



$C_{21}H_{28}N_4O_5$
416.48

13c-T

^{1}H-NMR (700 MHz, CD_3OD): δ = 1.90 (s, 1H, 7‘‘-H minor), 1.91 (s, 2H, 7‘‘-H major), 1.94–2.05 (m, 1H, 3‘-H_a), 2.07–2.18 (m, 1H, 3‘-H_b), 2.41–2.52 (m, 2H, 2‘‘-H), 3.00–3.09 (m, 1H, 3-H_a), 3.09–3.19 (m, 1H, 3-H_b), 3.22–3.29 (m, 1H, 4‘-H_a), 3.32–3.40 (m, 1H, 4‘-H_b), 3.41–3.48 (m, 2H, 3‘‘-H), 3.76 (s, 2H, 10-H major), 3.77 (s, 1H, 10-H minor), 3.94 (t, *J* = 5.6 Hz, 0.7H, 2‘-H major), 3.98 (dd, *J* = 7.0 Hz, 4.9 Hz, 0.3H, 2‘-H minor), 4.66 (t, *J* = 7.9 Hz, 0.7H, 2-H major), 4.72 (dd, *J* = 9.3 Hz, 5.8 Hz, 0.3H, 2-H minor), 5.35–5.38 (m, 1H, 6‘‘-H_a), 5.67 (s, 1H, 6‘‘-H_b), 6.87 (dd, *J* = 8.5 Hz, 6.5 Hz, 2H, 6-H, 8-H), 7.23 (dd, *J* = 12.3 Hz, 8.5 Hz, 2H, 5-H, 9-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 18.7 (C-7‘‘), 22.8 (C-3‘), 36.3, 36.3 (C-2‘‘), 36.9 (C-3‘‘), 38.0 (C-3), 38.9 (C-4‘), 54.5, 54.6 (C-2‘), 54.7, 54.8 (C-2), 55.6, 55.7 (C-10), 115.1, 115.1 (C-6, C-8), 120.8, 120.8 (C-6‘‘), 128.5 (C-4), 131.3, 131.5 (C-5, C-9), 141.0, 141.1 (C-5‘‘), 160.5 (C-7), 163.9 (C-1), 171.1 (C-4‘‘), 174.4 (C-1‘‘), 175.2 (C-1‘) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3268 (m, br), 2925 (m), 2854 (m), 2480 (w, br), 1654 (vs), 1609 (vs), 1546 (s), 1514 (vs), 1442 (s), 1395 (s), 1306 (m), 1248 (s), 1181 (m), 1032 (w), 592 (w), 555 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{21}H_{28}N_4O_5$: 417.2132; found: 417.2121.

$[\alpha]_D^{20}$ = + 70.4°·mL·dm^{-1}·g^{-1} (c = 0.108, MeOH).

R_f = 0.48 (CH_2Cl_2 / MeOH 3 : 1, UV).

Mp. 115 °C (decomposition); color change at 70 °C.

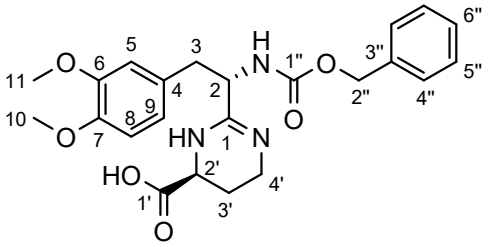
(*S*)-2-((*S*)-1-(((Benzyloxy)carbonyl)amino)-2-(3,4-dimethoxyphenyl)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (14d-D)

Synthesis according to **GP 2**:

Amide **15d-D** (729 mg, 2.03 mmol), MeOTf (0.33 mL, 479 mg, 2.92 mmol) in $CHCl_3$ (20 mL), 3 h reflux, 20 h rt.

EtOH (14 mL), DABA **16·2HCl** (390 mg, 2.04 mmol), 10 min RT, *i*Pr_2EtN (1.30 mL, 965 mg, 7.46 mmol), 23 h reflux.

Purification: Column chromatography (CH_2Cl_2 / MeOH 5 : 1, then 3 : 1). Slightly impure product **14d-D** (363 mg, 0.82 mmol, 40%) obtained as colorless solid.



$C_{23}H_{27}N_3O_6$
441.48

14d-D

^{1}H-NMR (700 MHz, CD_3OD): δ = 1.95–2.06 (m, 1H, 3‘-H_a), 2.08–2.20 (m, 1H, 3‘-H_b), 2.94–3.05 (m, 1H, 3-H_a), 3.08–3.21 (m, 1H, 3-H_b), 3.24–3.30 (m, 1H, 4‘-H_a), 3.34–3.41 (m, 1H, 4‘-H_b), 3.79 (d, *J* = 6.3 Hz, 6H, 10-H, 11-H), 3.95 (t, *J* = 5.7 Hz, 0.5H, 2‘-H major), 4.00 (t, *J* = 5.7 Hz, 0.4H, 2‘-H minor), 4.58 (t, *J* = 7.4 Hz, 0.5H, 2-H major), 4.67 (dd, *J* = 9.4 Hz, 5.0 Hz, 0.4H, 2-H minor), 4.98 (dd, *J* = 26.9 Hz, 12.4 Hz, 1H, 2‘‘-H_a), 5.04–5.13 (m, 1H, 2‘‘-H_b), 6.82–6.89 (m, 2H, 5-H, 9-H), 6.94 (s, 1H, 8-H), 7.21–7.36 (m, 5H, 4‘‘-H, 5‘‘-H, 6‘‘-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 22.8, 22.9 (C-3‘), 38.8, 38.9 (C-3), 38.9, 39.1 (C-4‘), 54.6, 54.7 (C-2‘), 55.8, 55.9 (C-2), 56.4, 56.4, 56.5, 56.5 (C-10, C-11), 68.0, 68.1 (C-2‘‘), 113.0, 113.0 (C-5, C-9), 114.0, 114.1 (C-8), 122.9, 123.0 (C-5, C-9), 128.7, 128.8, 128.8, 128.9, 129.1, 129.4, 129.5 (C-4, C-4‘‘, C-5‘‘, C-6‘‘), 137.8, 137.8 (C-3‘‘), 149.8, 149.8, 150.5, 150.6 (C-6, C-7), 158.0 (C-1‘‘), 164.3, 164.4 (C-1), 175.0, 175.0 (C-1‘) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3241 (m, br), 2933 (m), 1709 (s), 1656 (s), 1607 (vs), 1516 (vs), 1442 (s), 1420 (s), 1393 (s), 1350 (s), 1310 (s), 1261 (vs), 1240 (vs), 1214 (m), 1159 (s), 1142 (s), 1026 (vs), 810 (w), 759 (m), 743 (m), 698 (m), 596 (w), 555 (w), 459 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{23}H_{27}N_3O_6$: 442.1973; found: 442.1978.

$[\alpha]_D^{20}$ = + 48.9°·mL·dm^{-1}·g^{-1} (c = 0.139, MeOH + 3% concentrated HCl).

R_f = 0.26 (CH_2Cl_2 / MeOH 3 : 1, UV).

Mp. 187 °C (decomposition).

(*S*)-2-((*S*)-1-(3-((*tert*-Butoxycarbonyl)amino)propanamido)-2-(3,4-dimethoxyphenyl)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (23d-D)

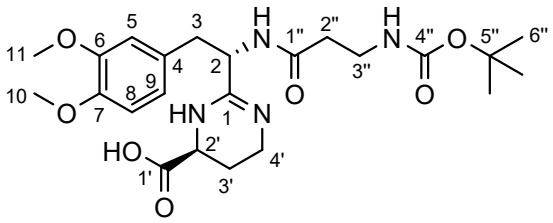
Synthesis according to **GP 3** (under N_2).

Activation of the acid: Boc-β-alanine **S2** (433 mg, 2.29 mmol), EDC·HCl (439 mg, 2.29 mmol), HOBt·H_2O (350 mg, 2.29 mmol) in dry DMF (12 mL) 1.5 h rt. Then *N*-methylmorphine (6.4 ml, 5.28 g, 57.6 mmol).

Deprotection: Ferribactin pre-chromophore derivative **14d-D** (1.00 g, 2.28 mmol) in 6 M hydrochloric acid (16.0 mL, 3.50 g, 96.0 mmol) 6 h 100 °C.

Coupling: Deprotected derivative dissolved and added in dry DMF (12 mL), 22 h rt.

Purification: Washed with CH_2Cl_2, product remains in water phase. Filtration over silica gel (Silicycle F60 silica gel) and Celite® (CH_2Cl_2 / MeOH 10 : 1 then CH_2Cl_2 / MeOH 5 : 1, then CH_2Cl_2 / MeOH 3 : 1). Product fraction mixed with 9 mL saturated Na_2CO_3 solution and 9 mL H_2O. Then washed with EtOAc (3 x 20 mL) and the aqueous phase dried under reduced pressure. The residue was treated with refluxing EtOH (100 mL) and washed with additional EtOH (50 mL). The ethanolic solution was dried under reduced pressure and the residue was treated with EtOAc (20 mL) overnight multiple times. After decanting and drying under reduced pressure, the product **23d-D** (380 mg, 794 µmol, 35%) was obtained as slightly orange foam.



$C_{23}H_{34}N_4O_7$
478.55

23d-D

^{1}H-NMR (700 MHz, CD_3OD): δ = 1.42 (s, 3H, 6''-H minor), 1.42 (s, 7H, 6''-H major), 1.95–2.04 (m, 1H, 3'-H_a), 2.07–2.17 (m, 1H, 3'-H_b), 2.36–2.44 (m, 2H, 2''-H), 3.00–3.08 (m, 1H, 3-H_a), 3.10–3.19 (m, 1H, 3-H_b), 3.19–3.29 (m, 2H, 3''-H), 3.33–3.41 (m, 2H, 4'-H), 3.80 (d, *J* = 3.7 Hz, 3H, 10-H), 3.84 (d, *J* = 3.9 Hz, 3H, 11-H), 3.91–3.95 (m, 0.6H, 2'-H major), 3.97 (dd, *J* = 6.9 Hz, 4.9 Hz, 0.4H, 2'-H minor), 4.66 (t, *J* = 7.9 Hz, 0.31H, major), 4.74 (dd, *J* = 9.1 Hz, 5.7 Hz, 0.25H minor), 6.79–7.02 (m, 3H, 5-H, 8-H, 9-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 23.0 (C-3‘), 28.7 (C-6‘‘), 37.0 (C-3‘‘), 37.6 (C-2‘‘), 38.6 (C-3), 39.3 (C-4‘), 54.5, 54.7 (C-2‘), 54.8, 54.9 (C-2), 56.4, 56.4 (C-11), 56.5, 56.6 (C-10), 80.2 (C-5‘‘), 113.0 (C-5, C-9), 114.0, 114.1(C-8), 122.8, 123.0 (C-5, C9), 129.5, 129.6 (C-4), 149.8, 149.8 (C-6, C-7), 150.5, 150.6 (C-6, C-7), 158.4 (C-4‘‘), 163.5, 163.6 (C-1), 174.4, 174.5 (C-1‘‘), 175.4 (C-1’) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3270 (m, br), 2974 (m), 2937 (m), 1654 (vs), 1611 (vs), 1516 (vs), 1442 (s), 1393 (vs), 1367 (s), 1308 (s), 1263 (vs), 1240 (vs), 1159 (vs), 1144 (s), 1026 (s), 804 (m), 763 (m), 620 (m), 555 (m), 463 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{23}H_{34}N_4O_7$: 479.2500; found: 479.2496.

$[\alpha]_D^{20}$ = + 66.7°·mL·dm^{-1}·g^{-1} (c = 0.114, MeOH).

R_f = 0.38 (CH_2Cl_2 / MeOH + Et_3N 3 : 1, UV).

Mp. 96 °C (decomposition).

(*S*)-2-((*S*)-2-(3,4-dimethoxyphenyl)-1-(3-methacrylamidopropanamido)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (13d-D)

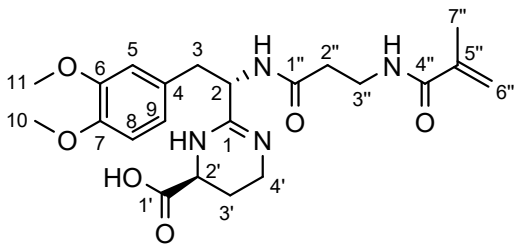
Synthesis according to **GP 3** (under N_2).

Activation of the acid: Methacrylic acid (0.06 mL, 61.2 mg, 711 µmol), EDC·HCl (133 mg, 694 µmol), HOBt·H_2O (105 mg, 686 µmol) in CH_2Cl_2 (3.5 mL) 1 h rt. Then *N*-methylmorphine (1.2 ml, 1.09 g, 10.8 mmol).

Deprotection: Ferribactin pre-chromophore derivative **23d-D** (329 mg, 688 µmol) in CH_2Cl_2 (1.0 mL) and MeOH (0.3 mL), TFA (1.0 mL, 1.48 g, 13.0 mmol) 2 h rt.

Coupling: Deprotected derivative dissolved and added in DMF (3.5 mL), 22 h rt.

Purification: Washed with CH_2Cl_2, product remains in water phase. Column chromatography (Silicycle F60 silica gel, CH_2Cl_2 / MeOH 3 : 1), Product **13d-D** (144 mg, 323 µmol, 47%) obtained as colorless glass.



$C_{22}H_{30}N_4O_6$
446.50

13d-D

^{1}H-NMR (700 MHz, CD_3OD): δ = 1.89 (s, 1.2H, 7‘‘-H minor), 1.90 (s, 1.8H, 7‘‘-H major), 1.98–2.18 (m, 2H, 3‘-H), 2.42–2.52 (m, 2H, 2‘‘-H), 2.99–3.21 (m, 2H, 3-H), 3.21–3.27 (m, 1H, 4‘-H_a), 3.34–3.41 (m, 1H, 4‘-H_b), 3.41 –3.48 (m, 2H, 3‘‘-H), 3.79 (d, *J* = 5.1 Hz, 3H, 10-H), 3.82 (d, *J* = 4.0 Hz, 3H, 11-H), 3.97 (t, *J* = 5.5 Hz, 0.6H, 2‘-H major), 4.01 (dd, *J* = 6.7 Hz, 5.0 Hz, 0.4H, 2‘-H minor), 4.67 (t, *J* = 8.0 Hz, 0.6H, 2-H major), 4.75 (dd, *J* = 9.4 Hz, 5.6 Hz, 0.4H, 2-H minor), 5.36 (t, *J* = 1.5 Hz, 0.4H, 6‘‘-H_a minor), 5.37 (t, *J* = 1.4 Hz, 0.6H, 6‘‘-H_a major), 5.67 (s, 0.4H, 6‘‘-H_b minor), 5.68 (s, 0.6H, 6‘‘-H_b major), 6.82–6.91 (m, 2H, 5-H, 9-H), 6.96 (dd, *J* = 6.4 Hz, 1.7 Hz, 1H, 8-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 18.8 (C-7‘‘), 22.7, 22.9 (C-3‘), 36.3, 36.3 (C-2‘‘), 36.9, 37.0 (C-3‘‘), 38.2, 38.5 (C-3), 38.8, 39.0 (C-4‘), 54.4, 54.6 (C-2‘), 54.9, 54.9 (C-2), 56.2, 56.2 (C-11), 56.4, 56.4 (C-10), 112.5, (C-5, C-9), 113.5, 113.8 (C-8), 120.9, (C-6‘‘), 122.7, 122.9, (C-5, C-9), 129.3, 129.4 (C-4), 140.9, 140.9 (C-5‘‘), 149.6, 149.7 (C-7), 150.3, 150.4 (C-6), 163.8, 164.0 (C-1), 171.0, 171.1 (C-4‘‘), 174.4, 174.6 (C-1‘‘), 175.2, 175.3 (C-1‘) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3245 (m, br), 2929 (m), 2478 (w), 1650 (vs), 1595 (vs), 1514 (vs), 1440 (vs), 1387 (vs), 1308 (s), 1261 (vs), 1238 (vs), 1208 (m), 1157 (s), 1142 (s), 1024 (s), 936 (w), 808 (m), 763 (m), 720 (w), 622 (m), 596 (m), 553 (m), 461 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{22}H_{30}N_4O_6$: 447.2238; found: 447.2230.

$[\alpha]_D^{20}$ = + 74.8°·mL·dm^{-1}·g^{-1} (c = 0.107, MeOH).

R_f = 0.07 (CH_2Cl_2 / MeOH 3 : 1, UV).

Mp. 120 °C (decomposition); color change at 70 °C.

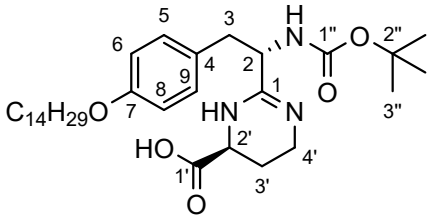
(*S*)-2-((*S*)-1-((*tert*-butoxycarbonyl)amino)-2-(4-(tetradecyloxy)phenyl)ethyl)-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid (S1a-T)

Synthesis according to **GP 2**:

Amide **S4b-T** (1.17 g, 2.45 mmol), MeOTf (0.42 mL, 609 mg, 3.71 mmol) in CH_2Cl_2 (25 mL), 3 h reflux, 19 h rt.

EtOH (17 mL), DABA **16·2HCl** (469 mg, 2.45 mmol), 10 min RT, *i*Pr_2EtN (1.50 mL, 1.11 g, 8.61 mmol), 20 h reflux.

Purification: Column chromatography (CH_2Cl_2 / MeOH 10 : 1, then 7 : 1). Product **S1a-T** (571 mg, 1.02 mmol, 42%) obtained as colorless solid.



$C_{32}H_{53}N_3O_5$
559.79

S1a-T

^{1}H-NMR (700 MHz, CD_3OD): δ = 0.90 (t, *J* = 7.0 Hz, 3H, Alkyl-H), 1.25–1.35 (m, 20H, Alkyl-H), 1.38 (s, 9H, 3''-H), 1.42–1.49 (m, 2H, Alkyl-H), 1.71–1.78 (m, 2H, Alkyl-H), 1.97–2.05 (m, 1H, 3'-H_a), 2.07–2.16 (m, 1H, 3'-H_b), 2.98 (dd, *J* = 14.0 Hz, 8.7 Hz, 1H, 3-H_a), 3.07 (dd, *J* = 14.0 Hz, 7.1 Hz, 1H, 3-H_b), 3.24–3.30 (m, 1H, 4'-H_a), 3.35–3.43 (m, 1H, 4'-H_b), 3.89–3.97 (m, 3H, 2'-H, Alkyl-H), 4.42–4.50 (m, 1H, 2-H), 6.85 (d, *J* = 8.1 Hz, 2H, 5-H, 9-H), 7.22 (d, *J* = 8.1 Hz, 2H, 6-H, 8-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 14.5 (Alkyl-C), 22.9 (C-3'), 23.7, 27.2 (Alkyl-C), 28.5 (C-3''), 30.4, 30.5, 30.5, 30.7, 30.8, 30.8, 31.2, 33.1 (Alkyl-C), 38.6 (C-4'), 38.9 (C-3), 54.6 (C-2'), 55.9 (C-2), 69.0 (Alkyl-C), 81.4 (C-2''), 115.7 (C-5, C-9), 128.5 (C-4), 131.6 (C-6, C-8), 157.2 (C-1''), 159.9 (C-7), 164.6 (C-1), 175.1 (C-1') ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3209 (w), 2919 (s), 2850 (s), 2352 (w), 2291 (w), 2256 (w), 2244 (w), 2203 (w), 2160 (w), 2119 (w), 2085 (w), 1667 (vs), 1656 (vs), 1611 (vs), 1514 (s), 1469 (m), 1383 (vs), 1369 (s), 1324 (m), 1308 (m), 1246 (s), 1171 (s), 1046 (m), 1024 (m), 997 (m), 881 (w), 828 (m), 789 (m), 720 (w), 659 (w), 604 (w), 575 (w), 536 (m) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{32}H_{53}N_3O_5$: 560.4058; found: 560.4059.

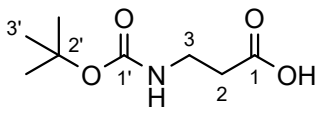
$[\alpha]_D^{20}$ = + 26.7°·mL·dm^{-1}·g^{-1} (c = 0.060, $CHCl_3$ / MeOH 1 : 1).

R_f = 0.15 (CH_2Cl_2 / MeOH 7 : 1, UV).

Mp. 202 °C (decomposition).

Boc-β-alanine (S2)

β-Alanine (2.5 g, 28.1 mmol), was dissolved in water (64 mL) and THF (130 mL), then 1 M NaOH solution (58.0 mL, 58.0 mmol) was added. Afterwards Boc_2O (6.84 g, 31.3 mmol) was added and the reaction stirred at rt for 17.5 h. The reaction mixture was washed with CH_2Cl_2 (1 x 50 mL). Then the pH value was adjusted to pH = 1 with 1 M hydrochloric acid. The mixture was extracted with EtOAc (3 x 1700 mL) and the combined organic phases were dried over Na_2SO_4 and filtered. After evaporation of the solvent under reduced pressure, **S2** (5.07 g, 26.8 mmol, 95%) was obtained as colorless solid.



$C_8H_{15}NO_4$
189.21

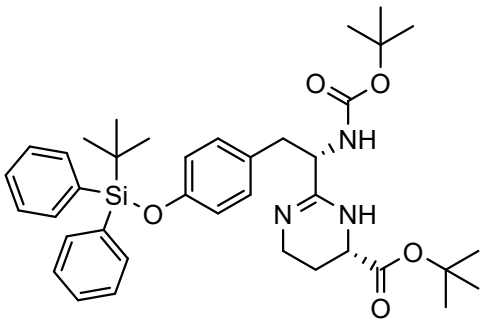
S2

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.44 (s, 9H, 3'-H), 2.46–2.61 (m, 2H, 3-H), 3.29–3.44 (m, 2H, 2-H), 5.12 (s, 0.6H, 3-NH major), 6.29 (s, 0.3H, 3-NH minor), 11.44 (s, 1H, COOH) ppm.

^{13}C-NMR (101 MHz, $CDCl_3$): δ = 28.5 (C-3'), 34.6, 36.0, 37.3 (C-2, C-3), 79.8, 81.3 (C-2'), 156.1, 157.7 (C-1'), 176.5, 177.6 (C-1) ppm.

Signal doubling occurs due to rotamers. The spectroscopic data match the literature data.[19]

Coupling attempt to S1b-T



$C_{38}H_{51}N_3O_5Si$
657.93

S1b-T

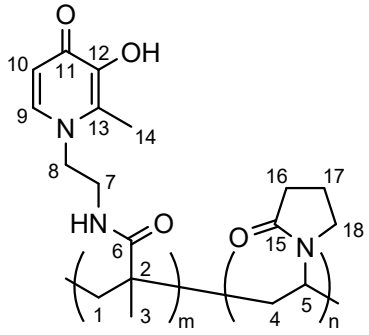
The *tert*-butyl protected DABA **S9** was used for the coupling reaction with **15a-T** too. The additional protecting group should decrease the polarity and increase the solubility in organic solvents. Indeed, the polarity in product **S1b-T** was decreased, leading to a mixture of product **S1b-T** (identified by MS) and side products that were not separable by column chromatography or crystallization, neither through extraction or washing.

2.6 Polymerization of the monomers

DIBI (MAHMP-NVP-copolymer, 10)

Synthesis according to **GP 4**.

N-[2-(3-hydroxy-2-methyl-4-oxopyridin-1(4H)-yl)ethyl]methacrylamide (MAHMP) **8** (150 mg, 634µmol), RAFT-agent **25** (22.7 mg, 109 µmol), NVP **9** (0.50 mL, 522 mg, 4.69 mmol), TMEDA (50 µL, 38.8 mg, 333 µmol) in water (2.0 mL), TBHP (70%, 60 µL, 55.8 mg, 433 µmol), 40 °C, 20 h. Purification as described in **GP 4**. Product **10** (573 mg, 83%) obtained as colorless solid.



10

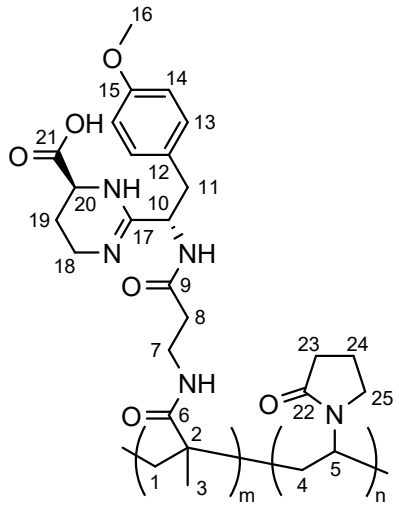
^{1}H-NMR (700 MHz, CD_3OD): δ = 1.19 (s, 20H, 3-H, overlap with MTBE), 1.43–1.93 (m, 18H, 1-H, 4-H), 1.94–2.12 (m, 17H, 17-H), 2.19–2.44 (m, 17H, 16-H), 2.45–2.54 (m, 3H, 14-H), 3.15–3.48 (m, 45H, 18-H overlap with MeOH), 3.54–4.00 (m, 9H, 5-H), 4.15 (s, 3H, 8-H), 6.40 (s, 1H, 9-H), 7.63 (s, 1H, 10-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 12.1 (C-14), 19.2 (C-17), 27.8 (C-2), 32.5 (C-16), 35.7, 36.6 (C-1, C-4), 43.4 (C-18), 45.4, 45.7, 46.7 (C-5), 53.9 (C-8), 112.5 (C-9), 124.4, 133.2 (C-13), 139.6 (C-10), 147.3 (C-12), 170.8 (C-11),177.9 (C-15) ppm.

Me-Tyr-ferribactin-pre-chromophore-monomer (29c-T)-NVP-copolymer (11c-T)

Synthesis according to **GP 4**.

Monomer **13c-T** (9.98 mg, 24.0 µmol), RAFT-agent **25** (0.83 mg, 3.98 µmol), NVP **9** (19.3 µL, 20.0 mg, 180 µmol), TMEDA (2.6 µL, 2.03 mg, 17.5 µmol) in water (150 µL), THBP (70%, 2.4 µL, 2.23 mg, 17.3 µmol), 40 °C, 19 h. Purification as described in **GP 4**. Product **11c-T** (20 mg, 65%) obtained as colorless solid.



11c-T

^{1}H-NMR (700 MHz, CD_3OD): δ = 1.43–1.92 (m, 19H, 1-H, 4-H), 1.93–2.16 (m, 20H, 24-H), 2.18–2.61 (m, 20H, 23-H), 3.00–3.51 (m, 35H, 25-H overlaps with MeOH), 3.67–4.20 (m, 11H, 5-H, 16-H, 20-H), 4.55–4.80 (m, 1H, 10-H), 6.87 (s, 2H, 14-H), 7.27 (s, 2H, 13-H) ppm.

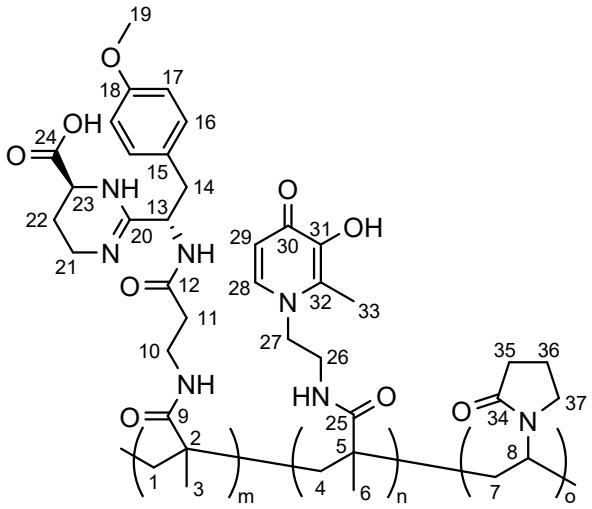
^{13}C-NMR (176 MHz, CD_3OD): δ = 19.2 (C-24), 32.5 (C-23), 35.5, 36.9, 37.0 (C-1, C-4), 43.3, 43.4, 43.5, 43.6 (C-25), 45.4, 45.5, 45.7 (C-5), 54.2 (C-10), 54.7 (C-20), 55.7 (C-16), 115.1, 115.2, 115.5 (C-14), 131.4, 131.8, 132.0 (C-13), 160.4 (C-15), 163.9 (C-17), 177.9, 177.9 (C-22) ppm.

Me-Tyr-ferribactin-pre-chromophore-monomer (29c-T)-MAHMP-NVP-copolymer (12c-T)

Monomer **13c-T** (10.7 mg, 25.7 µmol), MAHMP **8** (12.1 mg, 51.2 µmol), RAFT-agent **25** (2.8 mg, 13.4 µmol), NVP **9** (62.0 µL, 64.5 mg, 580 µmol), TMEDA (6.0 µL, 4.65 mg, 40.0 µmol) in water (260 µL), THBP (70%, 7.6 µL, 7.07 mg, 54.9 µmol), 40 °C, 20 h.

Purification as described in **GP 4**.

Product **12c-T** (63.9 mg, 71%) obtained as colorless solid.



12c-T

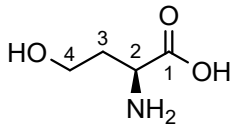
^{1}H-NMR (700 MHz, CD_3OD): δ = 1.39–1.92 (m, 46H, 1-H, 4-H, 7-H) 1.93–2.17 (m, 47H, 36-H) 2.17–2.45 (m, 43H, 35-H) 2.45–2.55 (m, 7H, 33-H) , 3.02–3.55 (m, 65H, 37-H, overlaps with MeOH), 3.55–4.07 (m, 25H, 8-H, 23-H), 4.07– 4.31 (m, 5H, 27-H), 4.65 (s, 1H, 13-H), 6.40 (s, 2H, 28-H), 6.87 (s, 2H, 17-H), 7.26 (s, 2H, 16-H), 7.64 (s, 2H, 29-H) ppm.

^{13}C-NMR (176 MHz, CD_3OD): δ = 12.1 (C-33), 19.2 (C-36), 32.5 (C-35), 35.5, 36.4, 36.7, 37.5 (C-1, C-4, C-7), 43.3 (C-37), 45.4, 45.7 (C-5), 53.8 (C-27), 54.5, 54.9 (C-13, C-23), 55.7 (C-19), 58.8 (C-23), 74.2, 93.7, 112.5, 112.9 (C-28), 115.1, 115.2 (C-17), 131.5 (C-16), 139.3, 139.5 (C-29), 147.2 (C-31), 160.4 (C-18), 164.0 (C-20), 170.7 (C-30), 177.9, 177.9 (C-34) ppm.

2.7 Homoserine derivatives

L-Homoserine (S10)

L-Methionine **S11** (25.0 g, 168 mmol) was suspended in water (470 mL) and MeOH (70 mL). Iodomethane (25.0 mL, 57.0 g, 402 mmol) was added and the mixture stirred at rt for 4 d. Then half of the solvent was evaporated under reduced pressure. After adding $NaHCO_3$ (14.1 g, 168 mmol) in water (24 mL), the reaction was refluxed for 18 h. Afterwards the solvent was evaporated under reduced pressure until an oily solution was obtained as crude product. The solution was added dropwise to a strongly stirred mixture of EtOH (700 mL) und acetone (90 mL). After all crude product was added, the mix was stirred additional 5 min, then rested 5 min. The obtained precipitate was filtered and dried. Homoserine **S10** (19.2 g, 161 mmol, 96%) was obtained as colorless powder.



$C_4H_9NO_3$
119.12

S10

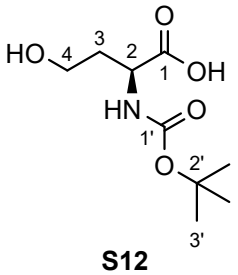
^{1}H-NMR (700 MHz, D_2O): δ = 1.97–2.06 (m, 1H, 3-H_a), 2.11–2.18 (m, 1H, 3-H_b), 3.72–3.81 (m, 2H, 4-H), 3.84 (dd, J = 7.6 Hz, 4.8 Hz, 1H, 2-H) ppm.

^{13}C-NMR (176 MHz, D_2O): δ = 32.1 (C-3), 53.4 (C-4), 58.6 (C-2), 174.4 (C-1) ppm.

The spectroscopic data match the literature data.[20]

(*tert*-Butoxycarbonyl)-L-homoserine (S12)

Homoserine **S10** (3.01 g, 25.2 mmol) was dissolved in water (57 mL), THF (115 mL) and 1 M NaOH solution (63.0 mL, 63.0 mmol). Boc_2O (6.07 g, 27.8 mmol) was added and the reaction stirred at rt for 19 h. Then the pH value was adjusted to pH = 2 with 1 M HCl and the mixture was extracted with CH_2Cl_2 (3 x 120 mL). The combined organic phases were dried over Na_2SO_4, filtered and the solvent evaporated under reduced pressure. The product **S12** (4.14 g, 18.9 mmol, 75%) was obtained as orange oil and used without further purification.



$C_9H_{17}NO_5$
219.24

S12

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.44 (s, 9H, 3‘-H), 1.78 (s, 3-H_a), 2.18 (s, 2H, 3-H_b), 3.65–3.85 (m, 2H, 4-Hz), 4.24 (ddd, J = 11.3 Hz, 9.3 Hz, 5.9 Hz, 1H, 2-H), 5.55 (d, J = 7.7 Hz, 1H, NH), 6.76 (s, 1H, OH) ppm.

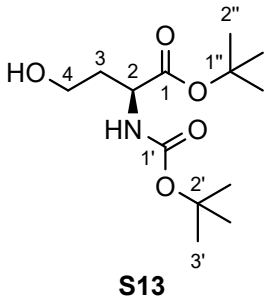
^{13}C-NMR (101 MHz, $CDCl_3$): δ = 28.4 (C-3‘), 35.5 (C-3), 50.8 (C-4), 58.6 (C-2), 80.7 (C-2‘), 156.7 (C-1‘), 175.5 (C-1) ppm.

The spectroscopic data match the literature data (Lit: DMSO-d_6), small deviations are caused by the solvent.[21]

***tert*-Butyl (*tert*-butoxycarbonyl)-L-homoserinate (S13)**

N,N’-diisopropyl-*O*-*tert*-butylisourea (DIC-O*t*Bu) was synthesized according to literature[22] and used without distillation.

The acid **S12** (3.13 g, 14.3 mmol) was dissolved in CH_2Cl_2 (72 mL) and treated with DIC-O*t*Bu (8.61 g, 43.0 mmol). The reaction was refluxed for 22 h and the precipitated solid was filtered out over Celite® and cotton. The now clear solvent was evaporated under reduced pressure and the crude product was purified by column chromatography (PE / EtOAc 2 : 1). Product **S13** (1.85 g, 6.72 mmol, 47%) was obtained as colorless oil.



$C_{13}H_{25}NO_5$
275.35

S13

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.45 (s, 9H, 3‘-H), 1.47 (s, 9H, 2‘‘-H), 1.52–1.67 (m, 1H, 3-H_a), 2.05–1.67 (m, 1H, 3-H_b), 3.56–3.76 (m, 2H, 4-H), 4.34 (ddd, *J* = 11.5 Hz, 7.9 Hz, 3.8 Hz, 1H, 2-H), 5.40 (d, *J* = 7.9 Hz, 1H, 2-NH) ppm.

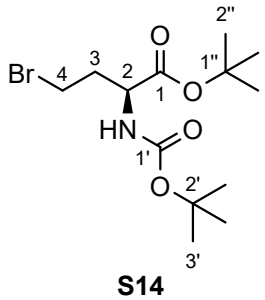
^{13}C-NMR (101 MHz, $CDCl_3$): δ = 28.0 (C-2‘‘), 28.3 (C-3‘), 36.5 (C-3), 51.1 (C-2), 58.4 (C-4), 80.3 (C-2‘), 82.3 (C-1‘‘), 156.7 (C1‘), 172.1 (C-1) ppm.

The spectroscopic data match the literature data.[23]

R_f = 0.29 (PE / EtOAc 2 : 1, anis aldehyde staining solution).

tert-Butyl-(*S*)-4-bromo-2-((*tert*-butoxycarbonyl)amino)butanoate (S14)

To the alcohol **S13** (1.09 g, 3.95 mmol) CBr_4 (1.31 g, 3.96 mmol) was added and both reactands were dissolved in CH_2Cl_2 (11 mL). After cooling to 0 °C, PPh_3 (1.05 g, 4.00 mmol) dissolved in CH_2Cl_2 (5 mL) was added dropwise. The flask was closed with a septum and the reaction stirred at rt for 3 h. Then the resulting solution was washed with water (1 x 15 mL) and saturated NaCl solution (1 x 15 mL). After drying over Na_2SO_4, filtration and evaporation of the solvent under reduced pressure, the crude product was obtained as yellow oil. Purification via filtration over silica gel and Celite® (PE / EtOAc 15 : 1) yielded the bromide **S14** (898 mg, 2.65 mmol, 67%) as colorless oil.



$C_{13}H_{24}BrNO_4$
338.24

S14

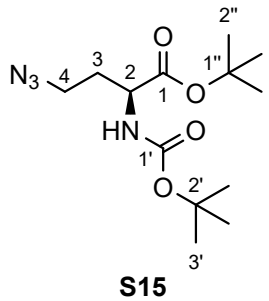
^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.45 (s, 9H, 3'-H), 1.47 (s, 9H, 2''-H), 2.10–2.23 (m, 1H, 3-H_a), 2.29–2.43 (m, 1H, 3-H_b), 3.34–3.48 (m, 2H, 4-H), 4.26 (s, 1H, 2-H), 5.09 (s, 1H, 2-NH) ppm

^{13}C-NMR (101 MHz, $CDCl_3$): δ = 28.1 (C-2''), 28.5 (C-3'), 28.5 (C-4), 36.5 (C-3), 53.4 (C-2), 80.2 (C-2'), 82.7 (C-1''), 155.5 (C-1'), 170.9 (C-1) ppm.

The spectroscopic data match the literature data.[24]

tert-Butyl-(*S*)-4-azido-2-((*tert*-butoxycarbonyl)amino)butanoate (S15)

The bromide **S14** (1.57 g, 4.64 mmol) was dissolved in DMSO (12 mL), then NaN_3 (906 mg, 13.9 mmol) was added. The reaction was stirred at 80 °C for 17 h. After cooling water (100 mL) was added and the reaction was extracted with EtOAc (3 x 80 mL). The combined organic phases were washed with water (2 x 100 mL), dried over Na_2SO_4, filtered and the solvent evaporated under reduced pressure. The azide **S15** (1.34 g, 4.48 mmol, 97%) was obtained as slightly orange oil.



$C_{13}H_{24}N_4O_4$
300.36

S15

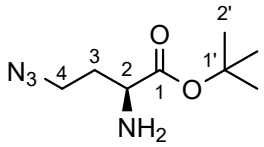
^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.44 (s, 9H, 3‘-H), 1.47 (s, 9H, 2‘‘-H), 1.88 (dq, *J* = 14.0 Hz, 7.0 Hz, 1H, 3-H_a), 2.08 (dd, *J* = 14.0 Hz, 6.8 Hz, 1H, 3-H_b), 3.39 (t, *J* = 6.8 Hz, 2H, 4-H), 4.25 (s, 1H, 2-H), 5.14 (s, 1H, 2-NH) ppm.

^{13}C-NMR (101 MHz, $CDCl_3$): δ = 28.1 (C-2‘‘), 28.4 (C-3‘), 32.2 (C-3), 48.0 (C-4), 52.0 (C-2), 80.1 (C-2‘), 82.6 (C-1‘‘), 155.5 (C-1‘), 171.2 (C-1) ppm.

The spectroscopic data match the literature data.[25]

***tert*-Butyl-(*S*)-2-amino-4-azidobutanoate (S16)**

The protected amino acid **S15** (632 mg, 2.10 mmol) was dissolved in CH_2Cl_2 (17 mL) and TFA (1.62 mL, 2.40 g, 21.0 mmol) was added dropwise. The reaction was stirred at rt for 3 h, then the pH value was adjusted to pH = 12 with 1 M NaOH solution. The reaction was extracted with CH_2Cl_2 (3 x 40 mL) and the combined organic phases were dried over Na_2SO_4, filtered and the solvent evaporated under reduced pressure. Product **S16** (342 mg, 1.71 mmol, 81%) was obtained as yellowish oil.



$C_8H_{16}N_4O_2$
200.24

S16

^{1}H-NMR (500 MHz, $CDCl_3$): δ = 1.46 (s, 9H, 2‘-H), 1.64–1.75 (m, 1H, 3-H_a), 1.93–2.02 (m, 1H, 3-H_b), 3.40 (dd, *J* = 8.5 Hz, 4.9 Hz, 1H, 2-H), 3.41–3.50 (m, 2H, 4-H) ppm.

^{13}C-NMR (126 MHz, $CDCl_3$): δ = 28.1 (C-2‘), 33.9 (C-3), 48.4 (C-4), 52.7 (C-2), 81.6 (C-1‘), 174.9 (C-1) ppm.

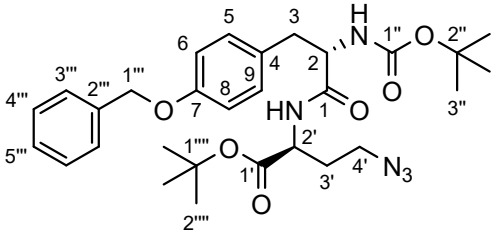
FT-IR (ATR): $\tilde{\nu}$ = 2978 (w), 2932 (w), 2093 (vs), 1724 (s), 1458 (w), 1393 (w), 1368 (m), 1251 (s), 1151 (vs), 1062 (w), 963 (w), 846 (s), 745 (w) cm^{-1}.

HRMS (ESI): m/z $[M+H]^+$ calculated for $C_8H_{16}N_4O_2$: 201.1346; found: 201.1346.

2.8 Homoserine dipeptides

tert-butyl (S)-4-azido-2-((S)-3-(4-(benzyloxy)phenyl)-2-((*tert*-butoxycarbonyl)amino)propanamido)butanoate (S17-T)

Acid **S6-T** (1.32 g, 3.56 mmol) and EDC·HCl (890 mg, 4.64 mmol) were dissolved in CH_2Cl_2 (37 mL) and stirred under N_2 at rt for 1 h. Then HOBt·H_2O (709 mg, 4.63 mmol) was added and the reaction stirred for additional 30 min. Amine **S16** (713 mg, 3.56 mmol) was dissolved in CH_2Cl_2 (10 mL) under N_2 and then added dropwise to the reaction. The reaction was stirred at rt for 2.5 d, then water (100 mL) was added and the resulting mixture extracted with CH_2Cl_2 (3 x 50 mL). The combined organic phases were washed with water (3 x 100 mL), dried over Na_2SO_4, filtered and the solvent evaporated under reduced pressure. The crude product was purified by column chromatography (PE / EtOAc 3 : 1) and the dipeptide **S17-T** (1.26 g, 2.28 mmol, 64%) was obtained as colorless, amorphous solid.



$C_{29}H_{39}N_5O_6$
553.66

S17-T

^{1}H-NMR (500 MHz, $CDCl_3$): δ = 1.42 (d, *J* = 3.4 Hz, 9H, 3‘‘-H), 1.45 (d, *J* = 3.0 Hz, 9H, 2‘‘‘‘-H), 1.79 (dq, *J* = 13.9 Hz, 6.8 Hz, 0.5H, 3‘-H_a minor), 1.88 (dq, *J* = 13.9 Hz, 6.8 Hz, 0.6H, 3‘-H_a major), 1.99 (dtd, *J* = 13.9 Hz, 6.8 Hz, 5.1 Hz, 0.5H, 3‘-H_b minor), 2.09 (dtd, *J* = 13.9 Hz, 6.8 Hz, 5.1 Hz, 0.6H, 3‘-H_b major), 3.01 (dd, *J* = 12.9 Hz, 6.7 Hz, 2H, 3-H), 3.08 (dt, *J* = 12.5 Hz, 6.9 Hz, 0.6H, 4‘-H_a minor), 3.16 (dt, *J* = 13.2 Hz, 6.7 Hz, 0.5H, 4‘-H_b minor), 3.26 (ddq, *J* = 19.5 Hz, 12.8 Hz, 6.8 Hz, 1H, 4‘-H major), 4.31 (s, 1H, 2-H), 4.42–4.51 (m, 1H, 2‘-H), 4.94–5.01 (m, 1H, 2-NH), 5.03 (d, *J* = 5.1 Hz, 2H, 1‘‘‘-H), 6.48–6.52 (m, 0.4H, 1-NH minor), 6.56 (d, *J* = 7.4 Hz, 0.5H, 1-NH major), 6.87–6.94 (m, 2H, 6-H, 8-H), 7.06–7.16 (m, 2H, 5-H, 9-H), 7.29–7.44 (m, 5H, 3‘‘‘-H bis 5‘‘‘-H) ppm. ^{13}C-NMR (126 MHz, $CDCl_3$): δ = 28.0, 28.0 (C-3‘‘), 28.4 (C-2‘‘‘‘), 31.6, 31.8 (C-3‘), 37.3, 37.7 (C-3), 47.5, 47.7 (C-4‘), 50.7, 50.8 (C-2‘), 56.1 (C-2), 70.1, 70.1 (C-1‘‘‘), 80.4 (C-2‘‘), 82.9 (C-1‘‘‘‘), 115.2, 115.2 (C-6, C-8), 127.6, 127.6, 128.1, 128.7 (Ar-C’s), 128.9 (C-4), 130.4, 130.5 (C-5, C-9), 137.1 (C-2‘‘‘), 155.5 (C-1‘‘), 158.0, 158.0 (C-7), 170.2, 170.4 (C-1‘), 171.2, 171.3 (C-1) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3300 (w, br), 2978 (w), 2932 (w), 2098 (s), 1730 (m), 1656 (s), 1612 (w), 1583 (w), 1510 (vs), 1455 (m), 1391 (m), 1367 (s), 1297 (m), 1242 (vs), 1156 (vs), 1041 (m), 1021 (m), 845 (m), 823 (w), 736 (m), 696 (m), 548 (w) cm^{-1}.

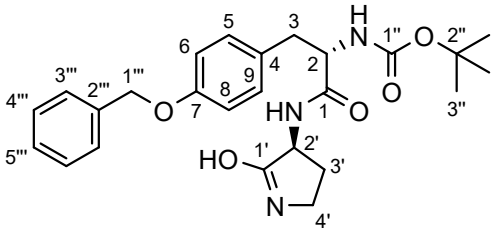
HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{29}H_{39}N_5O_6$: 554.2973; found: 554.2986.

$[\alpha]_D^{20}$ = + 5.4°·mL·dm^{-1}·g^{-1} (c = 0.147, $CHCl_3$).

Mp. 111 °C.

tert-Butyl-((*S*)-3-(4-(benzyloxy)phenyl)-1-(((*S*)-5-hydroxy-3,4-dihydro-2H-pyrrol-4-yl)amino)-1-oxopropan-2-yl)carbamate (S18-T)

Azide **S17-T** (200 mg, 361 µmol) was dissolved in dried, degassed toluene (3.8 mL). Bu_3P (0.10 mL, 82.0 mg, 405 µmol) was added and the reaction was stirred at 111 °C for 22 h. Afterwards the solvent was evaporated under reduced pressure and the resulting crude product was purified by column chromatography (CH_2Cl_2 / MeOH 20 : 1). Product **S18-T** (133 mg, 293 µmol, 81%) was obtained as colorless solid. The Bu_3P byproduct could not be separated completely.



$C_{25}H_{31}N_3O_5$
453.54

S18-T

^{1}H-NMR (700 MHz, $(CD_3)_2SO$): δ = 1.30 (d, J = 7.3 Hz, 8H, 3''-H), 1.61–1.68 (m, 0.6H, 3'-H_a major), 1.76–1.83 (m, 0.4H, 3'-H_a minor), 2.23–2.29 (m, 0.6H, 3'-H_b major), 2.29–2.35 (m, 0.4H, 3'-H_b minor), 2.63–2.70 (m, 0.8H, 3-H_a major + minor), 2.85 (dd, *J* = 13.7 Hz, 4.8 Hz, 0.6H, 3-H_b major), 2.91 (dd, *J* = 13.8 Hz, 4.0 Hz, 0.3H, 3-H_b minor), 3.13–3.17 (m, 1.2H, 4'-H major), 3.17–3.22 (m, 0.8H, 4'-H minor), 4.10 (td, *J* = 8.7 Hz, 4.0 Hz, 0.3H, 2-H minor), 4.14 (td, *J* = 8.8 Hz, 4.8 Hz, 0.5H, 2-H major), 4.23 (dt, *J* = 10.1 Hz, 8.1 Hz, 0.6H, 2'-H major), 4.30 (dt, *J* = 10.4 Hz, 8.3 Hz, 0.4H, 2'-H minor), 5.05 (s, 2H, 1'''-H), 6.74 (d, *J* = 8.7 Hz, 0.3H, 2-NH minor), 6.79 (d, *J* = 8.8 Hz, 0.5H, 2-NH major), 6.89 (t, *J* = 8.1 Hz, 2H, 6-H, 8-H), 7.12–7.24 (m, 2H, 5-H, 9-H), 7.29–7.34 (m, 1H, 5'''-H), 7.38 (ddd, *J* = 8.0 Hz, 6.7 Hz, 1.8 Hz, 2H, 4'''-H), 7.43 (ddd, *J* = 8.0 Hz, 2.9 Hz, 1.3 Hz, 2H, 3'''-H), 7.85 (s, 1H, 1'-OH), 8.12 (d, *J* = 8.3 Hz, 0.3H, 1-NH minor), 8.19 (d, *J* = 7.7 Hz, 0.6H, 1-NH major) ppm.

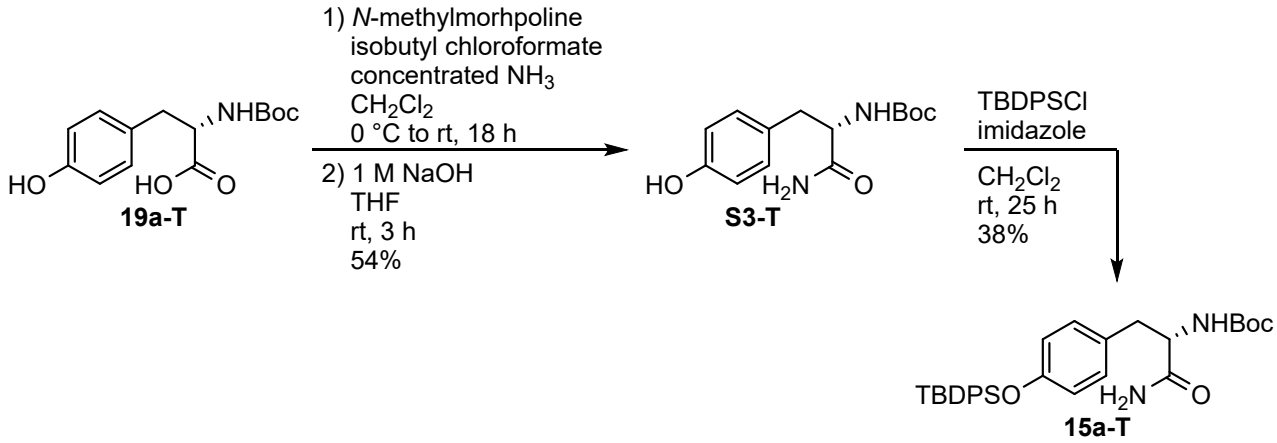
^{13}C-NMR (MHz, $(CD_3)_2SO$): δ = 28.1, 28.2 (C-3‘‘), 28.5 (C-3‘), 37.0, 37.0 (C-3), 38.0, 38.1 (C-4‘), 49.6, 49.6 (C-2‘), 55.6, 55.8 (C-2), 69.1, 69.1 (C-1‘‘‘), 77.9, 78.0 (C-2‘‘), 114.3, 114.3 (C-6, C-8), 127.6, 127.6, 127.7, 127.7, 128.4 (Ar-C’s), 130.2, 130.3 (C-5, C-9, C-4), 137.3 (C-2‘‘‘), 155.1, 155.2 (C-1‘‘), 156.9, 156.9 (C-7), 171.8, 171.8 (C-1), 174.3, 174.4 (C-1‘) ppm.

FT-IR (ATR): $\tilde{\nu}$ = 3329 (m), 3286 (m), 2980 (w), 2928 (w), 1712 (s), 1689 (vs), 1646 (vs), 1612 (m), 1584 (w), 1510 (vs), 1454 (m), 1439 (m), 1389 (s), 1366 (s), 1296 (s), 1239 (vs), 1164 (vs), 1110 (m), 1048 (m), 1016 (s), 908 (s), 859 (m), 823 (m), 777 (m), 728 (vs), 695 (vs), 645 (s), 603 (s), 549 (s), 516 (m), 503 (m), 463 (w) cm^{-1}.

HRMS (ESI): m/z $[M+Na]^+$ calculated for $C_{25}H_{31}N_3O_5$: 476.2156; found: 476.2155.

3. Further details of the pre-chromophore synthesis

To obtain **15a-T** the amide **S3-T** had to be synthesized as shown in Scheme S1.



Scheme S1: Synthesis of TBDPS and Boc protected tyrosine amide **15a-T**.

The amide **S3-T** was synthesized by treatment of the Boc-protected **19a-T** with isobutyl chloroformate, then with an excess of concentrated NH3 solution (25%wt). During the reaction a carbonate side product was observed, which was partly hydrolyzed with 1 M NaOH in THF. Thus 54% of amide **S3-T** were obtained. The free phenol group was then protected with TBDPSCl, yielding 38% of **15a-T**.

To obtain the ferribactin pre-chromophore derivatives, different reaction conditions were tested. The coupling of the methylated amide **15c-T** was performed according to Abdallah with Et_3OBF_4, then DABA **16** and yielded 15% of methylated **14c-T**.[7] The coupling of methylated amide **15c-T** was performed according to Jones with MeOTf, then DABA **16** as well.[26] Thus 73% of methylated **14c-T** as colourless solid were obtained. Due to its higher yield, this method was used for all couplings to the pre-chromophores. For the silyl-protected amides **15a-T** and **15b-D** the use of CH_2Cl_2 as solvent in the first reaction step was sufficient. Due to their higher polarity the methyl-protected amides **15c-T** and **15d-D** needed a solvent change to $CHCl_3$, increasing the yields from 39% to 73% for **14c-T** and from 11% to 40% for **14d-D**.

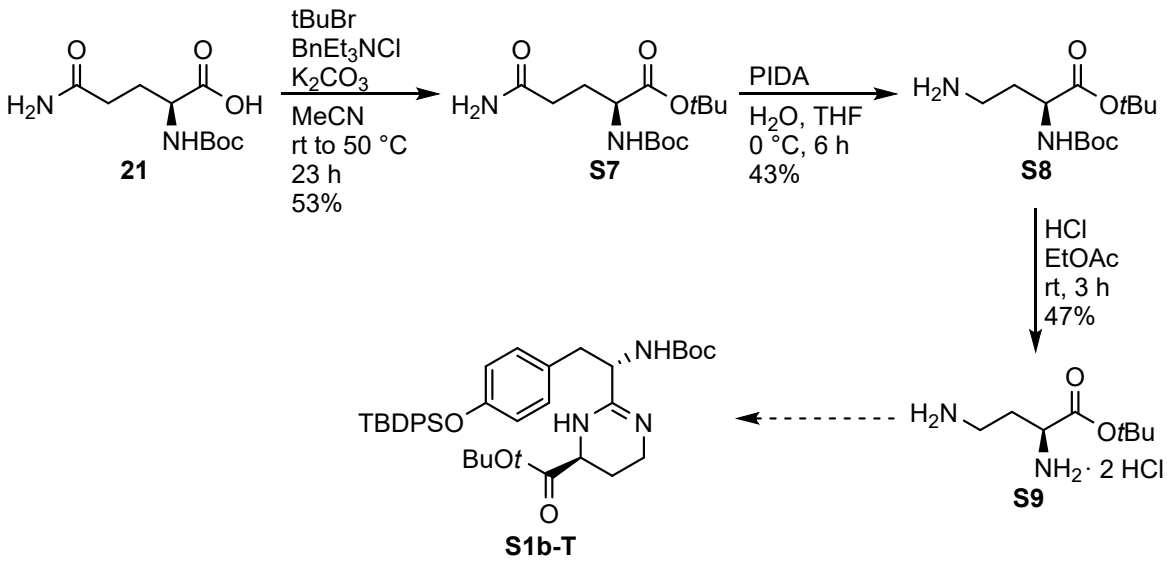
The results confirmed that the MeOTf procedure by Jones worked not only for the truncated molecules without stereogenic centers, but as well for the amino acid based silyl-protected (**15a-T**, **15b-D**), methyl-protected (**15c-T**, **15d-D**) and alkyl-protected

(**S4b-T**) precursors to get the corresponding ferribactin pre-chromophores.[26] Compared to the iminothioester route by Jones, which yielded 34% over 4 steps from the free acid to the tetrahydropyrimidine unit, the number of steps was reduced and the combined yields were between 11% and 40% (over 2 steps).[27] Abdallah reported the coupling to methyl-protected **14c-T** with 41% (*S*-isomer), whereas in this work 73% were achieved.[7]
Characterization of the ferribactin pre-chromophores **14d-D** and **S1a-T** by NMR indicated the presence of rotamers (for details see Figure S1 and the corresponding text).

For the coupling with the spacer **S2** the pre-chromophore derivatives had to be deprotected. The deprotection of the methyl-protected, Cbz-containing derivatives **14c-T** and **14d-D** was attempted via catalytic hydrogenation with palladium as reported by Ishihara.[28] No reliable results were obtained by test reactions with this method. Ghorai[29] reported a deprotection method of Cbz with 6 M HCl under reflux and Jones[27] showed with other tetrahydropyrimidine amino acids that the tetrahydropyrimidine moiety is robust enough to withstand 5 M HCl at 100 °C.

To introduce a polymerizable side group, the Boc deprotection with TFA performed with the silyl-protected (**23a-T**, **23b-D**) and methyl-protected (**23c-T**, **23d-D**) spacer derivatives and the coupling with freshly distilled methacryloyl chloride was attempted. However, no conversion was detected. Therefore, coupling was performed with activated methacrylic acid (with EDC·HCl and HOBt) which led to the desired silyl-protected monomers **13a-T** in 80% and **13b-D** in 49% and methyl-protected monomers **13c-T** in 68% and **13d-D** in 47% yield.

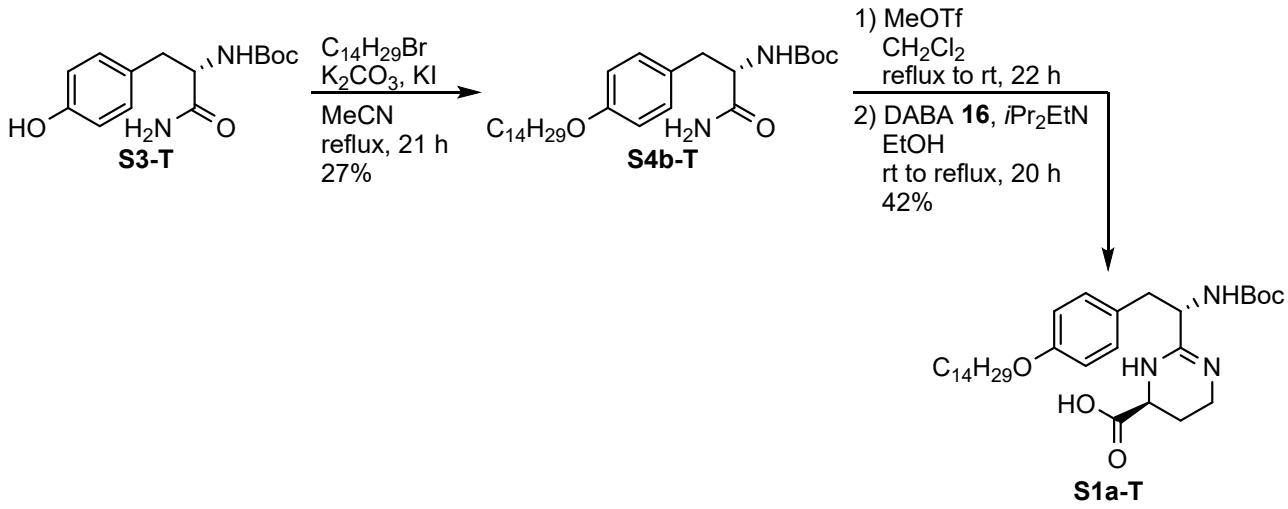
For the synthesis of esterified pre-chromophore derivatives *tert*-butyl protected DABA **S9** was prepared (Scheme S2)



Scheme S2: Synthesis of *tert*-butyl protected DABA **S9** and corresponding pre-chromophore derivative **S1b-T**.

Therefore, Boc-protected glutamine **21** was stirred with *t*BuBr, yielding *tert*-butyl ester **S7** in 53%.[30] Then an alternative Hofmann rearrangement reaction with PIDA was performed to yield the amine **S8** in 43%.[31] Afterwards Boc deprotection of **S8** was performed with freshly prepared HCl in EtOAc, which yielded diamine **S9** as dihydrochloride in 47%.[32] Then, **S9** was used for the coupling reaction with **15a-T**. Product **S1b-T** could only be identified by MS, since it could not been purified. The additional protecting group decreased the polarity and increased the solubility in organic solvents as expected. But, due to this change, side products were not separable by column chromatography or crystallization, neither through extraction nor washing.

For investigation of the influence of a long alkyl chain on the properties of the target molecule **14-T**, the amide **S3-T** was alkylated with $C_{14}H_{29}Br$ to obtain the alkylated amide **S4b-T** in 27% yield (Scheme S3).

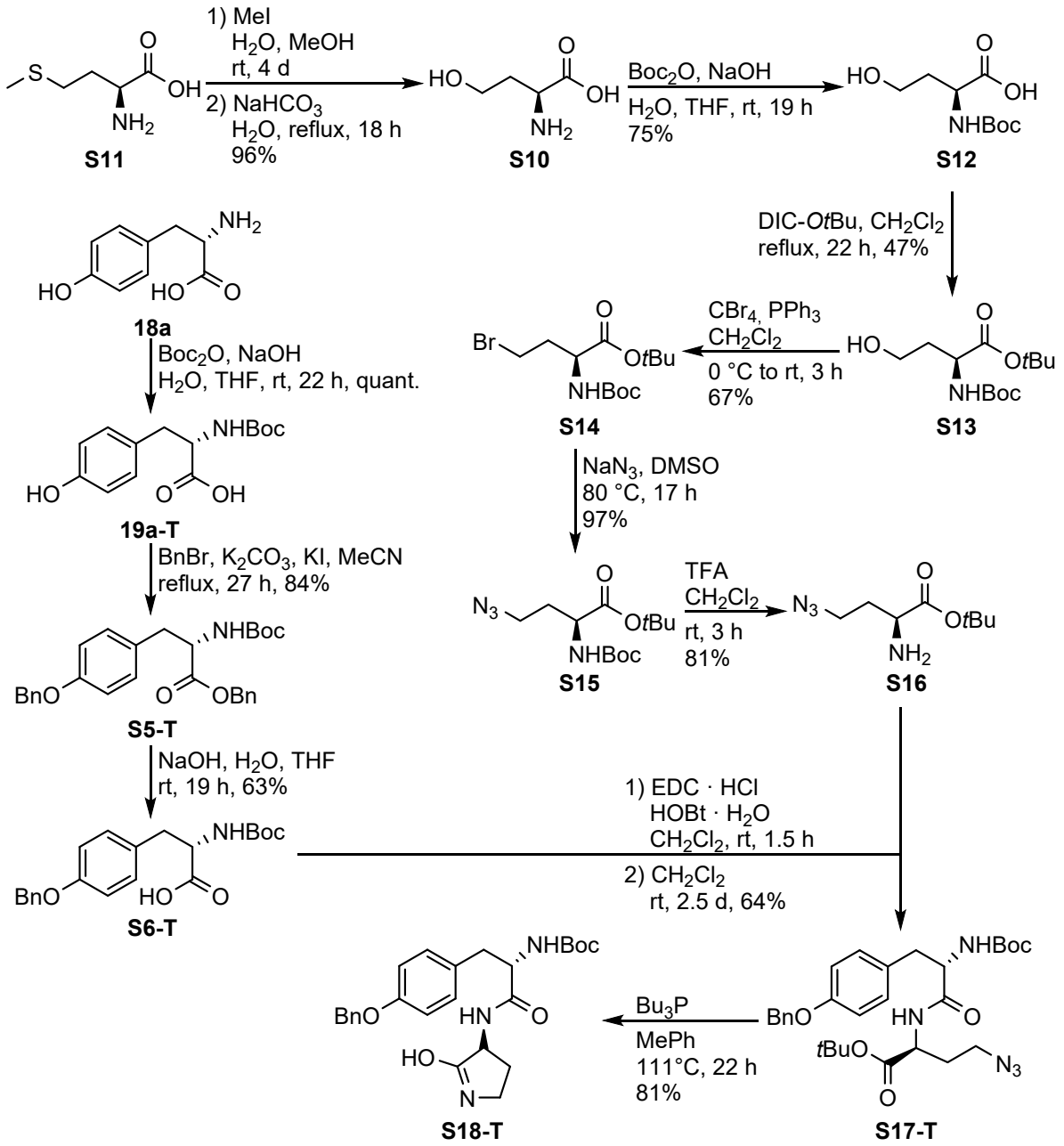


Scheme S3: Synthesis of alkylated ferribactin pre-chromophore **S1a-T**.

Afterwards the amide **S4b-T** was methylated with MeOTf in CH_2Cl_2, then coupled with DABA **16** and yielded 42% of **S1a-T**.

4. Aza-Wittig approach

In addition to the iminoether coupling, the synthesis of the ferribactin pre-chromophore **14-T** via a tyrosine **18a** and homoserine **S10** based route was attempted, shown in Scheme S3.



Scheme S4: Aza-Wittig approach leading to the Iminol **S10-T**.

To get the desired protected tyrosine **S6-T**, tyrosine **18a** was first stirred with Boc_2O and NaOH as base, modifying known literature[33]. This gave Boc-tyrosine **19a-T** in quantitative yield. Then **19a-T** was treated with BnBr in the presence of K_2CO_3 and KI in a modified known procedure[8] and yielded the fully benzylated derivative **S5-T** in

84%. The derivative **S5-T** had to be saponified with NaOH according to literature[34], yielding the free acid **S6-T** in 63% yield.

For the homoserine based derivatives, first homoserine **S10** had to be synthesized. According to a known procedure[35] methionine **S11** was methylated with iodomethane and in a second step dimethylsulfide was substituted by water by refluxing the intermediate with $NaHCO_3$. This led to homoserine **S10** in 96% yield. The purification by precipitation in EtOH / acetone turned out to be difficult. The solvent mixture must be stirred fast, while the oily crude product must be added dropwise (fast) in order to a get colorless powder. If the crude product was added too fast, or the mixture was stirred to slow, a colorless slimy substance precipitated, and the precipitation had to be done a second time. The homoserine **S10** was then protected with Boc_2O and NaOH as base and yielded Boc-homoserine **S12** in 75%. The Boc-homoserine **S12** was then esterified with *N,N'*-diisopropyl-*O*-*tert*-butylisourea (DIC-O*t*Bu) according to literature[36] and yielded **S13** in 47%. Afterwards the hydroxyl group of **S13** was treated with CBr_4 and PPh_3 in a literature[37] known Appel reaction to give the bromide **S14** in 67% yield. The bromide of **S14** was substituted in a known procedure[38] with NaN3 and yielded the azide **S14** in 97%. Deprotection of the Boc group of **S15** with trifluoroacetic acid (TFA) in a known procedure[39] then led to the desired homoserine derivative **S16** in 81% yield. The carbon to nitrogen ratio in **S16** is 2.5 (below 3), indicating that **S16** is potentially explosive and should be handled with care[40]. Thus, the azide **S16** was directly used in the following reaction.

The tyrosine derivative **S6-T** was activated with EDC·HCl and HOBt·H_2O, then azide **S16** was added for the peptide coupling in a known procedure[41]. The reaction yielded **S17-T** in 64%. Afterwards, an intramolecular Aza-Wittig reaction of **S17-T** with Bu_3P in toluene at 111 °C was performed, modifying a known procedure[42], to get the ferribactin pre-chromophor **14-T**, but instead the reaction yielded the iminol **S18-T** in 81%. Instead of the amide, the generated aza-ylide attacked the more reactive ester moiety. The reaction temperature was elevated (111 °C) to force the amide to reaction and the *tert*-butyl ester was introduced to provide a sterical hinderance for the ester, but the reaction still favors the more reactive ester over the less reactive amide.

5. NMR studies on 14d-D and S1a-T

During the synthesis and characterization of the ferrribactin pre-chromophore series **14a-T**, **14b-D**, **14c-T**, **14d-D** and **S1a-T** a signal doubling of the stereogenic centers was observed in some ^{1}H NMR spectra of the tyrosine-based (**14c-T, S1a-T**) and DOPA-based derivatives (**14d-D**). Previous studies by Abdallah[7] showed two distinguishable signal sets for the (*S*,*S*)- and the (*R*,*S*)-diastereomers of **14c-T**. These could (in good approximation) fit the observations, but the performed reactions should not be basic enough to racemise the amino acid derivatives. To test this hypothesis ^{1}H NMR experiments were conducted, and the results are shown in Figure S1.

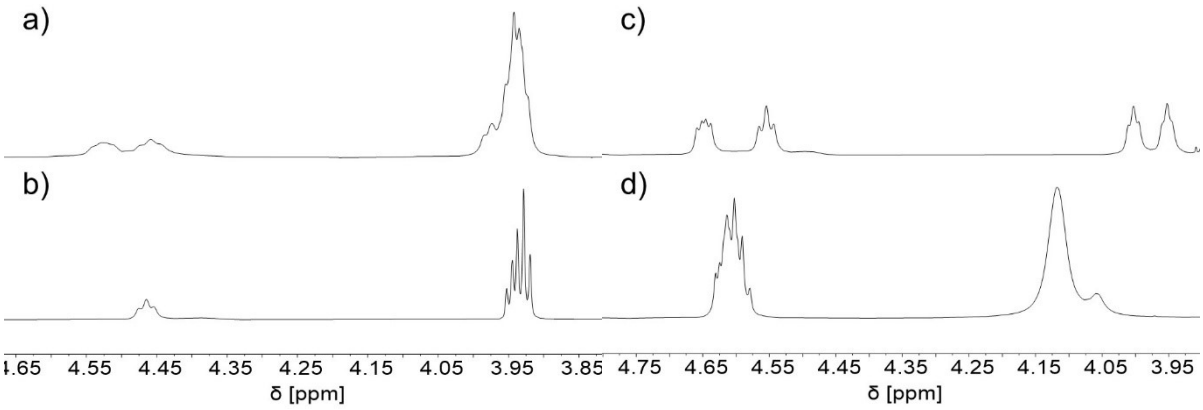


Figure S1: Section of the stereocenters of two ^{1}H NMR measurements of the same batch of **S1a-T** in MeOD-d_4 in different tubes. a) 500 MHz NMR, b) 700 MHz NMR (stereocenter at 3.93 ppm overlaps with another proton). Section of the stereocenters of two ^{1}H NMR measurements of **14d-D** at 700 MHz, c) MeOD-d_4, d) substance of the NMR in methanol recovered and measured in DMSO-d_6.

The derivative **14d-D** showed signal doubling in CD_3OD at the 700 MHz (Figure S1c). The NMR sample was recovered by evaporating the deuterated solvent and subsequent dissolved in DMSO-d_6. to be measured again at 700 MHz. This time the signal doubling for the proton at 4.63 ppm was not observed and a slightly doubled signal with a distinctively lower second signal at 4.12 ppm. The derivative **S1a-T** was measured at 500 MHz and 700 MHz in deuterated methanol (Figure S1a and b). Both NMR-tubes were filled with compound of the same batch, so no difference was expected. The ^{1}H NMR at 500 MHz showed a clear signal doubling at 4.47 ppm and probably a second one at 3.95 ppm (Figure S1a), that is overlapping with another proton signal. In contrast the proton NMR at 700 MHz just showed a single signal set

for both signals (Figure S1b). Thus, the observed signal doubling is not the result of a diastereomeric mixture, but of rotamers.

6. UV-VIS spectroscopy

UV-VIS measurements were performed on the UV-2600 UV-VIS spectrometer by Shimadzu. The cuvette was filled with 1 mL of dissolved monomer **13a-T**, **13b-D**, **13c-T** and **13d-D** in MeOH with the molar concentrations of **13a-T**: 64.9 µM; **13b-D**: 92.7 µM; **13c-T**: 122.5 µM; **13d-D**: 112.0 µM. Then $FeCl_3 \cdot 6H_2O$ dissolved in MeOH (4 mM) was added stepwise (in µL amounts with an Eppendorf pipette), mixed and measured to get the spectra with the shown molar amounts of Fe^{3+}. The deprotection of **13a-T** and **13b-D** was carried out by adding 1 µL TBAF (70% in water) to 2 mL of the substance solutions and stirring for 20 h at rt. The excess TBAF and byproducts were not removed from the solutions before the measurements.

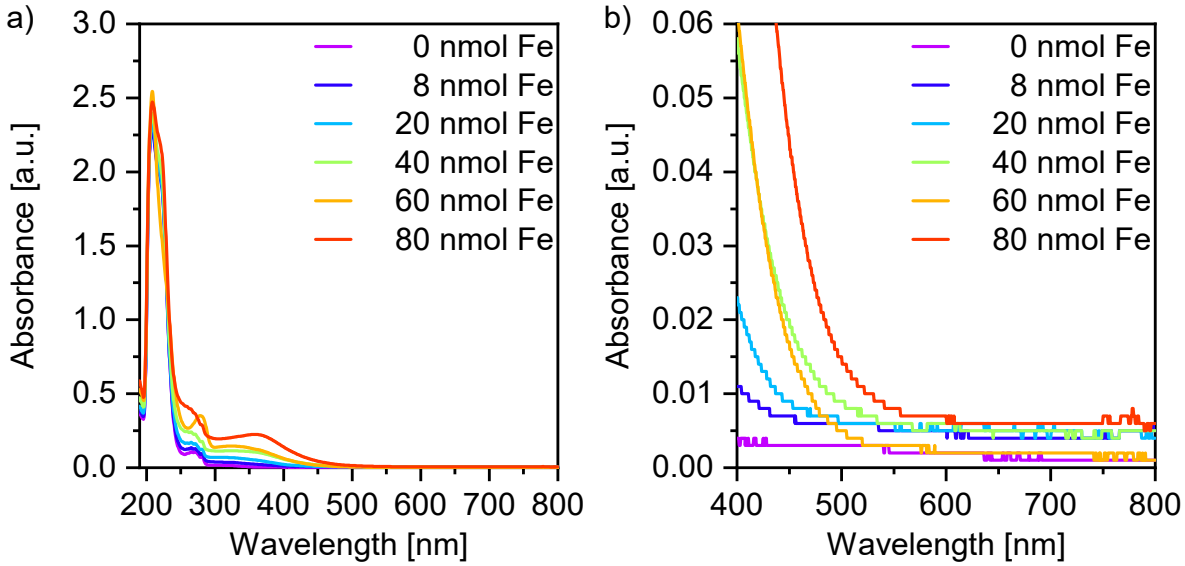


Figure S2: a) UV-VIS spectra of **13a-T** with different molar amounts of Fe^{3+}. b) Zoom into the spectra between 400 and 800 nm.

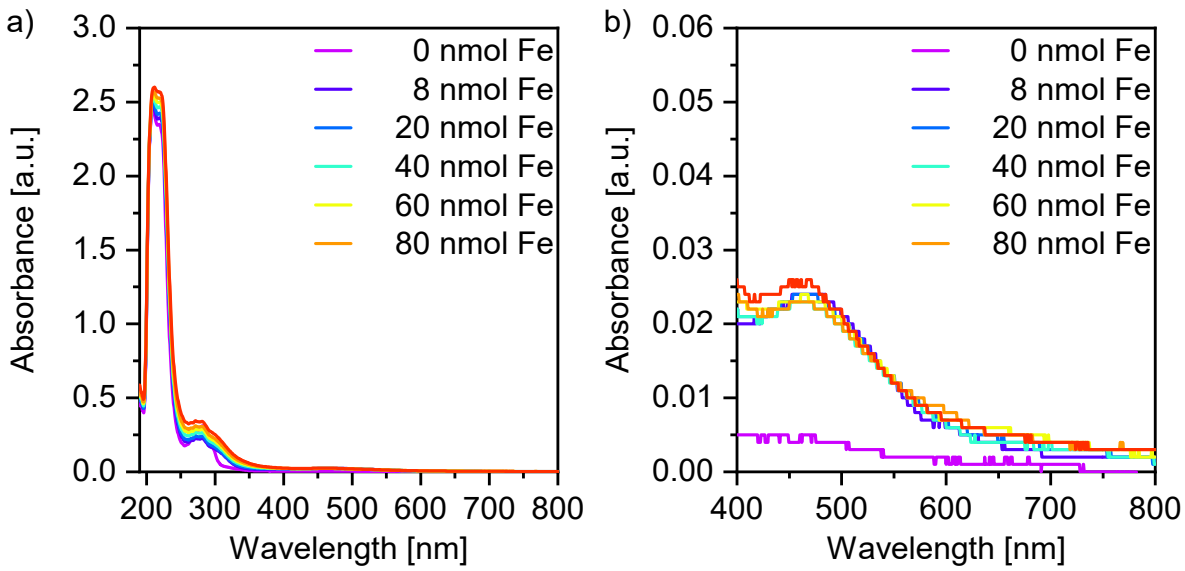


Figure S3: a) UV-VIS spectra of **24a-T** with different molar amounts of Fe^{3+}. b) Zoom into the spectra between 400 and 800 nm.

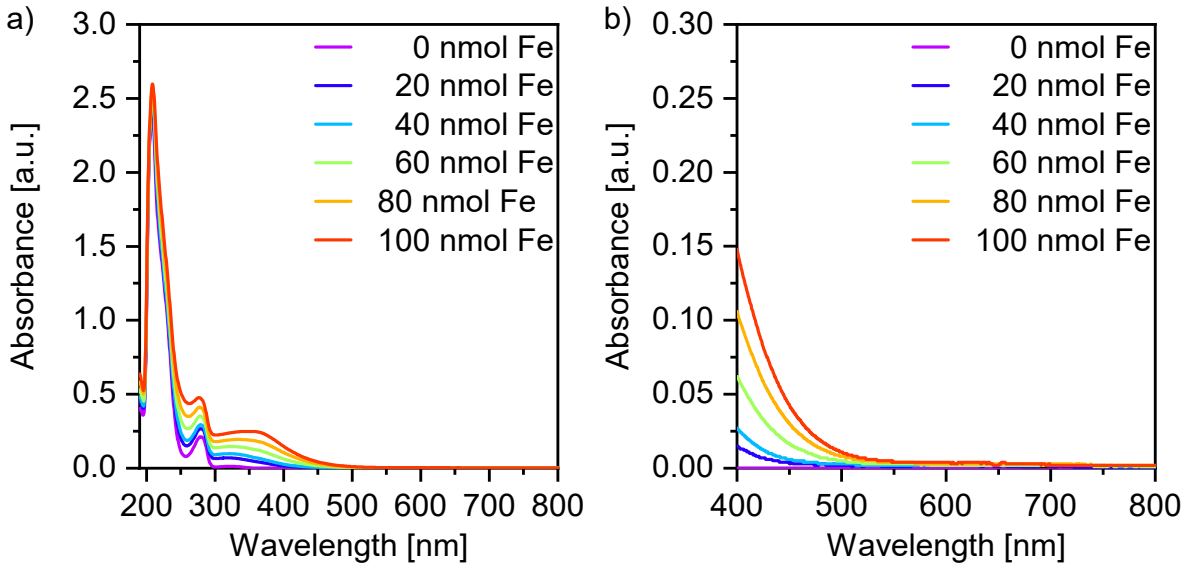


Figure S4: a) UV-VIS spectra of **13b-D** with different molar amounts of Fe^{3+}. b) Zoom into the spectra between 400 and 800 nm.

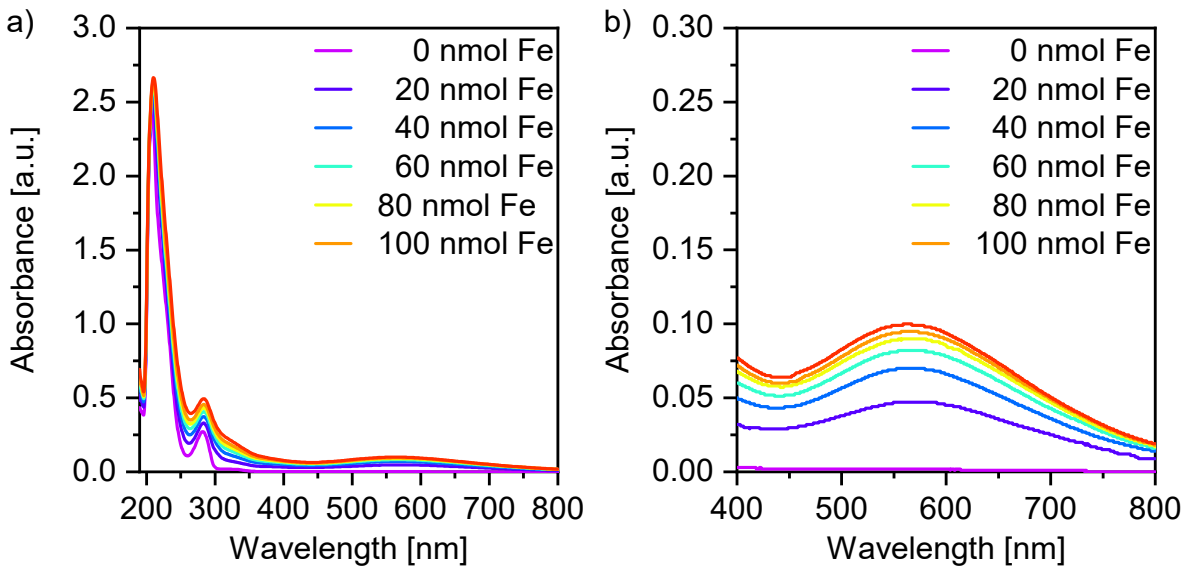


Figure S5: a) UV-VIS spectra of **24b-D** with different molar amounts of Fe^{3+}. b) Zoom into the spectra between 400 and 800 nm.

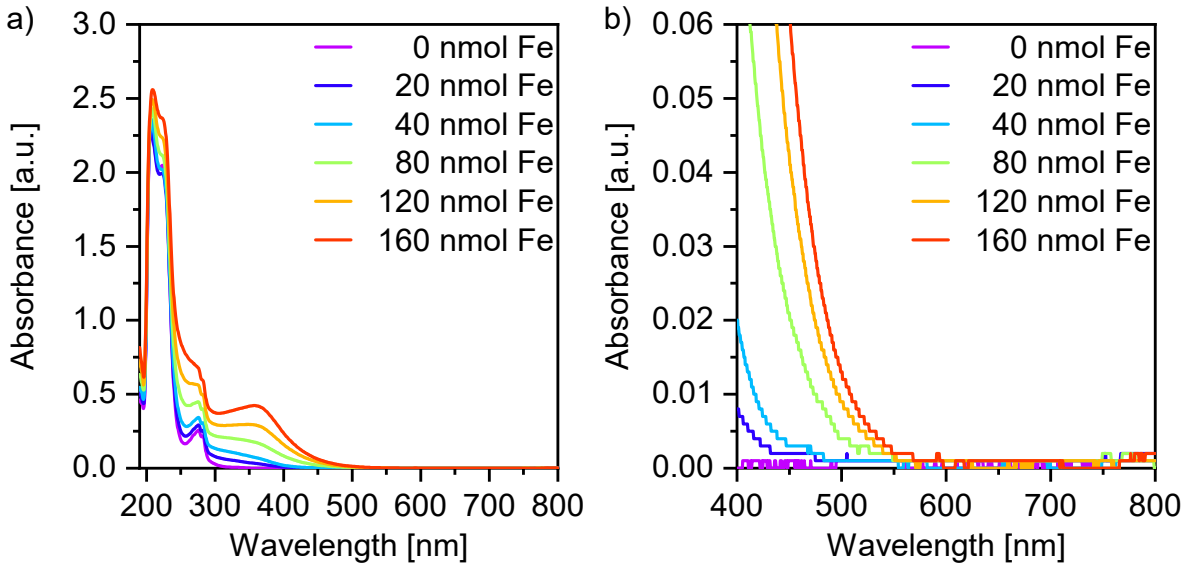


Figure S6: a) UV-VIS spectra of **13c-T** with different molar amounts of Fe^{3+}. b) Zoom into the spectra between 400 and 800 nm.

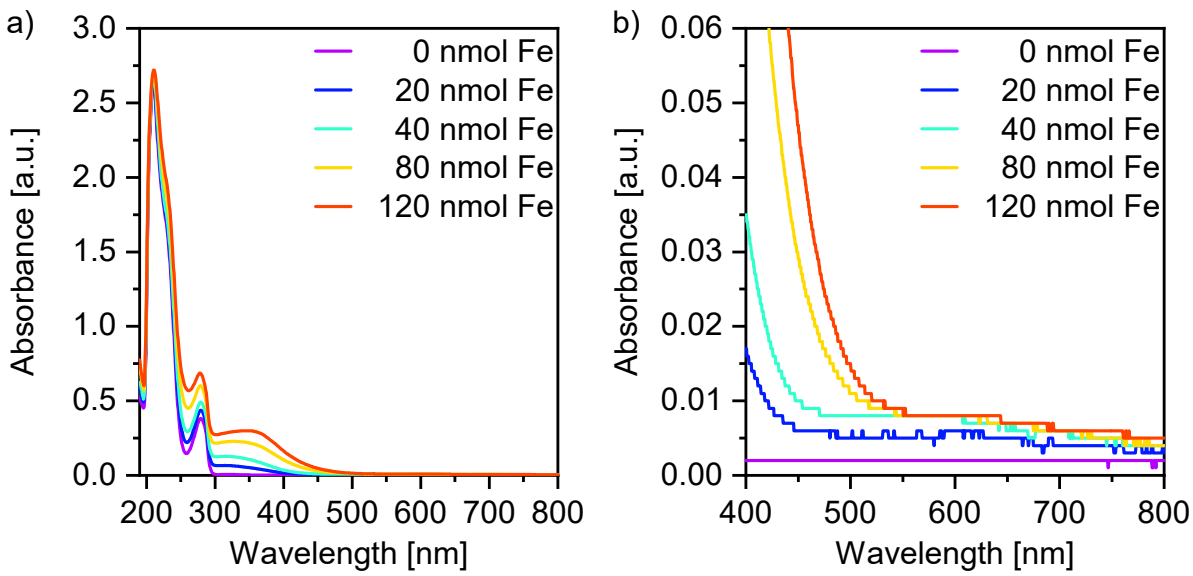


Figure S7: a) UV-VIS spectra of **13d-D** with different molar amounts of Fe^{3+}. b) Zoom into the spectra between 400 and 800 nm.

7. Polymer attributes

The MALDI spectra showed a typical polymer distribution (see MALDI spectra). The signal distance in all MALDI spectra is around 111 mass units, which corresponds to the mass of one NVP-molecule **9**. Since polyvinylpyrrolidone (PVP) is the backbone of the polymer and thus more abundant, this was expected.

Table S1: MALDI signal and estimated compositions of **10**, **11c-T** and **12c-T**.

Entry	Polymer	MALDI Signals [*m/z*]	Estimated composition (ratio of **8** : **9**)
1	**10**	~800 (start)	1 x MAHMP **8**, 5 x NVP **9**
		2137.1 (max)	2 x MAHMP **8**, 14 x NVP **9** (1 : 7)
		~6000 (end)	6 x MAHMP **8**, 42 x NVP **9** (1 : 7) or
			7 x MAHMP **8**, 39 x NVP **9** (1 . 5.6)
2	**11c-T**	~800 (start)	1 x **13c-T**, 3 x NVP **9**
		1805.7 (max)	1 x **13c-T**, 11 x NVP **9** (1 : 11)
		4231.3 (end)	4 x **13c-T**, 22 x NVP **9** (1 : 5.5)
3	**12c-T**	1030.7 (start, spike)	- [a]
		1586.4 (max)	1 x **13c-T**, 2 x MAHMP **8**, 5 x NVP **9**
		~6000 (end)	- [a]

[a] only calculated for maximum, due to uncertainty with 3 monomers.

For **10** the MALDI distribution starts at an *m/z* value of around 800 and ends due to the signal to noise ratio around 6000, with a maximum at 2137.1 (Table S1, entry 1). Rough estimations for the composition were calculated. The obtained values correspond to small oligomers containing 1 x MAHMP **8** and 5 x NVP **9** (plus additional end-groups) at the beginning of the MALDI spectrum up to small polymers containing 6 x MAHMP **8** and 42 x NVP **9** (1 : 7 assumed ratio) or 7 x MAHMP **8** and around 39 x NVP **9** (1 . 5.6 assumed ratio) at the at the end of the spectrum. The maximum equals 2 x MAHMP **8** and 14 x NVP **9** (1 : 7 assumed ratio). The ratio of **8** / **9** in the test reaction solution was 1 : 7.4 and data from ^{1}H NMR suggests a ratio of 1 : 8 incorporated in the polymer. The relative molecular weight for **10** synthesized by Ang with a reaction solution ratio of **8** / **9** of 1 : 5 was determined to be 2298, which is in the same order of magnitude.[43] For **11c-T** the MALDI distribution starts at an m/z value of around 800 and ends due to the signal to noise ratio at 4231.3, with a maximum at 1805.7 (entry 2). This corresponds to small oligomers containing 1 x **13c-T** and 3 x NVP **9** at the beginning of the MALDI spectrum up to small polymers containing 4 x **13c-T** and 22 x NVP **9** (1 : 5.5

assumed ratio) at the at the end of the spectrum. The maximum equals 1 x **13c-T** and 11 x NVP **9** (1 : 11 assumed ratio). The ratio of **13c-T** / **9** in the test reaction solution was 1 : 7.5 and data from ^{1}H NMR suggests a ratio of 1 : 10 incorporated in the polymer. For the mixed polymer **12c-T** the MALDI distribution starts with a spike at an *m/z* value of 1030.7, then goes into a vague polymer distribution at 1254.1 and ends due to the signal to noise ratio at around 6000, with a maximum at 1586.4 (entry 3). Due to the use of three monomers **13c-T**, MAHMP **8** and NVP **9** deductions to the assumed incorporated amounts of monomers though the MALDI spectrum are less certain. The shown maximum could contain 1 x **13c-T**, 2 x MAHMP **8** and 5 x NVP **9**, but could also be one of the monomers with a certain amount of NVP **9**. Suggestions with the ^{1}H NMR spectrum are less accurate as well, due to overlapping signals, the suggested ratio of **13c-T** / **8** / **9** is 1 : 1.8 : 46.7 (2.8 : 16.6 for monomers / NVP **9**), while the ratio in the reaction mixture was 1 : 2 : 22.6 (3 : 7.5 for monomers / NVP **9**). DOSY spectra are a 2D spectra, showing the cross signals of the ^{1}H NMR and the diffusion coefficient. All polymers showed one signal set corresponding to one average diffusion coefficient, indicating that all monomers are included in one copolymer and no homopolymers were created (see ESI, Chapter 8).

Table S2: Average diffusion coefficients [a] of polymers **10**, **11c-T** and **12c-T**.

Entry	Polymer	Average diffusion coefficient [a] [m^2/s]
1	**10**	2.25×10^{-10}
2	**11c-T**	1.24×10^{-10}
3	**12c-T**	7.12×10^{-11}

[a] determined with DOSY-NMR.

The average diffusion coefficient for **10** is 2.25×10^{-10} m^2/s (Table S2, entry 1). The value for **11c-T** is 1.24×10^{-10} m^2/s and for **12c-T** is 7.12×10^{-11} m^2/s (entries 2, 3). The extracted values are roughly in between the reported ones for NVP **9** (7.5×10^{-10} m^2/s) and PVP (9 kDa, 7.4×10^{-11} m^2/s).[44] They are also clearly smaller than the diffusion coefficients of the solvents MeOD with around 1.31×10^{-9} m^2/s and D_2O with around 2.34×10^{-9} m^2/s which was expected due to the vast difference in weight and thus size. Gel permeation chromatography (GPC) with the synthesized polymers **10**, **11c-T** and **12c-T** was not possible due to incompatibility of the polymers with the solvents and GPC columns available. Thus, no PDI and no average molecular weights was reported.

8. Biological tests

8.1 Cytotoxicity

Cytotoxicity of compounds was evaluated with the murine fibroblast cell line L929 and the alamarBlue™ viability assay, which is based on the reduction of blue, nonfluorescent resazurin to red, highly fluorescent resorufin. All incubation steps were performed in a cell culture incubator at 37 °C and 10% CO_2.

Approximately 1000 L929 cells/54 µL were seeded in each well of a sterile, cell culture treated 96-well microtiter plate. The plate was incubated overnight to allow the cells to adhere and was loaded with 6 µL test substance solutions in different concentrations afterwards. After an incubation period of 3 d 5 µL of the alamarBlue™ solution (500 µM resazurin solution) were added and the plate was incubated for another 3 – 4 h. Finally, the fluorescence was determined with the Spark Multimode Microplate Reader from Tecan (excitation wavelength 540 nm, emission wavelength 600 nm).

Experiments were repeated independently twice with duplicates on the microtiter plate for the monomers **13a-T**, **13b-D**, **13c-T**, **13d-D** and triplicates on each microtiter plate for the polymers **10**, **11c-T** and **12c-T**. Wells without cells were used as positive control (blank; no viable cells: maximum effect on viability), and wells with cells but without compounds were the negative control (no effect on viability). Chlorhexidine as known cytotoxic reference compound was used as positive control compound.

The averages of the positive (blank) and negative controls were used to normalize the effects of the compounds according to:

100% x (value – blank) / (negative control – blank). Then the averages for all data points per substance and concentration were calculated, as well as the standard deviations (displayed as error bars), and plotted against the concentration.

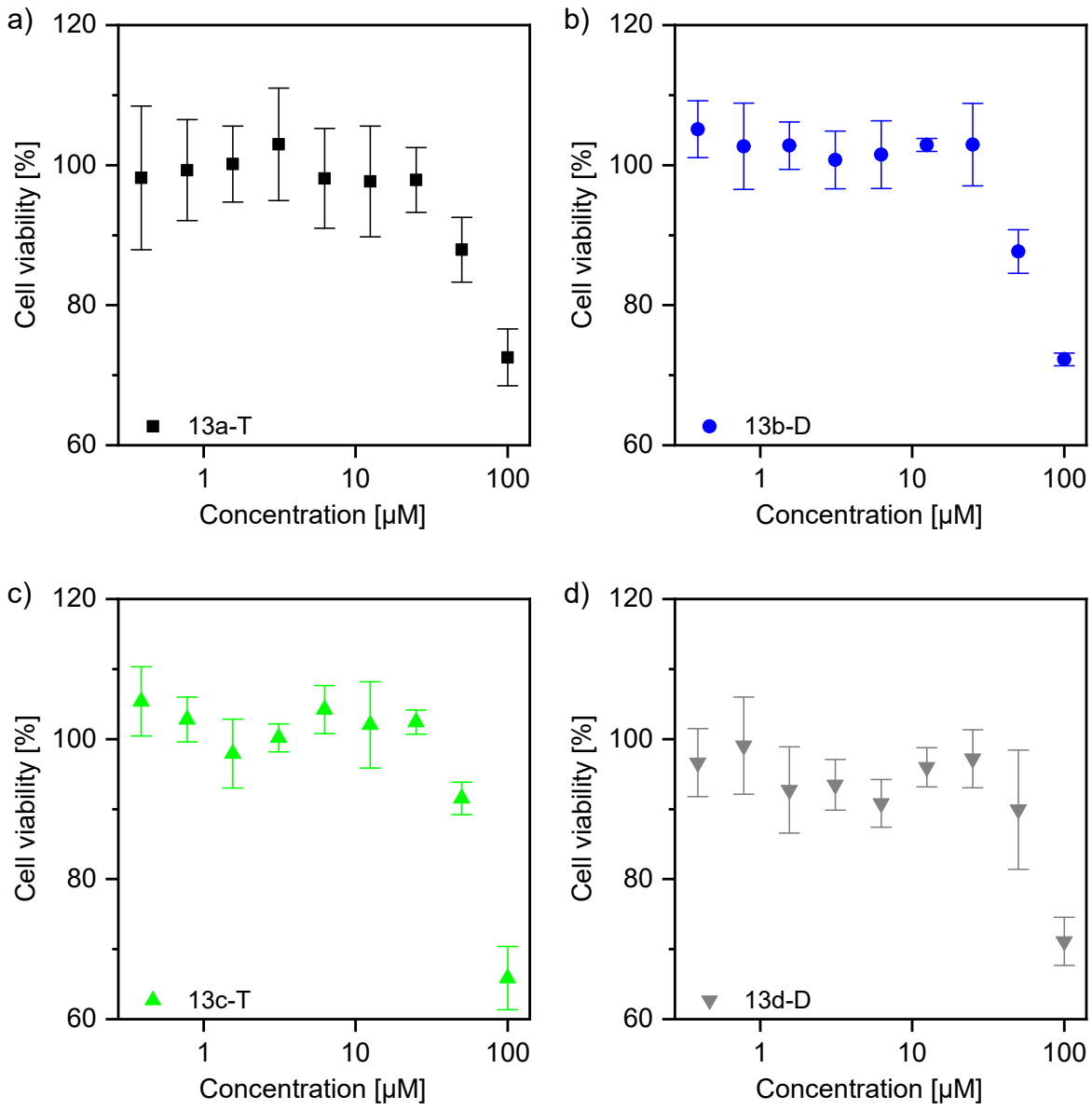


Figure S8: Cell viability of L929 incubated with the monomers **13a-T**, **13b-D**, **13c-T** and **13d-D** at different concentrations. a) monomer **13a-T**, b) monomer **13b-D**, c) monomer **13c-T**, d) monomer **13d-D**.

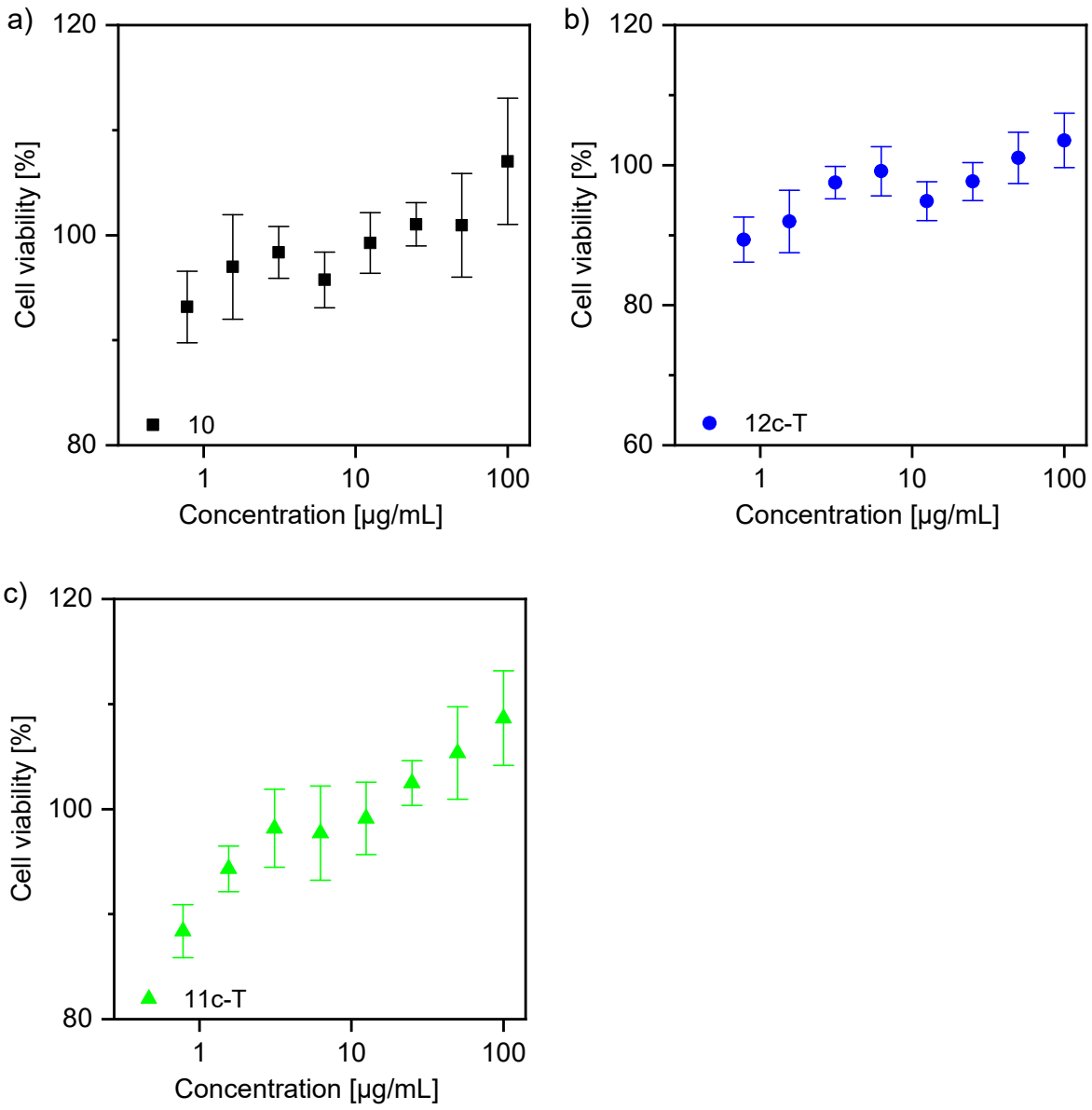


Figure S9: Cell viability of L929 incubated with the polymers **10**, **12c-T** and **11c-T** at different concentrations. a) polymer **10**, b) polymer **12c-T**, c) polymer **11c-T**.

8.2 Antibacterial activity

The antibacterial activity tests were performed with the bacteria *Escherichia coli* wild type (WT) (DSM 1103 / ATCC 25922), *Escherichia coli* ΔTolC (JW5503-1, parent strain BW25113), *Staphylococcus aureus* (USA300), *Klebsiella pneumoniae* (DSM 681 / ATCC 10031) and *Pseudomonas aeruginosa* (DSM 1117 / ATCC 27853). OD_{600}-values of overnight cultures were determined with the Eppendorf BioSpectrometer®, of microtiter plates with the Epoch2 – microtiterplate reader (Agilent).

The bacterial cultures were cultivated over night with the Benchtop Orbital Shaker (Thermo Scientific™ MaxQ™ 4000) at 37 °C and 150 rpm. The overnight cultures were diluted in 20 mL fresh TBS medium to obtain an OD_{600} = 0.1. This culture was allowed to grow to an OD_{600} = 0.5 to obtain the preculture. The preculture was again diluted with fresh TBS medium to an OD_{600} = 0.02. 6 µL of the compound solutions in different concentrations were transferred to each well of a sterile 384-well plate (Corning® 3701) and 54 µL of the diluted preculture (OD_{600} = 0.02) were added, to obtain a total volume of 60 µL. The plate was incubated without shaking at 37 °C for 21 - 24 h. The OD_{600} values were determined with the microtiterplate spectrophotometer Epoch 2 (Agilent).

On each 384well microtiter plate quadruplicate measurements were done for each sample, and for each bacterial strain 2 microtiter plates were used for the monomers **13a-T**, **13b-D**, **13c-T**, **13d-D**, and 3 for the polymers **10**, **11c-T** and **12c-T**, resulting in 8 and 12, respectively, single values per sample and bacterial strain.

Wells without bacteria were used as blank (positive control: no bacterial growth) and wells with cells but without compounds were the negative control (no antibiotic activity, full bacterial growth).

All data were normalized with respect to the average blank and negative control values according to:

100% x (value – blank) / (negative control – blank).

On the *P. aeruginosa* plate some positive control wells were obviously contaminated so that for the average blank only wells with OD_{600} < 0.2 were considered.

Then the average for all data points per substance and concentration were calculated, as well as the standard deviation (displayed as error bars), and plotted against the concentration.

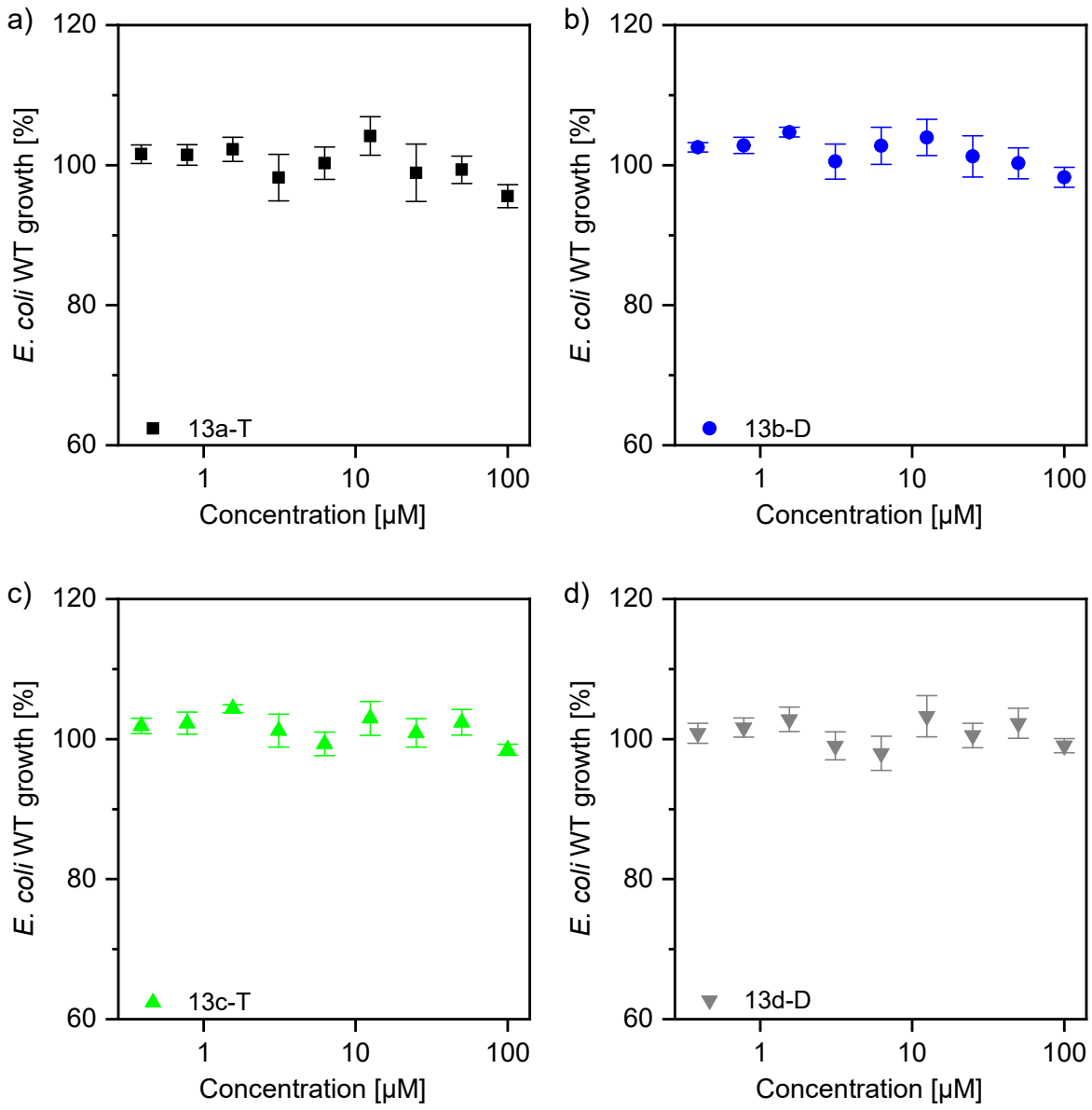


Figure S10: Growth of *E. coli* WT incubated with the monomers **13a-T**, **13b-D**, **13c-T** and **13d-D** at different concentrations. a) monomer **13a-T**, b) monomer **13b-D**, c) monomer **13c-T**, d) monomer **13d-D**.

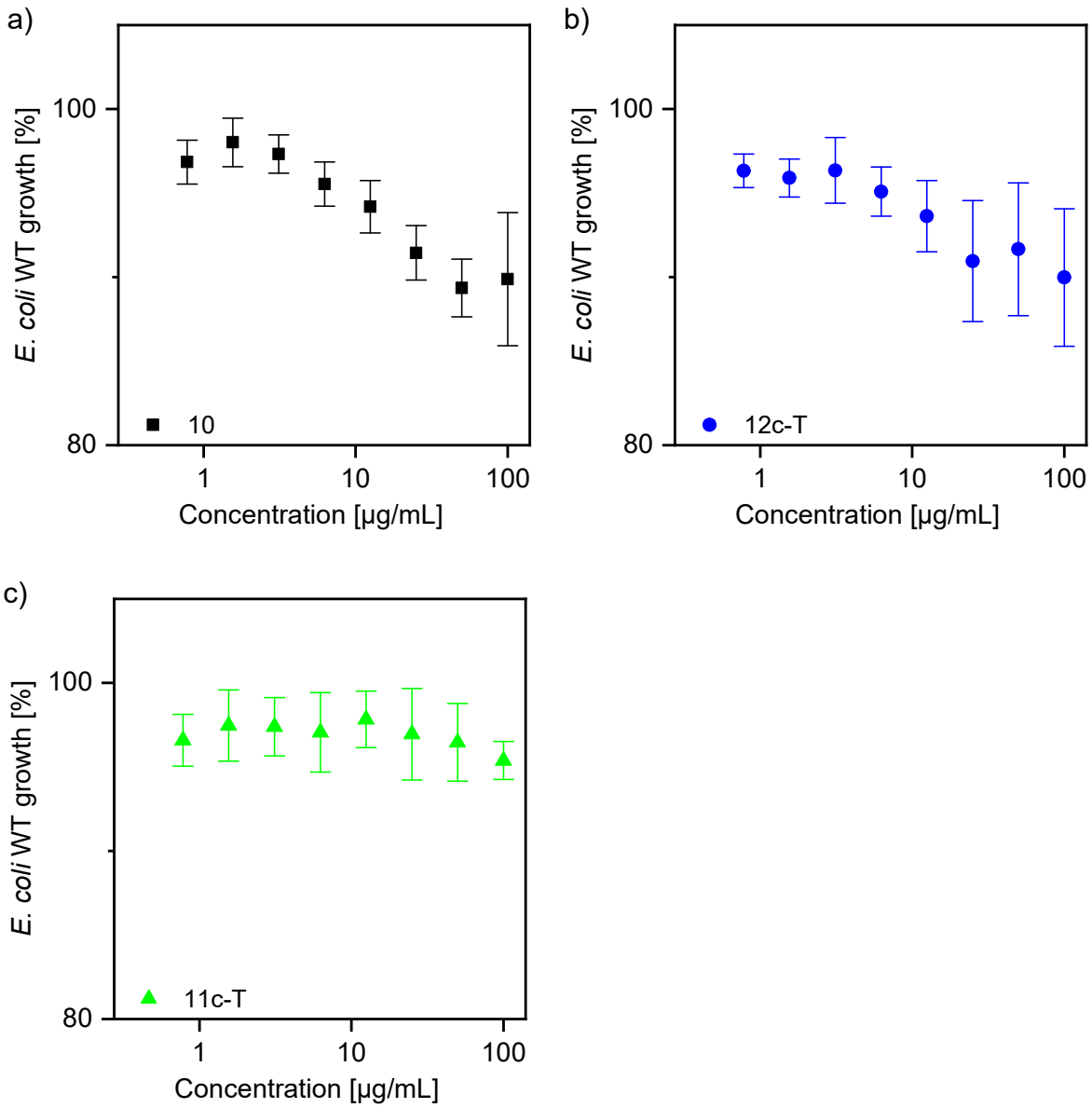


Figure S11: Growth of *E. coli* WT incubated with the polymers **10**, **12c-T** and **11c-T** at different concentrations. a) polymer **10**, b) polymer **12c-T**, c) polymer **11c-T**.

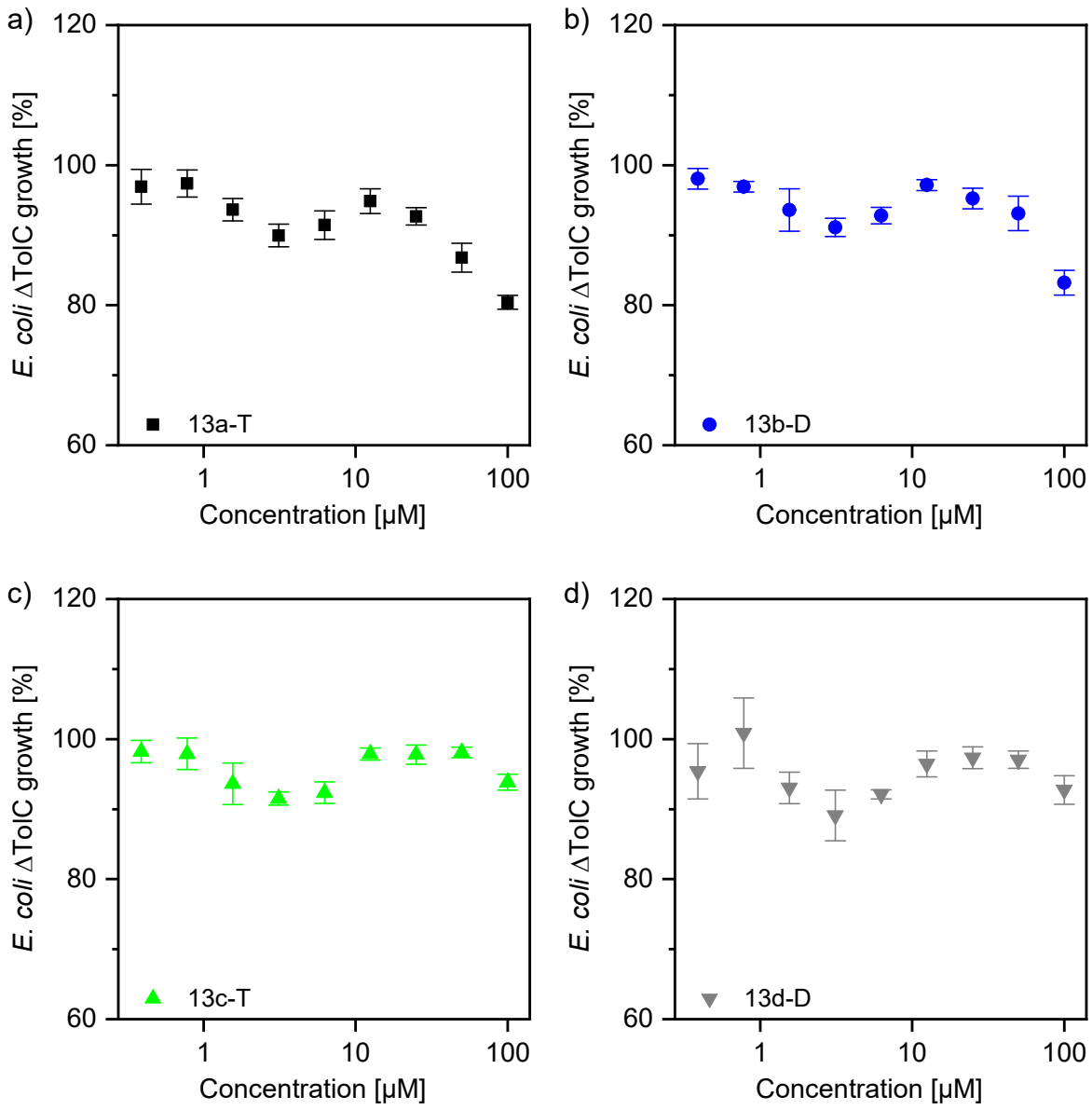


Figure S12: Growth of *E. coli* ΔTolC incubated with the monomers **13a-T**, **13b-D**, **13c-T** and **13d-D** at different concentrations. a) monomer **13a-T**, b) monomer **13b-D**, c) monomer **13c-T**, d) monomer **13d-D**.

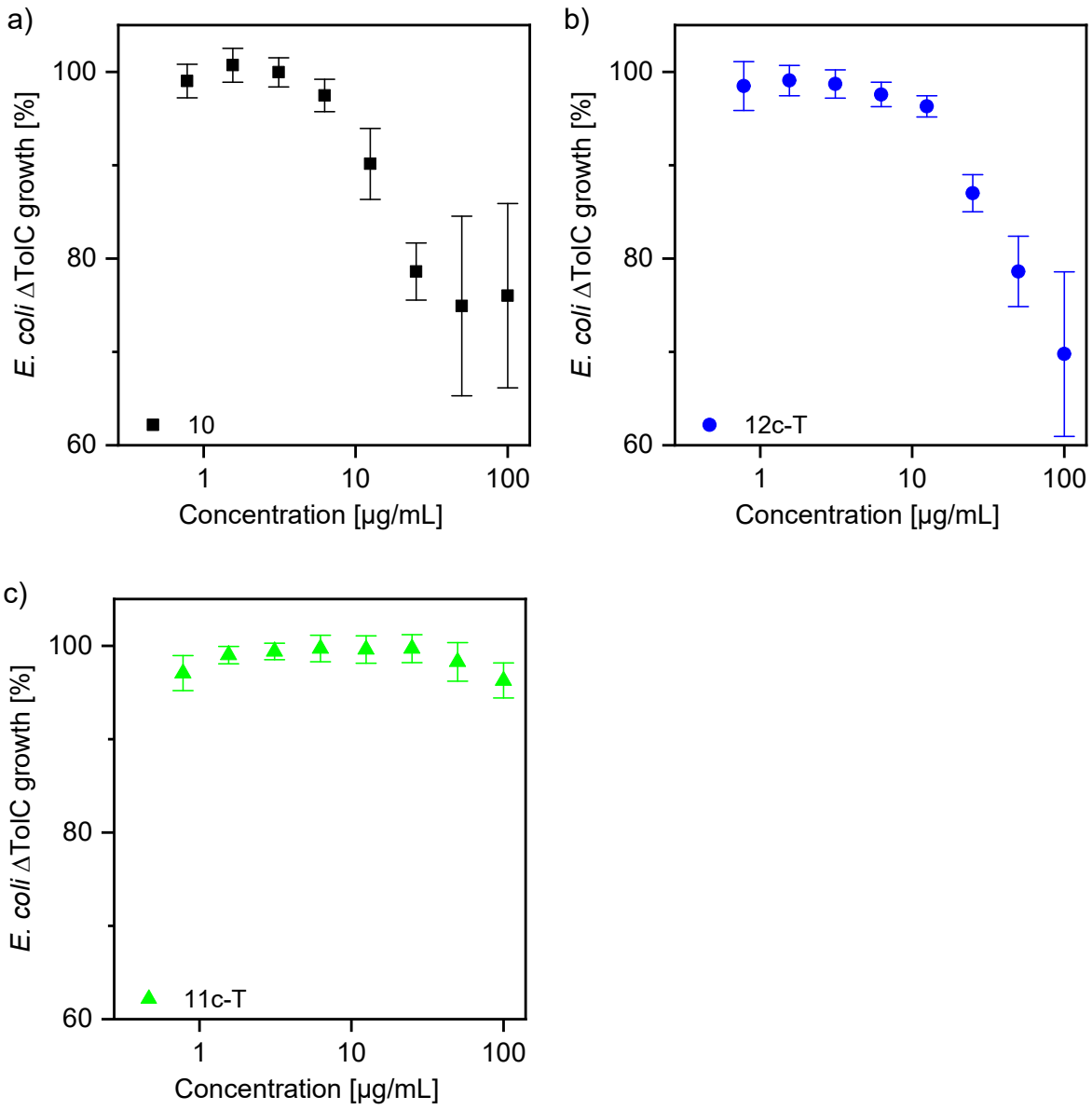


Figure S13: Growth of *E. coli* ΔTolC incubated with the polymers **10**, **12c-T** and **11c-T** at different concentrations. a) polymer **10**, b) polymer **12c-T**, c) polymer **11c-T**.

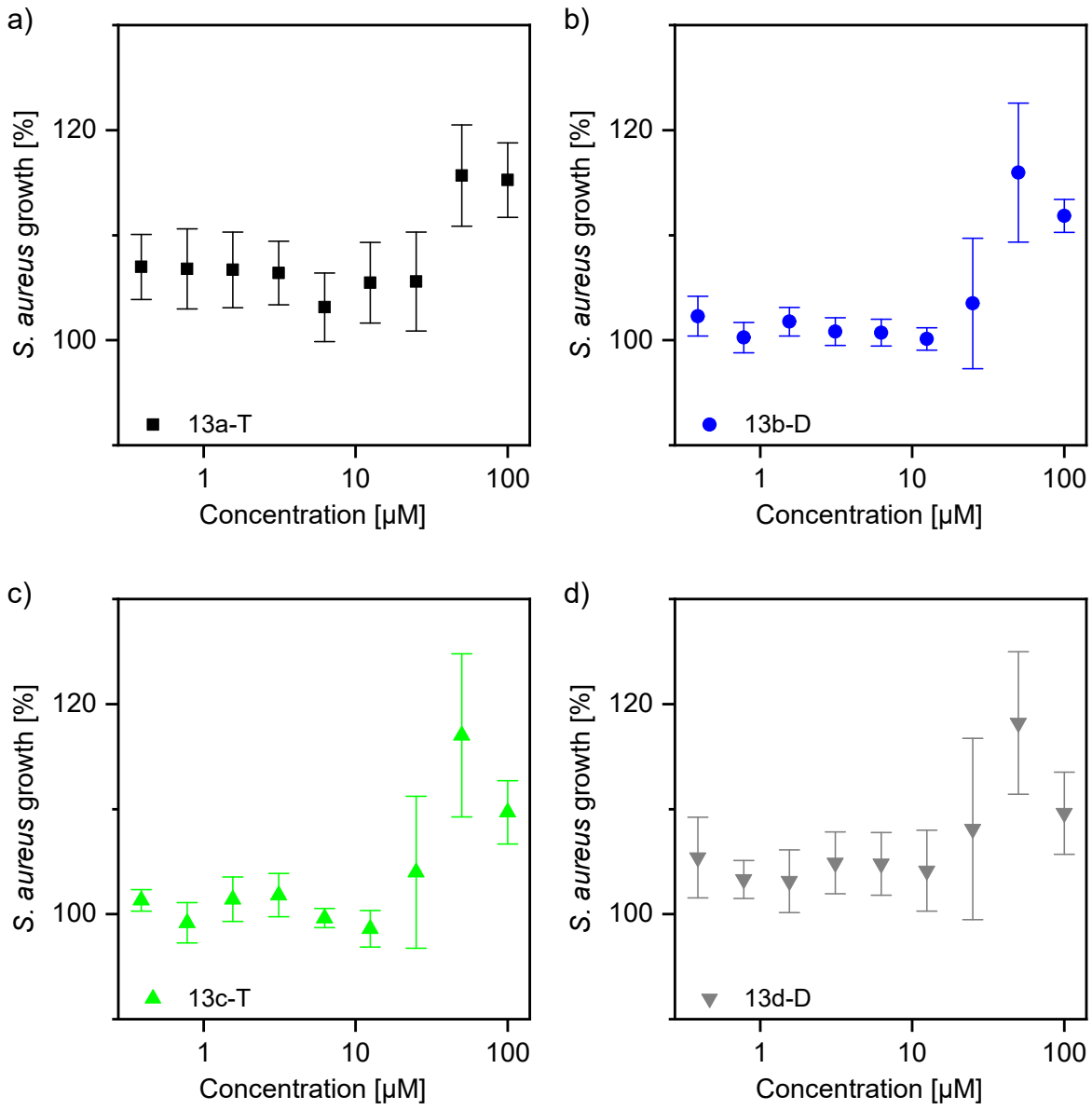


Figure S14: Growth of *S. aureus* incubated with the monomers **13a-T**, **13b-D**, **13c-T** and **13d-D** at different concentrations. a) monomer **13a-T**, b) monomer **13b-D**, c) monomer **13c-T**, d) monomer **13d-D**.

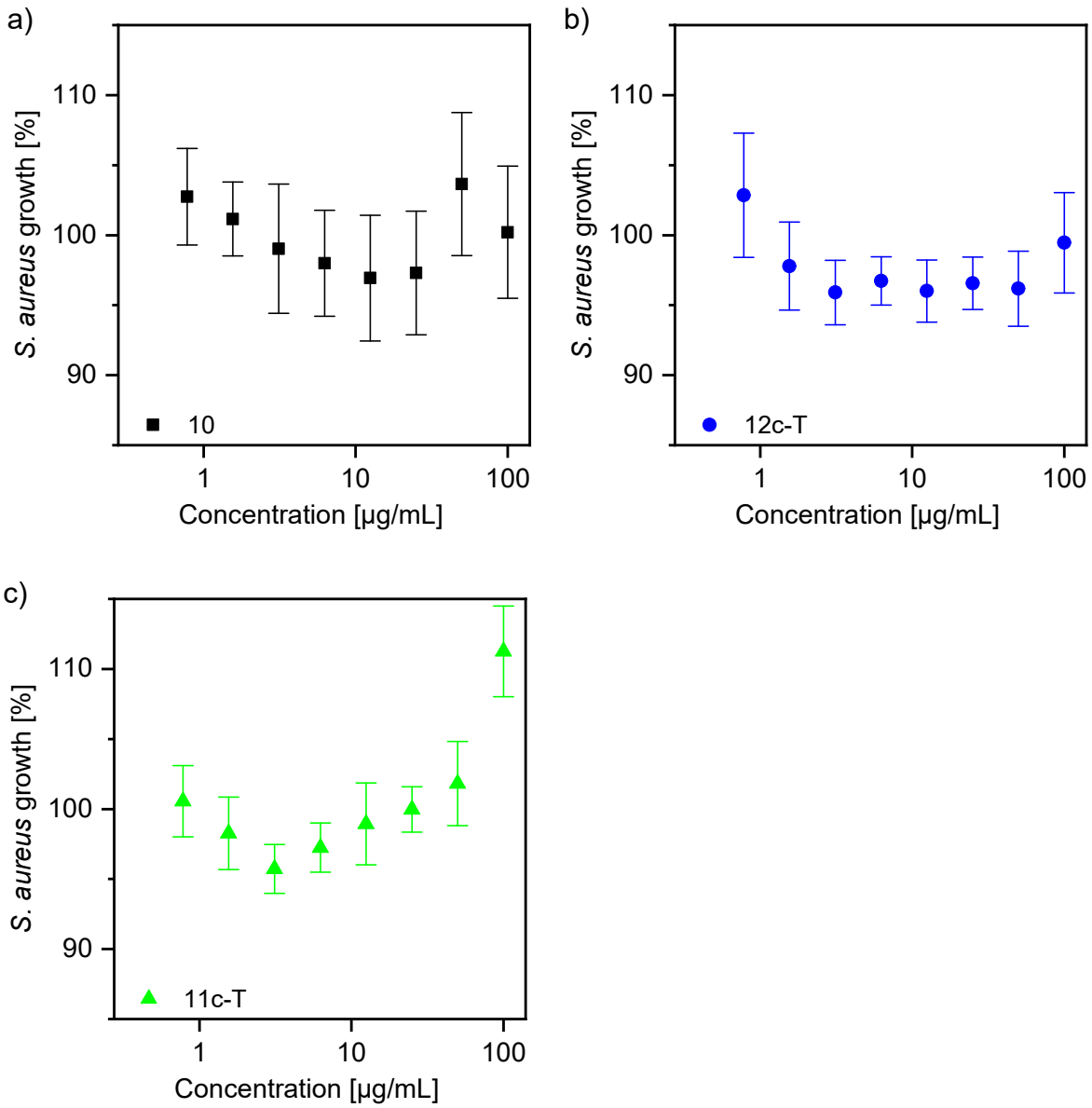


Figure S15: Growth of *S. aureus* incubated with the polymers **10**, **12c-T** and **11c-T** at different concentrations. a) polymer **10**, b) polymer **12c-T**, c) polymer **11c-T**.

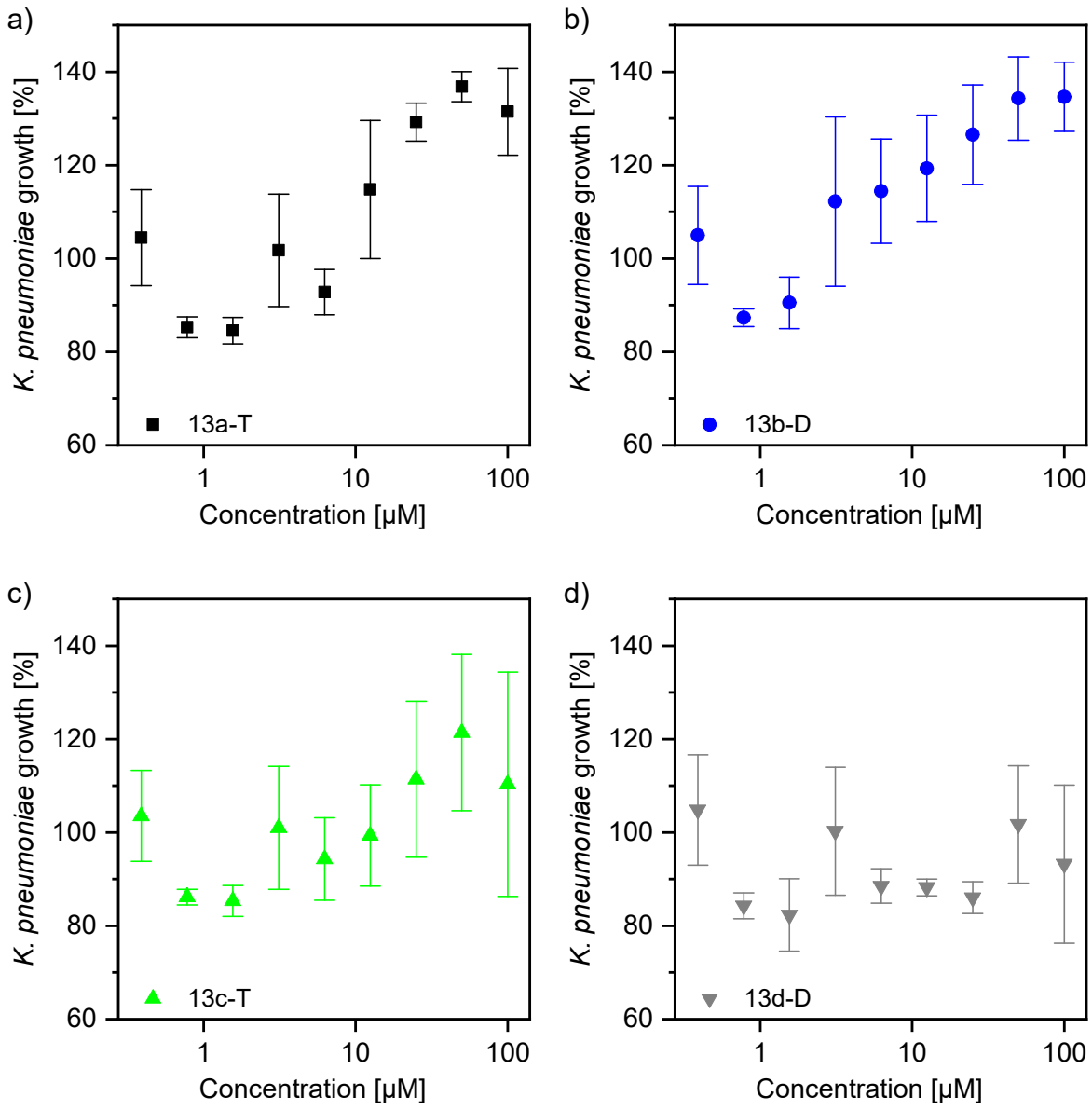


Figure S16: Growth of *K. pneumoniae* incubated with the monomers **13a-T**, **13b-D**, **13c-T** and **13d-D** at different concentrations. a) monomer **13a-T**, b) monomer **13b-D**, c) monomer **13c-T**, d) monomer **13d-D**.

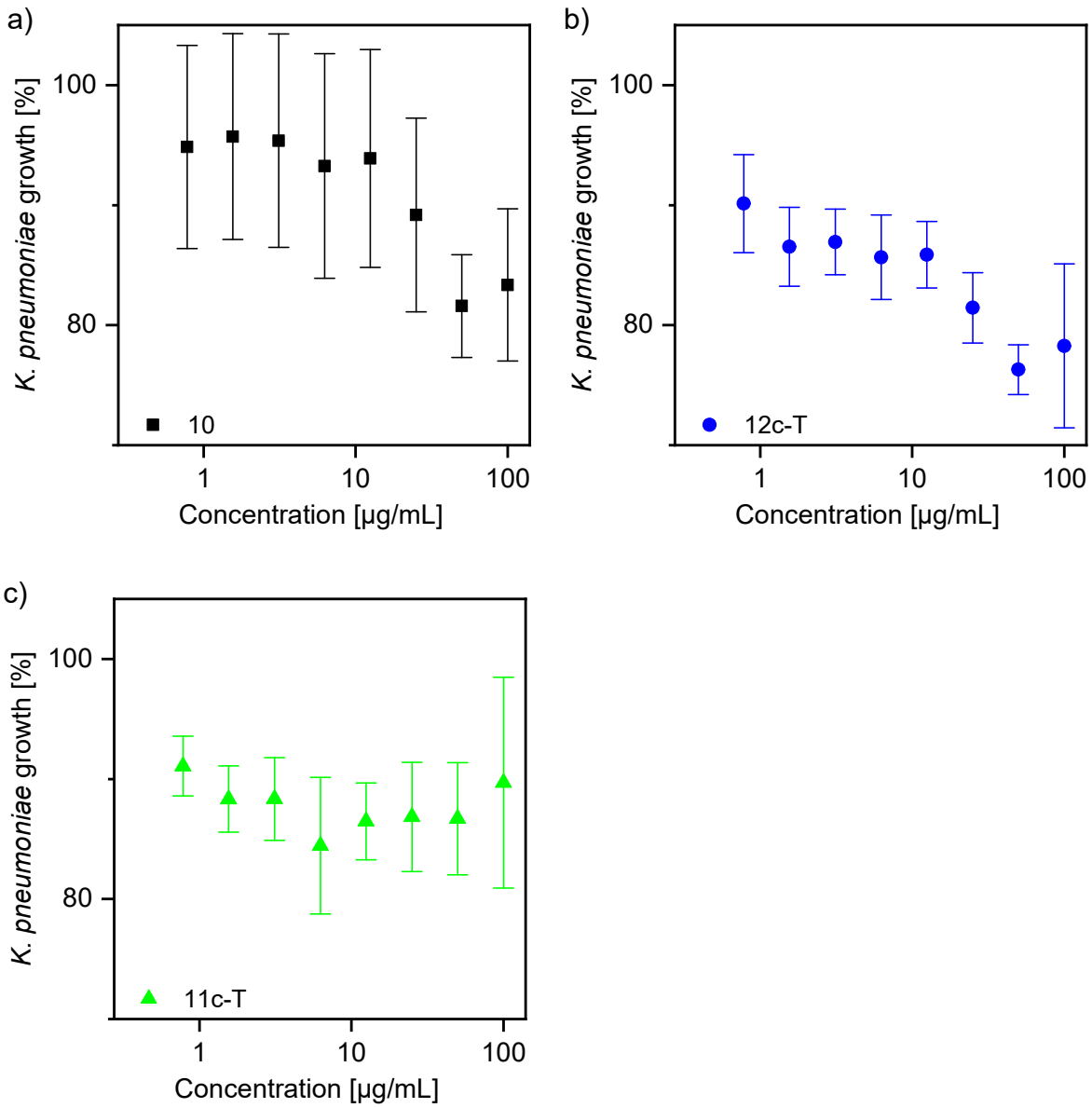


Figure S17: Growth of *K. pneumoniae* incubated with the polymers **10**, **12c-T** and **11c-T** at different concentrations. a) polymer **10**, b) polymer **12c-T**, c) polymer **11c-T**.

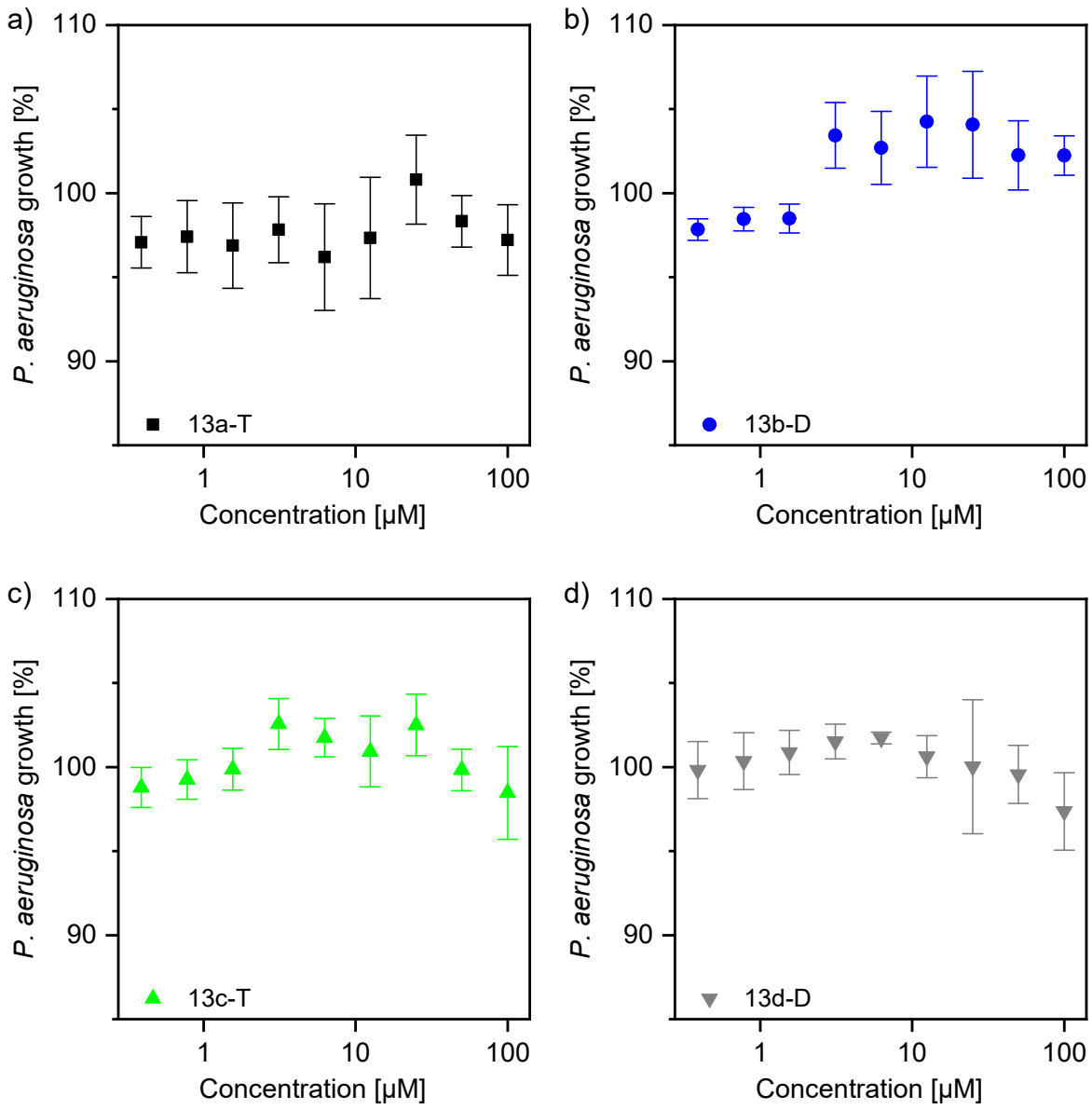


Figure S18: Growth of *P. aeruginosa* incubated with the monomers **13a-T**, **13b-D**, **13c-T** and **13d-D** at different concentrations. a) monomer **13a-T**, b) monomer **13b-D**, c) monomer **13c-T**, d) monomer **13d-D**.

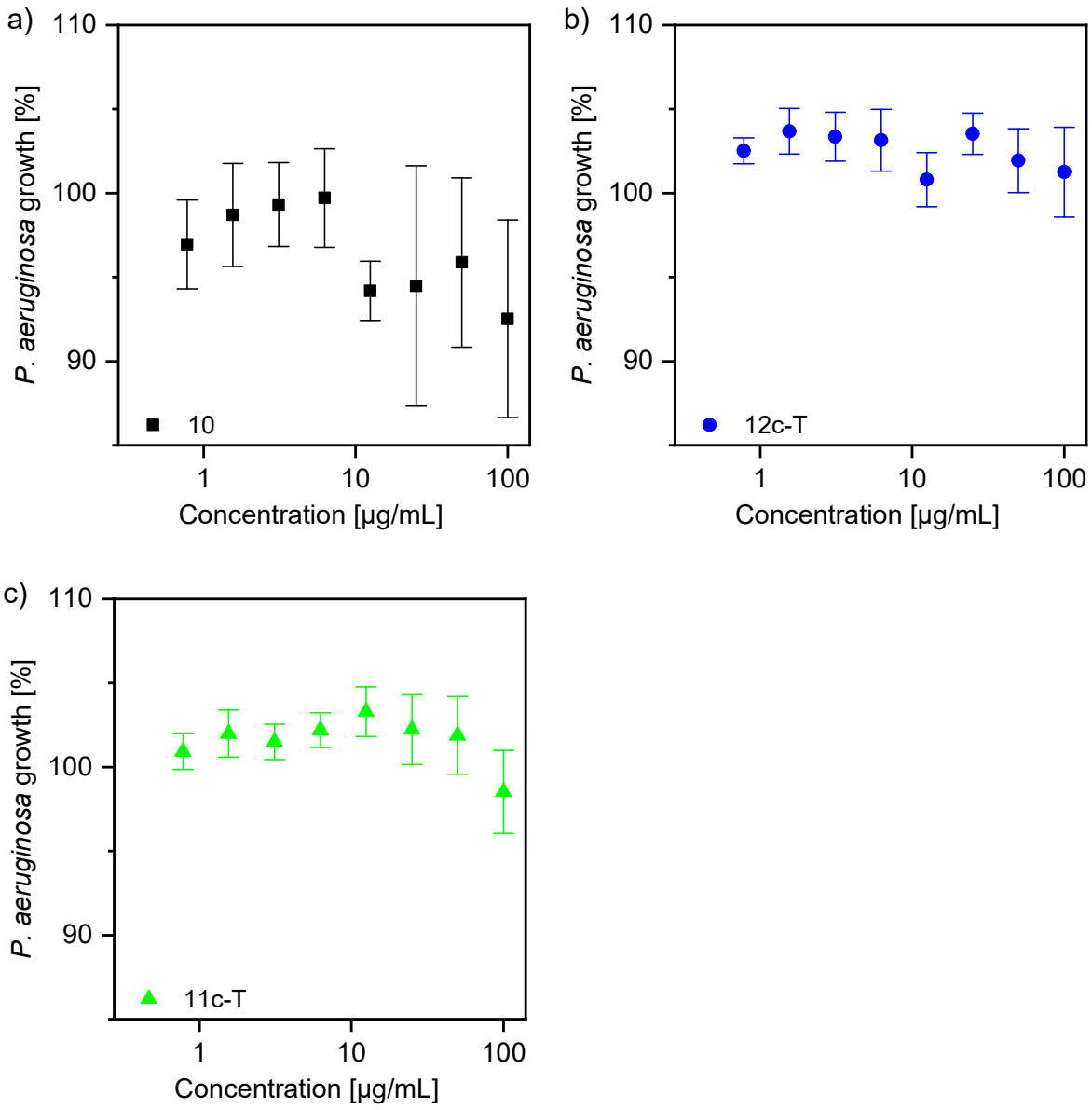
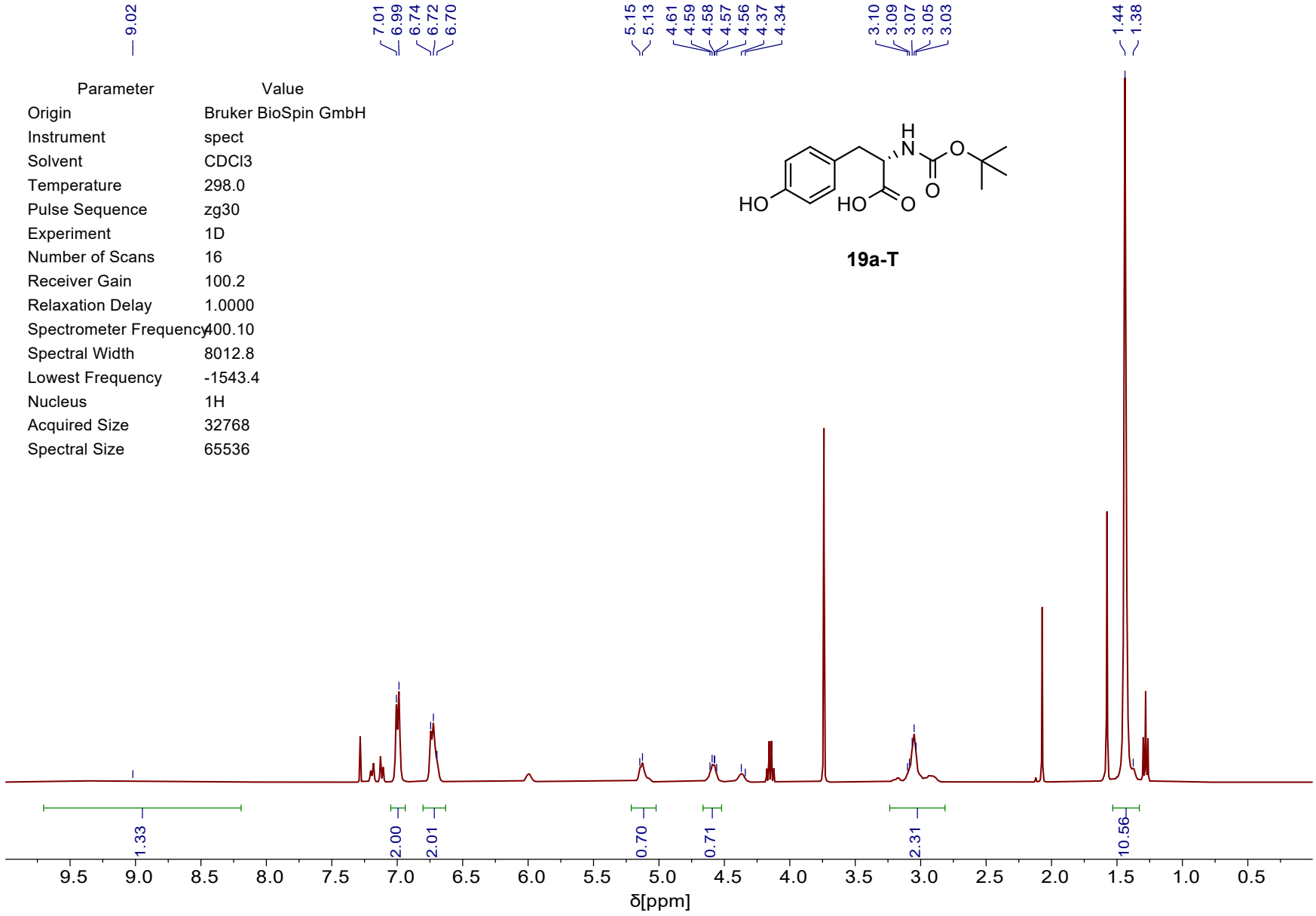
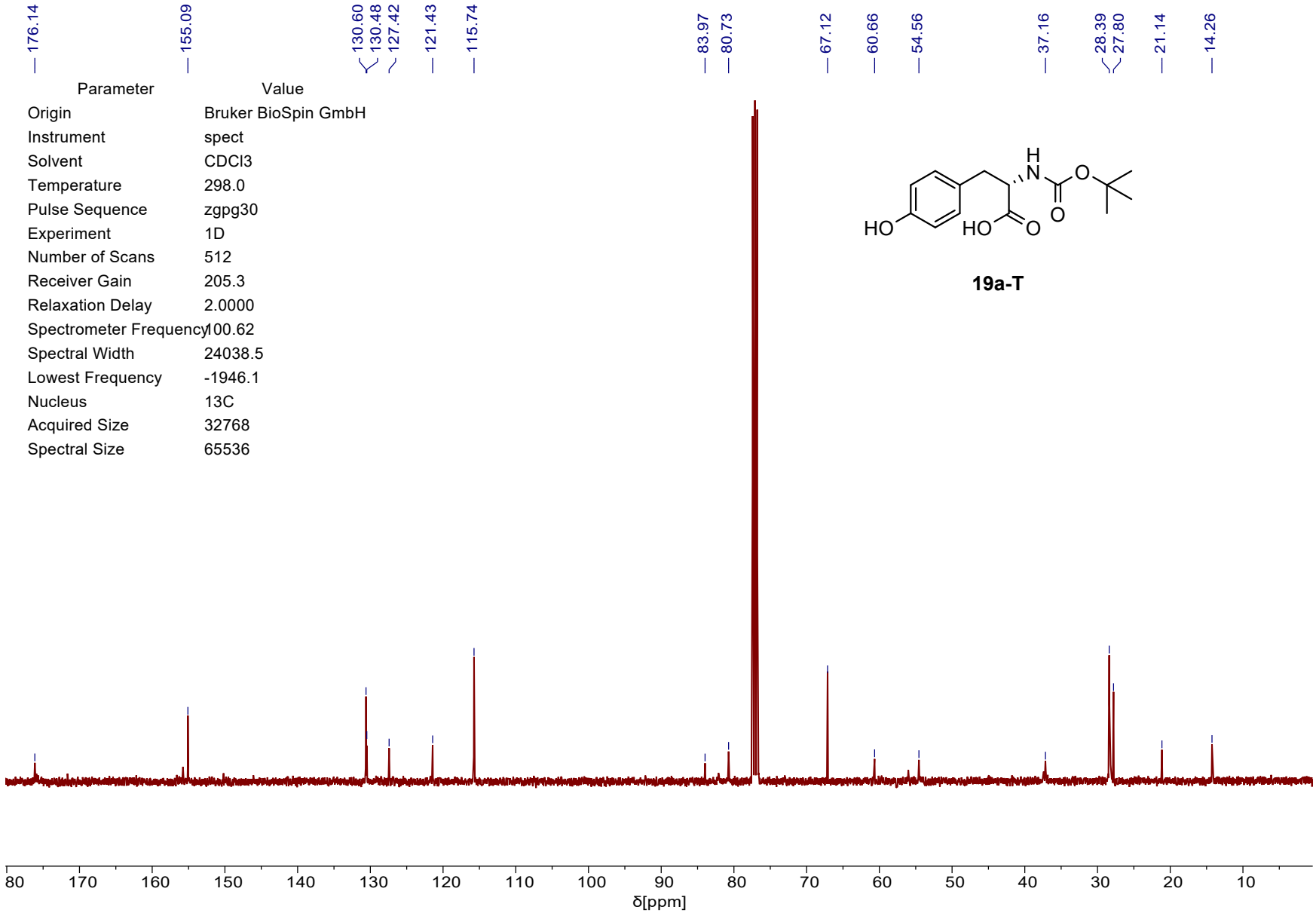
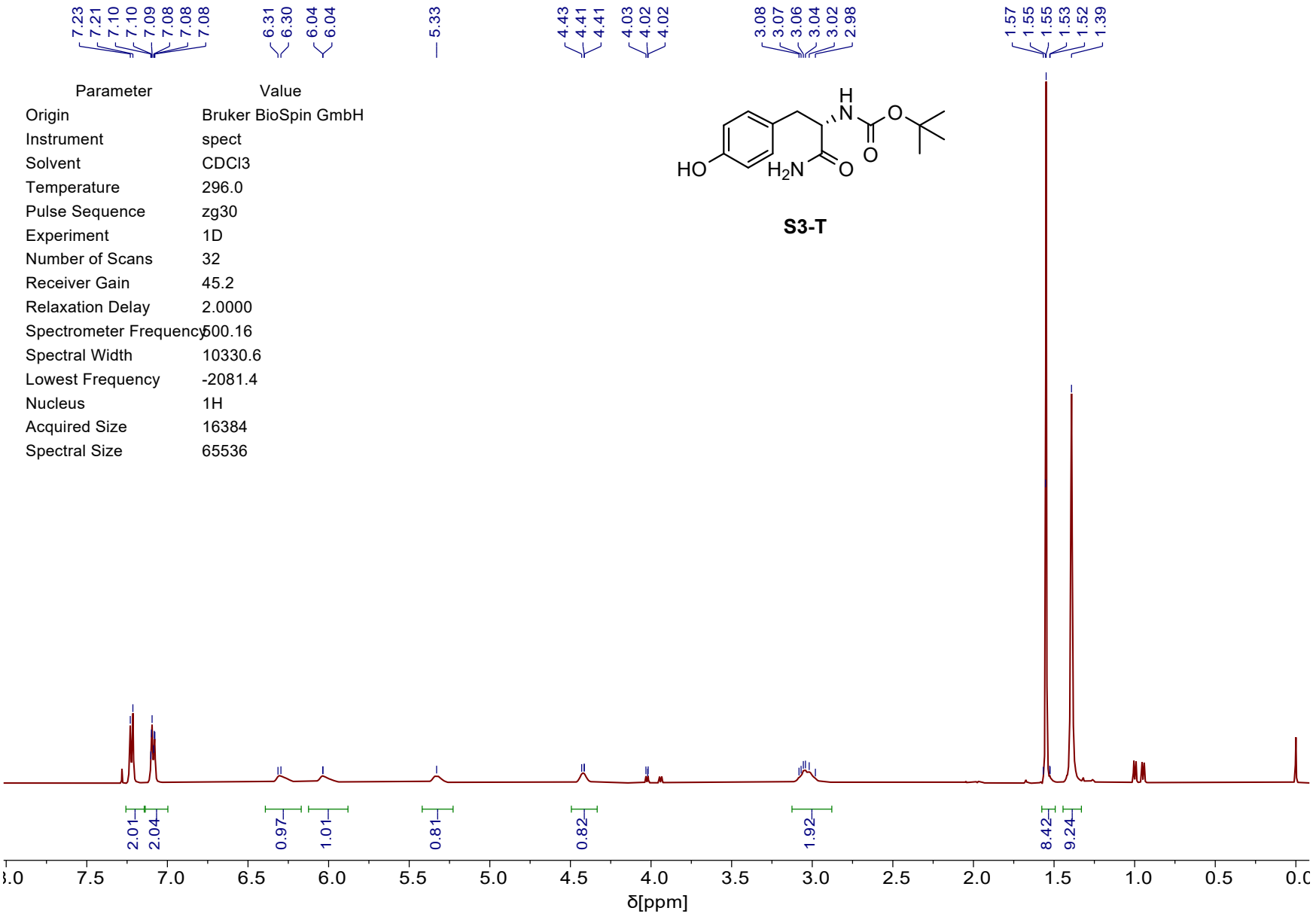


Figure S19: Growth of *P. aeruginosa* incubated with the polymers **10**, **12c-T** and **11c-T** at different concentrations. a) polymer **10**, b) polymer **12c-T**, c) polymer **11c-T**.

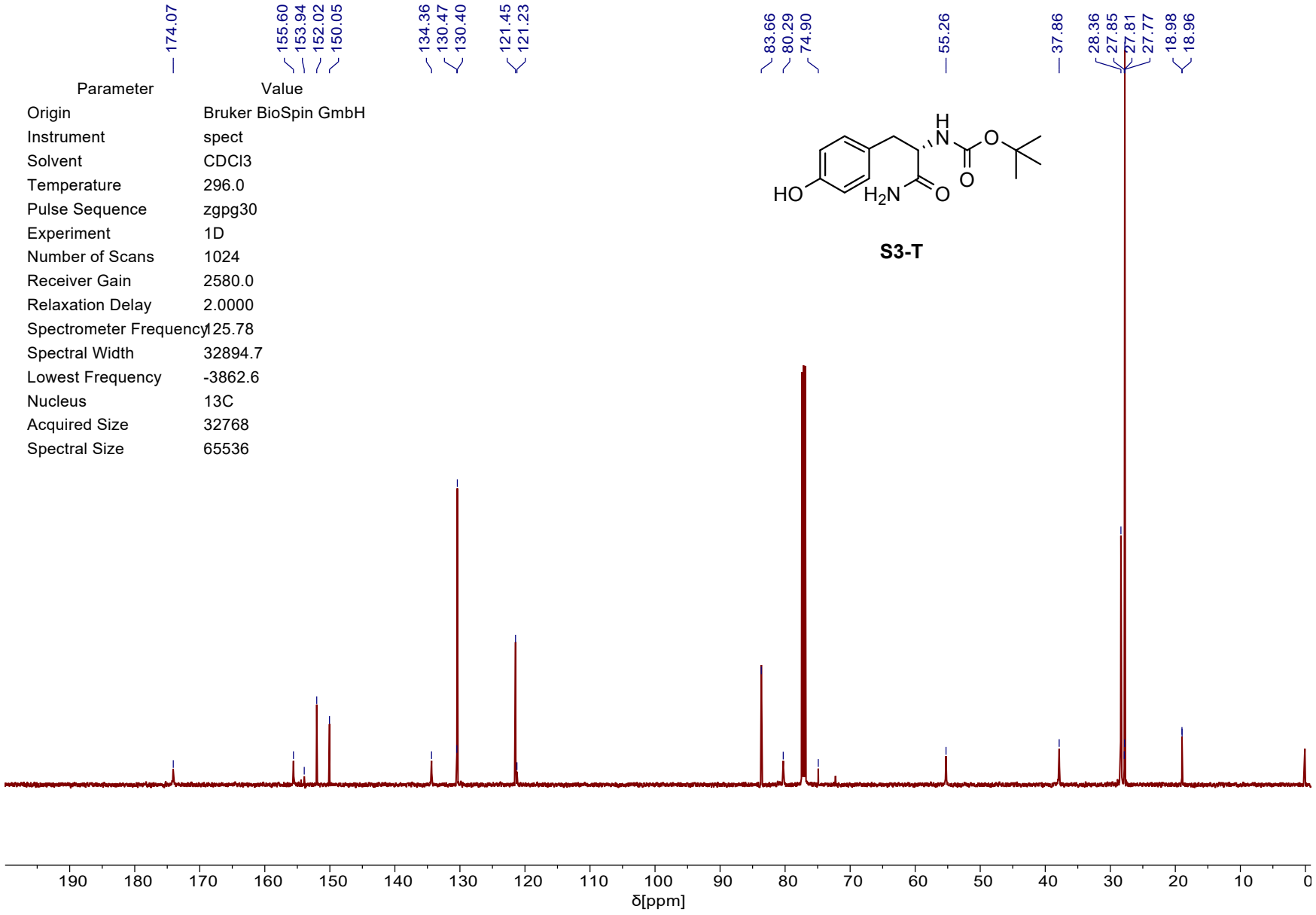
9. NMR spectra


9.02
7.01
6.99
6.74
6.72
6.70
5.15
5.13
4.61
4.59
4.58
4.57
4.56
4.37
4.34
3.10
3.09
3.07
3.05
3.03
1.44
1.38
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 100.2
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1543.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
HO
HO
H
N
O
O
O
19a-T
1.33
2.00
2.01
0.70
0.71
2.31
10.56
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]


176.14
155.09
130.60
130.48
127.42
121.43
115.74
83.97
80.73
67.12
60.66
54.56
37.16
28.39
27.80
21.14
14.26
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1946.1
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
HO
HO
O
O
H
N
O
19a-T
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]


7.23
7.21
7.10
7.10
7.09
7.08
7.08
7.08
6.31
6.30
6.04
6.04
5.33
4.43
4.41
4.41
4.03
4.02
4.02
3.08
3.07
3.06
3.04
3.02
2.98
1.57
1.55
1.55
1.53
1.52
1.39
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 32
Receiver Gain 45.2
Relaxation Delay 2.0000
Spectrometer Frequency 500.16
Spectral Width 10330.6
Lowest Frequency -2081.4
Nucleus 1H
Acquired Size 16384
Spectral Size 65536
HO
H2N
H
N
O
O
O
2.01
2.04
0.97
1.01
0.81
0.82
1.92
8.42
9.24
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]

S3-T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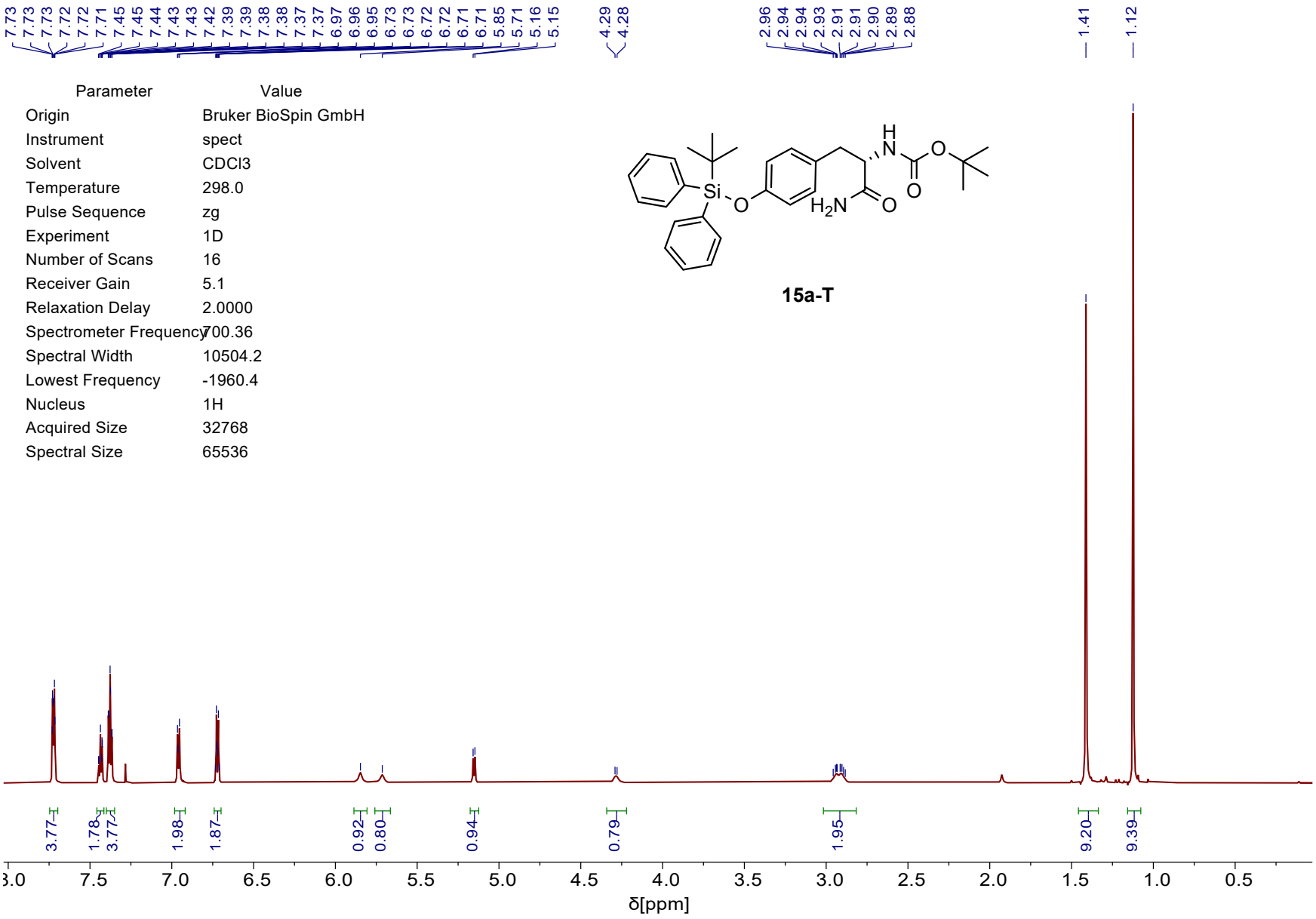
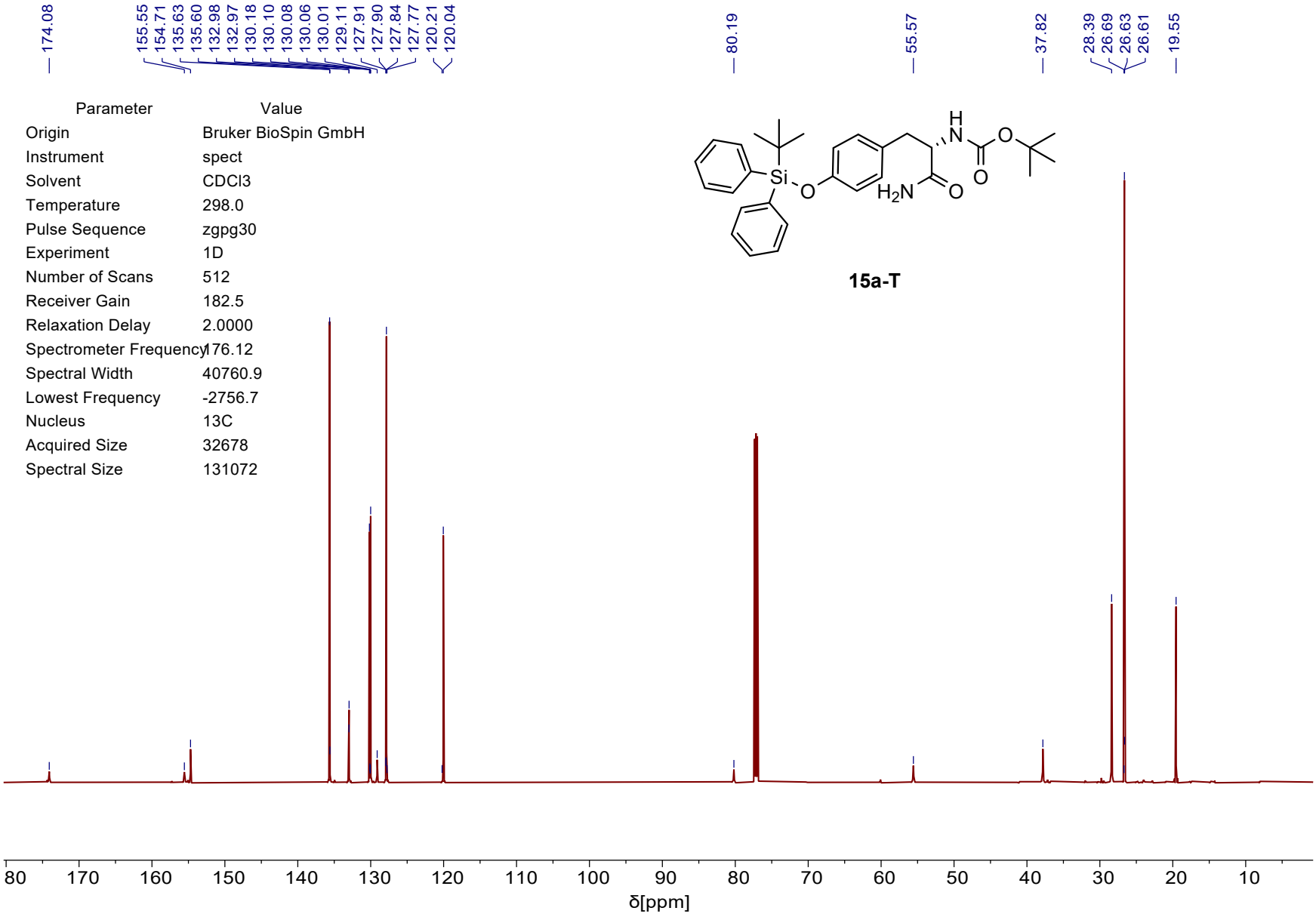
155.60
153.94
152.02
150.05
134.36
130.47
130.40
121.45
121.23
83.66
80.29
74.90
55.26
37.86
28.36
27.85
27.81
27.77
18.98
18.96
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1024
Receiver Gain 2580.0
Relaxation Delay 2.0000
Spectrometer Frequency 125.78
Spectral Width 32894.7
Lowest Frequency -3862.6
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
HO
H2N
O
N
H
O
O
S3-T
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ[ppm]


7.73 7.73 7.73 7.72 7.72 7.71 7.45 7.45 7.44 7.43 7.43 7.42 7.39 7.39 7.38 7.38 7.37 7.37 6.97 6.96 6.95 6.73 6.72 6.72 6.71 6.71 5.85 5.71 5.16 5.15
4.29 4.28
2.96 2.94 2.94 2.93 2.91 2.91 2.90 2.89 2.88
1.41
1.12
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Experiment 1D
Number of Scans 16
Receiver Gain 5.1
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
15a-T
3.77 1.78 3.77 1.98 1.87 0.92 0.80 0.94 0.79 1.95 9.20 9.39
δ[ppm]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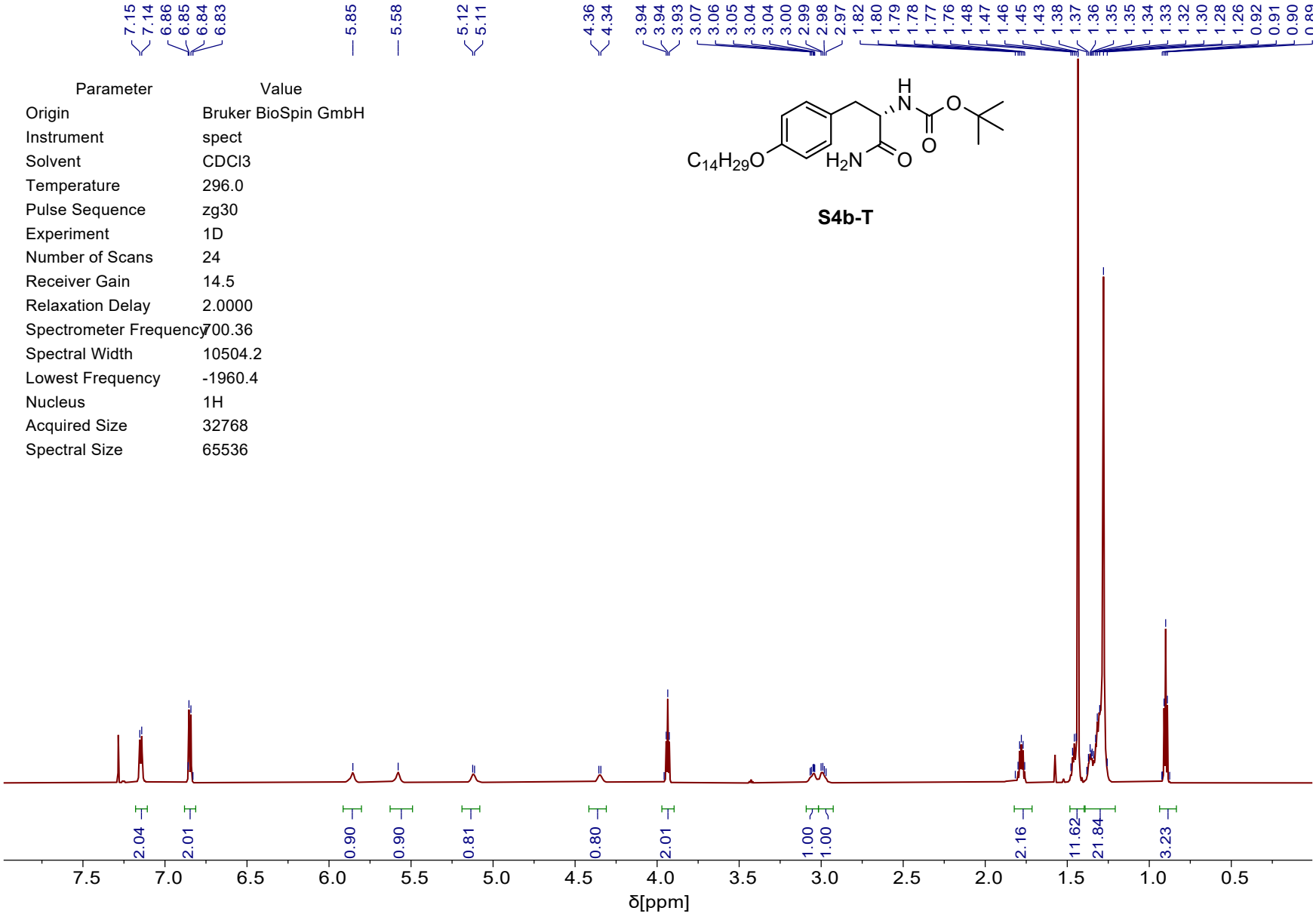
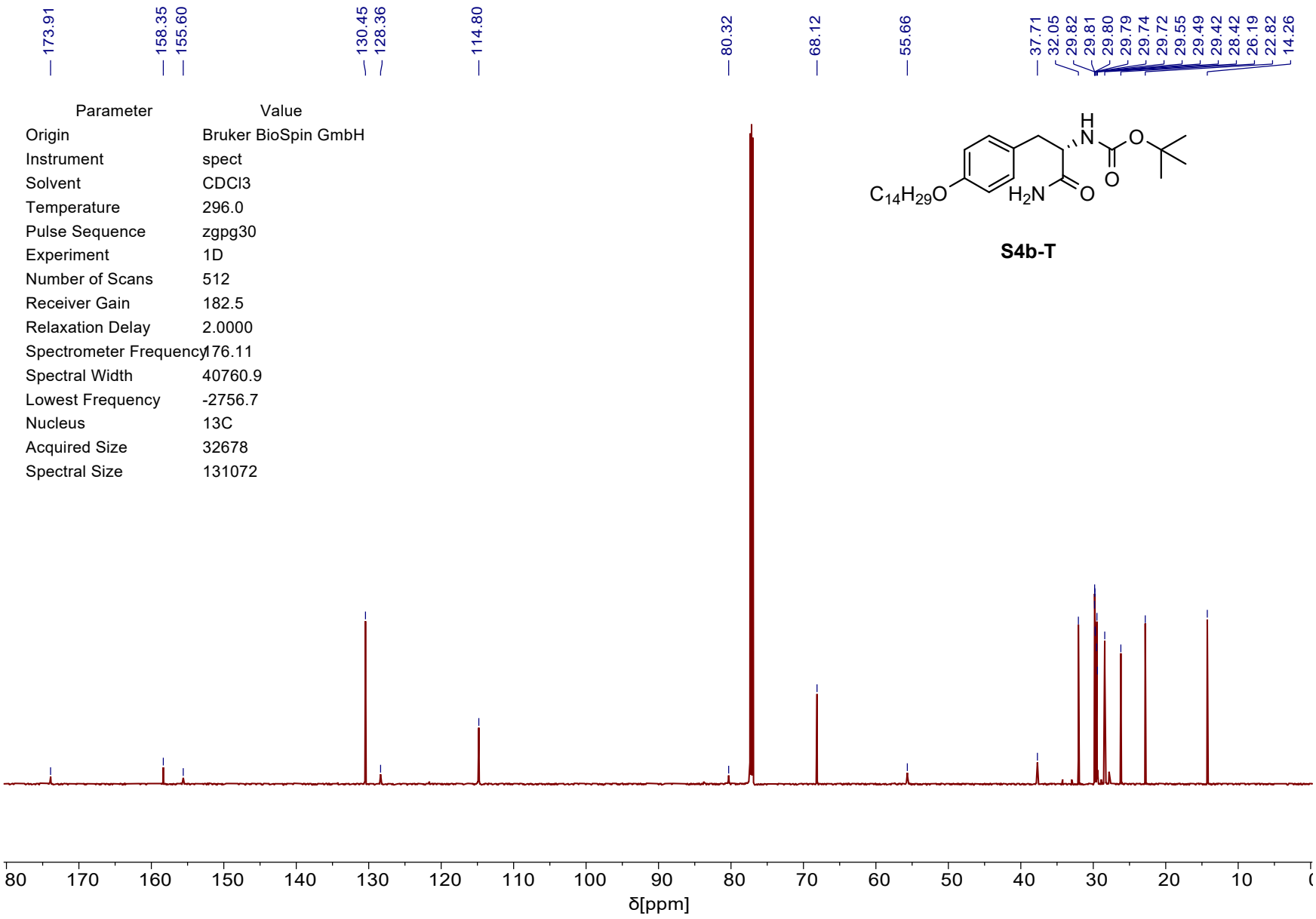
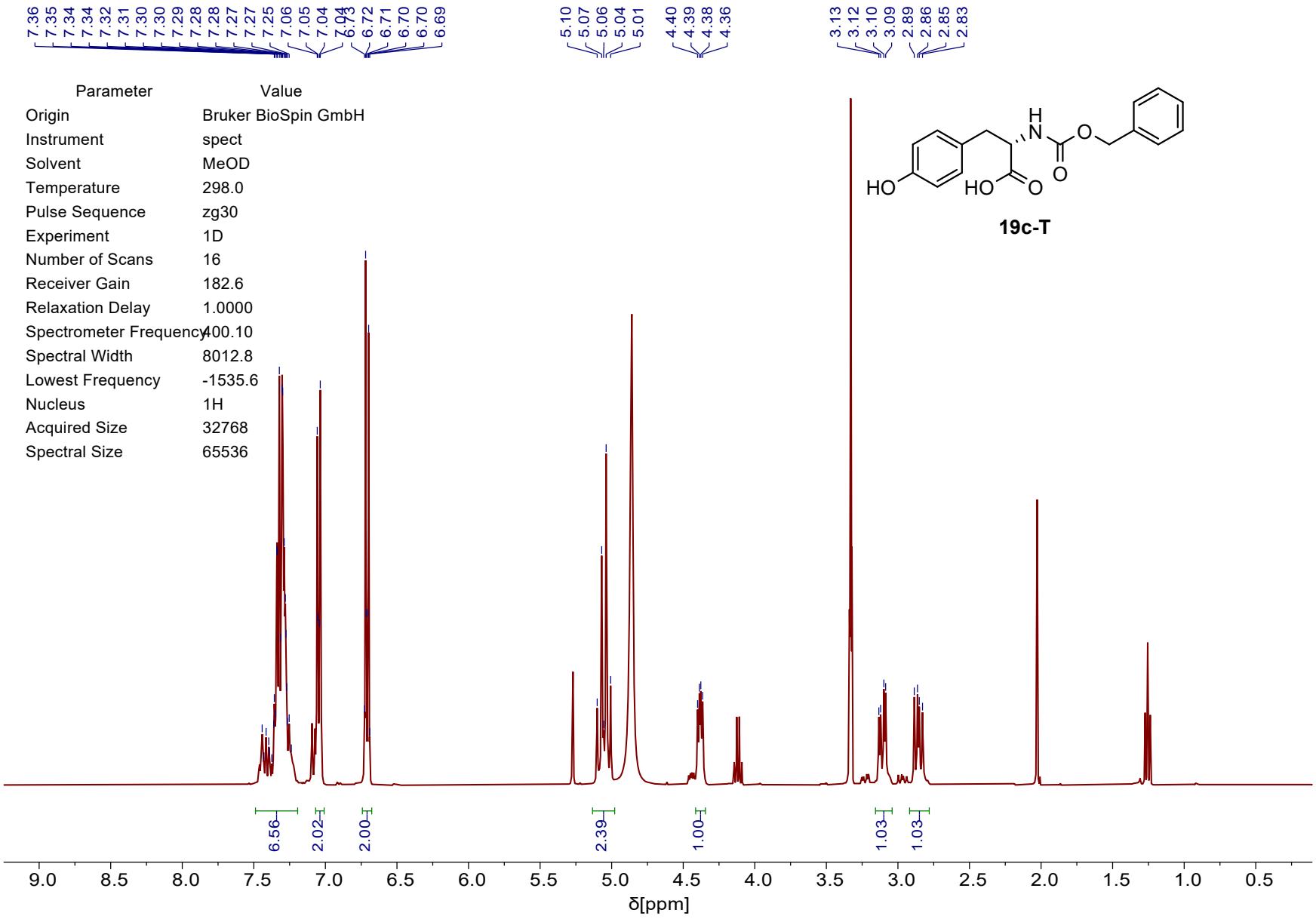
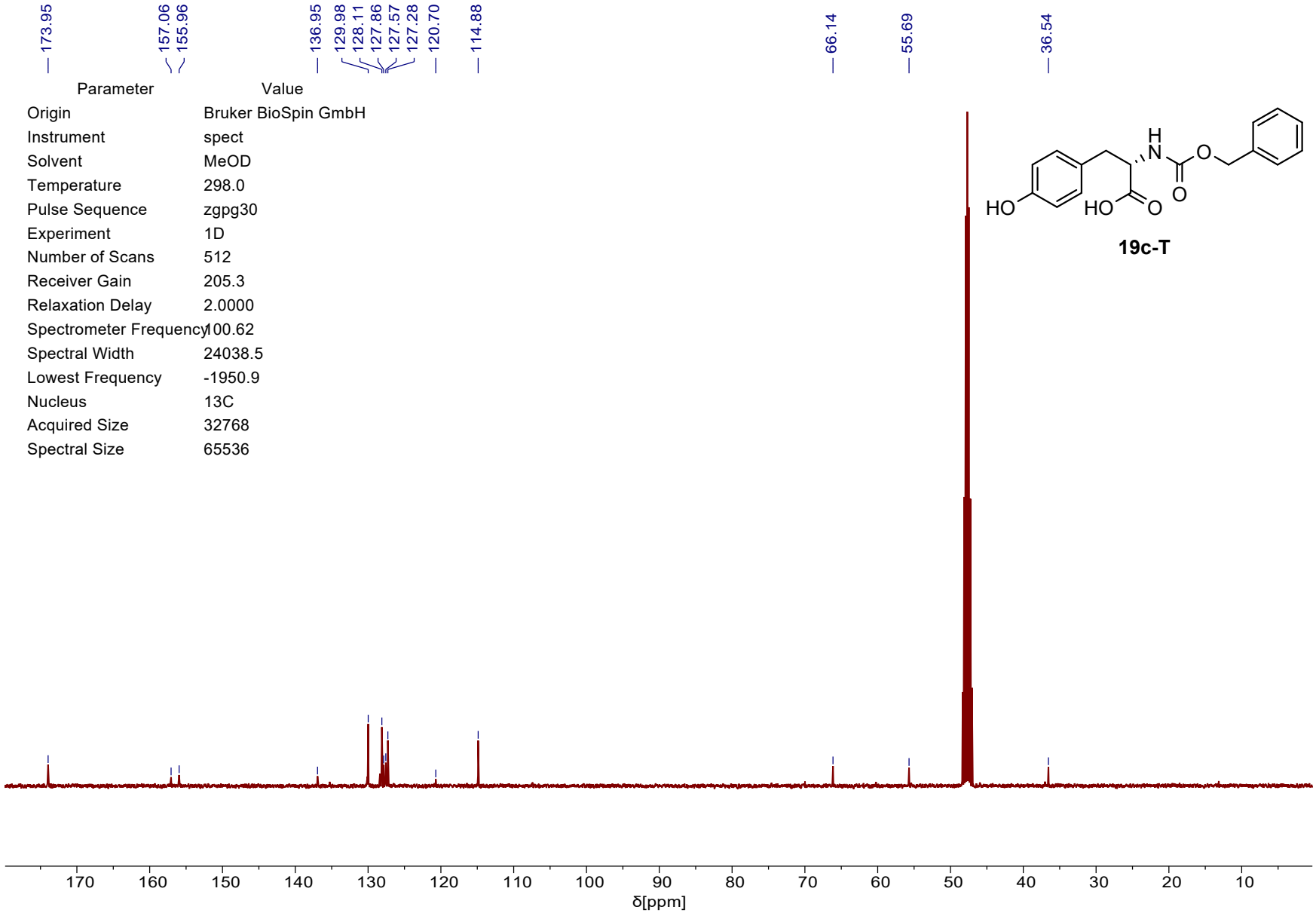
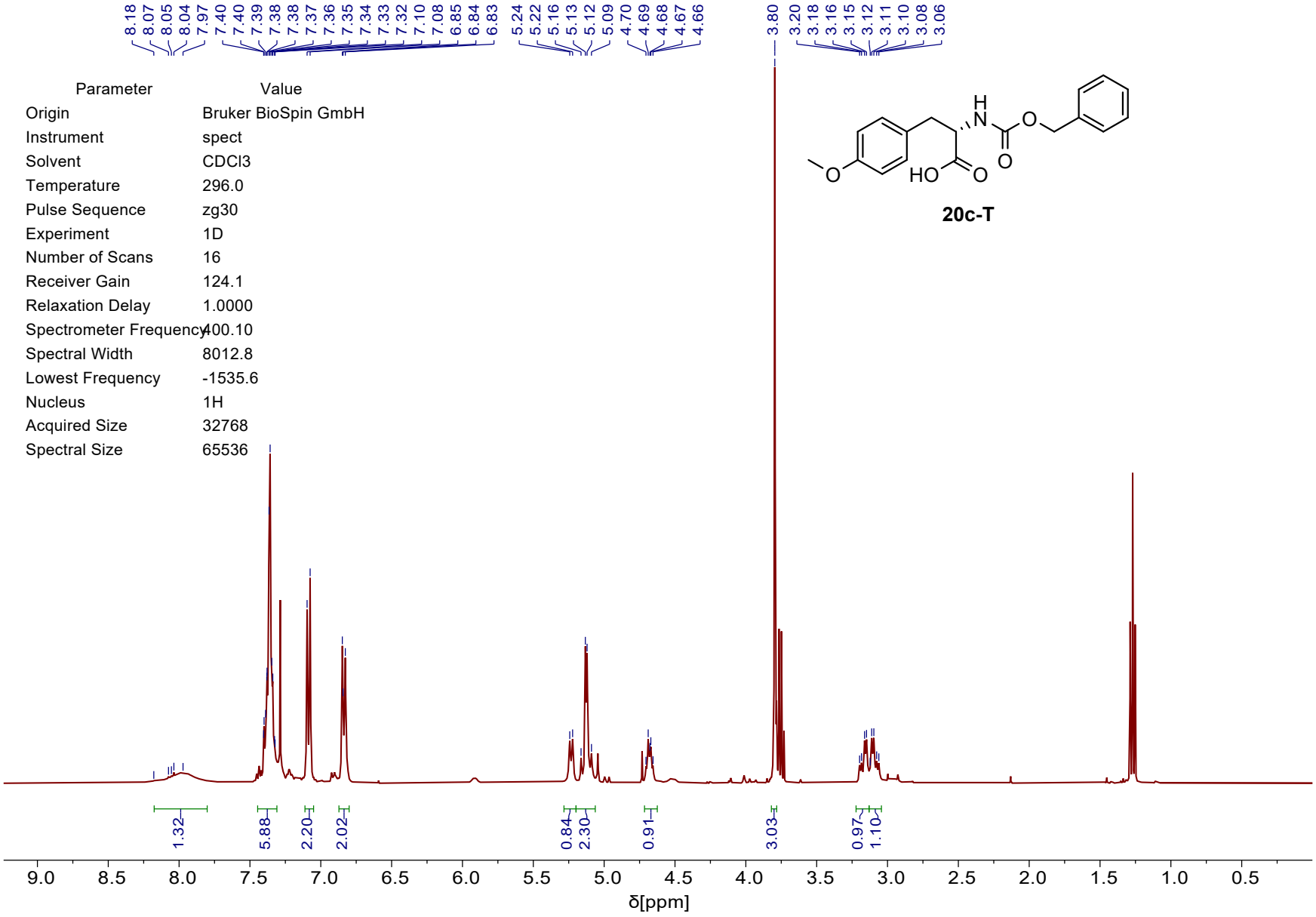
155.55
154.71
135.63
135.60
132.98
132.97
130.18
130.10
130.08
130.06
130.01
129.11
127.91
127.90
127.84
127.77
120.21
120.04
80.19
55.57
37.82
28.39
26.69
26.63
26.61
19.55
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
15a-T
δ[ppm]

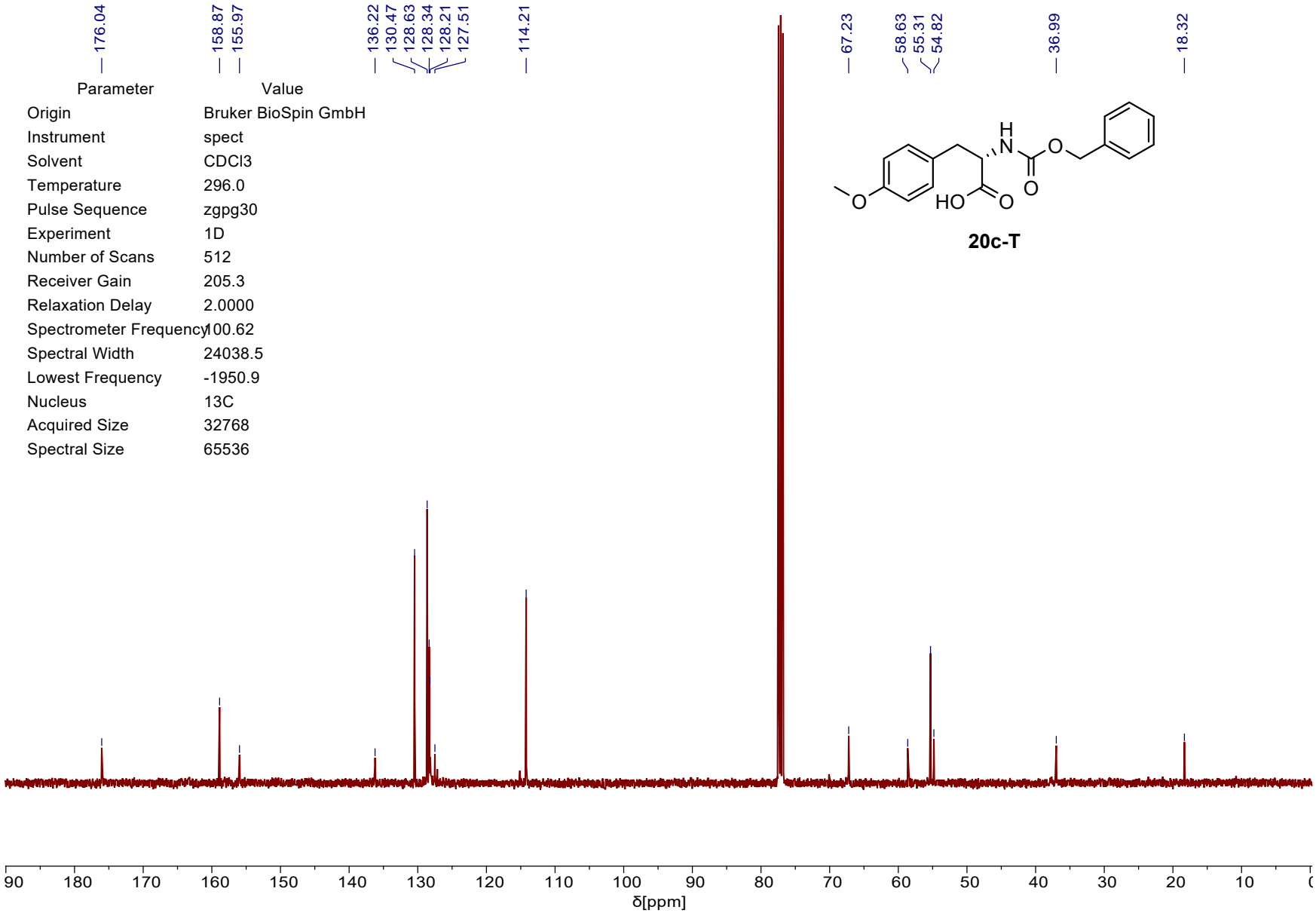

7.15
7.14
6.86
6.85
6.84
6.83
5.85
5.58
5.12
5.11
4.36
4.34
3.94
3.94
3.93
3.07
3.06
3.05
3.04
3.04
3.00
2.99
2.98
2.97
1.82
1.80
1.79
1.78
1.77
1.76
1.48
1.47
1.46
1.45
1.43
1.38
1.37
1.36
1.35
1.35
1.34
1.33
1.32
1.30
1.28
1.26
0.92
0.91
0.90
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 14.5
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
H
N
O
O
C14H29O
H2N
O
S4b-T
2.04
2.01
0.90
0.90
0.81
0.80
2.01
1.00
1.00
2.16
11.62
21.84
3.23
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]

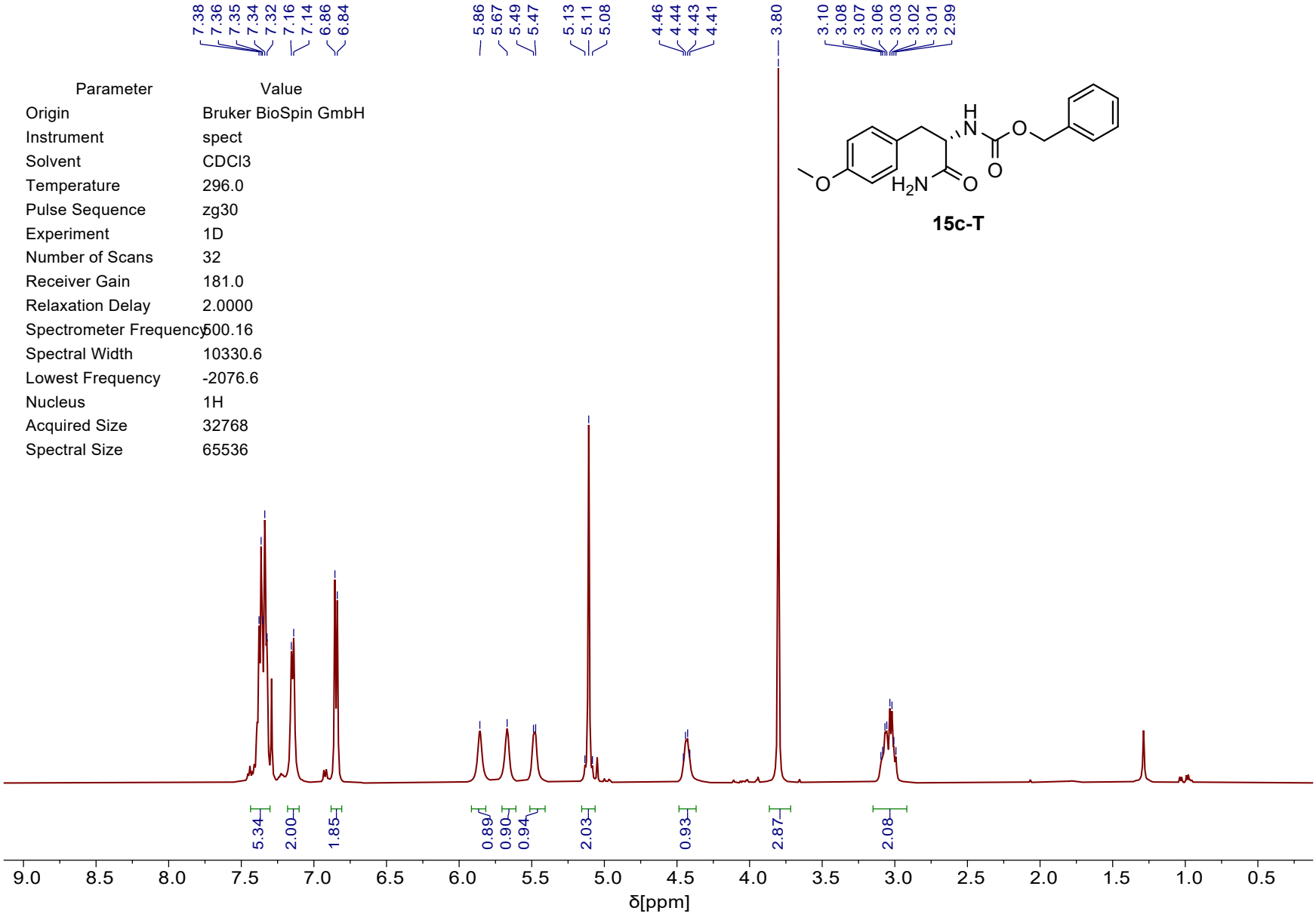

173.91
158.35
155.60
130.45
128.36
114.80
80.32
68.12
55.66
37.71
32.05
29.82
29.81
29.80
29.79
29.74
29.72
29.55
29.49
29.42
28.42
26.19
22.82
14.26
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.11
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
C14H29O
H2N
S4b-T
δ[ppm]

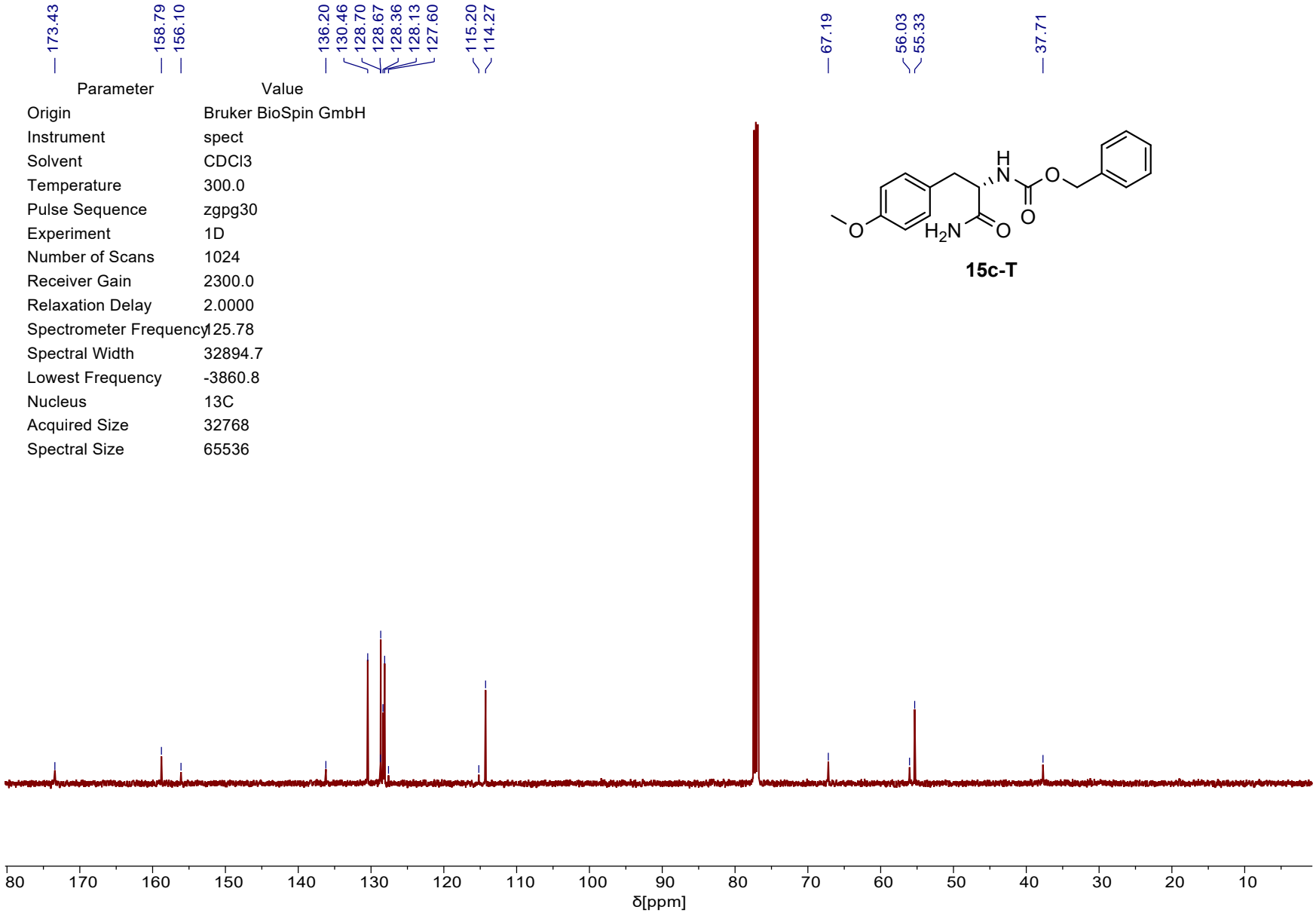

7.36 7.35 7.34 7.34 7.32 7.31 7.30 7.30 7.29 7.28 7.28 7.27 7.27 7.25 7.06 7.05 7.04 7.04 6.73 6.72 6.71 6.70 6.70 6.69
5.10 5.07 5.06 5.04 5.01
4.40 4.39 4.38 4.36
3.13 3.12 3.10 3.09 2.89 2.86 2.85 2.83
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 182.6
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1535.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
HO
HO
O
H
N
O
O
19c-T
6.56
2.02
2.00
2.39
1.00
1.03
1.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
δ[ppm]

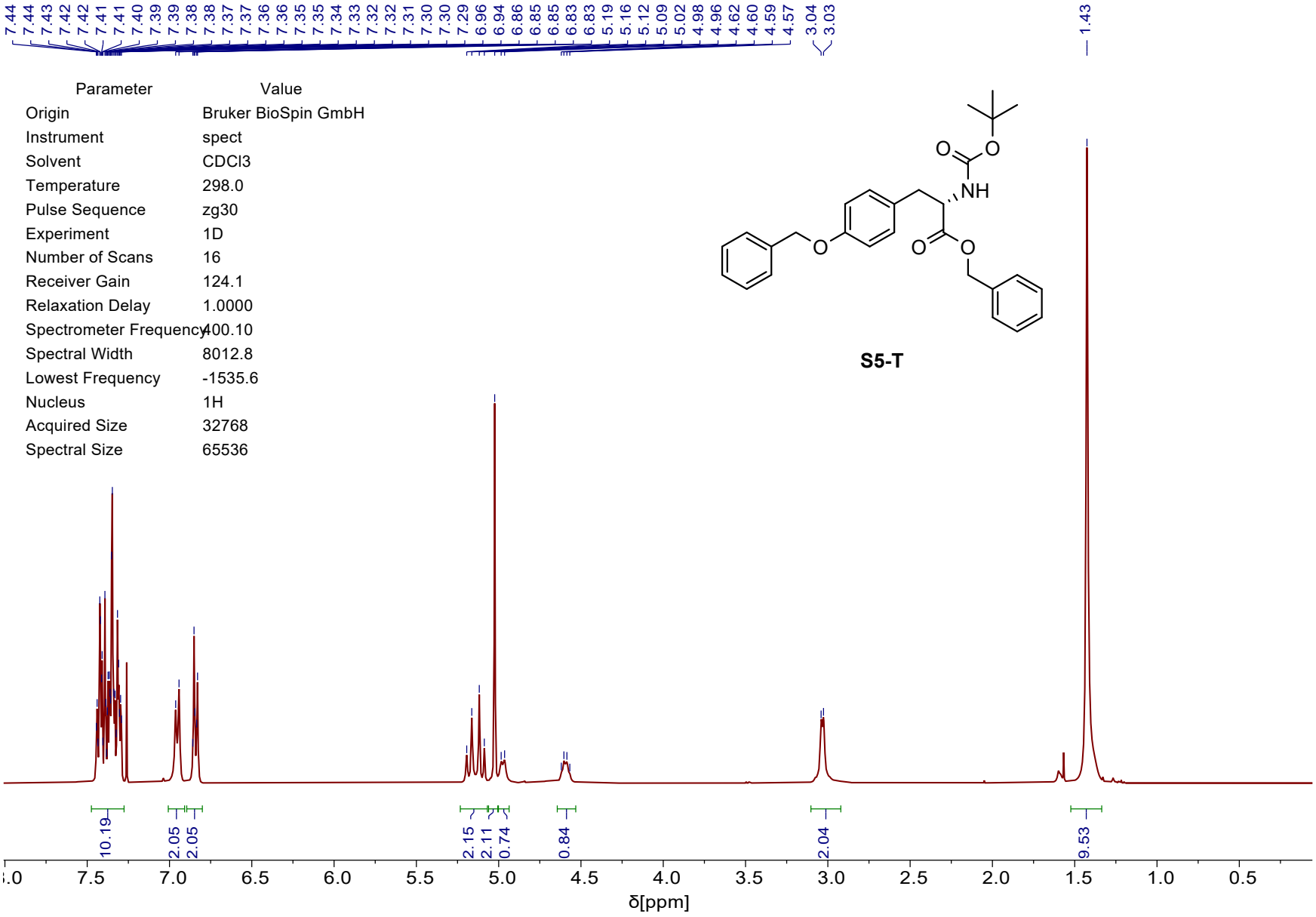

173.95
157.06
155.96
136.95
129.98
128.11
127.86
127.57
127.28
120.70
114.88
66.14
55.69
36.54
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
HO
HO
O
H
N
O
O
19c-T
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

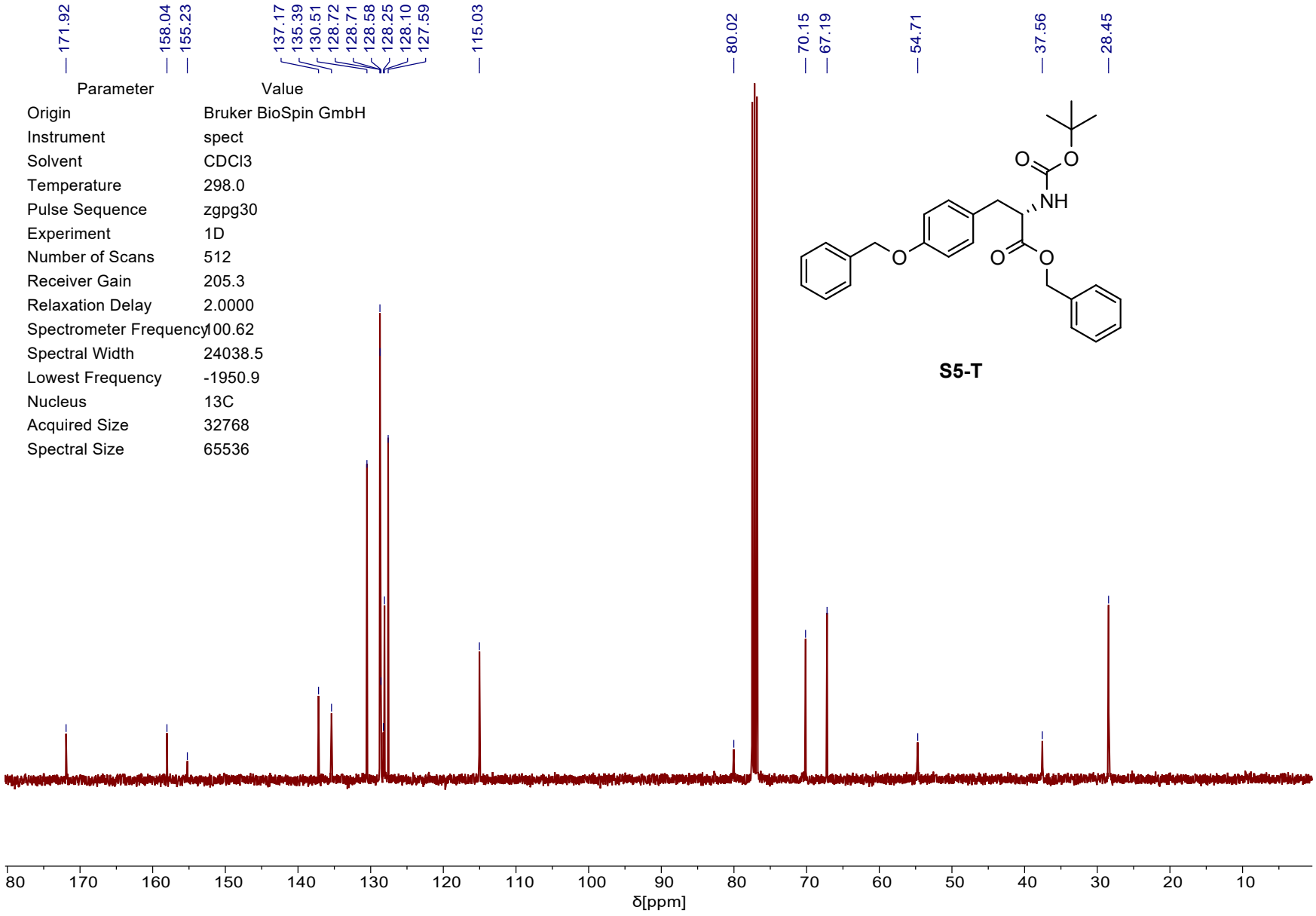

8.18 8.07 8.05 8.04 7.97 7.40 7.40 7.39 7.38 7.38 7.37 7.36 7.35 7.34 7.33 7.32 7.10 7.08 6.85 6.84 6.83
5.24 5.22 5.16 5.13 5.12 5.09 4.70 4.69 4.68 4.67 4.66
3.80
3.20 3.18 3.16 3.15 3.12 3.11 3.10 3.08 3.06
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 124.1
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1535.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
H
N
O
O
O
HO
O
20c-T
1.32 5.88 2.20 2.02 0.84 2.30 0.91 3.03 0.97 1.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
δ[ppm]

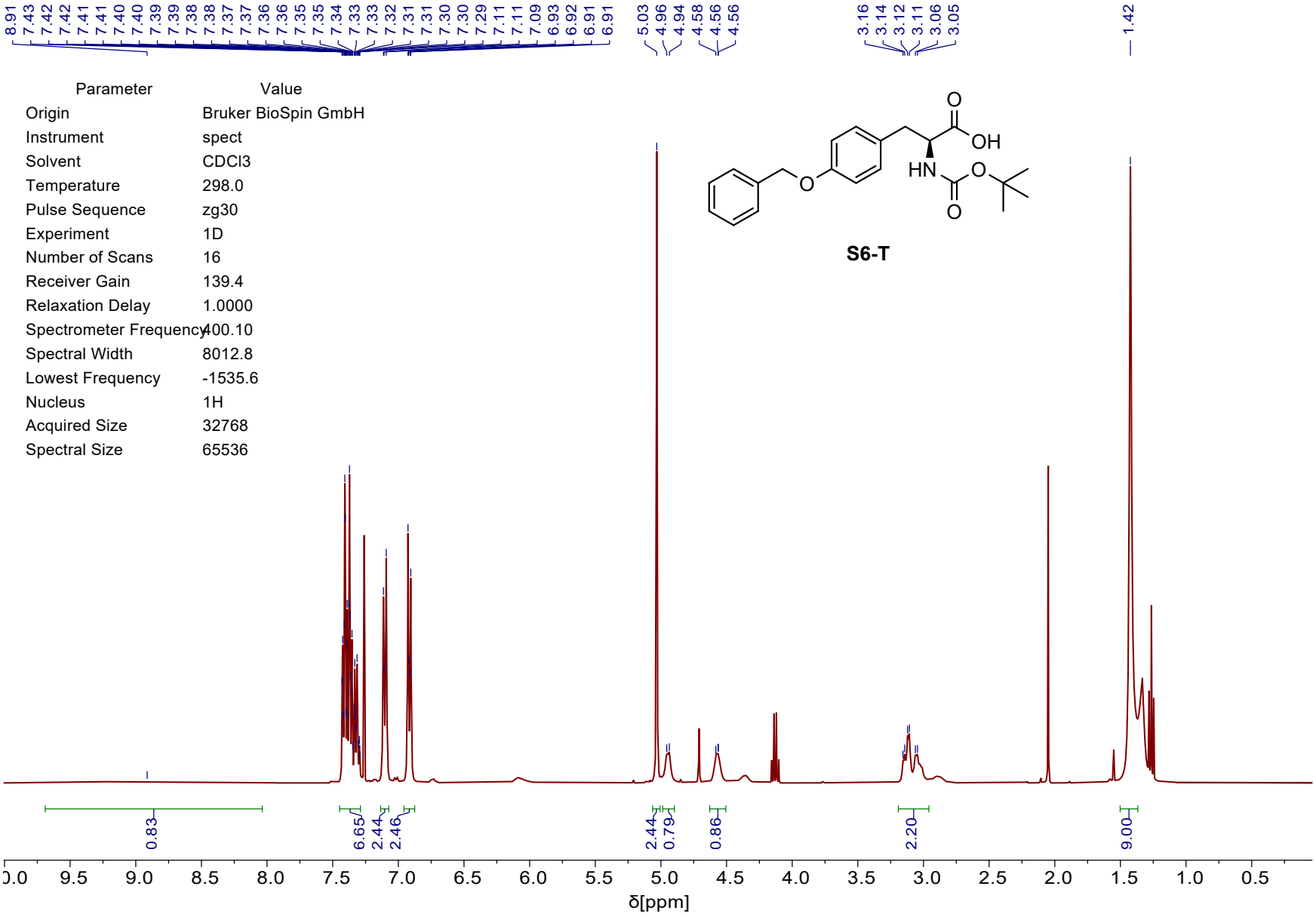

176.04
158.87
155.97
136.22
130.47
128.63
128.34
128.21
127.51
114.21
67.23
58.63
55.31
54.82
36.99
18.32
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
20c-T
δ[ppm]

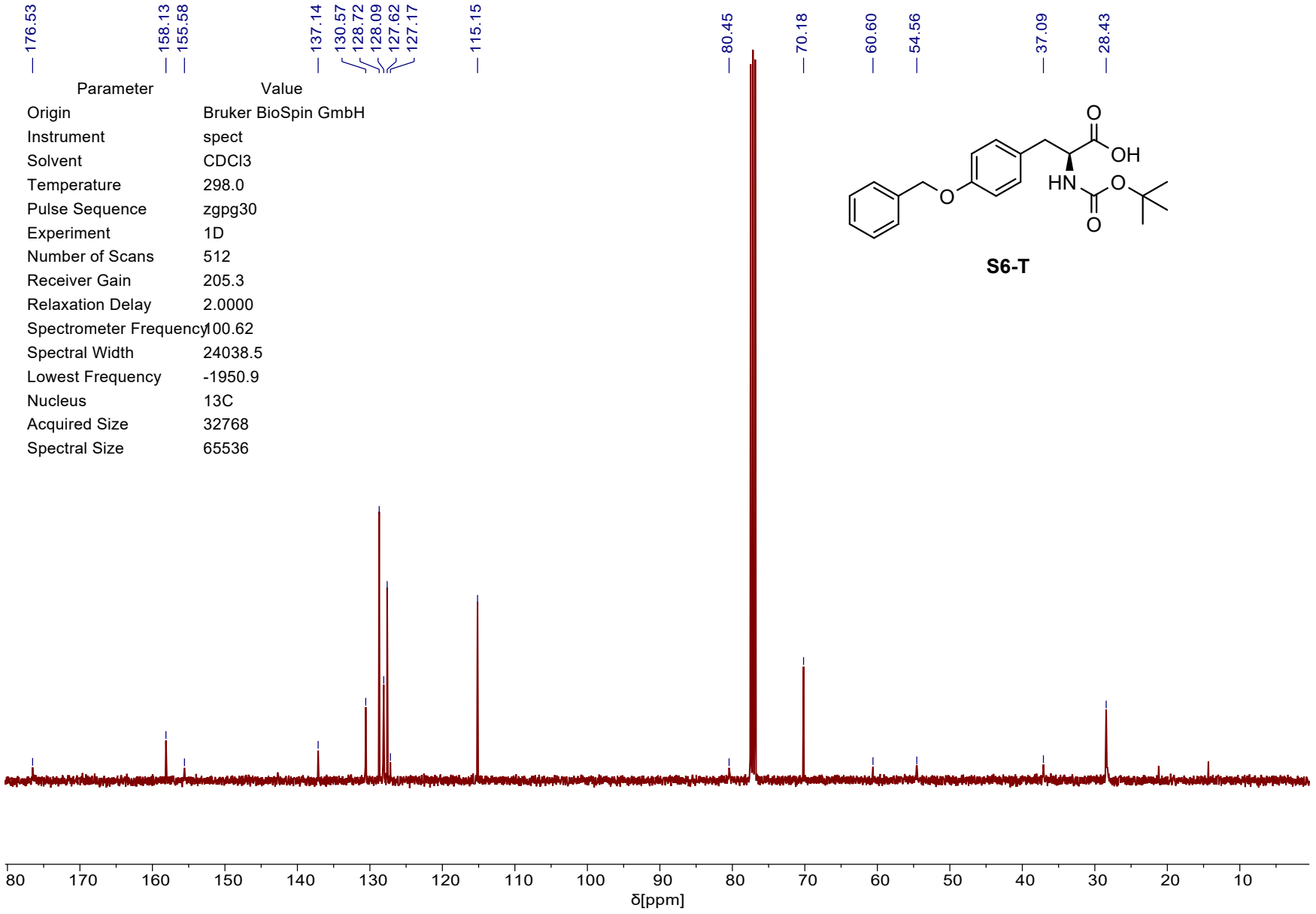

7.38
7.36
7.35
7.34
7.32
7.16
7.14
6.86
6.84
5.86
5.67
5.49
5.47
5.13
5.11
5.08
4.46
4.44
4.43
4.41
3.80
3.10
3.08
3.07
3.06
3.03
3.02
3.01
2.99
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 32
Receiver Gain 181.0
Relaxation Delay 2.0000
Spectrometer Frequency 500.16
Spectral Width 10330.6
Lowest Frequency -2076.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
15c-T
5.34
2.00
1.85
0.89
0.90
0.94
2.03
0.93
2.87
2.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]

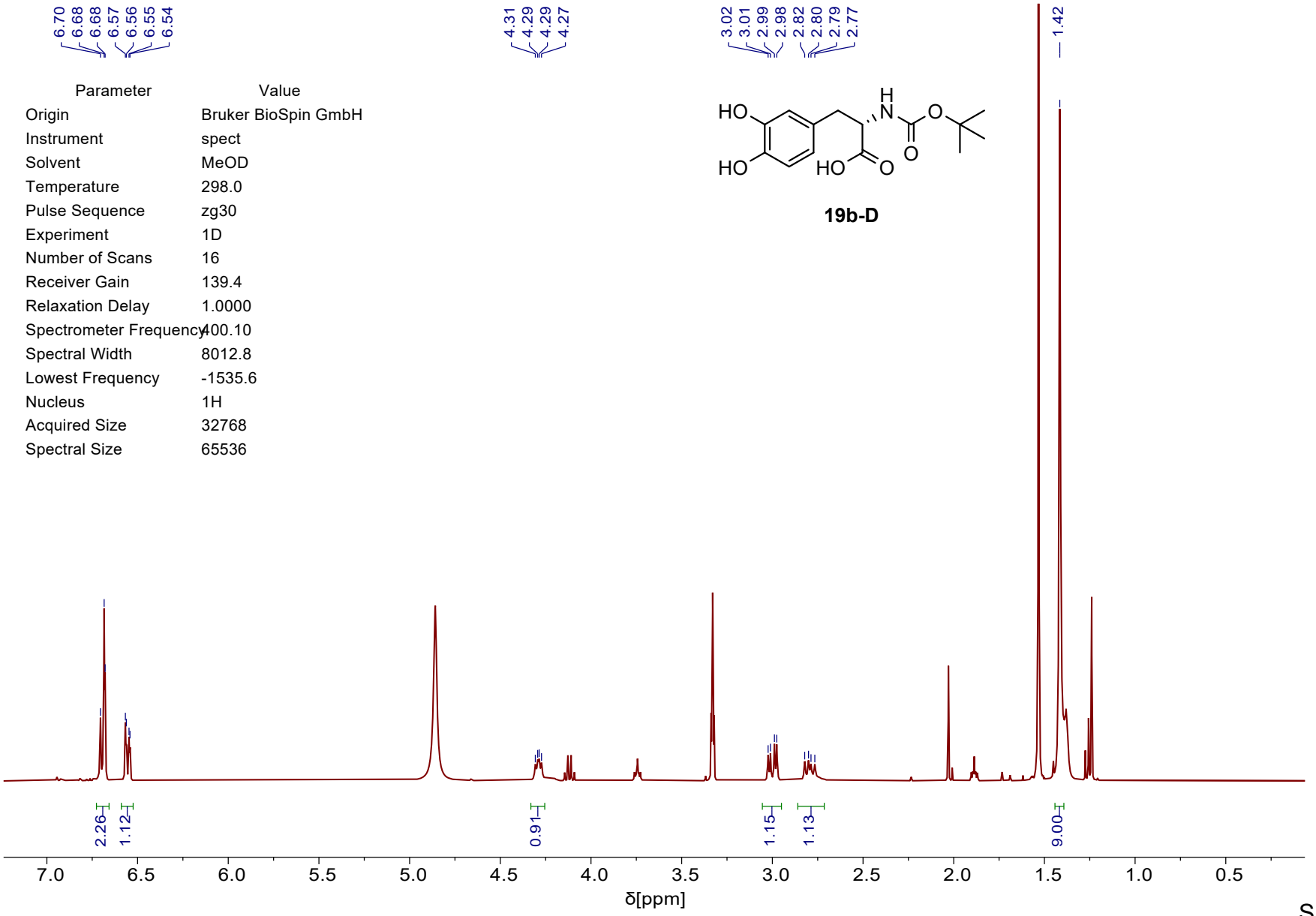

173.43
158.79
156.10
136.20
130.46
128.70
128.67
128.36
128.13
127.60
115.20
114.27
67.19
56.03
55.33
37.71
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1024
Receiver Gain 2300.0
Relaxation Delay 2.0000
Spectrometer Frequency 125.78
Spectral Width 32894.7
Lowest Frequency -3860.8
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
H
N
O
O
O
O
H_2N
15c-T
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

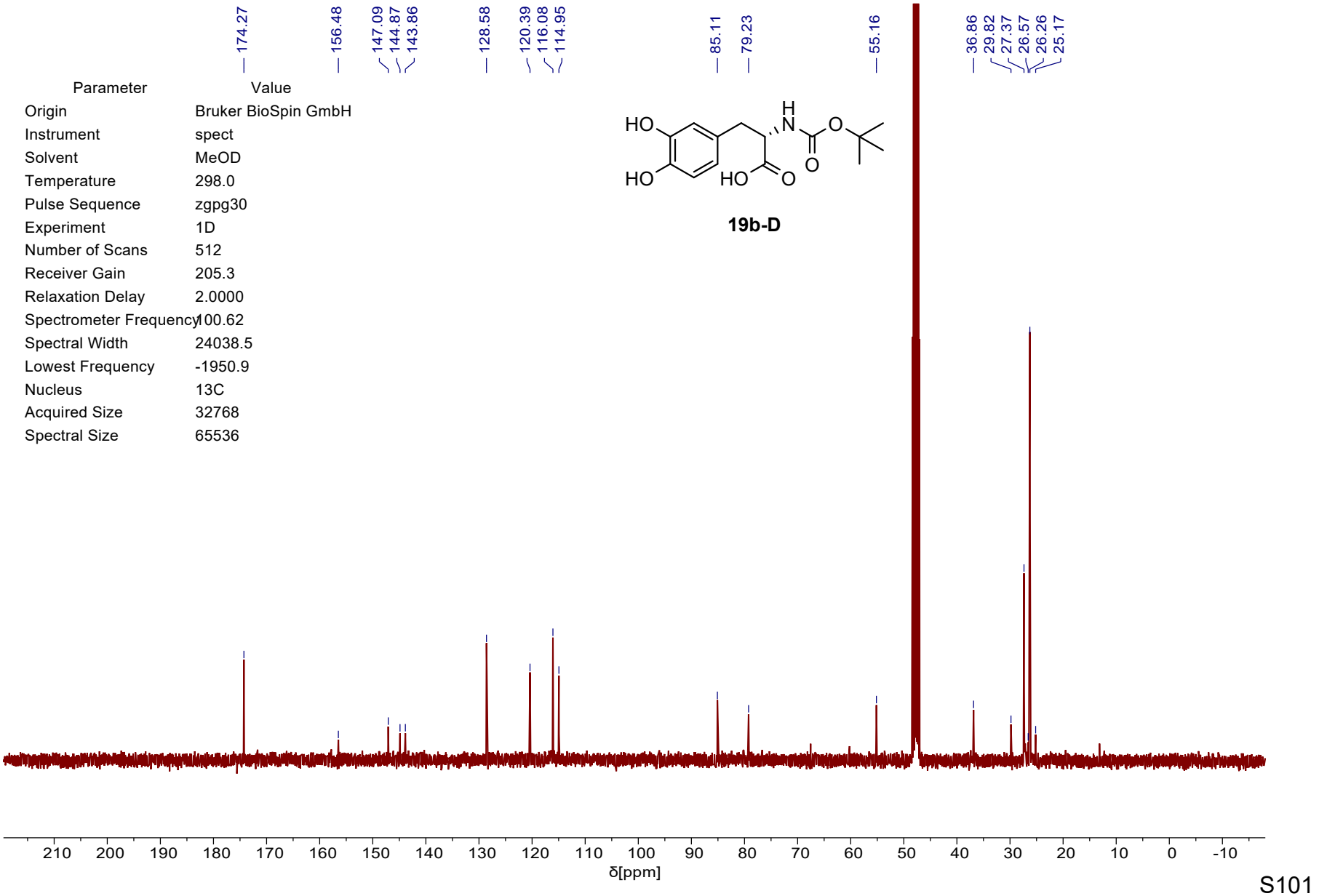

7.44 7.44 7.43 7.42 7.42 7.41 7.41 7.40 7.39 7.39 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.33 7.32 7.32 7.31 7.30 7.30 7.29 6.96 6.94 6.86 6.85 6.85 6.83 6.83 5.19 5.16 5.12 5.09 5.02 4.98 4.96 4.62 4.60 4.59 4.57 3.04 3.03 1.43
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 124.1
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1535.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
O
O
NH
O
O
O
S5-T
10.19
2.05
2.05
2.15
2.11
0.74
0.84
2.04
9.53
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]

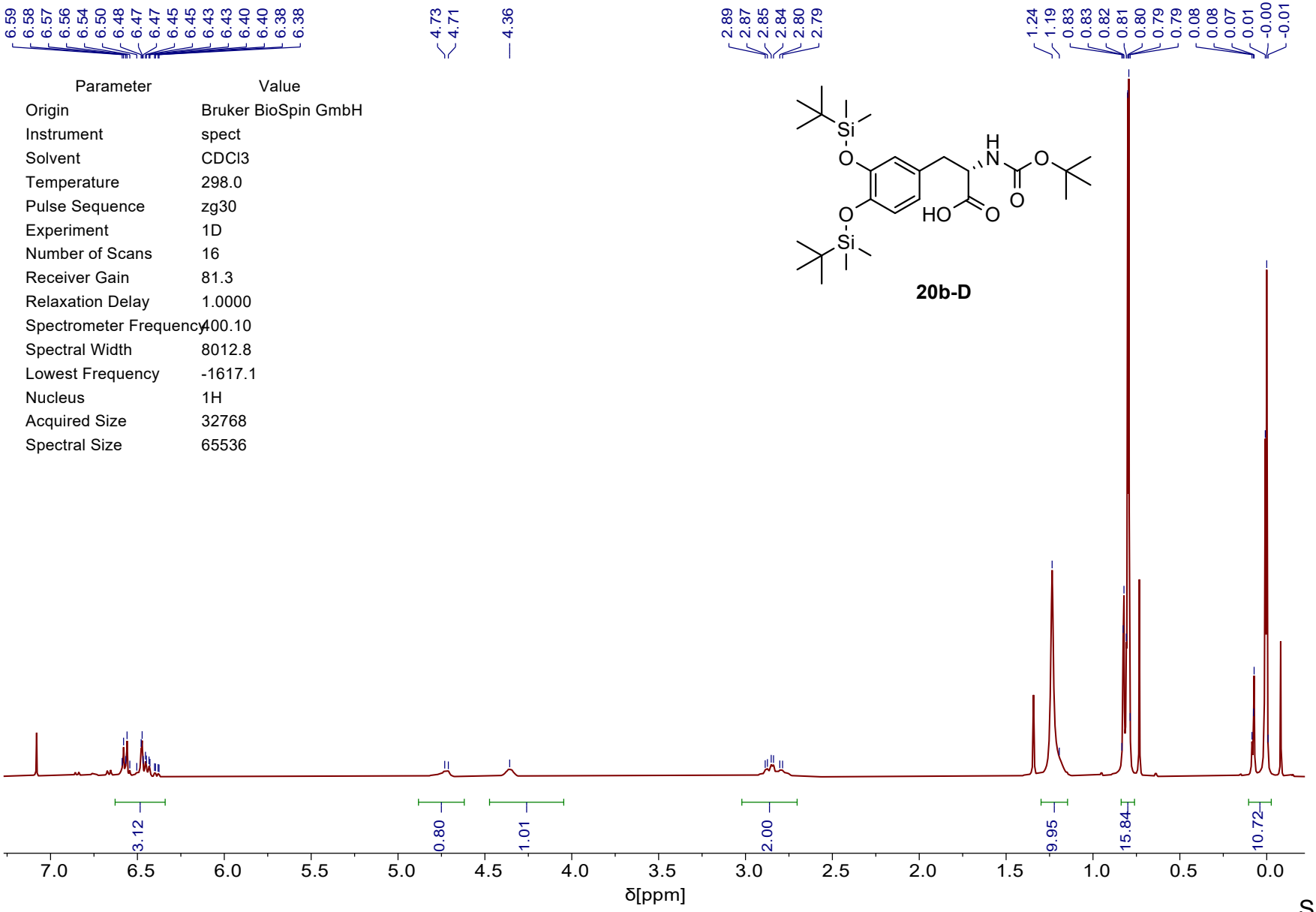

171.92
158.04
155.23
137.17
135.39
130.51
128.72
128.71
128.58
128.25
128.10
127.59
115.03
80.02
70.15
67.19
54.71
37.56
28.45
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
S5-T
δ[ppm]

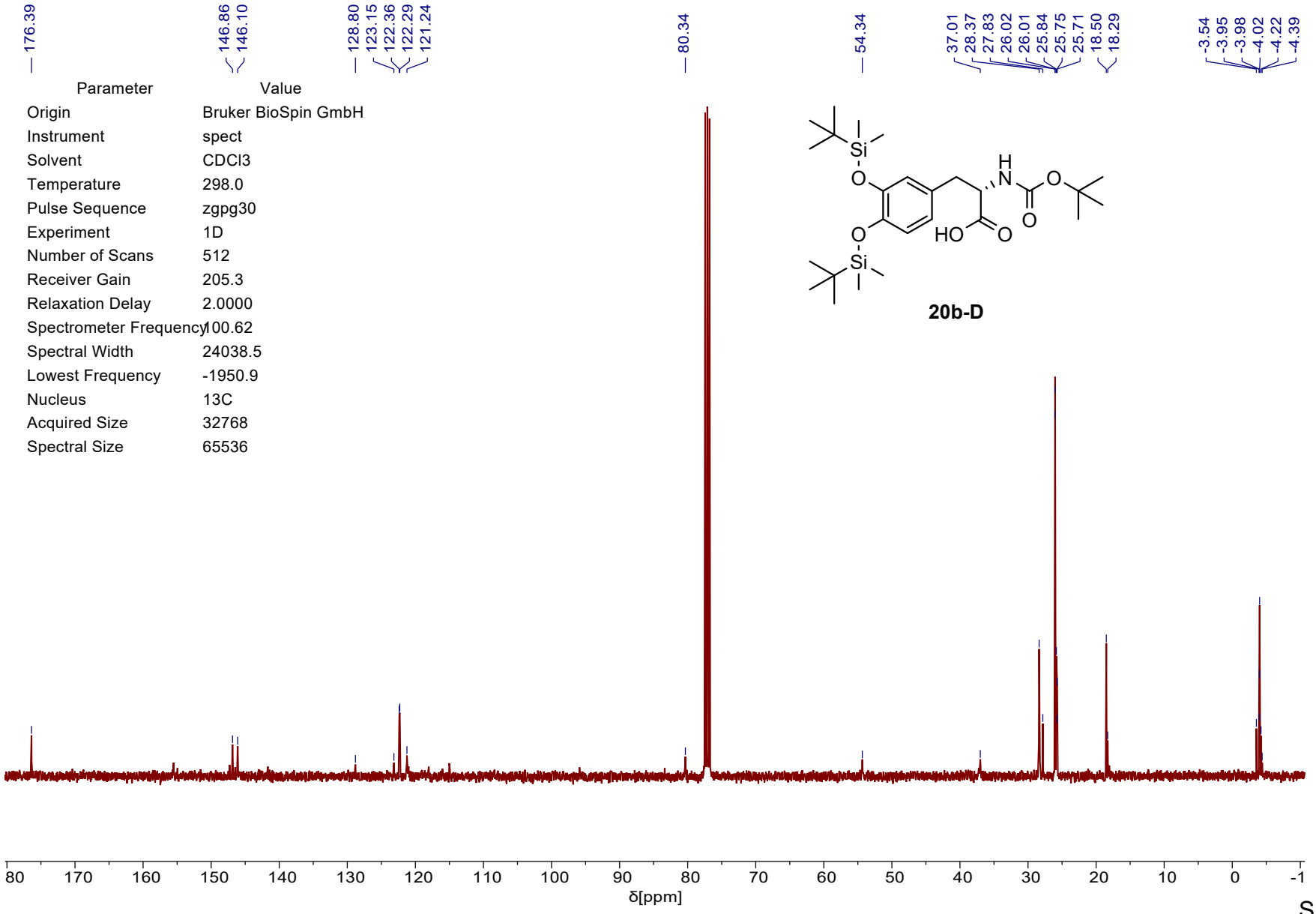

8.91 7.43 7.42 7.42 7.41 7.41 7.40 7.40 7.39 7.39 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.33 7.33 7.32 7.31 7.31 7.30 7.30 7.29 7.11 7.11 7.09 6.93 6.92 6.91 6.91
5.03 4.96 4.94 4.58 4.56 4.56
3.16 3.14 3.12 3.11 3.06 3.05
1.42
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 139.4
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1535.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
O
OH
HN
O
O
O
S6-T
0.83
6.65
2.44
2.46
2.44
0.79
0.86
2.20
9.00
δ[ppm]

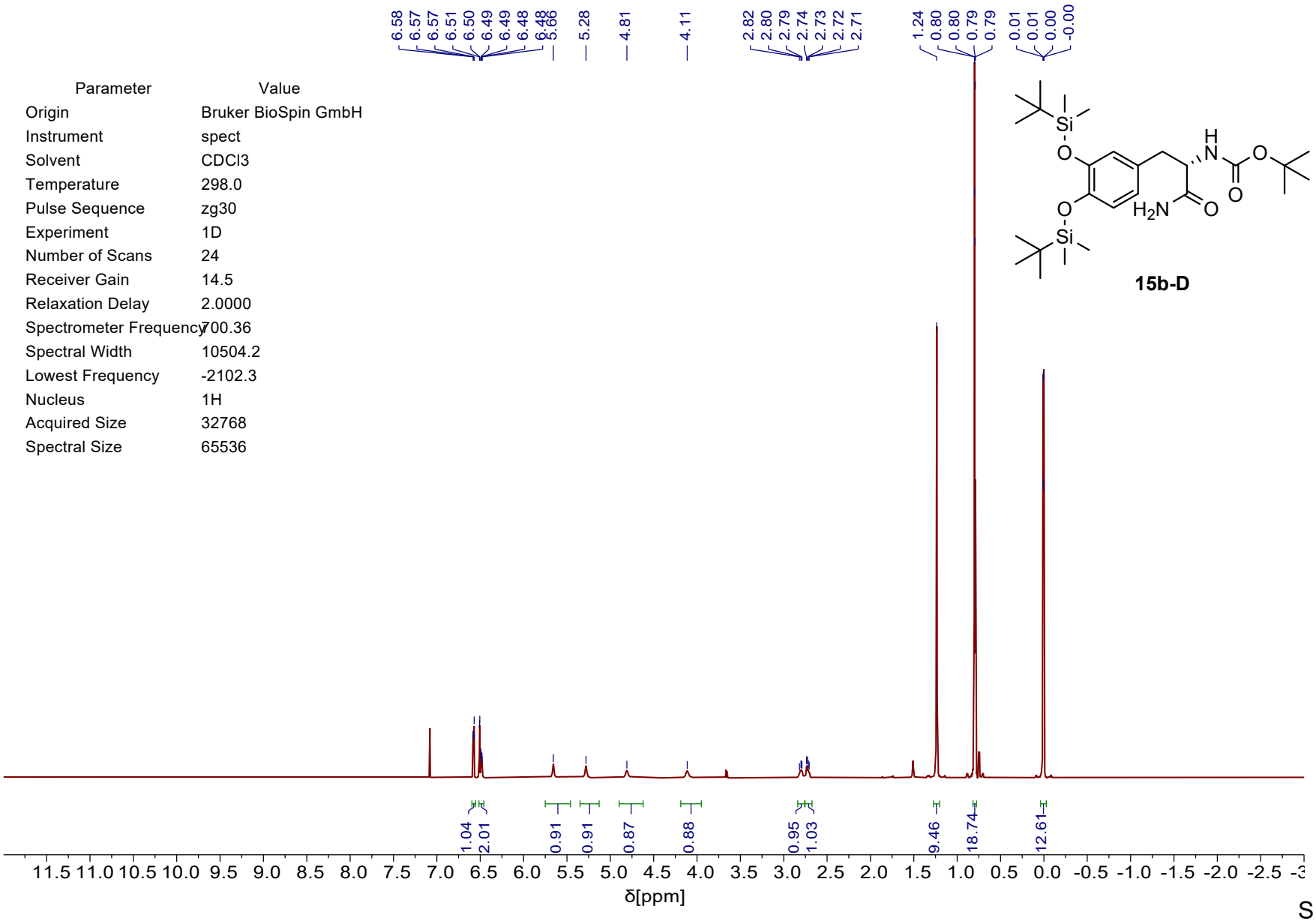

176.53
158.13
155.58
137.14
130.57
128.72
128.09
127.62
127.17
115.15
80.45
70.18
60.60
54.56
37.09
28.43
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
O
OH
HN
O
O
O
S6-T
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

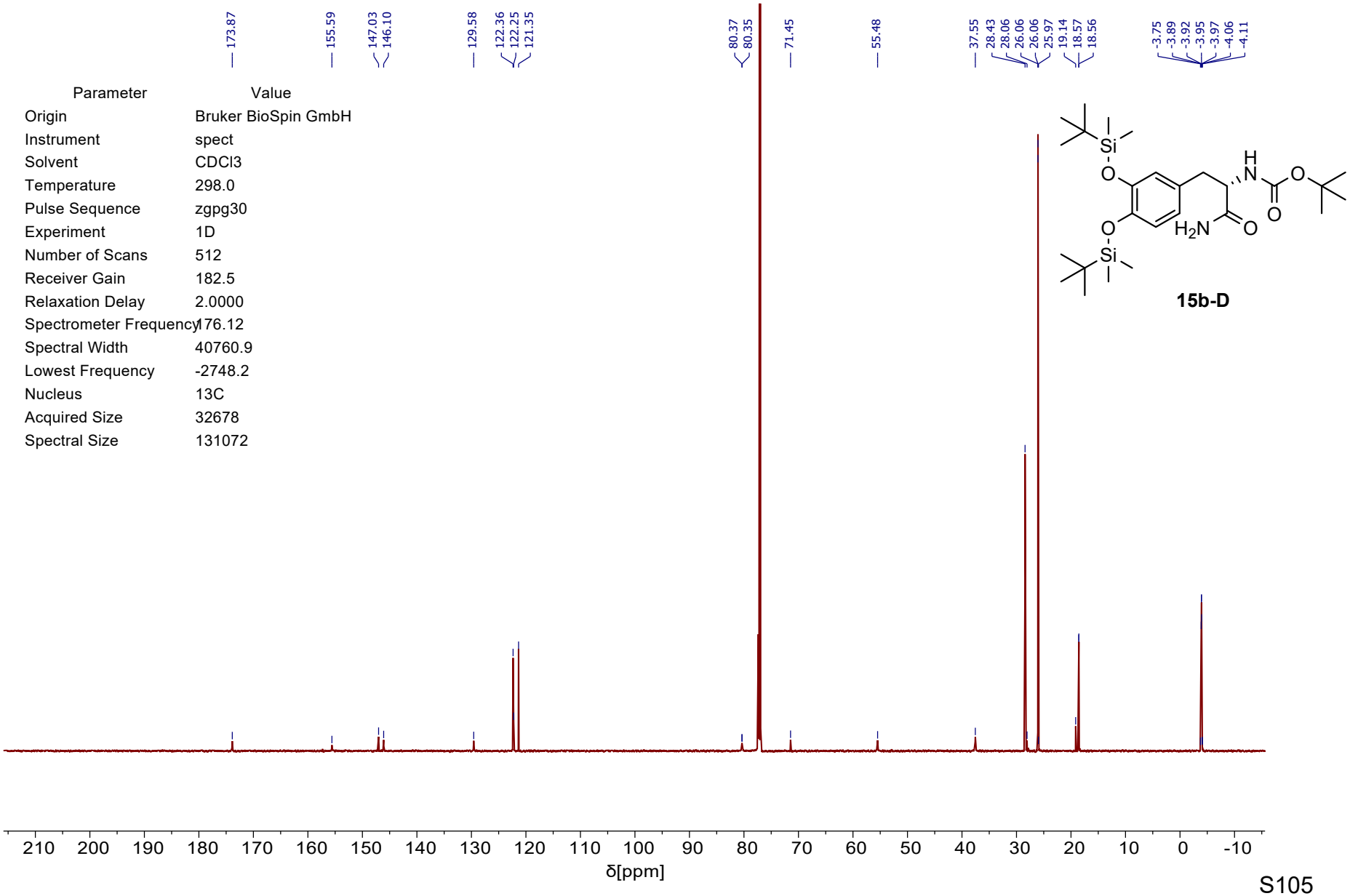

6.70
6.68
6.68
6.57
6.56
6.55
6.54
4.31
4.29
4.29
4.27
3.02
3.01
2.99
2.98
2.82
2.80
2.79
2.77
1.42
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 139.4
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1535.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
HO
HO
H
N
O
O
HO
O
19b-D
2.26
1.12
0.91
1.15
1.13
9.00
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]

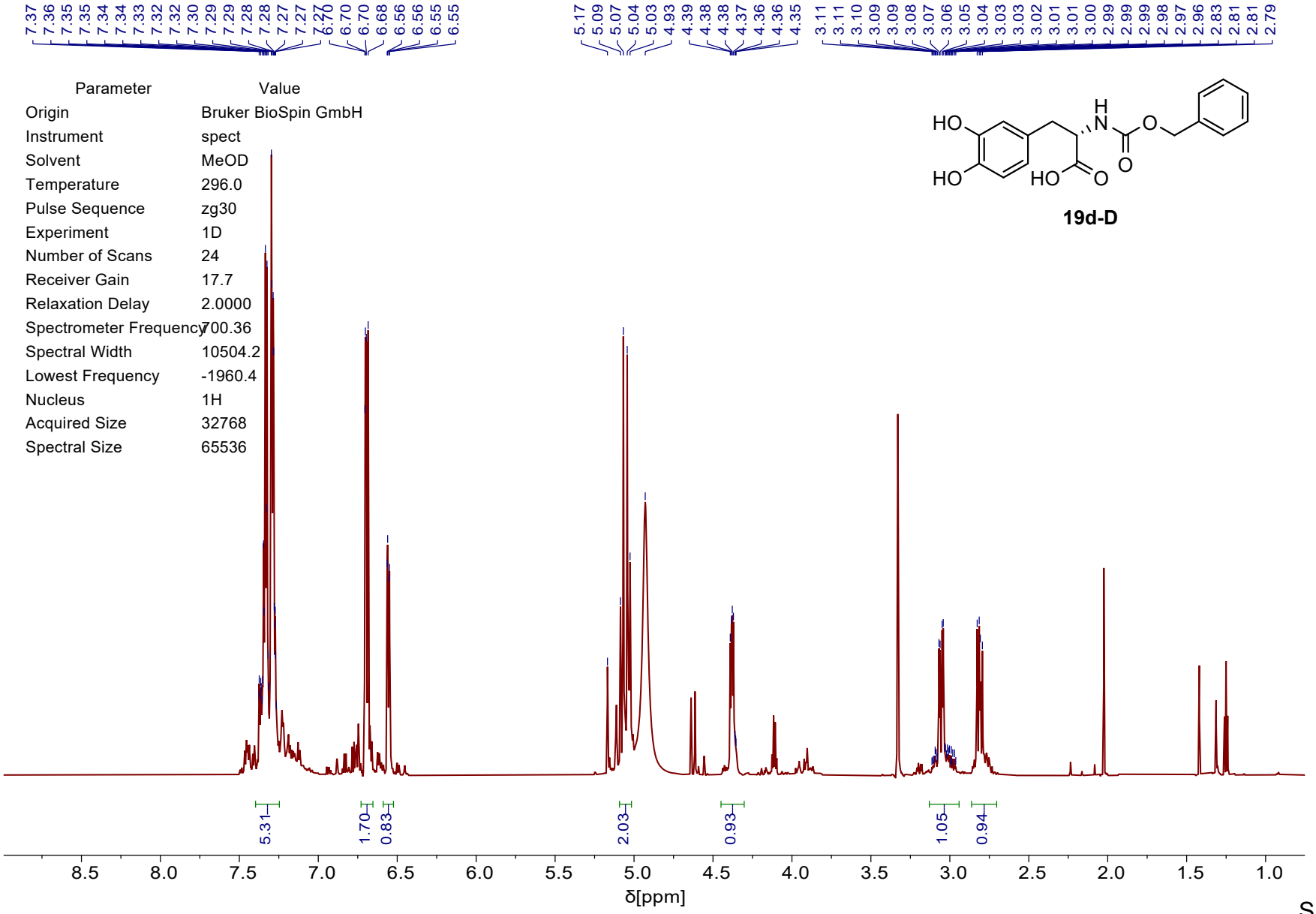

174.27
156.48
147.09
144.87
143.86
128.58
120.39
116.08
114.95
85.11
79.23
55.16
36.86
29.82
27.37
26.57
26.26
25.17
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
HO
HO
HO
O
H
N
O
O
19b-D
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
δ[ppm]

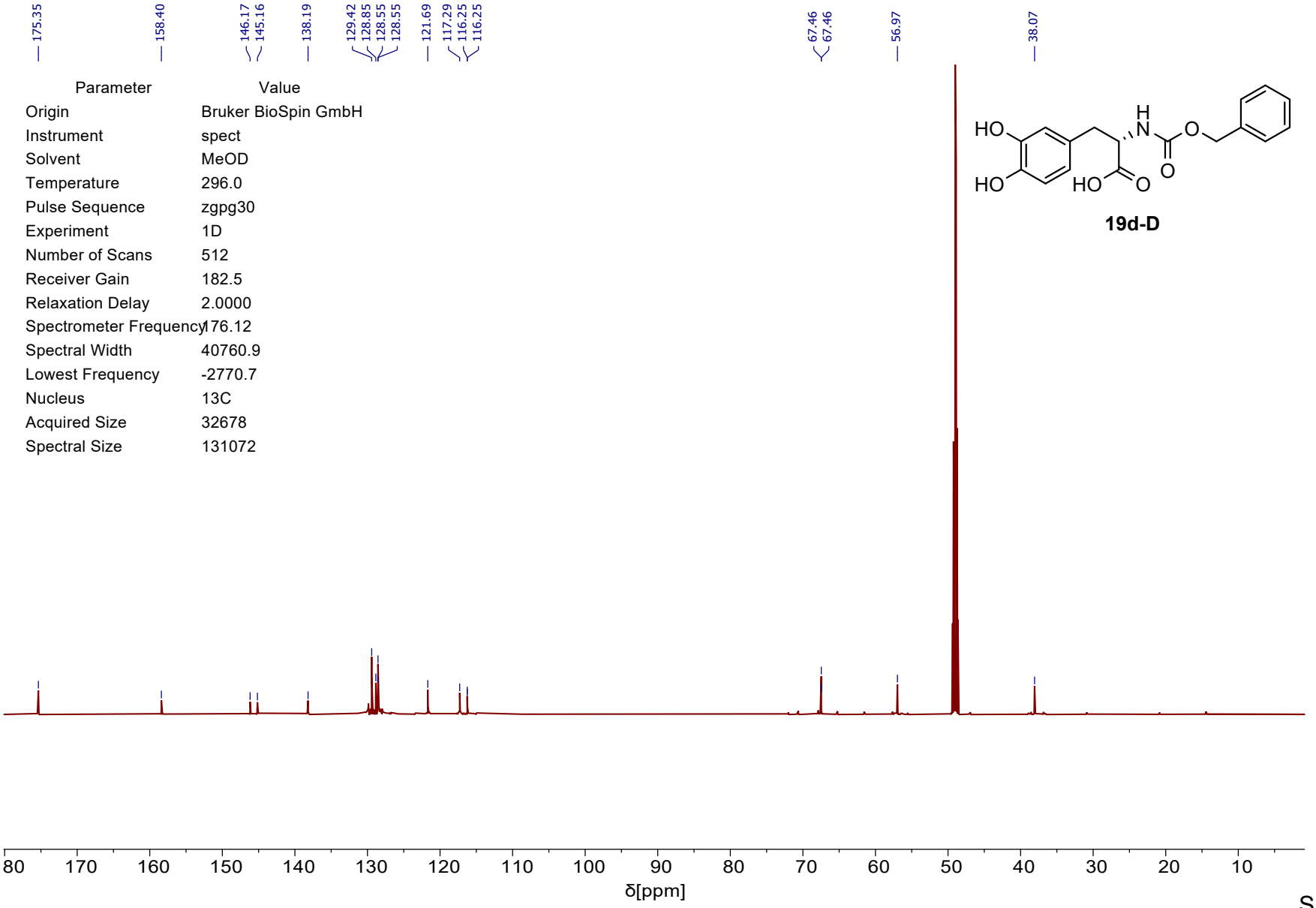

6.59 6.58 6.57 6.56 6.54 6.50 6.48 6.47 6.47 6.45 6.45 6.43 6.43 6.40 6.40 6.38 6.38
4.73 4.71
4.36
2.89 2.87 2.85 2.84 2.80 2.79
1.24 1.19 0.83 0.83 0.82 0.81 0.80 0.79 0.79 0.08 0.08 0.07 0.01 -0.00 -0.01
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 81.3
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1617.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
Si
O
H
N
O
O
HO
O
O
Si
20b-D
3.12
0.80
1.01
2.00
9.95
15.84
10.72
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ[ppm]

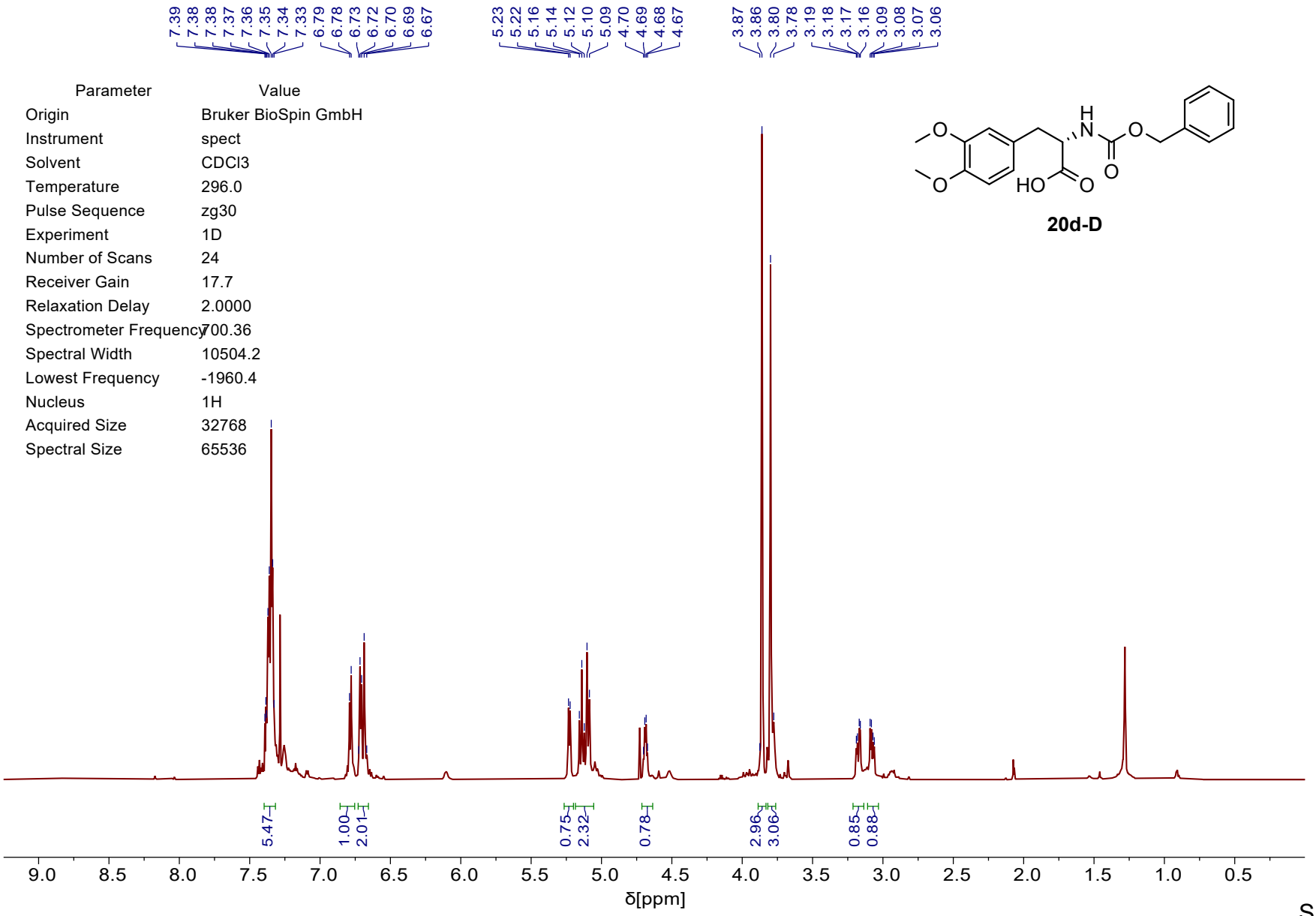

176.39
146.86
146.10
128.80
123.15
122.36
122.29
121.24
80.34
54.34
37.01
28.37
27.83
26.02
26.01
25.84
25.75
25.71
18.50
18.29
-3.54
-3.95
-3.98
-4.02
-4.22
-4.39
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
20b-D
δ[ppm]

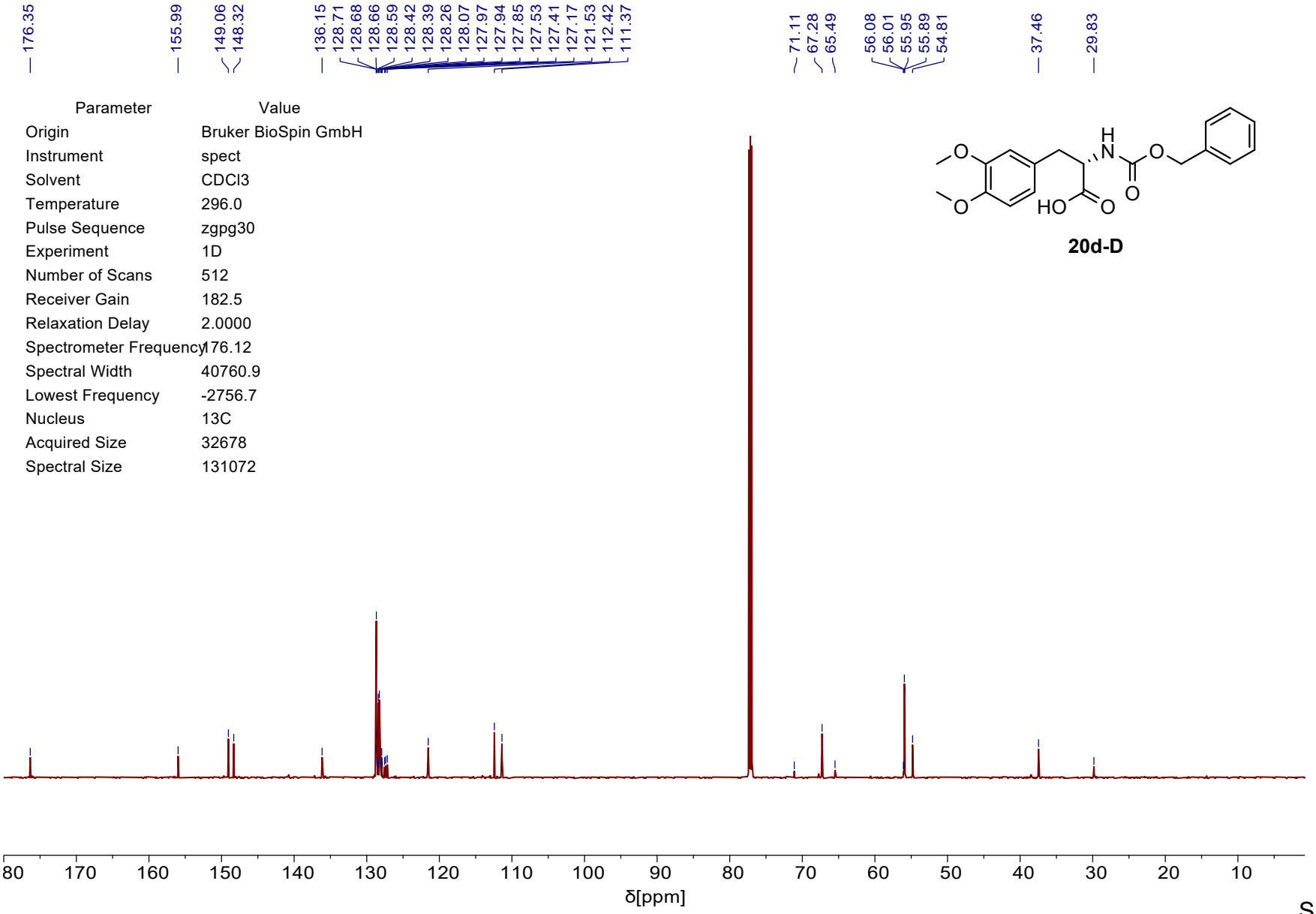

6.58
6.57
6.57
6.51
6.50
6.49
6.49
6.48
6.48
6.46
5.28
4.81
4.11
2.82
2.80
2.79
2.74
2.73
2.72
2.71
1.24
0.80
0.80
0.79
0.79
0.01
0.01
0.00
-0.00
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 14.5
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -2102.3
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
15b-D
1.04
2.01
0.91
0.91
0.87
0.88
0.95
1.03
9.46
18.74
12.61
δ[ppm]

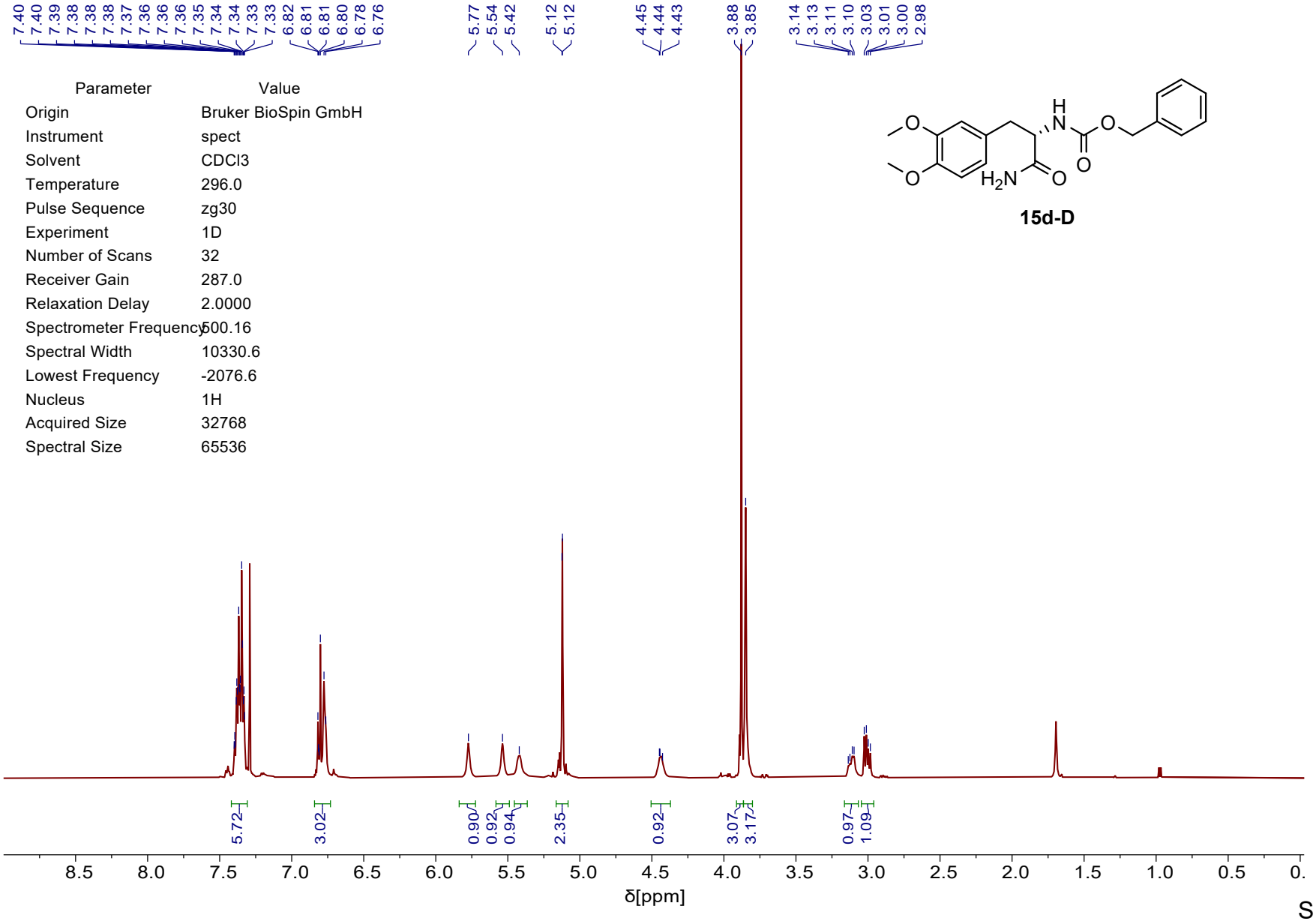

173.87
155.59
147.03
146.10
129.58
122.36
122.25
121.35
80.37
80.35
71.45
55.48
37.55
28.43
28.06
26.06
26.06
25.97
19.14
18.57
18.56
-3.75
-3.89
-3.92
-3.95
-3.97
-4.06
-4.11
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2748.2
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
15b-D
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
δ[ppm]

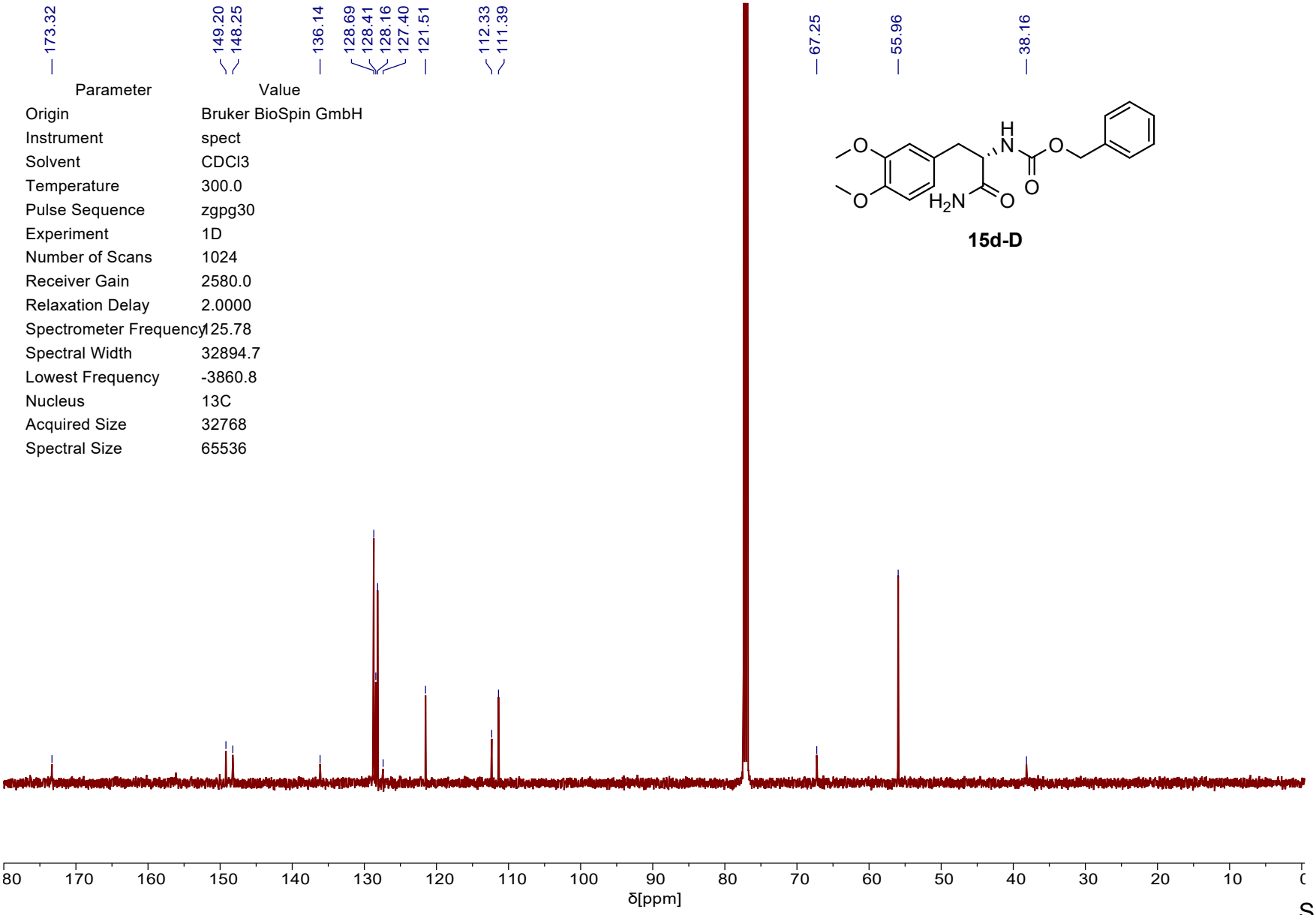

7.37 7.36 7.35 7.35 7.34 7.34 7.33 7.32 7.32 7.30 7.29 7.29 7.28 7.28 7.27 7.27 7.27 6.70 6.70 6.68 6.56 6.56 6.55 6.55
5.17 5.09 5.07 5.04 5.03 4.93 4.39 4.38 4.38 4.37 4.36 4.36 4.35
3.11 3.11 3.10 3.09 3.09 3.08 3.07 3.06 3.05 3.04 3.03 3.03 3.02 3.01 3.01 3.00 2.99 2.99 2.99 2.98 2.97 2.96 2.83 2.81 2.81 2.79
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 17.7
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
HO
HO
HO
O
H
N
O
O
19d-D
5.31
1.70
0.83
2.03
0.93
1.05
0.94
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
δ[ppm]


175.35
158.40
146.17
145.16
138.19
129.42
128.85
128.55
128.55
121.69
117.29
116.25
116.25
67.46
67.46
56.97
38.07
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2770.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
HO
HO
H
N
O
O
HO
O
19d-D
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

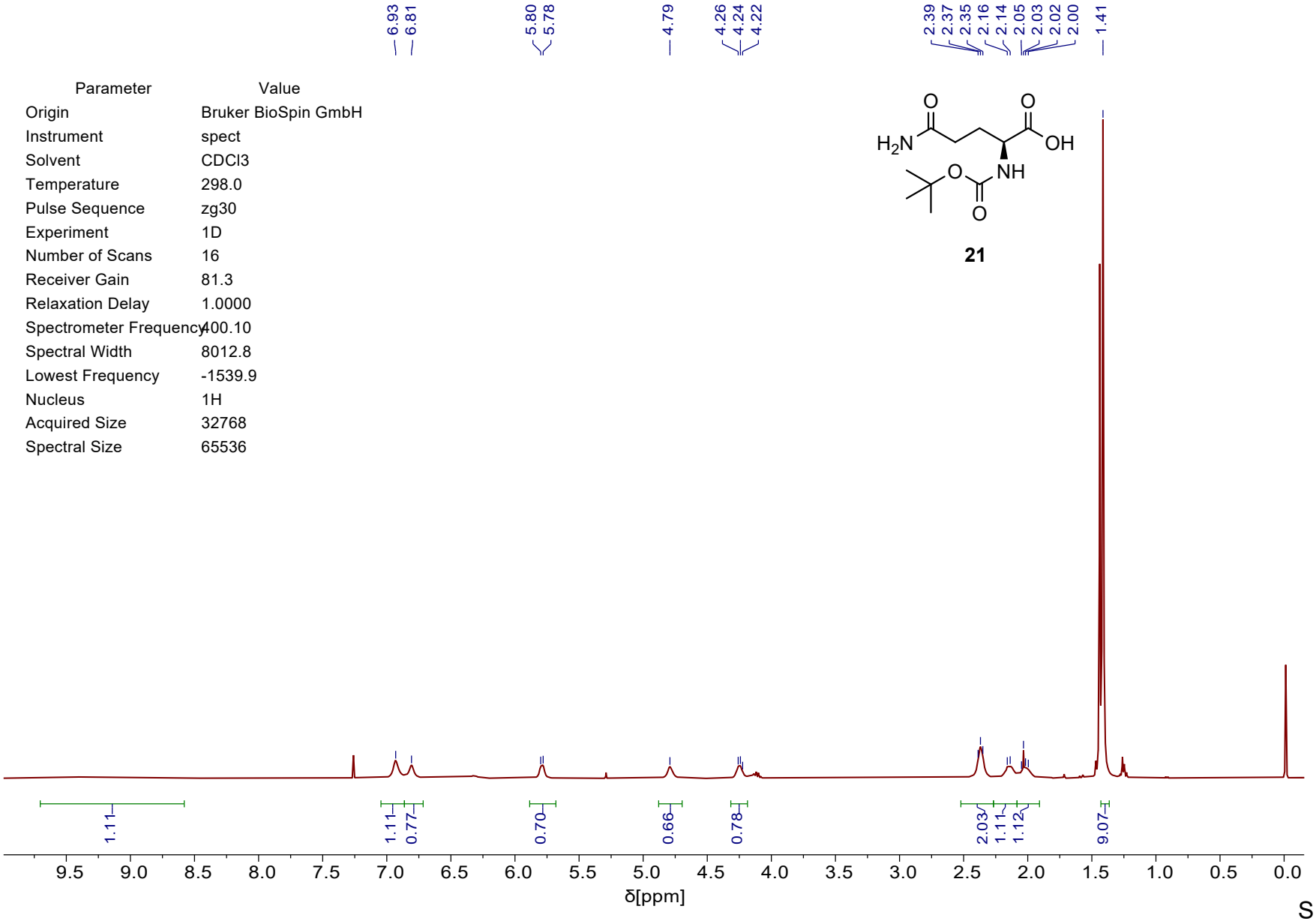

7.39 7.38 7.38 7.37 7.36 7.35 7.34 7.33 6.79 6.78 6.73 6.72 6.70 6.69 6.67
5.23 5.22 5.16 5.14 5.12 5.10 5.09 4.70 4.69 4.68 4.67
3.87 3.86 3.80 3.78 3.19 3.18 3.17 3.16 3.09 3.08 3.07 3.06
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 17.7
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
20d-D
5.47 1.00 2.01 0.75 2.32 0.78 2.96 3.06 0.85 0.88
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
δ[ppm]

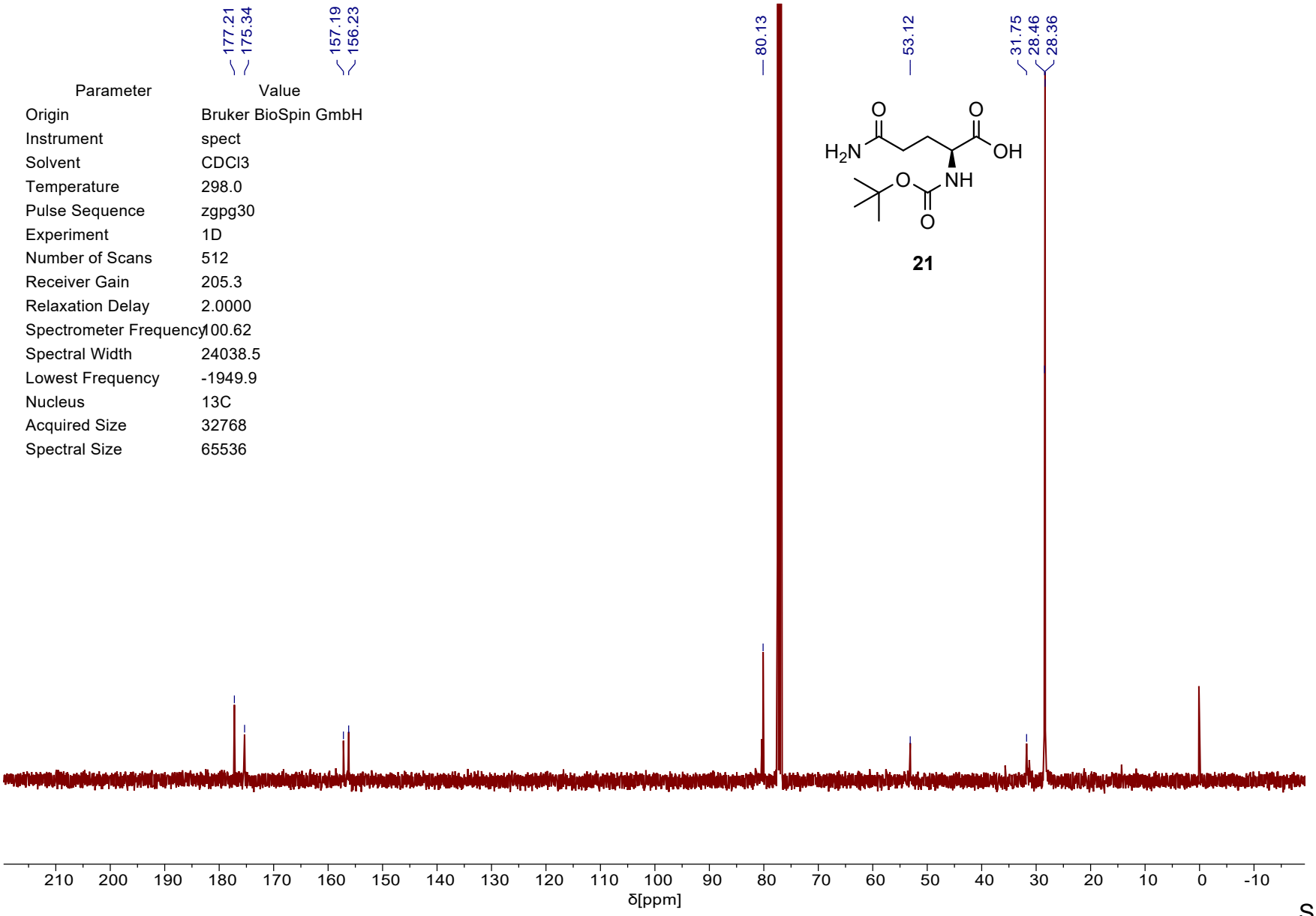

176.35
155.99
149.06
148.32
136.15
128.71
128.68
128.66
128.59
128.42
128.39
128.26
128.07
127.97
127.94
127.85
127.53
127.41
127.17
121.53
112.42
111.37
71.11
67.28
65.49
56.08
56.01
55.95
55.89
54.81
37.46
29.83
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
20d-D
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

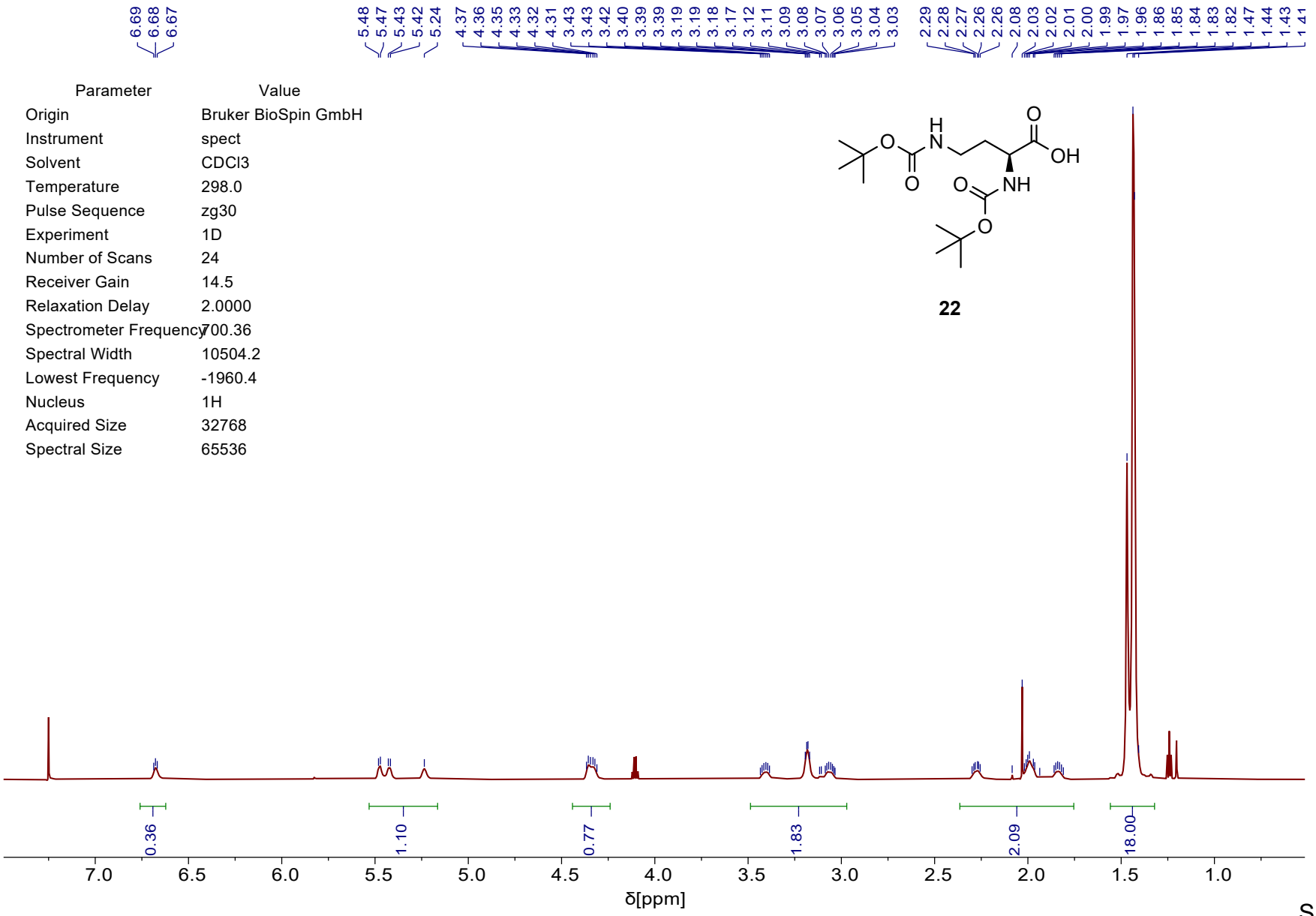

7.40 7.40 7.39 7.38 7.38 7.38 7.37 7.36 7.36 7.36 7.35 7.34 7.34 7.33 7.33 6.82 6.81 6.81 6.80 6.78 6.76
5.77 5.54 5.42 5.12 5.12 4.45 4.44 4.43 3.88 3.85 3.14 3.13 3.11 3.10 3.03 3.01 3.00 2.98
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 32
Receiver Gain 287.0
Relaxation Delay 2.0000
Spectrometer Frequency 500.16
Spectral Width 10330.6
Lowest Frequency -2076.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
15d-D
5.72 3.02 0.90 0.92 0.94 2.35 0.92 3.07 3.17 0.97 1.09
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
δ[ppm]

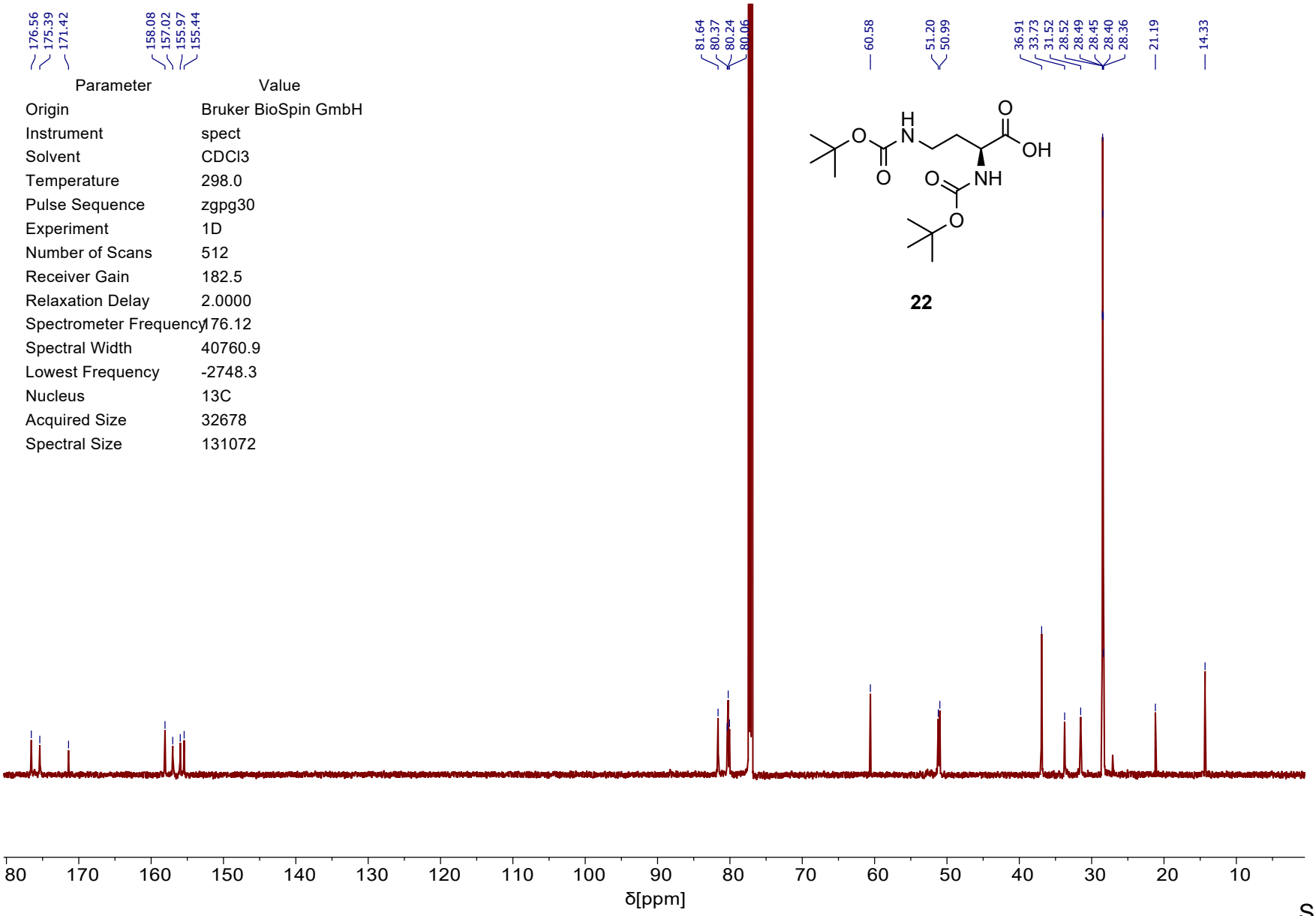

173.32
149.20
148.25
136.14
128.69
128.41
128.16
127.40
121.51
112.33
111.39
67.25
55.96
38.16
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1024
Receiver Gain 2580.0
Relaxation Delay 2.0000
Spectrometer Frequency 125.78
Spectral Width 32894.7
Lowest Frequency -3860.8
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
δ[ppm]

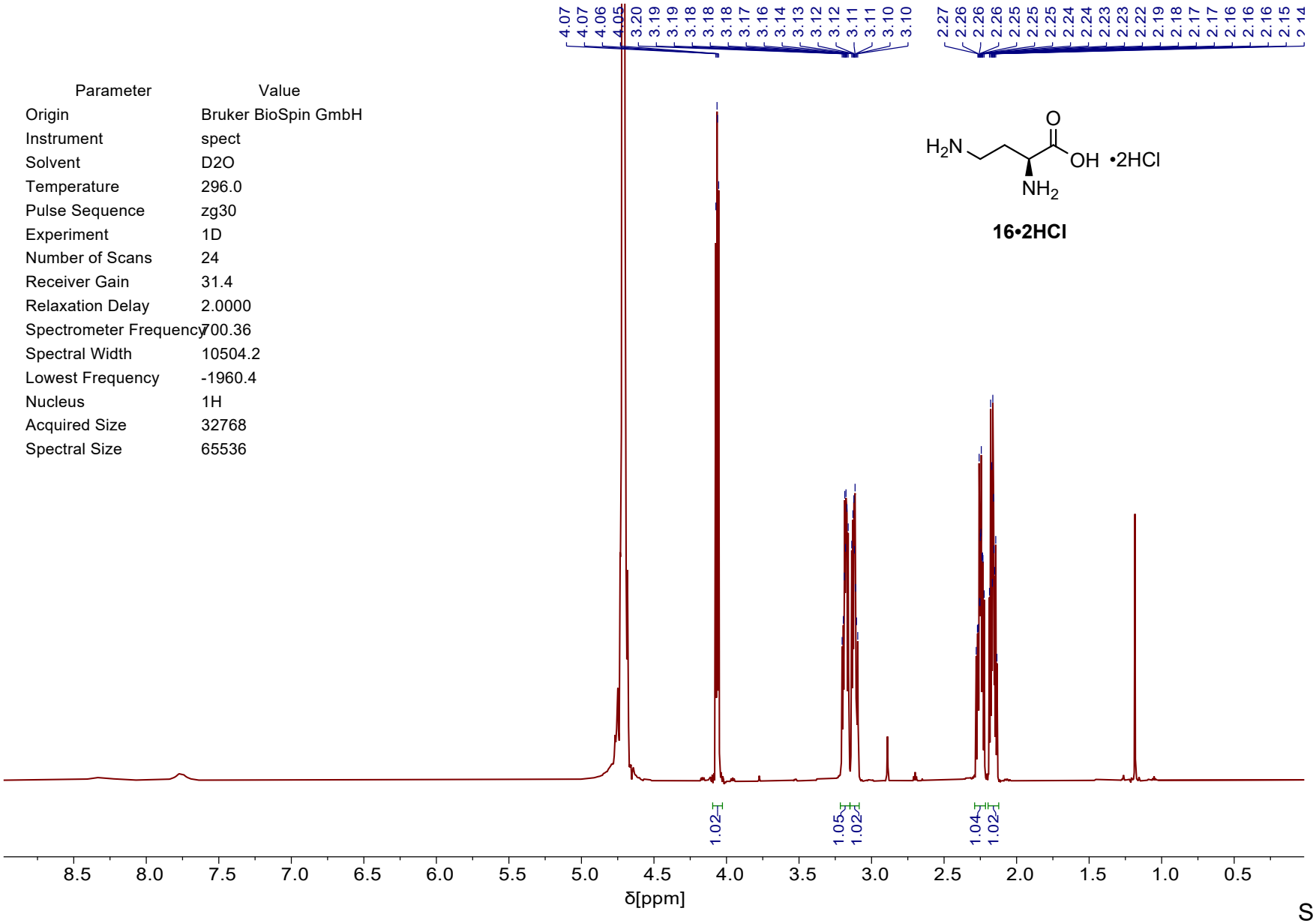
15d-D

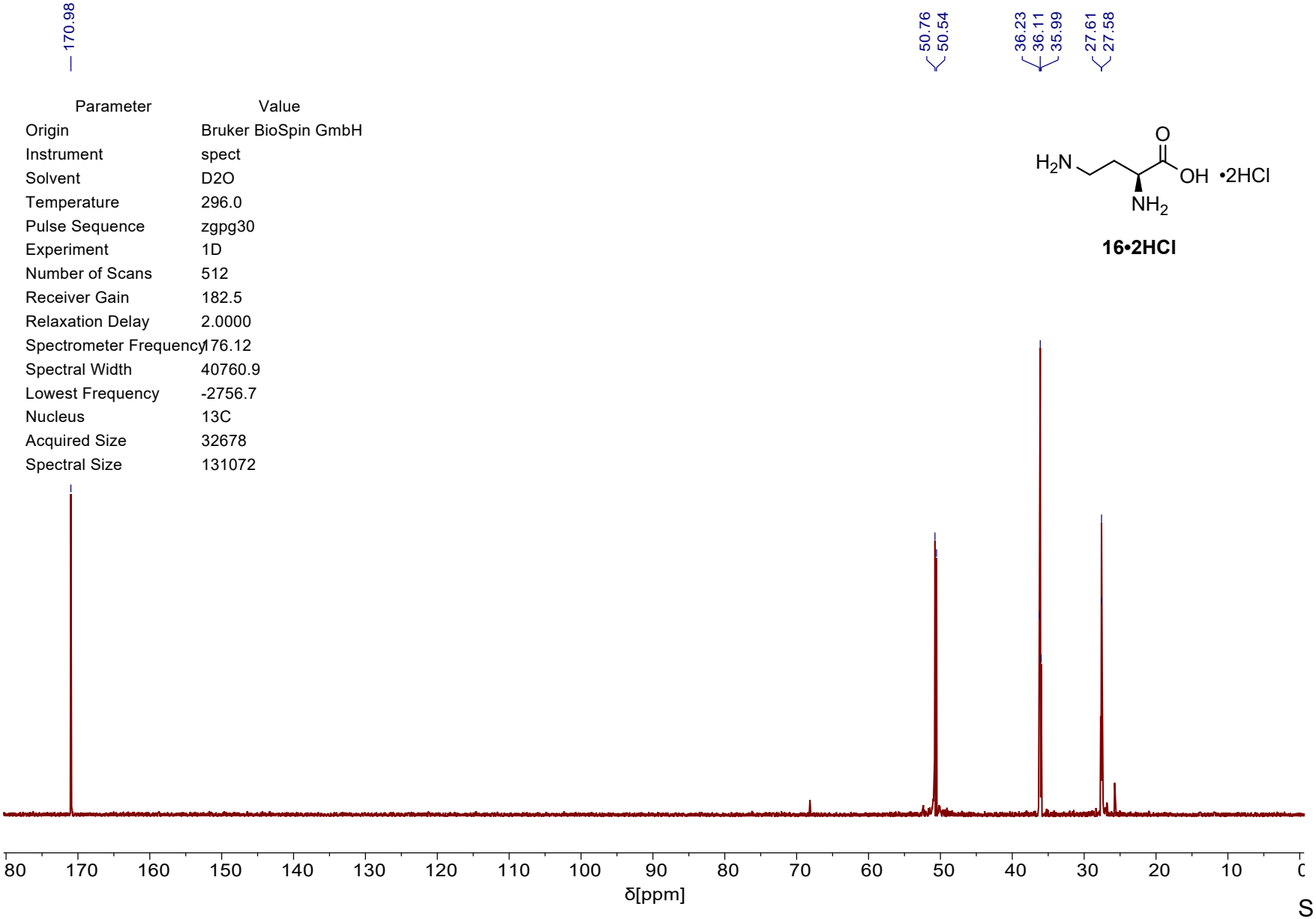

6.93
6.81
5.80
5.78
4.79
4.26
4.24
4.22
2.39
2.37
2.35
2.16
2.14
2.05
2.03
2.02
2.00
1.41
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 81.3
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1539.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
O
O
H2N
OH
NH
O
O
21
1.11
1.11
0.77
0.70
0.66
0.78
2.03
1.11
1.12
9.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ[ppm]

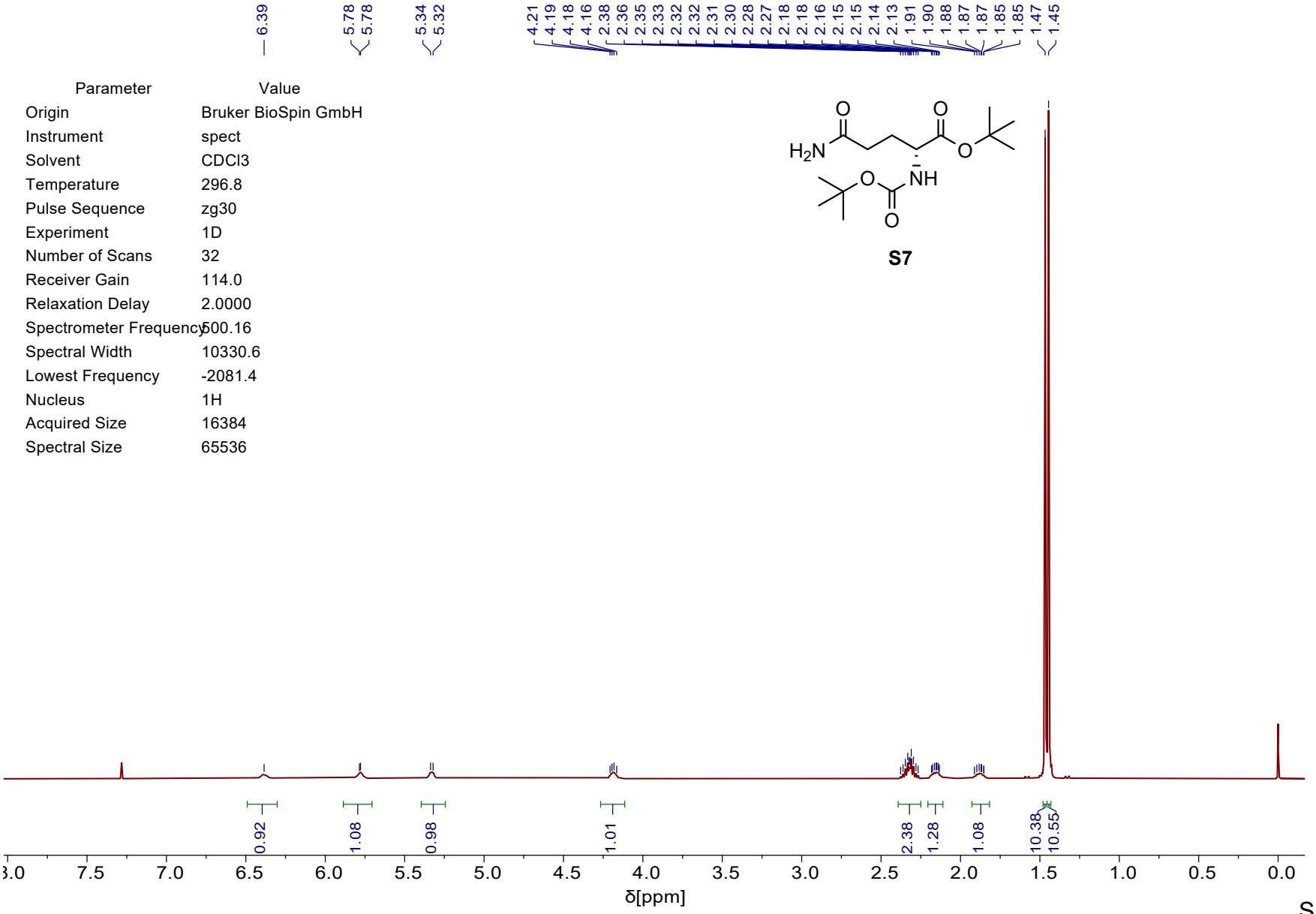

177.21
175.34
157.19
156.23
80.13
53.12
31.75
28.46
28.36
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1949.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
O
O
H2N
OH
O
NH
O
21
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
δ[ppm]

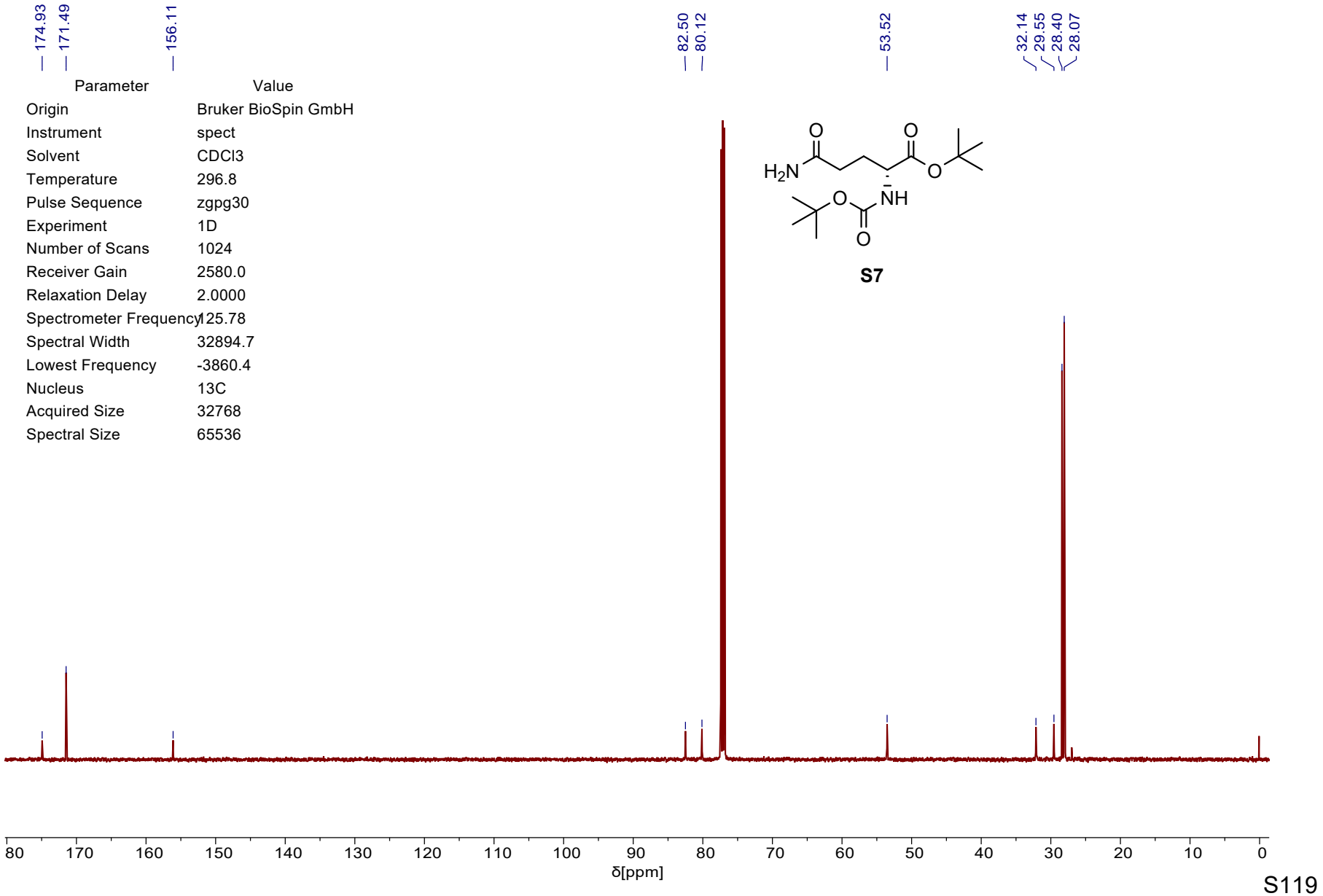

6.69 6.68 6.67
5.48 5.47 5.43 5.42 5.24
4.37 4.36 4.35 4.33 4.32 4.31 3.43 3.43 3.42 3.40 3.39 3.39 3.19 3.19 3.18 3.17 3.12 3.11 3.09 3.08 3.07 3.06 3.05 3.04 3.03
2.29 2.28 2.27 2.26 2.26 2.08 2.03 2.02 2.01 2.00 1.99 1.97 1.96 1.86 1.85 1.84 1.83 1.82 1.47 1.44 1.43 1.41
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 14.5
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
O
H
N
O
O
OH
O
NH
O
22
0.36
1.10
0.77
1.83
2.09
18.00
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
δ[ppm]

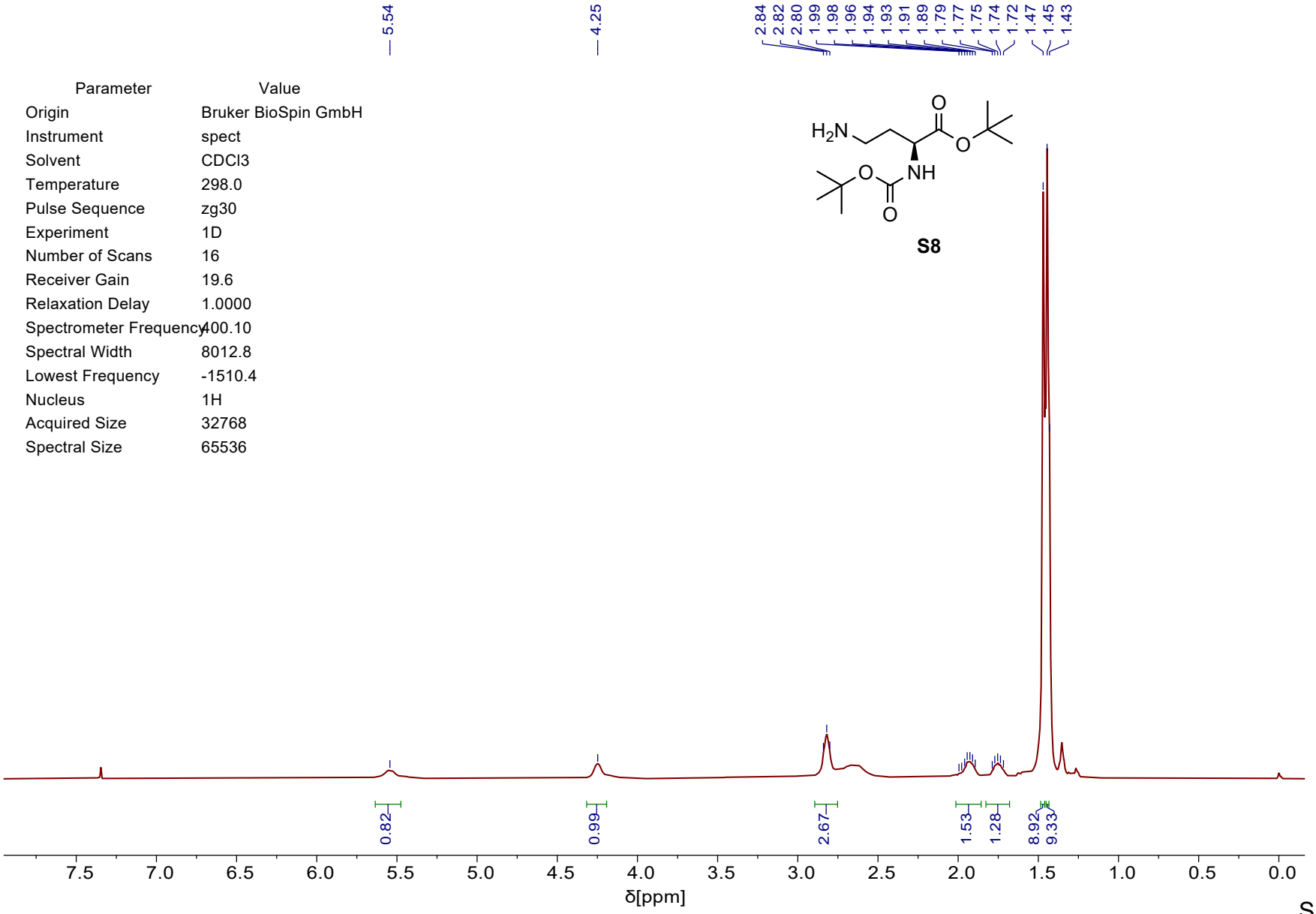

176.56
175.39
171.42
158.08
157.02
155.97
155.44
81.64
80.37
80.24
80.06
60.58
51.20
50.99
36.91
33.73
31.52
28.52
28.49
28.45
28.40
28.36
21.19
14.33
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2748.3
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
22
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

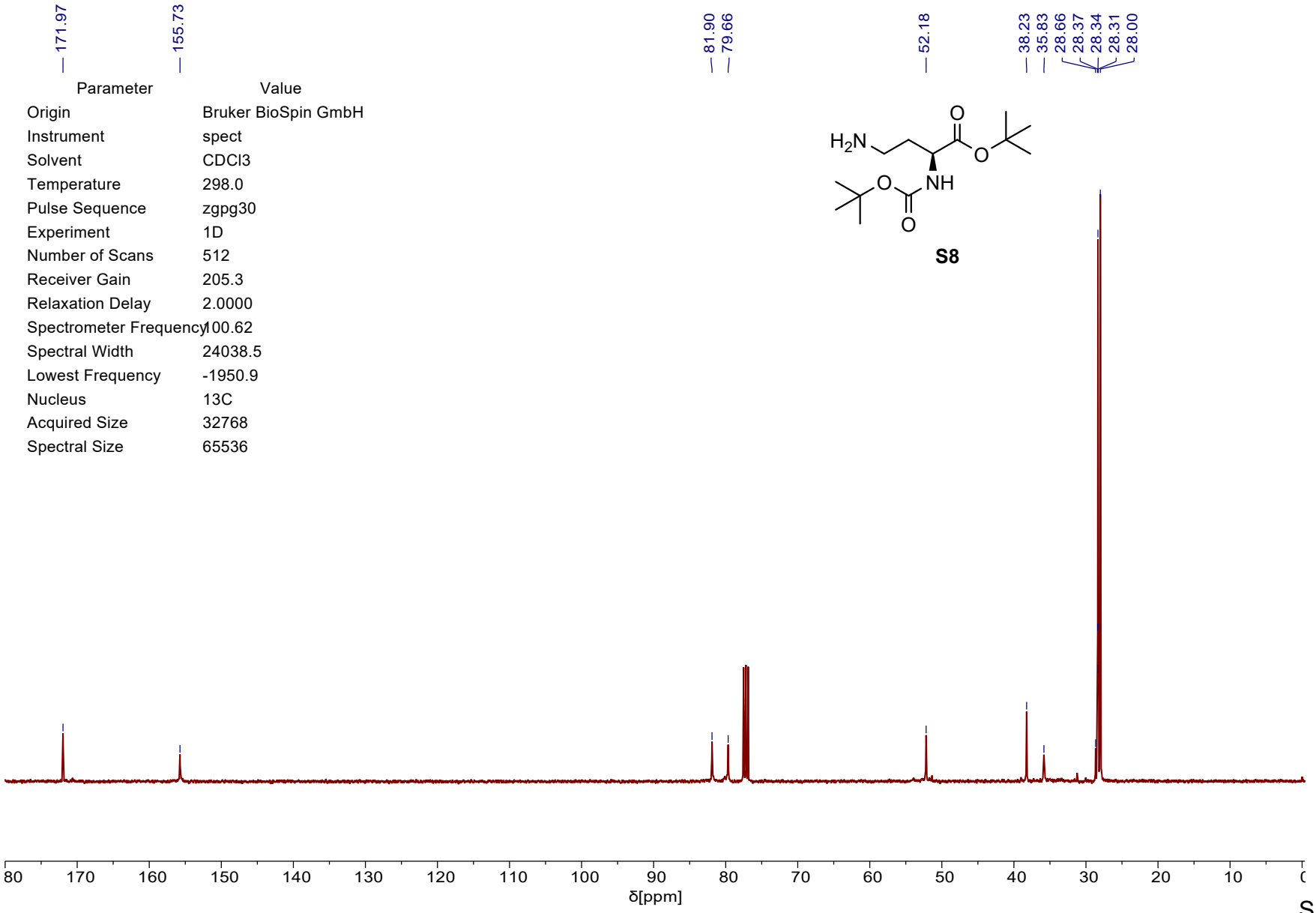

4.07 4.07 4.06 4.05 3.20 3.19 3.19 3.18 3.18 3.18 3.17 3.16 3.14 3.13 3.12 3.12 3.11 3.11 3.10 3.10
2.27 2.26 2.26 2.26 2.25 2.25 2.24 2.24 2.23 2.23 2.22 2.19 2.18 2.17 2.17 2.16 2.16 2.15
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent D2O
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 31.4
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
O
H2N
OH •2HCl
NH2
16•2HCl
1.02
1.05
1.02
1.04
1.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
δ[ppm]

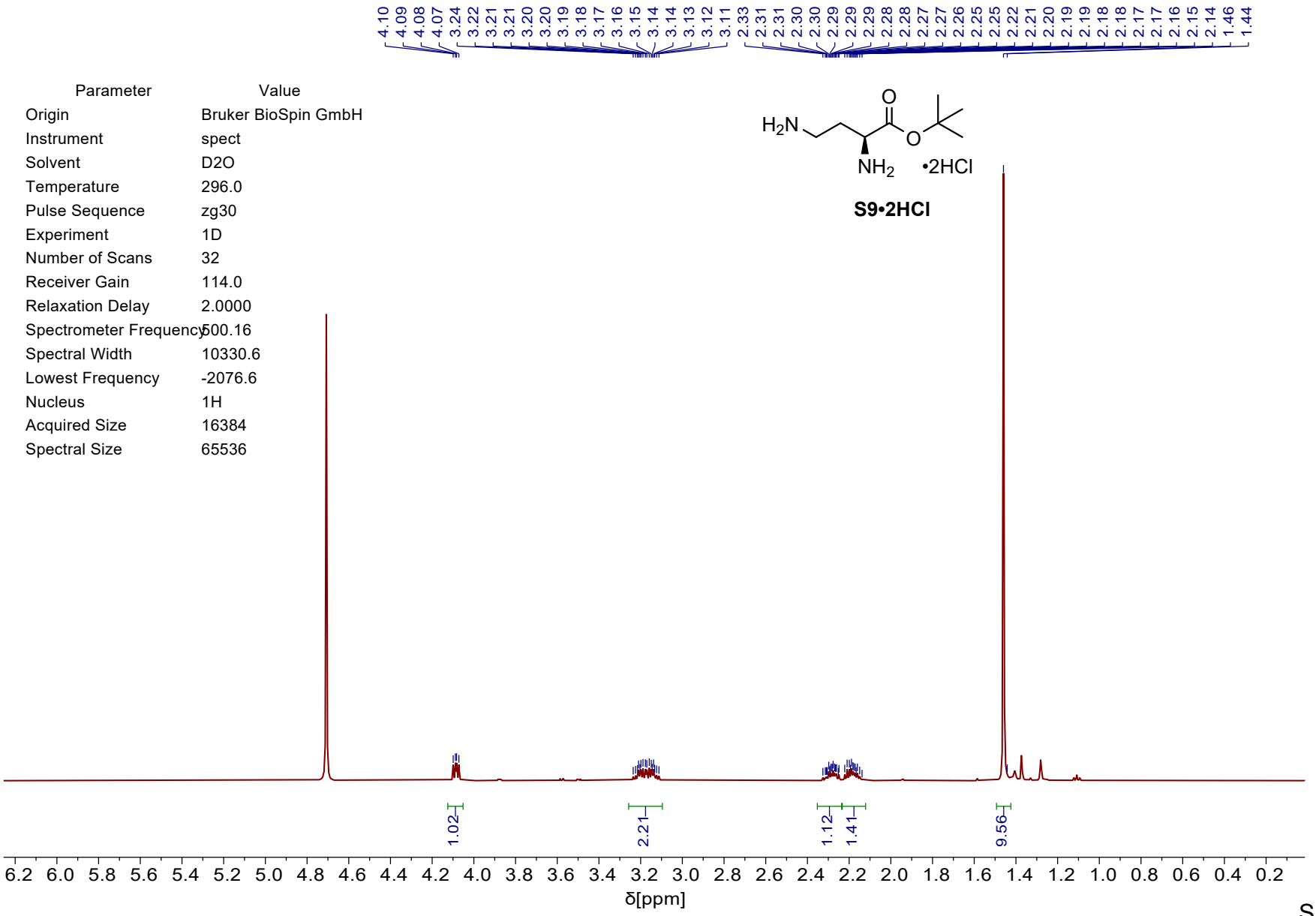

170.98
50.76
50.54
36.23
36.11
35.99
27.61
27.58
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent D2O
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
O
H2N
OH •2HCl
NH2
16•2HCl
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ[ppm]

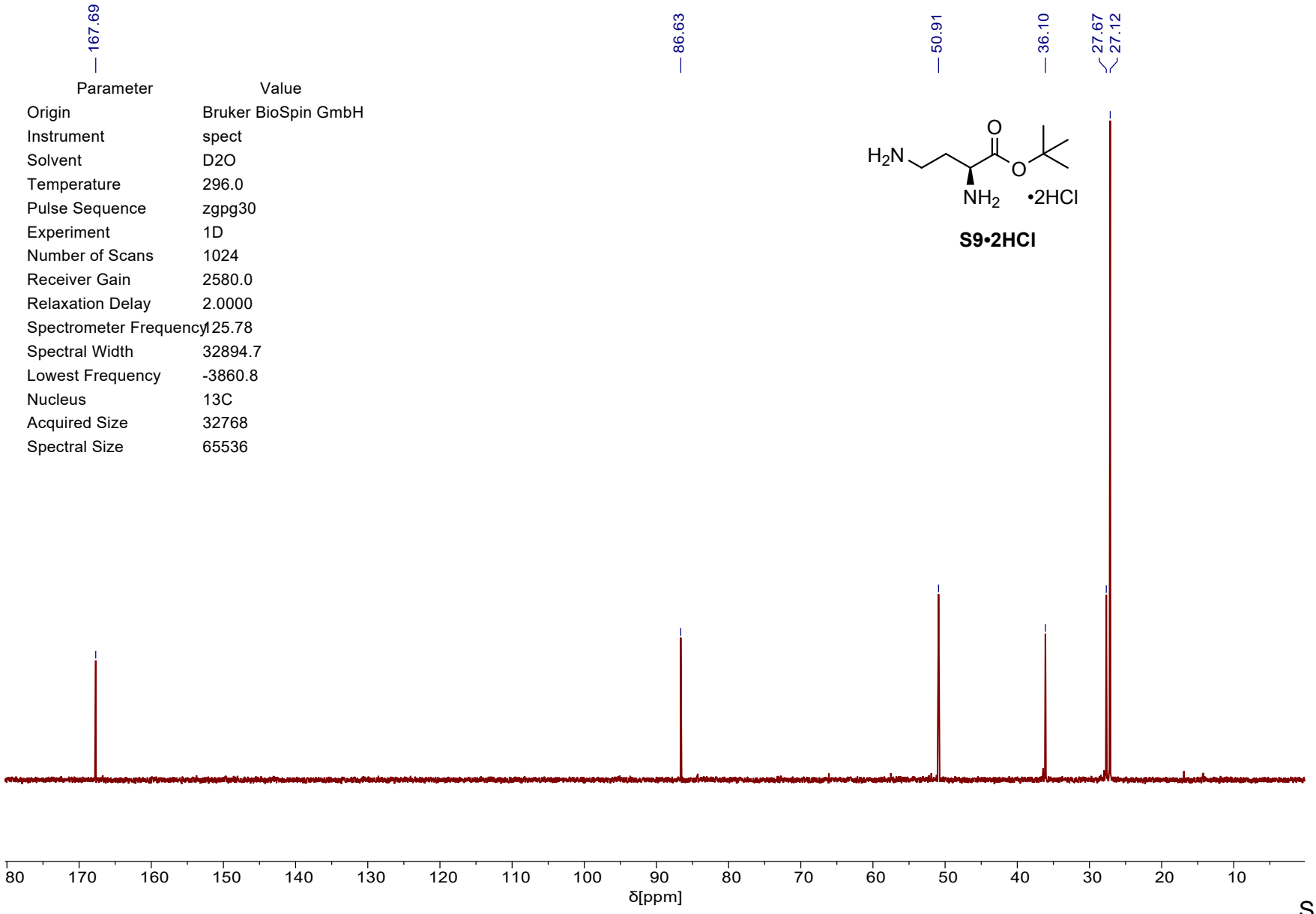

6.39
5.78
5.78
5.34
5.32
4.21
4.19
4.18
4.16
2.38
2.36
2.35
2.33
2.32
2.32
2.31
2.30
2.28
2.27
2.18
2.18
2.16
2.15
2.15
2.14
2.13
1.91
1.90
1.88
1.87
1.87
1.85
1.85
1.47
1.45
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.8
Pulse Sequence zg30
Experiment 1D
Number of Scans 32
Receiver Gain 114.0
Relaxation Delay 2.0000
Spectrometer Frequency 500.16
Spectral Width 10330.6
Lowest Frequency -2081.4
Nucleus 1H
Acquired Size 16384
Spectral Size 65536
S7
0.92
1.08
0.98
1.01
2.38
1.28
1.08
10.38
10.55
δ[ppm]

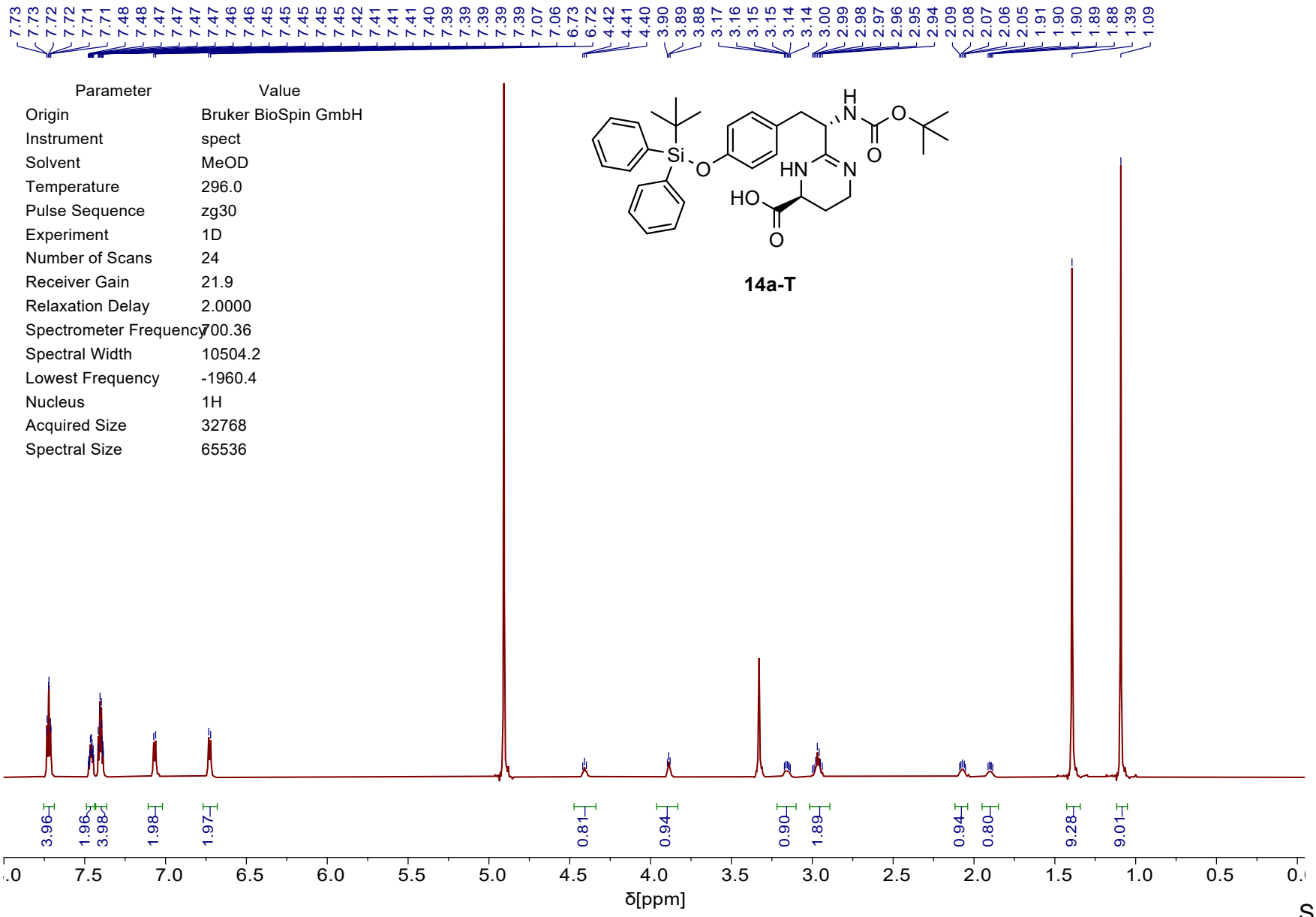

174.93
171.49
156.11
82.50
80.12
53.52
32.14
29.55
28.40
28.07
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.8
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1024
Receiver Gain 2580.0
Relaxation Delay 2.0000
Spectrometer Frequency 125.78
Spectral Width 32894.7
Lowest Frequency -3860.4
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
S7
δ[ppm]

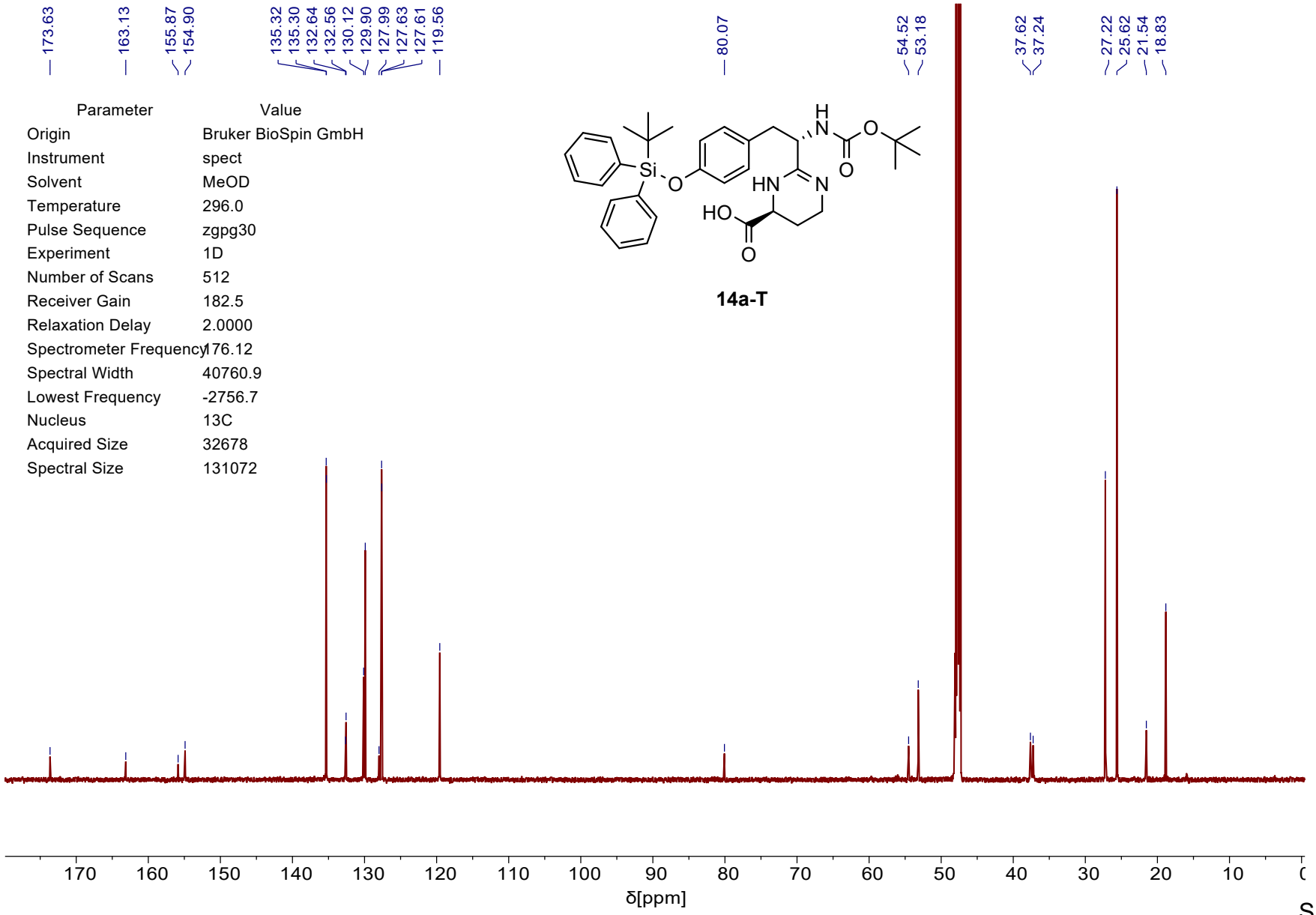

5.54
4.25
2.84
2.82
2.80
1.99
1.98
1.96
1.94
1.93
1.91
1.89
1.79
1.77
1.75
1.74
1.72
1.47
1.45
1.43
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 19.6
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1510.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
H2N
O
O
NH
O
O
S8
0.82
0.99
2.67
1.53
1.28
8.92
9.33
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ[ppm]

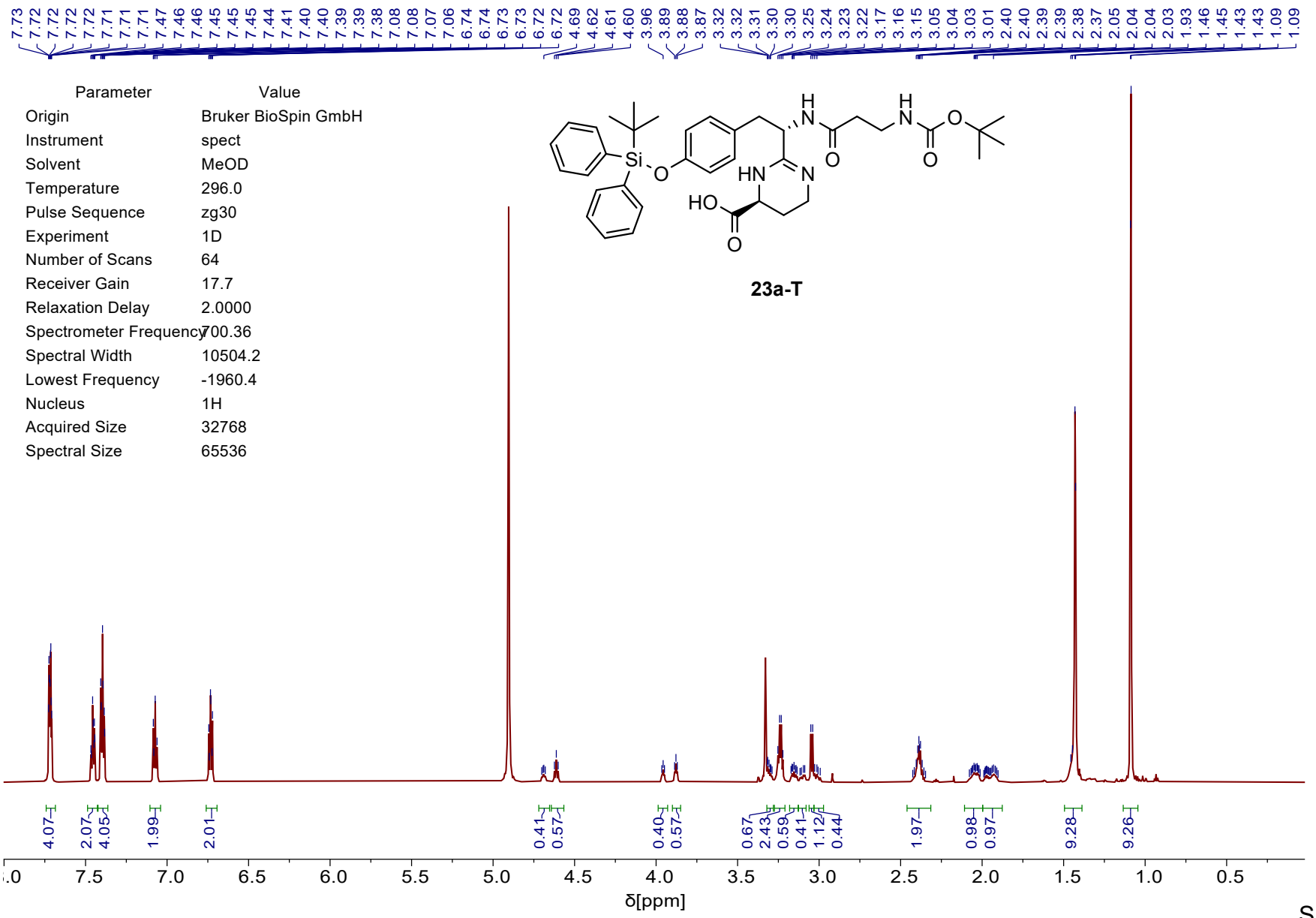

171.97
155.73
81.90
79.66
52.18
38.23
35.83
28.66
28.37
28.34
28.31
28.00
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
S8
δ[ppm]

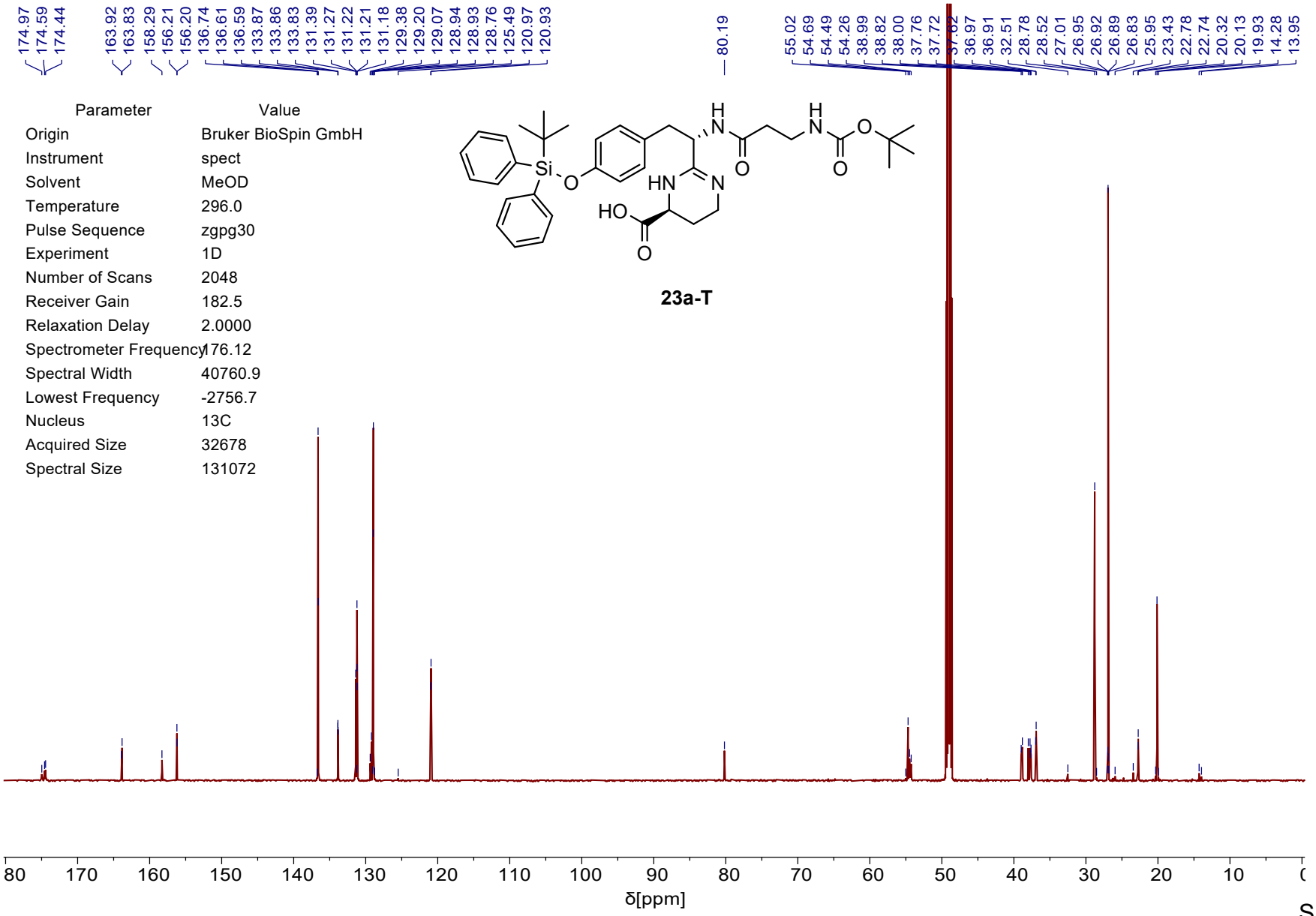

4.10 4.09 4.08 4.07 3.24 3.22 3.21 3.21 3.20 3.20 3.19 3.18 3.17 3.16 3.15 3.14 3.14 3.13 3.12 3.11 2.33 2.31 2.31 2.30 2.30 2.29 2.29 2.29 2.28 2.28 2.27 2.27 2.26 2.25 2.25 2.22 2.21 2.20 2.19 2.19 2.18 2.18 2.17 2.17 2.16 2.15 2.14 1.46 1.44
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent D2O
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 32
Receiver Gain 114.0
Relaxation Delay 2.0000
Spectrometer Frequency 500.16
Spectral Width 10330.6
Lowest Frequency -2076.6
Nucleus 1H
Acquired Size 16384
Spectral Size 65536
H2N
O
O
NH2
•2HCl
S9•2HCl
1.02
2.21
1.12
1.41
9.56
6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4 0.2
δ[ppm]

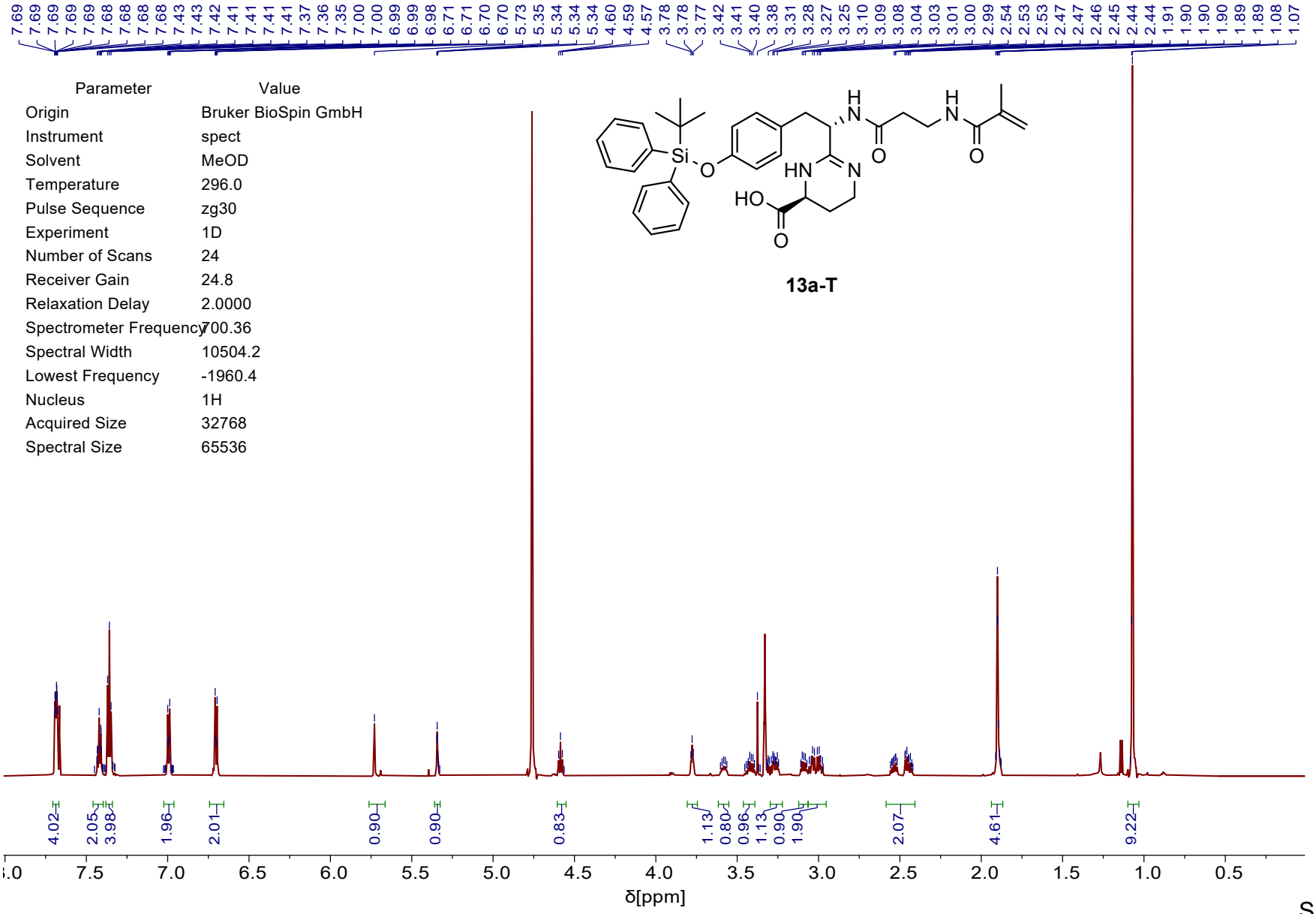

167.69
86.63
50.91
36.10
27.67
27.12
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent D2O
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1024
Receiver Gain 2580.0
Relaxation Delay 2.0000
Spectrometer Frequency 125.78
Spectral Width 32894.7
Lowest Frequency -3860.8
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
H2N
O
O
NH2
•2HCl
S9•2HCl
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

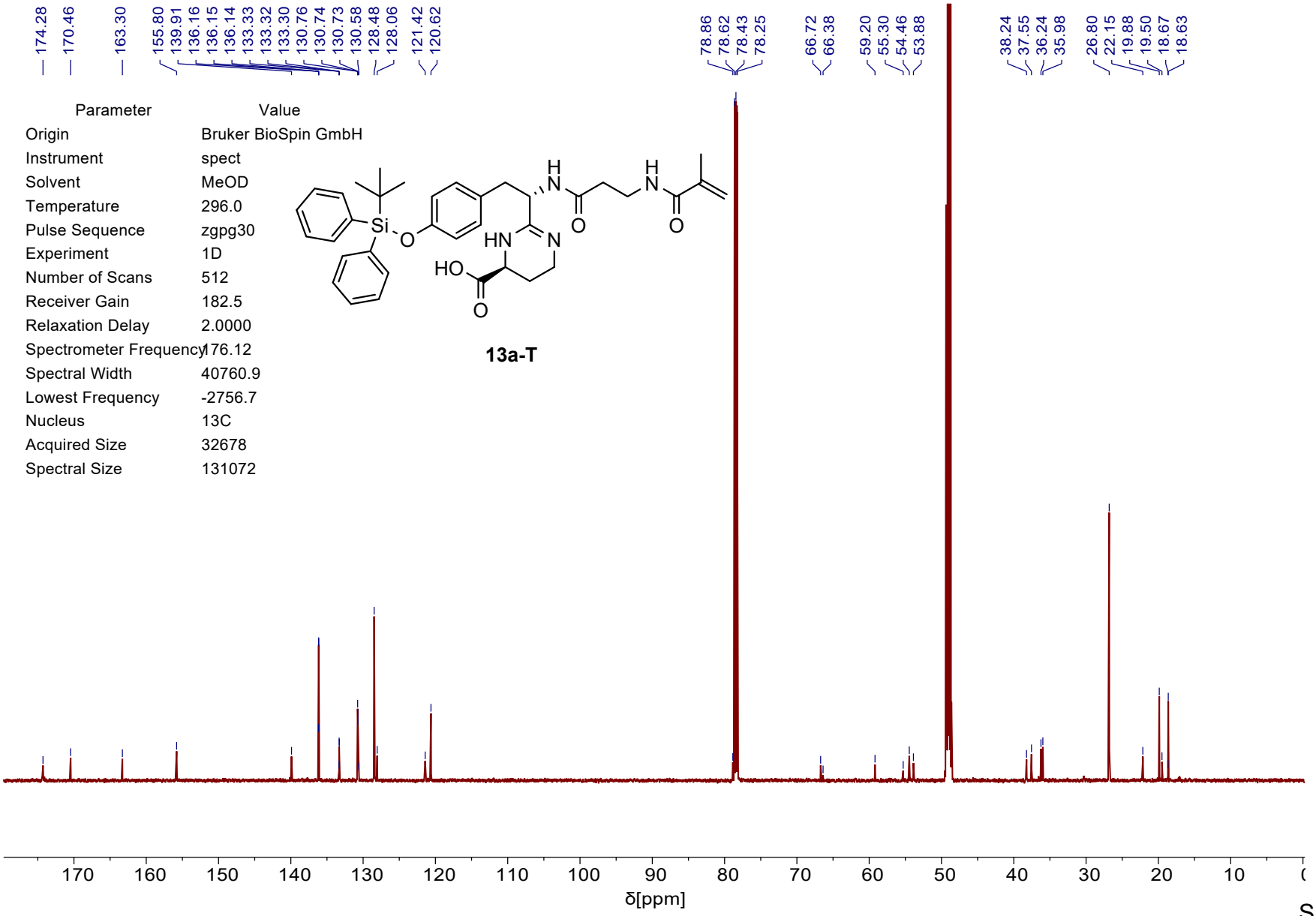

7.73 7.73 7.72 7.72 7.71 7.71 7.48 7.48 7.47 7.47 7.47 7.47 7.46 7.46 7.45 7.45 7.45 7.45 7.45 7.42 7.41 7.41 7.41 7.40 7.39 7.39 7.39 7.39 7.07 7.06 6.73 6.72 4.42 4.41 4.40 3.90 3.89 3.88 3.17 3.16 3.15 3.15 3.14 3.14 3.00 2.99 2.98 2.97 2.96 2.95 2.94 2.09 2.08 2.07 2.06 2.05 1.91 1.90 1.90 1.89 1.88 1.39 1.09
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 21.9
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
14a-T
3.96 1.96 3.98 1.98 1.97 0.81 0.94 0.90 1.89 0.94 0.80 9.28 9.01
δ[ppm]

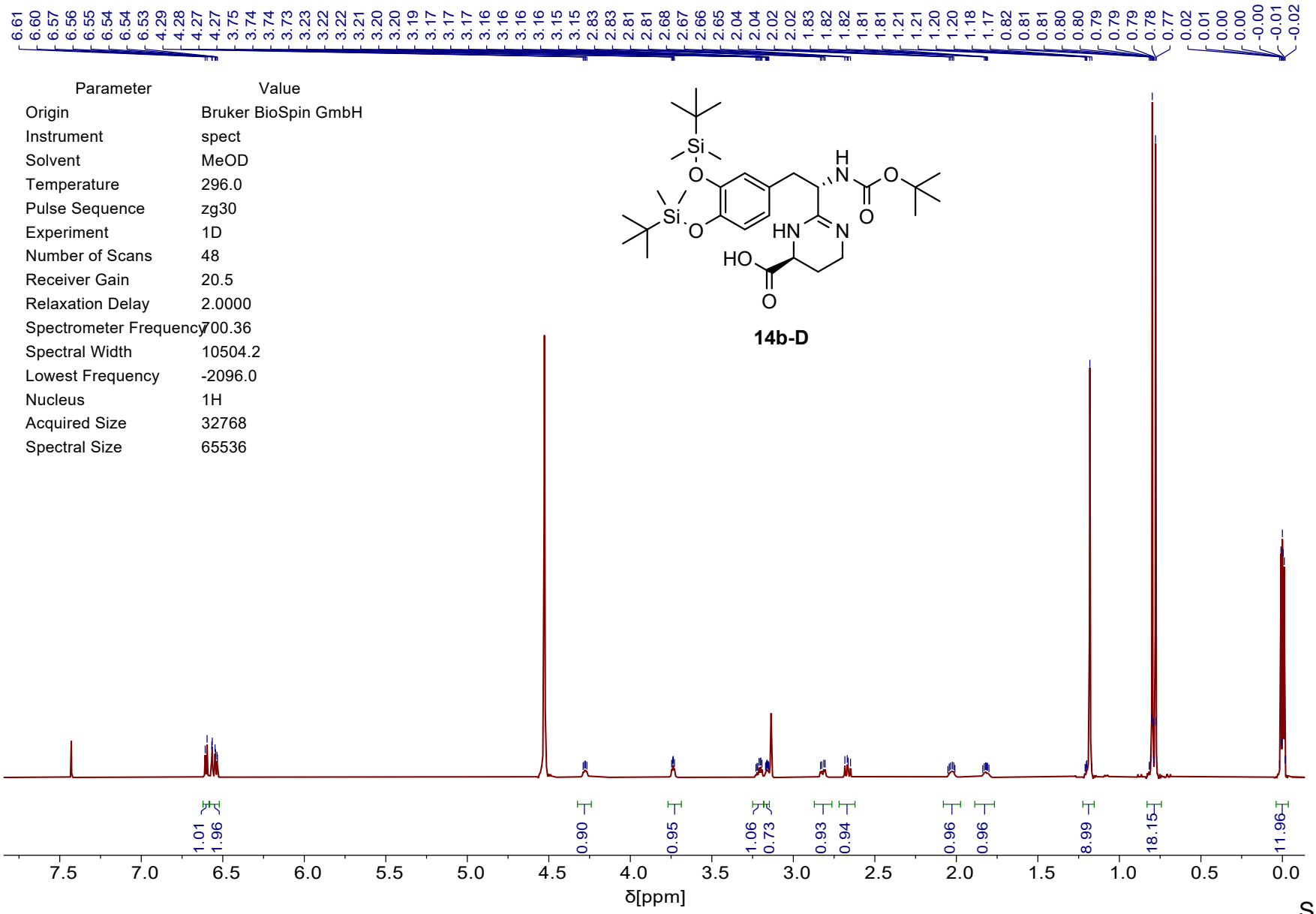

173.63
163.13
155.87
154.90
135.32
135.30
132.64
132.56
130.12
129.90
127.99
127.63
127.61
119.56
80.07
54.52
53.18
37.62
37.24
27.22
25.62
21.54
18.83
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
Si
O
HN
N
H
N
O
O
HO
O
14a-T
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ[ppm]

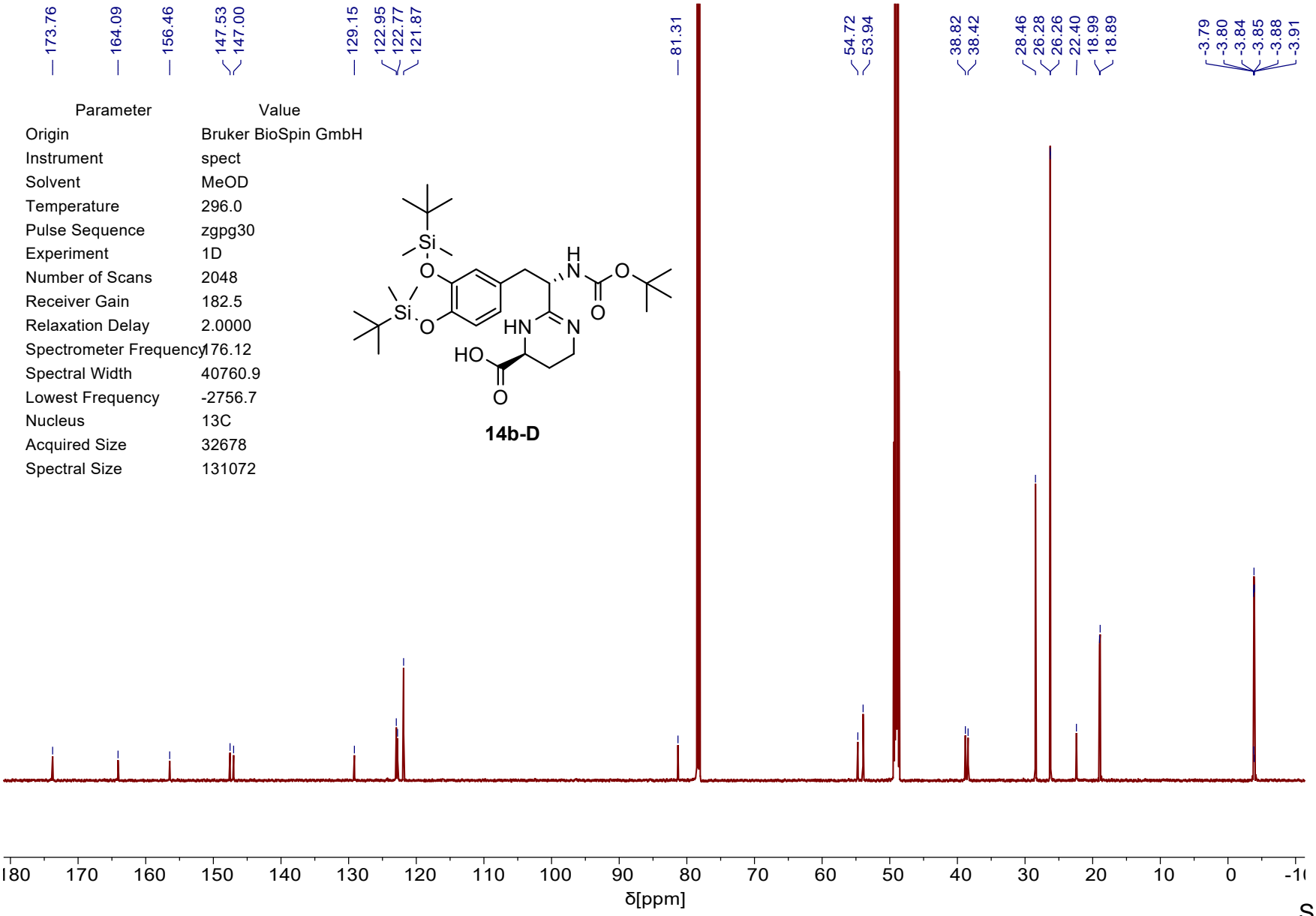

7.73 7.72 7.72 7.72 7.72 7.71 7.71 7.71 7.47 7.46 7.46 7.45 7.45 7.45 7.44 7.41 7.40 7.40 7.39 7.39 7.38 7.08 7.08 7.07 7.06 6.74 6.74 6.73 6.73 6.72 6.72 4.69 4.62 4.61 4.60 3.96 3.89 3.88 3.87 3.32 3.32 3.31 3.30 3.30 3.25 3.24 3.23 3.22 3.17 3.16 3.15 3.05 3.04 3.03 3.01 2.40 2.40 2.39 2.39 2.38 2.37 2.05 2.04 2.04 2.03 1.93 1.46 1.45 1.43 1.43 1.09 1.09
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 64
Receiver Gain 17.7
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
23a-T
4.07 2.07 4.05 1.99 2.01 0.41 0.57 0.40 0.57 0.67 2.43 0.59 0.41 1.12 0.44 1.97 0.98 0.97 9.28 9.26
δ[ppm]

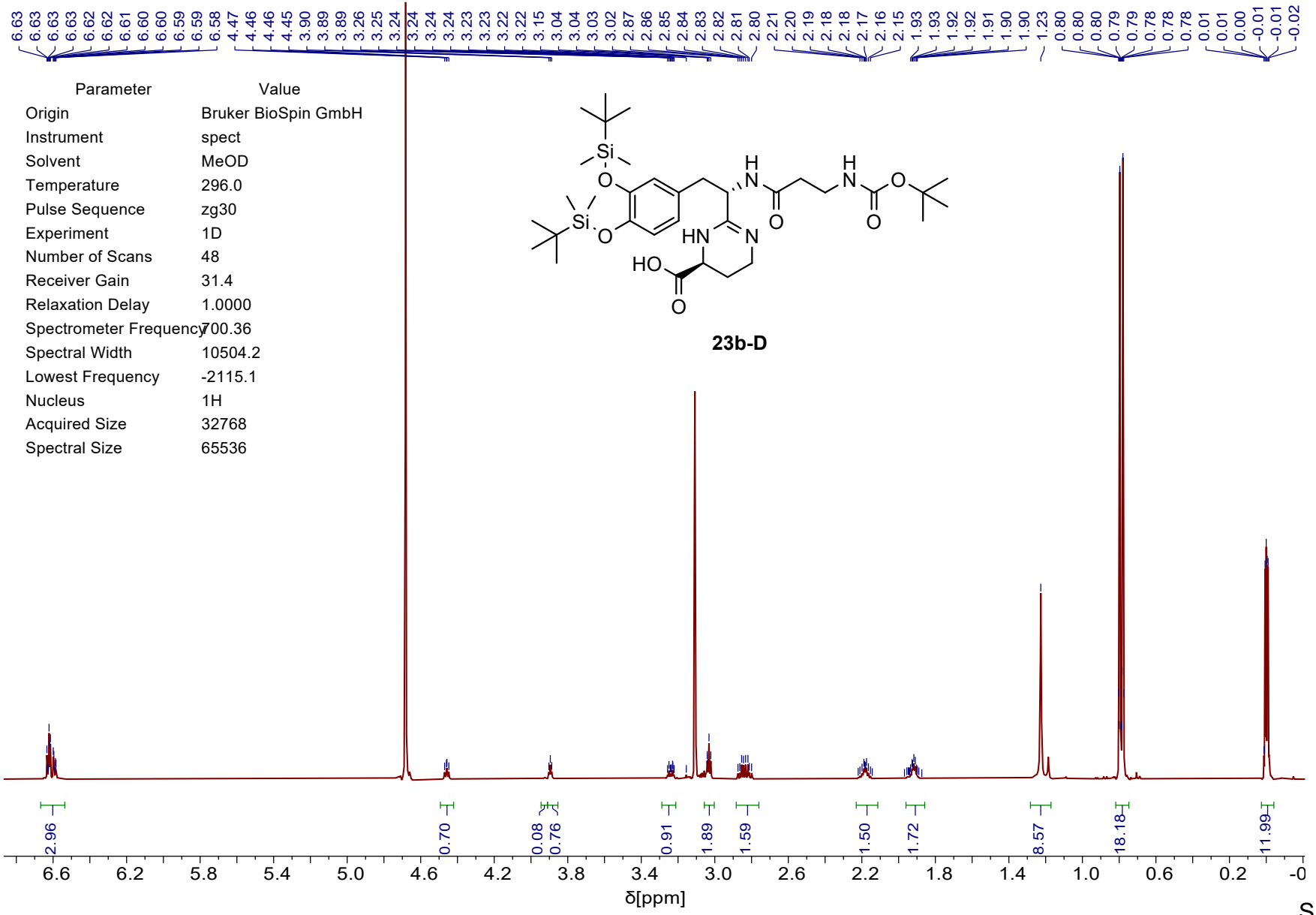

174.97
174.59
174.44
163.92
163.83
158.29
156.21
156.20
136.74
136.61
136.59
133.87
133.86
133.83
131.39
131.27
131.22
131.21
131.18
129.38
129.20
129.07
128.94
128.93
128.76
125.49
120.97
120.93
80.19
55.02
54.69
54.49
54.26
38.99
38.82
38.00
37.76
37.72
37.62
36.97
36.91
32.51
28.78
28.52
27.01
26.95
26.92
26.89
26.83
25.95
23.43
22.78
22.74
20.32
20.13
19.93
14.28
13.95
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 2048
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
23a-T
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

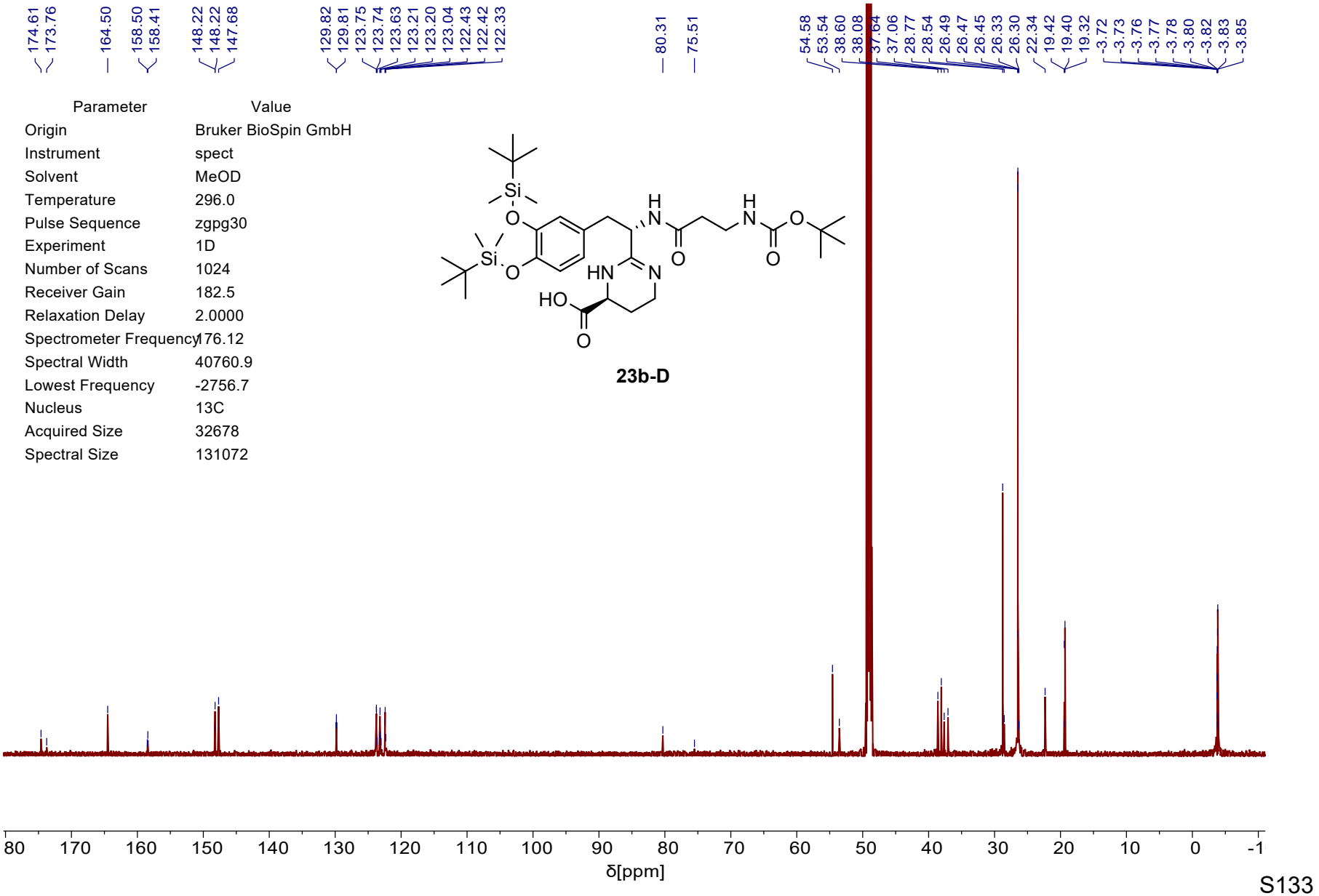

7.69 7.69 7.69 7.69 7.69 7.68 7.68 7.68 7.68 7.43 7.43 7.42 7.41 7.41 7.41 7.41 7.37 7.36 7.35 7.00 7.00 6.99 6.99 6.98 6.71 6.71 6.70 6.70 5.73 5.35 5.34 5.34 5.34 4.60 4.59 4.57 3.78 3.78 3.77 3.42 3.41 3.40 3.38 3.31 3.28 3.27 3.25 3.10 3.09 3.08 3.04 3.03 3.01 3.00 2.99 2.54 2.53 2.53 2.47 2.47 2.46 2.45 2.44 2.44 1.91 1.90 1.90 1.90 1.89 1.89 1.08 1.07
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 24.8
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
13a-T
4.02 2.05 3.98 1.96 2.01 0.90 0.90 0.83 1.13 0.80 0.96 1.13 0.90 1.90 2.07 4.61 9.22
δ[ppm]


174.28
170.46
163.30
155.80
139.91
136.16
136.15
136.14
133.33
133.32
133.30
130.76
130.74
130.73
130.58
128.48
128.06
121.42
120.62
78.86
78.62
78.43
78.25
66.72
66.38
59.20
55.30
54.46
53.88
38.24
37.55
36.24
35.98
26.80
22.15
19.88
19.50
18.67
18.63
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
13a-T
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ[ppm]


6.61 6.60 6.57 6.56 6.55 6.54 6.54 6.53 4.29 4.28 4.27 4.27 3.75 3.74 3.74 3.73 3.23 3.22 3.21 3.20 3.20 3.19 3.17 3.17 3.17 3.16 3.16 3.16 3.16 3.15 3.15 2.83 2.81 2.81 2.68 2.67 2.66 2.65 2.04 2.04 2.02 2.02 1.83 1.82 1.81 1.81 1.21 1.21 1.20 1.20 1.18 1.17 0.82 0.81 0.81 0.80 0.80 0.79 0.79 0.79 0.78 0.77 0.02 0.01 0.00 0.00 -0.00 -0.01 -0.02
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 48
Receiver Gain 20.5
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -2096.0
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
Si
O
Si
O
H
N
O
O
HN
N
HO
O
14b-D
1.01 1.96 0.90 0.95 1.06 0.73 0.93 0.94 0.96 0.96 8.99 18.15 11.96
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ[ppm]


173.76
164.09
156.46
147.53
147.00
129.15
122.95
122.77
121.87
81.31
54.72
53.94
38.82
38.42
28.46
26.28
26.26
22.40
18.99
18.89
-3.79
-3.80
-3.84
-3.85
-3.88
-3.91
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 2048
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
Si
O
Si
O
H
N
O
O
HN
N
HO
O
14b-D
δ[ppm]


6.63 6.63 6.63 6.63 6.62 6.62 6.61 6.60 6.60 6.59 6.59 6.58 4.47 4.46 4.46 4.45 3.90 3.89 3.89 3.26 3.25 3.24 3.24 3.24 3.24 3.24 3.23 3.22 3.22 3.15 3.04 3.04 3.03 3.02 2.87 2.86 2.85 2.84 2.83 2.82 2.81 2.80 2.21 2.20 2.19 2.18 2.18 2.17 2.16 2.15 1.93 1.93 1.92 1.92 1.91 1.90 1.90 1.23 0.80 0.80 0.80 0.79 0.79 0.78 0.78 0.78 0.01 0.01 0.00 -0.01 -0.01 -0.02
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 48
Receiver Gain 31.4
Relaxation Delay 1.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -2115.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
Si
O
Si
O
H
N
O
HN
N
HO
O
H
N
O
O
23b-D
2.96 0.70 0.08 0.76 0.91 1.89 1.59 1.50 1.72 8.57 18.18 11.99
6.6 6.2 5.8 5.4 5.0 4.6 4.2 3.8 3.4 3.0 2.6 2.2 1.8 1.4 1.0 0.6 0.2 -0
δ[ppm]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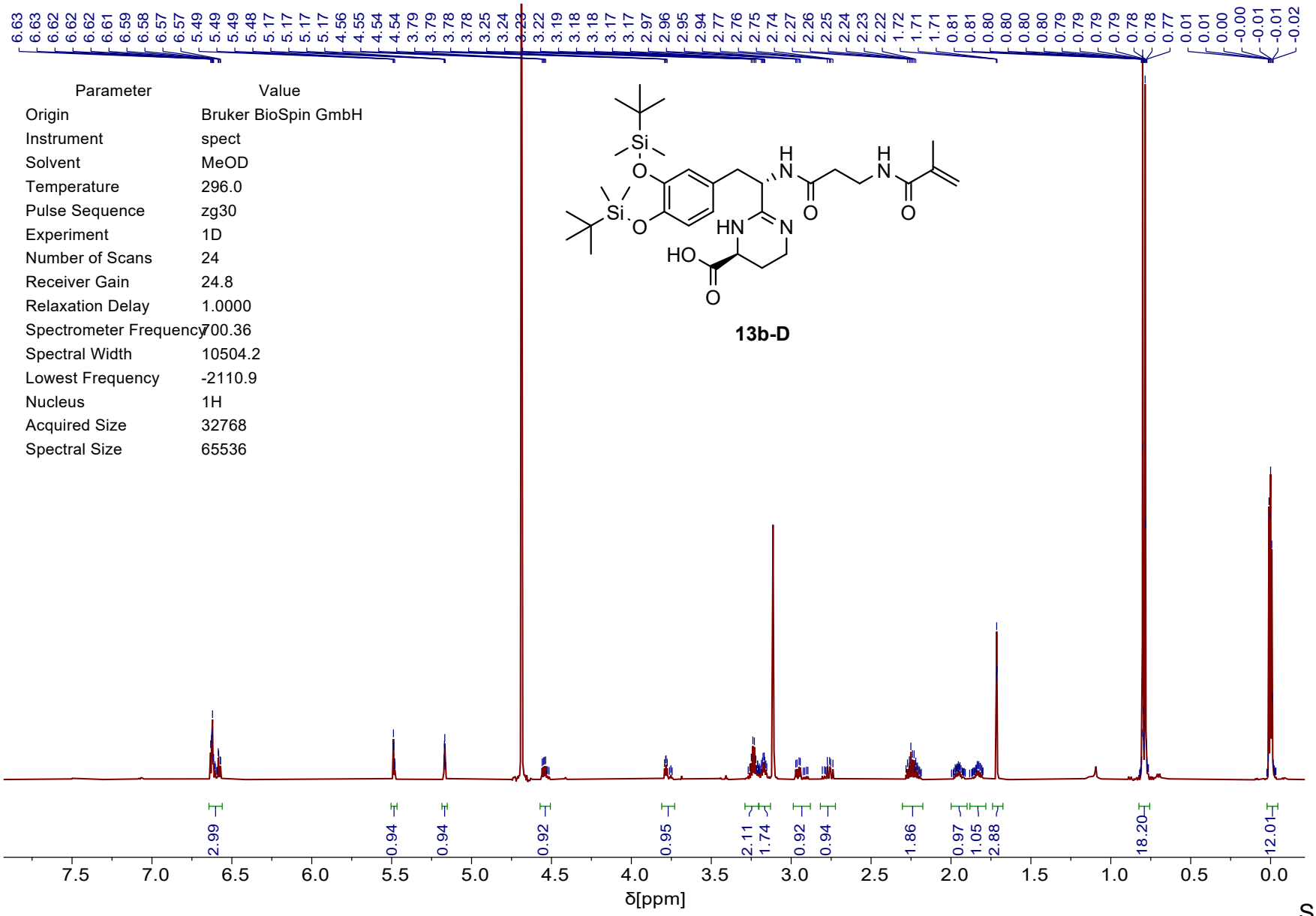
173.76
164.50
158.50
158.41
148.22
148.22
147.68
129.82
129.81
123.75
123.74
123.63
123.21
123.20
123.04
122.43
122.42
122.33
80.31
75.51
54.58
53.54
38.60
38.08
37.64
37.06
28.77
28.54
26.49
26.47
26.45
26.33
26.30
22.34
19.42
19.40
19.32
-3.72
-3.73
-3.76
-3.77
-3.78
-3.80
-3.82
-3.83
-3.85
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1024
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
23b-D
δ[ppm]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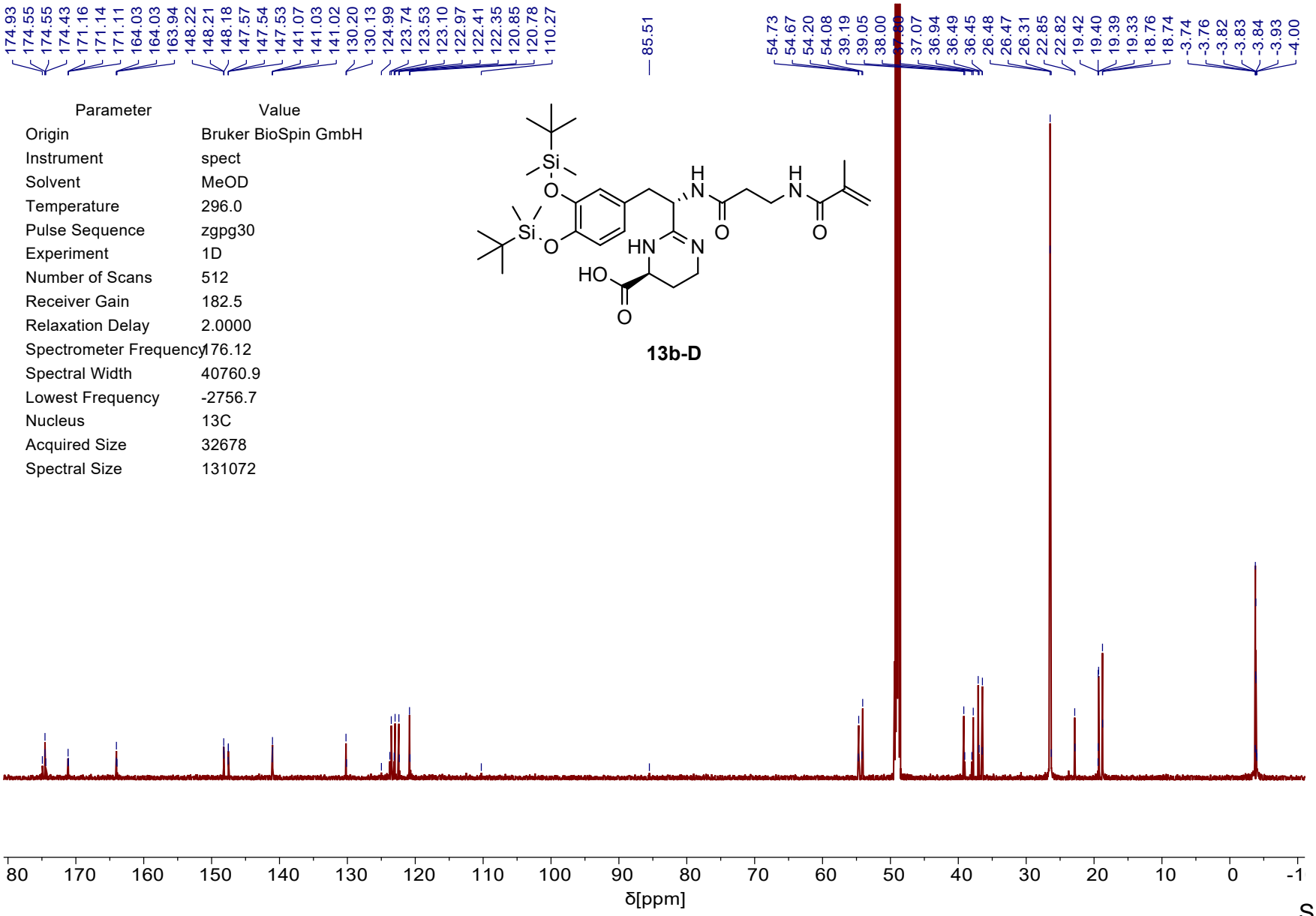
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 24.8
Relaxation Delay 1.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -2110.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
Si
O
Si
O
H
N
O
H
N
O
HN
N
HO
O
2.99 0.94 0.94 0.92 0.95 2.11 1.74 0.92 0.94 1.86 0.97 1.05 2.88 18.20 12.01
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ[ppm]

13b-D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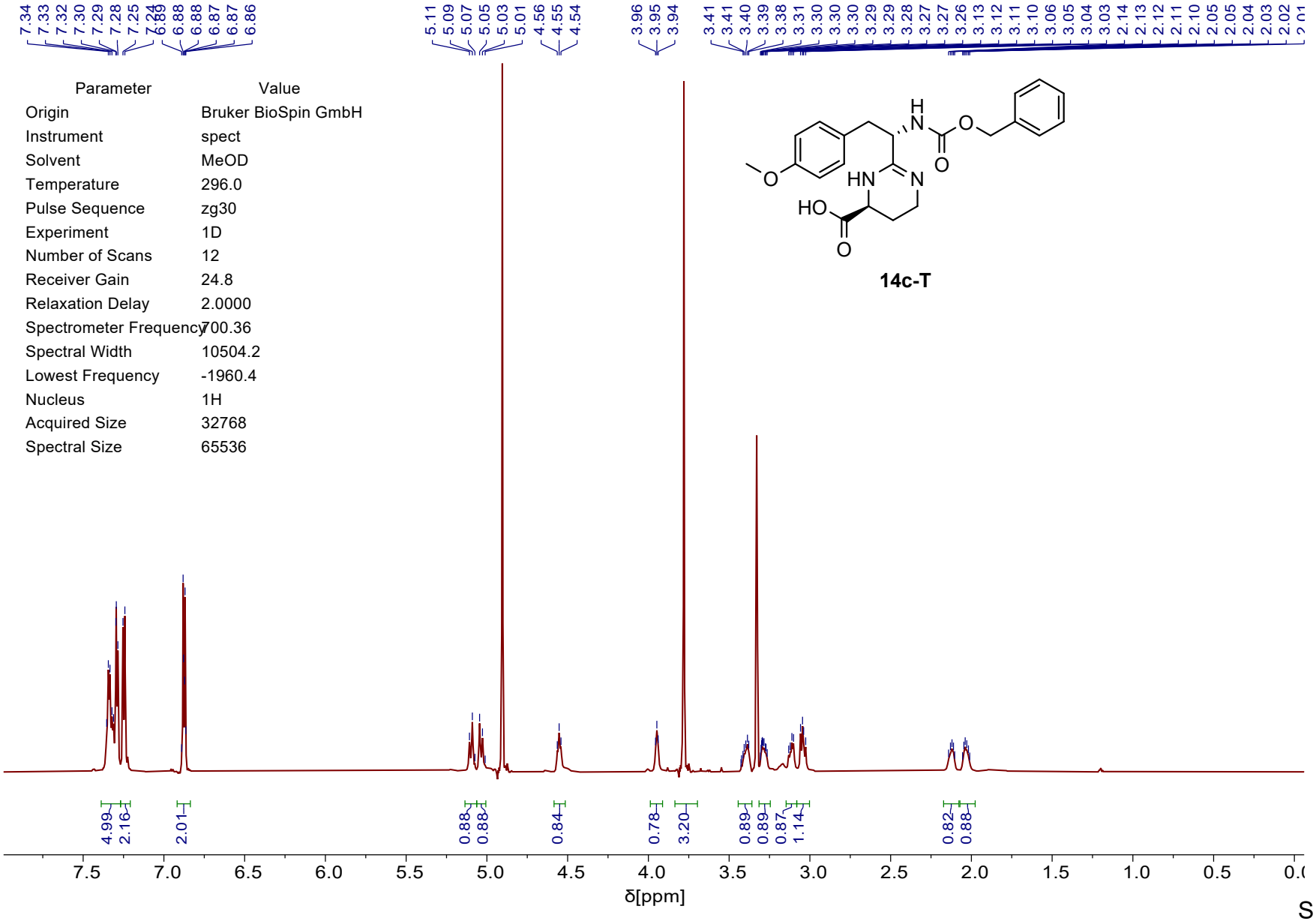
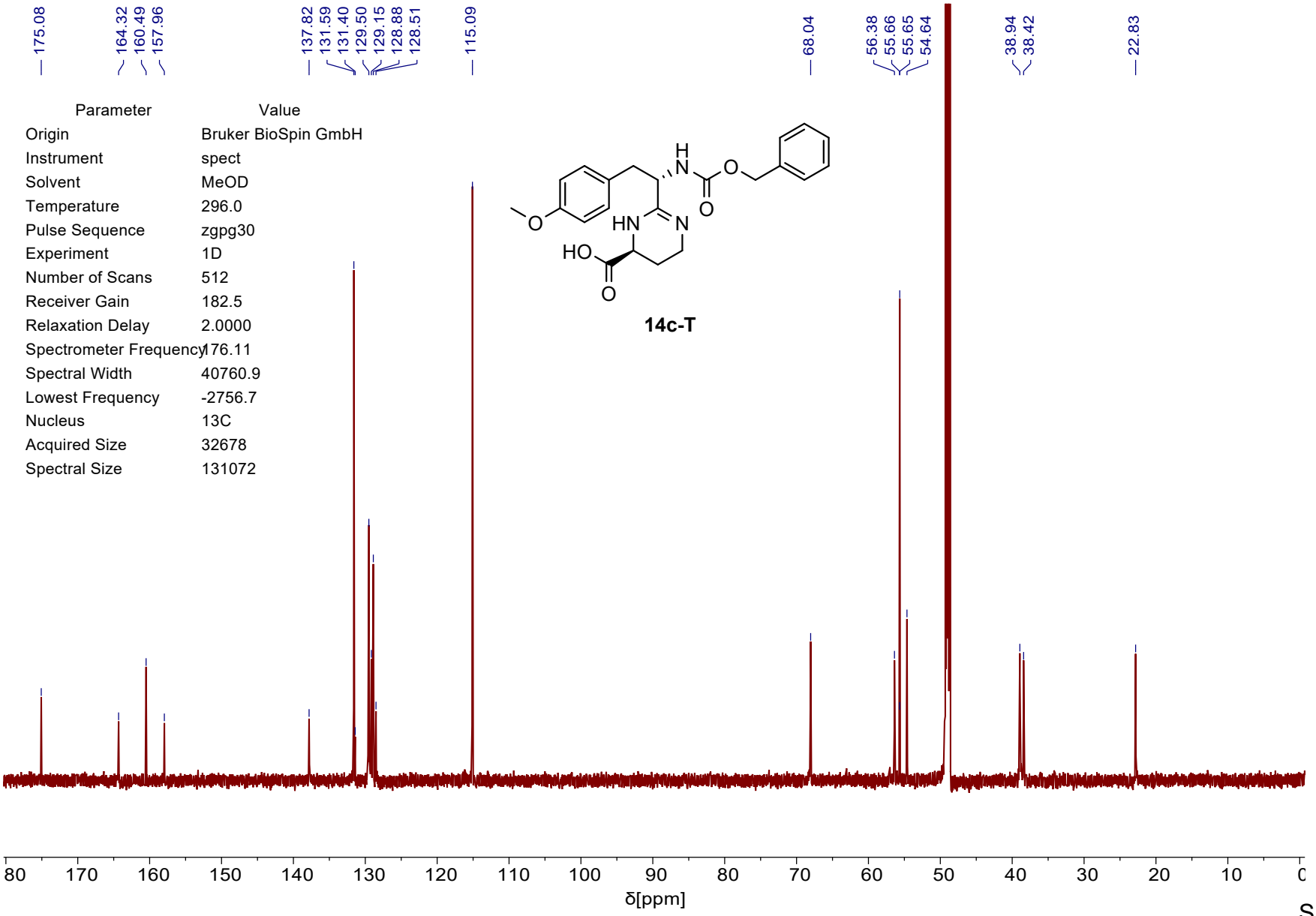
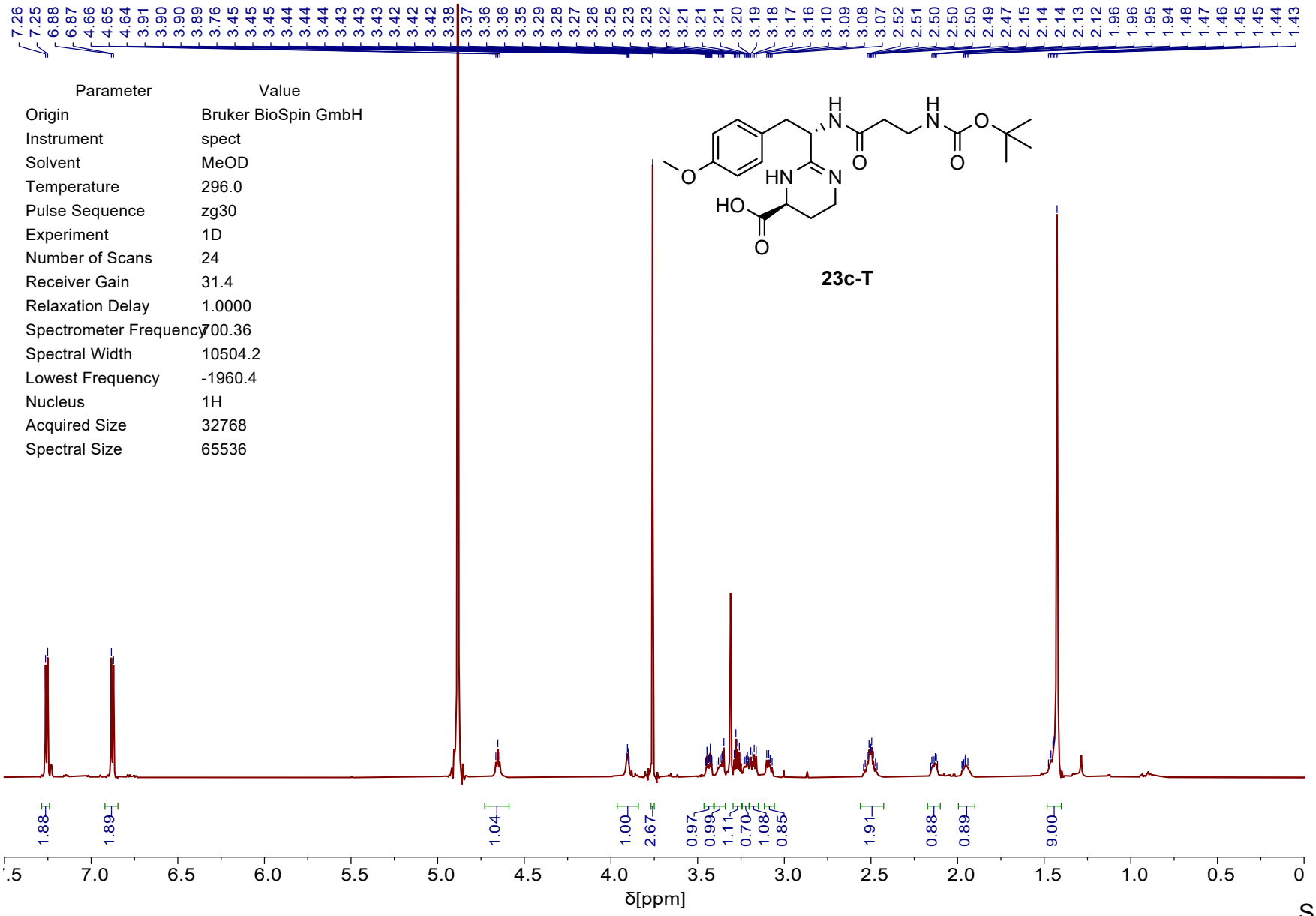
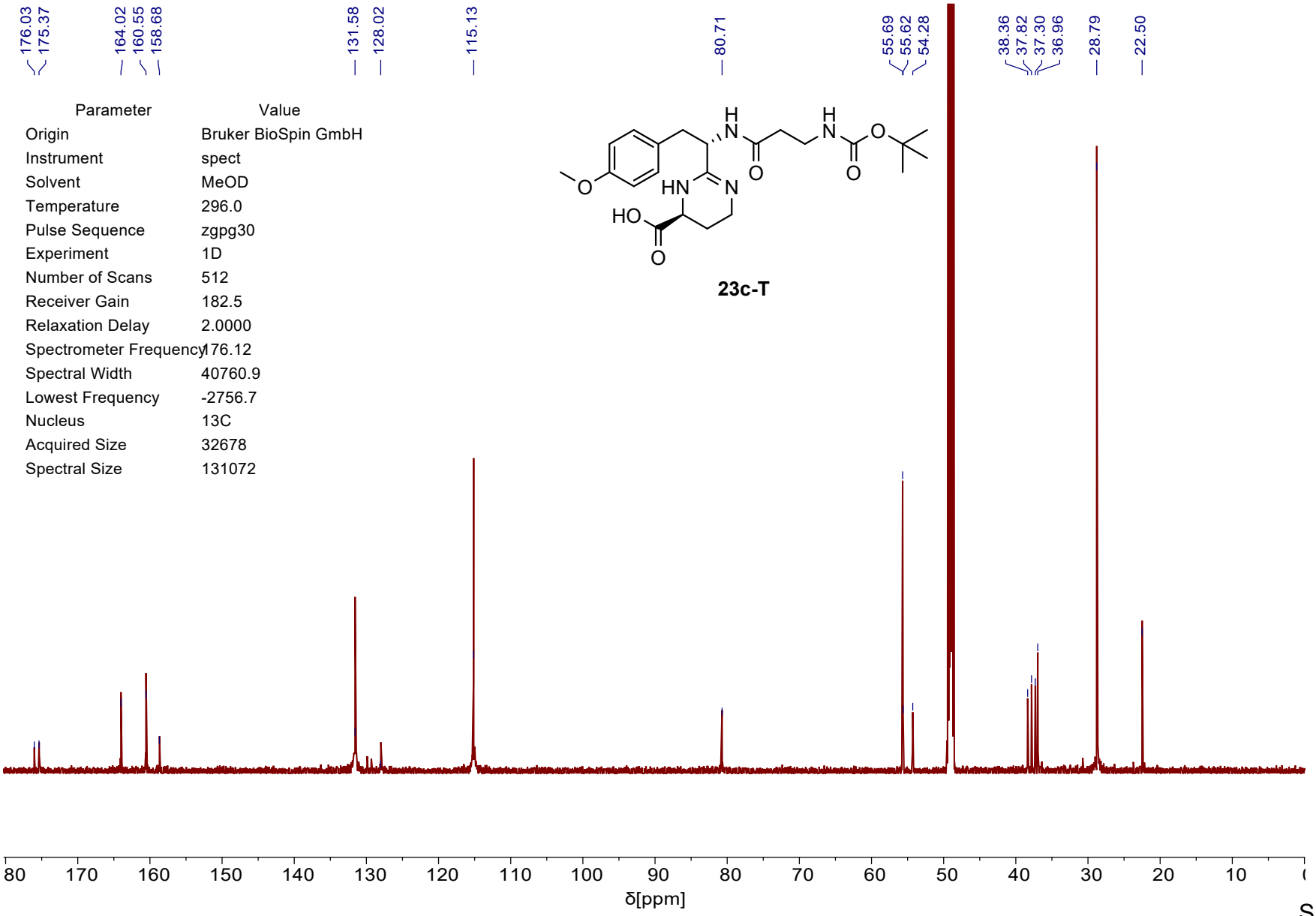
174.55
174.55
174.43
171.16
171.14
171.11
164.03
164.03
163.94
148.22
148.21
148.18
147.57
147.54
147.53
141.07
141.03
141.02
130.20
130.13
124.99
123.74
123.53
123.10
122.97
122.41
122.35
120.85
120.78
110.27
85.51
54.73
54.67
54.20
54.08
39.19
39.05
38.00
37.90
37.07
36.94
36.49
36.45
26.48
26.47
26.31
22.85
22.82
19.42
19.40
19.39
19.33
18.76
18.74
-3.74
-3.76
-3.82
-3.83
-3.84
-3.93
-4.00
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
Si
O
Si
O
HN
N
H
N
O
H
N
O
HO
O
13b-D
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
δ[ppm]


7.34 7.33 7.32 7.30 7.29 7.28 7.25 6.88 6.88 6.87 6.87 6.86
5.11 5.09 5.07 5.05 5.03 5.01 4.56 4.55 4.54
3.96 3.95 3.94
3.41 3.41 3.40 3.39 3.38 3.31 3.30 3.30 3.30 3.29 3.29 3.28 3.27 3.27 3.26 3.13 3.12 3.11 3.10 3.06 3.05 3.04 3.03 2.14 2.13 2.12 2.11 2.10 2.05 2.05 2.04 2.03 2.02
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 12
Receiver Gain 24.8
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
H
N
O
O
O
HN
N
HO
O
14c-T
4.99 2.16 2.01 0.88 0.88 0.84 0.78 3.20 0.89 0.89 0.87 1.14 0.82 0.88
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
δ[ppm]


175.08
164.32
160.49
157.96
137.82
131.59
131.40
129.50
129.15
128.88
128.51
115.09
68.04
56.38
55.66
55.65
54.64
38.94
38.42
22.83
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.11
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
14c-T
δ[ppm]


7.26 7.25 6.88 6.87 4.66 4.65 4.64 3.91 3.90 3.90 3.89 3.76 3.45 3.45 3.45 3.44 3.44 3.44 3.43 3.43 3.43 3.42 3.42 3.42 3.38 3.37 3.36 3.36 3.35 3.29 3.28 3.27 3.26 3.25 3.23 3.23 3.22 3.21 3.21 3.21 3.20 3.19 3.18 3.17 3.16 3.10 3.09 3.08 3.07 2.52 2.51 2.50 2.50 2.50 2.49 2.47 2.15 2.14 2.14 2.13 2.12 1.96 1.96 1.95 1.94 1.48 1.47 1.46 1.45 1.45 1.44 1.43
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 31.4
Relaxation Delay 1.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
H N
N
O
O
O
HN
N
HO
O
23c-T
1.88 1.89 1.04 1.00 2.67 0.97 0.99 1.11 0.70 1.08 0.85 1.91 0.88 0.89 9.00
.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
δ[ppm]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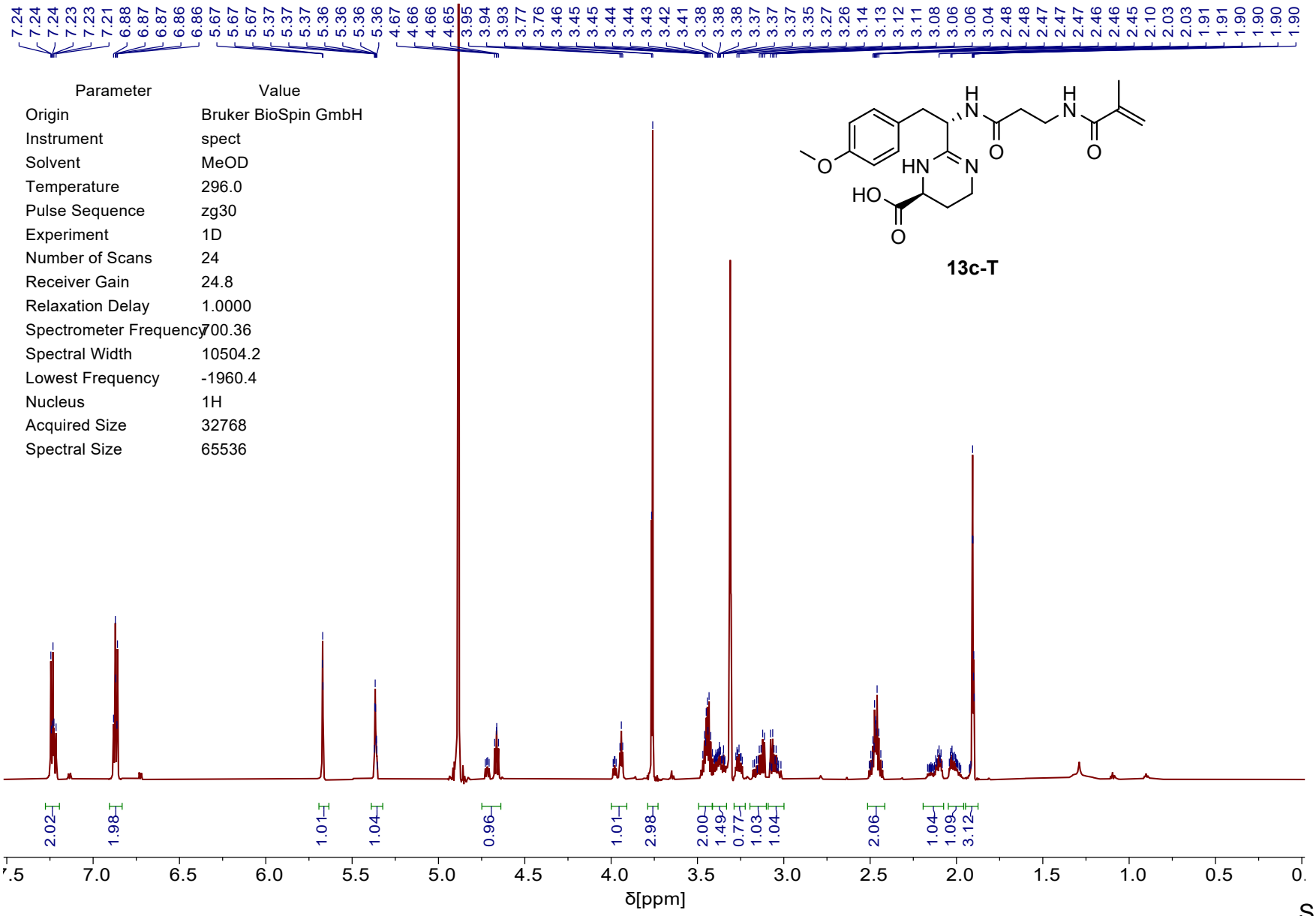
175.37
164.02
160.55
158.68
131.58
128.02
115.13
80.71
55.69
55.62
54.28
38.36
37.82
37.30
36.96
28.79
22.50
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
23c-T
δ[ppm]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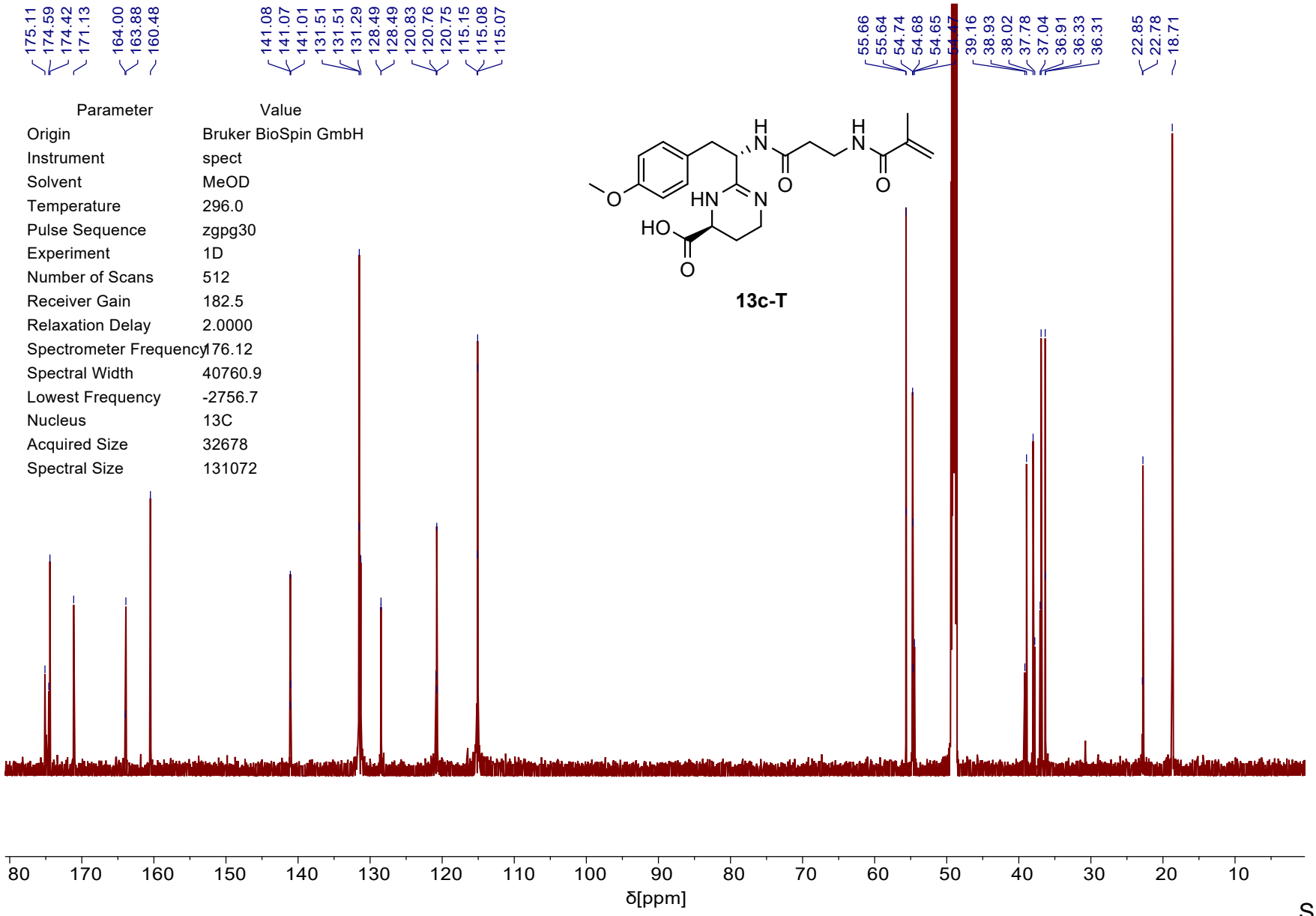
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 24.8
Relaxation Delay 1.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
H N H N O O O HN N HO O
13c-T
2.02 1.98 1.01 1.04 0.96 1.01 2.98 2.00 1.49 0.77 1.03 1.04 2.06 1.04 1.09 3.12
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
δ[ppm]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174.42
171.13
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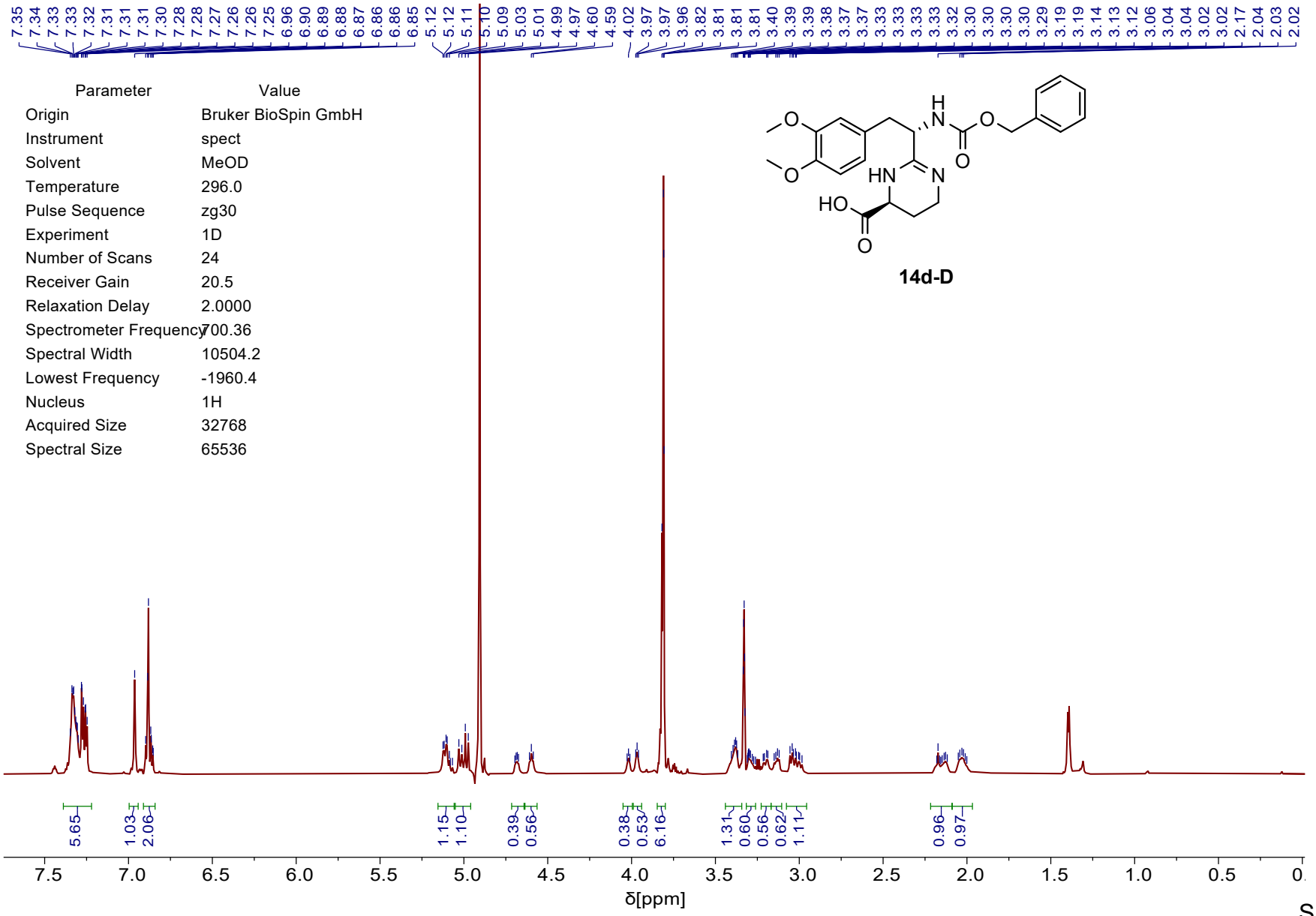
163.88
160.48
141.08
141.07
141.01
131.51
131.51
131.29
128.49
128.49
120.83
120.76
120.75
115.15
115.08
115.07
55.66
55.64
54.74
54.68
54.65
54.47
39.16
38.93
38.02
37.78
37.04
36.91
36.33
36.31
22.85
22.78
18.71
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
13c-T
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]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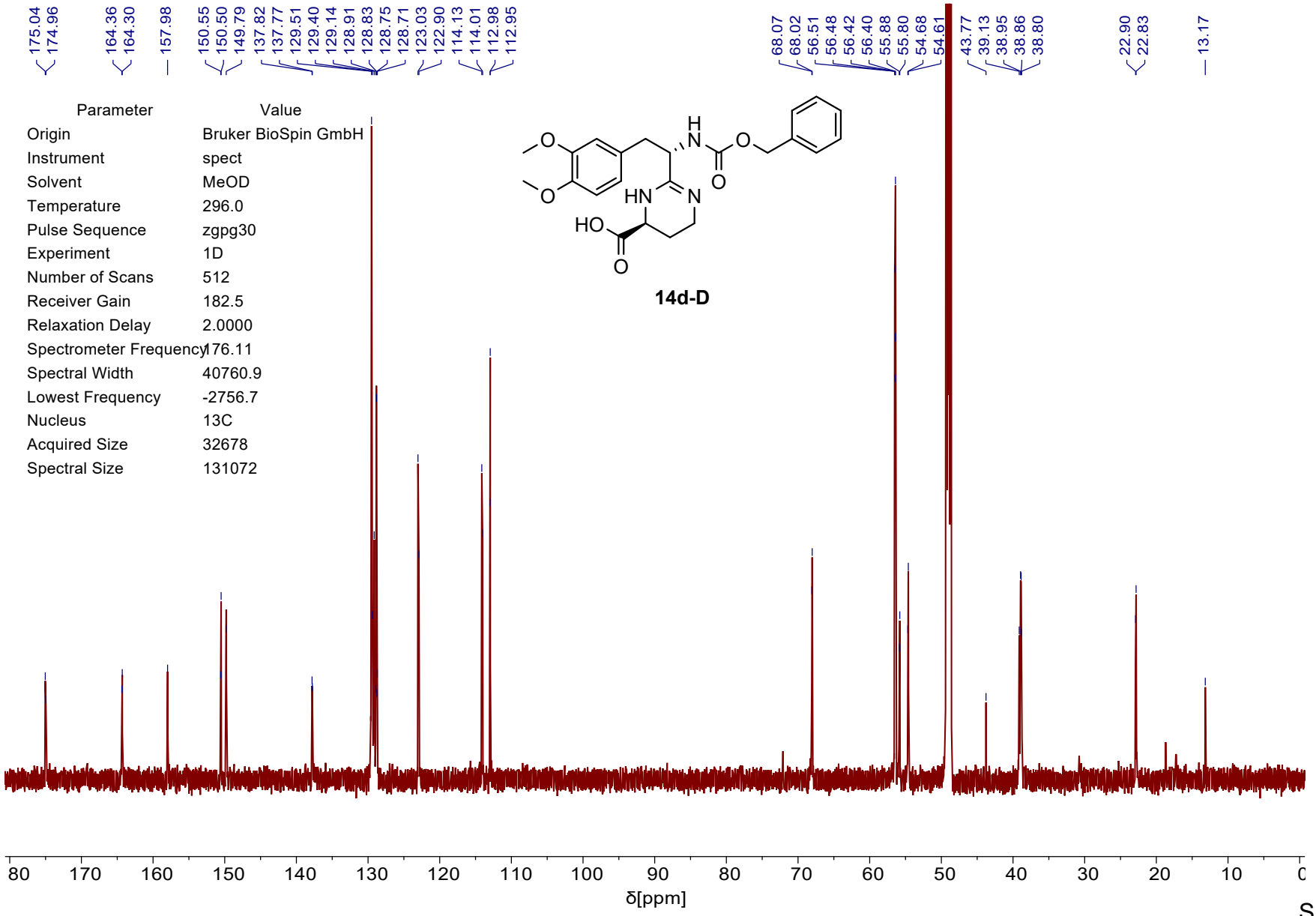
5.12 5.12 5.11 5.10 5.09 5.03 5.01 4.99 4.97 4.60 4.59
4.02 3.97 3.97 3.96 3.82 3.81 3.81 3.81 3.40 3.39 3.39 3.38 3.37 3.37 3.33 3.33 3.33 3.33 3.32 3.30 3.30 3.30 3.30 3.29 3.19 3.19 3.14 3.13 3.12 3.06 3.04 3.04 3.02 3.02 2.17 2.04 2.03 2.02
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 20.5
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
O
O
O
H
N
O
O
HN
N
HO
O
14d-D
5.65 1.03 2.06 1.15 1.10 0.39 0.56 0.38 0.53 6.16 1.31 0.60 0.56 0.62 1.11 0.96 0.97
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
δ[ppm]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164.36
164.30
157.98
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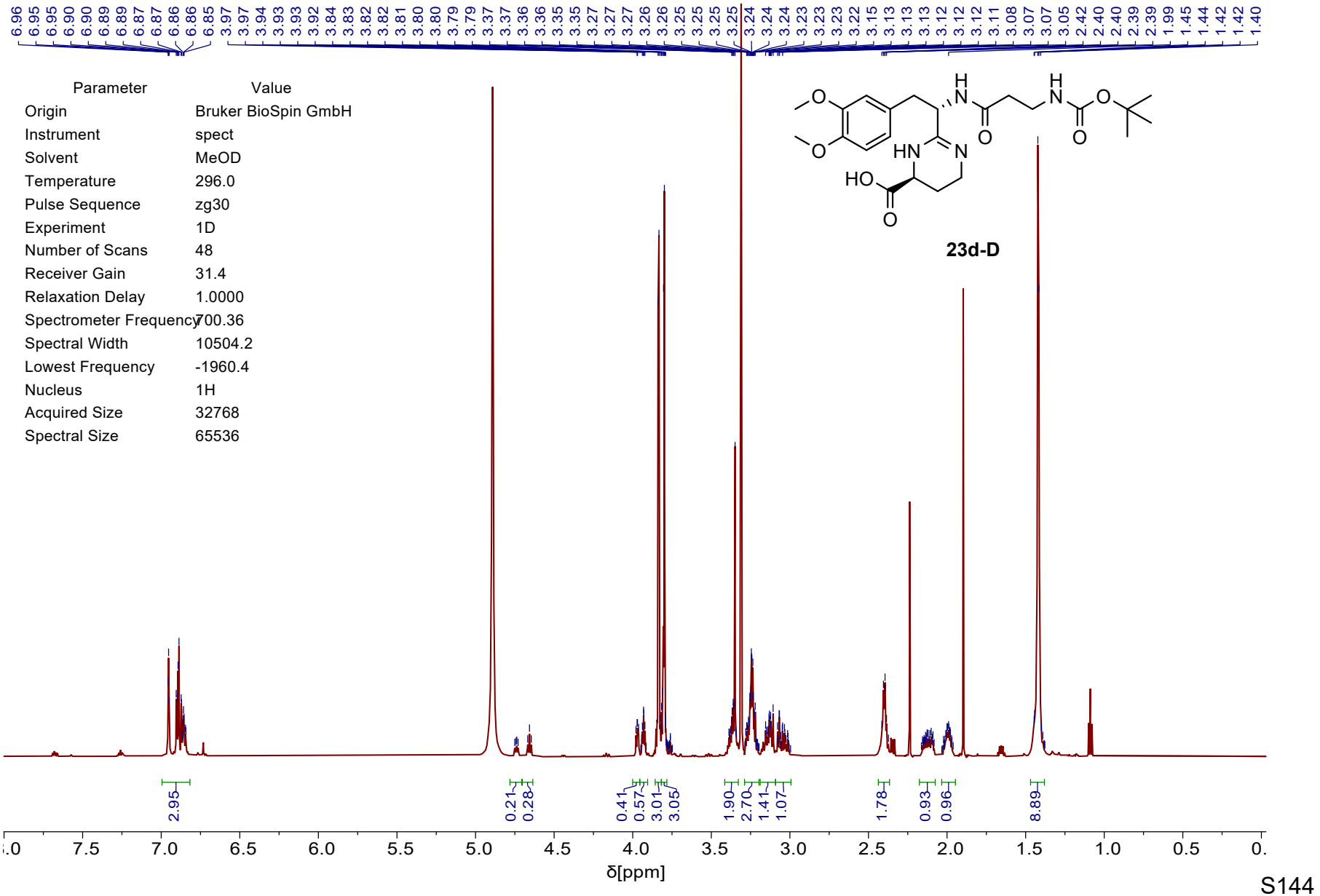
150.50
149.79
137.82
137.77
129.51
129.40
129.14
128.91
128.83
128.75
128.71
123.03
122.90
114.13
114.01
112.98
112.95
68.07
68.02
56.51
56.48
56.42
56.40
55.88
55.80
54.68
54.61
43.77
39.13
38.95
38.86
38.80
22.90
22.83
13.17
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.11
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
14d-D
δ[ppm]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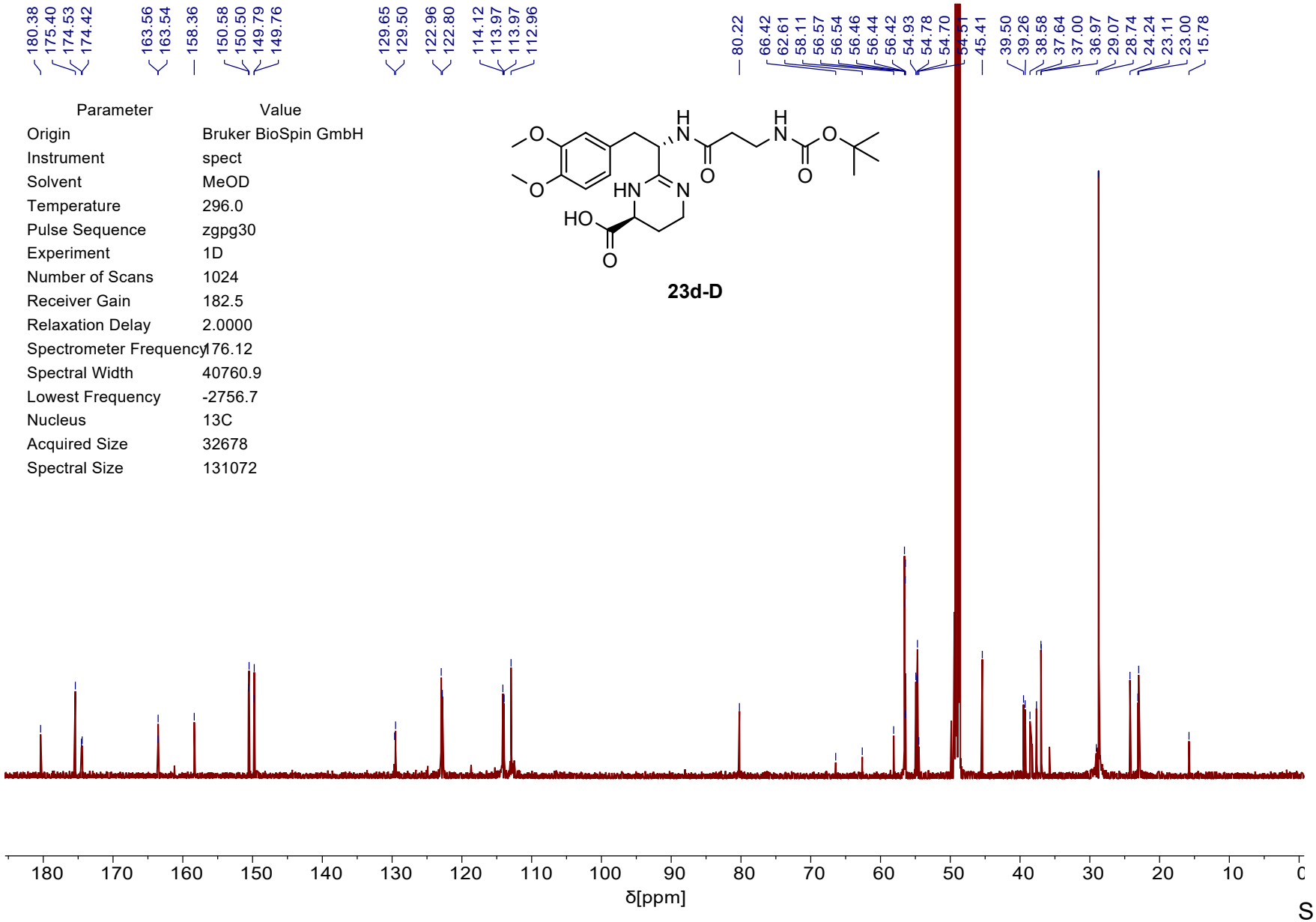
3.97 3.97 3.94 3.93 3.93 3.92 3.84 3.83 3.82 3.82 3.81 3.80 3.80 3.79 3.79 3.37 3.37 3.36 3.36 3.35 3.35 3.27 3.27 3.27 3.26 3.26 3.25 3.25 3.25 3.24 3.24 3.24 3.23 3.23 3.22 3.15 3.13 3.13 3.12 3.12 3.12 3.11 3.08 3.07 3.07 3.05 2.42 2.40 2.40 2.39 2.39 1.99 1.45 1.44 1.42 1.42 1.40
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 48
Receiver Gain 31.4
Relaxation Delay 1.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
23d-D
2.95 0.21 0.28 0.41 0.57 3.01 3.05 1.90 2.70 1.41 1.07 1.78 0.93 0.96 8.89
δ[ppm]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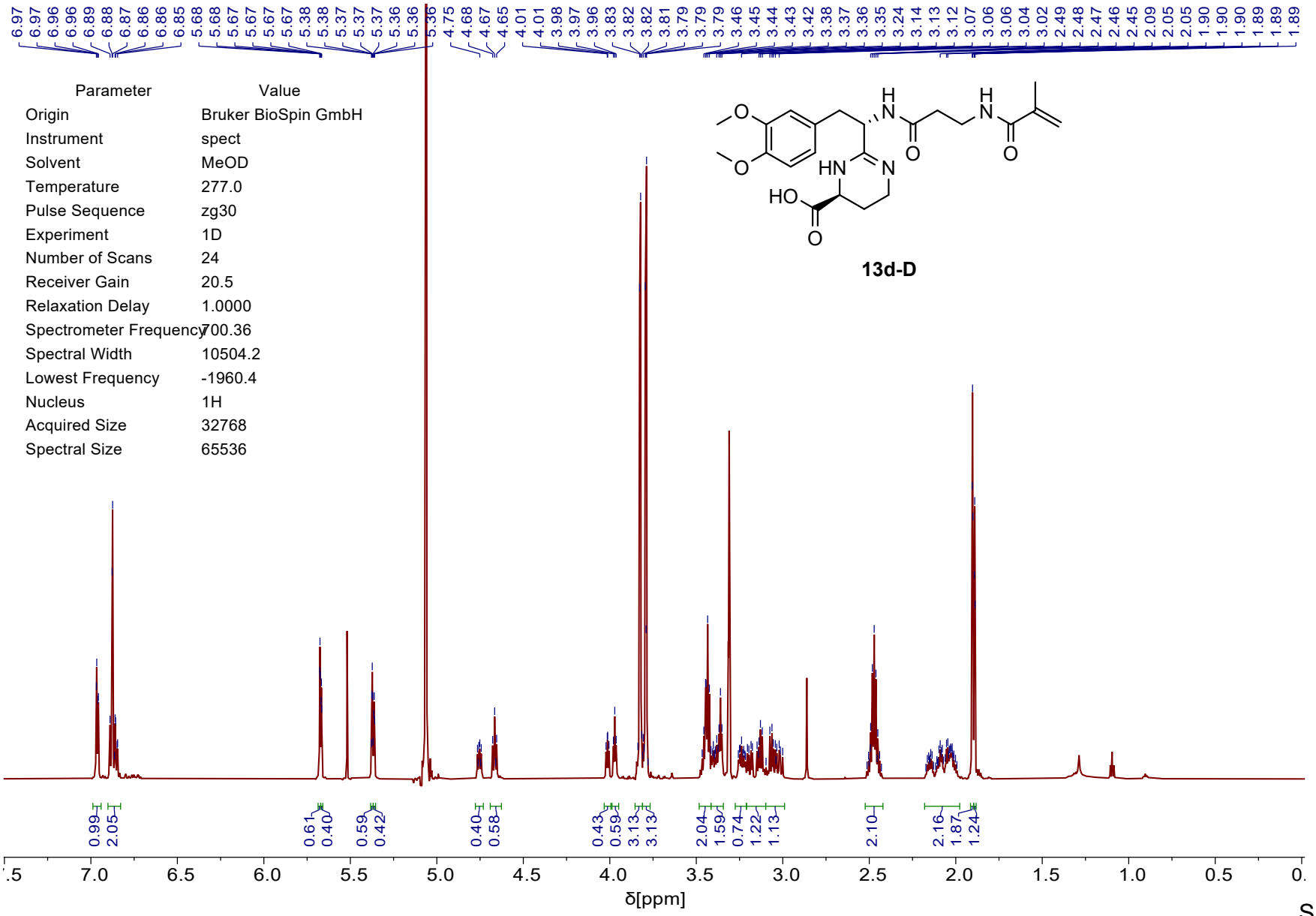
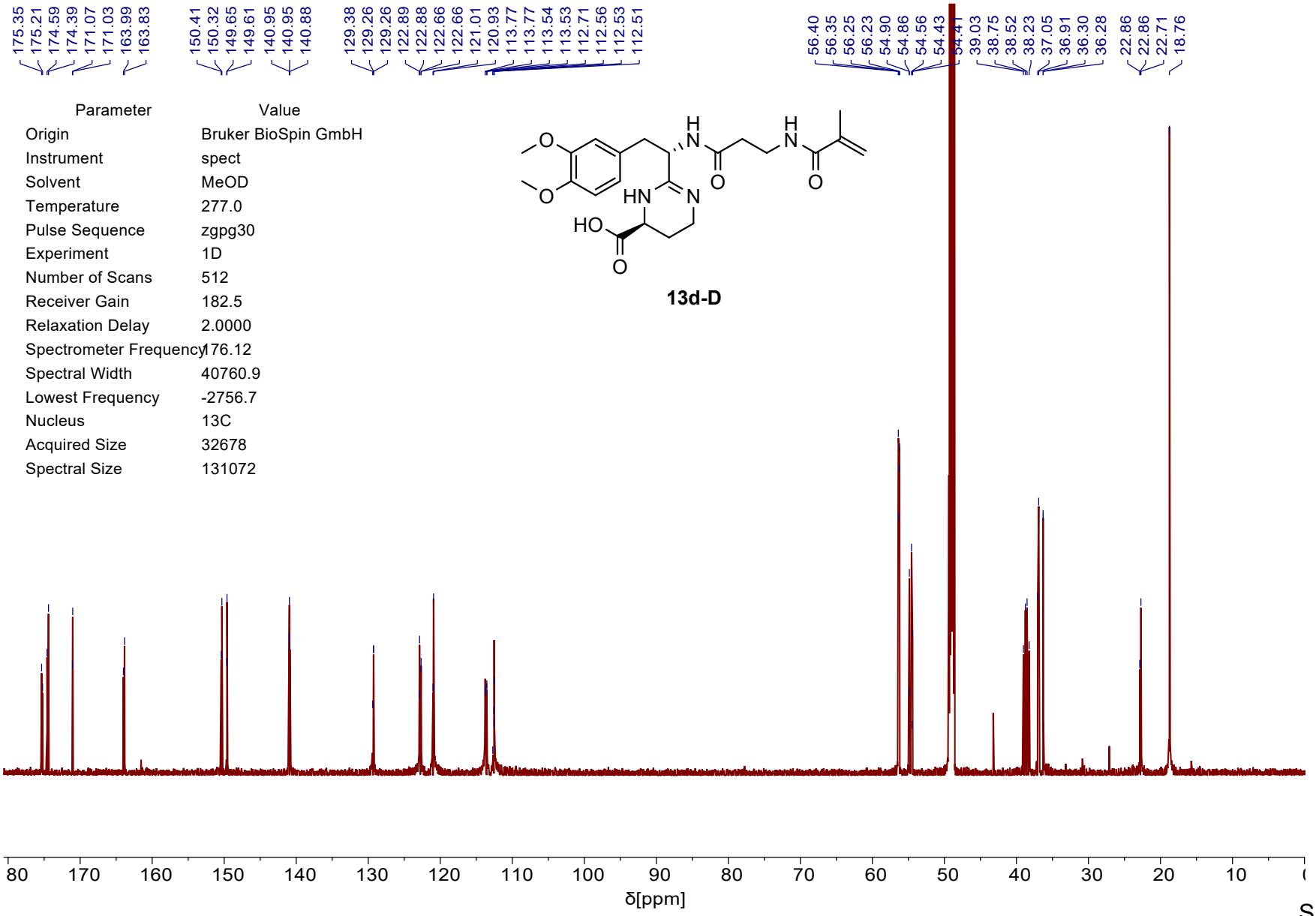
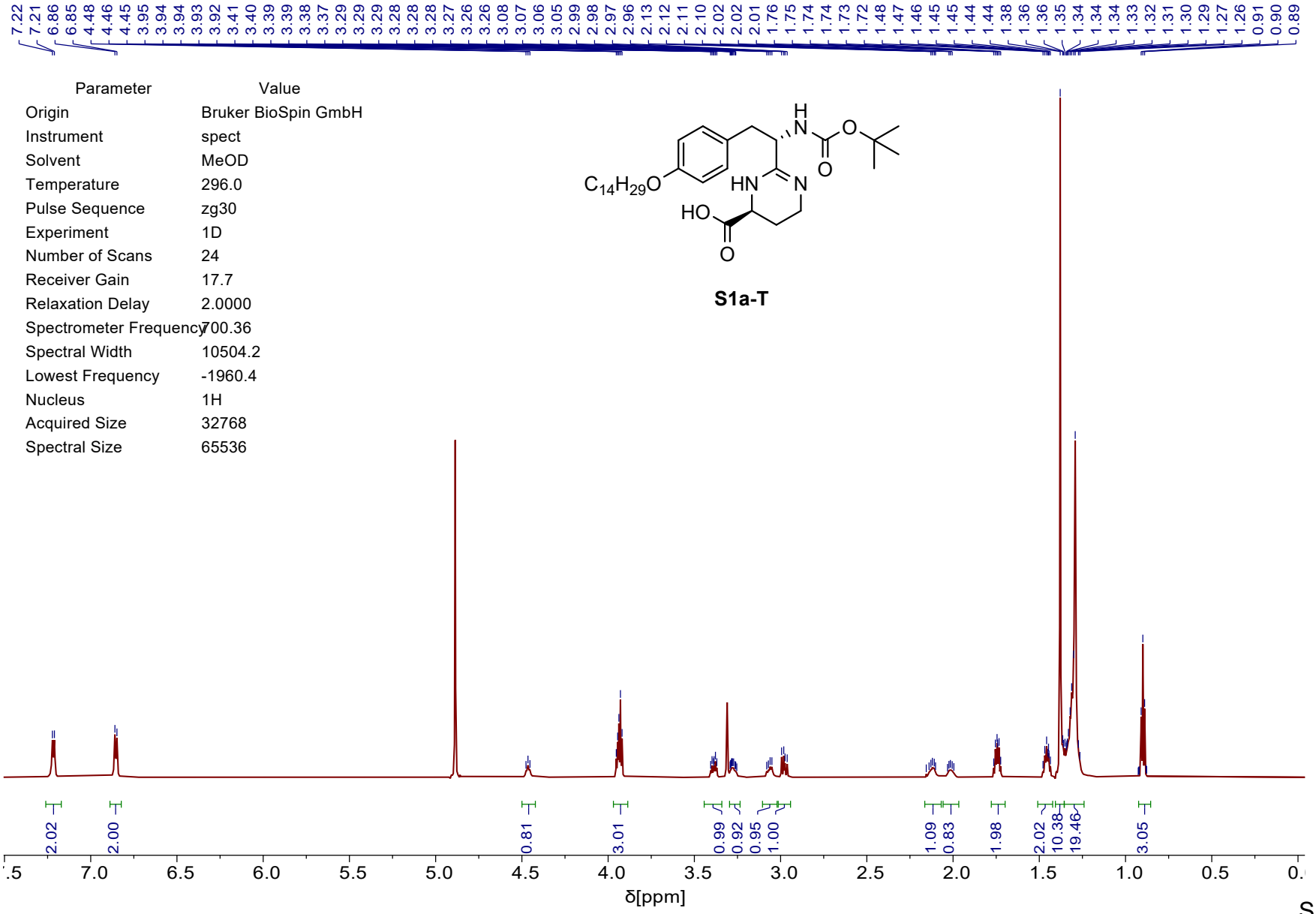
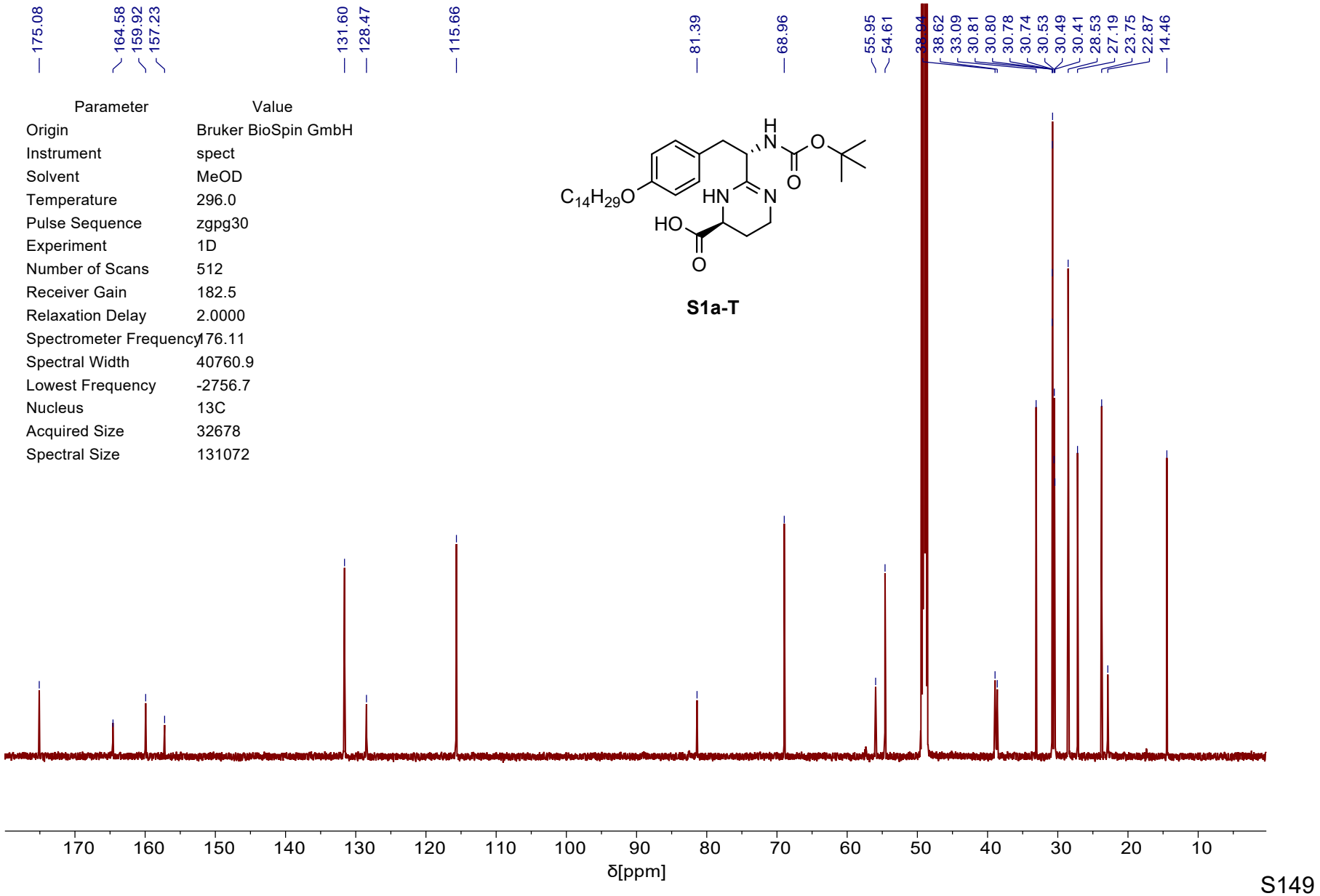
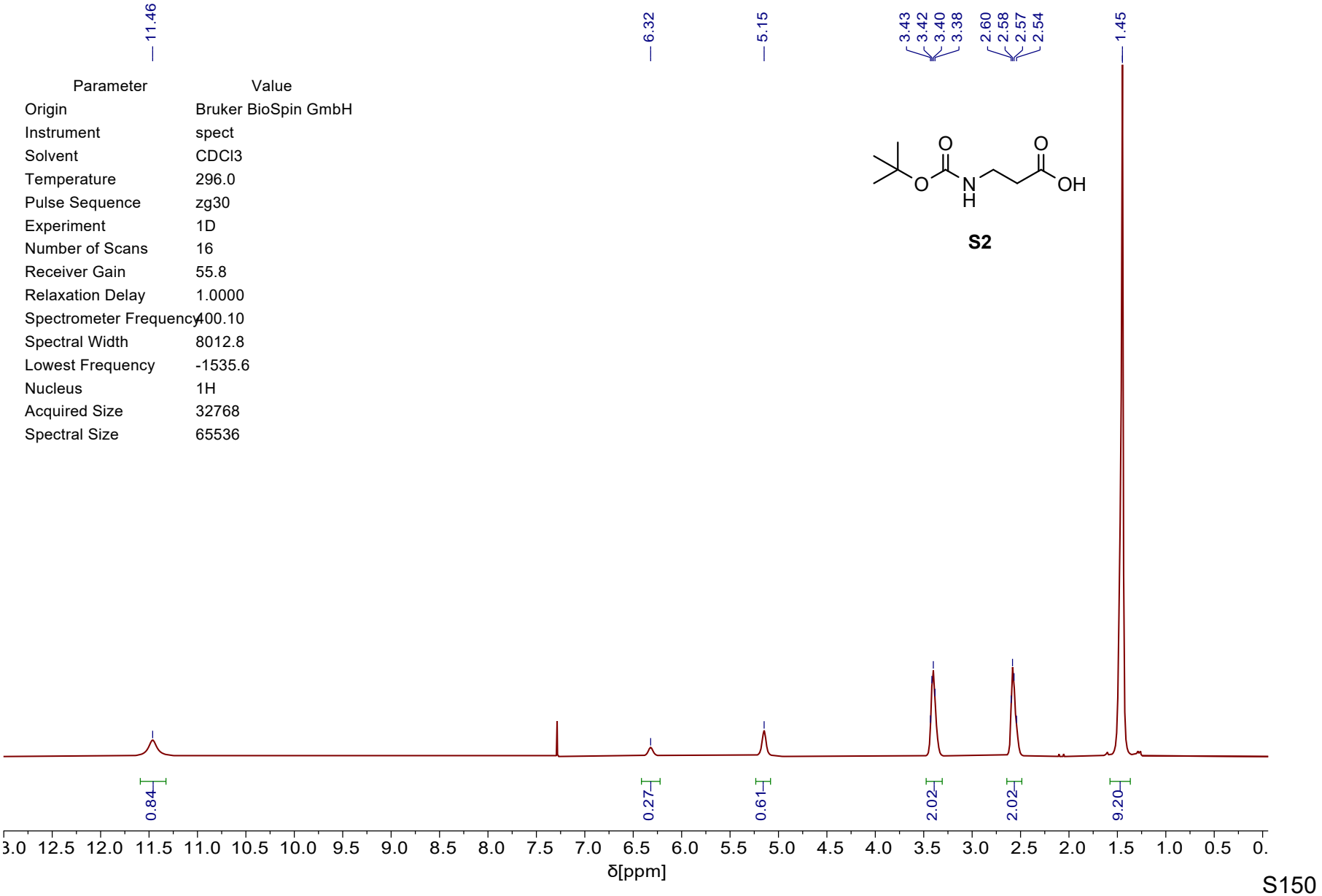
174.53
174.42
163.56
163.54
158.36
150.58
150.50
149.79
149.76
129.65
129.50
122.96
122.80
114.12
113.97
113.97
112.96
80.22
66.42
62.61
58.11
56.57
56.54
56.46
56.44
56.42
54.93
54.78
54.70
34.51
45.41
39.50
39.26
38.58
37.64
37.00
36.97
29.07
28.74
24.24
23.11
23.00
15.78
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1024
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
23d-D
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ[ppm]

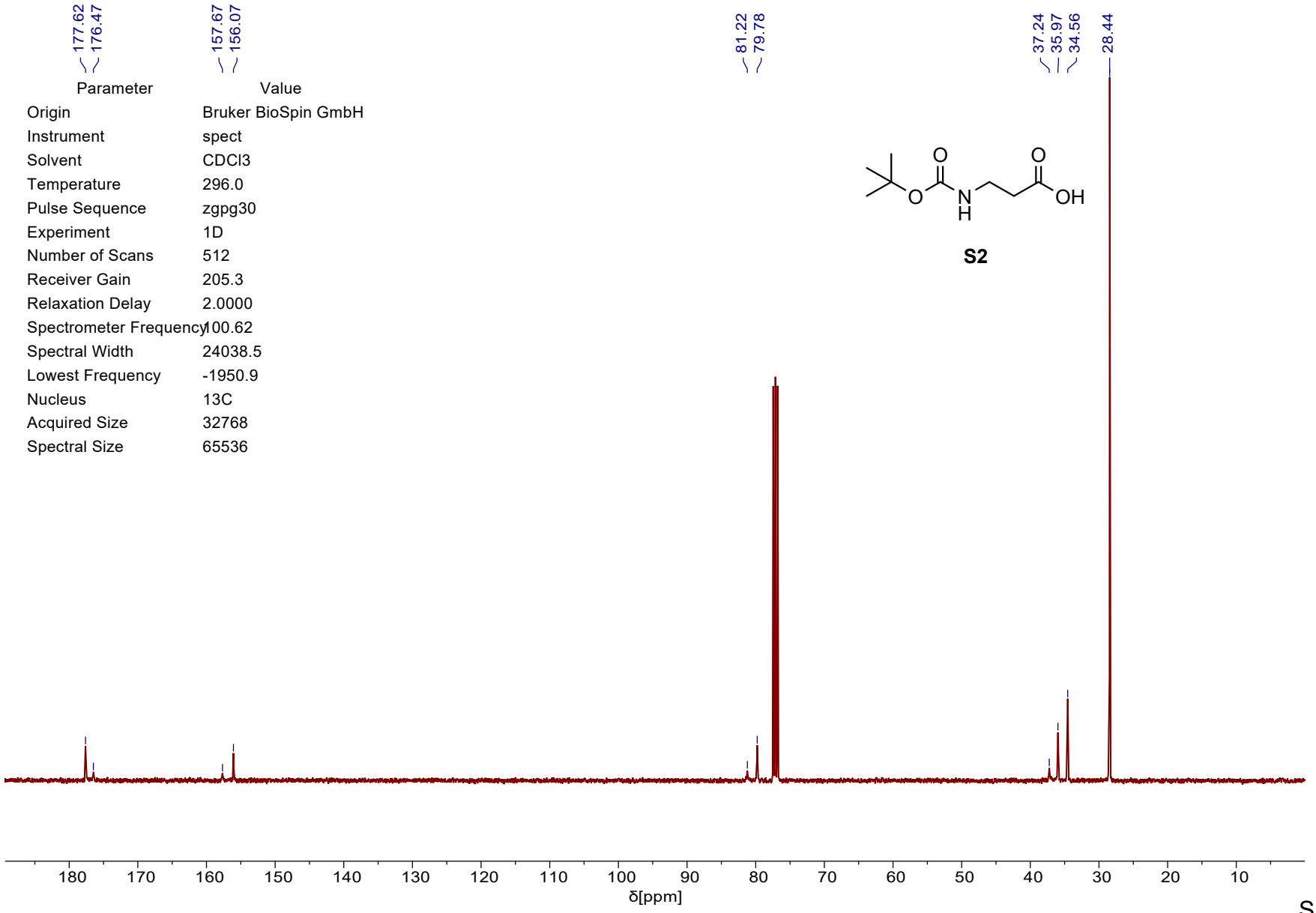

6.97 6.97 6.96 6.96 6.89 6.88 6.87 6.86 6.86 6.85 5.68 5.68 5.67 5.67 5.67 5.67 5.38 5.38 5.37 5.37 5.37 5.36 5.36 5.36 4.75 4.68 4.67 4.65 4.01 4.01 3.98 3.97 3.96 3.83 3.82 3.82 3.81 3.79 3.79 3.79 3.46 3.45 3.44 3.43 3.42 3.38 3.37 3.36 3.35 3.24 3.14 3.13 3.12 3.07 3.06 3.06 3.04 3.02 2.49 2.48 2.47 2.46 2.45 2.09 2.05 2.05 1.90 1.90 1.89 1.89 1.89
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 277.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 20.5
Relaxation Delay 1.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
13d-D
0.99 2.05 0.61 0.40 0.59 0.42 0.40 0.58 0.43 0.59 3.13 3.13 2.04 1.59 0.74 1.22 1.13 2.10 2.16 1.87 1.24
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
δ[ppm]

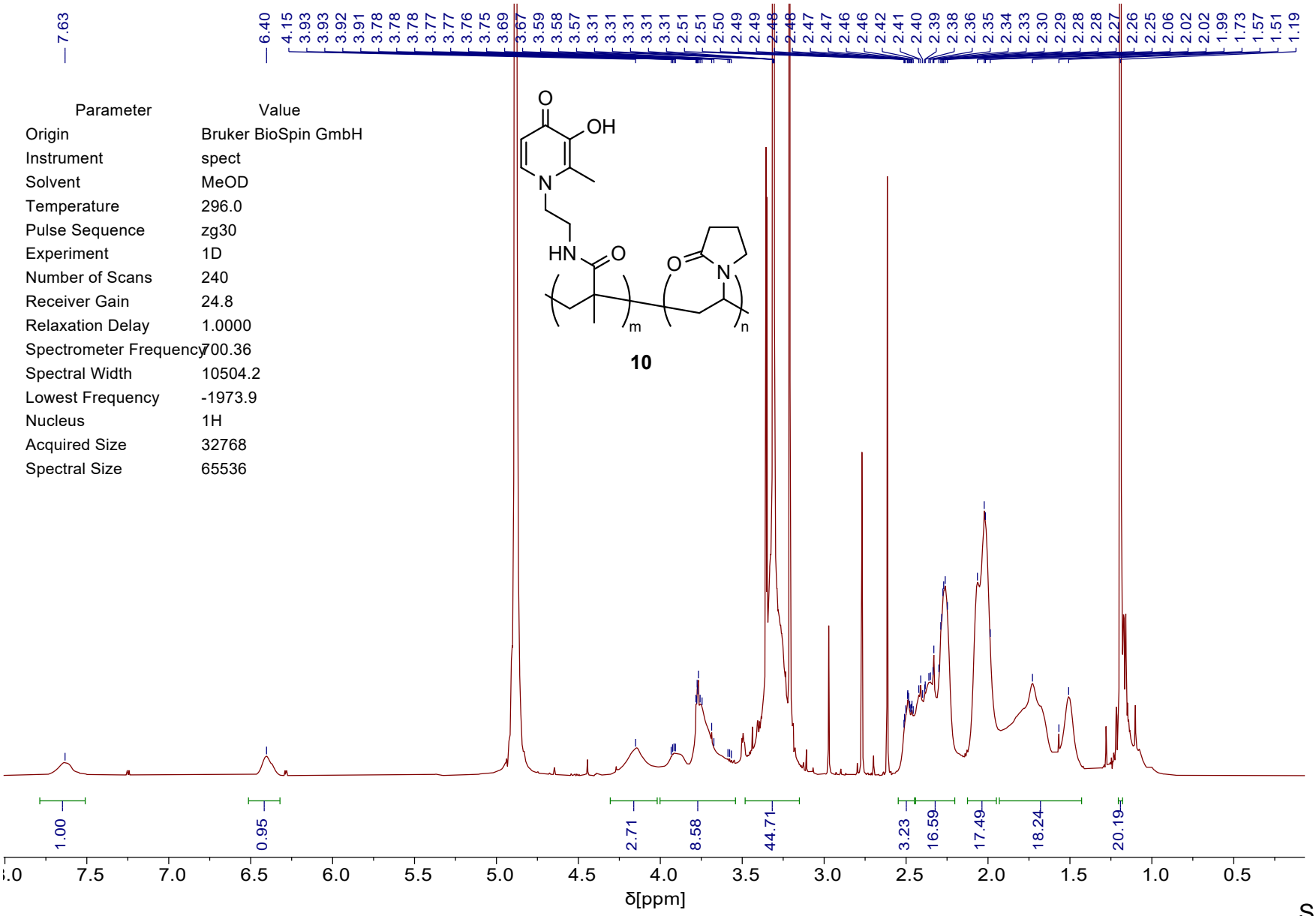

175.35
175.21
174.59
174.39
171.07
171.03
163.99
163.83
150.41
150.32
149.65
149.61
140.95
140.95
140.88
129.38
129.26
129.26
122.89
122.88
122.66
122.66
121.01
120.93
113.77
113.77
113.54
113.53
112.71
112.56
112.53
112.51
56.40
56.35
56.25
56.23
54.90
54.86
54.56
54.43
54.41
39.03
38.75
38.52
38.23
37.05
36.91
36.30
36.28
22.86
22.86
22.71
18.76
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 277.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
13d-D
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ[ppm]

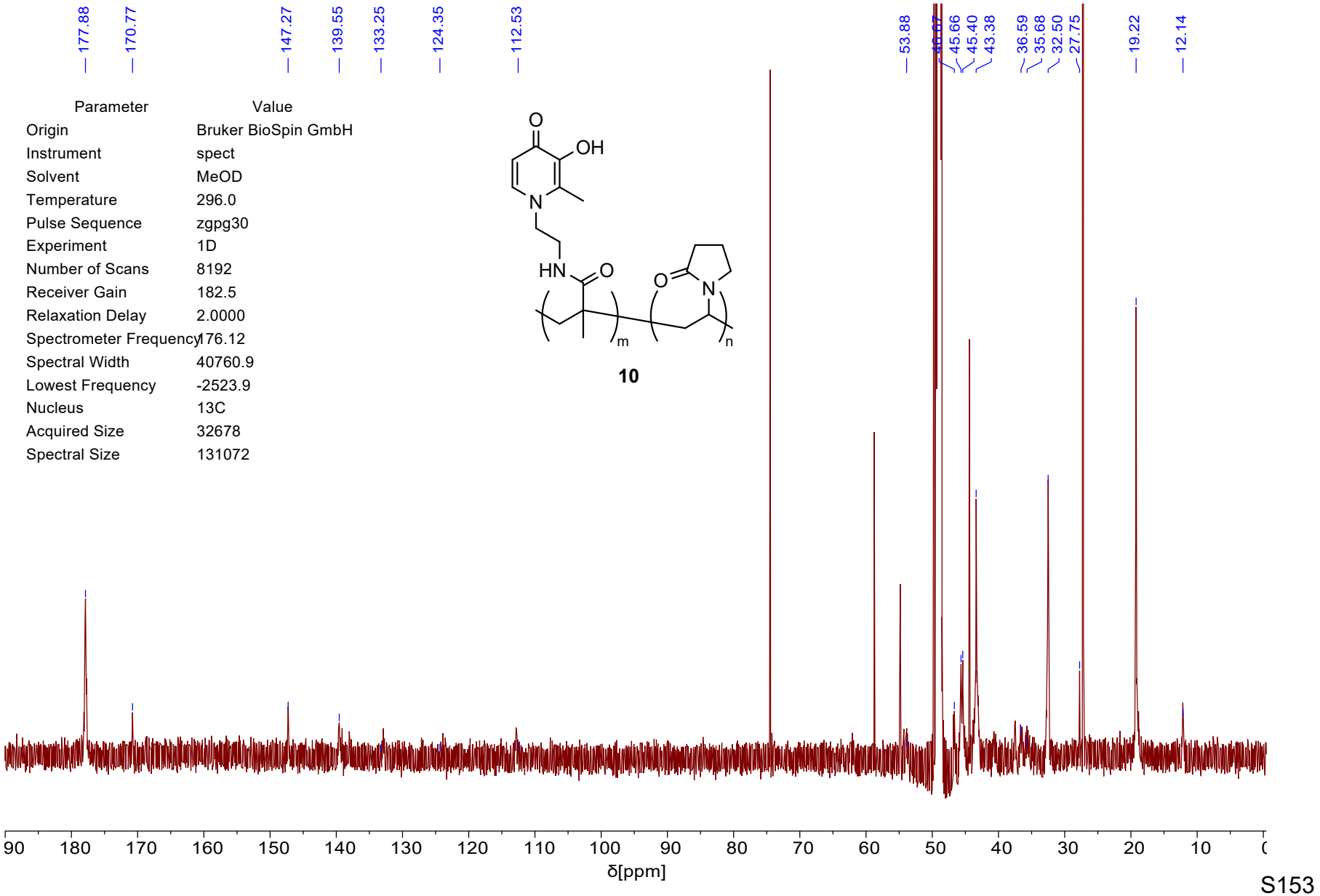

7.22 7.21 6.86 6.85 4.48 4.46 4.45 3.95 3.94 3.94 3.93 3.92 3.41 3.40 3.39 3.39 3.38 3.37 3.29 3.29 3.29 3.28 3.28 3.28 3.27 3.26 3.26 3.08 3.07 3.06 3.05 2.99 2.98 2.97 2.96 2.13 2.12 2.11 2.10 2.02 2.02 2.01 1.76 1.75 1.74 1.74 1.73 1.72 1.48 1.47 1.46 1.45 1.45 1.44 1.44 1.38 1.36 1.36 1.35 1.34 1.34 1.34 1.33 1.32 1.31 1.30 1.29 1.27 1.26 0.91 0.90 0.89
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 24
Receiver Gain 17.7
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1960.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
H
N
O
O
C14H29O
HN
N
HO
O
S1a-T
2.02 2.00 0.81 3.01 0.99 0.92 0.95 1.00 1.09 0.83 1.98 2.02 10.38 19.46 3.05
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
δ[ppm]

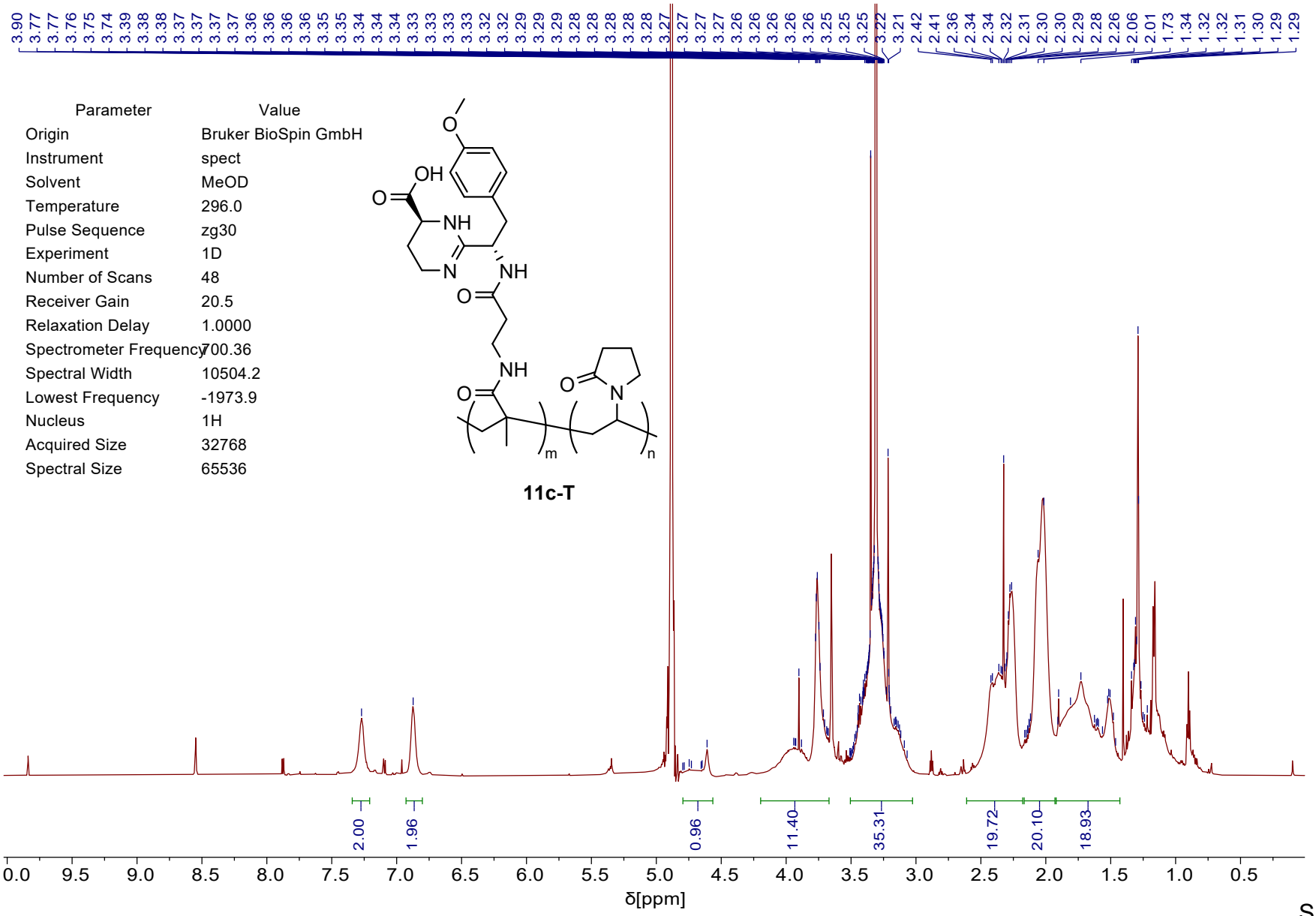

175.08
164.58
159.92
157.23
131.60
128.47
115.66
81.39
68.96
55.95
54.61
39.94
38.62
33.09
30.81
30.80
30.78
30.74
30.53
30.49
30.41
28.53
27.19
23.75
22.87
14.46
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.11
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
H
N
O
O
C14H29O
HN
N
HO
O
S1a-T
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ[ppm]

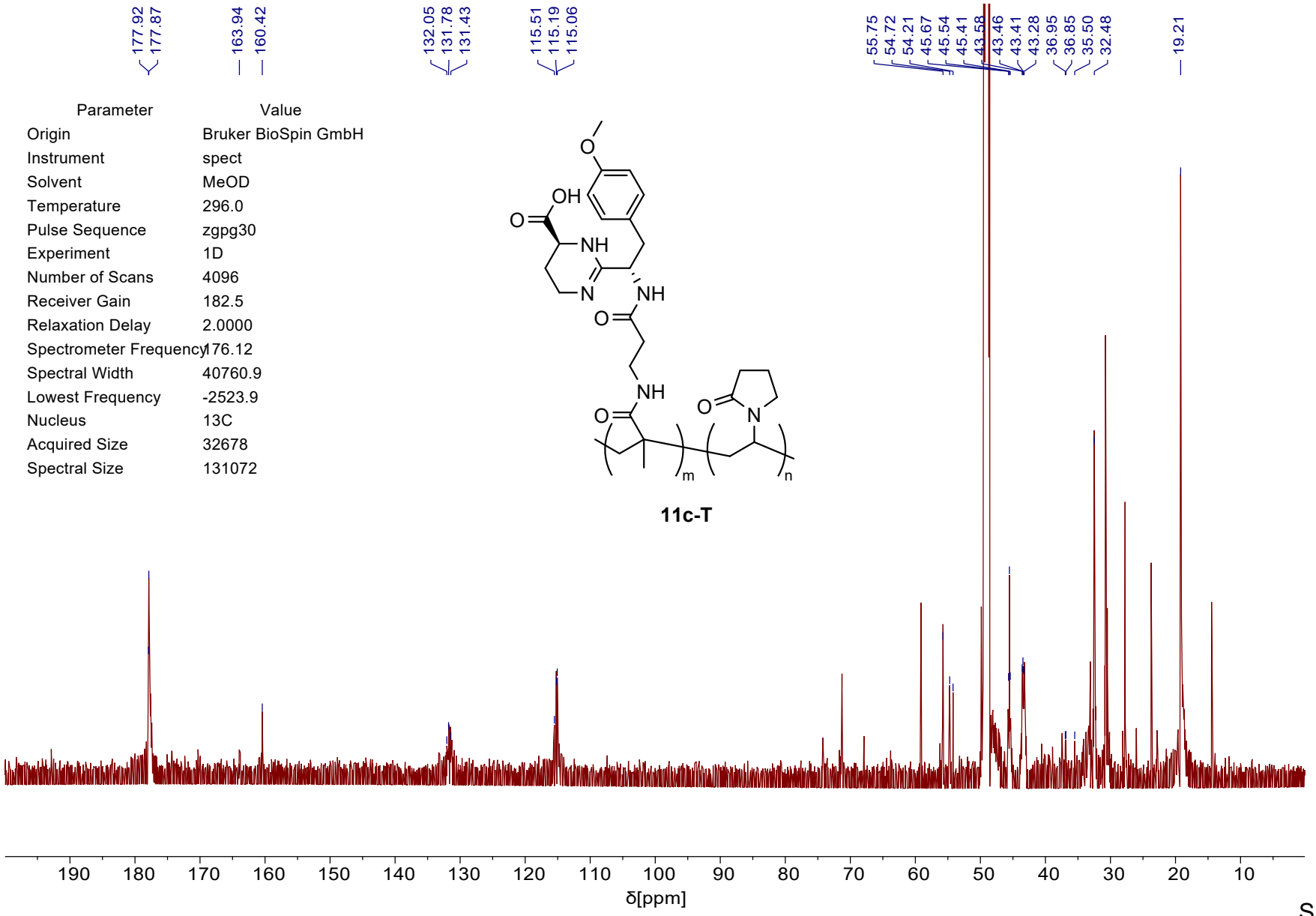

11.46
6.32
5.15
3.43
3.42
3.40
3.38
2.60
2.58
2.57
2.54
1.45
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 55.8
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1535.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
O
O
O
N
H
OH
S2
0.84
0.27
0.61
2.02
2.02
9.20
δ[ppm]

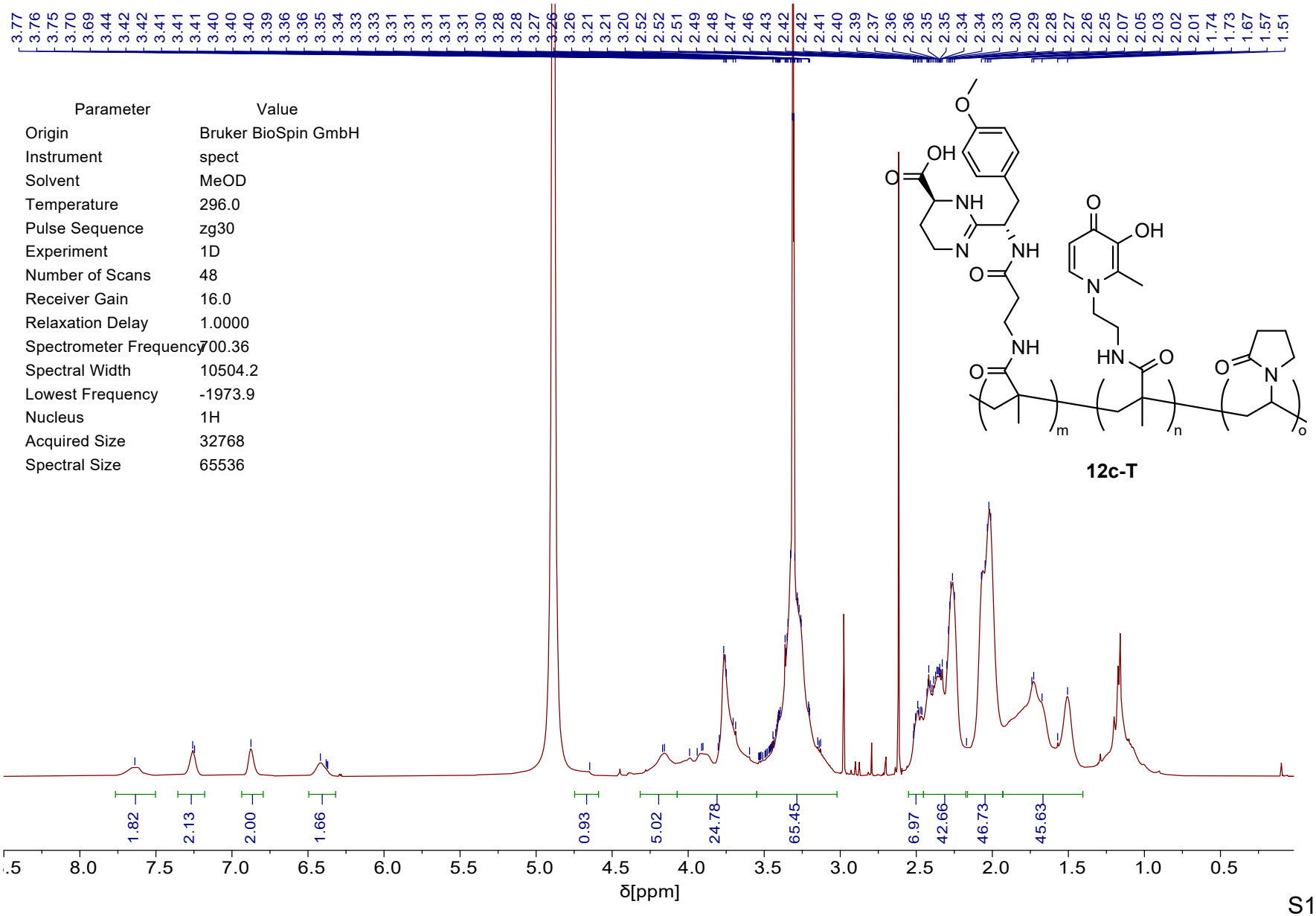

177.62
176.47
157.67
156.07
81.22
79.78
37.24
35.97
34.56
28.44
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
O
O
O
N
H
OH
S2
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

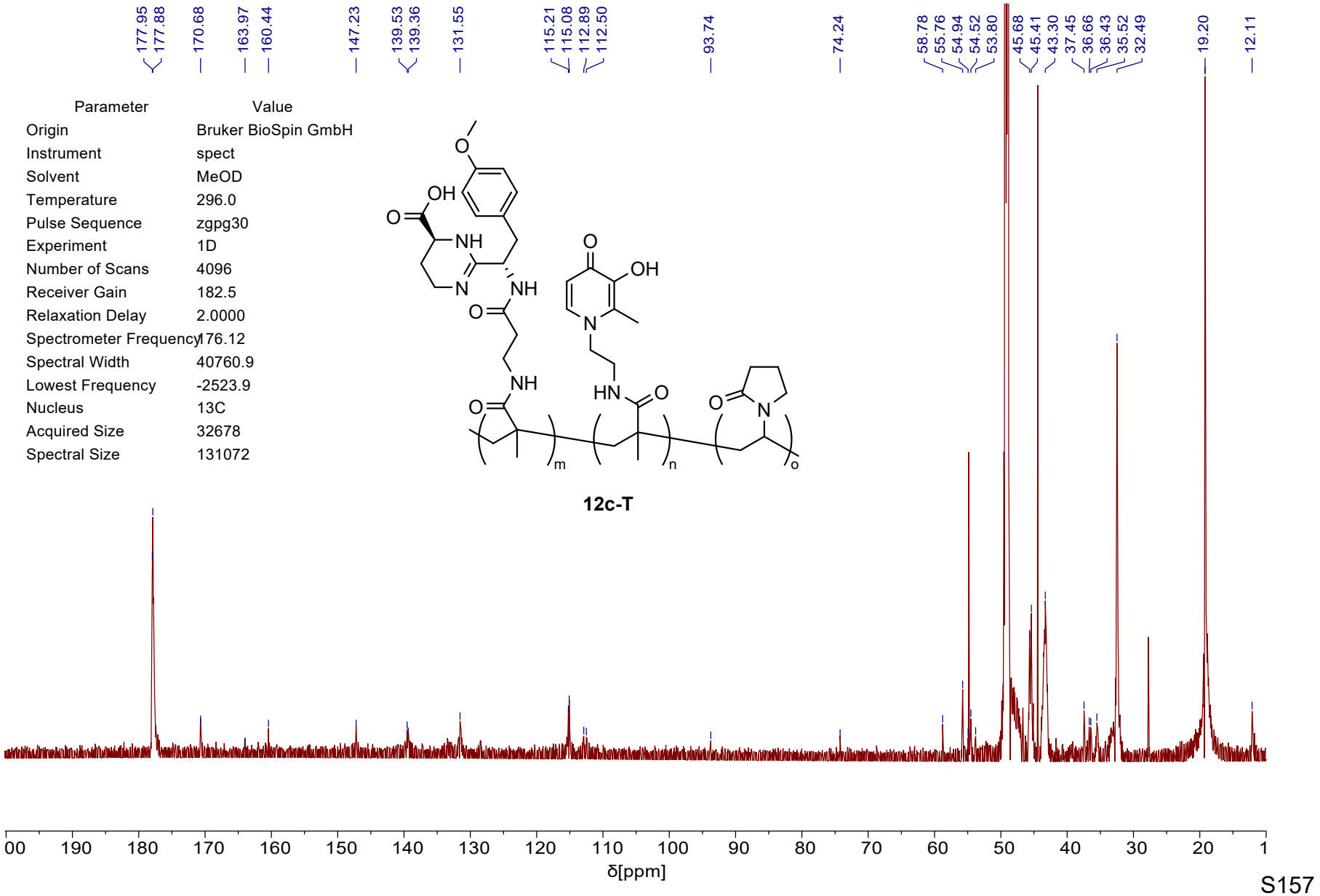

7.63
6.40
4.15 3.93 3.93 3.92 3.91 3.78 3.78 3.78 3.77 3.77 3.76 3.75 3.69 3.67 3.59 3.58 3.57 3.31 3.31 3.31 3.31 2.51 2.51 2.50 2.49 2.49 2.48 2.48 2.47 2.47 2.46 2.46 2.42 2.41 2.40 2.39 2.38 2.36 2.35 2.34 2.33 2.30 2.29 2.28 2.28 2.27 2.26 2.25 2.06 2.02 2.02 1.99 1.73 1.57 1.51 1.19
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 240
Receiver Gain 24.8
Relaxation Delay 1.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1973.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
O
OH
N
HN
O
O
N
m
n
10
1.00
0.95
2.71
8.58
44.71
3.23
16.59
17.49
18.24
20.19
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
δ[ppm]

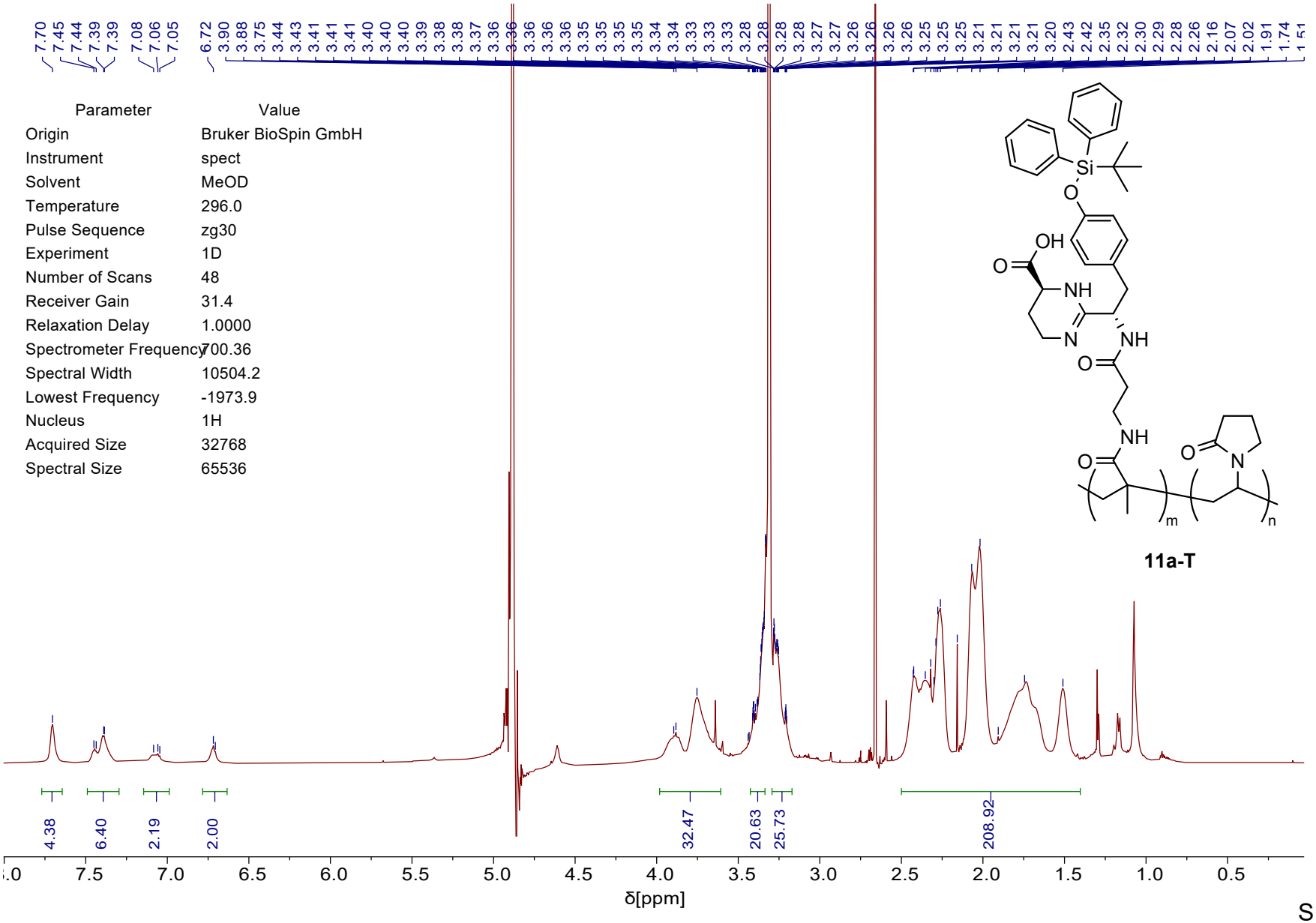

177.88
170.77
147.27
139.55
133.25
124.35
112.53
53.88
46.67
45.66
45.40
43.38
36.59
35.68
32.50
27.75
19.22
12.14
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 8192
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2523.9
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
O
OH
N
HN
O
O
N
m
n
10
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]


Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 48
Receiver Gain 20.5
Relaxation Delay 1.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1973.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
11c-T
2.00
1.96
0.96
11.40
35.31
19.72
20.10
18.93
δ[ppm]

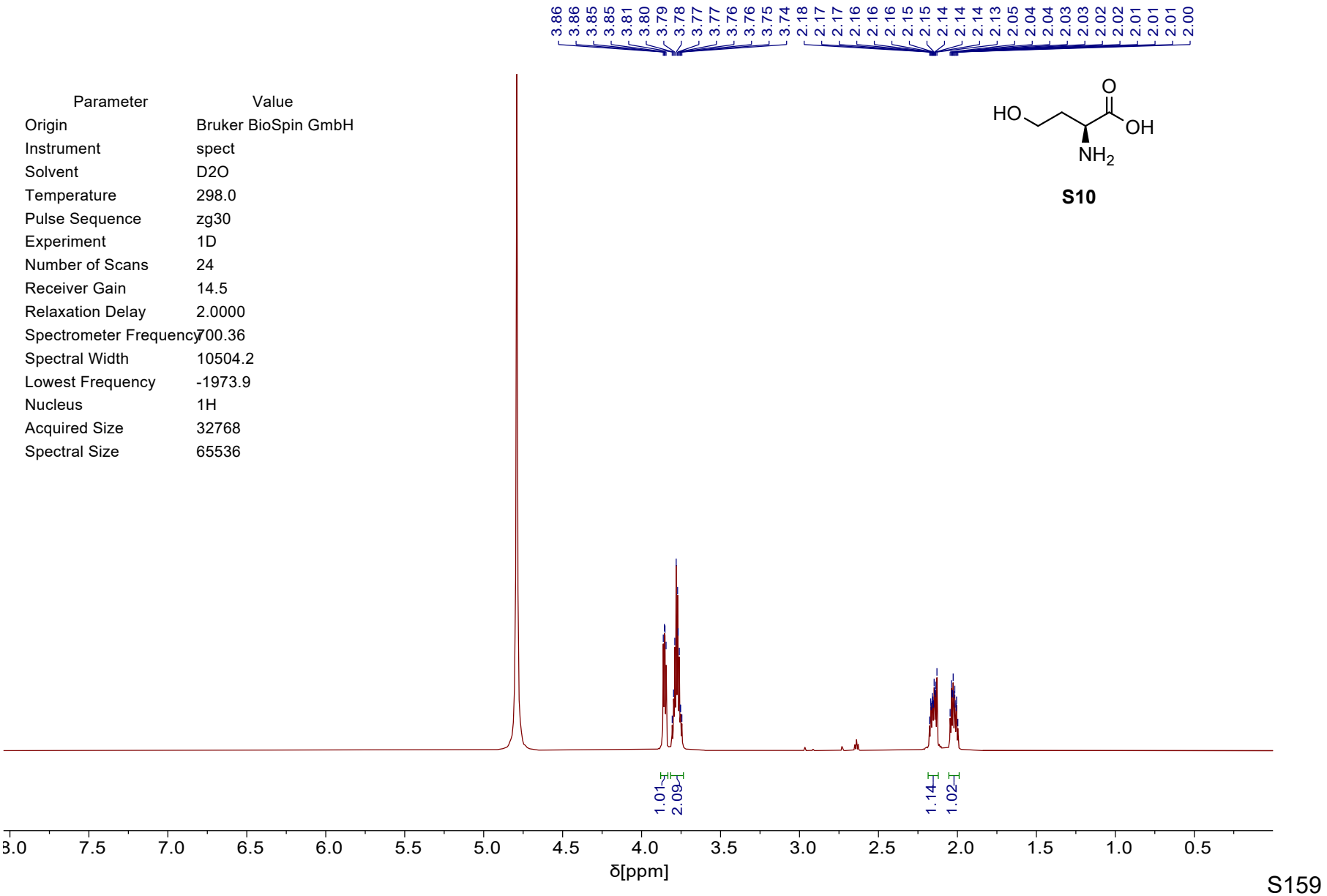

177.92
177.87
163.94
160.42
132.05
131.78
131.43
115.51
115.19
115.06
55.75
54.72
54.21
45.67
45.54
45.41
43.58
43.46
43.41
43.28
36.95
36.85
35.50
32.48
19.21
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 4096
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2523.9
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
11c-T
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]


3.77 3.76 3.75 3.70 3.69 3.44 3.42 3.42 3.41 3.41 3.41 3.40 3.40 3.40 3.39 3.36 3.36 3.35 3.34 3.33 3.33 3.31 3.31 3.31 3.31 3.31 3.30 3.28 3.28 3.27 3.26 3.26 3.21 3.20 2.52 2.52 2.51 2.49 2.48 2.47 2.46 2.43 2.42 2.42 2.41 2.40 2.39 2.37 2.36 2.36 2.35 2.34 2.34 2.33 2.30 2.29 2.28 2.27 2.26 2.25 2.07 2.05 2.03 2.02 2.01 1.74 1.73 1.67 1.57 1.51
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 48
Receiver Gain 16.0
Relaxation Delay 1.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1973.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
12c-T
1.82 2.13 2.00 1.66 0.93 5.02 24.78 65.45 6.97 42.66 46.73 45.63
δ[ppm]

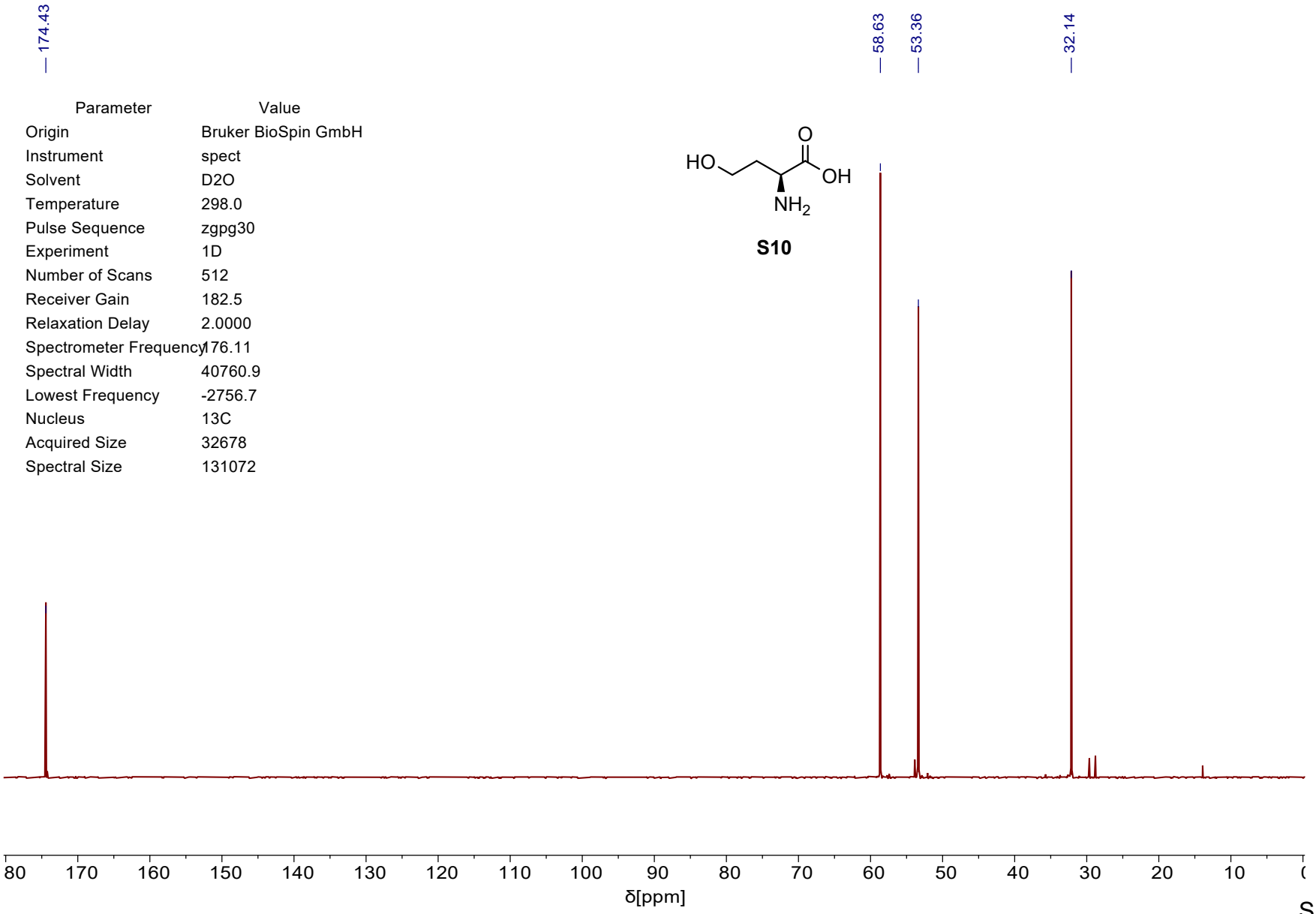

177.95
177.88
170.68
163.97
160.44
147.23
139.53
139.36
131.55
115.21
115.08
112.89
112.50
93.74
74.24
58.78
55.76
54.94
54.52
53.80
45.68
45.41
43.30
37.45
36.66
36.43
35.52
32.49
19.20
12.11
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 4096
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2523.9
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
12c-T
δ[ppm]

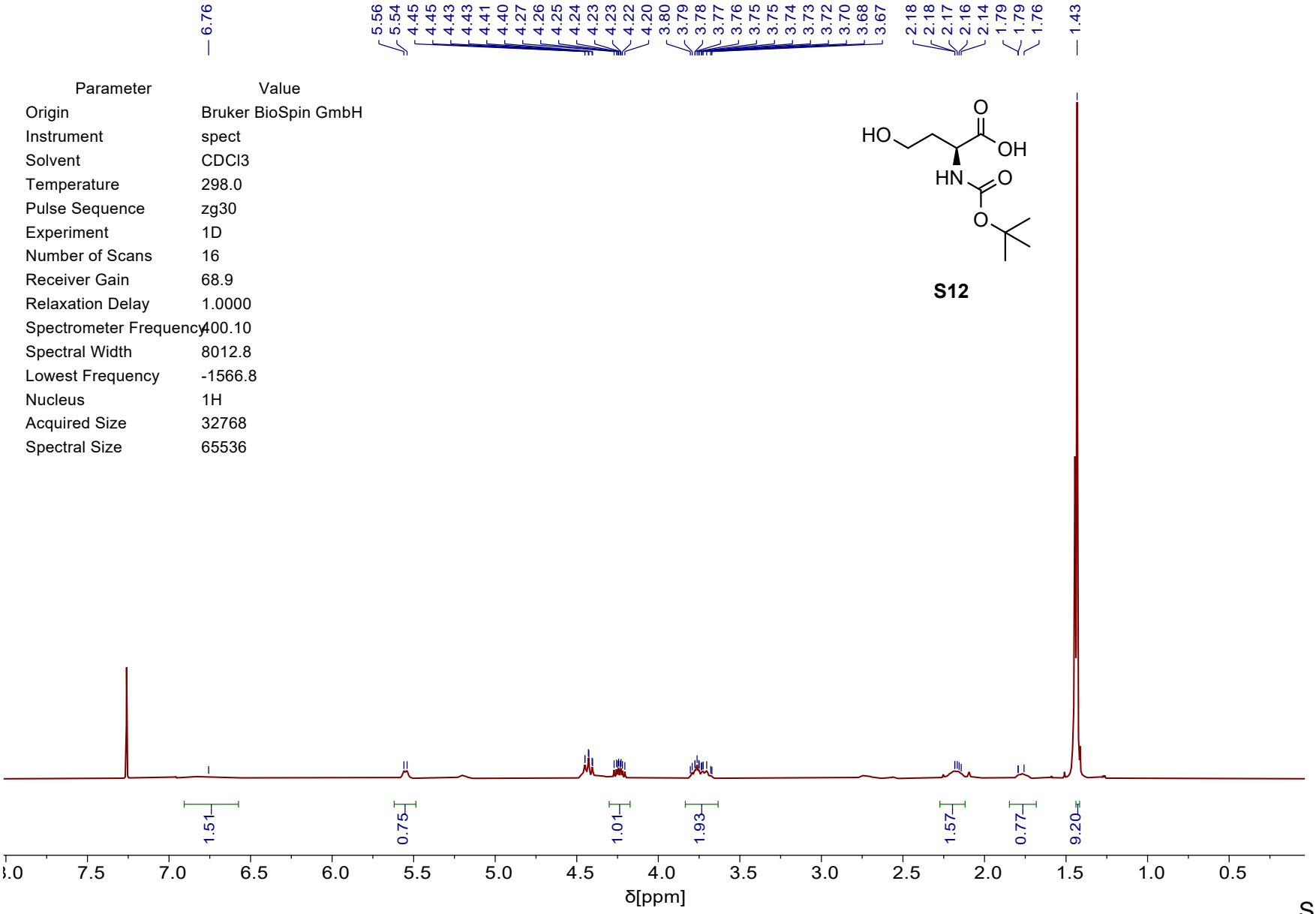

Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent MeOD
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 48
Receiver Gain 31.4
Relaxation Delay 1.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1973.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
11a-T
4.38
6.40
2.19
2.00
32.47
20.63
25.73
208.92
δ[ppm]

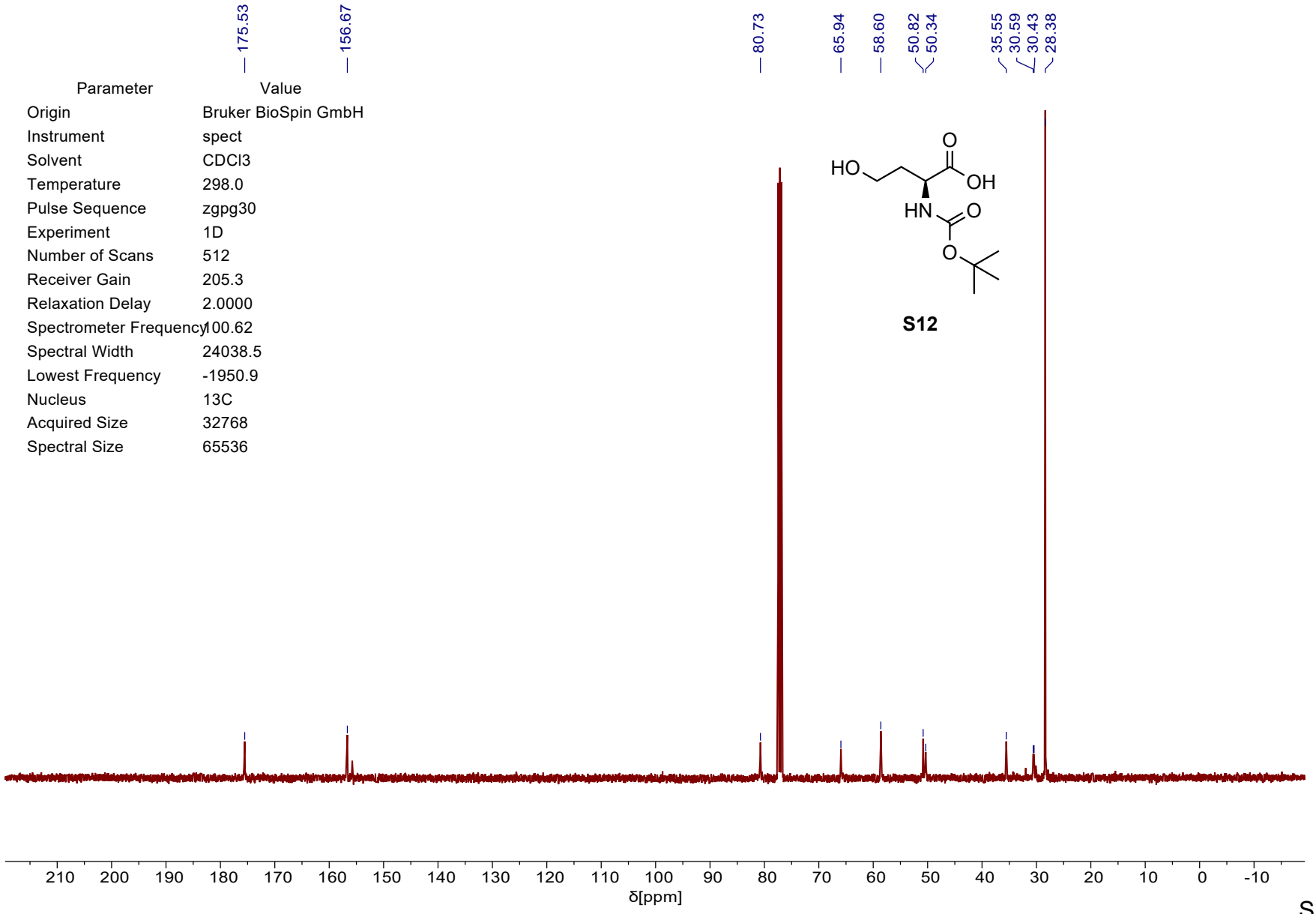
Parameter	Value
Origin	Bruker BioSpin GmbH
Instrument	spect
Solvent	D2O
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	24
Receiver Gain	14.5
Relaxation Delay	2.0000
Spectrometer Frequency	700.36
Spectral Width	10504.2
Lowest Frequency	-1973.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



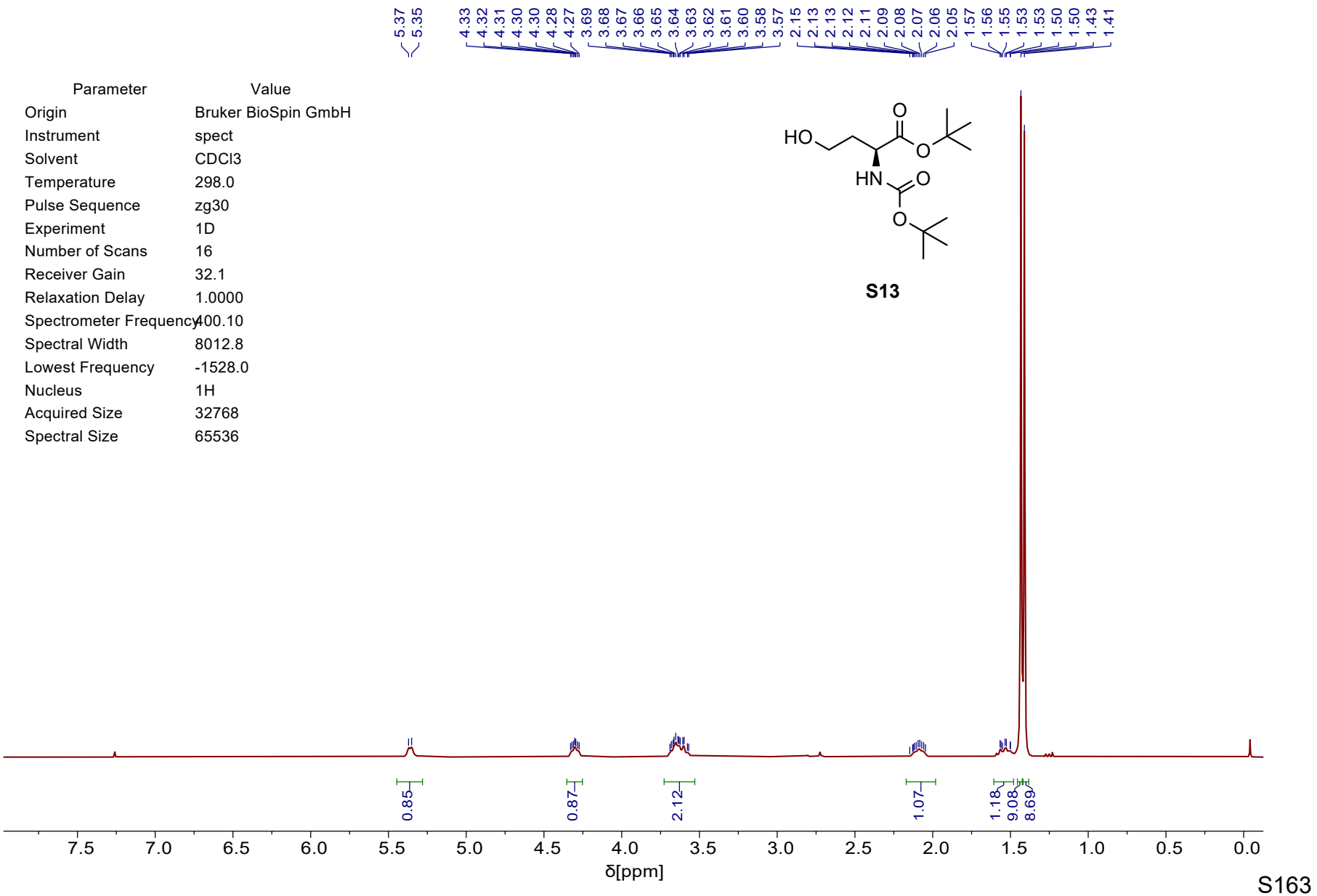
S10


174.43
58.63
53.36
32.14
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent D2O
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.11
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
HO
O
OH
NH2
S10
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

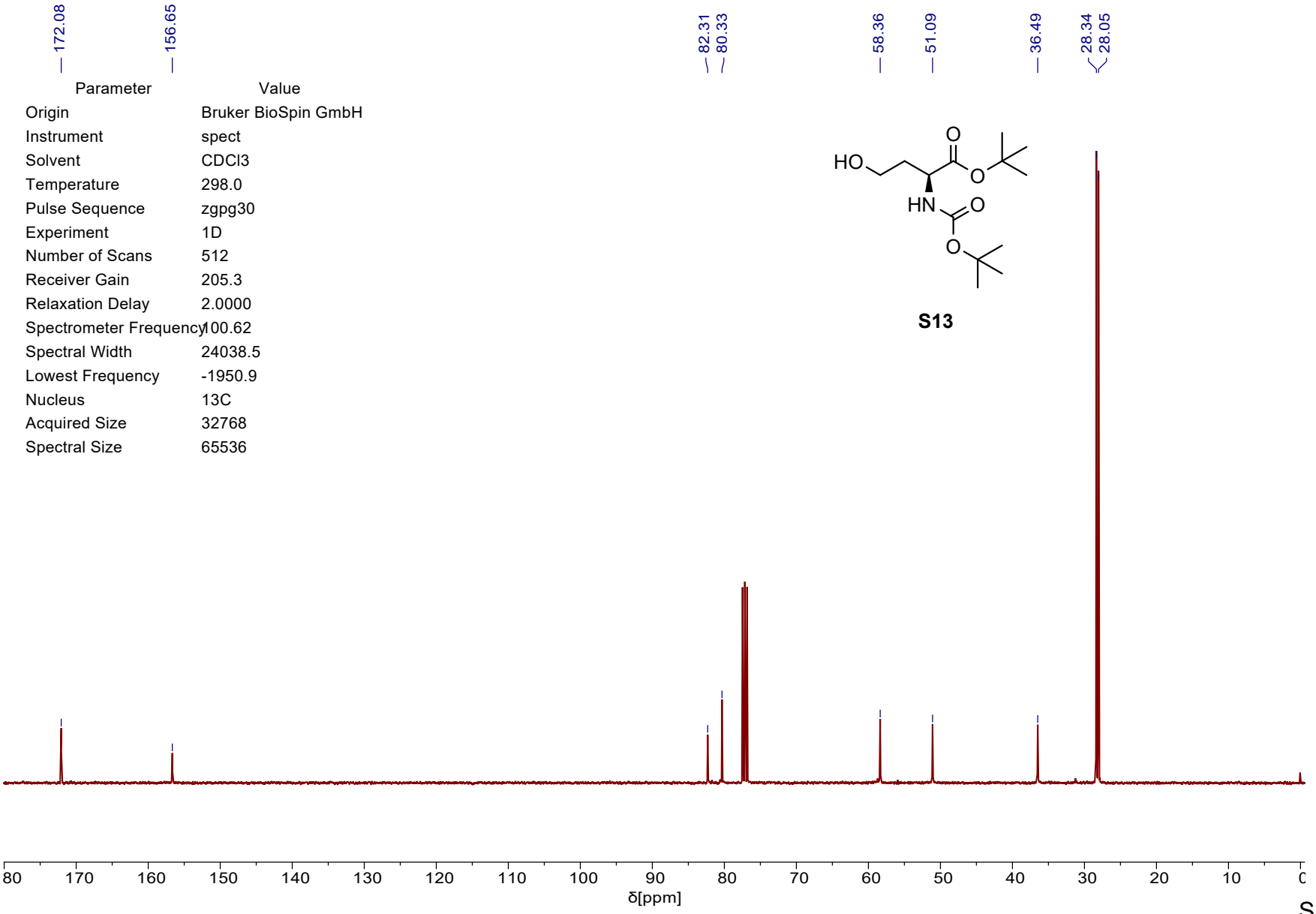

6.76
5.56
5.54
4.45
4.45
4.43
4.43
4.41
4.40
4.27
4.26
4.25
4.24
4.23
4.23
4.22
4.20
3.80
3.79
3.78
3.77
3.76
3.75
3.75
3.74
3.73
3.72
3.70
3.68
3.67
2.18
2.18
2.17
2.16
2.14
1.79
1.79
1.76
1.43
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 68.9
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1566.8
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
HO
O
OH
HN
O
O
S12
1.51
0.75
1.01
1.93
1.57
0.77
9.20
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]

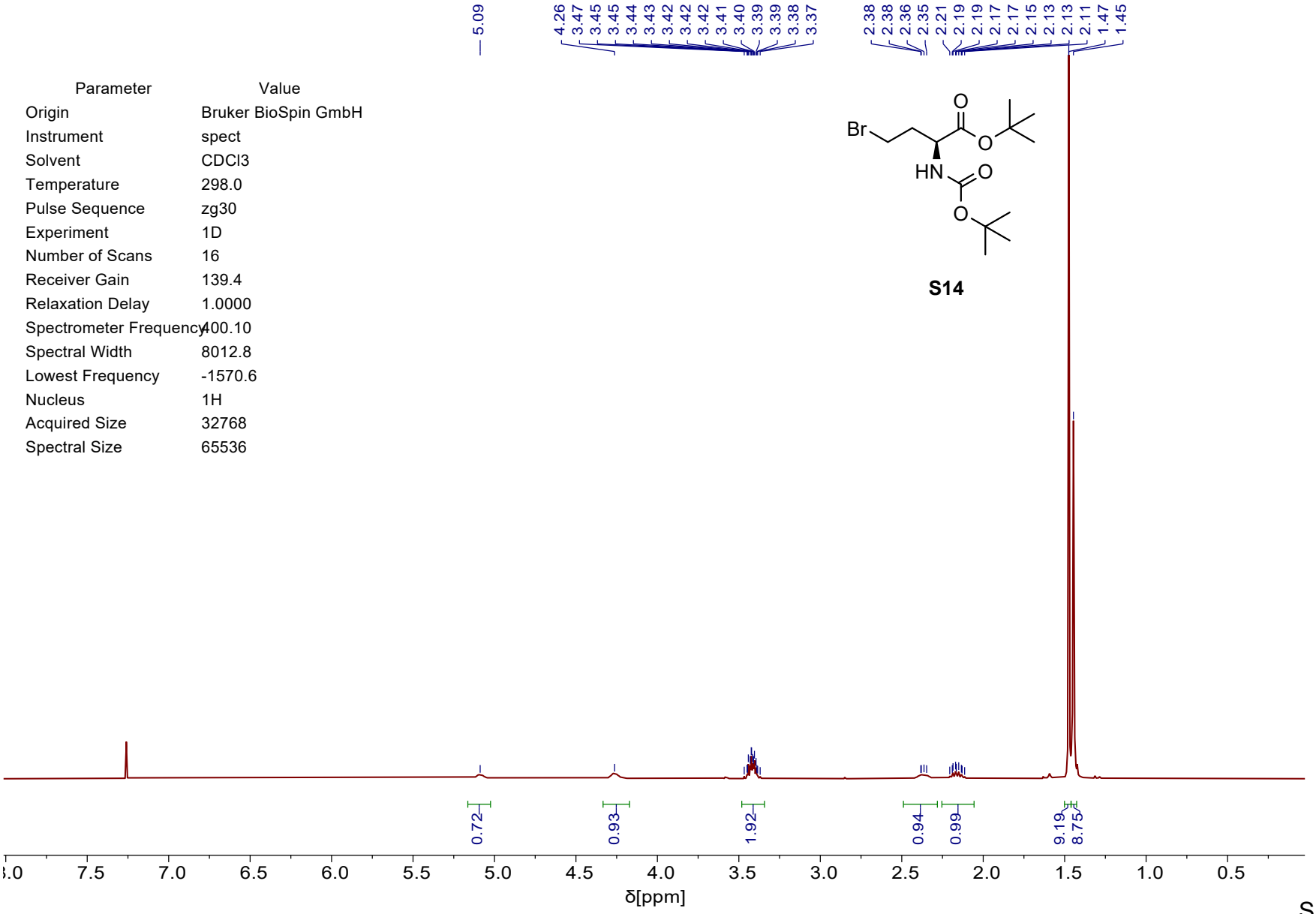

175.53
156.67
80.73
65.94
58.60
50.82
50.34
35.55
30.59
30.43
28.38
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
HO
O
OH
HN
O
O
S12
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
δ[ppm]

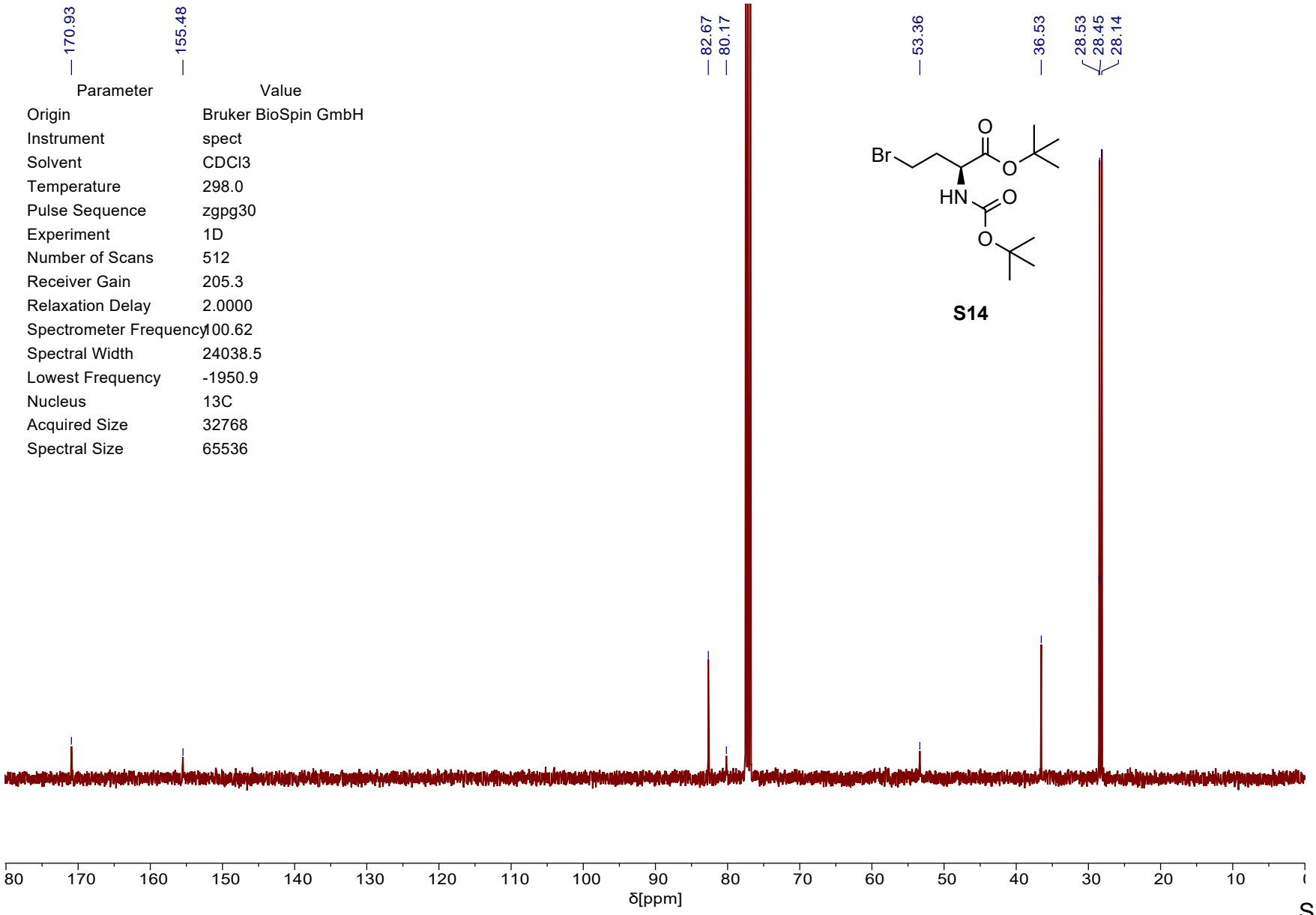
Parameter	Value
Origin	Bruker BioSpin GmbH
Instrument	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	32.1
Relaxation Delay	1.0000
Spectrometer Frequency	400.10
Spectral Width	8012.8
Lowest Frequency	-1528.0
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

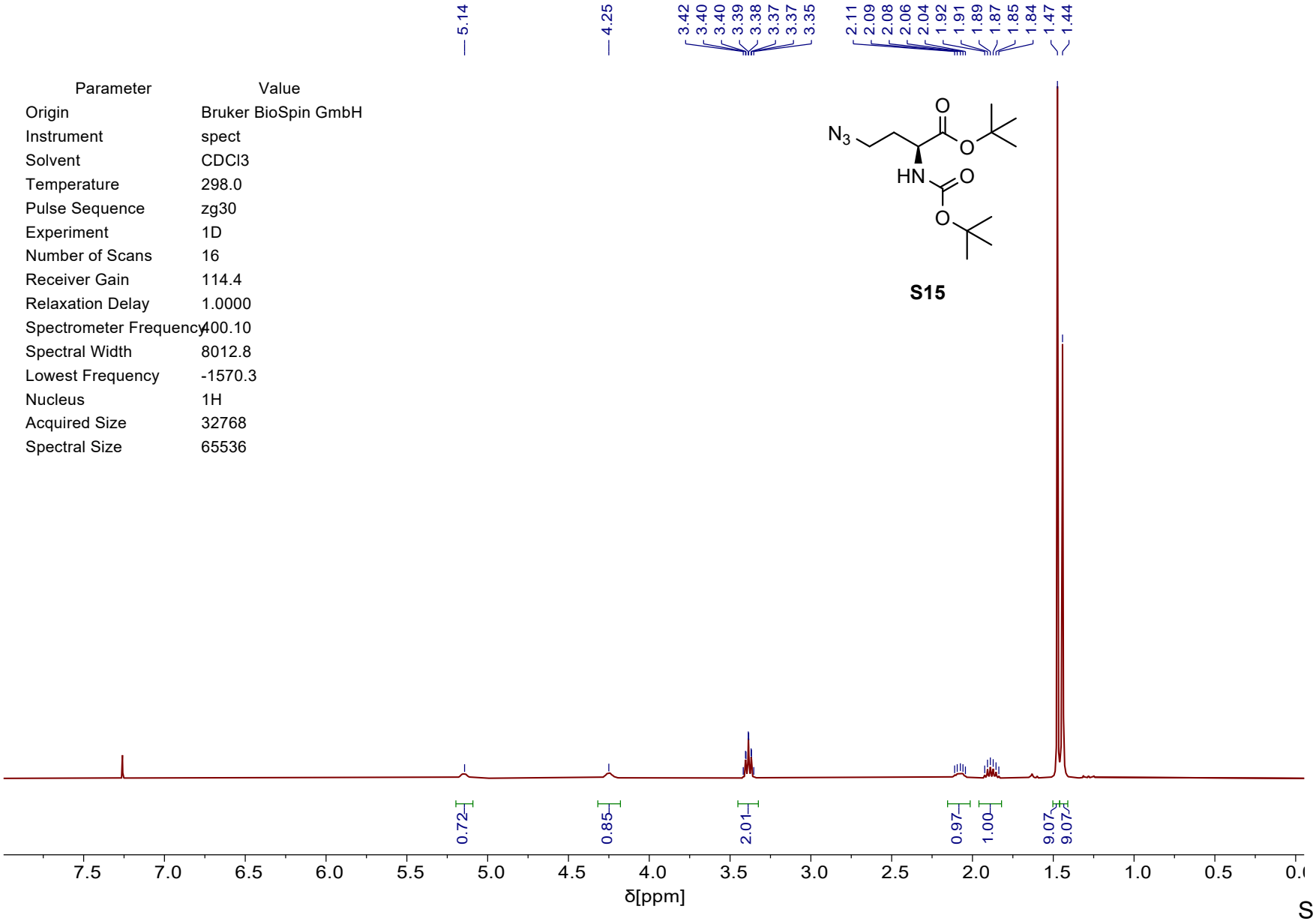


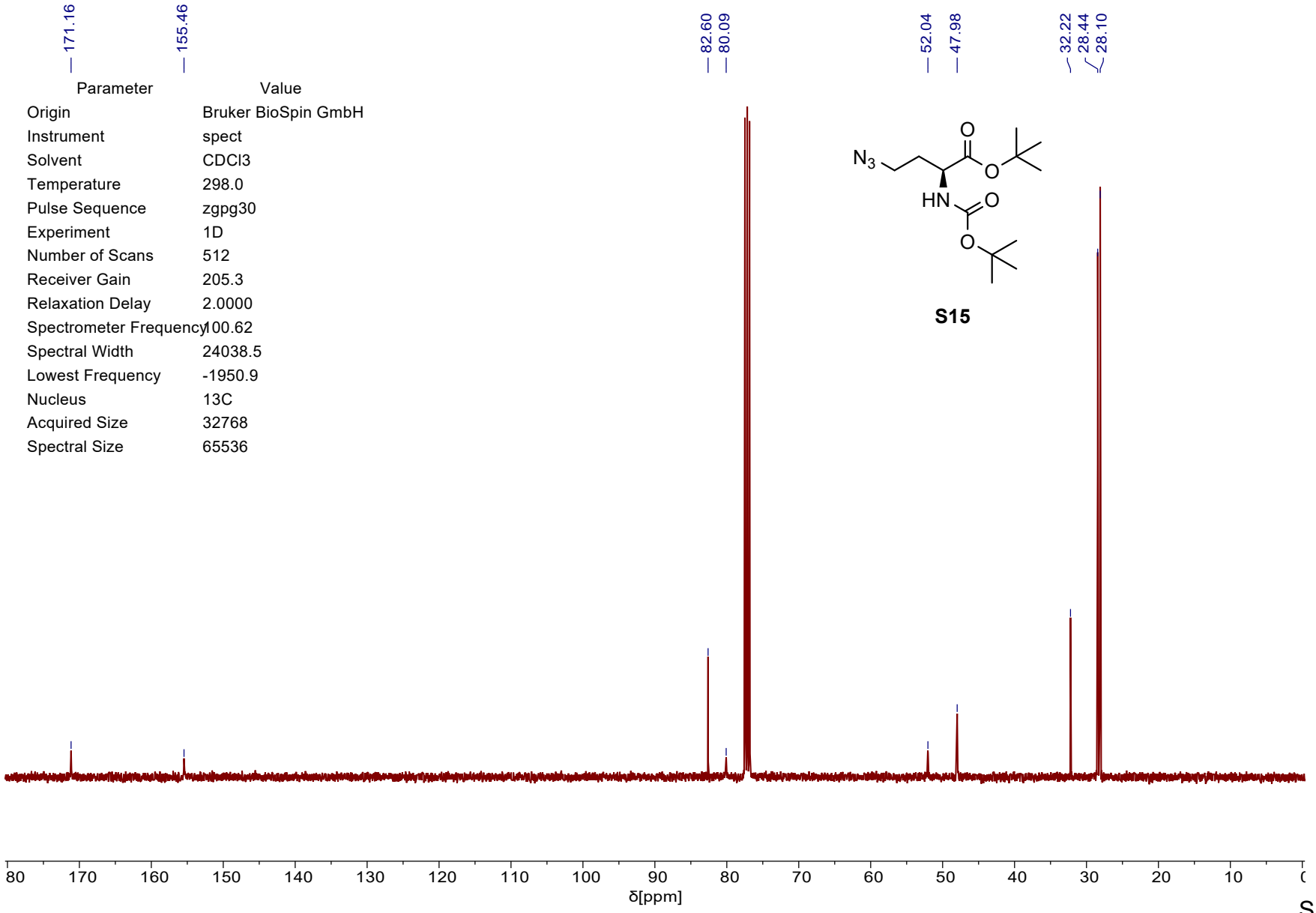
S13


172.08
156.65
82.31
80.33
58.36
51.09
36.49
28.34
28.05
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
HO
O
O
HN
O
O
S13
δ[ppm]

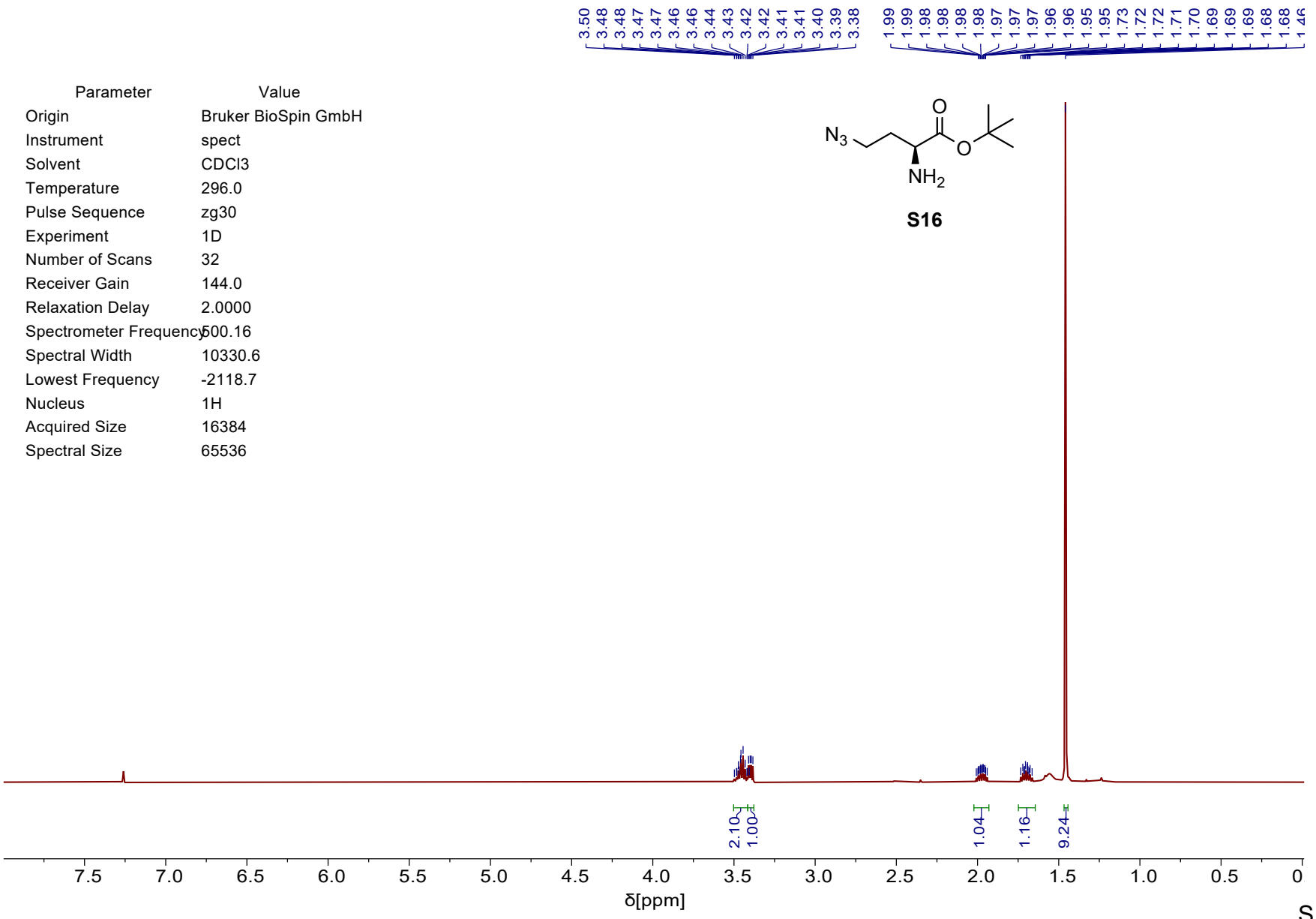

5.09
4.26
3.47
3.45
3.45
3.44
3.43
3.42
3.42
3.42
3.41
3.40
3.39
3.39
3.38
3.37
2.38
2.38
2.36
2.35
2.21
2.19
2.19
2.17
2.17
2.15
2.13
2.13
2.11
1.47
1.45
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 139.4
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1570.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
Br
O
O
HN
O
O
S14
0.72
0.93
1.92
0.94
0.99
9.19
8.75
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]

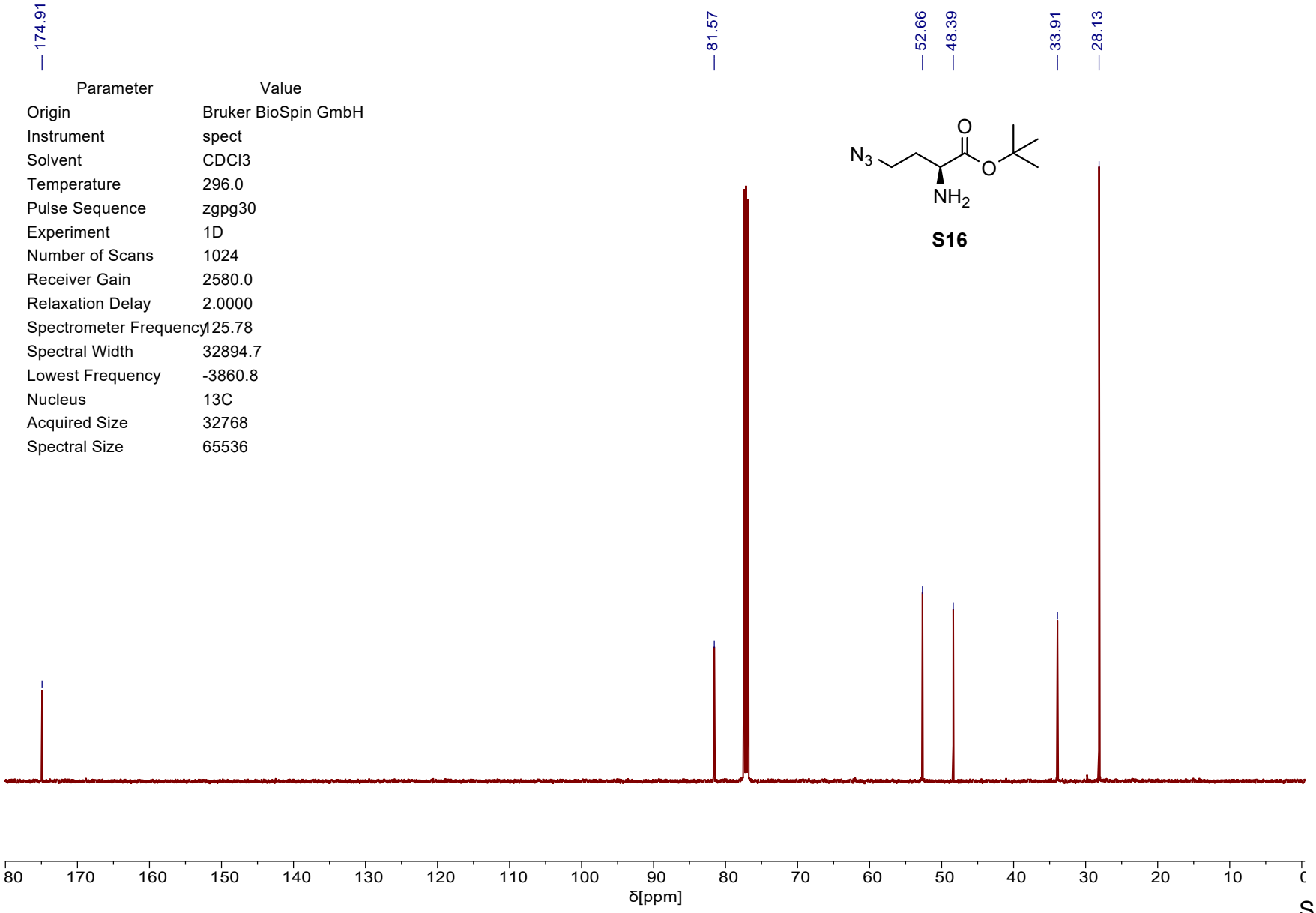

170.93
155.48
82.67
80.17
53.36
36.53
28.53
28.45
28.14
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
Br
HN
O
O
O
O
S14
δ[ppm]

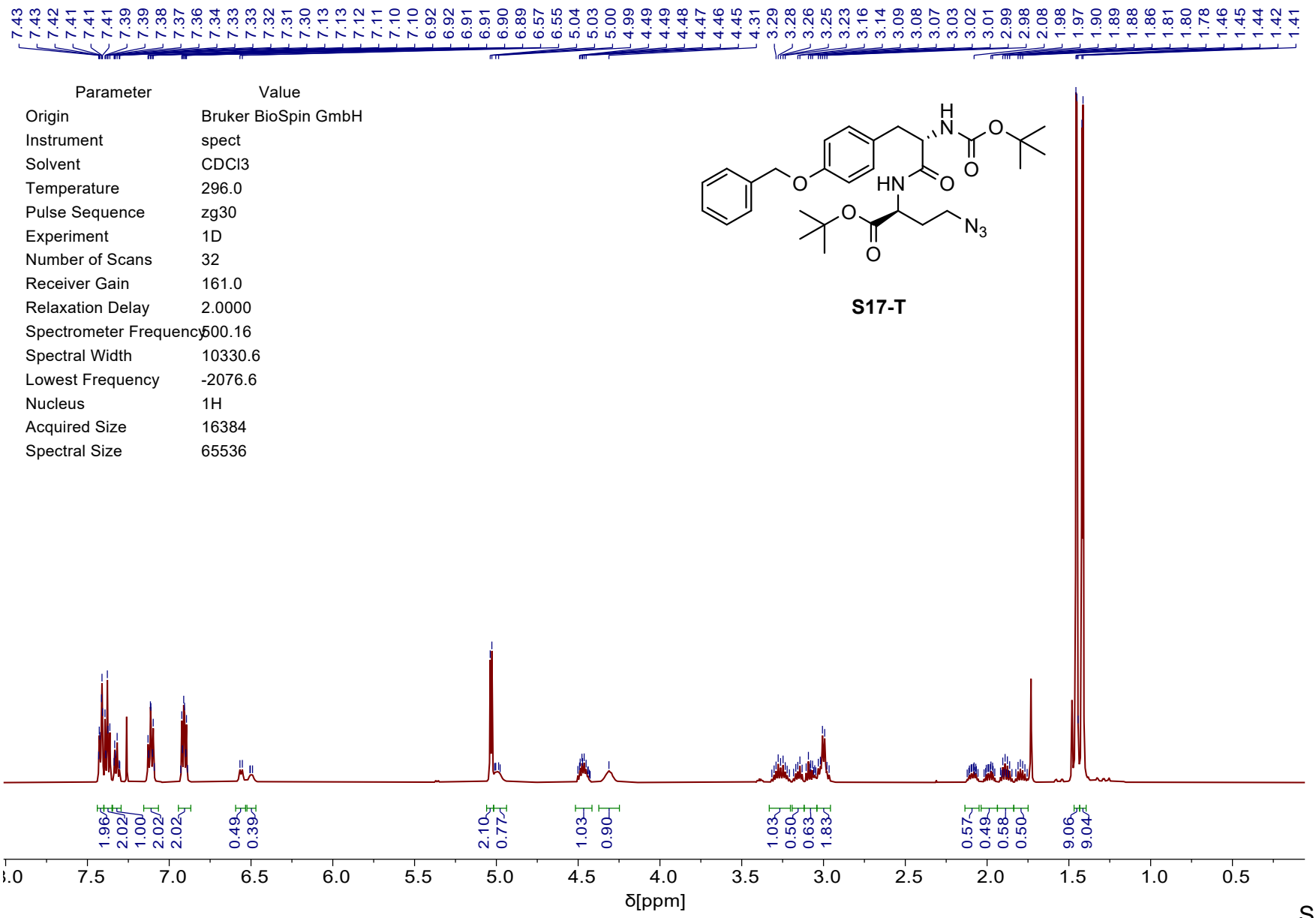

5.14
4.25
3.42
3.40
3.40
3.39
3.38
3.37
3.37
3.35
2.11
2.09
2.08
2.06
2.04
1.92
1.91
1.89
1.87
1.85
1.84
1.47
1.44
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 114.4
Relaxation Delay 1.0000
Spectrometer Frequency 400.10
Spectral Width 8012.8
Lowest Frequency -1570.3
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
N3
HN
O
O
O
O
S15
0.72
0.85
2.01
0.97
1.00
9.07
9.07
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]

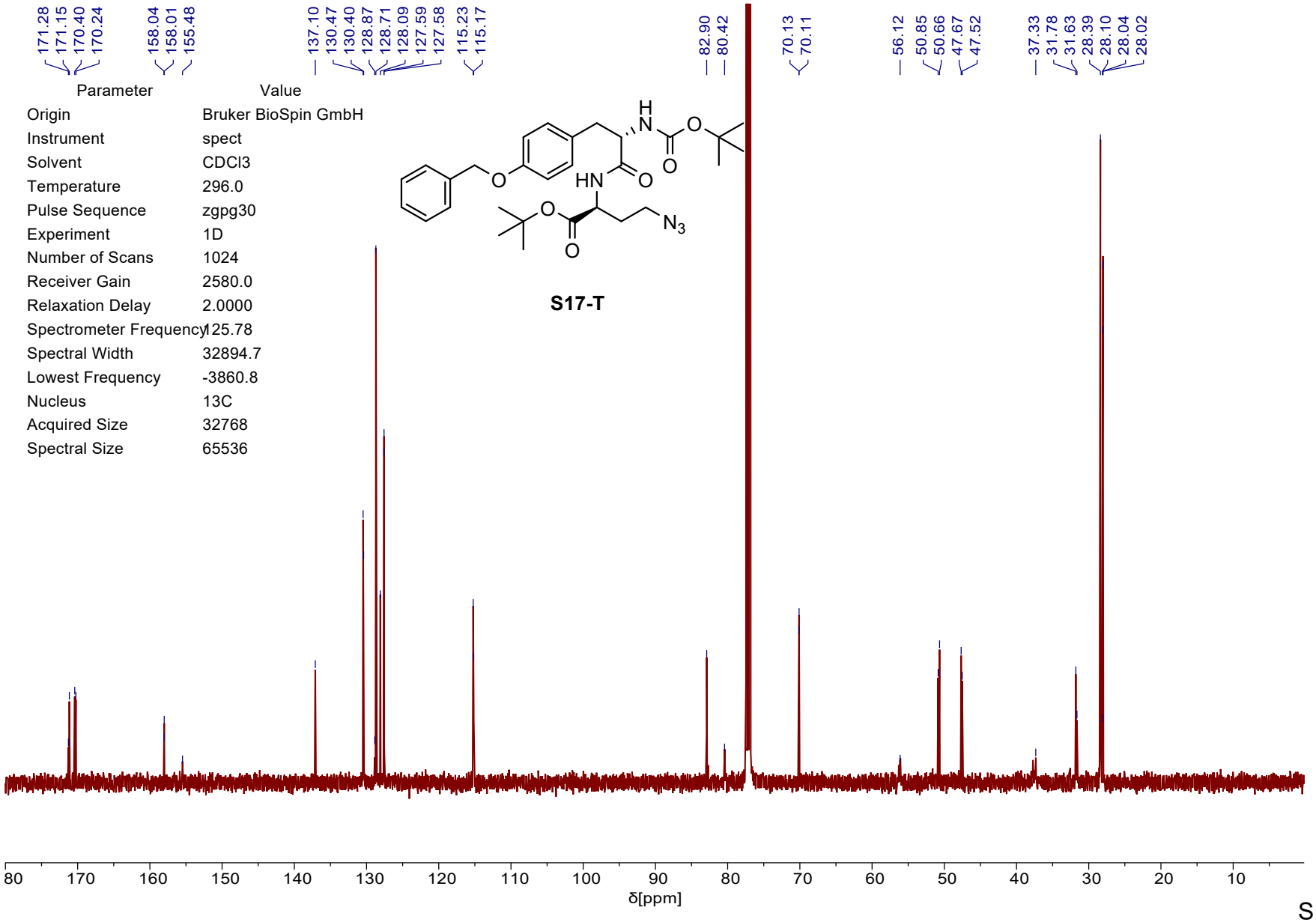

171.16
155.46
82.60
80.09
52.04
47.98
32.22
28.44
28.10
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 205.3
Relaxation Delay 2.0000
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1950.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
N3
HN
O
O
O
O
S15
δ[ppm]

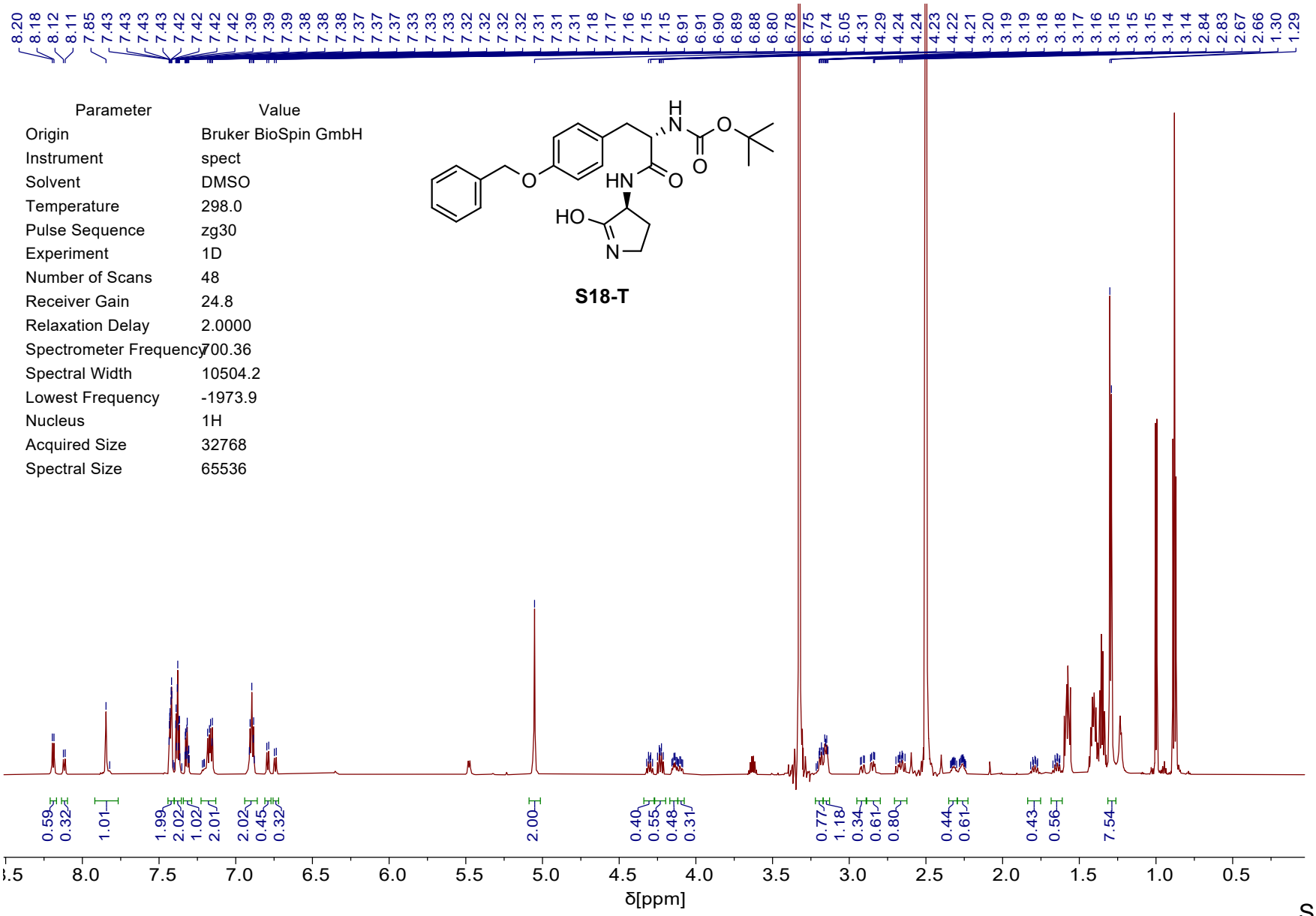
Parameter	Value
Origin	Bruker BioSpin GmbH
Instrument	spect
Solvent	CDCl3
Temperature	296.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	32
Receiver Gain	144.0
Relaxation Delay	2.0000
Spectrometer Frequency	500.16
Spectral Width	10330.6
Lowest Frequency	-2118.7
Nucleus	1H
Acquired Size	16384
Spectral Size	65536

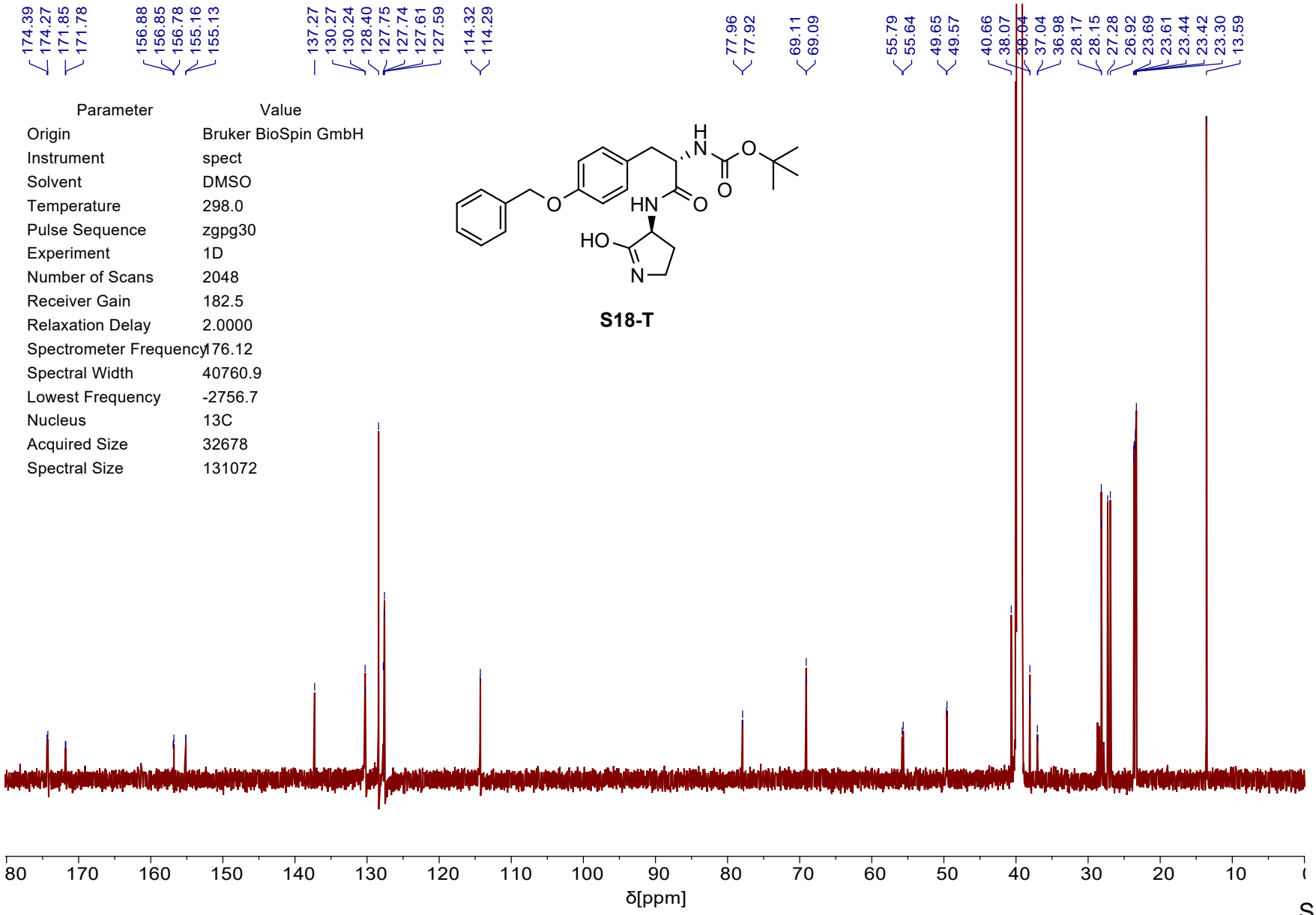



174.91
81.57
52.66
48.39
33.91
28.13
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1024
Receiver Gain 2580.0
Relaxation Delay 2.0000
Spectrometer Frequency 125.78
Spectral Width 32894.7
Lowest Frequency -3860.8
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
N3
O
O
NH2
S16
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ[ppm]

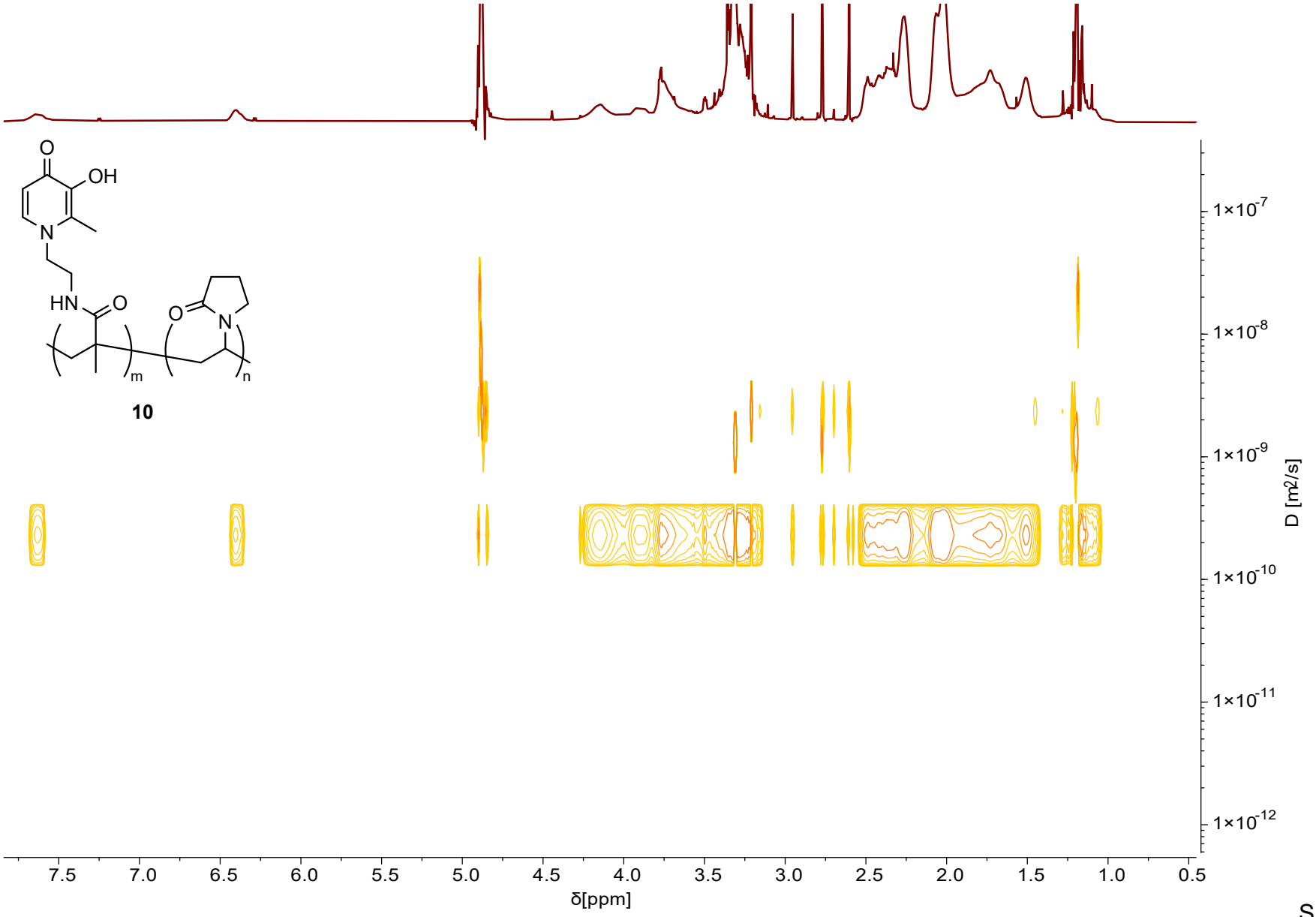

7.43 7.43 7.42 7.41 7.41 7.41 7.39 7.39 7.38 7.37 7.36 7.34 7.33 7.33 7.32 7.31 7.30 7.13 7.13 7.12 7.11 7.10 7.10 7.10 6.92 6.92 6.91 6.91 6.90 6.89 6.57 6.55 5.04 5.03 5.00 4.99 4.49 4.49 4.48 4.47 4.46 4.45 4.31
3.29 3.28 3.26 3.25 3.23 3.16 3.14 3.09 3.08 3.07 3.03 3.02 3.01 2.99 2.98 2.08 1.98 1.97 1.90 1.89 1.88 1.86 1.81 1.80 1.78 1.46 1.45 1.44 1.42 1.41
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 32
Receiver Gain 161.0
Relaxation Delay 2.0000
Spectrometer Frequency 500.16
Spectral Width 10330.6
Lowest Frequency -2076.6
Nucleus 1H
Acquired Size 16384
Spectral Size 65536
H
N
O
O
O
HN
O
O
O
N3
O
S17-T
1.96 2.02 1.00 2.02 2.02 0.49 0.39 2.10 0.77 1.03 0.90 1.03 0.50 0.63 1.83 0.57 0.49 0.58 0.50 9.06 9.04
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
δ[ppm]

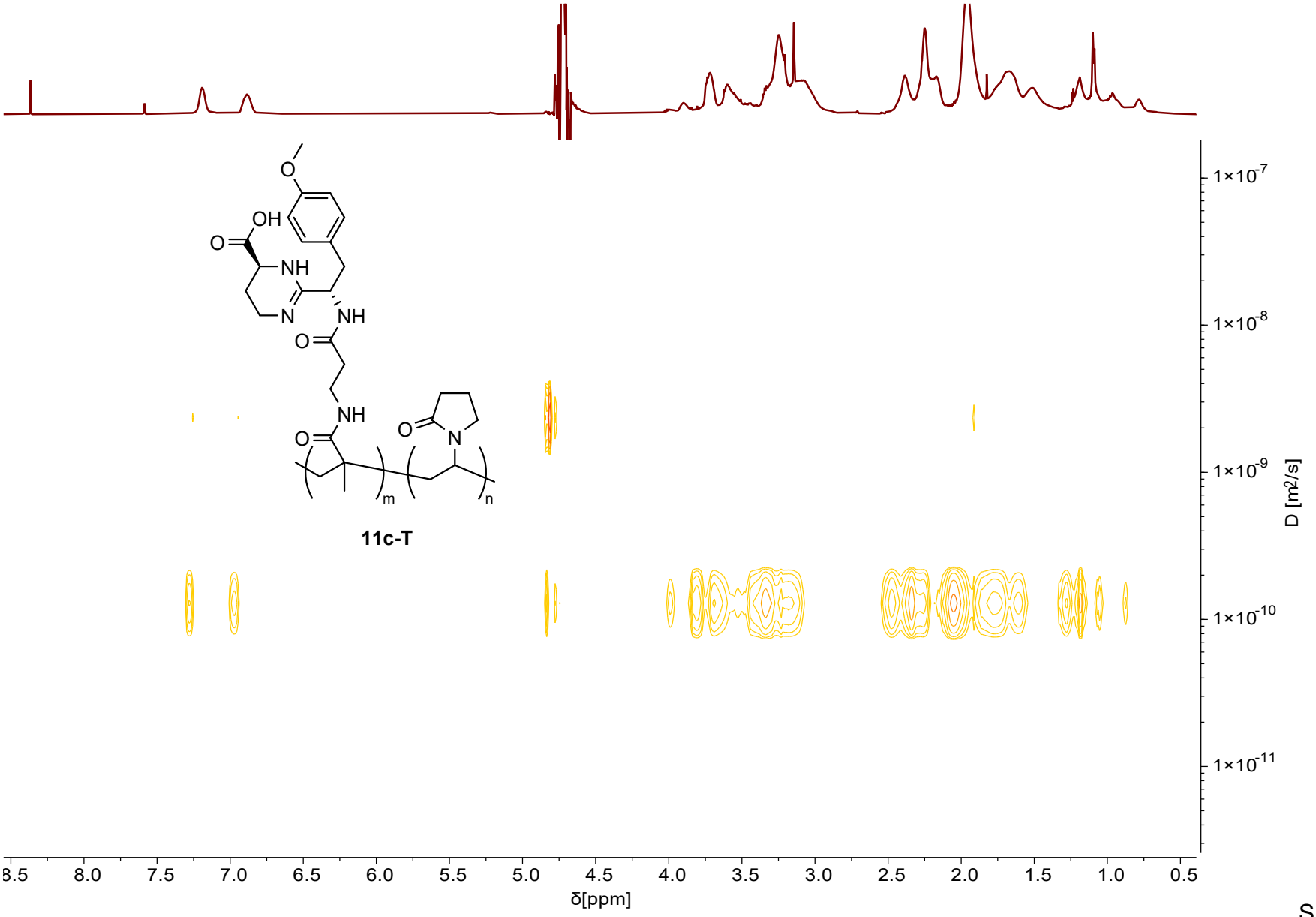

171.28
171.15
170.40
170.24
158.04
158.01
155.48
137.10
130.47
130.40
128.87
128.71
128.09
127.59
127.58
115.23
115.17
82.90
80.42
70.13
70.11
56.12
50.85
50.66
47.67
47.52
37.33
31.78
31.63
28.39
28.10
28.04
28.02
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent CDCl3
Temperature 296.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1024
Receiver Gain 2580.0
Relaxation Delay 2.0000
Spectrometer Frequency 125.78
Spectral Width 32894.7
Lowest Frequency -3860.8
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
S17-T
δ[ppm]

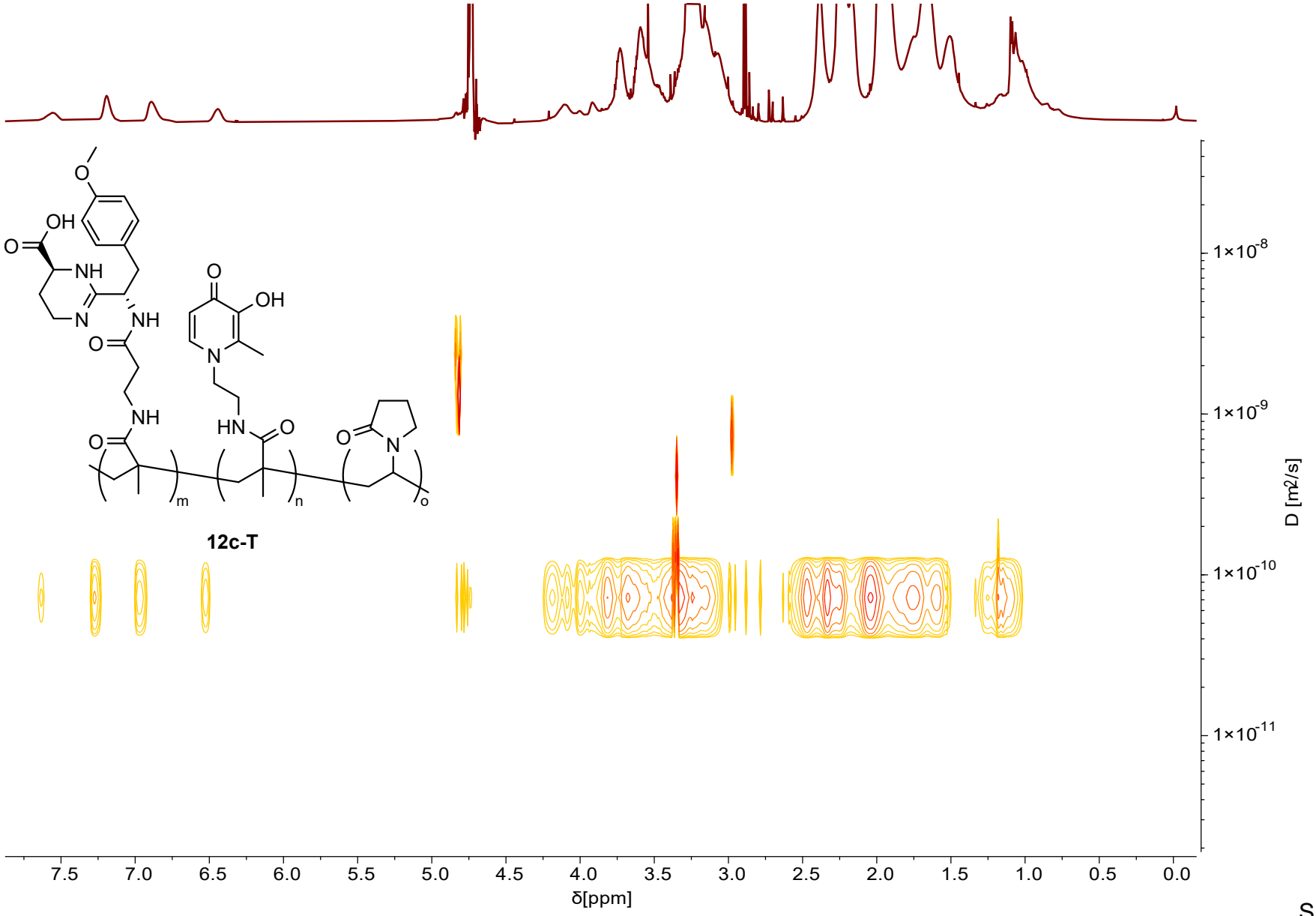

8.20 8.18 8.12 8.11 7.85 7.43 7.43 7.43 7.43 7.42 7.42 7.42 7.42 7.39 7.39 7.39 7.38 7.38 7.38 7.37 7.37 7.37 7.33 7.33 7.33 7.32 7.32 7.32 7.32 7.31 7.31 7.31 7.18 7.17 7.16 7.15 7.15 6.91 6.91 6.90 6.89 6.88 6.80 6.78 6.75 6.74 5.05 4.31 4.29 4.24 4.24 4.23 4.22 4.21 3.20 3.19 3.19 3.18 3.18 3.17 3.16 3.15 3.15 3.15 3.14 3.14 2.84 2.83 2.67 2.66 1.30 1.29
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent DMSO
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 48
Receiver Gain 24.8
Relaxation Delay 2.0000
Spectrometer Frequency 700.36
Spectral Width 10504.2
Lowest Frequency -1973.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
H N O O O HN O HO N
S18-T
0.59 0.32 1.01 1.99 2.02 1.02 2.01 2.02 0.45 0.32 2.00 0.40 0.55 0.48 0.31 0.77 1.18 0.34 0.61 0.80 0.44 0.61 0.43 0.56 7.54
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
δ[ppm]


174.39
174.27
171.85
171.78
156.88
156.85
156.78
155.16
155.13
137.27
130.27
130.24
128.40
127.75
127.74
127.61
127.59
114.32
114.29
77.96
77.92
69.11
69.09
55.79
55.64
49.65
49.57
40.66
38.07
38.04
37.04
36.98
28.17
28.15
27.28
26.92
23.69
23.61
23.44
23.42
23.30
13.59
Parameter Value
Origin Bruker BioSpin GmbH
Instrument spect
Solvent DMSO
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 2048
Receiver Gain 182.5
Relaxation Delay 2.0000
Spectrometer Frequency 176.12
Spectral Width 40760.9
Lowest Frequency -2756.7
Nucleus 13C
Acquired Size 32678
Spectral Size 131072
H
N
O
O
O
HN
O
HO
N
S18-T
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ[ppm]

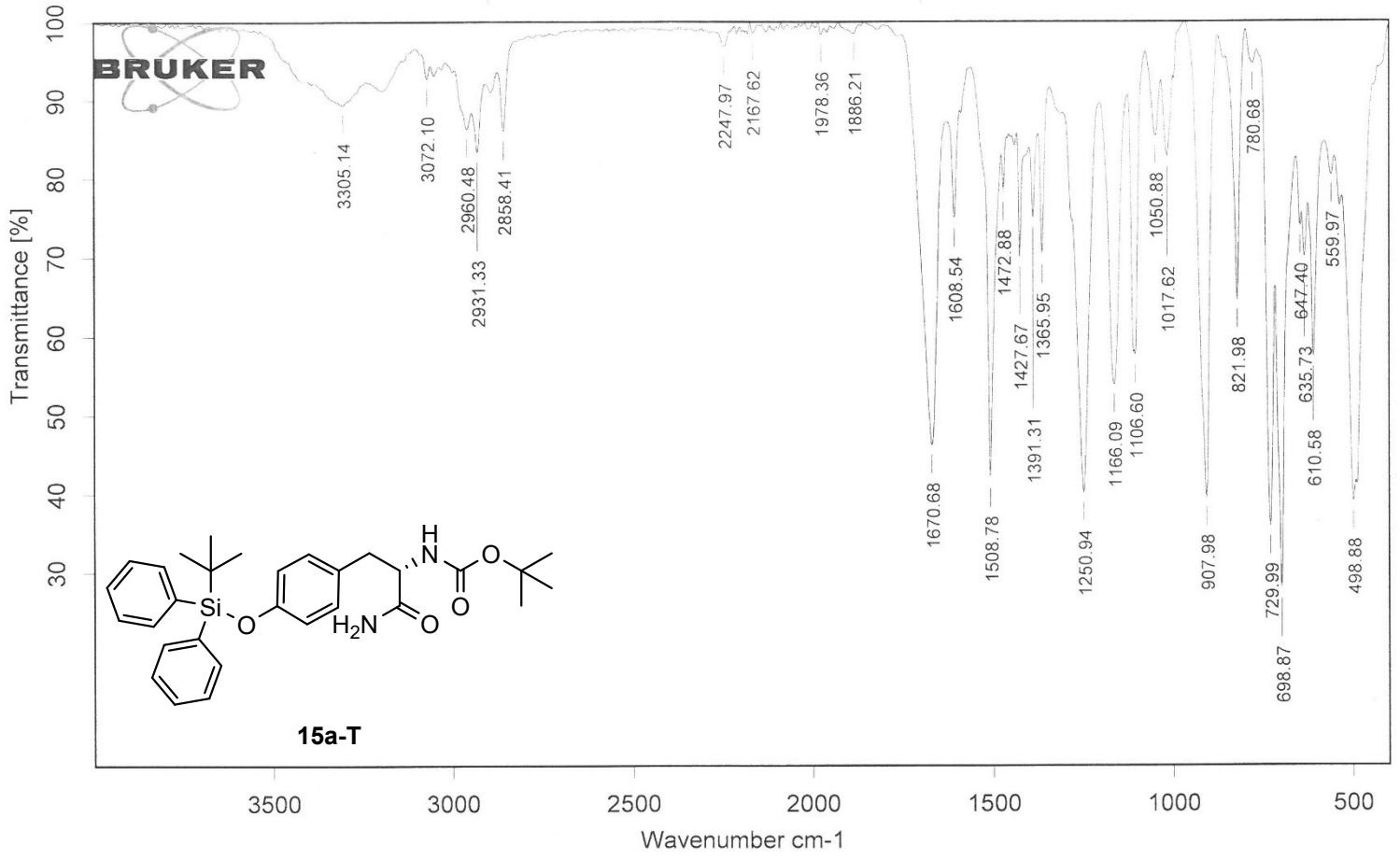
10. DOSY spectra


O
OH
N
HN
O
O
N
m
n
10
1×10-7
1×10-8
1×10-9
1×10-10
1×10-11
1×10-12
D [m2/s]
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]

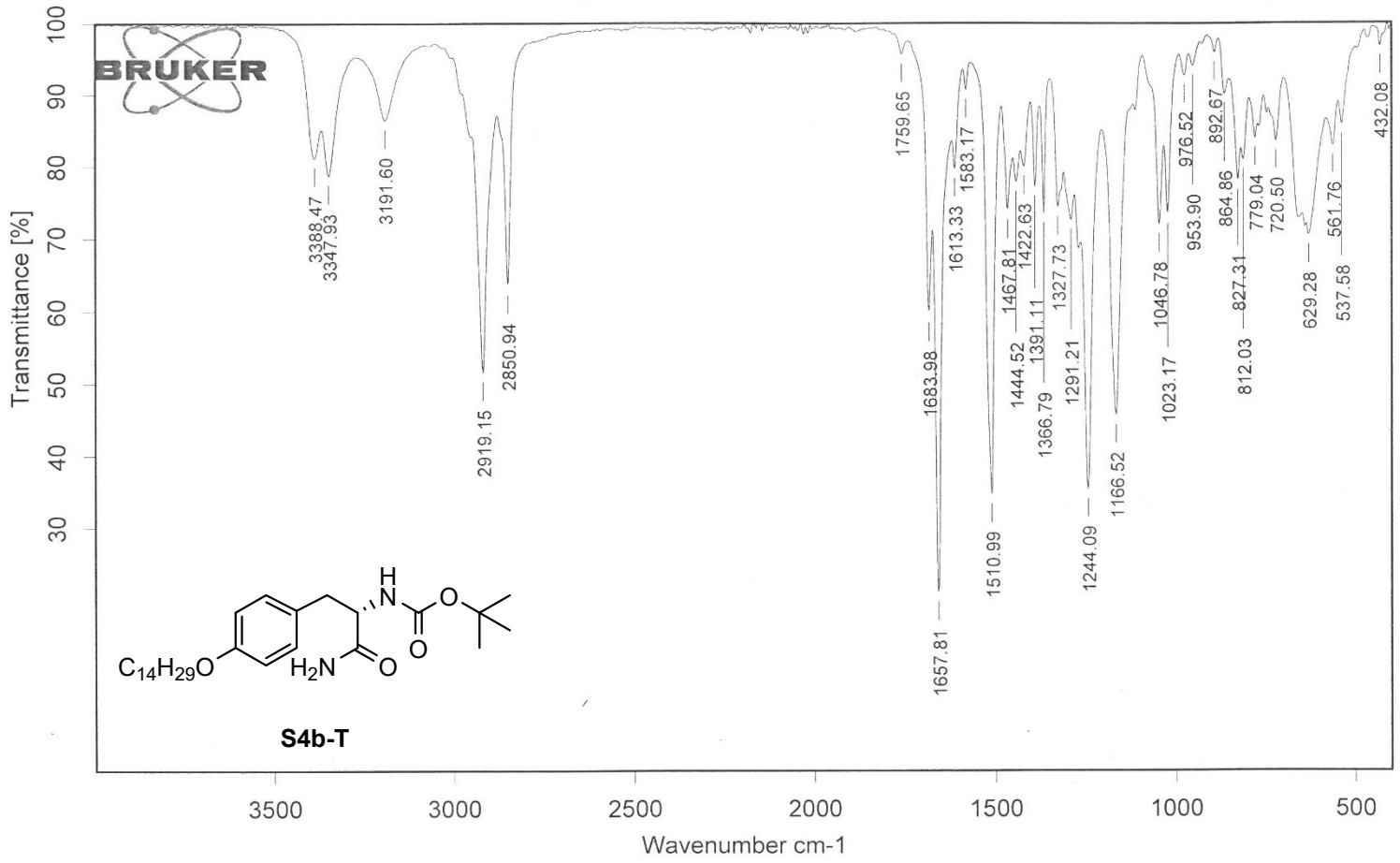

11c-T
1×10-7
1×10-8
1×10-9
1×10-10
1×10-11
D [m2/s]
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ[ppm]


12c-T
1×10-8
1×10-9
1×10-10
1×10-11
D [m2/s]
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ[ppm]

11. IR spectra

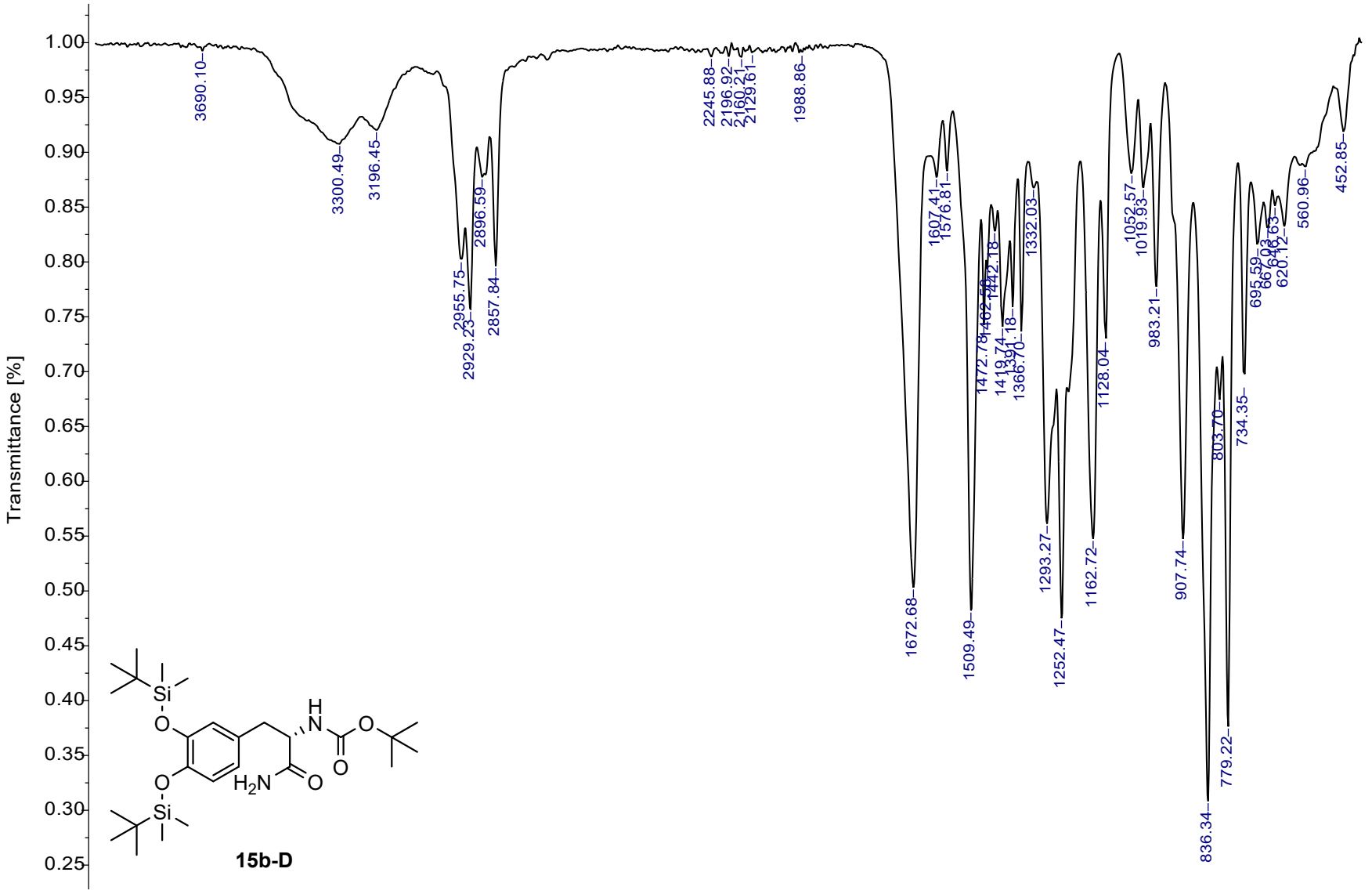


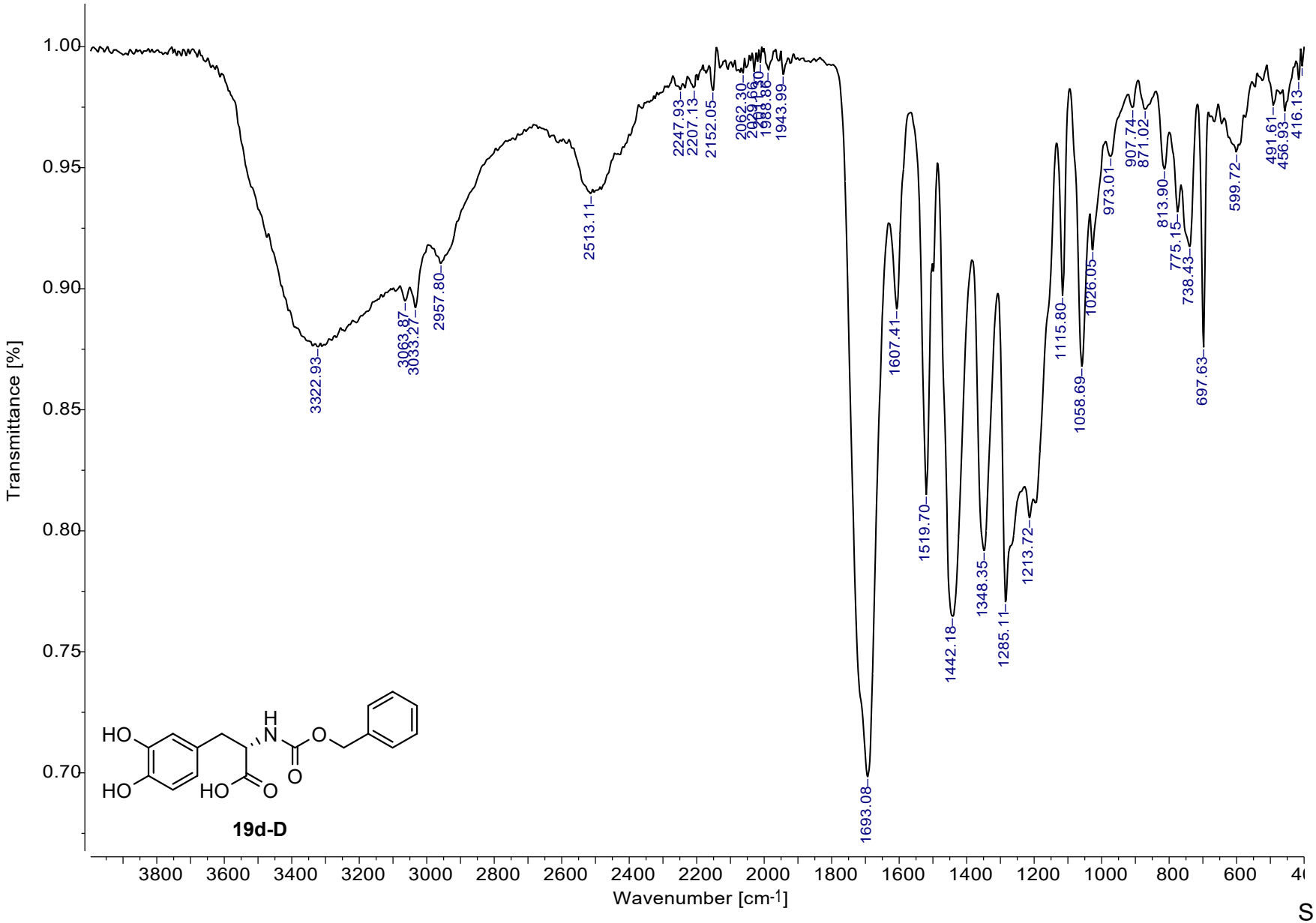
C:\Service\Greulich\GRE-215-F3-voll.0	Greulich/GRE-215-F3-voll	in CDCl3	01.07.2020

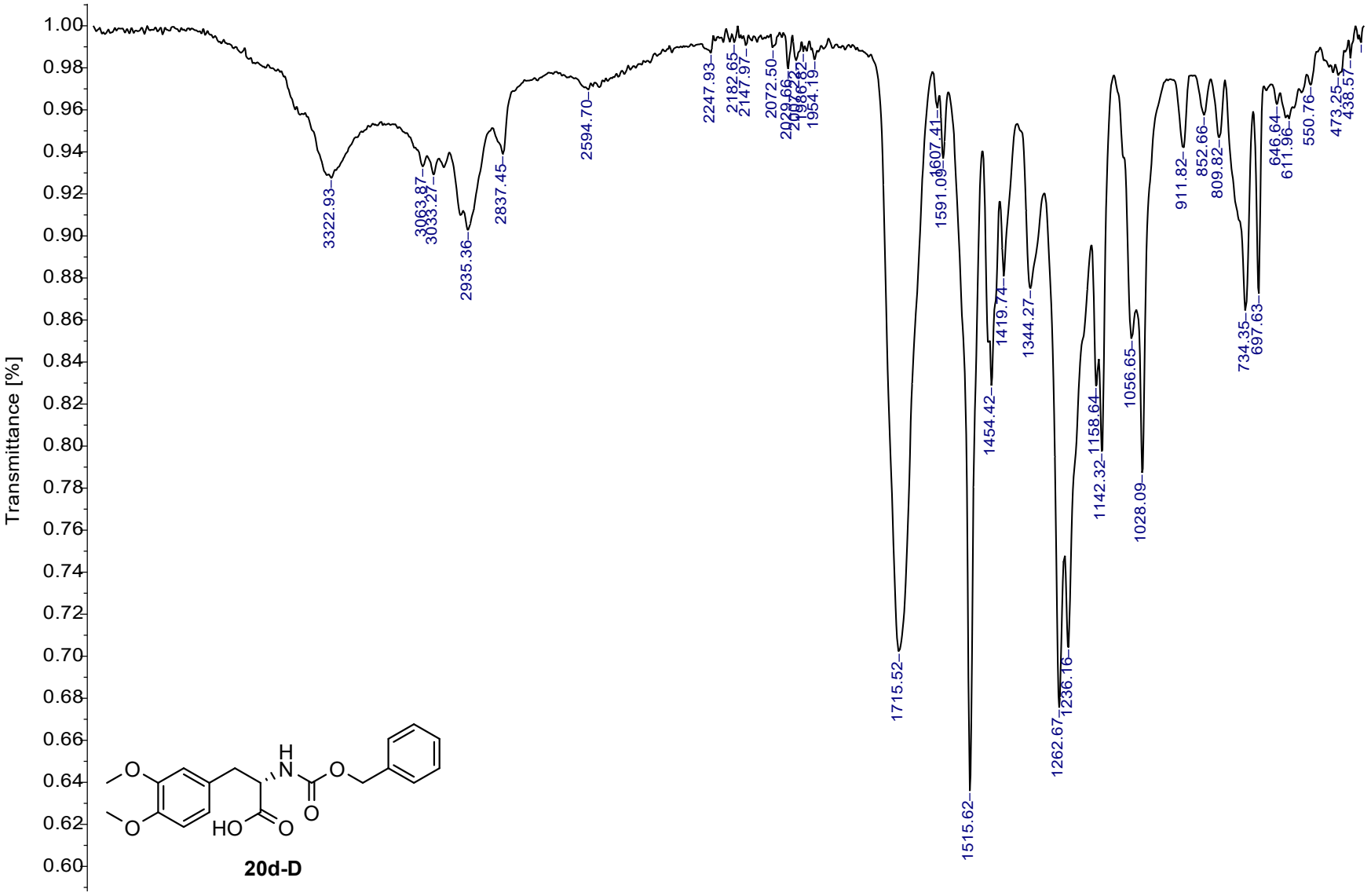


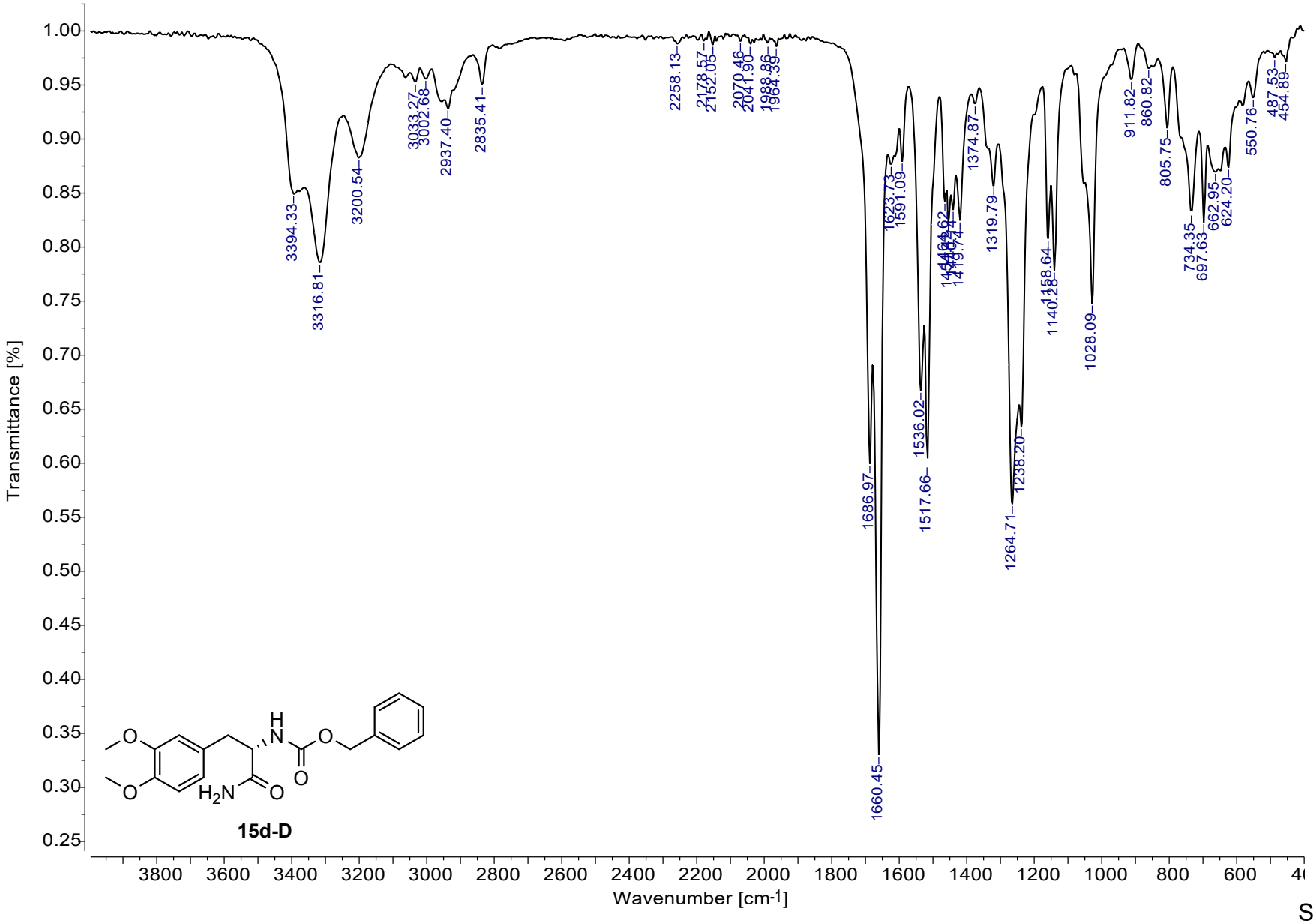
S4b-T

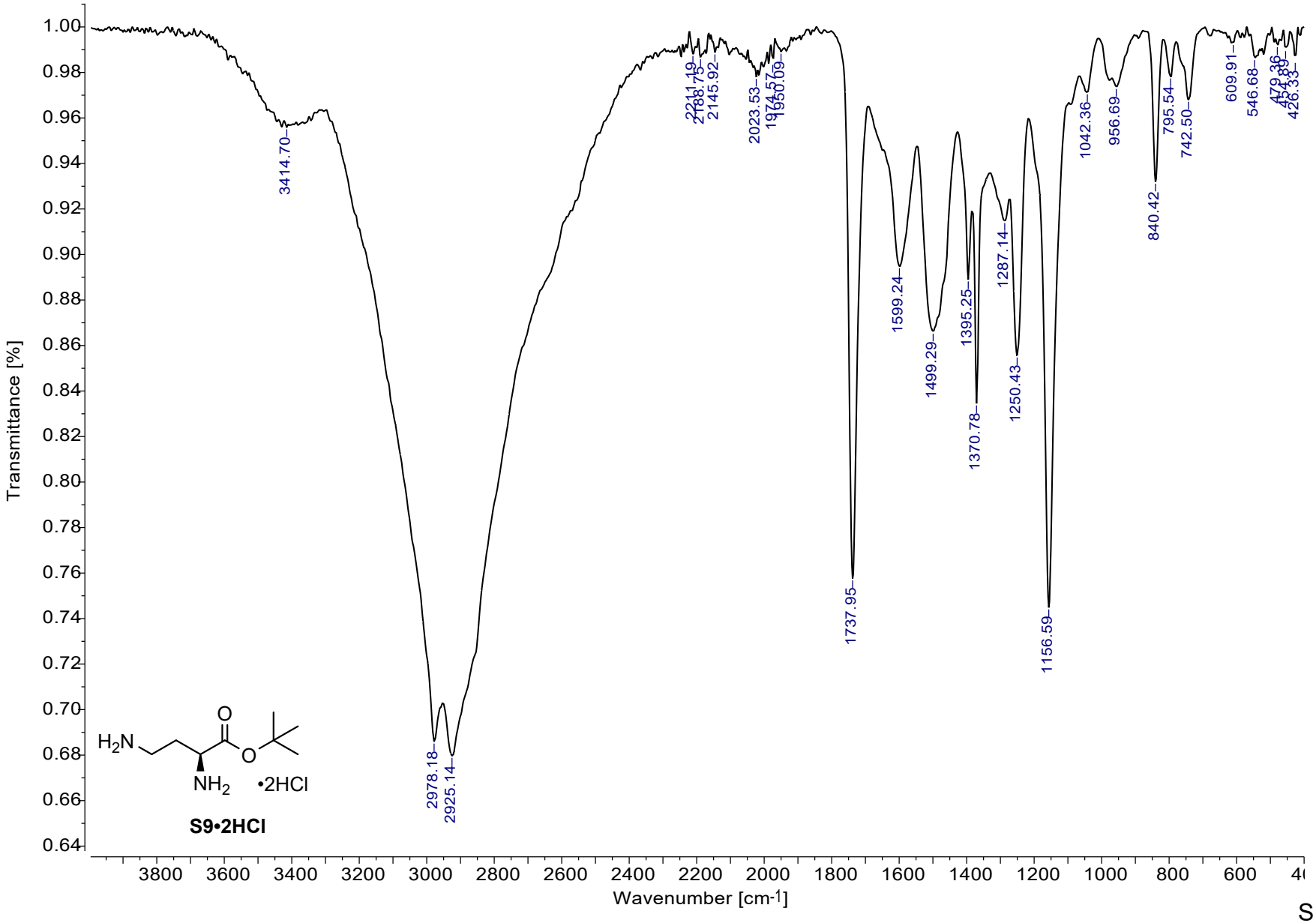
C:\Service\Greulich\GRE-527-P63voll.0	Greulich/GRE-527-P63voll	in CDCl3	05.07.2023

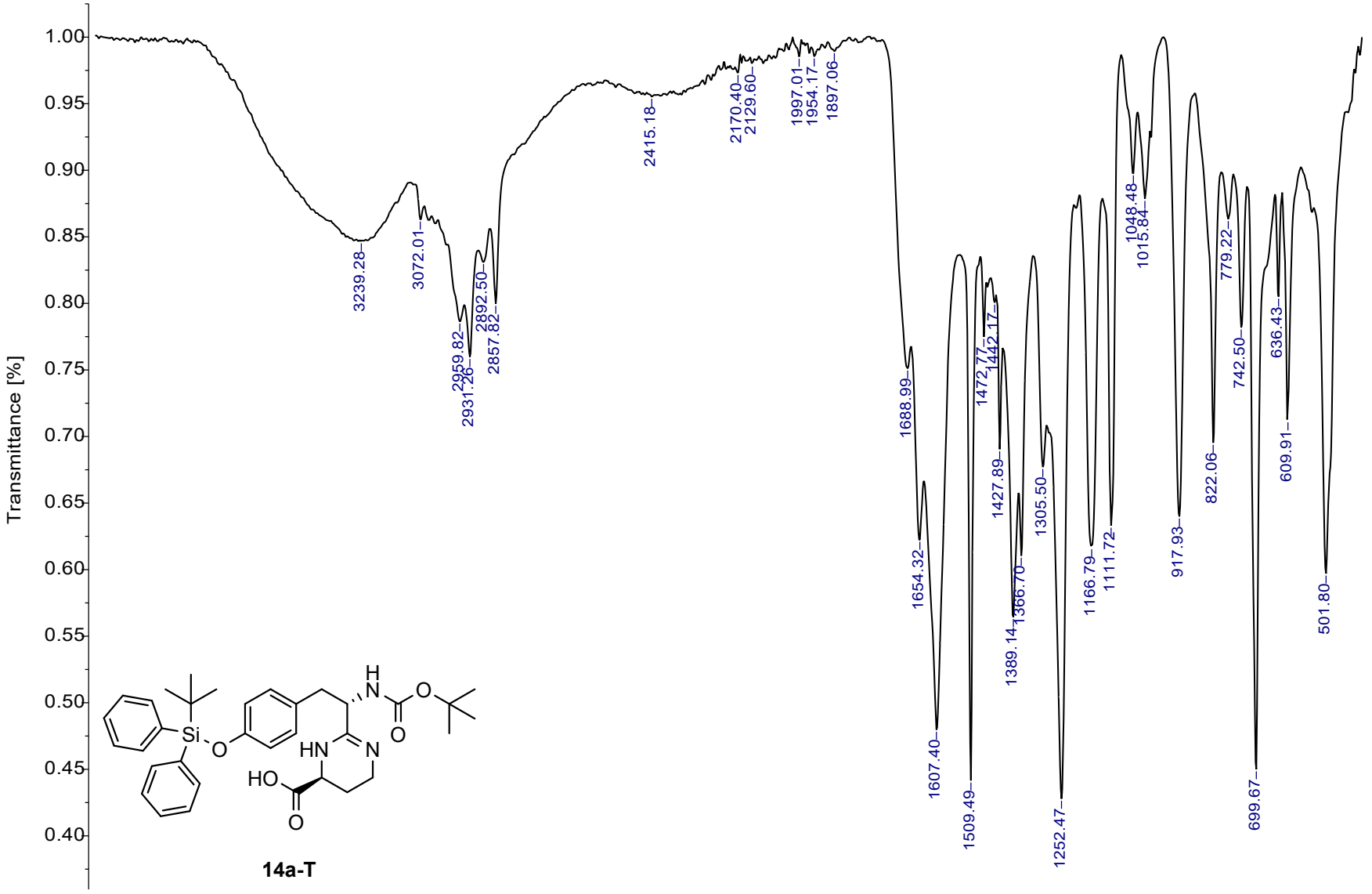

Transmittance [%]
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
3690.10
3300.49
3196.45
2955.75
2929.23
2896.59
2857.84
2245.88
2196.92
2160.21
2129.61
1988.86
1672.68
1607.41
1576.81
1509.49
1472.78
1462.50
1442.18
1419.74
1393.18
1366.70
1332.03
1293.27
1252.47
1162.72
1128.04
1052.57
1019.63
983.21
907.74
836.34
803.70
779.22
734.35
695.59
667.63
620.12
560.96
452.85
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]
Si
O
O
Si
H
N
O
O
H2N
O
15b-D


Transmittance [%]
1.00
0.95
0.90
0.85
0.80
0.75
0.70
3322.93
3063.87
3033.27
2957.80
2513.11
2247.93
2207.13
2152.05
2062.30
1943.99
1693.08
1607.41
1519.70
1442.18
1348.35
1285.11
1213.72
1115.80
1058.69
1026.05
973.01
907.74
871.02
813.90
775.15
738.43
697.63
599.72
491.61
456.93
416.13
HO
HO
HO
O
H
N
O
O
19d-D
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]

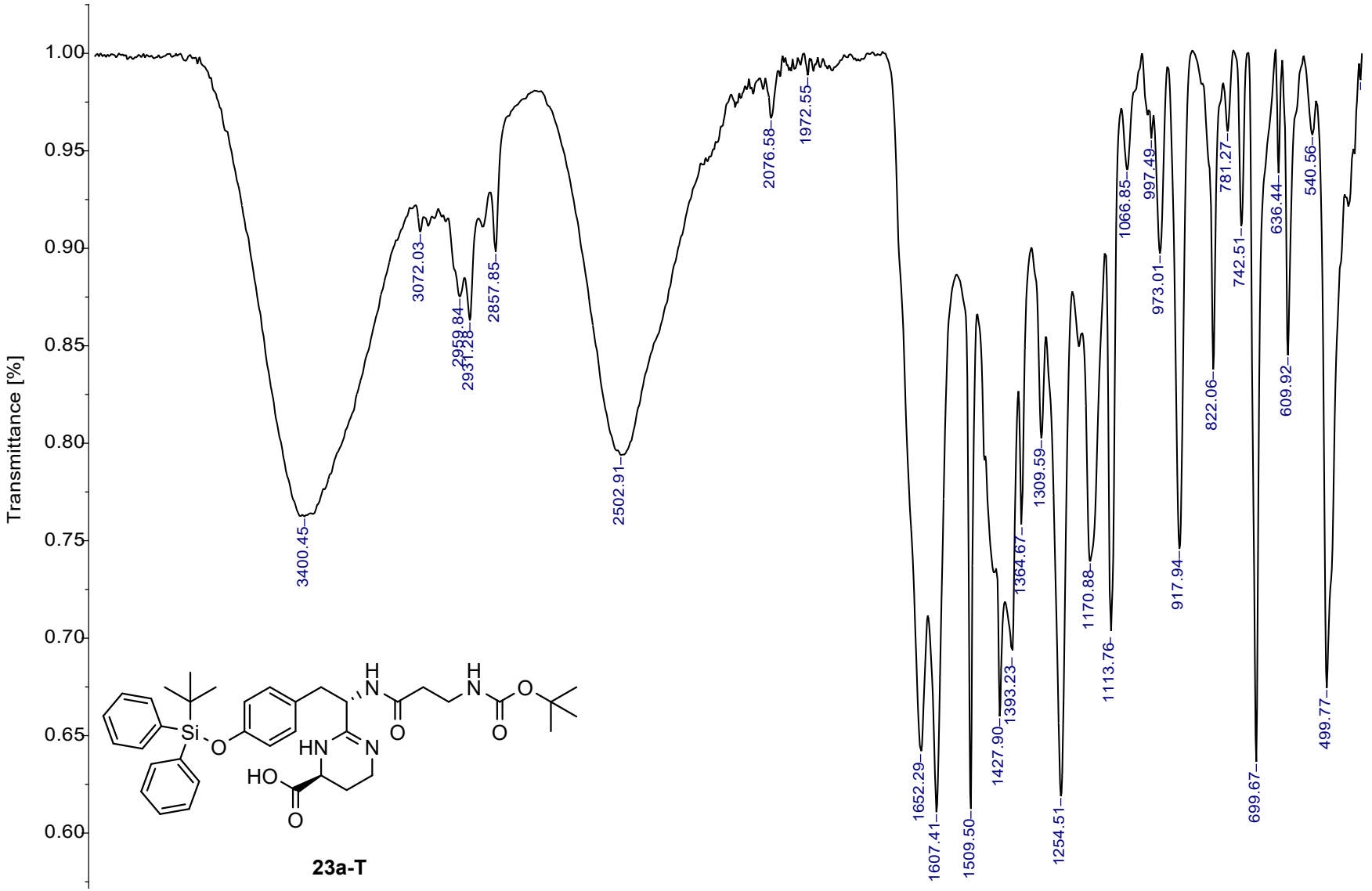

Transmittance [%]
1.00
0.98
0.96
0.94
0.92
0.90
0.88
0.86
0.84
0.82
0.80
0.78
0.76
0.74
0.72
0.70
0.68
0.66
0.64
0.62
0.60
3322.93
3063.87
3033.27
2935.36
2837.45
2594.70
2247.93
2182.65
2147.97
2072.50
2029.66
2006.22
1954.19
1715.52
1607.41
1591.09
1515.62
1454.42
1419.74
1344.27
1262.67
1236.16
1158.64
1142.32
1056.65
1028.09
911.82
852.66
809.82
734.35
697.63
646.64
611.96
550.76
473.25
438.57
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]
O
O
H
N
O
O
HO
O
20d-D


Transmittance [%]
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]
3394.33
3316.81
3200.54
3033.27
3002.68
2937.40
2835.41
2258.13
2178.57
2152.05
2070.46
2041.90
1988.86
1964.39
1686.97
1660.45
1623.73
1591.09
1536.02
1517.66
1374.87
1319.79
1264.71
1238.20
1168.64
1140.28
1028.09
911.82
860.82
805.75
734.35
697.63
662.95
624.20
550.76
487.53
454.89
O
O
O
H
N
O
O
H2N
15d-D


Transmittance [%]
1.00
0.98
0.96
0.94
0.92
0.90
0.88
0.86
0.84
0.82
0.80
0.78
0.76
0.74
0.72
0.70
0.68
0.66
0.64
3414.70
2978.18
2925.14
2211.19
2188.75
2145.92
2023.53
1974.57
1950.09
1737.95
1599.24
1499.29
1395.25
1370.78
1287.14
1250.43
1156.59
1042.36
956.69
840.42
795.54
742.50
609.91
546.68
479.36
454.89
426.33
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]
H2N
O
O
NH2
•2HCl
S9•2HCl


Transmittance [%]
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
3239.28
3072.01
2959.82
2931.26
2892.50
2857.82
2415.18
2170.40
2129.60
1997.01
1954.17
1897.06
1688.99
1654.32
1607.40
1509.49
1472.77
1442.17
1427.89
1389.14
1366.70
1305.50
1252.47
1166.79
1111.72
1048.48
1015.84
917.93
822.06
779.22
742.50
699.67
636.43
609.91
501.80
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]
Si
O
HN
N
H
N
O
O
HO
O

14a-T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0.60
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2502.91
2076.58
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1607.41
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1427.90
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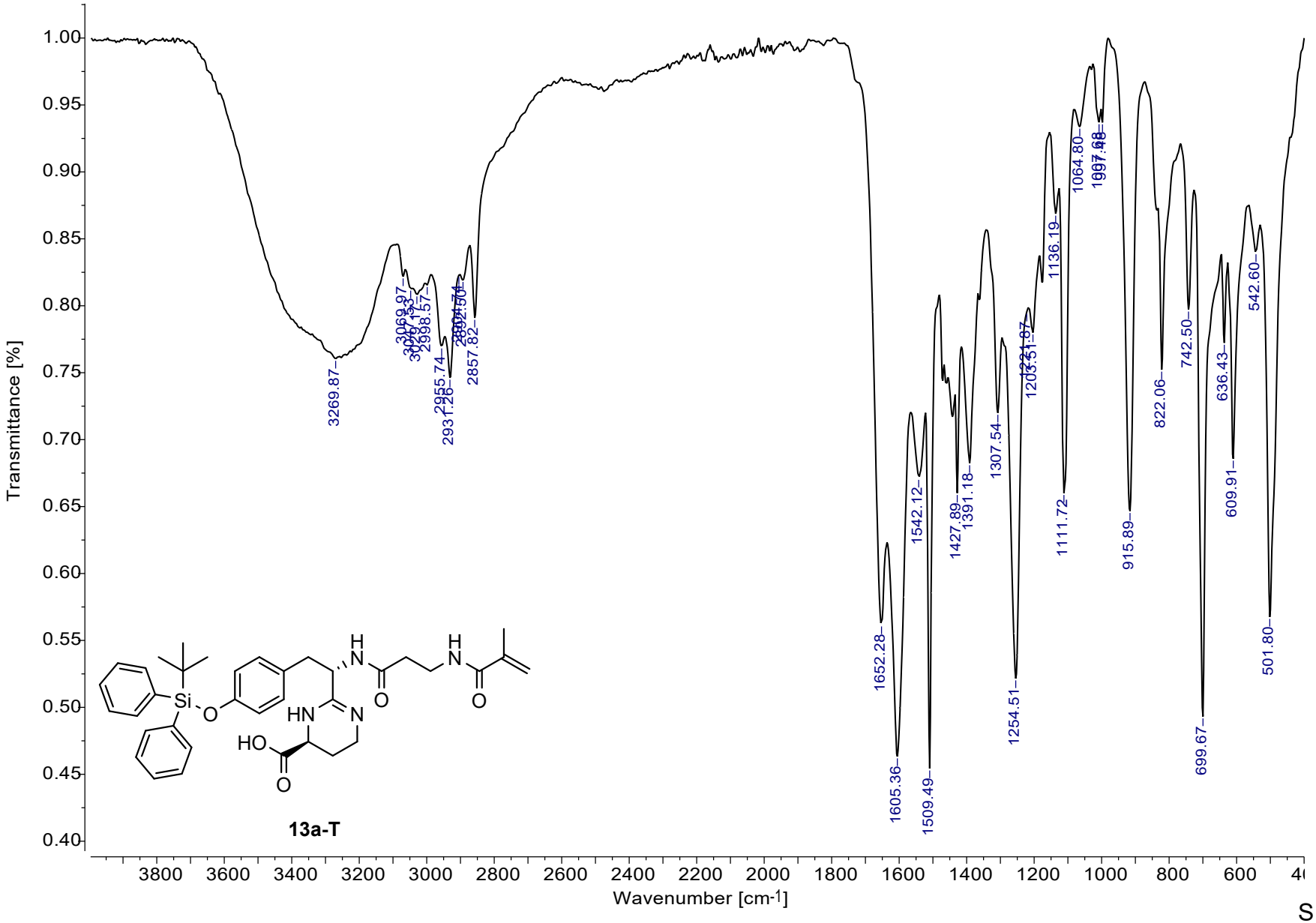
1309.59
1254.51
1170.88
1113.76
1066.85
997.49
973.01
917.94
822.06
781.27
742.51
699.67
636.44
609.92
540.56
499.77
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]
Si
O
HN
N
HO
O
H
N
O
O
H
N
O
O

23a-T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0.80
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0.55
0.50
0.45
0.40
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]
3269.87
2998.57
2955.74
2857.82
1652.28
1605.36
1542.12
1509.49
1427.89
1391.18
1307.54
1254.51
1136.19
1111.72
1064.80
915.89
822.06
742.50
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542.60
501.80
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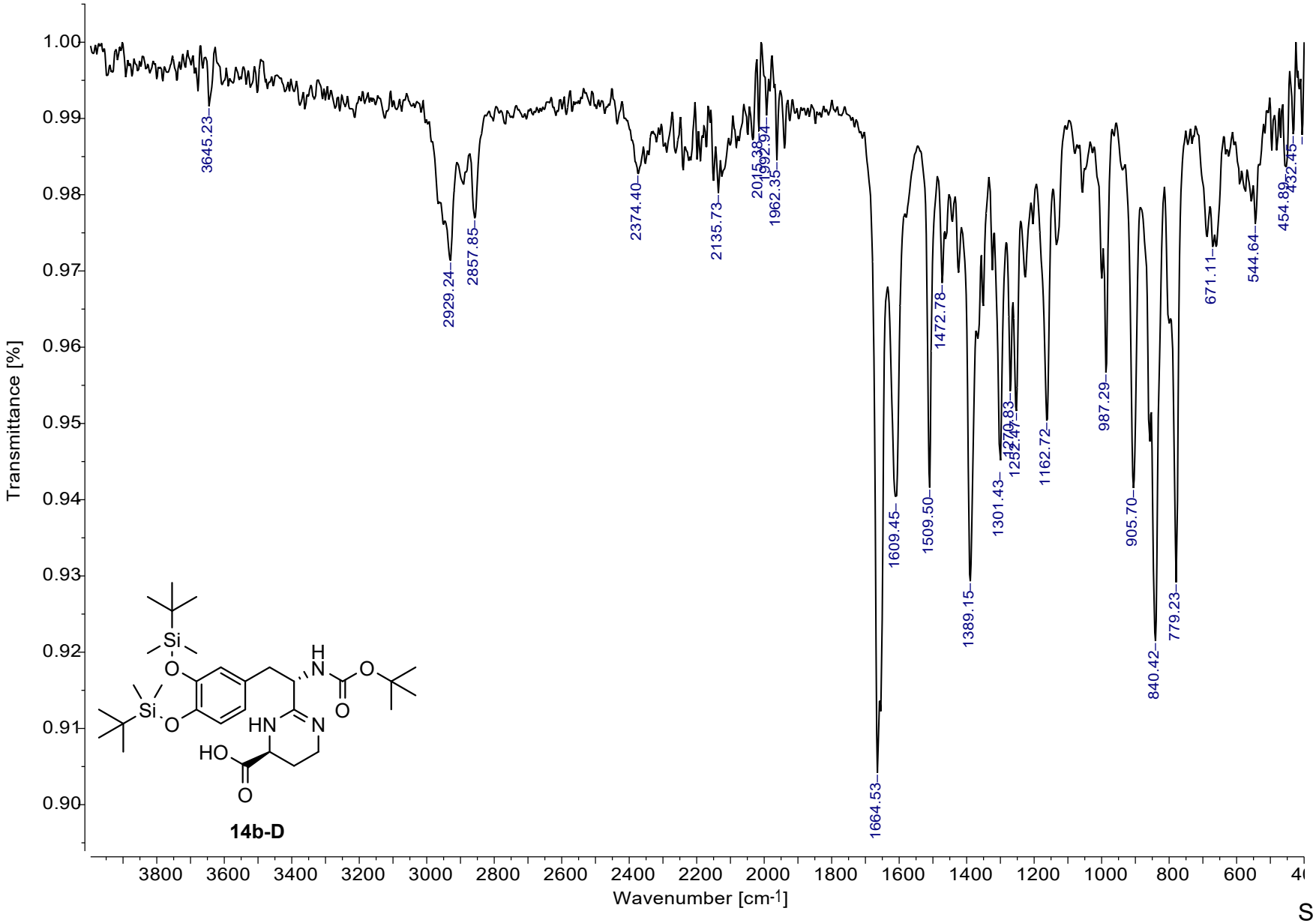
O
HN
N
H
N
O
HO
O
13a-T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0.90
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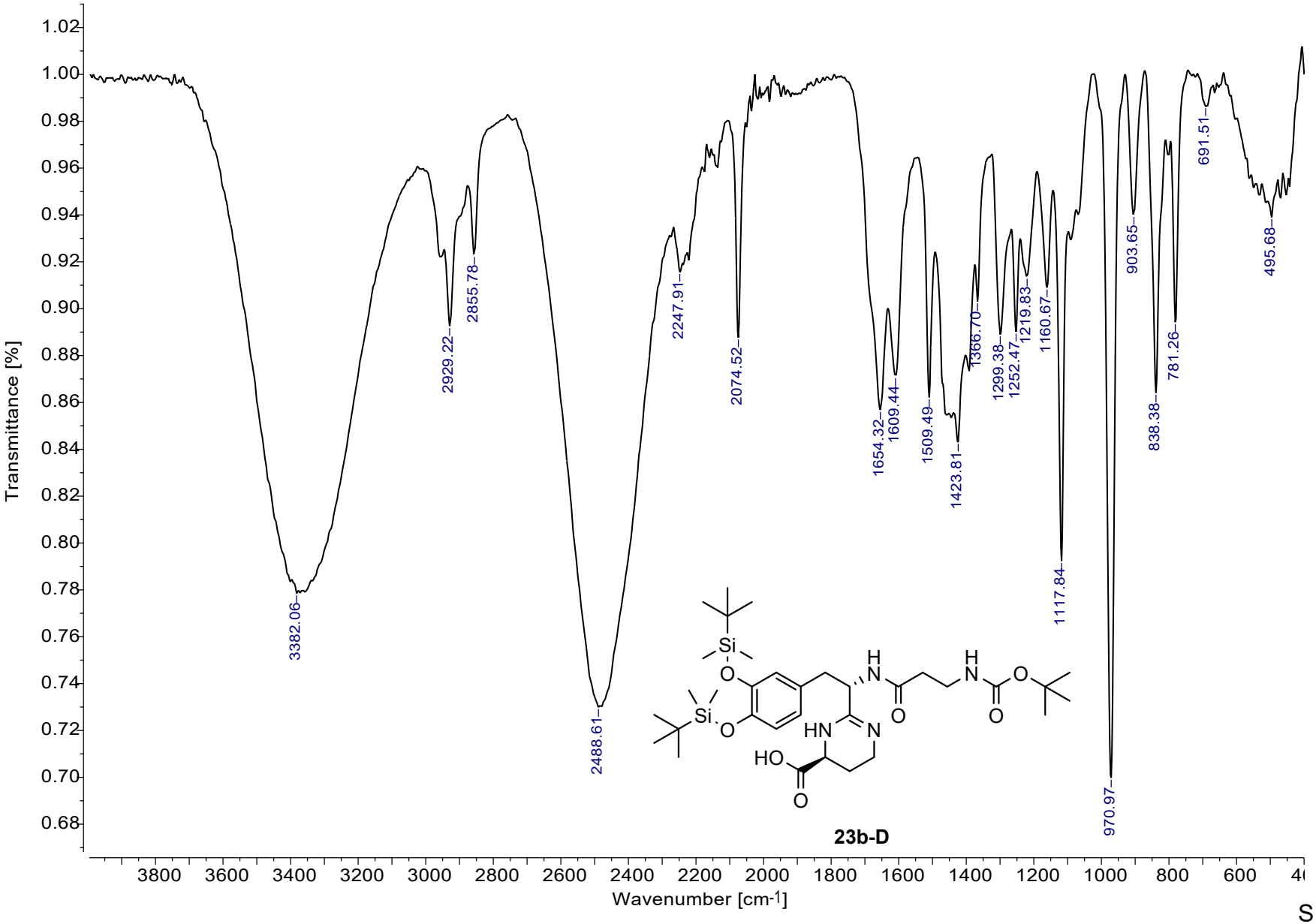
2929.24
2857.85
2374.40
2135.73
2015.38
1992.94
1962.35
1664.53
1609.45
1509.50
1472.78
1389.15
1301.43
1270.83
1252.47
1162.72
987.29
905.70
840.42
779.23
671.11
544.64
454.89
432.45
Si
O
Si
O
H
N
O
O
HN
N
HO
O
14b-D
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]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0.76
0.74
0.72
0.70
0.68
3382.06
2929.22
2855.78
2488.61
2247.91
2074.52
1654.32
1609.44
1509.49
1423.81
1366.70
1299.38
1252.47
1219.83
1160.67
1117.84
970.97
903.65
838.38
781.26
691.51
495.68
Si
O
Si
O
H
N
O
H
N
O
O
HN
N
HO
O
3800
3600
3400
3200
3000
2800
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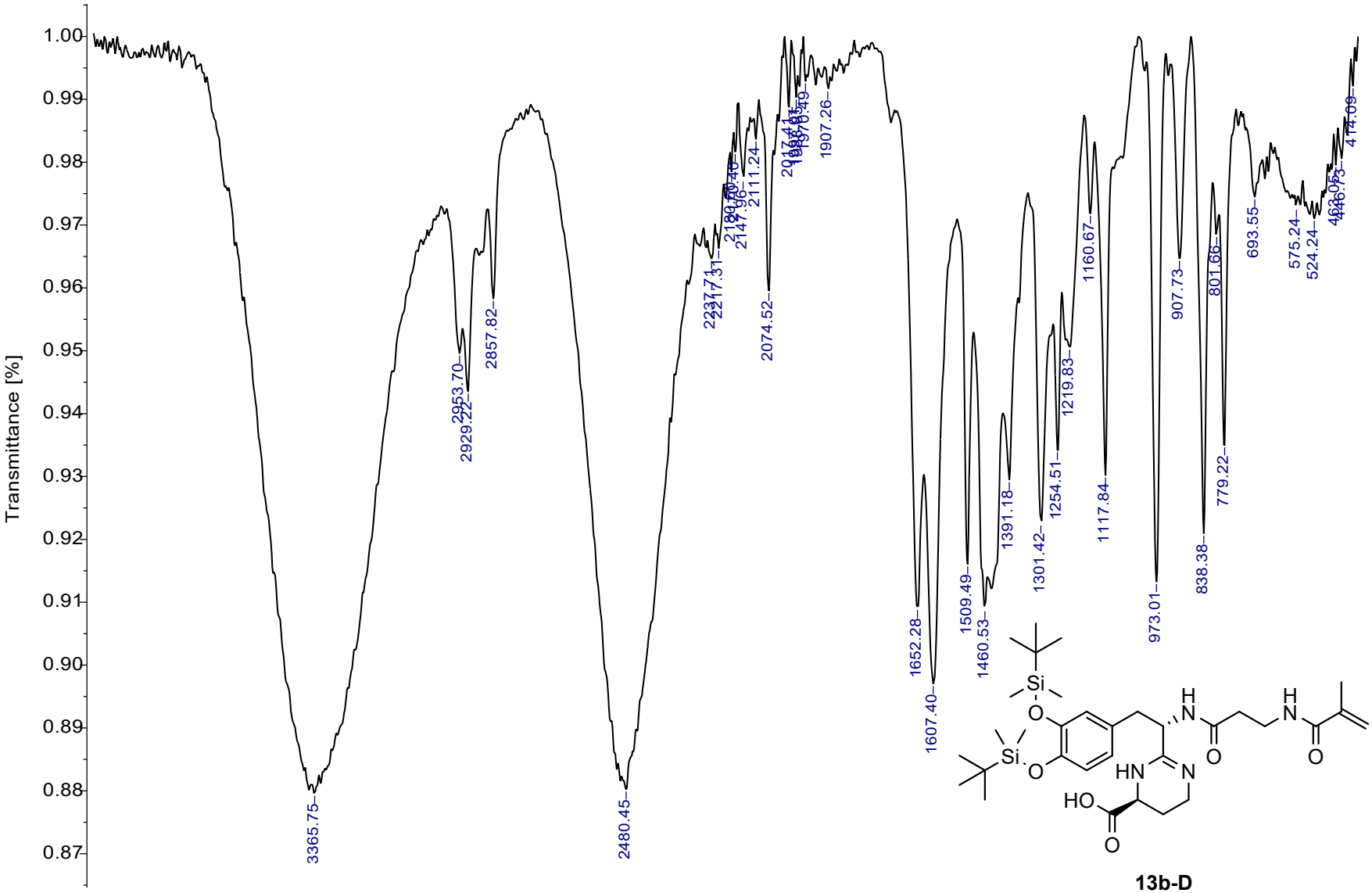
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]

23b-D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0.87
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2074.52
2017.41
1907.26
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1301.42
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1117.84
973.01
907.73
838.38
801.66
779.22
693.55
575.24
524.24
463.05
446.73
414.09
Si
O
Si
O
H
N
O
H
N
O
HN
N
HO
O
3800
3600
3400
3200
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2800
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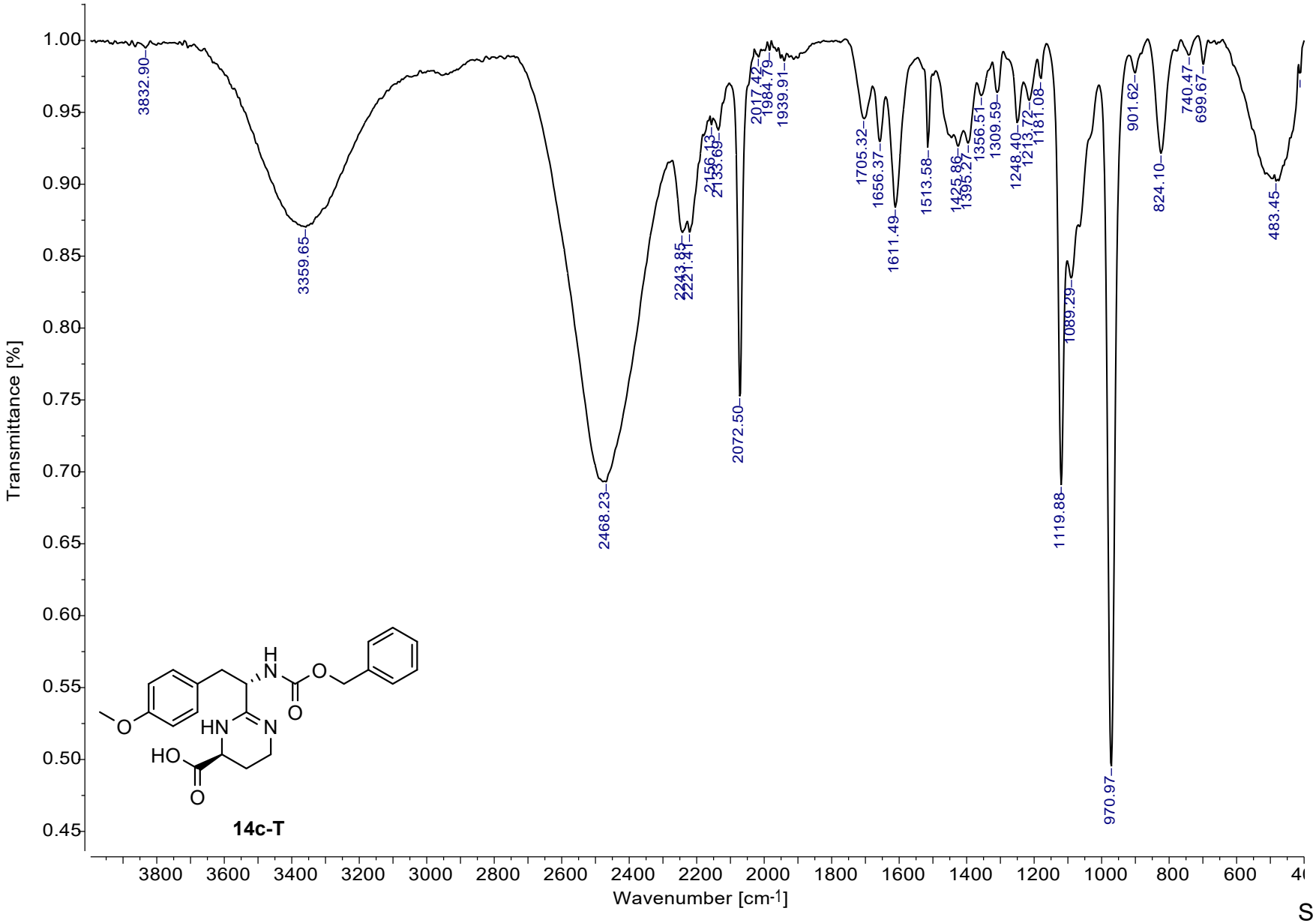
600
Wavenumber [cm-1]

13b-D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1705.32
1656.37
1611.49
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1248.40
1213.72
1181.08
1119.88
1089.29
970.97
901.62
824.10
740.47
699.67
483.45
3800
3600
3400
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2800
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2400
2200
2000
1800
1600
1400
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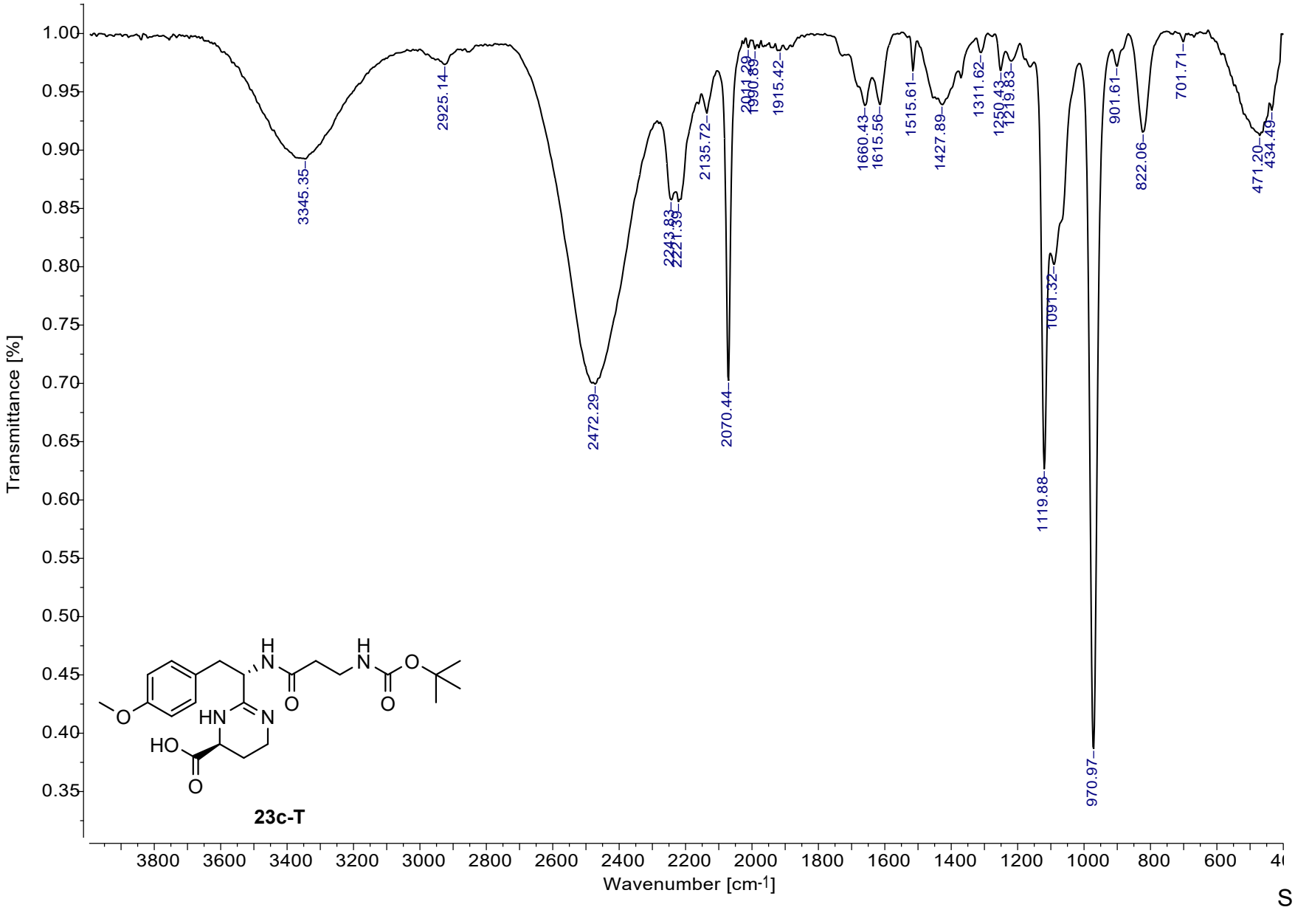
1000
800
600
Wavenumber [cm-1]
14c-T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1427.89
1311.62
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901.61
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471.20
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3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
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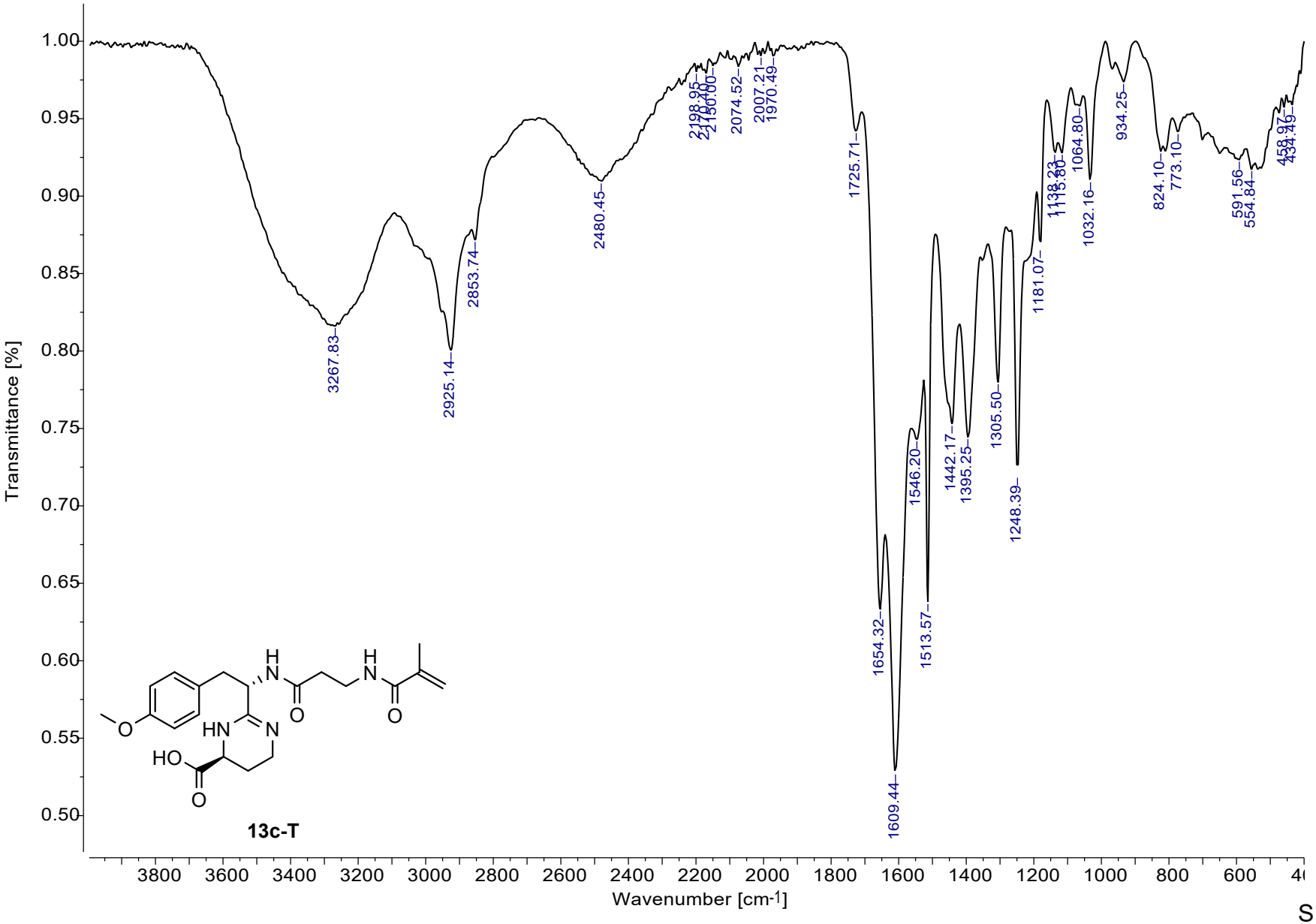
800
600
Wavenumber [cm-1]
HO
HN
N
O
H
N
O
O
O
O
23c-T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0.50
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2150.00
2074.52
2007.21
1970.49
1725.71
1654.32
1609.44
1546.20
1513.57
1442.17
1395.25
1305.50
1248.39
1181.07
1138.23
1115.80
1064.80
1032.16
934.25
824.10
773.10
591.56
554.84
458.97
434.49
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]
HO
O
HN
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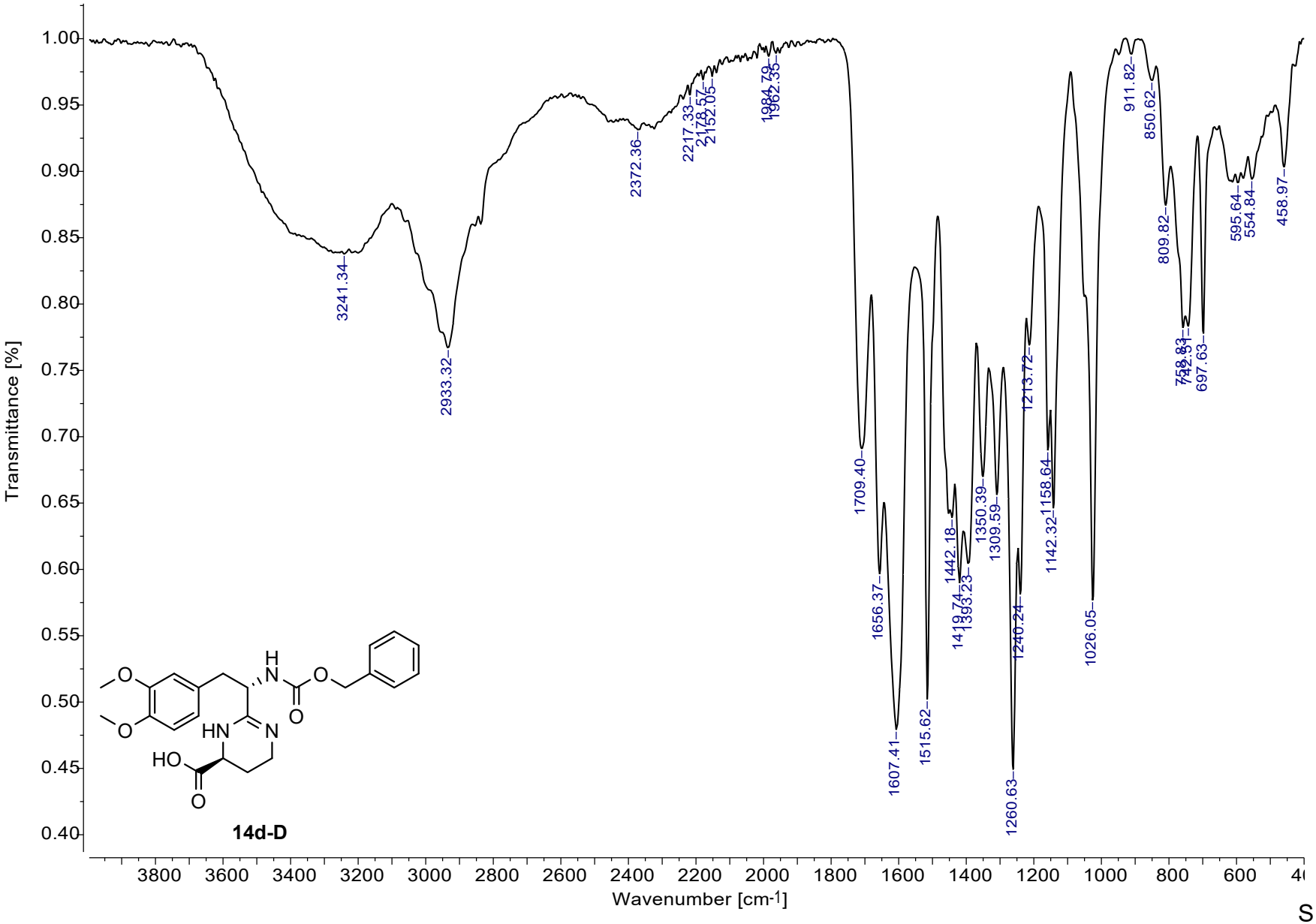
N
O
H
N
O
O
13c-T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0.45
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3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]
3241.34
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2178.57
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1984.79
1962.33
1709.40
1656.37
1607.41
1515.62
1442.18
1419.74
1393.23
1350.39
1309.59
1260.63
1240.24
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1158.64
1142.32
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911.82
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809.82
758.83
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554.84
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N
O
O
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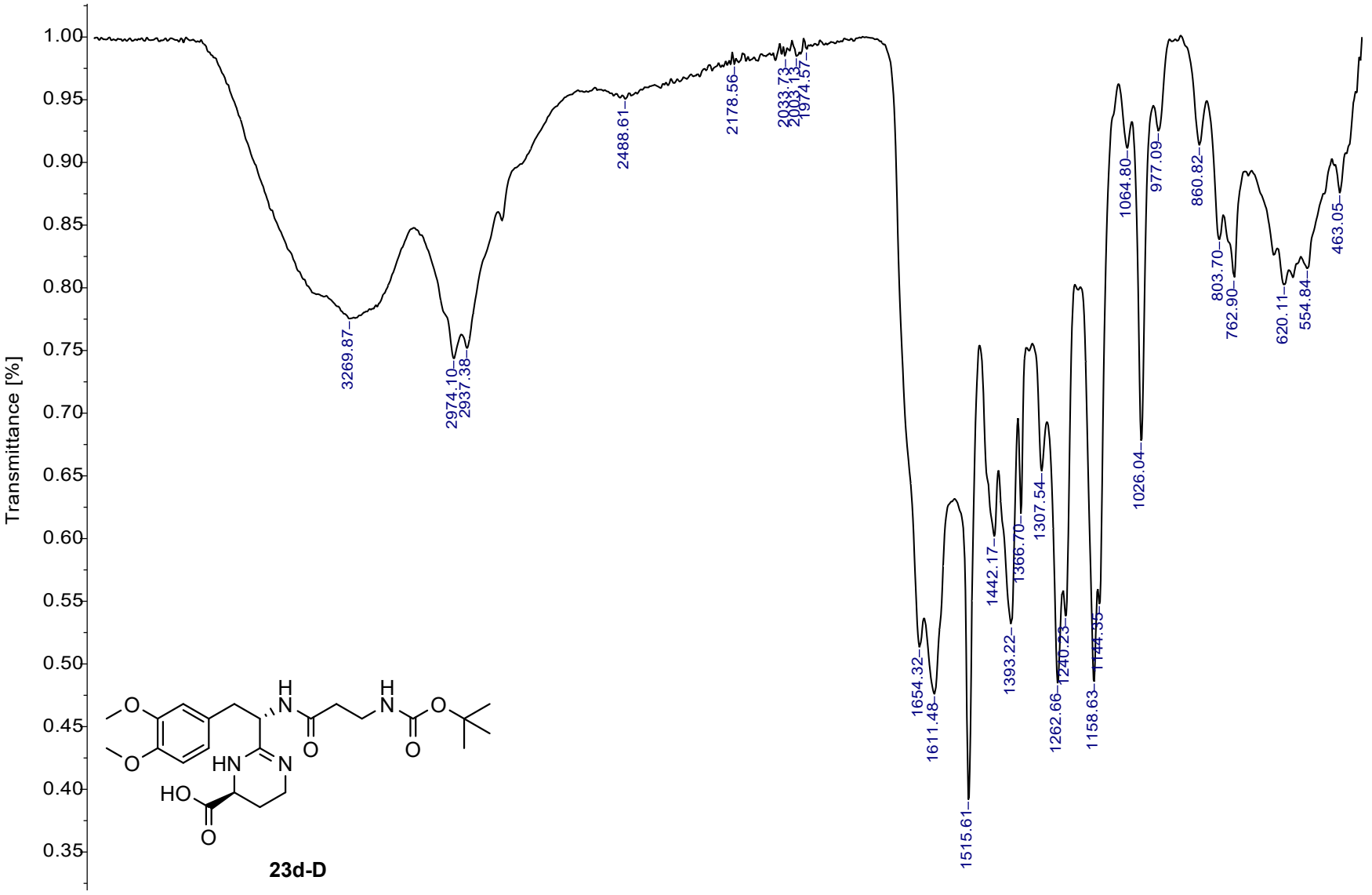
O
O
14d-D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0.60
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0.45
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0.35
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2974.10
2937.38
2488.61
2178.56
2033.73
2003.13
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1654.32
1611.48
1515.61
1442.17
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1240.23
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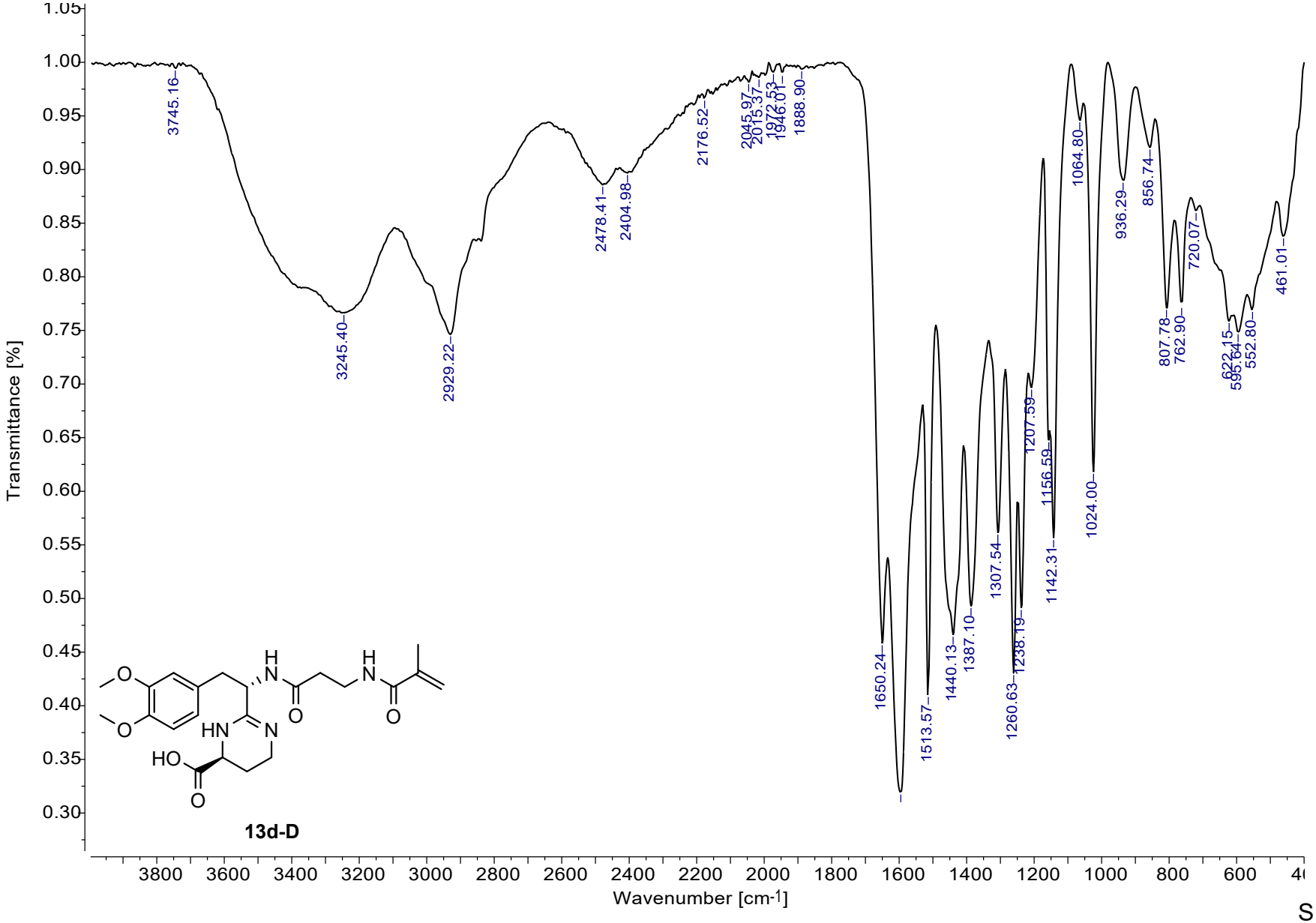
1144.35
1064.80
1026.04
977.09
860.82
803.70
762.90
620.11
554.84
463.05
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumber [cm-1]
23d-D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2015.37
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1946.01
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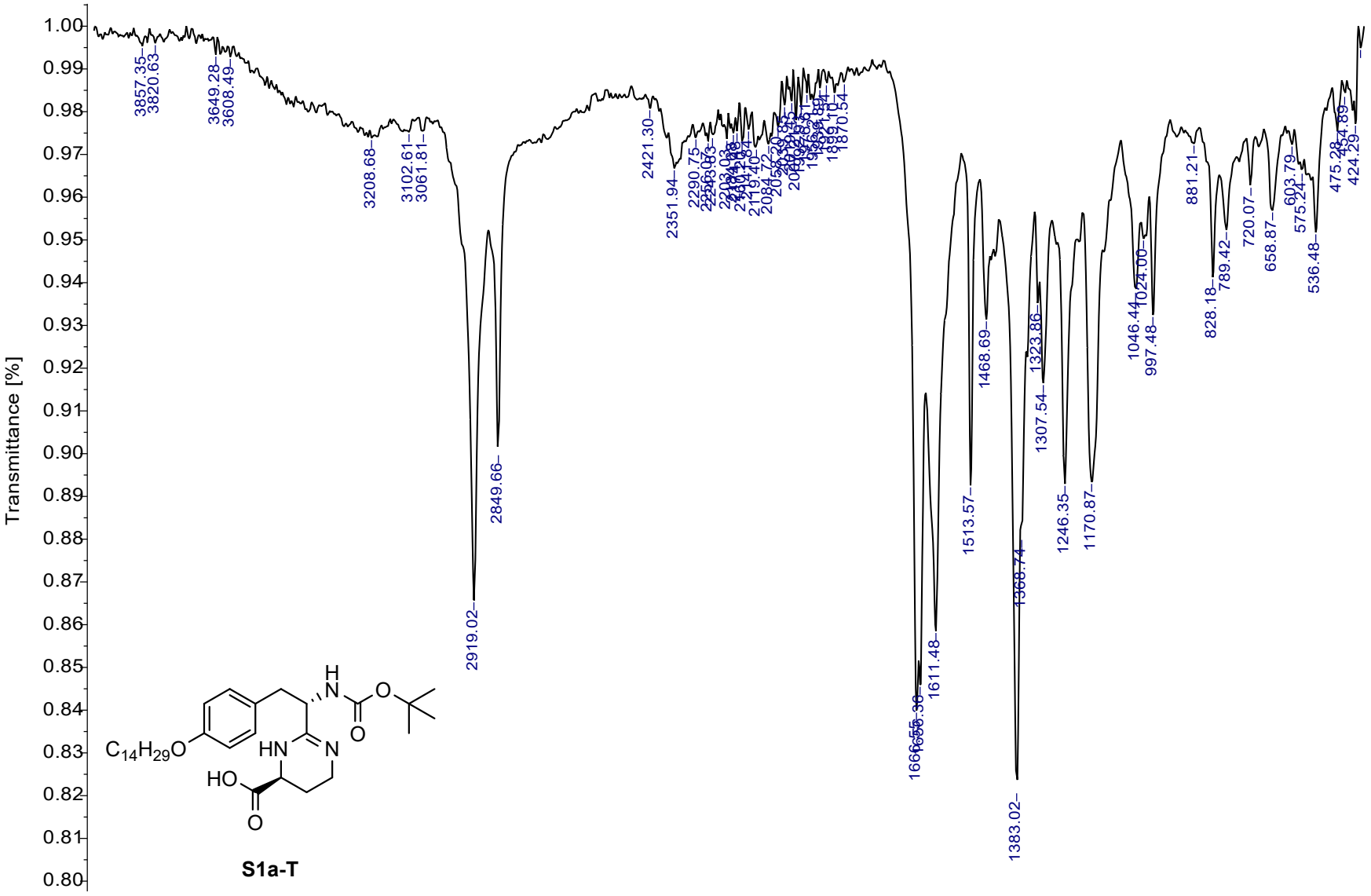
595.64
552.80
461.01
13d-D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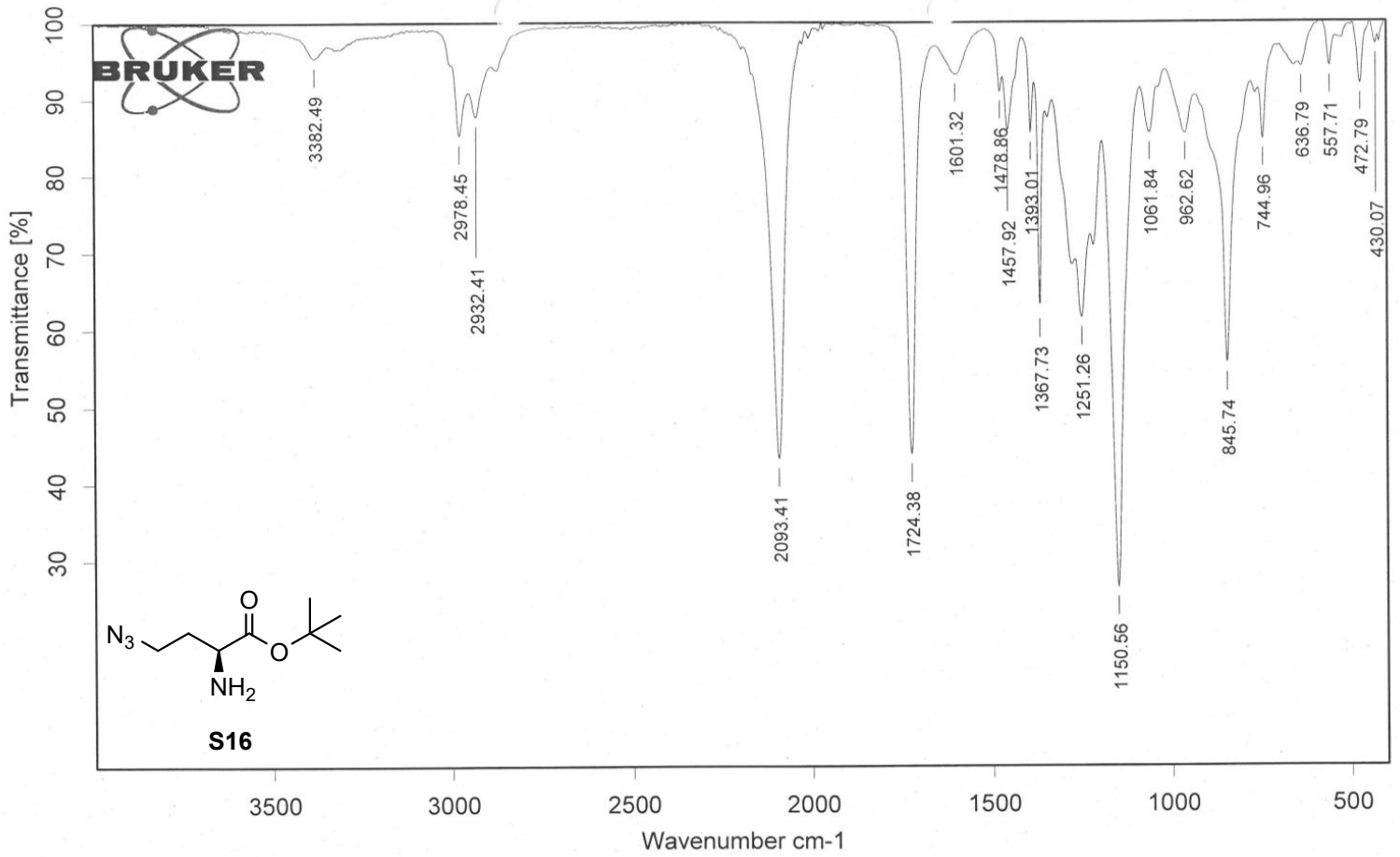
S1a-T



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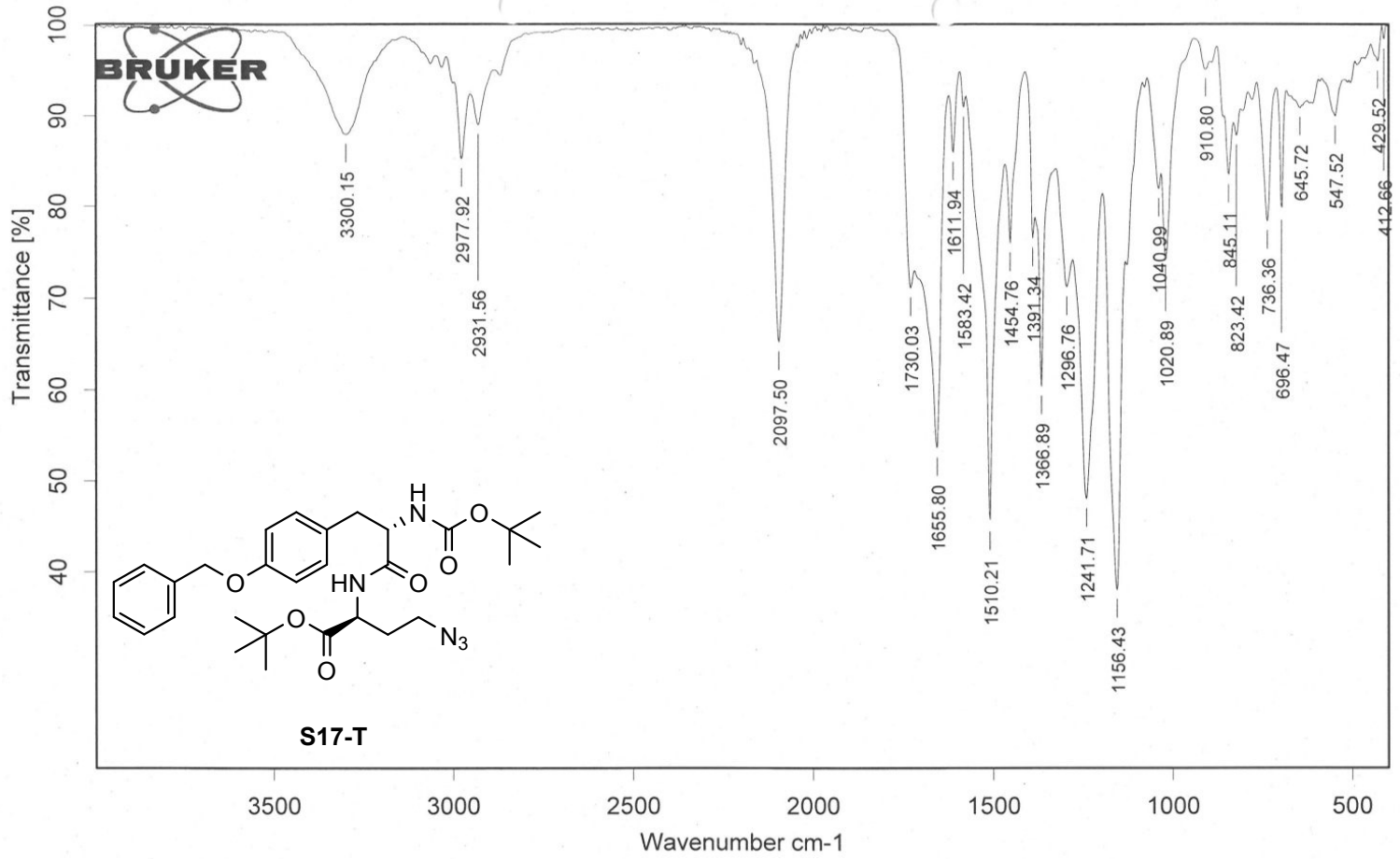
Seite 1 von 1



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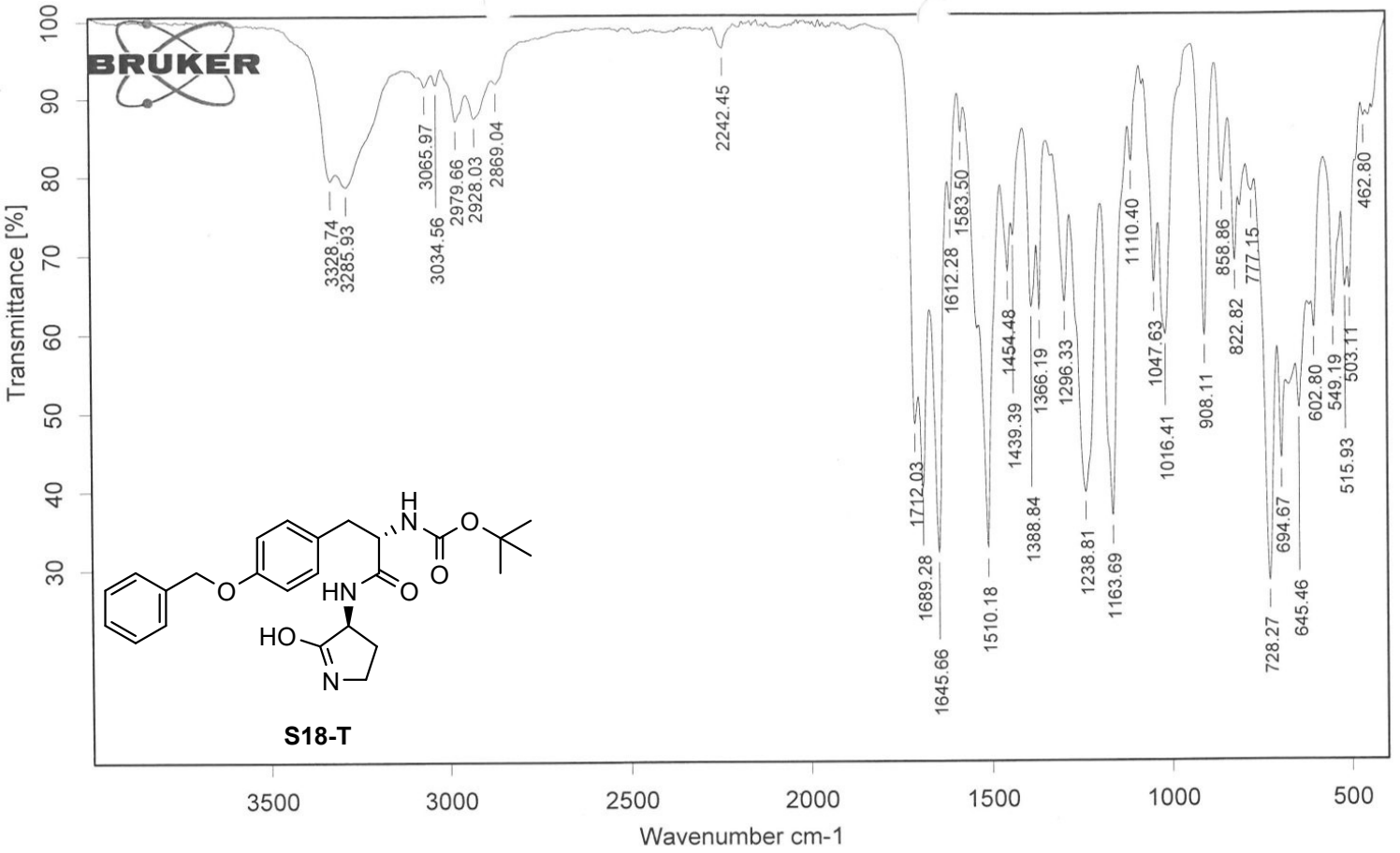
P26

Seite 1 von 1



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P36

Seite 1 von 1

12. Mass spectra

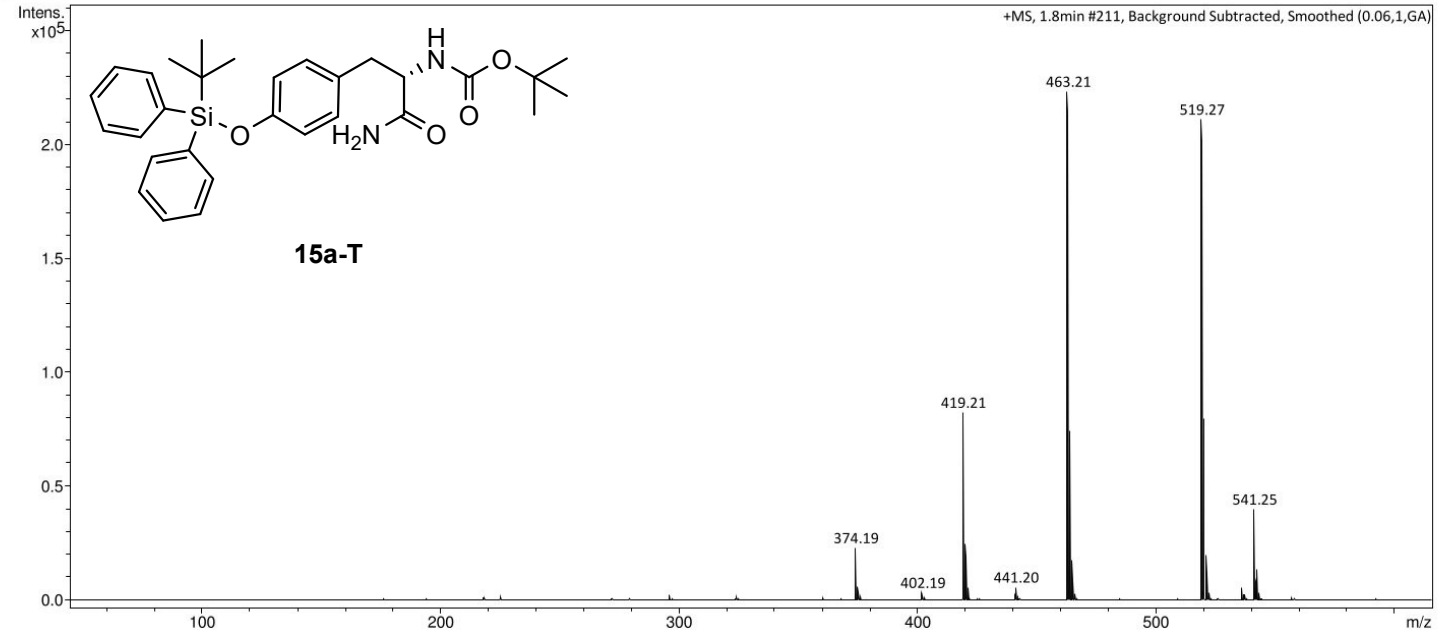
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE215-F3-Voll_1_01_26074.d			Acquisition Date	7/1/2020 2:16:44 PM
Method	tune-low-oktober-2019.m			Operator	BDAL@DE
Sample Name	Greulich-GRE215-F3-Voll			Instrument	micrOTOF-Q 228888.00043
Comment					

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



15a-T

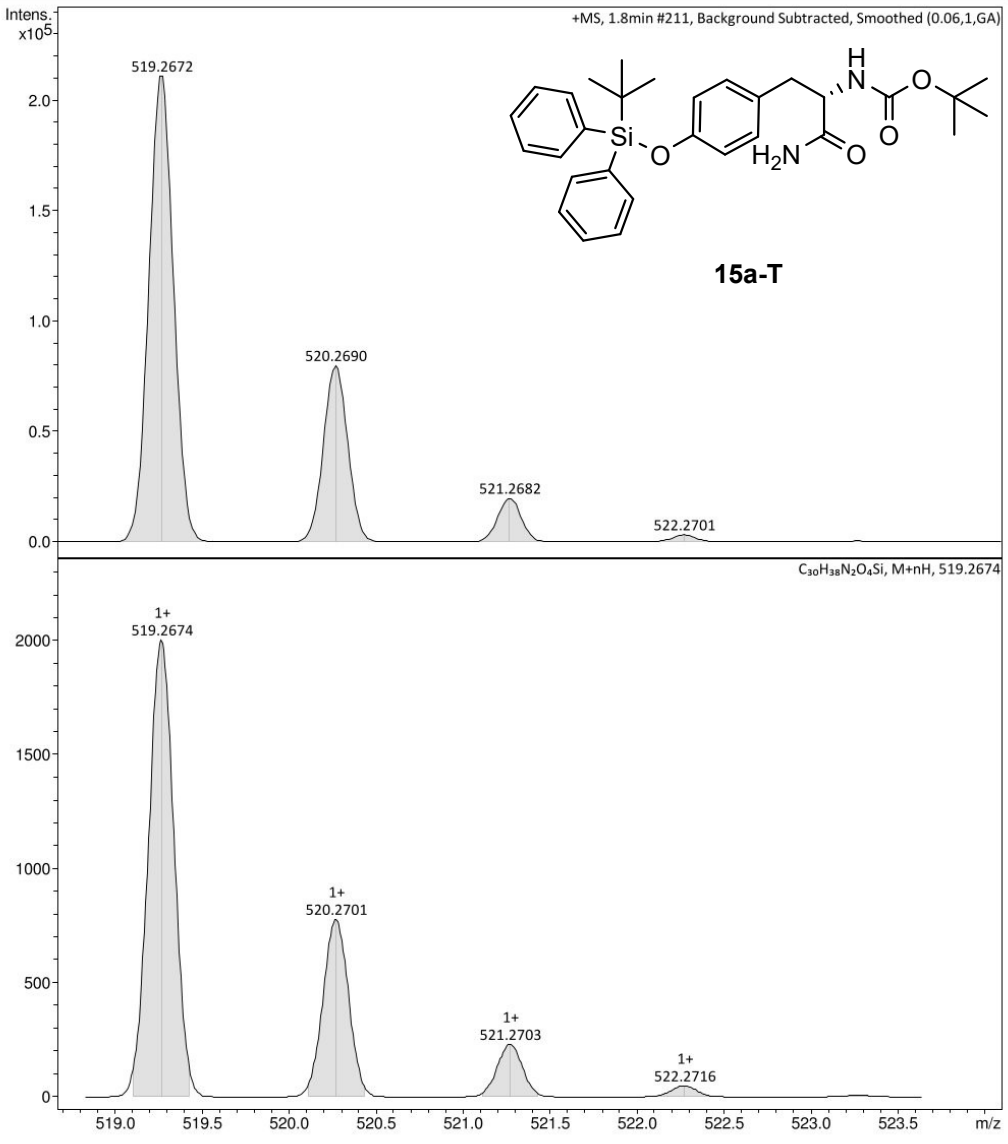
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE215-F3-Voll_1_01_26074.d	Acquisition Date	7/1/2020 2:16:44 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE215-F3-Voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.2 printed: 7/1/2020 2:26:19 PM Page 1 of 1

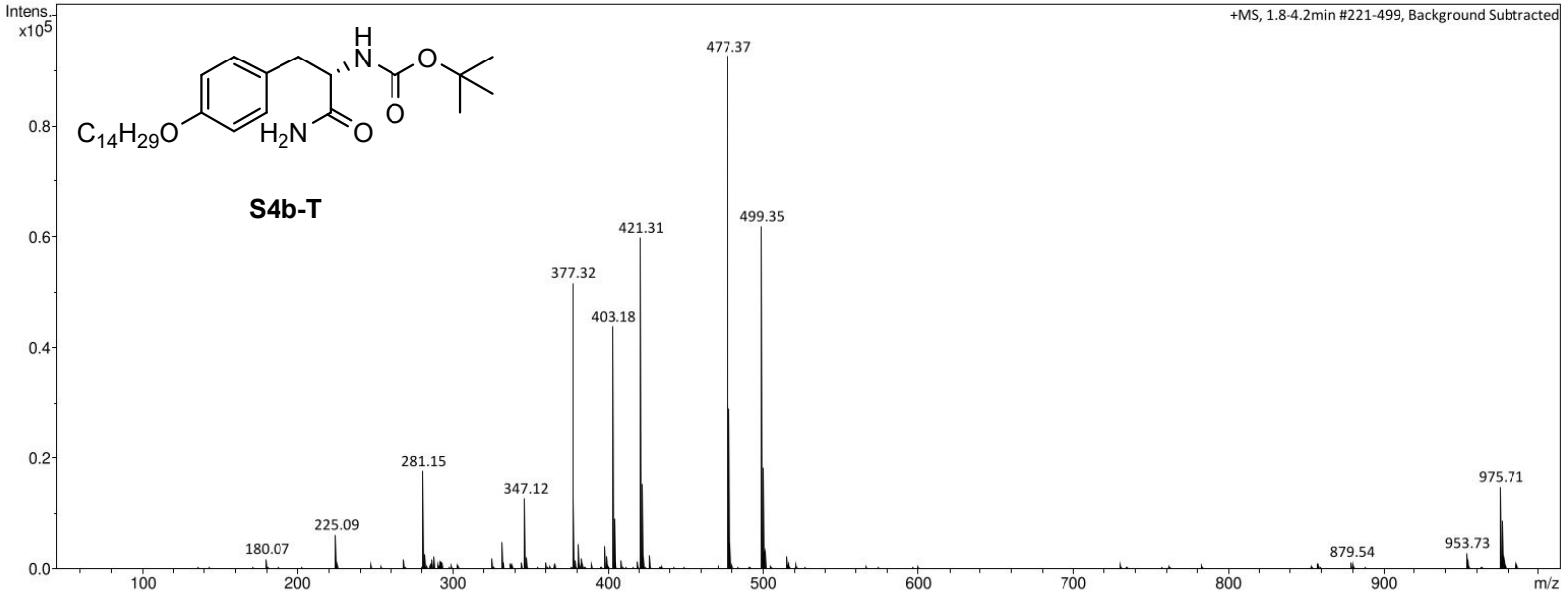
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich_GRE527-P36_voll_5_01_3115.d	Acquisition Date	7/6/2023 8:46:48 AM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich_GRE527-P36_voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.2 printed: 7/6/2023 9:16:24 AM by: BDAL@DE Page 1 of 1

Massenspektrometrie - Universität Stuttgart

Analysis Info

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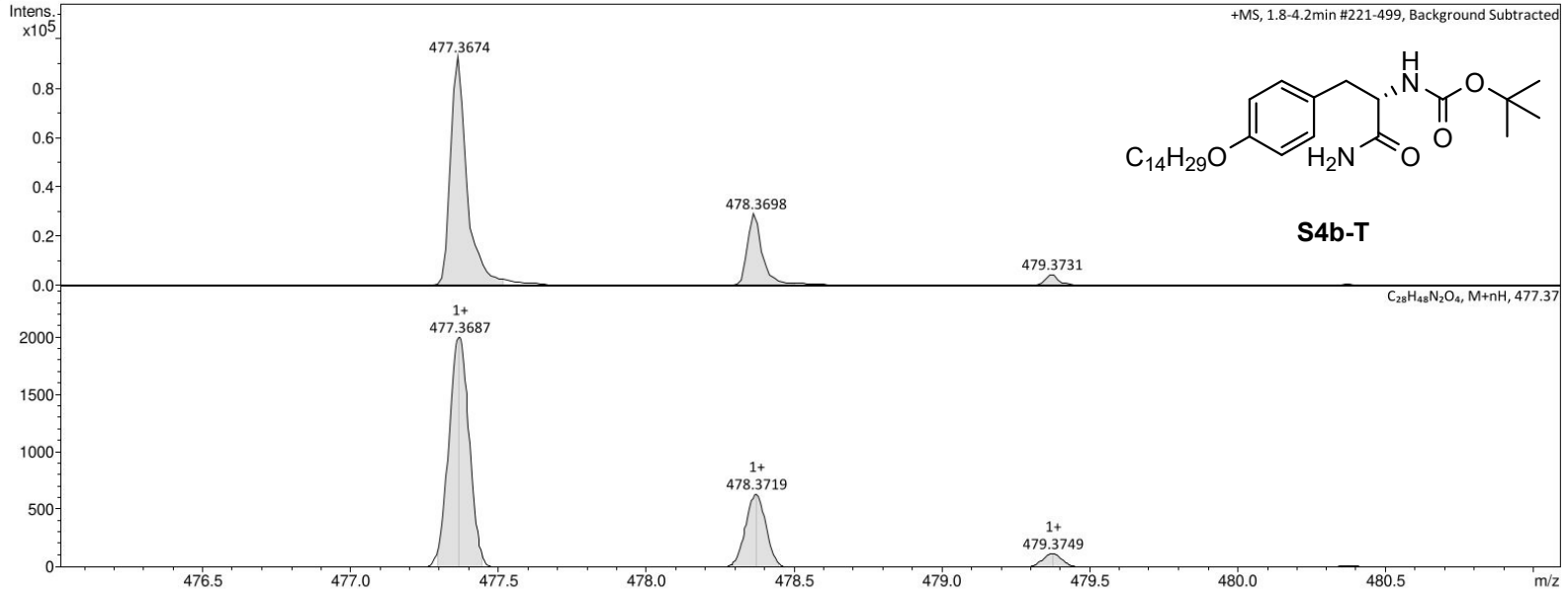
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich_GRE527-P36_voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



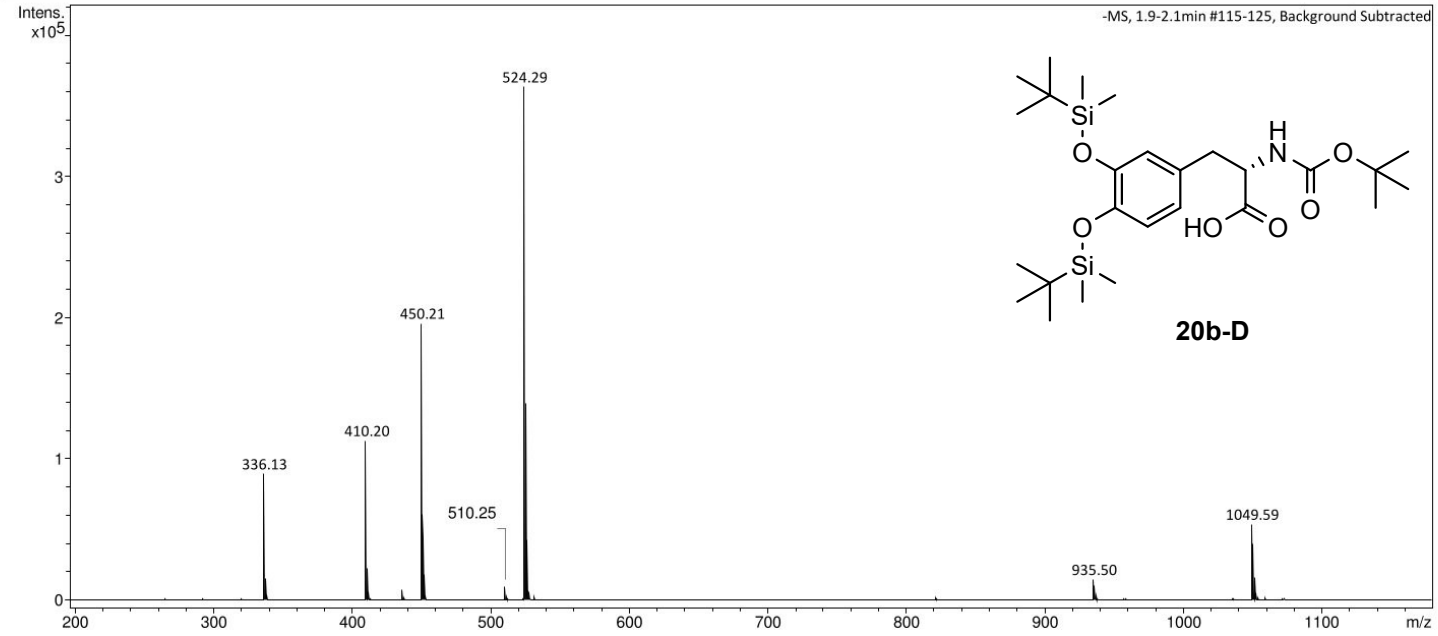
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE403-Säule-F2_11_01_37860.d	Acquisition Date	4/21/2022 4:32:04 PM
Method	tune-low-neg-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE403-Säule-F2	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	34 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.2 printed: 4/21/2022 4:56:25 PM Page 1 of 1

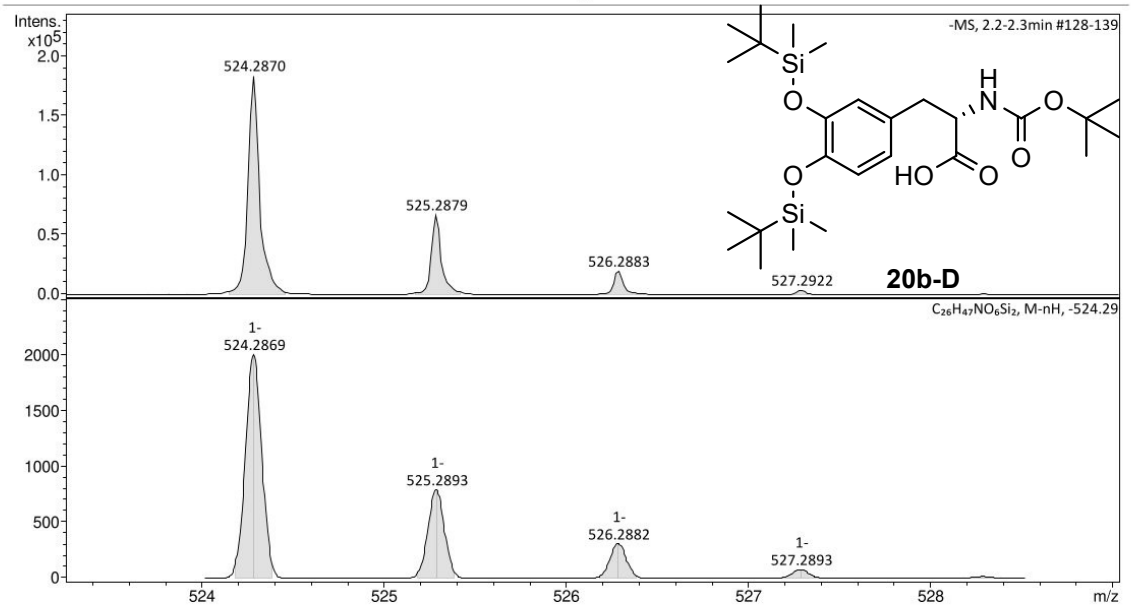
Massenspektrometrie - Universität Stuttgart

Analysis Info

		Acquisition Date	4/21/2022 4:32:04 PM
Analysis Name	C:\Data\2022\Laschat_2022\Greulich-GRE403-Säule-F2_11_01_37860.d		
Method	tune-low-neg-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE403-Säule-F2	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	34 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



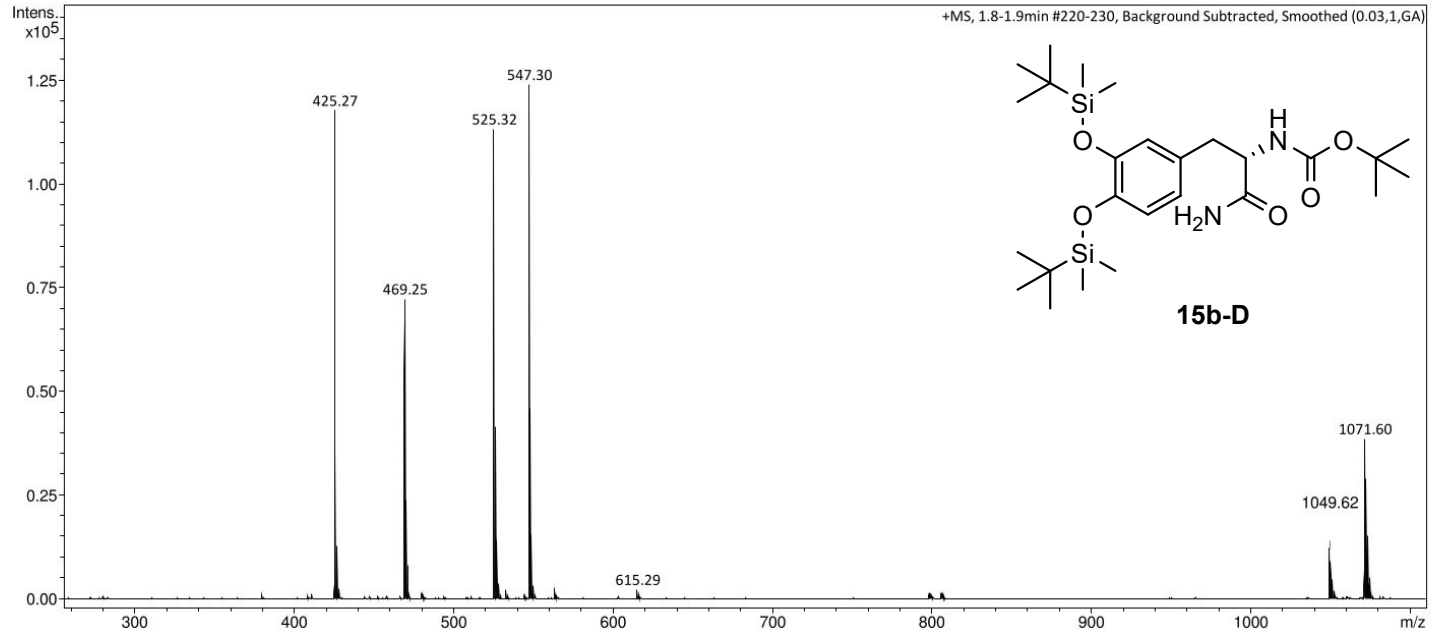
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE404F1_2_01_38335.d	Acquisition Date	5/20/2022 11:13:23 AM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE404F1	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



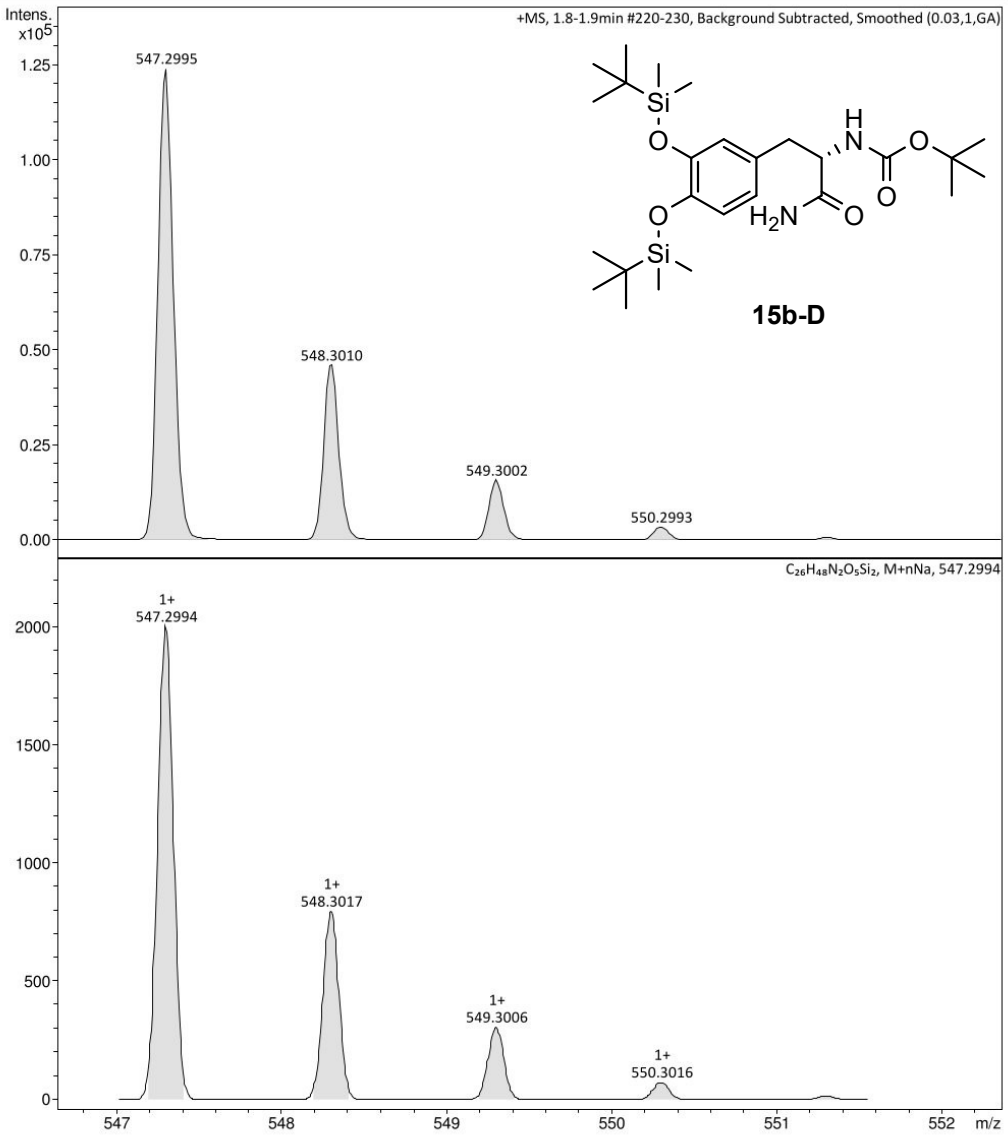
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE404F1_2_01_38335.d	Acquisition Date	5/20/2022 11:13:23 AM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE404F1	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



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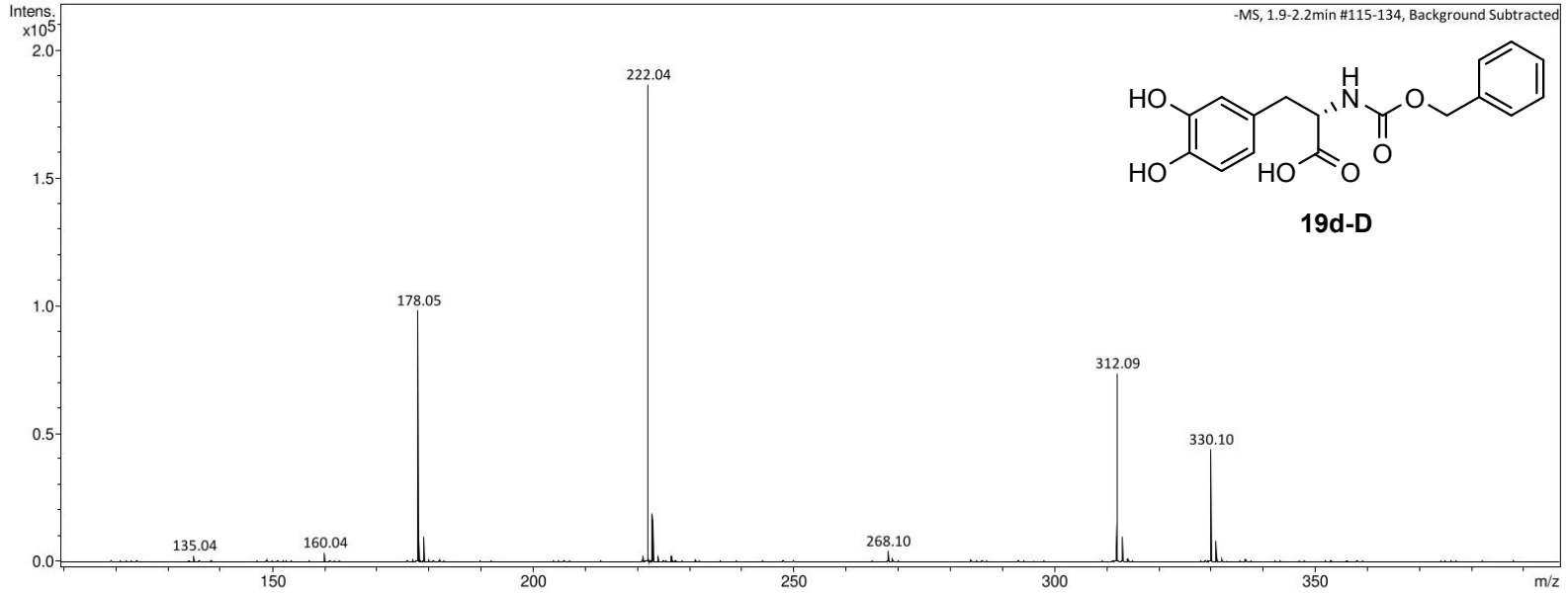
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE483-P52_9_01_771.d	Acquisition Date	2/10/2023 1:58:46 PM
Method	tune-low-neg-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE483-P52	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	34 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



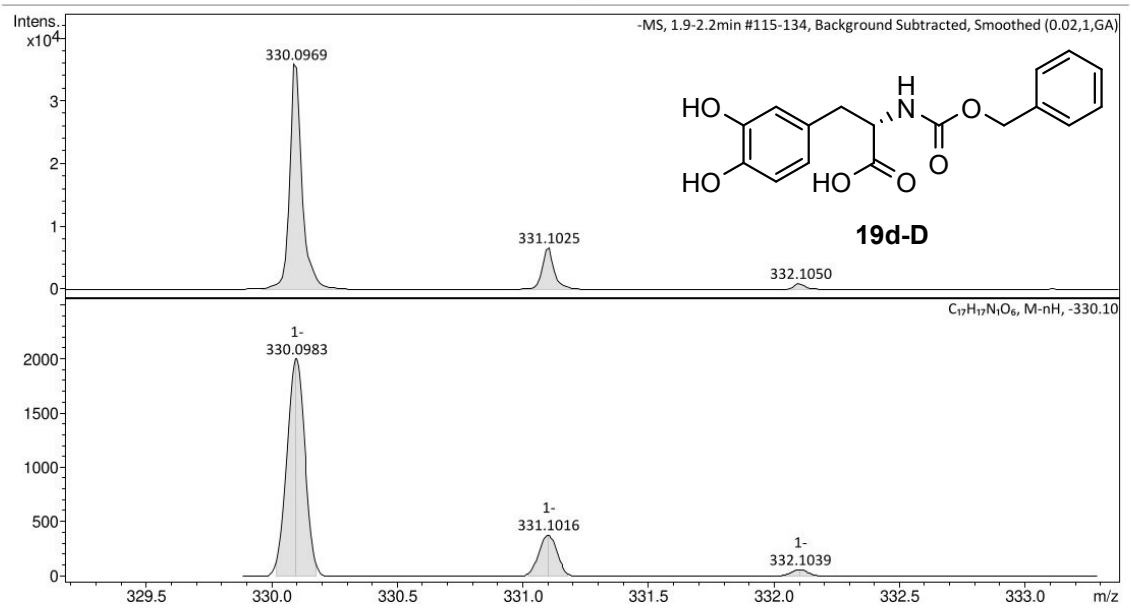
Massenspektrometrie - Universität Stuttgart

Analysis Info

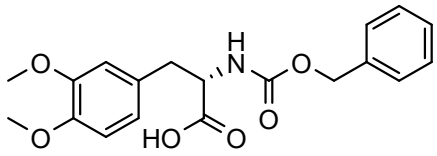
		Acquisition Date	2/10/2023 1:58:46 PM
Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE483-P52_9_01_771.d		
Method	tune-low-neg-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE483-P52	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

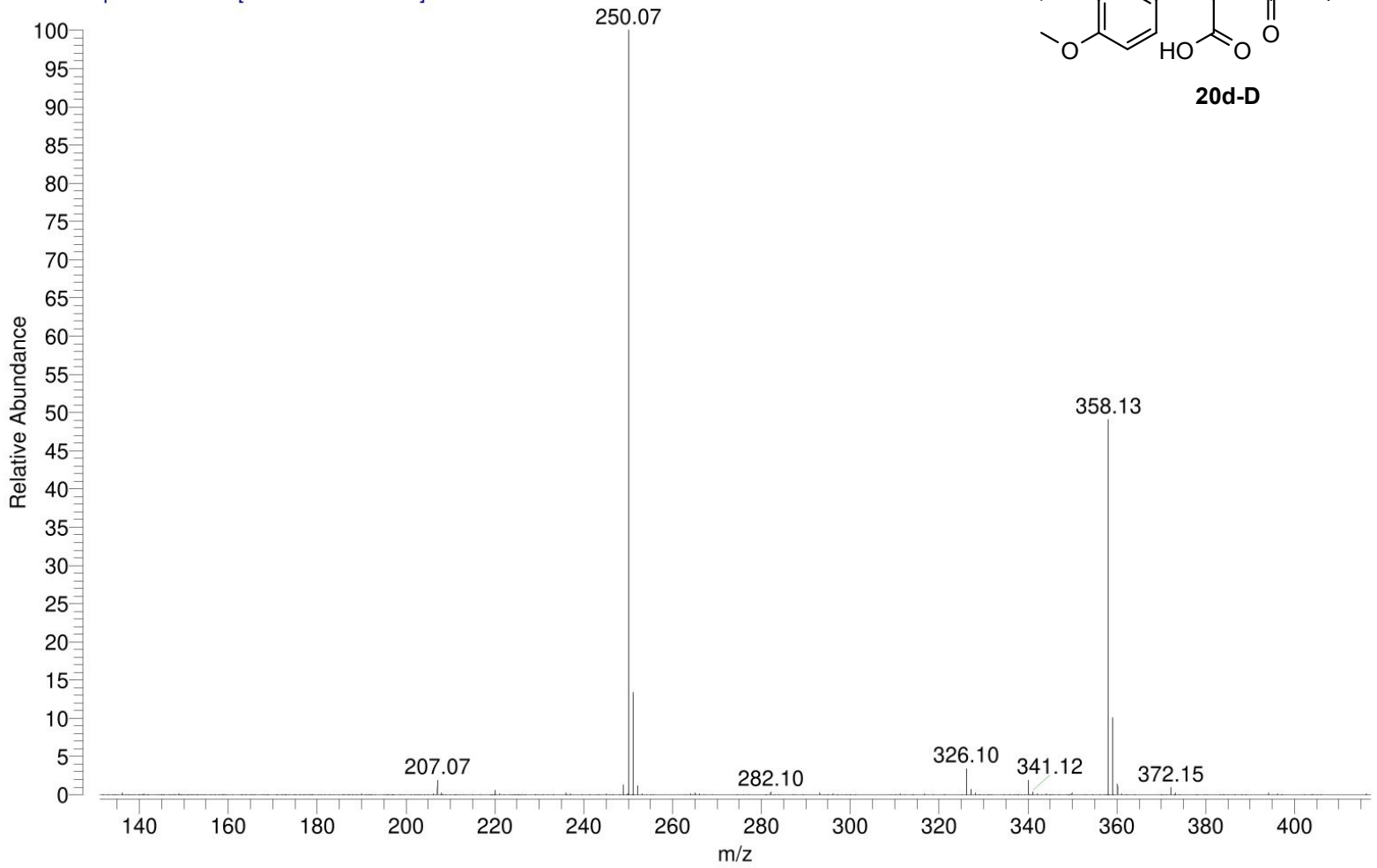
Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	34 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



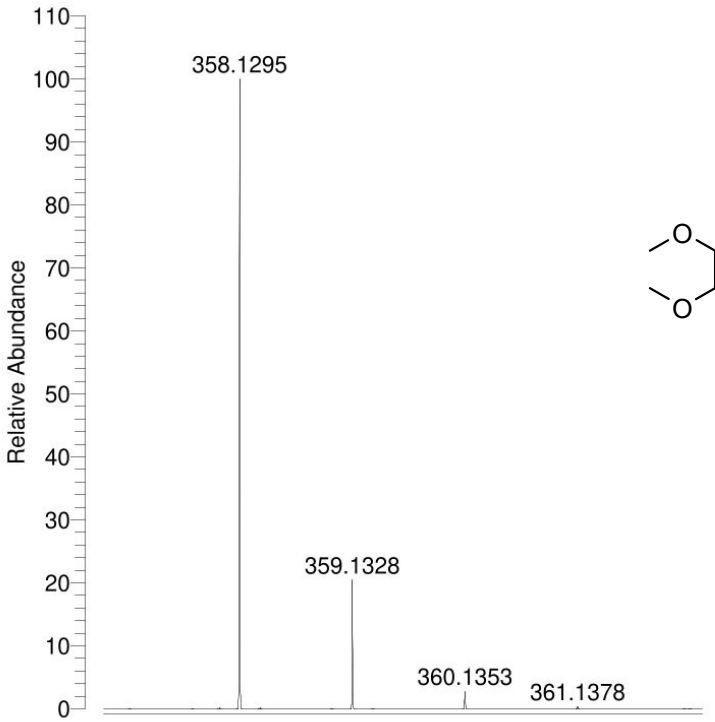
D:\2024\...\Greulich-GRE-489-P53_98 01/12/24 10:27:41
ESI negativ am Exactive Plus GRE-489-P53
Greulich-GRE-489-P53_98 #50-72 RT: 0.22-0.32 AV: 23 SB: 64 0.10-0.19 , 0.40-0.59 NL: 9.43E7
T: FTMS - p ESI Full ms [50.0000-750.0000]



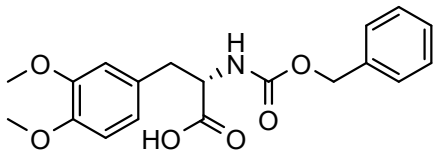
20d-D



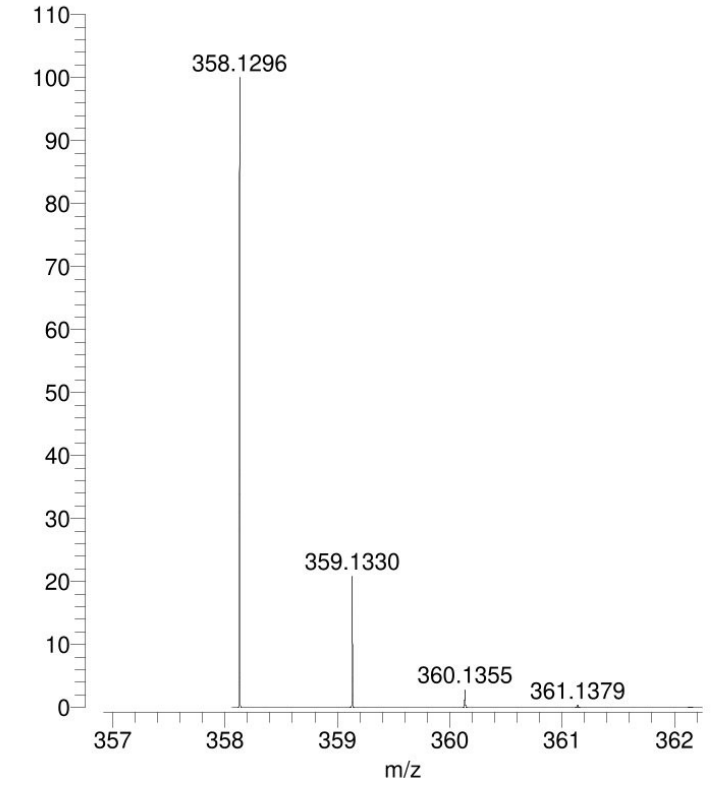
D:\2024\...\Greulich-GRE-489-P53_98 01/12/24 10:27:41
ESI negativ am Exactive Plus GRE-489-P53



NL:
4.63E7
Greulich-GRE-489-P53_98#50-72 RT: 0.22-0.32 AV: 23 SB: 64 0.10-0.19 , 0.40-0.59 T: FTMS - p ESI Full ms [50.0000-750.0000]



20d-D



NL:
1.87E4
$C_{19}H_{20}N_1O_6$:
$C_{19}H_{20}N_1O_6$
p (gss, s /p:40) Chrg -1
R: 70000 Res .Pwr . @FWHM

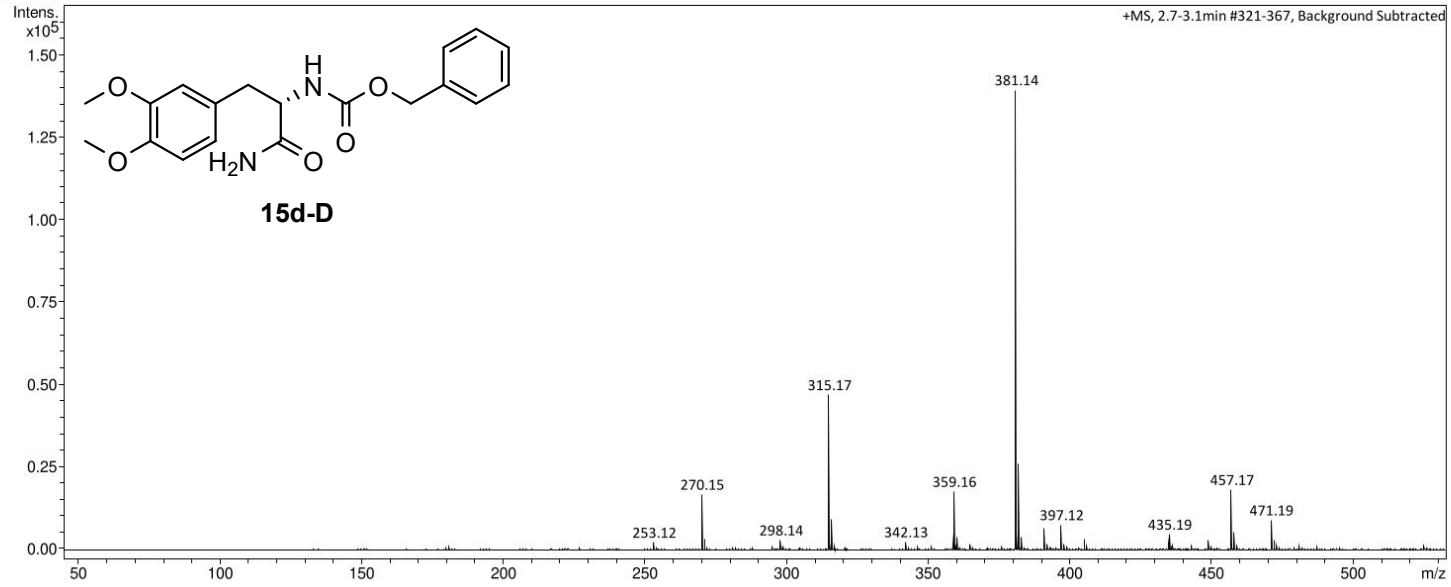
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE492-P55Voll_1_01_1056.d	Acquisition Date	2/28/2023 4:01:10 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE492-P55 Voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



15d-D

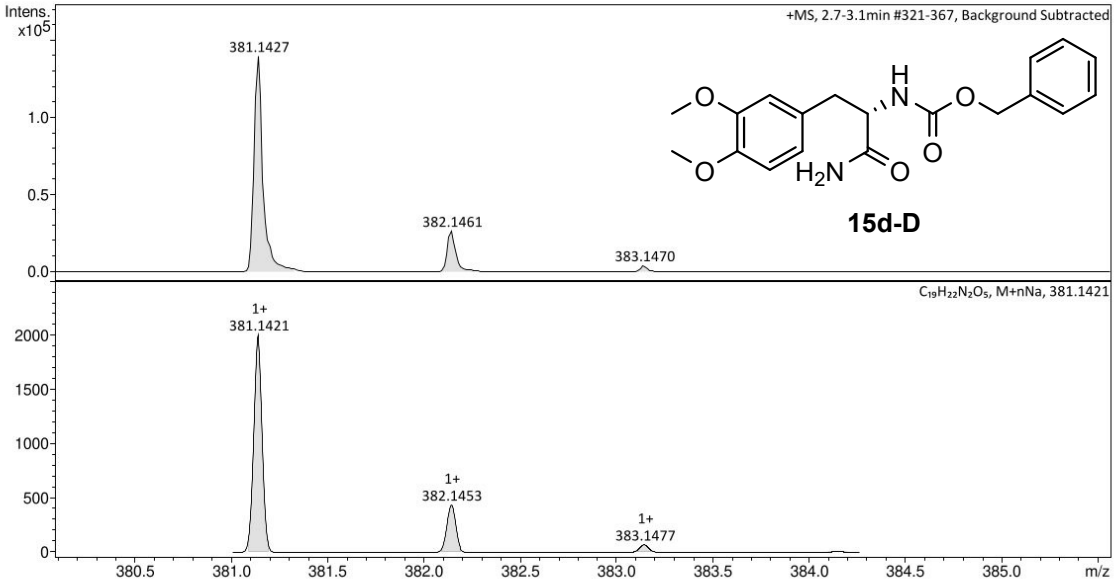
Massenspektrometrie - Universität Stuttgart

Analysis Info

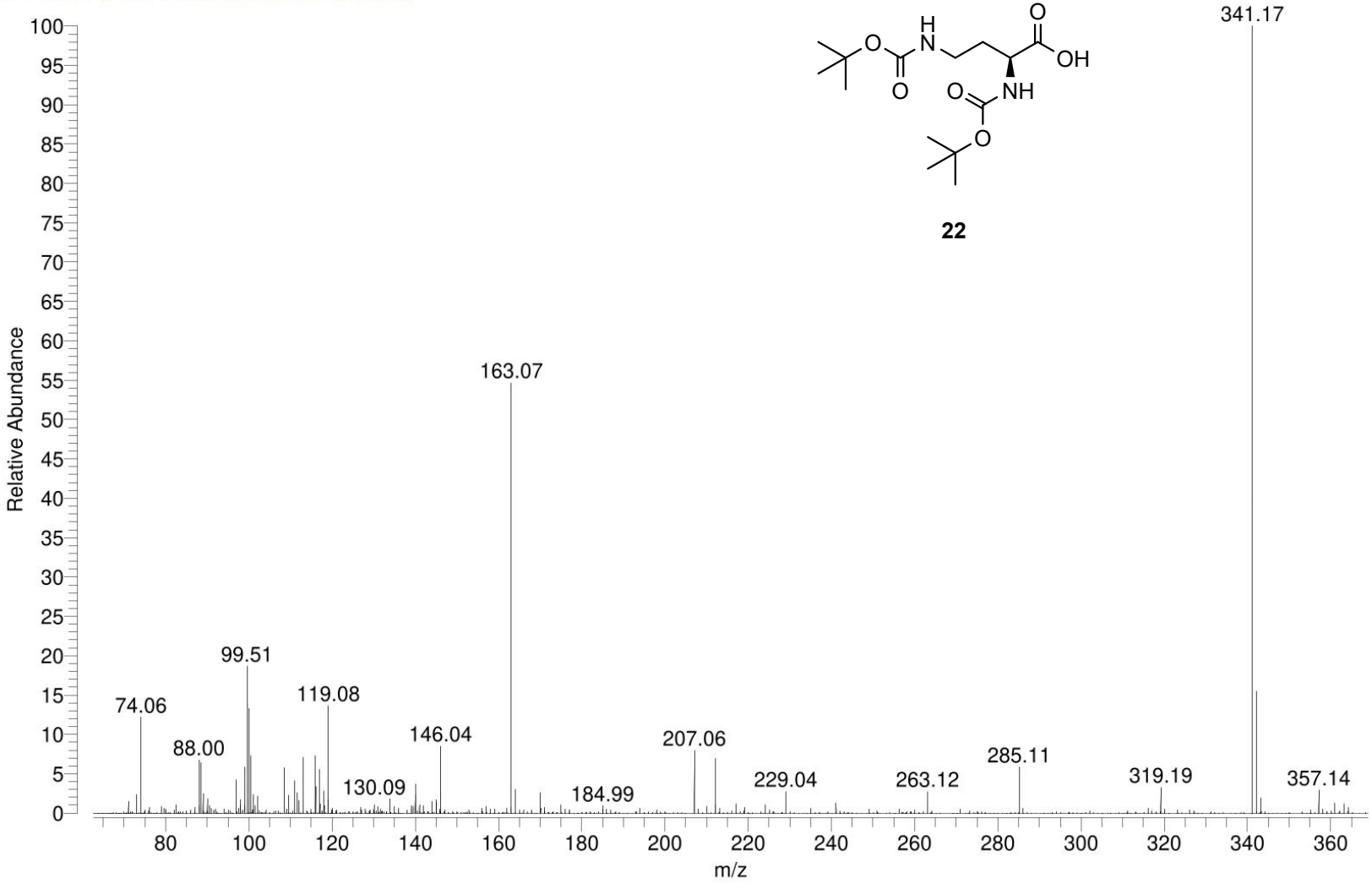
Acquisition Date	2/28/2023 4:01:10 PM		
Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE492-P55Voll_1_01_1056.d		
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE492-P55 Voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

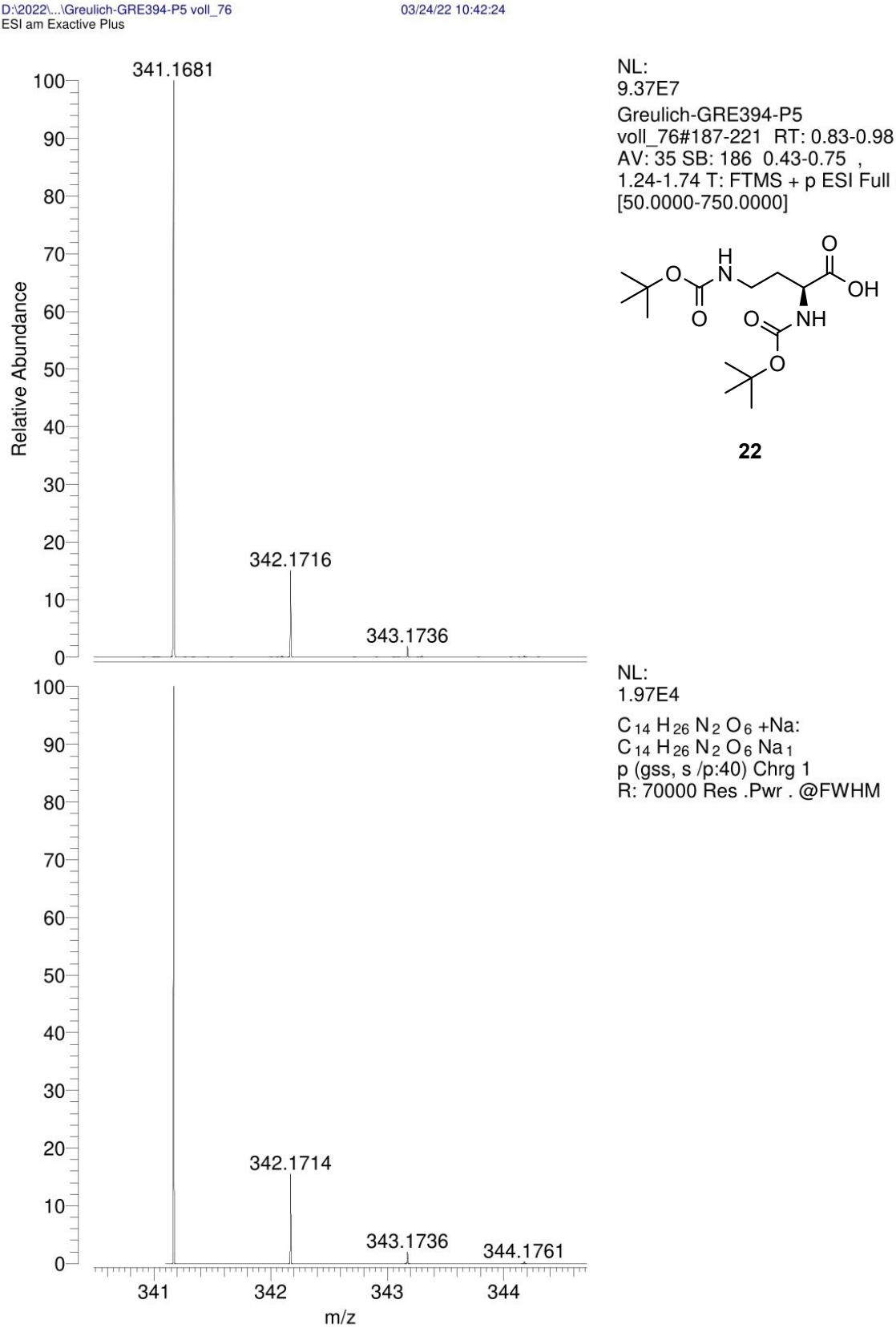
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



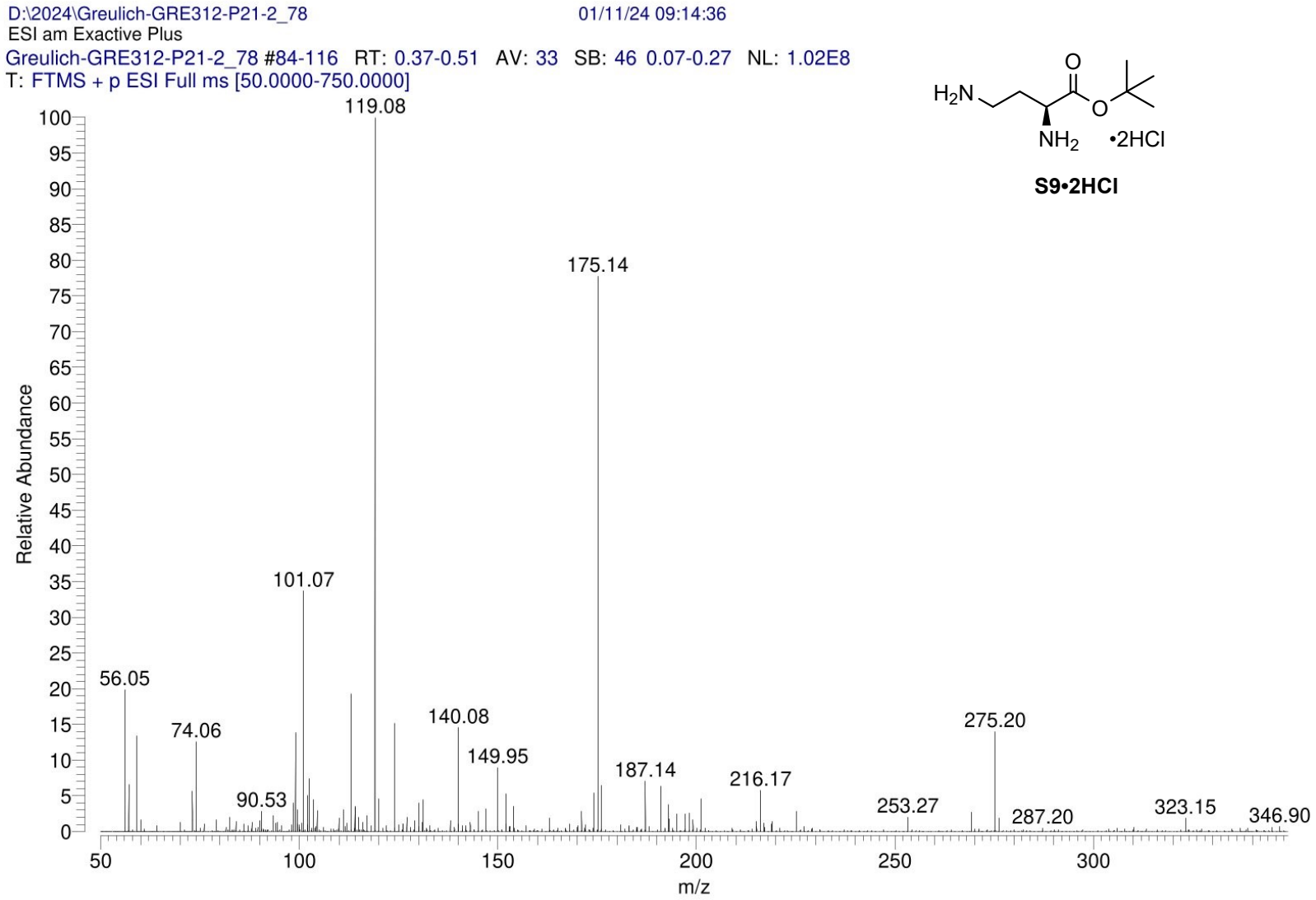
D:\2022\...\Greulich-GRE394-P5 voll_76 03/24/22 10:42:24
ESI am Exactive Plus
Greulich-GRE394-P5 voll_76 #197-209 RT: 0.87-0.93 AV: 13 SB: 10 0.49-0.53 NL: 1.24E8
T: FTMS + p ESI Full ms [50.0000-750.0000]



22


D:\2022\...\Greulich-GRE394-P5 voll_76
03/24/22 10:42:24
ESI am Exactive Plus
341.1681
342.1716
343.1736
Relative Abundance
NL:
9.37E7
Greulich-GRE394-P5
voll_76#187-221 RT: 0.83-0.98
AV: 35 SB: 186 0.43-0.75 ,
1.24-1.74 T: FTMS + p ESI Full ms
[50.0000-750.0000]
NL:
1.97E4
C14 H26 N2 O6 +Na:
C14 H26 N2 O6 Na1
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM
342.1714
343.1736
344.1761
m/z

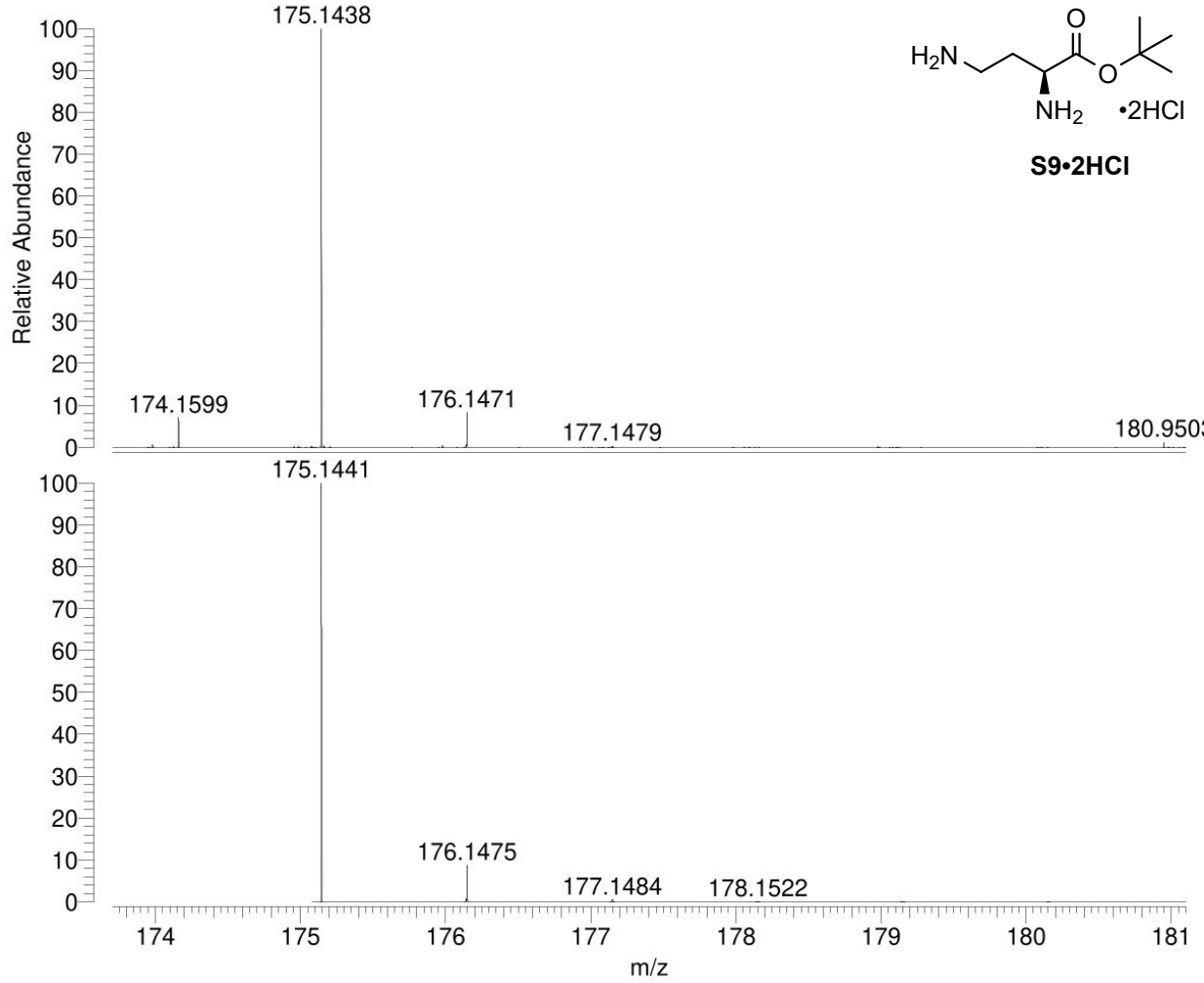
22


D:\2024\Greulich-GRE312-P21-2_78
01/11/24 09:14:36
ESI am Exactive Plus
Greulich-GRE312-P21-2_78 #84-116 RT: 0.37-0.51 AV: 33 SB: 46 0.07-0.27 NL: 1.02E8
T: FTMS + p ESI Full ms [50.0000-750.0000]
119.08
175.14
101.07
56.05
74.06
140.08
149.95
90.53
187.14
216.17
253.27
275.20
287.20
323.15
346.90
Relative Abundance
m/z
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
50
100
150
200
250
300

O
H2N
O
NH2
•2HCl

S9•2HCl

D:\2024\Greulich-GRE312-P21-2_78 01/11/24 09:14:36
ESI am Exactive Plus



S9•2HCl

NL:
7.90E7
Greulich-GRE312-P21-2_78#84-116 RT: 0.37-0.51
AV: 33 SB: 46 0.07-0.27 T:
FTMS + p ESI Full ms
[50.0000-750.0000]

NL:
2.12E4
$C_8H_{18}N_2O_2$ +H:
$C_8H_{19}N_2O_2$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

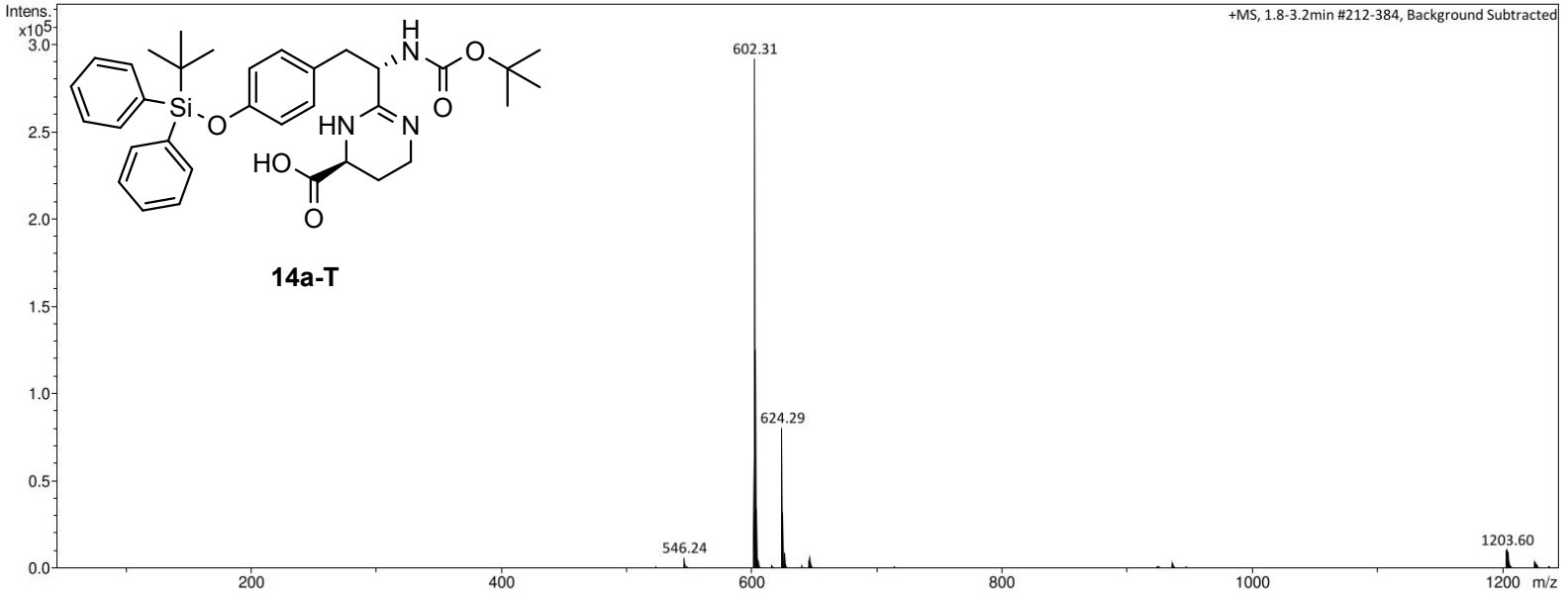
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE528-P11a_13_01_3338.d	Acquisition Date	7/18/2023 2:29:46 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE528-P11a	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



14a-T

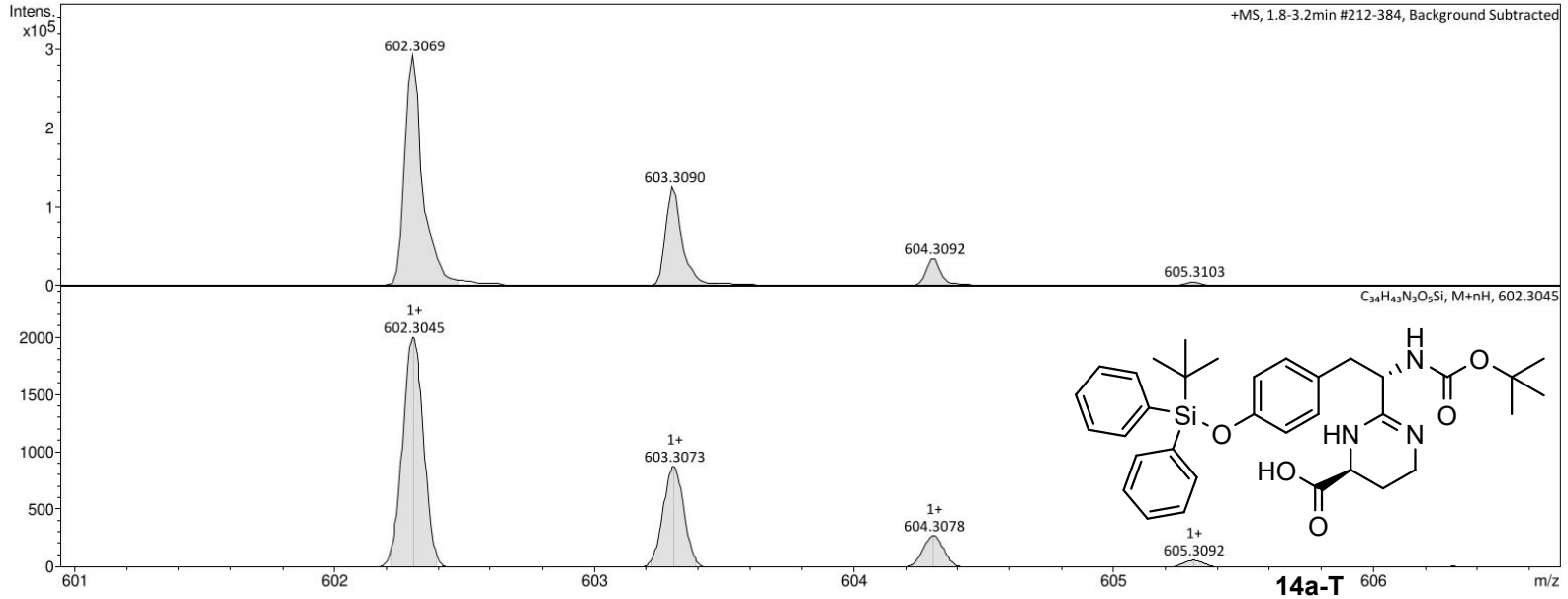
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE528-P11a_13_01_3338.d	Acquisition Date	7/18/2023 2:29:46 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE528-P11a	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



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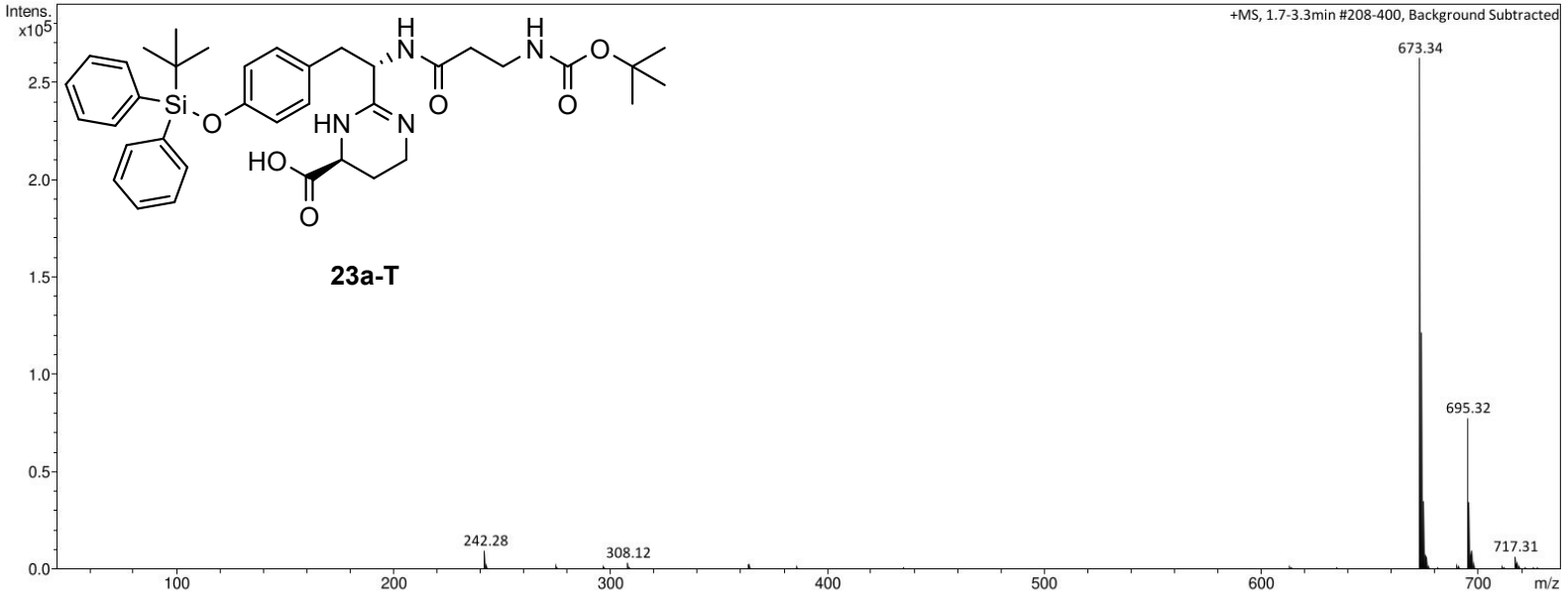
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE519-P61avoll_14_01_2556.d	Acquisition Date	6/12/2023 12:22:28 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE519-P61avoll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



23a-T

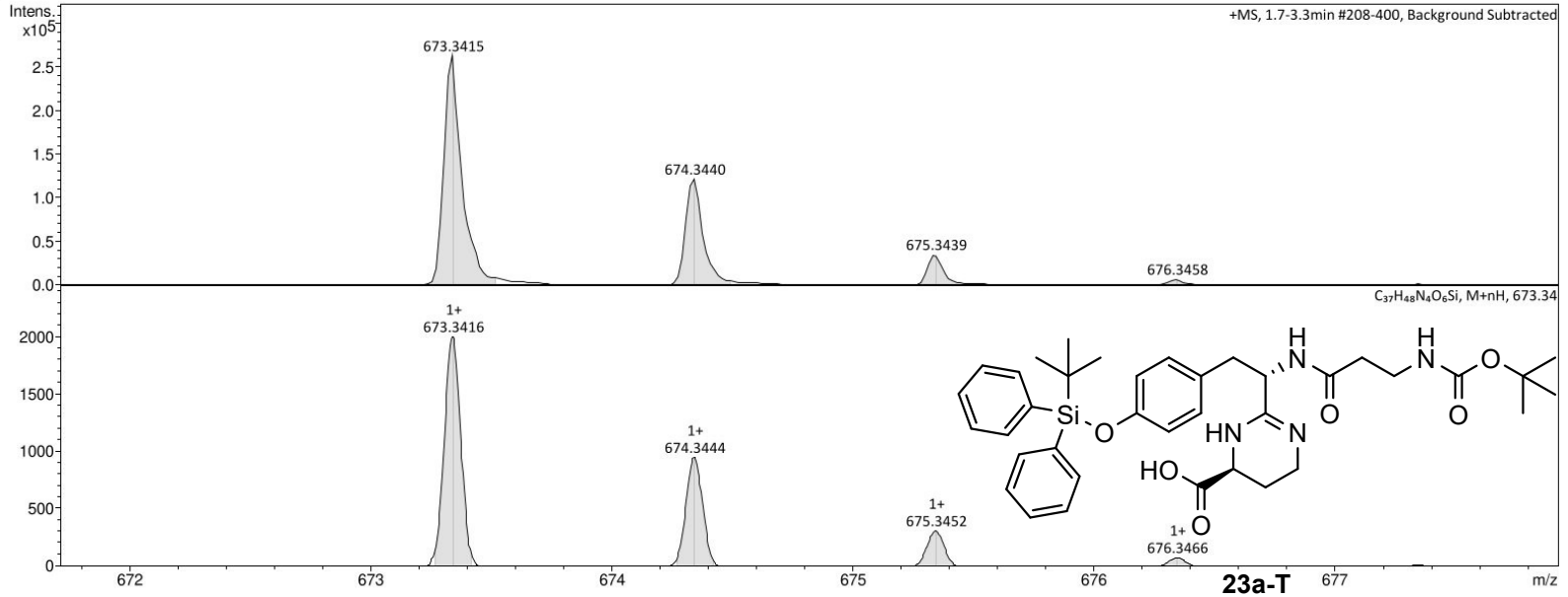
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE519-P61avoll_14_01_2556.d	Acquisition Date	6/12/2023 12:22:28 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE519-P61avoll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



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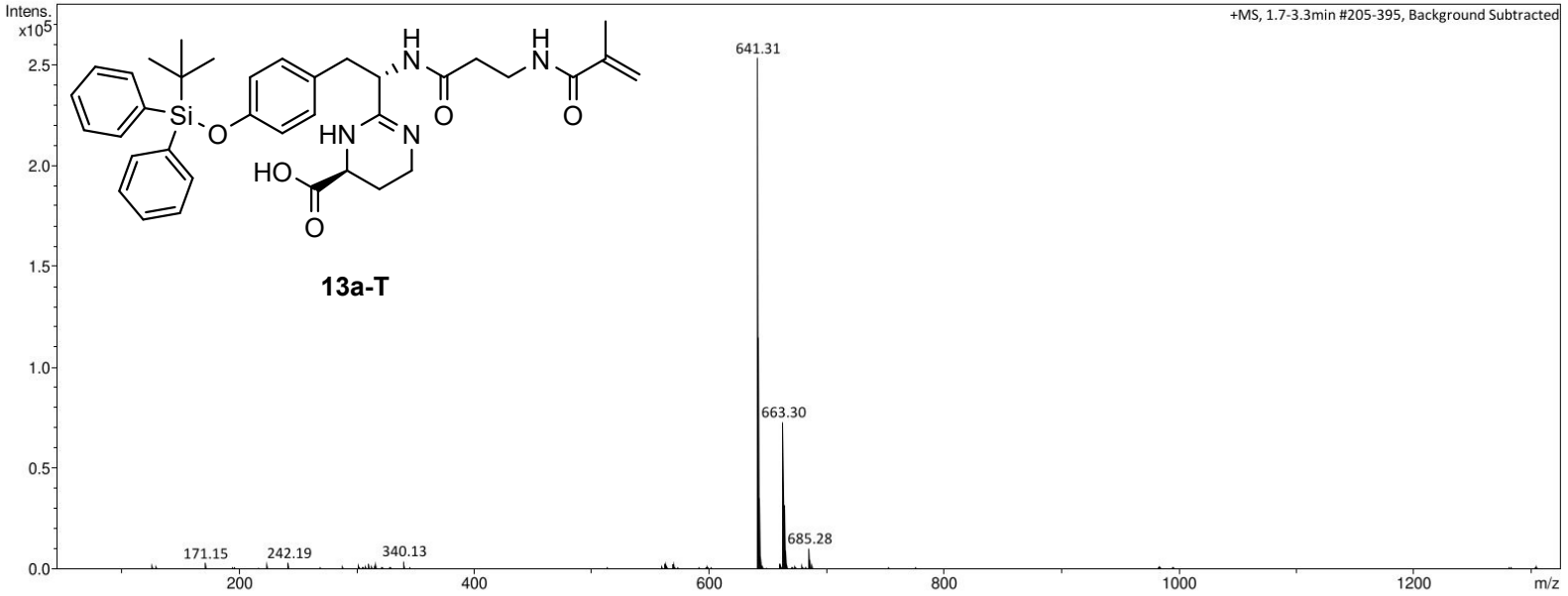
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE543-P62aVoll_2_01_3728.d	Acquisition Date	8/4/2023 9:50:40 AM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE543-P62a Voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



13a-T

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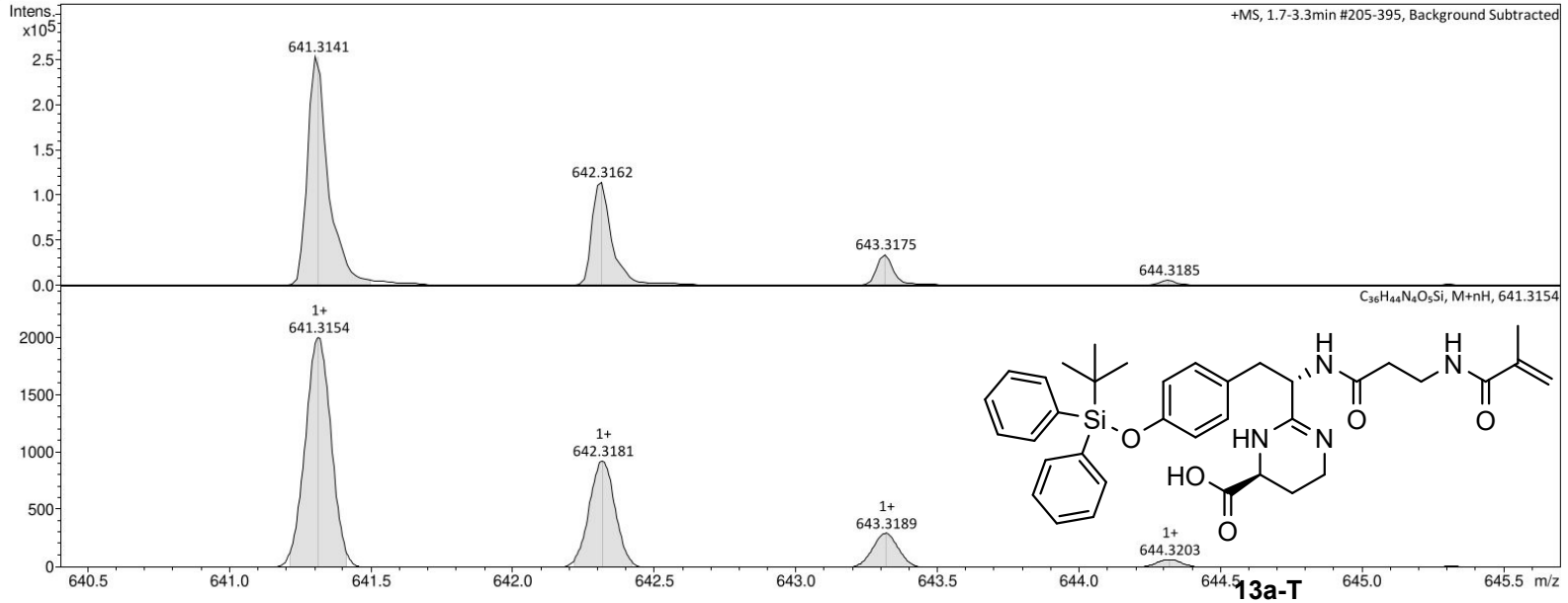
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE543-P62aVoll_2_01_3728.d	Acquisition Date	8/4/2023 9:50:40 AM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE543-P62a Voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



13a-T

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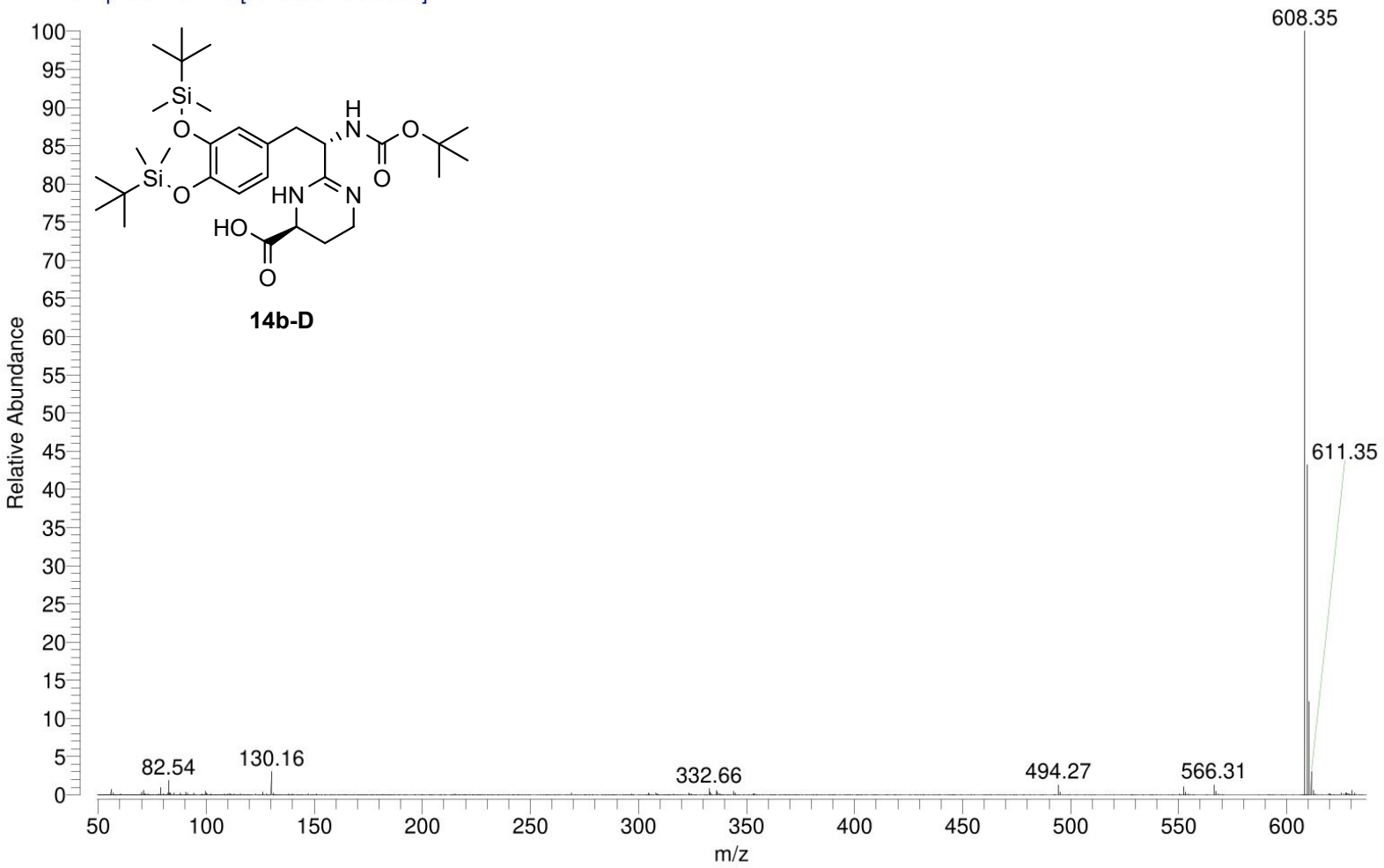
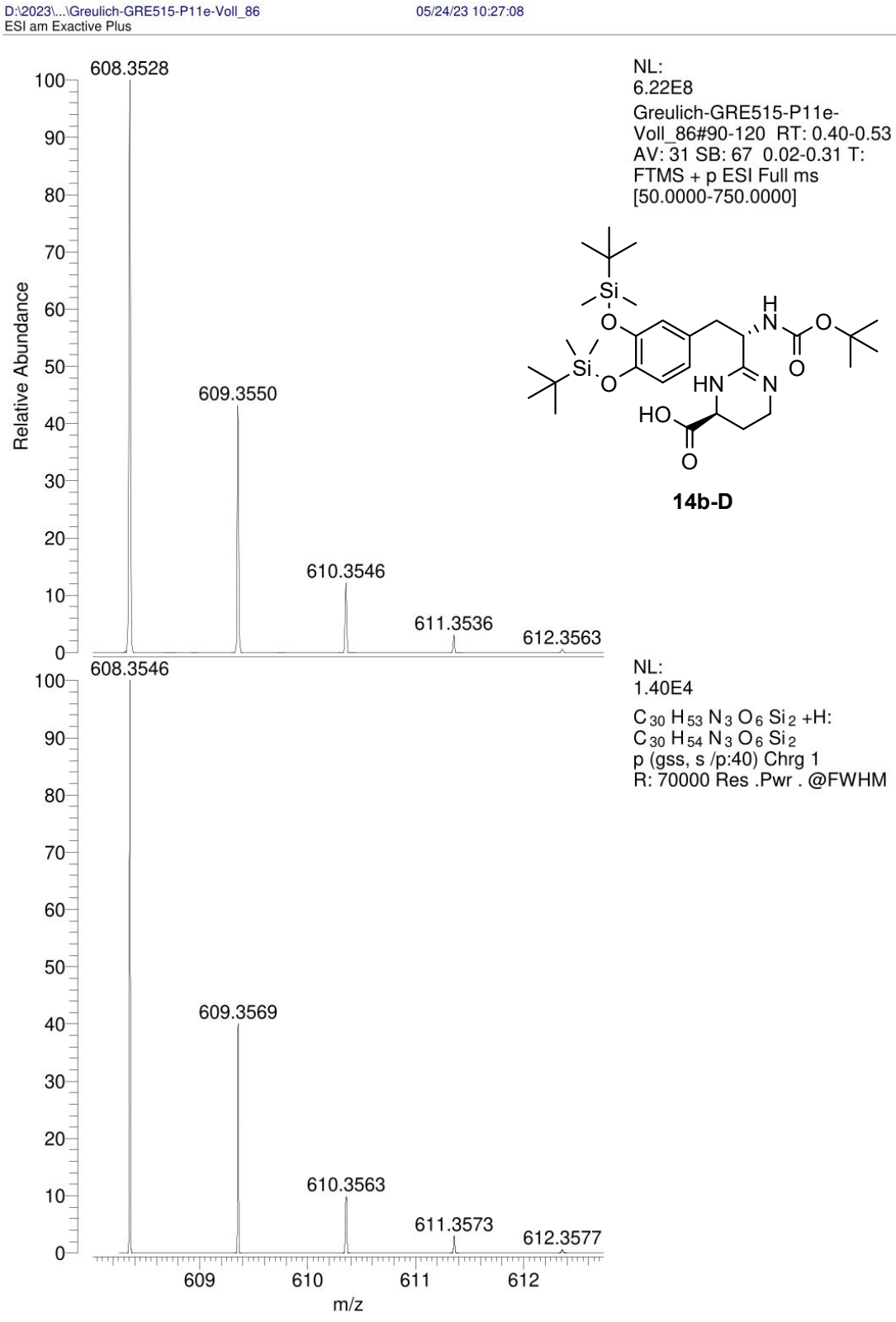
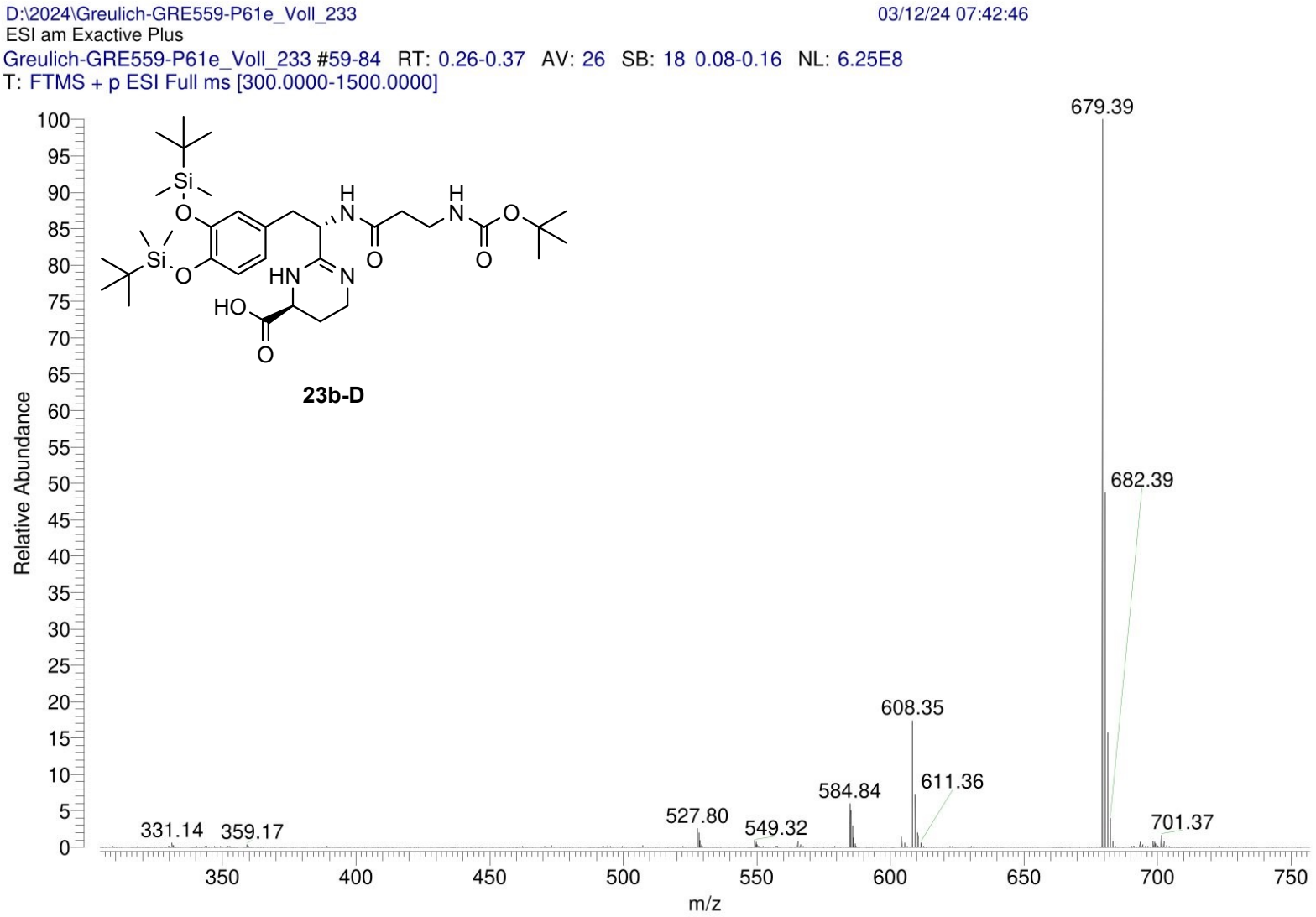
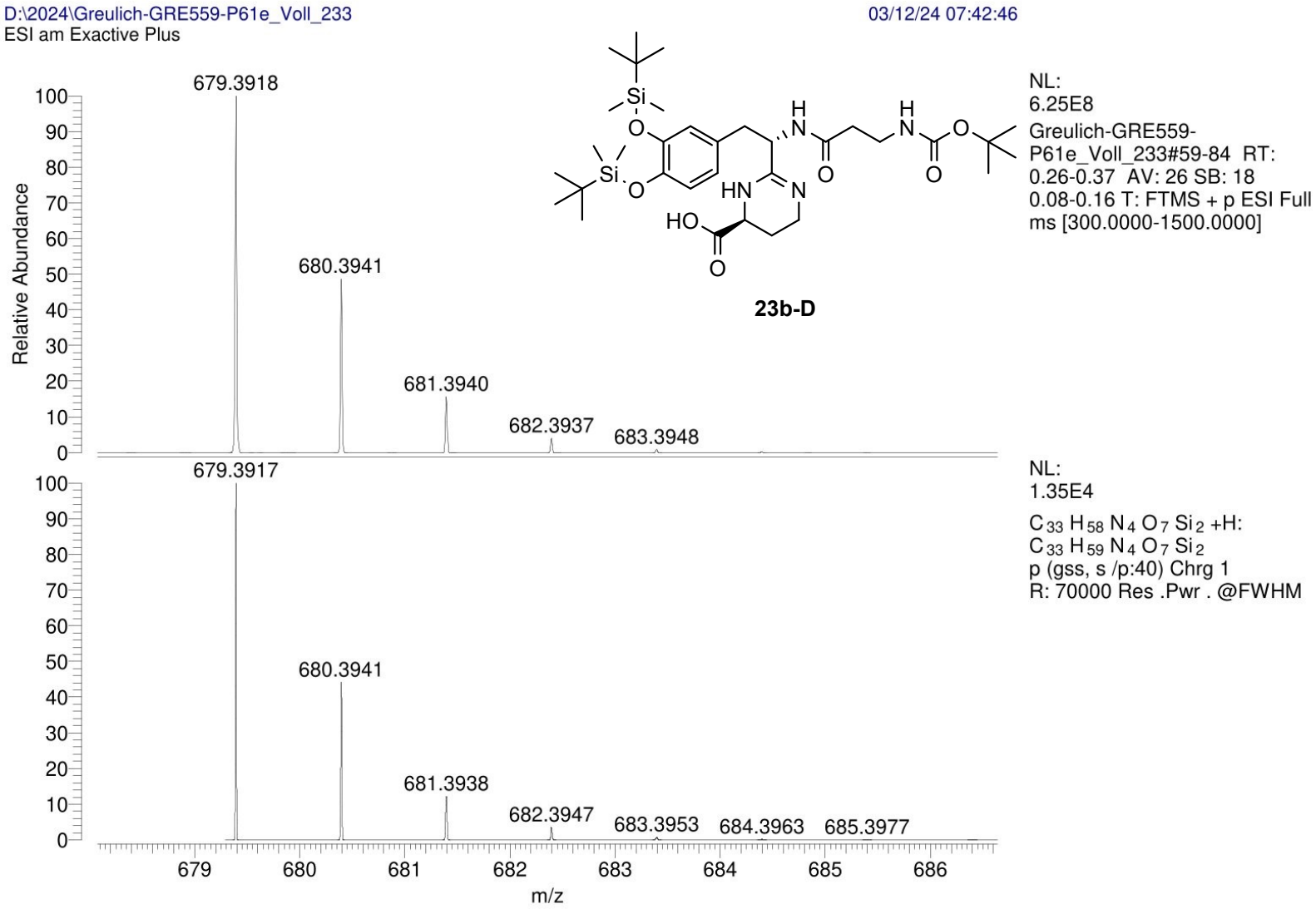
D:\2023\...\Greulich-GRE515-P11e-Voll_86 05/24/23 10:27:08
ESI am Exactive Plus
Greulich-GRE515-P11e-Voll_86 #90-120 RT: 0.40-0.53 AV: 31 SB: 67 0.02-0.31 NL: 6.22E8
T: FTMS + p ESI Full ms [50.0000-750.0000]

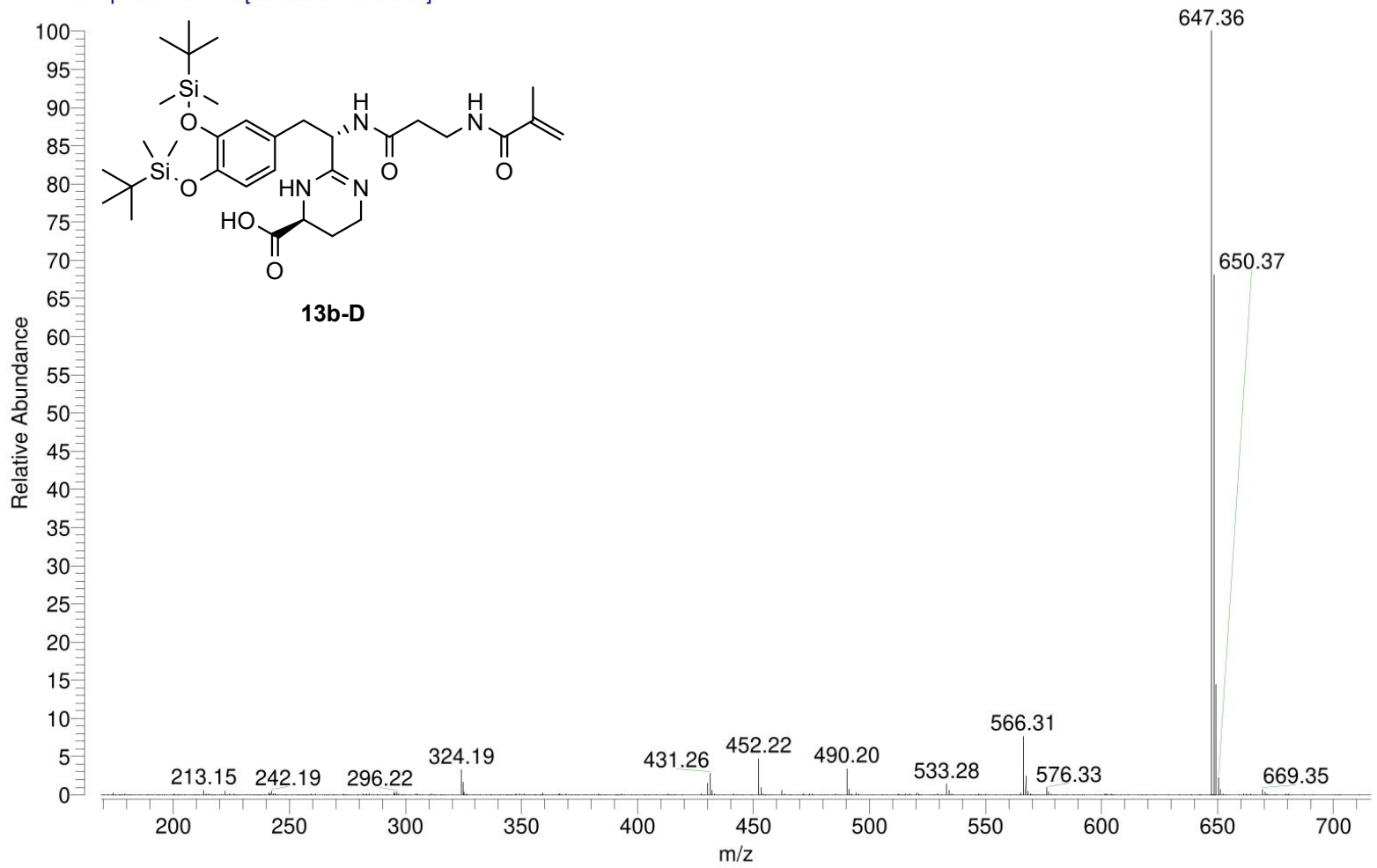



D:\2023\...\Greulich-GRE515-P11e-Voll_86 05/24/23 10:27:08
ESI am Exactive Plus
608.3528
609.3550
610.3546
611.3536
612.3563
NL:
6.22E8
Greulich-GRE515-P11e-Voll_86#90-120 RT: 0.40-0.53 AV: 31 SB: 67 0.02-0.31 T: FTMS + p ESI Full ms [50.0000-750.0000]
14b-D
608.3546
609.3569
610.3563
611.3573
612.3577
NL:
1.40E4
C30 H53 N3 O6 Si2 +H:
C30 H54 N3 O6 Si2
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM
Relative Abundance
m/z

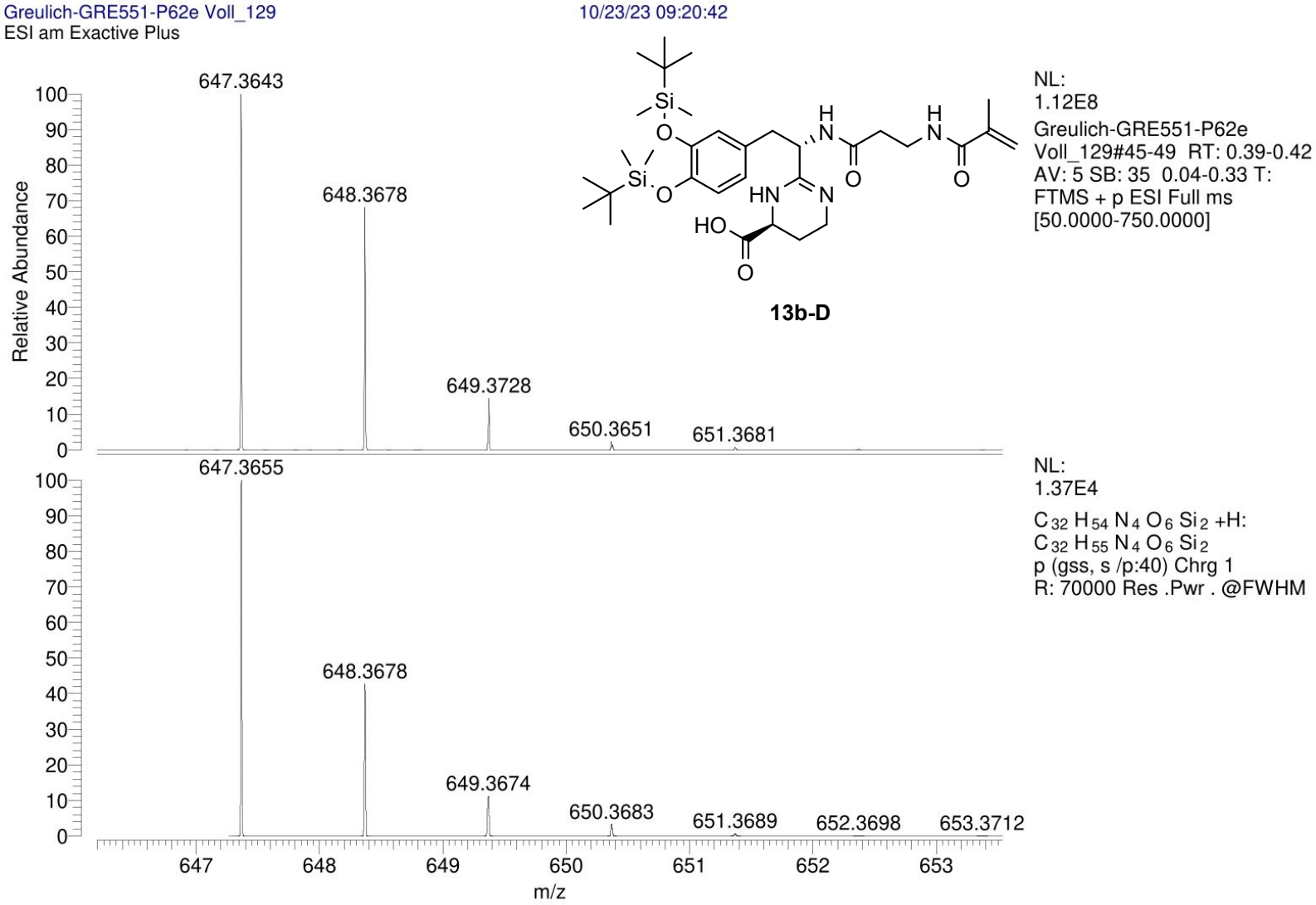

D:\2024\Greulich-GRE559-P61e_Voll_233
03/12/24 07:42:46
ESI am Exactive Plus
Greulich-GRE559-P61e_Voll_233 #59-84 RT: 0.26-0.37 AV: 26 SB: 18 0.08-0.16 NL: 6.25E8
T: FTMS + p ESI Full ms [300.0000-1500.0000]
23b-D
Relative Abundance
m/z
679.39
682.39
608.35
611.36
584.84
527.80
549.32
331.14
359.17
701.37


D:\2024\Greulich-GRE559-P61e_Voll_233
03/12/24 07:42:46
ESI am Exactive Plus
679.3918
680.3941
681.3940
682.3937
683.3948
Relative Abundance
NL:
6.25E8
Greulich-GRE559-P61e_Voll_233#59-84 RT: 0.26-0.37 AV: 26 SB: 18 0.08-0.16 T: FTMS + p ESI Full ms [300.0000-1500.0000]
23b-D
679.3917
680.3941
681.3938
682.3947
683.3953
684.3963
685.3977
NL:
1.35E4
C33 H58 N4 O7 Si2 +H:
C33 H59 N4 O7 Si2
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM
m/z

Greulich-GRE551-P62e Voll_129 10/23/23 09:20:42
ESI am Exactive Plus
Greulich-GRE551-P62e Voll_129 #45-49 RT: 0.39-0.42 AV: 5 SB: 35 0.04-0.33 NL: 1.12E8
T: FTMS + p ESI Full ms [50.0000-750.0000]



13b-D


Greulich-GRE551-P62e Voll_129
ESI am Exactive Plus
10/23/23 09:20:42
647.3643
648.3678
649.3728
650.3651
651.3681
Relative Abundance
NL:
1.12E8
Greulich-GRE551-P62e
Voll_129#45-49 RT: 0.39-0.42
AV: 5 SB: 35 0.04-0.33 T:
FTMS + p ESI Full ms
[50.0000-750.0000]
13b-D
647.3655
648.3678
649.3674
650.3683
651.3689
652.3698
653.3712
NL:
1.37E4
C32 H54 N4 O6 Si2 +H:
C32 H55 N4 O6 Si2
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM
m/z

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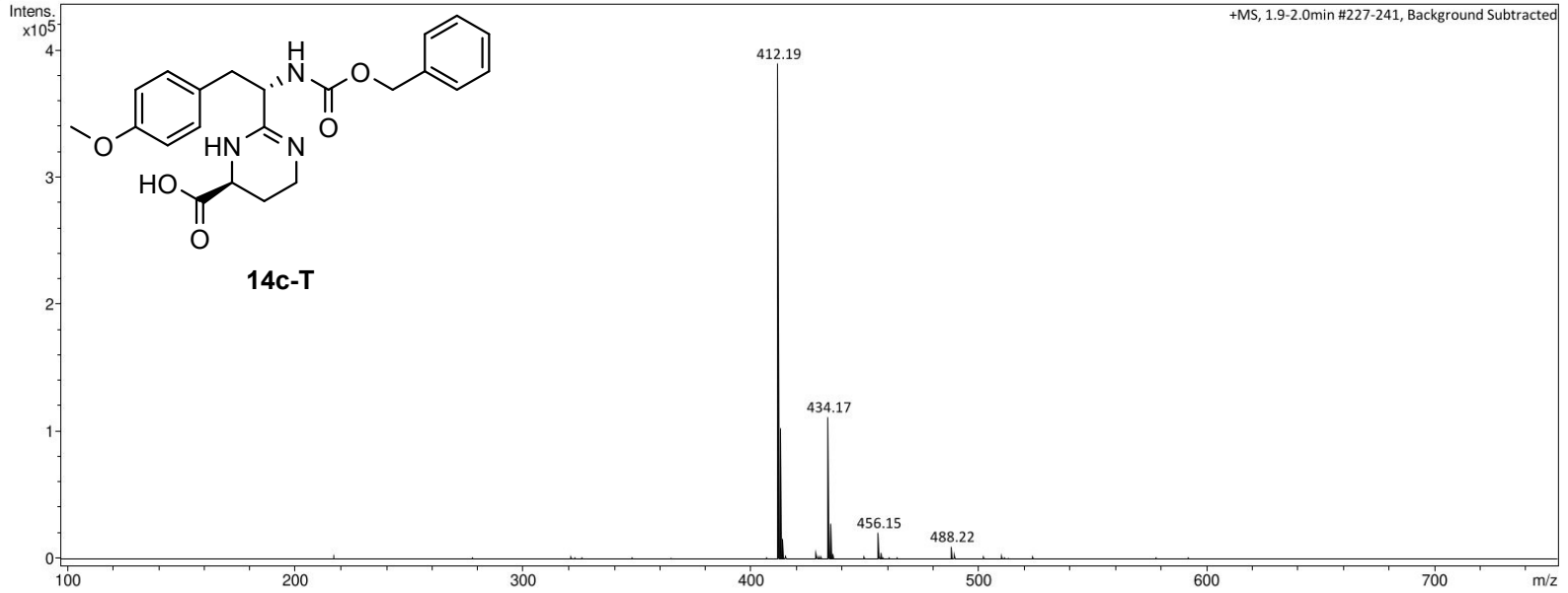
Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE487-P11gUmkrist_5_01_1256.d	Acquisition Date	3/14/2023 10:21:36 AM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE487-P11gUmkrist	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



14c-T

Bruker Compass DataAnalysis 4.2 printed: 3/14/2023 1:11:27 PM by: BDAL@DE Page 1 of 1

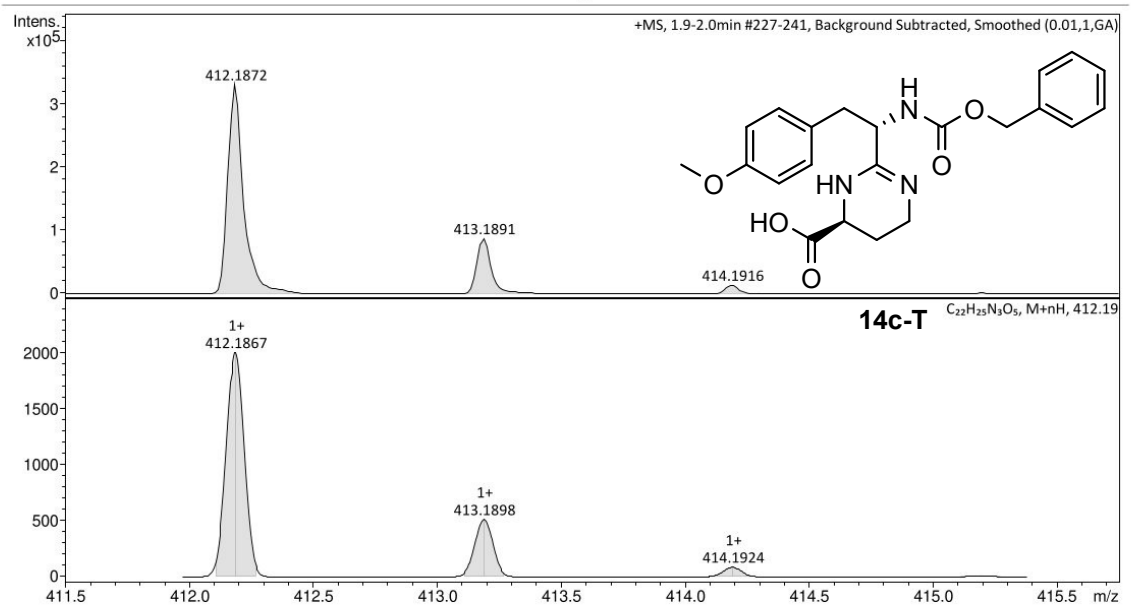
Massenspektrometrie - Universität Stuttgart

Analysis Info

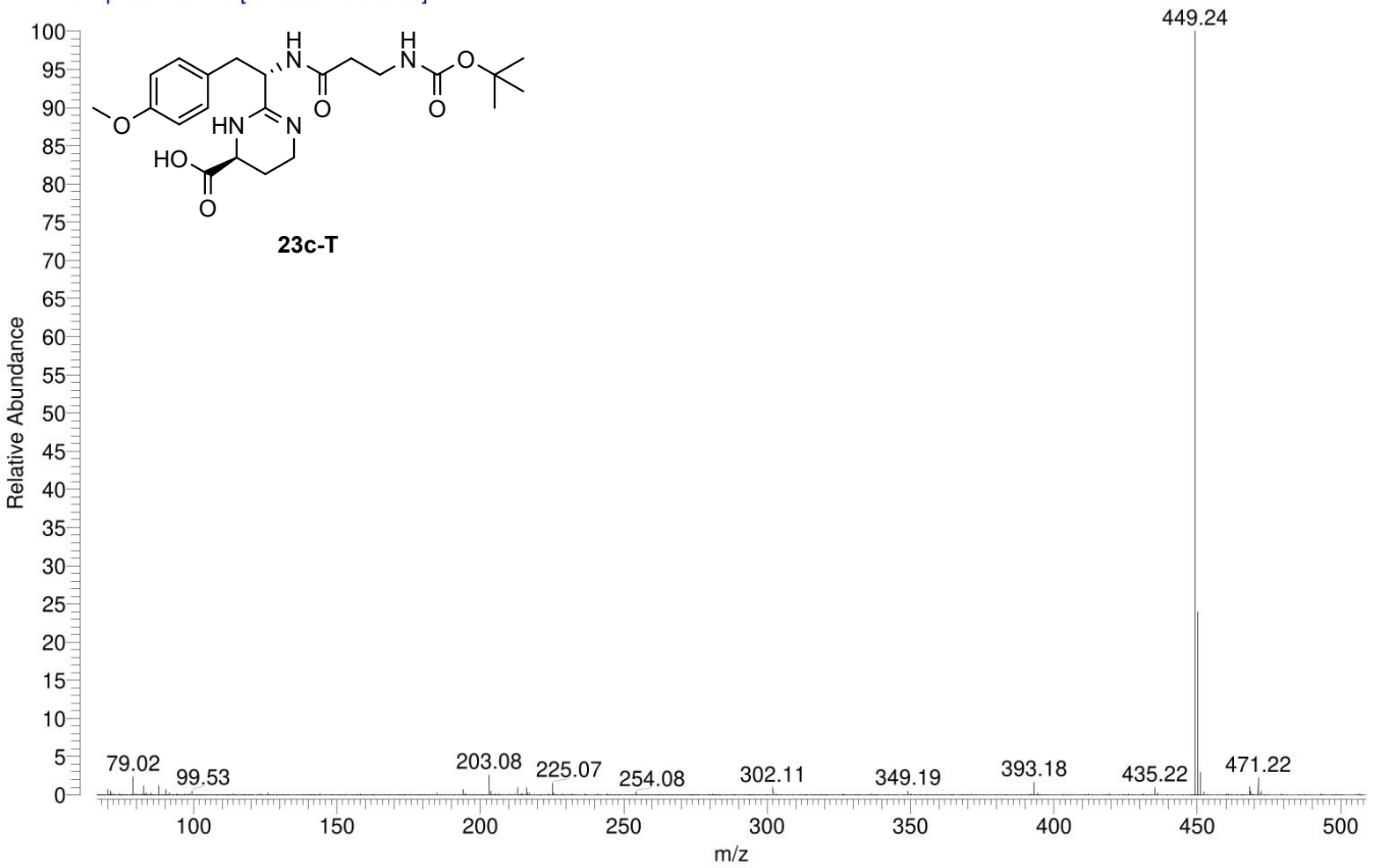
		Acquisition Date	3/14/2023 10:21:36 AM
Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE487-P11gUmkrist_5_01_1256.d		
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE487-P11gUmkrist	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



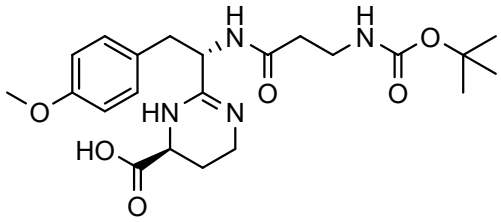
D:\2023\Greulich-GRE547-P61g voll_423 09/26/23 09:31:19
ESI am Exactive Plus
Greulich-GRE547-P61g voll_423 #23-38 RT: 0.19-0.32 AV: 16 SB: 11 0.04-0.12 NL: 1.51E9
T: FTMS + p ESI Full ms [50.0000-750.0000]



23c-T

D:\2023\Greulich-GRE547-P61g voll_423
ESI am Exactive Plus

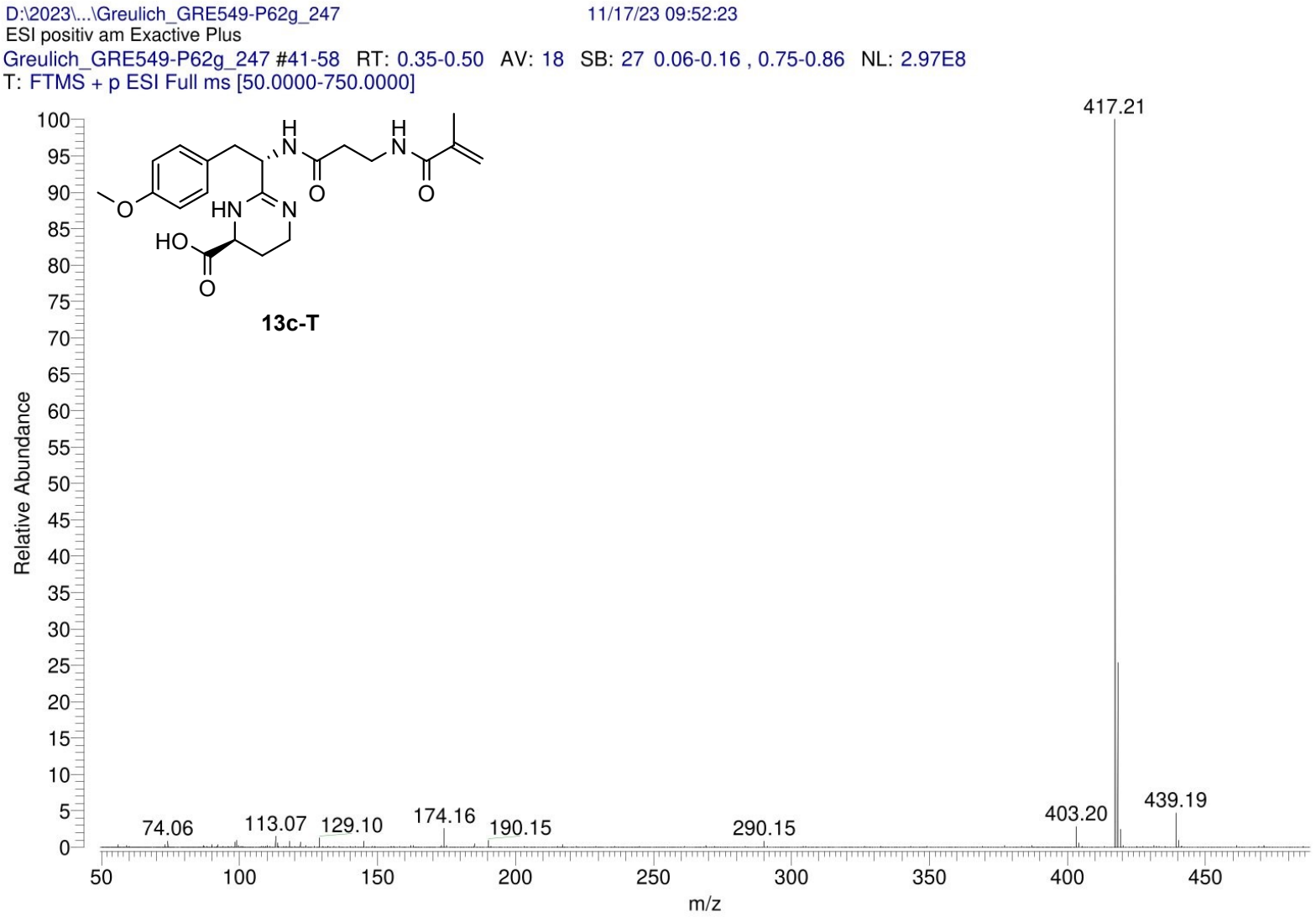
09/26/23 09:31:19

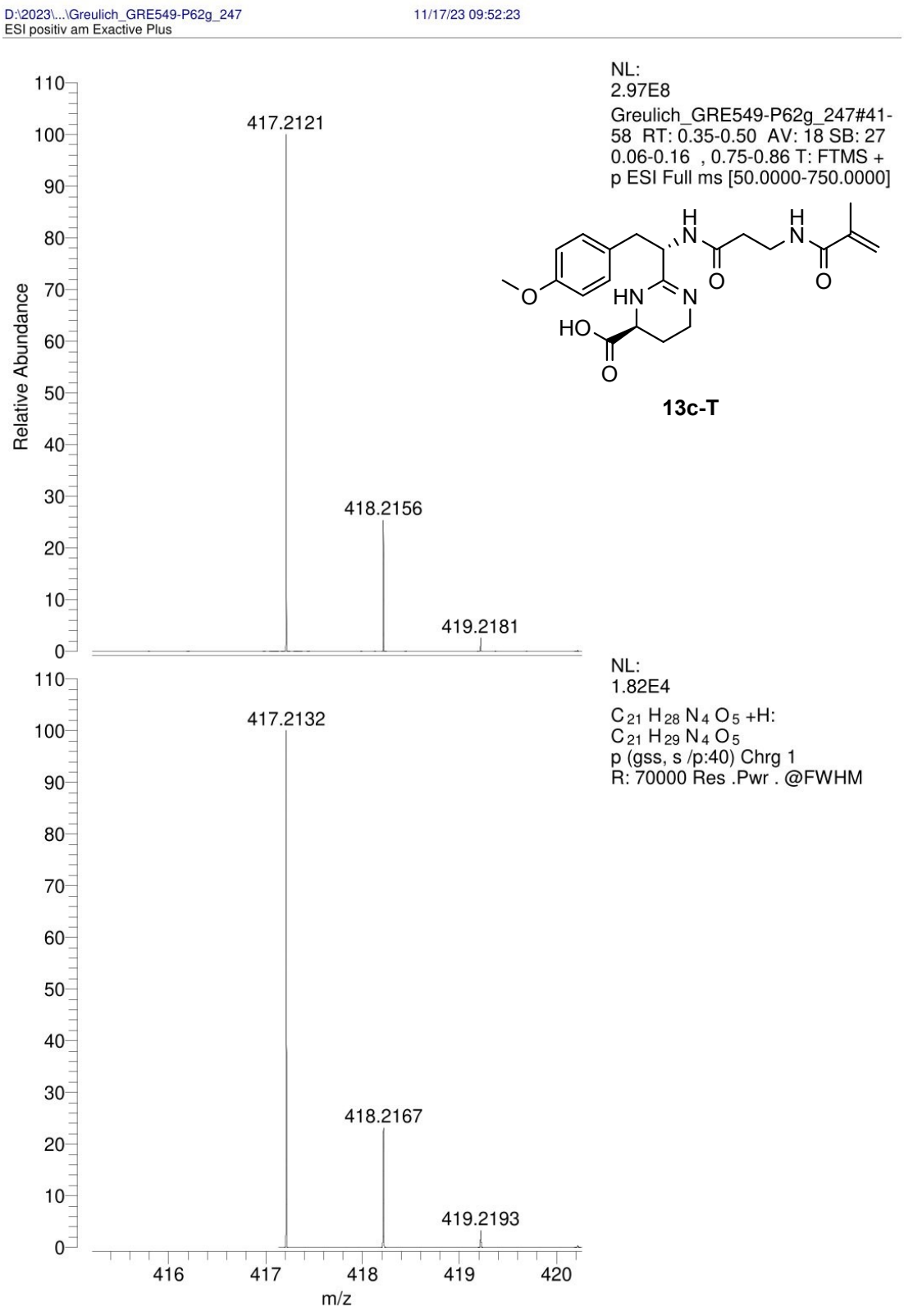


23c-T

NL:
1.51E9
Greulich-GRE547-P61g
voll_423#23-38 RT: 0.19-0.32
AV: 16 SB: 11 0.04-0.12 T:
FTMS + p ESI Full ms
[50.0000-750.0000]

NL:
1.79E4
$C_{22}H_{32}N_4O_6$ +H:
$C_{22}H_{33}N_4O_6$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM


D:\2023\...\Greulich_GRE549-P62g_247
11/17/23 09:52:23
ESI positiv am Exactive Plus
Greulich_GRE549-P62g_247 #41-58 RT: 0.35-0.50 AV: 18 SB: 27 0.06-0.16 , 0.75-0.86 NL: 2.97E8
T: FTMS + p ESI Full ms [50.0000-750.0000]
13c-T
Relative Abundance
m/z
417.21
439.19
403.20
74.06
113.07
129.10
174.16
190.15
290.15


D:\2023\...\Greulich_GRE549-P62g_247
11/17/23 09:52:23
ESI positiv am Exactive Plus
NL:
2.97E8
Greulich_GRE549-P62g_247#41-58 RT: 0.35-0.50 AV: 18 SB: 27 0.06-0.16 , 0.75-0.86 T: FTMS + p ESI Full ms [50.0000-750.0000]
13c-T
Relative Abundance
417.2121
418.2156
419.2181
NL:
1.82E4
C21 H28 N4 O5 +H:
C21 H29 N4 O5
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM
417.2132
418.2167
419.2193
m/z

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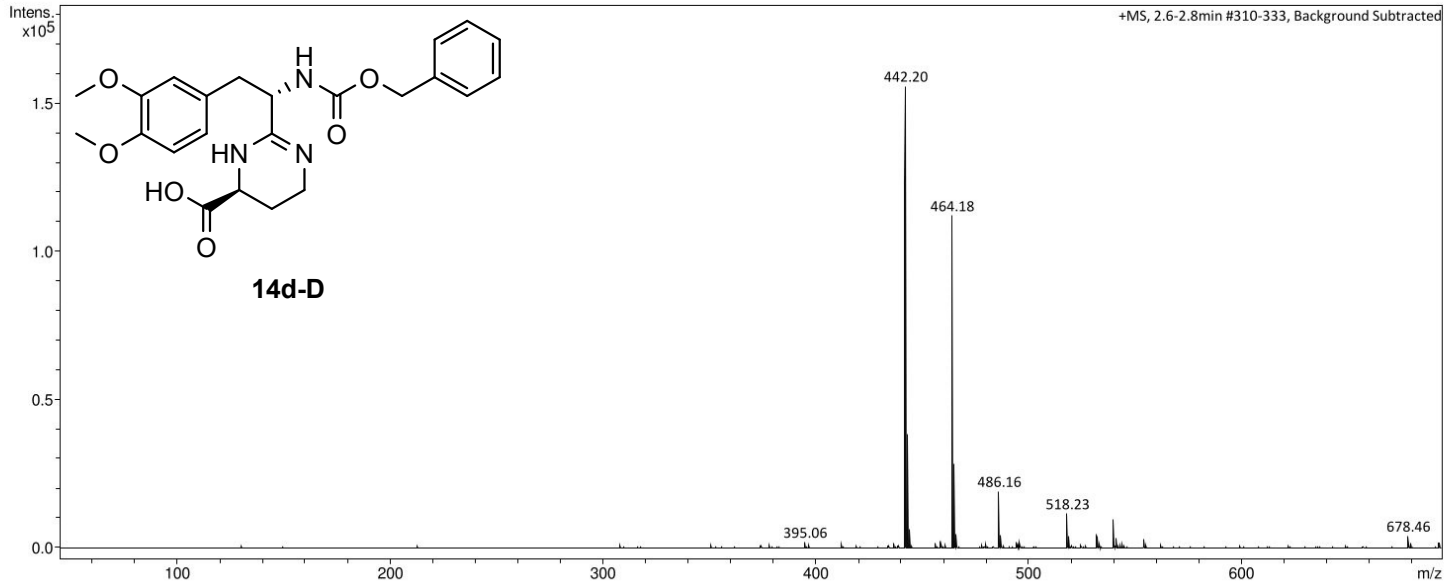
Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE501F1_3_01_1190.d	Acquisition Date	3/8/2023 3:01:56 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE501F1	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



14d-D

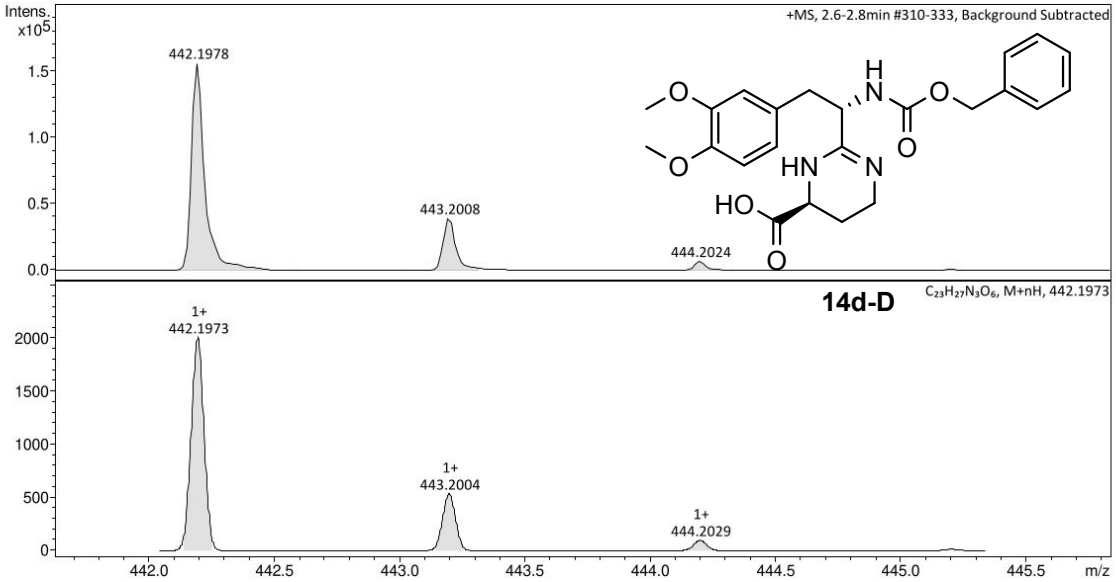
Massenspektrometrie - Universität Stuttgart

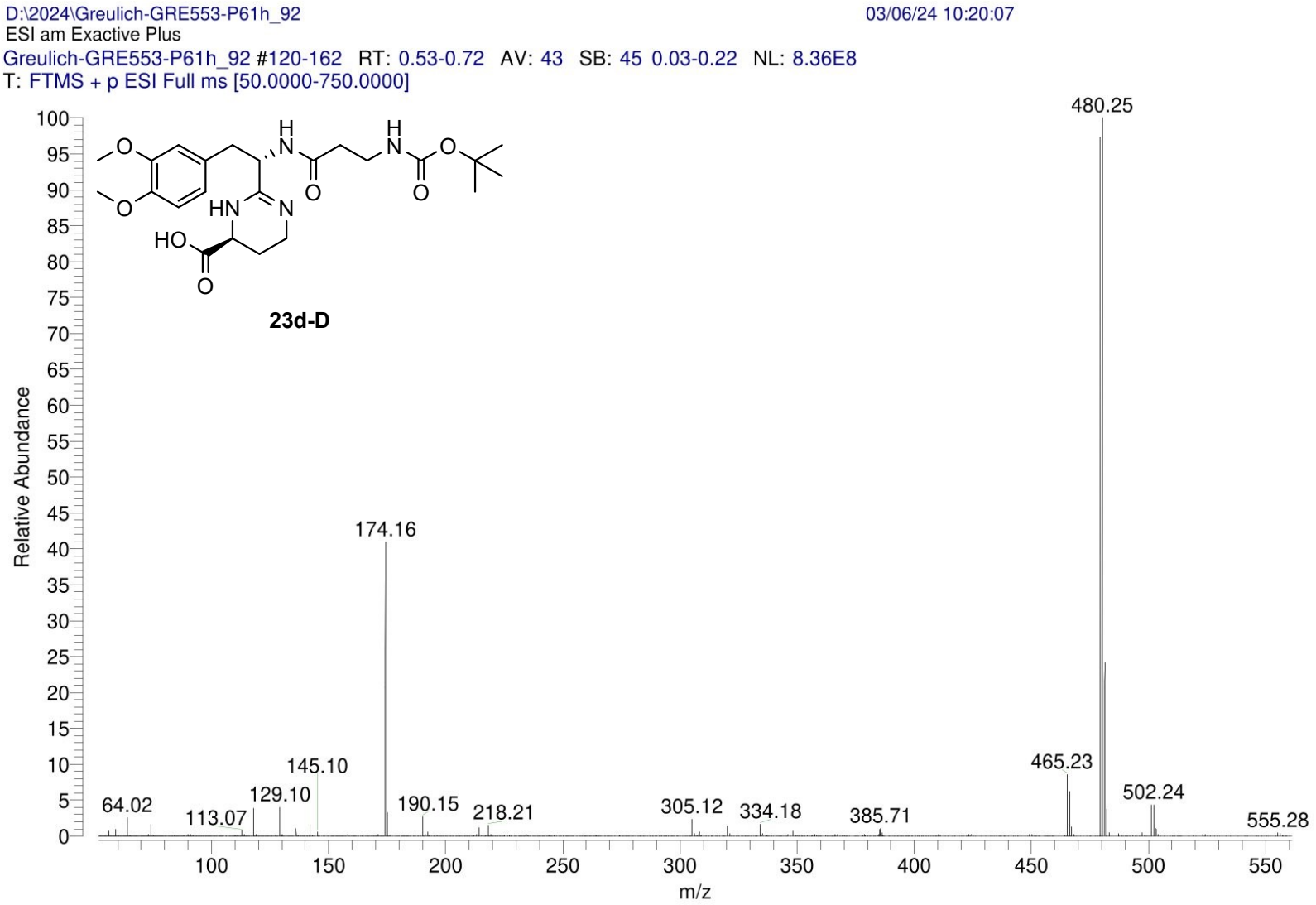
Analysis Info

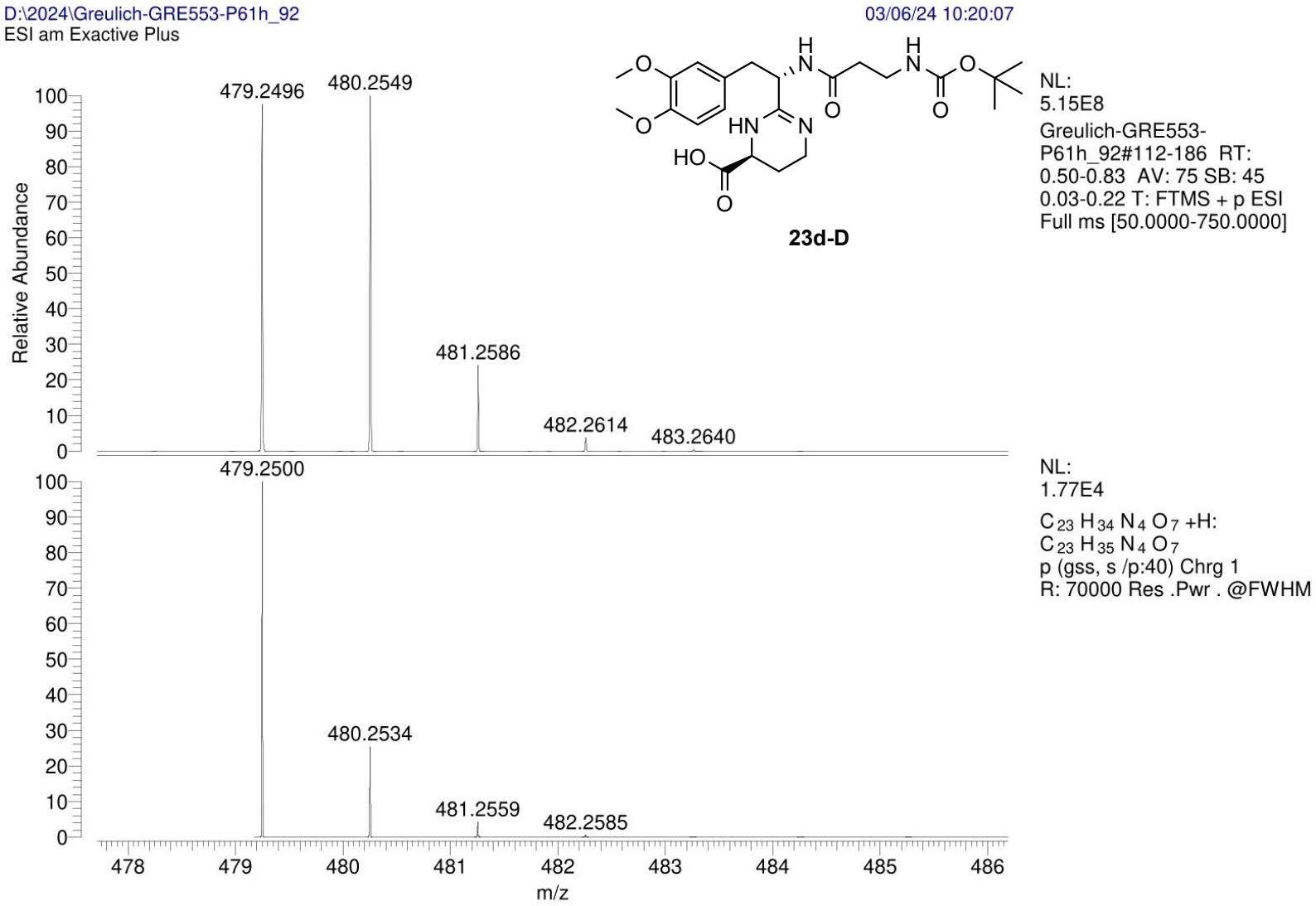
Analysis Name	C:\Data\2023\laschat_2023\Greulich-GRE501F1_3_01_1190.d	Acquisition Date	3/8/2023 3:01:56 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE501F1	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

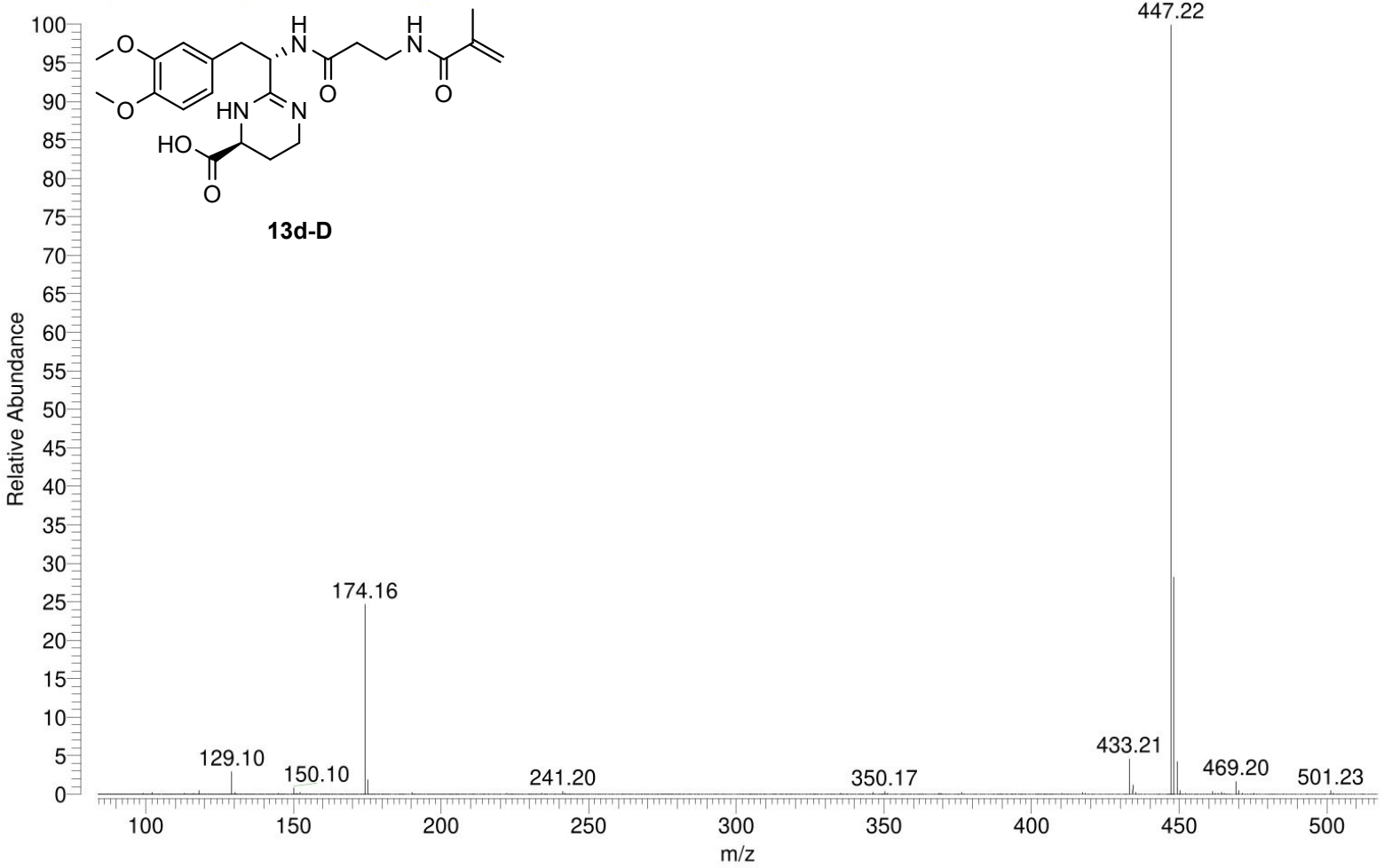
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste

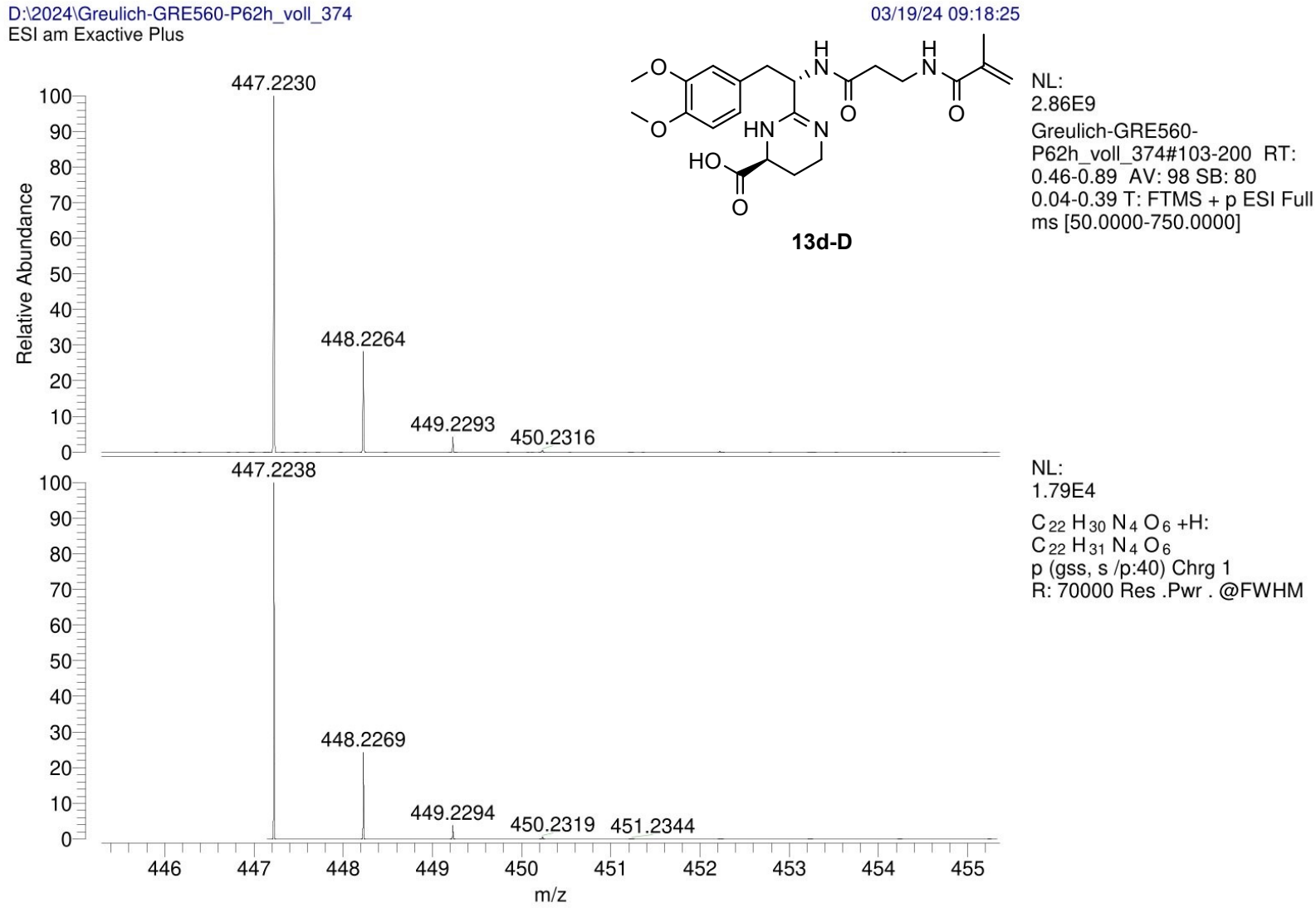



D:\2024\Greulich-GRE553-P61h_92
03/06/24 10:20:07
ESI am Exactive Plus
Greulich-GRE553-P61h_92 #120-162 RT: 0.53-0.72 AV: 43 SB: 45 0.03-0.22 NL: 8.36E8
T: FTMS + p ESI Full ms [50.0000-750.0000]
23d-D
Relative Abundance
m/z
480.25
174.16
145.10
129.10
64.02
113.07
190.15
218.21
305.12
334.18
385.71
465.23
502.24
555.28


D:\2024\Greulich-GRE553-P61h_92
ESI am Exactive Plus
03/06/24 10:20:07
23d-D
NL:
5.15E8
Greulich-GRE553-P61h_92#112-186 RT: 0.50-0.83 AV: 75 SB: 45 0.03-0.22 T: FTMS + p ESI Full ms [50.0000-750.0000]
479.2496
480.2549
481.2586
482.2614
483.2640
NL:
1.77E4
C23 H34 N4 O7 +H:
C23 H35 N4 O7
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM
479.2500
480.2534
481.2559
482.2585
Relative Abundance
m/z

D:\2024\Greulich-GRE560-P62h_voll_374 03/19/24 09:18:25
ESI am Exactive Plus
Greulich-GRE560-P62h_voll_374 #103-200 RT: 0.46-0.89 AV: 98 SB: 80 0.04-0.39 NL: 2.86E9
T: FTMS + p ESI Full ms [50.0000-750.0000]




D:\2024\Greulich-GRE560-P62h_voll_374
03/19/24 09:18:25
ESI am Exactive Plus
13d-D
NL:
2.86E9
Greulich-GRE560-P62h_voll_374#103-200 RT: 0.46-0.89 AV: 98 SB: 80 0.04-0.39 T: FTMS + p ESI Full ms [50.0000-750.0000]
NL:
1.79E4
C22 H30 N4 O6 +H:
C22 H31 N4 O6
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM
Relative Abundance
m/z
447.2230
448.2264
449.2293
450.2316
447.2238
448.2269
449.2294
450.2319
451.2344

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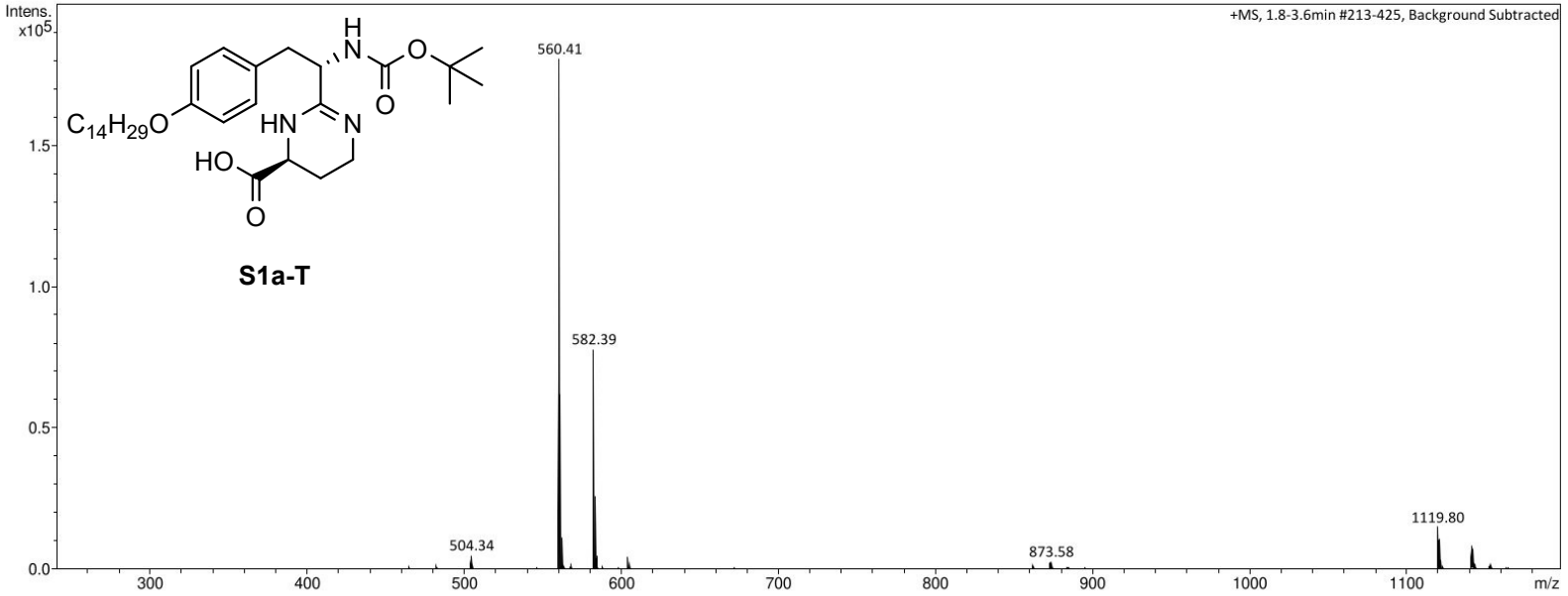
Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich_GRE534-P11i_voll_11_01_3081.d	Acquisition Date	7/4/2023 11:36:51 AM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich_GRE534-P11i_voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



S1a-T

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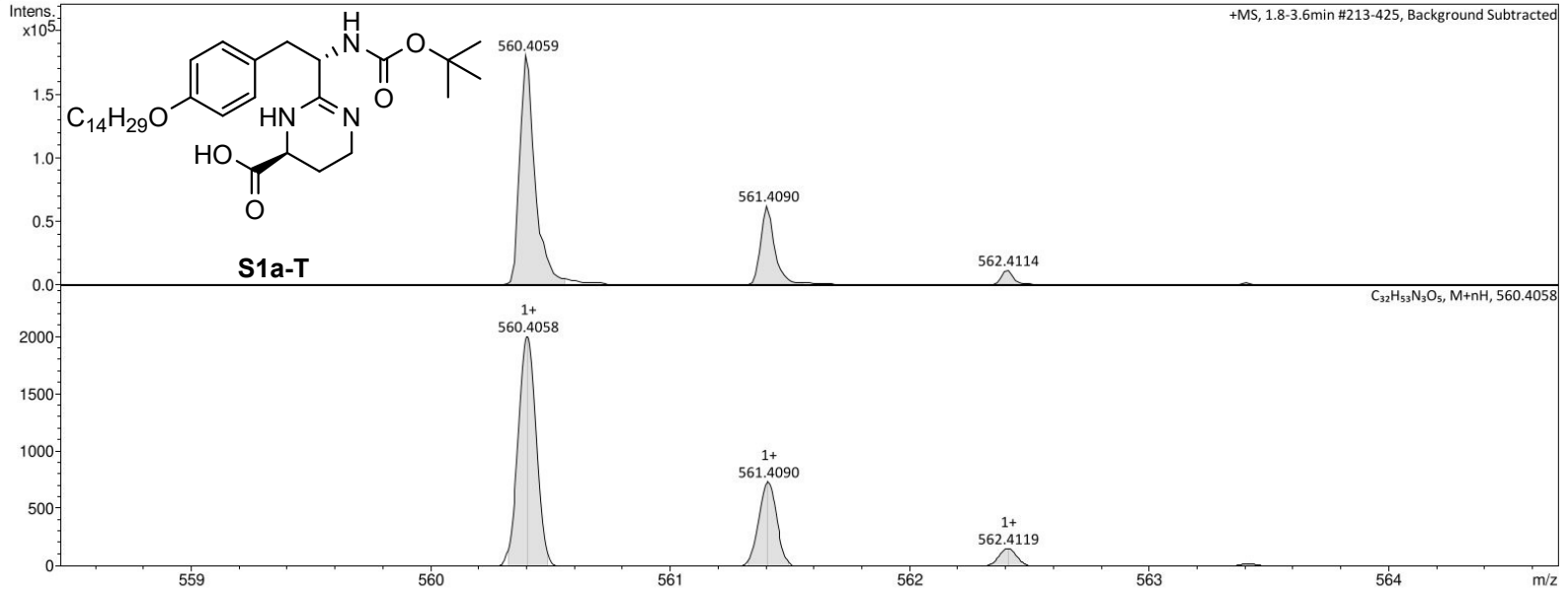
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	C:\Data\2023\laschat_2023\Greulich_GRE534-P11i_voll_11_01_3081.d	Acquisition Date	7/4/2023 11:36:51 AM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich_GRE534-P11i_voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



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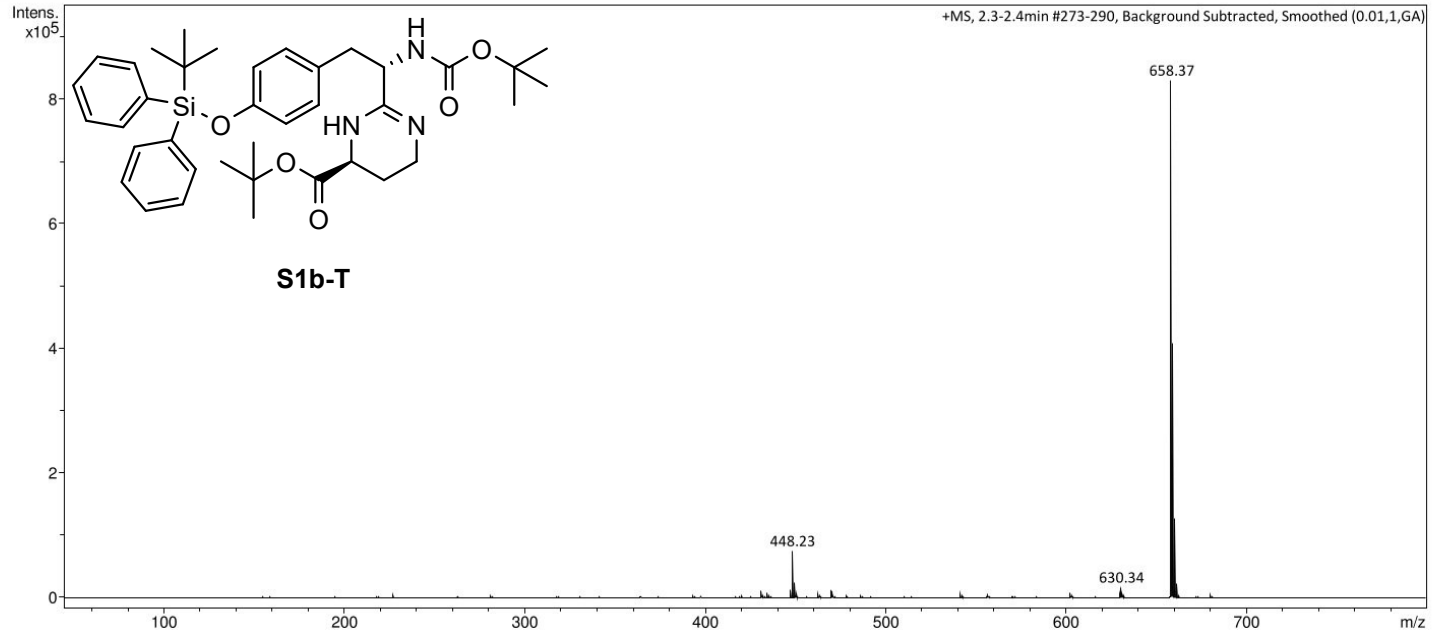
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE332 F1_3_01_34469.d	Acquisition Date	9/8/2021 3:27:04 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE332 F1	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



S1b-T

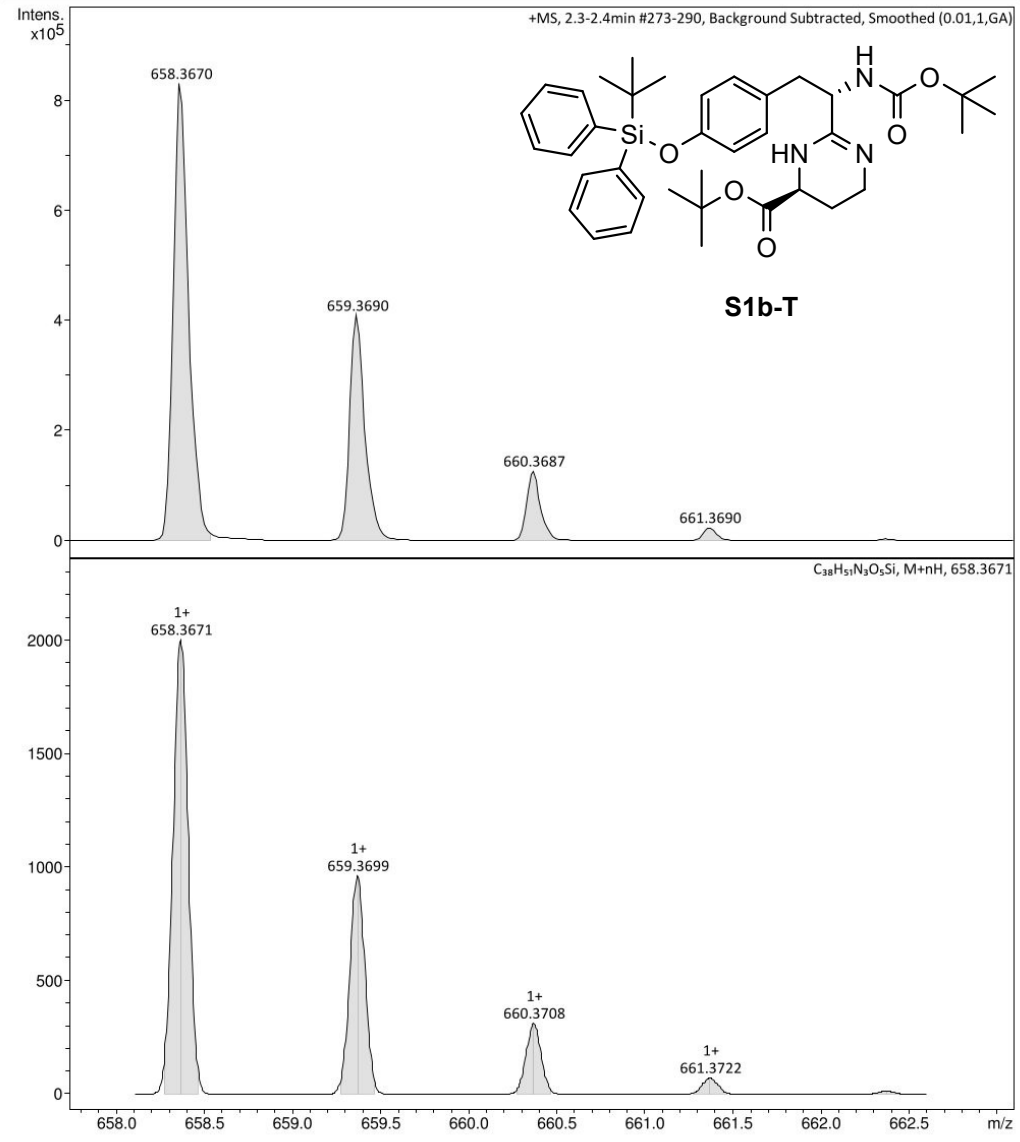
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE332 F1_3_01_34469.d	Acquisition Date	9/8/2021 3:27:04 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE332 F1	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



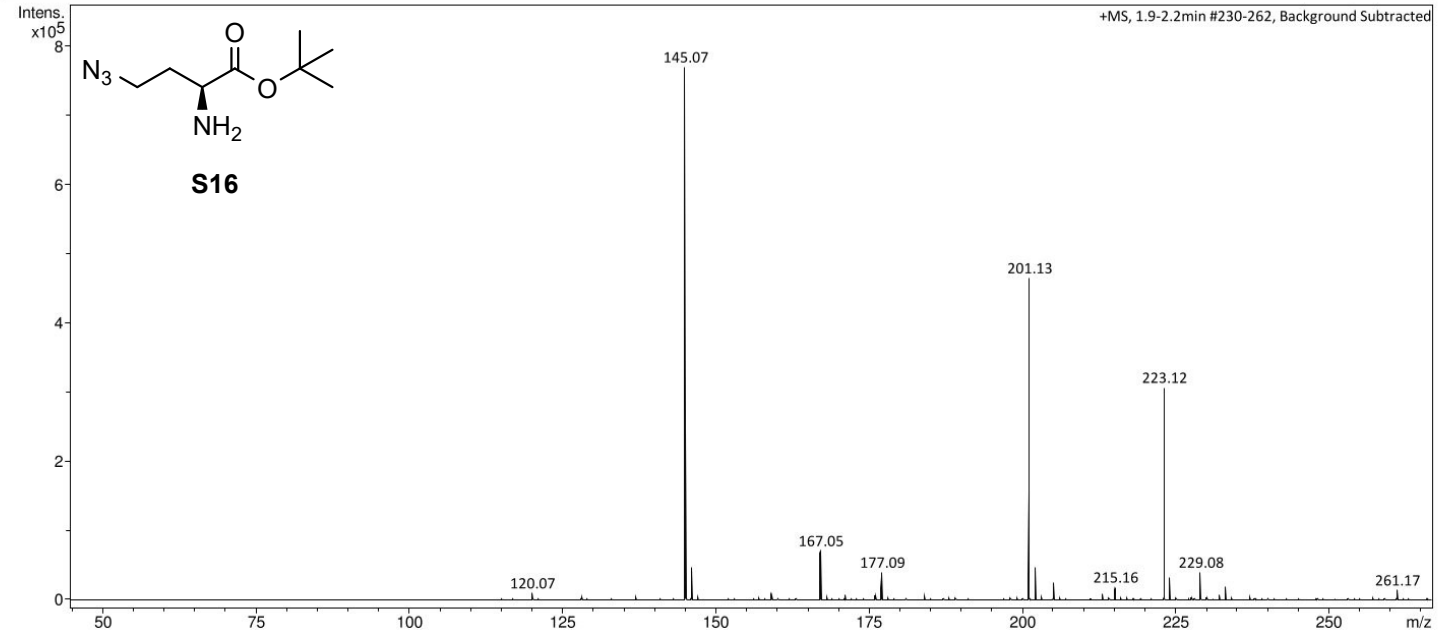
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE345-P30 Voll_1_01_33946.d	Acquisition Date	8/16/2021 2:17:16 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE345-P30 Voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



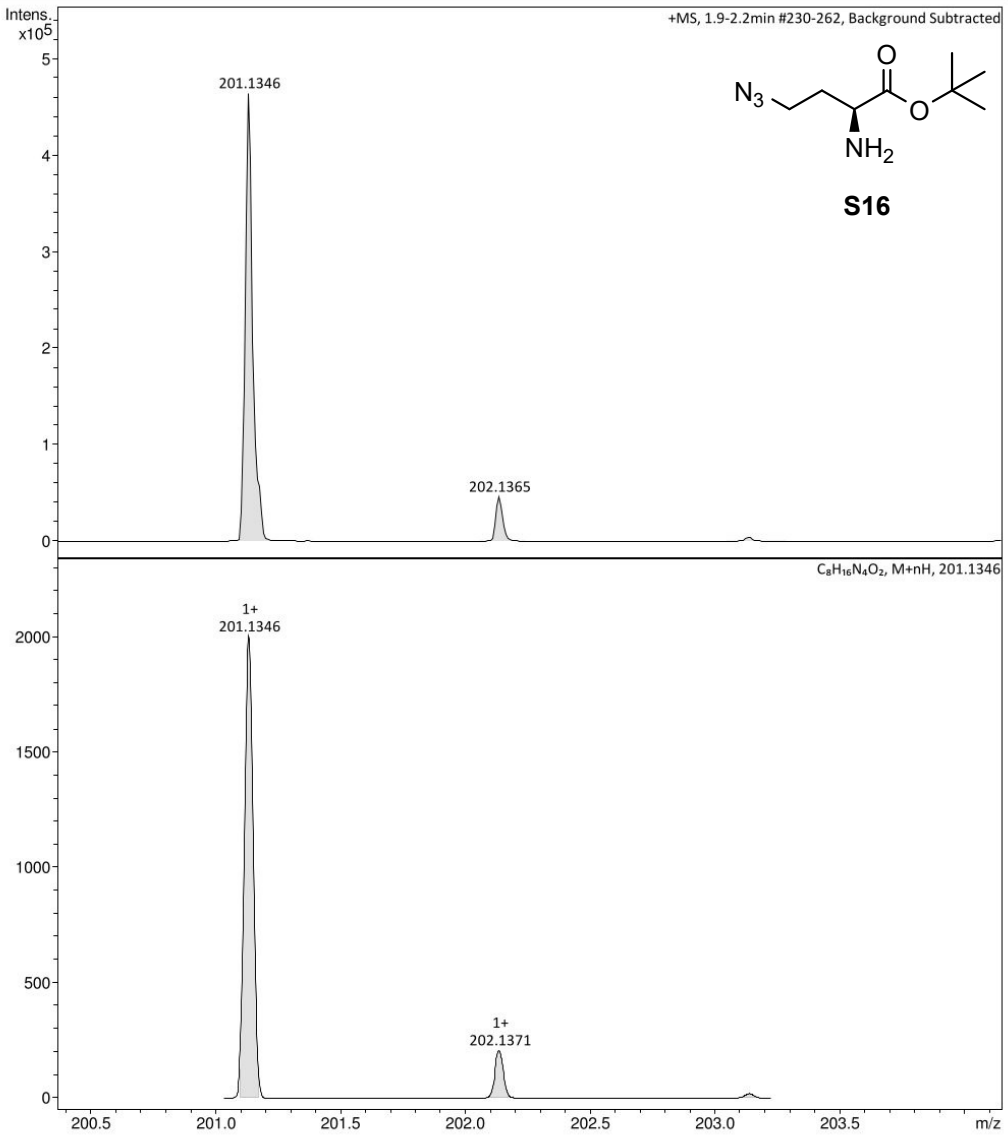
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE345-P30 Voll_1_01_33946.d	Acquisition Date	8/16/2021 2:17:16 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE345-P30 Voll	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



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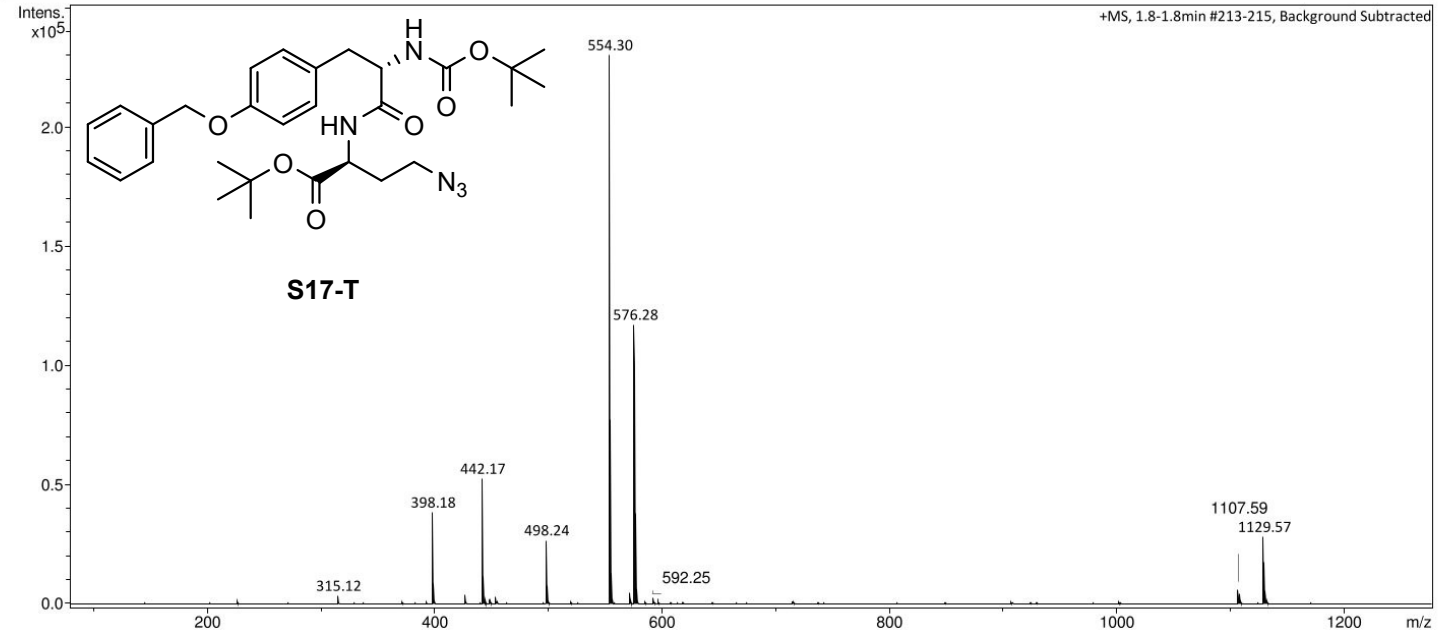
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE346F2_8_01_34227.d	Acquisition Date	8/23/2021 3:56:32 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE346F2	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



S17-T

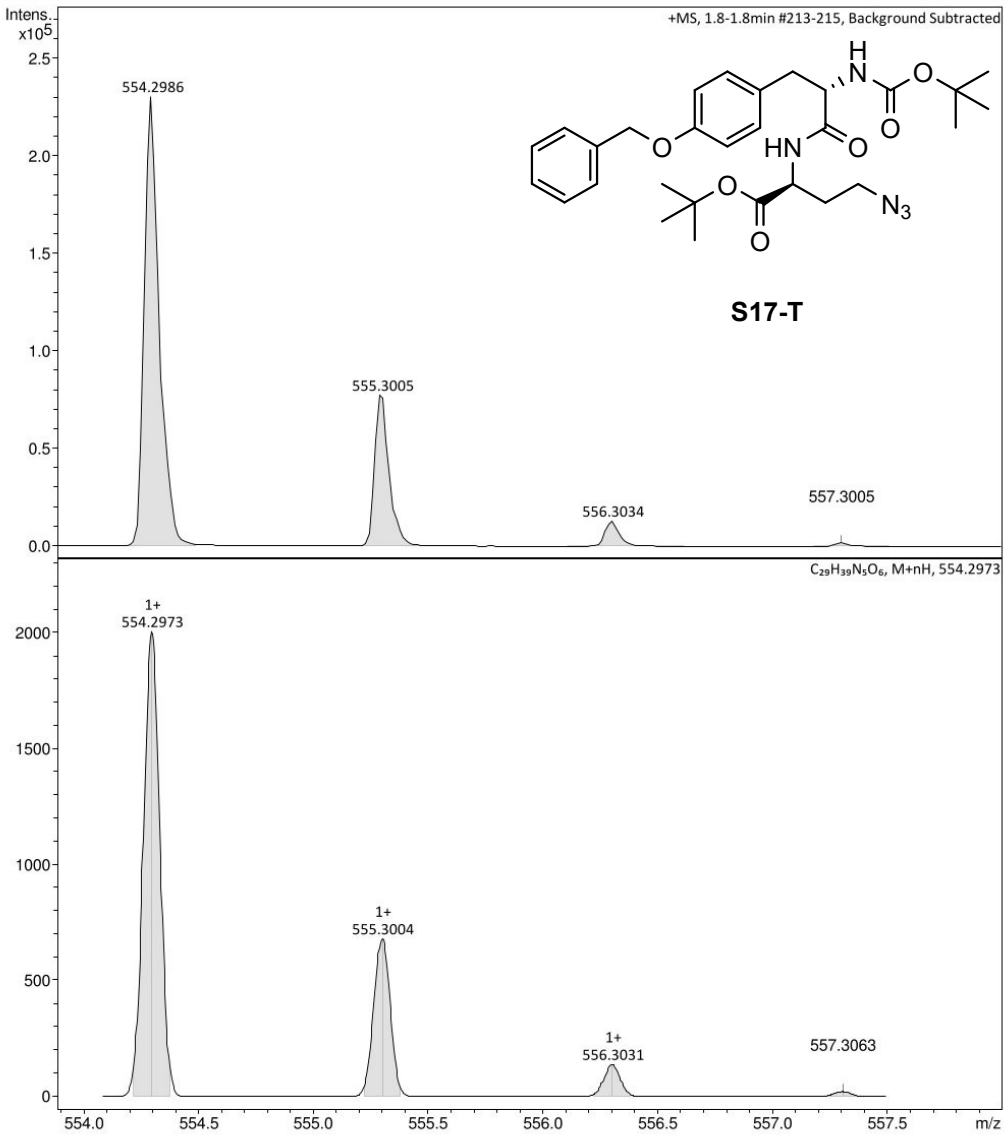
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE346F2_8_01_34227.d	Acquisition Date	8/23/2021 3:56:32 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE346F2	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.2 printed: 8/23/2021 4:22:42 PM Page 1 of 1

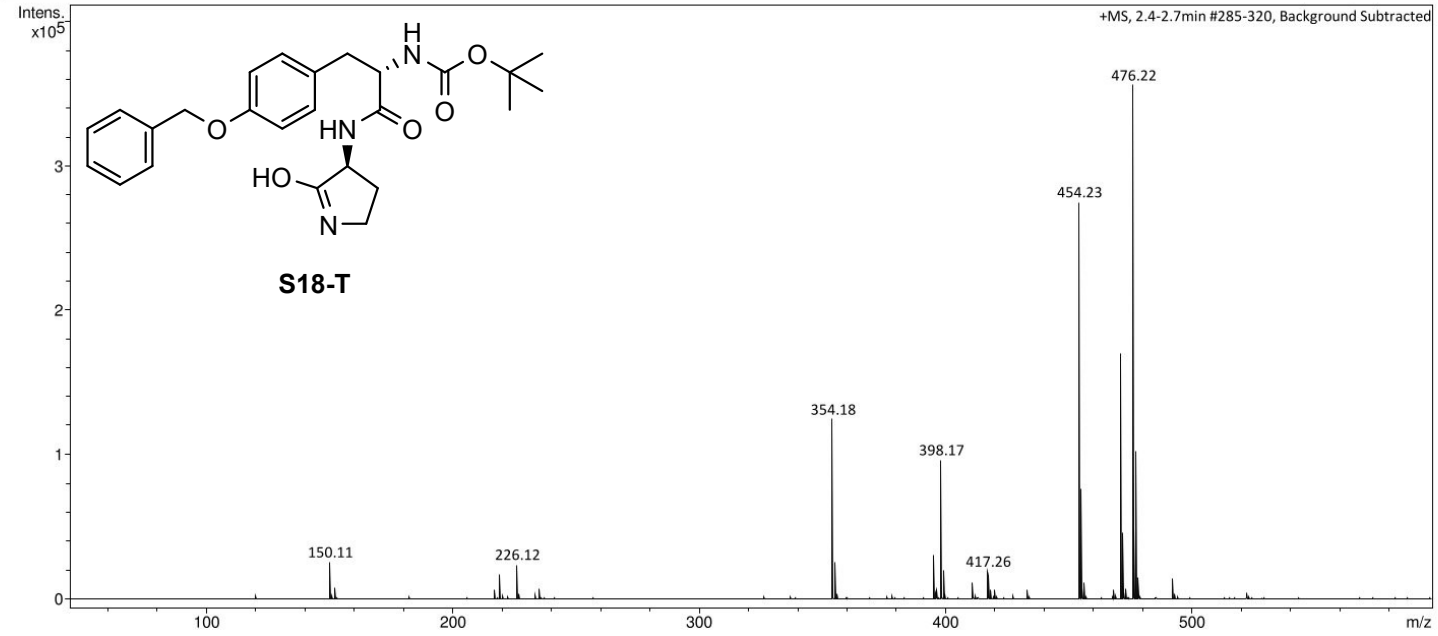
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Greulich-GRE-367 Glas B12_1_01_36078.d	Acquisition Date	12/2/2021 1:48:34 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE-367 Glas B12	Instrument	micrOTOF-Q 228888.00043
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



S18-T

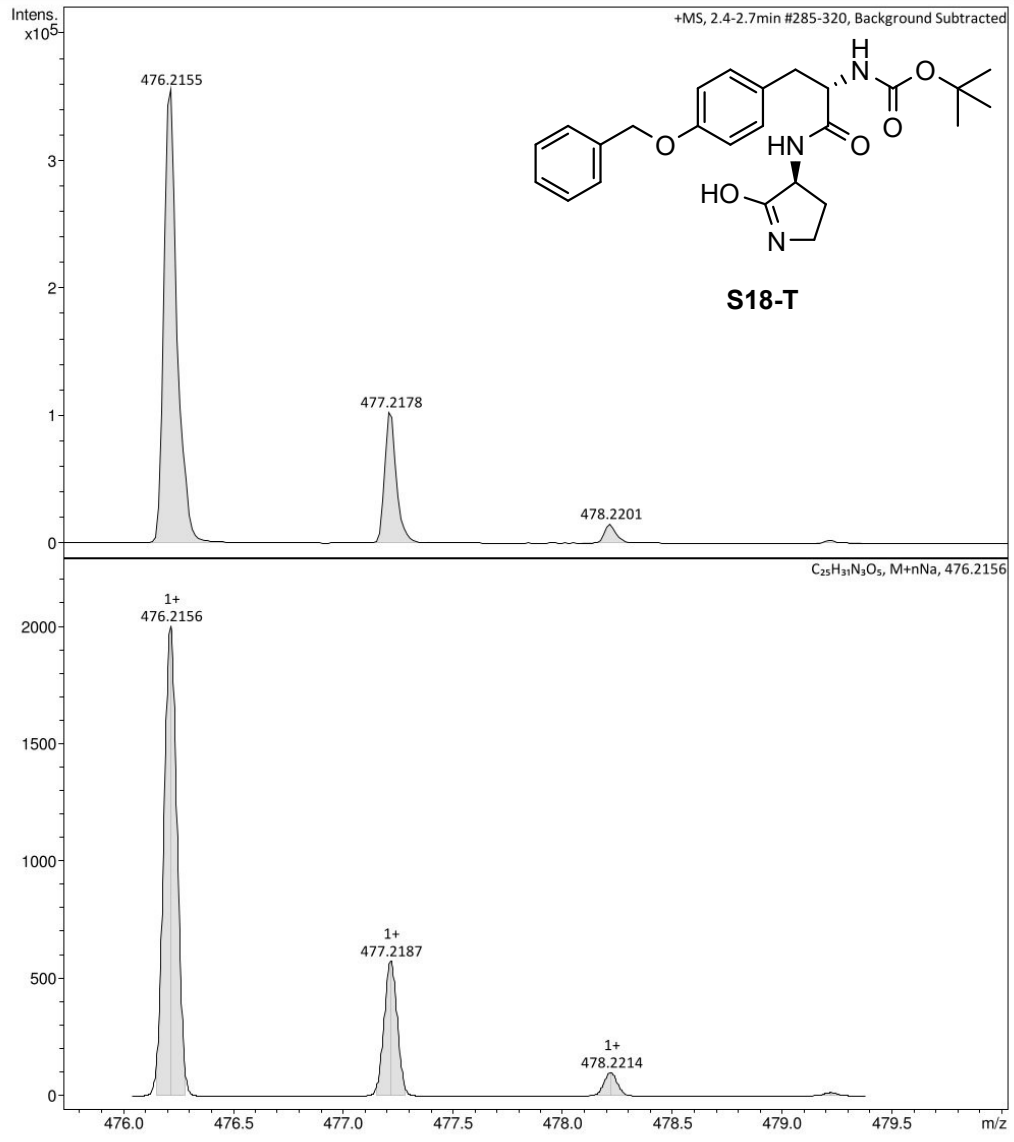
Massenspektrometrie - Universität Stuttgart

Analysis Info

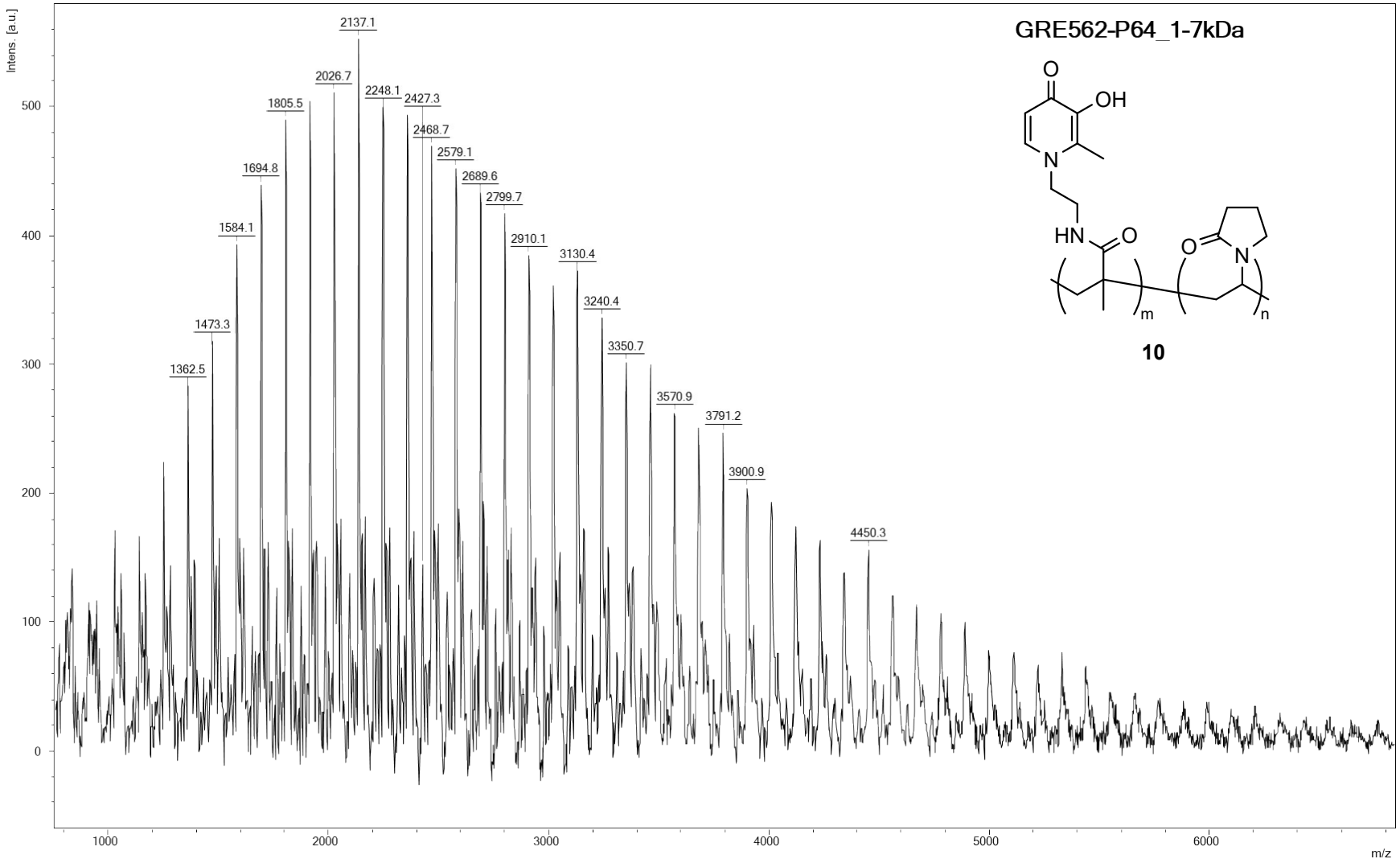
Analysis Name	Greulich-GRE-367 Glas B12_1_01_36078.d	Acquisition Date	12/2/2021 1:48:34 PM
Method	tune-low-oktober-2019.m	Operator	BDAL@DE
Sample Name	Greulich-GRE-367 Glas B12	Instrument	micrOTOF-Q 228888.00043
Comment			

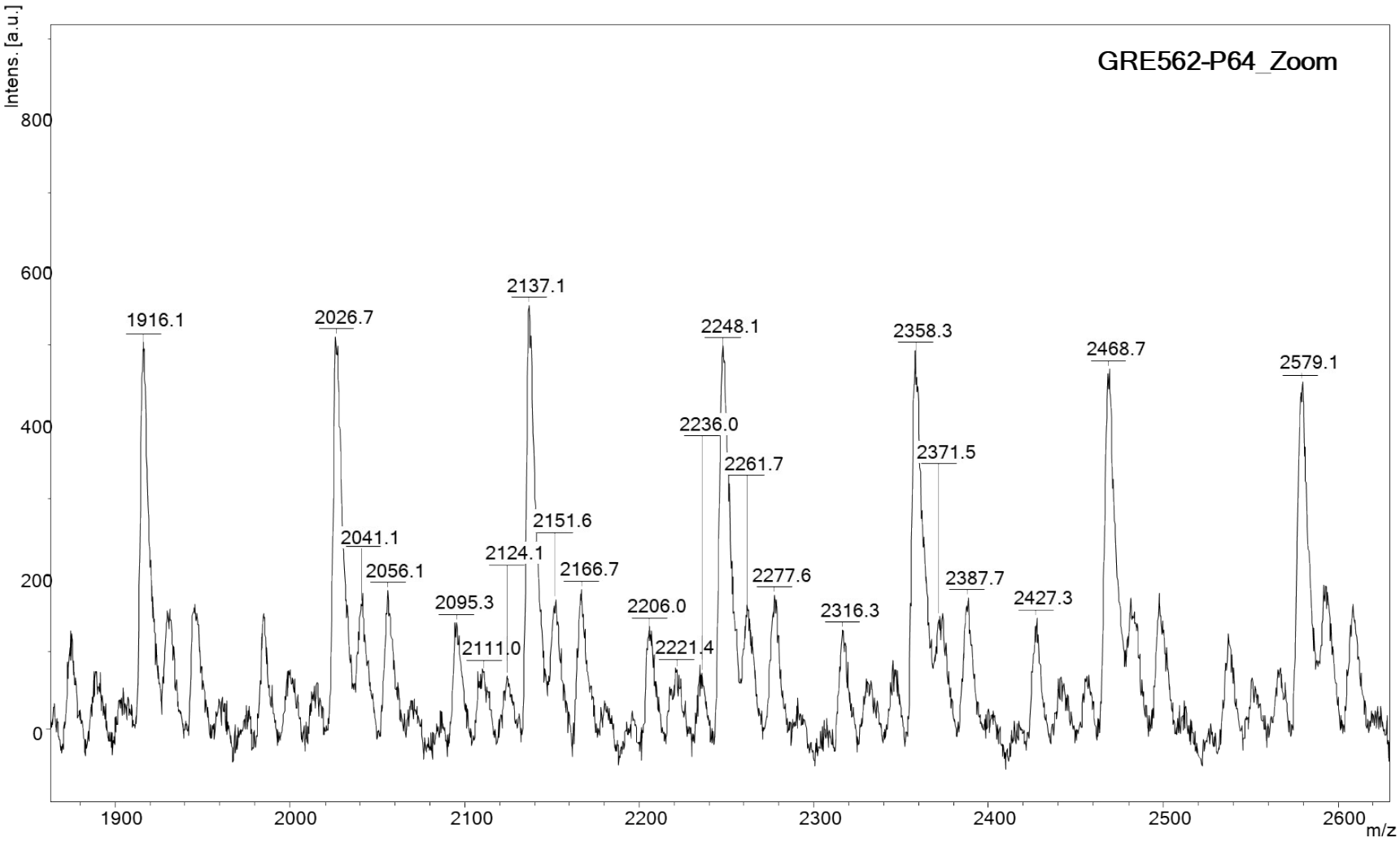
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste



13. MALDI spectra




GRE562-P64_Zoom
Intens. [a.u.]
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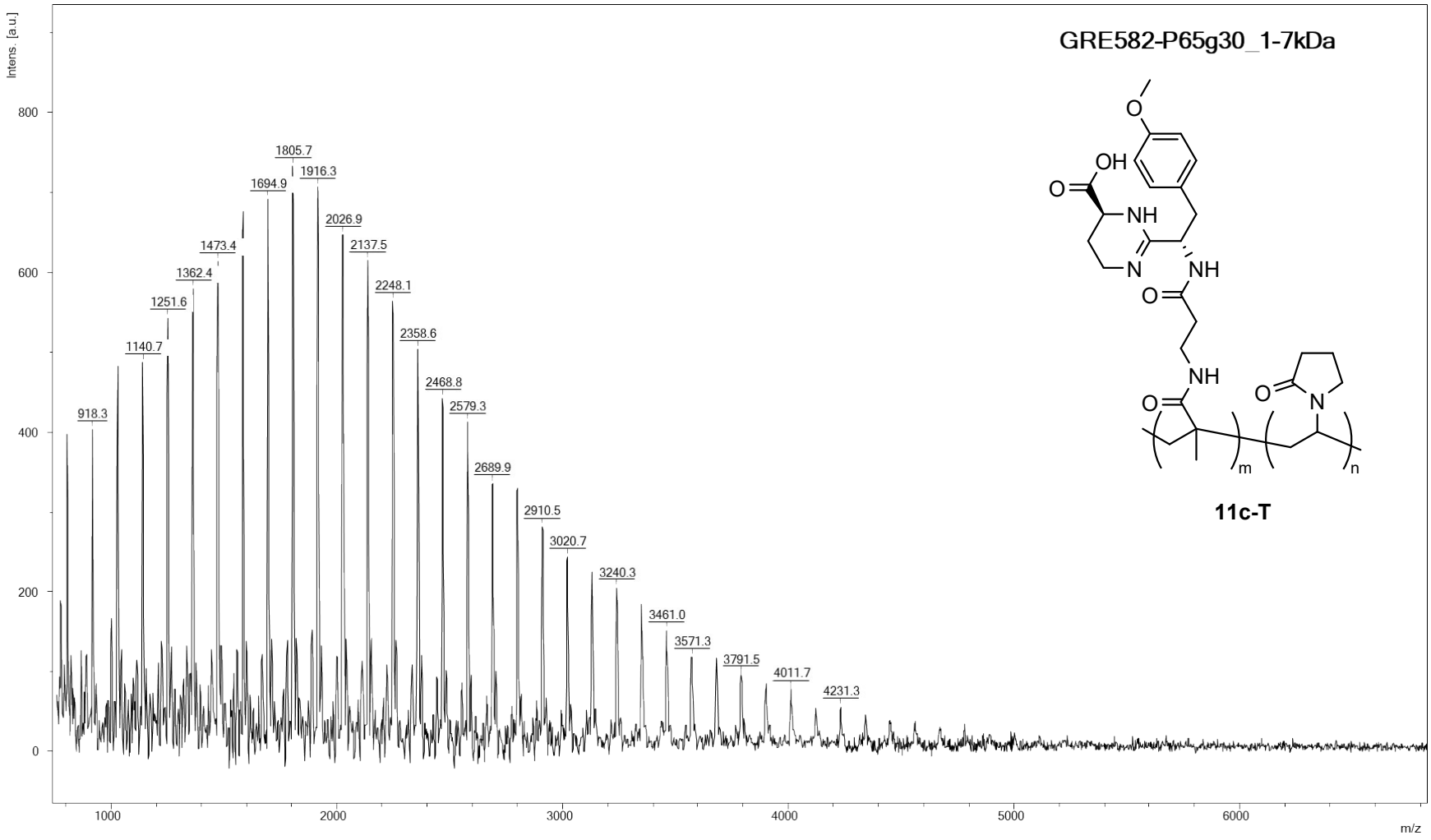
600
400
200
0
1900
2000
2100
2200
2300
2400
2500
2600
m/z
1916.1
2026.7
2137.1
2248.1
2358.3
2468.7
2579.1
2236.0
2261.7
2371.5
2041.1
2056.1
2151.6
2124.1
2166.7
2277.6
2387.7
2095.3
2111.0
2206.0
2221.4
2316.3
2427.3


GRE582-P65g30_1-7kDa
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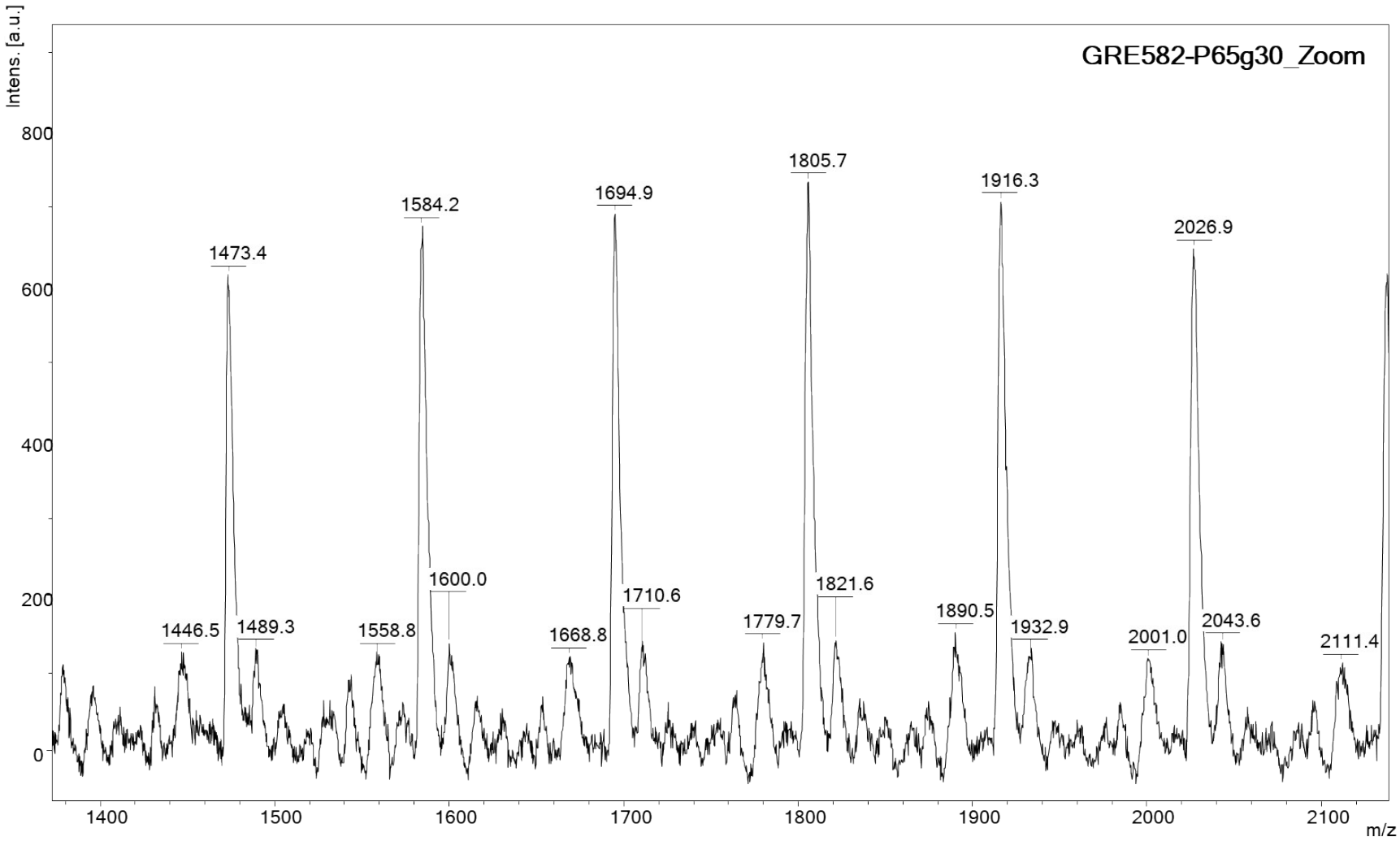
600
400
200
0
1000
2000
3000
4000
5000
6000
m/z
1805.7
1916.3
1694.9
2026.9
1473.4
2137.5
1362.4
2248.1
1251.6
2358.6
1140.7
2468.8
918.3
2579.3
2689.9
2910.5
3020.7
3240.3
3461.0
3571.3
3791.5
4011.7
4231.3
OH
O
NH
N
NH
O
NH
O
O
N
m
n
11c-T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Intens. [a.u.]
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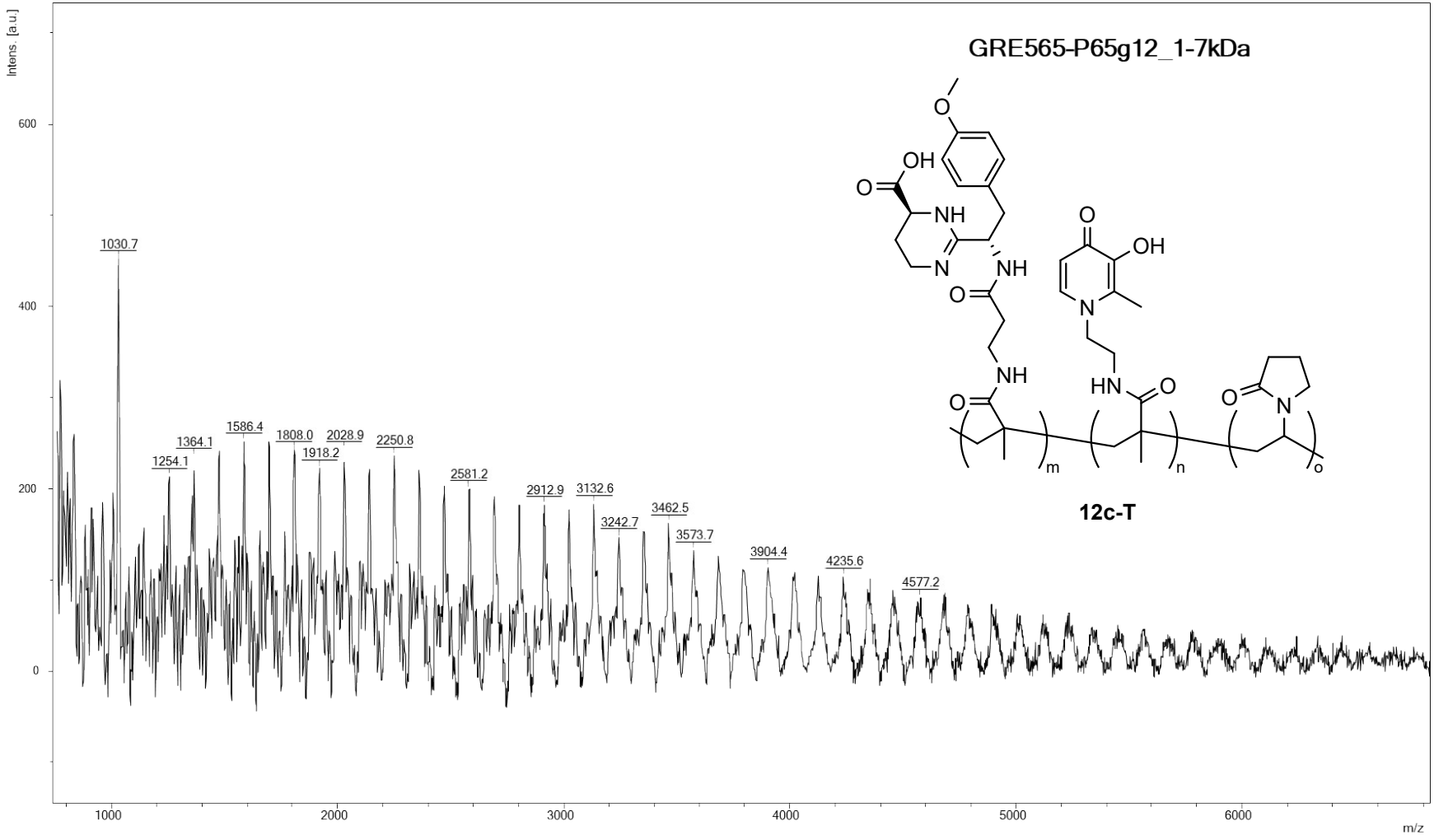
600
400
200
0
1400
1500
1600
1700
1800
1900
2000
2100
m/z
1446.5
1473.4
1489.3
1558.8
1584.2
1600.0
1668.8
1694.9
1710.6
1779.7
1805.7
1821.6
1890.5
1916.3
1932.9
2001.0
2026.9
2043.6
2111.4


GRE565-P65g12_1-7kDa
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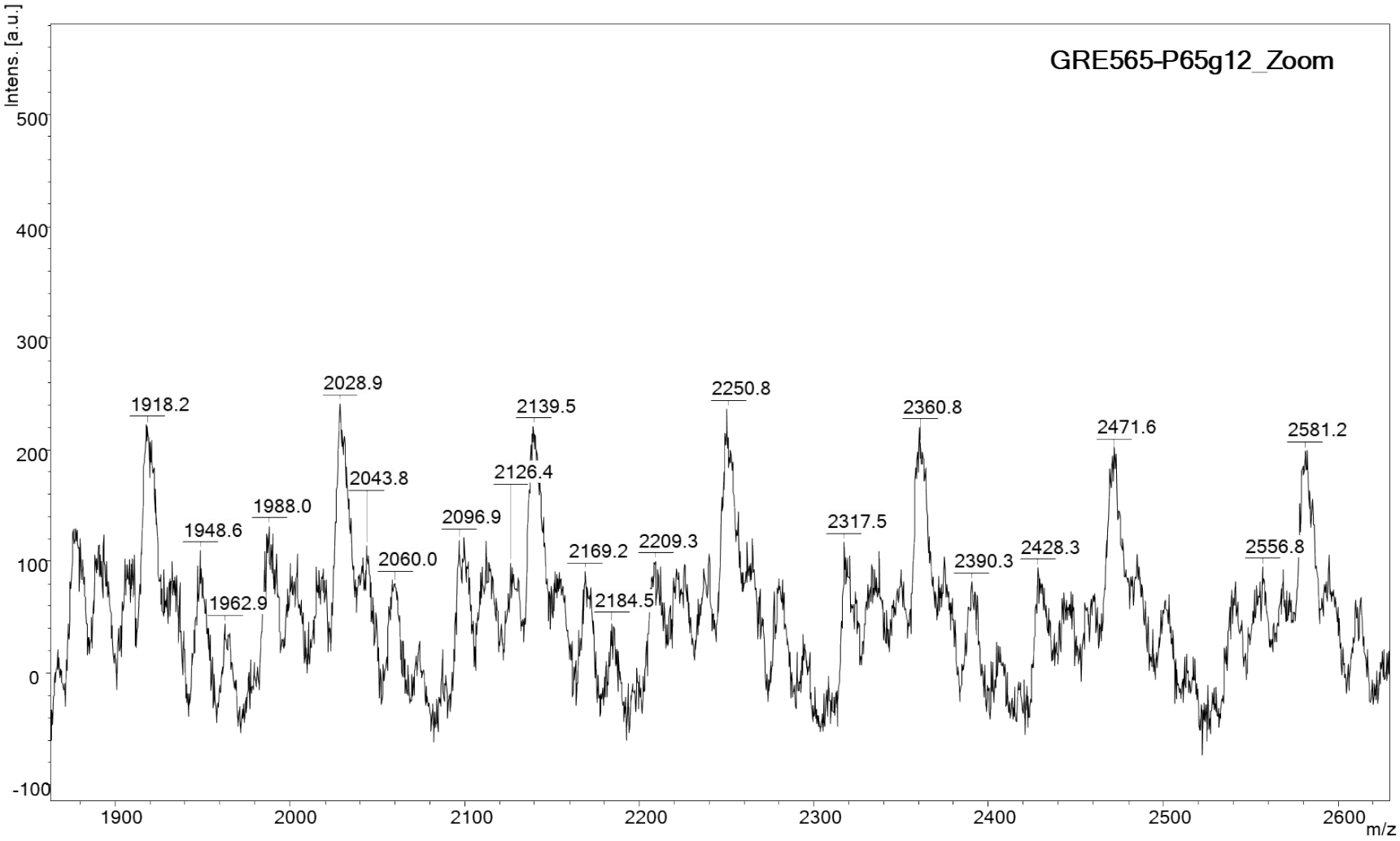
600
400
200
0
1030.7
1254.1
1364.1
1586.4
1808.0
1918.2
2028.9
2250.8
2581.2
2912.9
3132.6
3242.7
3462.5
3573.7
3904.4
4235.6
4577.2
1000
2000
3000
4000
5000
6000
m/z
12c-T


GRE565-P65g12_Zoom
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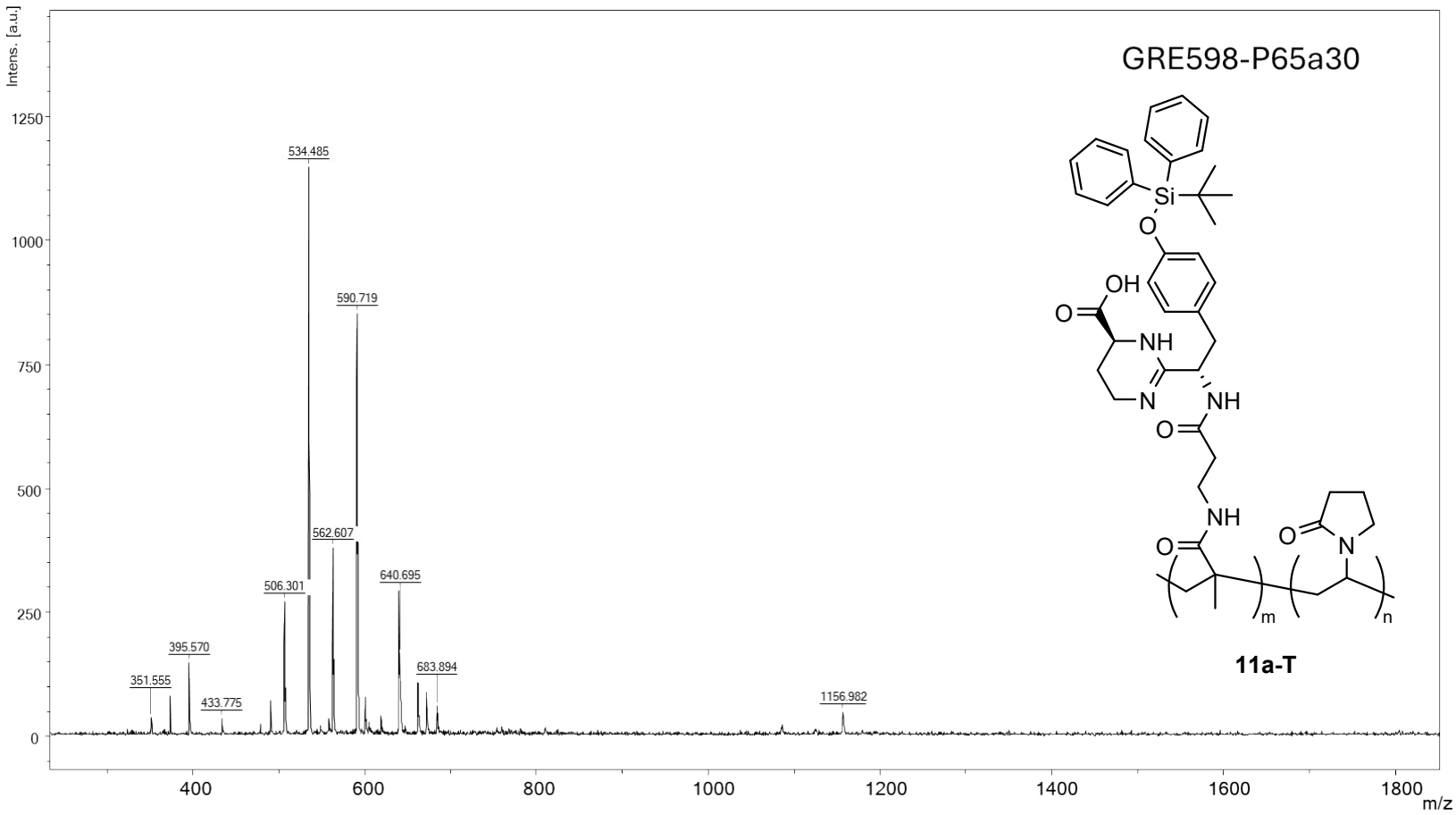
500
400
300
200
100
0
-100
1900
2000
2100
2200
2300
2400
2500
2600
m/z
1918.2
1948.6
1962.9
1988.0
2028.9
2043.8
2060.0
2096.9
2126.4
2139.5
2169.2
2184.5
2209.3
2250.8
2317.5
2360.8
2390.3
2428.3
2471.6
2556.8
2581.2


GRE598-P65a30
Intens. [a.u.]
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750
500
250
0
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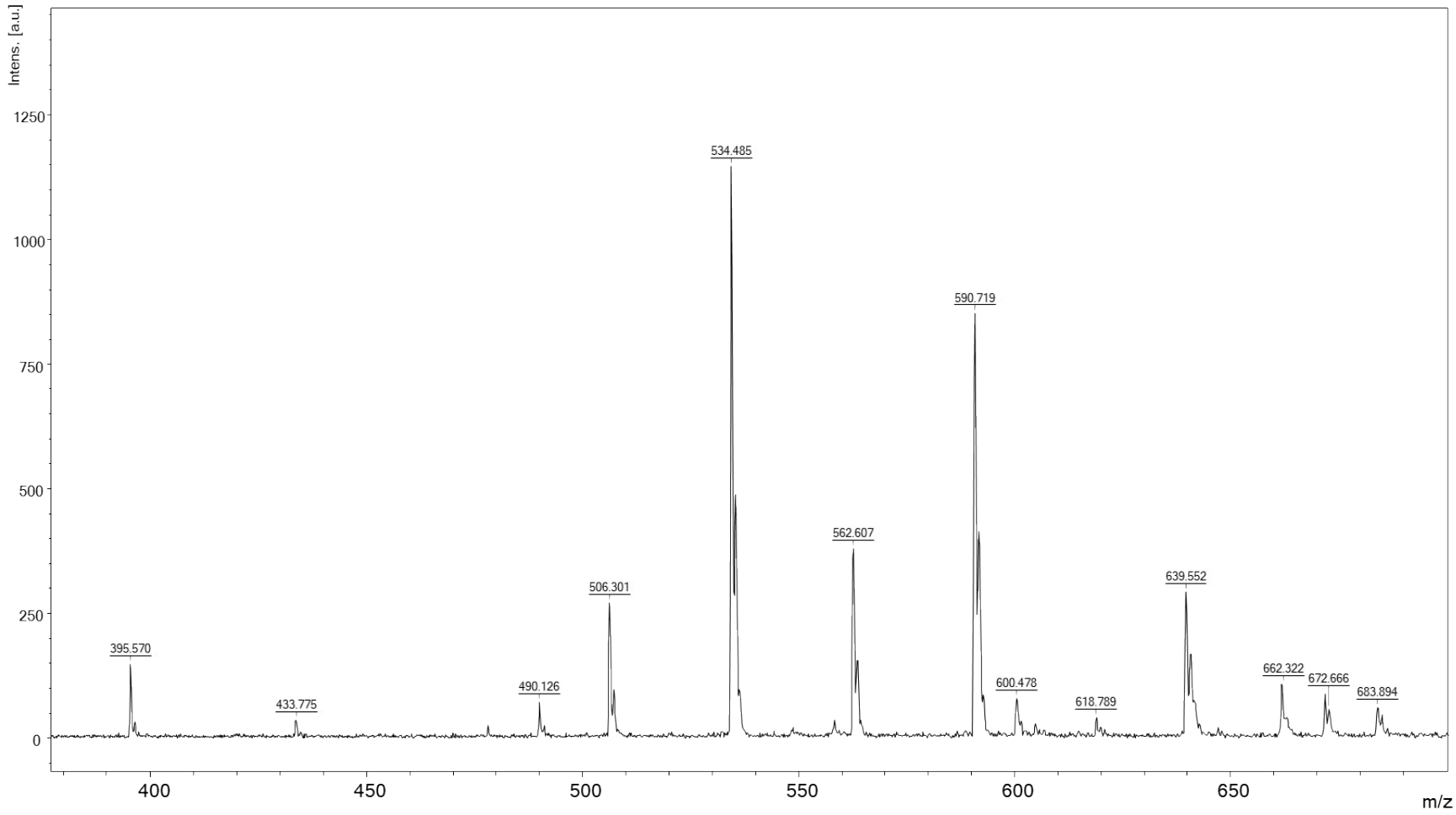
590.719
562.607
506.301
640.695
395.570
683.894
351.555
433.775
1156.982
400
600
800
1000
1200
1400
1600
1800
m/z
OH
O
NH
N
NH
O
NH
O
O
N
m
n
11a-T


Intens. [a.u.]
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1000
750
500
250
0
534.485
590.719
562.607
506.301
639.552
395.570
433.775
490.126
600.478
618.789
662.322
672.666
683.894
400
450
500
550
600
650
m/z

14. Biological tests – raw data

14.1 Cytotoxicity

17.03.2025 Polymers

	Gre562-**10**			Gre65-**12c-T**			Gre82-**11c-T**				only cells		
										Chlorhexidine		no cells	mg/mL
<>	1	2	3	4	5	6	7	8	9	10	11	12	
A	46804	48331	48615	49068	48006	45388	49184	50909	48544	11345	47343	6539	0,1
B	50601	45586	46796	46104	48893	45675	47112	47969	52020	12030	46317	6551	0,05
C	47400	46807	47945	44643	47808	46395	47504	49351	47245	10795	48063	6491	0,025
D	48520	45991	46182	44051	44762	44719	44612	46954	47174	24558	48747	6520	0,0125
E	43627	45915	44493	44687	48408	46808	43120	46977	45398	45878	45829	6483	0,0063
F	45405	46784	46688	45510	45204	44744	43941	46435	45847	44099	48483	6611	0,0031
G	42275	47943	45657	42380	42222	45294	44216	43682	45268	44752	46411	32251	0,0016
H	44456	42376	46555	44430	40569	42589	41613	42009	43669	44254	45320	35762	0,0008
												DMSO control	

17.03.2025 Monomers

	µM	100	50	25	12,5	6,25	3,125	1,56	0,78	0,39	Chlorhexidine	only cells	no cells
	<>	1	2	3	4	5	6	7	8	9	10	11	12
Gre543-**13a-T**	A	37380	39459	42565	39700	40236	42210	42509	40895	41085	7788	46005	6396
	B	34295	40403	45228	43992	45688	47900	44576	45533	49232	11842	42353	6418
Gre551-**13b-D**	C	34157	41718	45822	45968	44349	46017	45428	44078	46552	10423	46980	6326
	D	35139	41164	43986	46807	44274	43562	45093	44135	45337	18122	45412	6374
Gre556-**13c-T**	E	31492	41036	45991	43362	46685	45548	41617	44985	46925	44791	47617	6343
	F	34895	42552	45597	45117	45163	45276	44364	45698	44698	45021	45790	6620
Gre560-**13d-D**	G	34605	46480	45959	42836	42949	44365	42712	44521	46785	46111	44983	34330
	H	36165	39357	42207	43417	40788	41559	41169	45593	43503	41317	44444	34075
													DMSO control

21.03.2025 Polymers

	Gre562-**10**			Gre65-**12c-T**			Gre82-**11c-T**			Chlorhexidine	only cells	no cells	mg/mL
<>	1	2	3	4	5	6	7	8	9	10	11	12	
A	49931	53038	48899	49301	47943	47593	49200	48852	52899	14785	47762	6515	0,1
B	48435	44152	45644	45324	46988	48384	46476	48621	49505	22082	44152	6556	0,05
C	47811	45289	46126	43742	45685	45068	47989	46335	46456	13499	46183	6466	0,025
D	46999	45248	44220	46217	43754	43020	44067	46593	47394	31685	47561	6476	0,0125
E	45767	43985	44861	46764	46307	43874	43940	46671	47262	46340	47663	6469	0,00625
F	47030	44149	44922	45955	45925	45501	44601	45918	47715	44559	44948	6593	0,003125
G	45239	46991	43516	43591	40692	45428	42945	44035	45117	45376	45953	30956	0,00156
H	44241	42146	42762	42400	40693	42684	40054	41012	42705	48870	43050	28550	0,00078
												DMSO control	

21.03.2025 Monomers

	µM	100	50	25	12,5	6,25	3,125	1,56	0,78	0,39	Chlorhexidine	only cells	no cells
	<>	1	2	3	4	5	6	7	8	9	10	11	12
Gre543-**13a-T**	A	33073	43607	47094	47192	44920	45409	46807	45277	40251	13180	46635	6347
	B	33898	39136	43262	46914	47649	50556	47761	48619	48014	14905	43230	6356
Gre551-**13b-D**	C	34470	40919	50090	46472	48652	47869	48119	49065	48406	14321	46454	6249
	D	34426	38424	46093	46685	46501	45157	47144	48354	49141	29235	45116	6295
Gre556-**13c-T**	E	29914	41433	46410	46383	48587	44381	46409	47287	49457	47834	45519	6296
	F	31912	43211	47215	49739	47593	46538	45788	47842	48746	47142	46872	6511
Gre560-**13d-D**	G	33013	42272	45714	45529	43221	44090	46269	48709	44527	46898	43624	34345
	H	32632	37628	43184	43384	40156	41247	39951	41162	41384	41423	44741	33902
													DMSO control

14.2 Antimicrobial experiments

Layout 1 (polymers)

Concen. [mg/mL]		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
0,1	A B	GRE 562-**10**						GRE 565-**12c-T**						GRE 582-**11c-T**						Chlorhexidin (10µg/ml)		PBS+Medium		PBS+Medium	
0,05	C D	1:2	1:2	1:2				1:2	1:2	1:2				1:2	1:2	1:2				1:2					
0,025	E F	1:2	1:2	1:2				1:2	1:2	1:2				1:2	1:2	1:2				1:2					
0,0125	G H	1:2	1:2	1:2				1:2	1:2	1:2				1:2	1:2	1:2				1:2					
0,00625	I J	1:2	1:2	1:2				1:2	1:2	1:2				1:2	1:2	1:2				1:2					
0,00312	K L	1:2	1:2	1:2				1:2	1:2	1:2				1:2	1:2	1:2				1:2					
0,00156	M N	1:2	1:2	1:2				1:2	1:2	1:2				1:2	1:2	1:2				1:2				1% DMSO	
0,00078	O P	1:2	1:2	1:2				1:2	1:2	1:2				1:2	1:2	1:2				1:2					

Layout 2 (monomers)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	GRE 543-**13a-T**		1:2		1:2		1:2		1:2		1:2		1:2		1:2		1:2		Chlorhexidin (10µg/ml)		**PBS+Medium**		**PBS+Medium**	
B																								
C																			1:2					
D																								
E	GRE 551-**13b-D**		1:2		1:2		1:2		1:2		1:2		1:2		1:2		1:2		1:2					
F																								
G																			1:2					
H																								
I	GRE 556-**13c-T**		1:2		1:2		1:2		1:2		1:2		1:2		1:2		1:2		1:2					
J																								
K																			1:2					
L																								
M	GRE 560-**13d-D**		1:2		1:2		1:2		1:2		1:2		1:2		1:2		1:2		1:2				1% DMSO	
N																								
O																			1:2					
P																								
Concentration (µM)	**100**		**50**		**25**		**13**		**6,25**		**3,125**		**1,56**		**0,78**		**0,39**						PBS+Medium without cells	

E. coli WT

Layout N.1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	1,17	1,08	1,221	1,182	1,069	1,087	1,204	1,092	1,204	1,082	1,074	1,092	1,177	1,187	1,195	1,175	1,2	1,204	0,051	0,051	1,201	1,231	0,05	0,053
B	1,06	1,096	1,138	1,109	1,107	1,121	1,104	1,091	1,085	1,168	1,082	1,176	1,181	1,175	1,181	1,163	1,177	1,21	0,051	0,051	1,229	1,27	0,051	0,052
C	1,077	1,116	1,135	1,132	1,13	1,12	1,218	1,199	1,182	1,112	1,119	1,093	1,194	1,207	1,221	1,167	1,214	1,239	0,053	0,051	1,228	1,274	0,051	0,053
D	1,093	1,131	1,128	1,073	1,114	1,116	1,087	1,109	1,095	1,187	1,104	1,189	1,165	1,15	1,211	1,168	1,223	1,22	0,052	0,052	1,209	1,276	0,051	0,052
E	1,126	1,156	1,146	1,157	1,124	1,119	1,217	1,11	1,096	1,1	1,108	1,11	1,165	1,25	1,214	1,194	1,23	1,235	0,052	0,052	1,243	1,27	0,052	0,051
F	1,109	1,133	1,181	1,124	1,145	1,143	1,101	1,128	1,101	1,177	1,13	1,215	1,167	1,159	1,228	1,157	1,23	1,22	0,053	0,055	1,226	1,274	0,05	0,051
G	1,158	1,203	1,184	1,186	1,152	1,139	1,158	1,149	1,151	1,169	1,154	1,173	1,204	1,238	1,211	1,193	1,253	1,235	1,209	1,159	1,24	1,284	0,05	0,051
H	1,166	1,185	1,183	1,188	1,151	1,16	1,128	1,14	1,157	1,205	1,168	1,222	1,19	1,21	1,224	1,184	1,223	1,209	1,232	1,231	1,214	1,268	0,051	0,05
I	1,173	1,206	1,194	1,194	1,175	1,183	1,176	1,174	1,167	1,175	1,189	1,195	1,19	1,265	1,219	1,193	1,227	1,232	1,168	1,21	1,219	1,271	0,053	0,052
J	1,171	1,214	1,206	1,167	1,194	1,169	1,17	1,163	1,18	1,189	1,174	1,231	1,165	1,166	1,215	1,177	1,215	1,201	1,182	1,185	1,181	1,243	0,053	0,051
K	1,188	1,217	1,21	1,211	1,192	1,203	1,182	1,183	1,185	1,204	1,191	1,193	1,192	1,223	1,213	1,196	1,225	1,238	1,239	1,247	1,21	1,304	0,052	0,052
L	1,189	1,224	1,227	1,222	1,22	1,199	1,178	1,189	1,184	1,237	1,182	1,255	1,187	1,183	1,23	1,176	1,233	1,217	1,253	1,183	1,215	1,284	0,051	0,051
M	1,199	1,235	1,218	1,227	1,244	1,217	1,201	1,19	1,192	1,185	1,192	1,193	1,209	1,228	1,225	1,195	1,244	1,237	1,274	1,266	1,212	1,275	1,206	1,199
N	1,189	1,233	1,233	1,21	1,196	1,2	1,183	1,189	1,174	1,203	1,172	1,225	1,169	1,161	1,218	1,19	1,226	1,22	1,265	1,265	1,202	1,26	1,214	1,194
O	1,178	1,224	1,213	1,222	1,216	1,211	1,204	1,209	1,201	1,2	1,217	1,207	1,197	1,21	1,221	1,202	1,223	1,225	1,266	1,276	1,206	1,255	1,222	1,201
P	1,174	1,191	1,207	1,198	1,206	1,194	1,185	1,186	1,197	1,192	1,172	1,189	1,169	1,179	1,206	1,172	1,201	1,192	1,238	1,231	1,181	1,234	1,193	1,198

E. coli WT

Layout N.2	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	1,144	1,145	1,182	1,166	1,176	1,142	1,22	1,284	1,176	1,198	1,178	1,149	1,248	1,223	1,229	1,222	1,211	1,208	0,05	0,05	1,199	1,181	0,049	0,05
B	1,155	1,181	1,22	1,183	1,248	1,131	1,241	1,291	1,222	1,265	1,21	1,228	1,261	1,255	1,252	1,215	1,227	1,226	0,051	0,05	1,216	1,206	0,05	0,05
C	1,139	1,173	1,218	1,238	1,23	1,24	1,224	1,285	1,214	1,183	1,211	1,113	1,256	1,226	1,238	1,218	1,233	1,227	0,051	0,05	1,214	1,23	0,049	0,051
D	1,143	1,193	1,201	1,216	1,256	1,16	1,226	1,3	1,232	1,22	1,196	1,234	1,2	1,225	1,249	1,198	1,261	1,238	0,051	0,051	1,227	1,217	0,049	0,051
E	1,214	1,193	1,258	1,186	1,196	1,216	1,237	1,292	1,212	1,253	1,232	1,16	1,258	1,255	1,252	1,256	1,254	1,234	0,052	0,051	1,228	1,204	0,05	0,051
F	1,168	1,199	1,199	1,193	1,263	1,161	1,238	1,288	1,288	1,291	1,199	1,233	1,265	1,26	1,252	1,217	1,231	1,24	1,023	0,052	1,228	1,212	0,05	0,05
G	1,178	1,197	1,214	1,213	1,244	1,231	1,222	1,289	1,247	1,222	1,228	1,188	1,281	1,263	1,257	1,238	1,25	1,238	0,944	1,103	1,208	1,217	0,051	0,051
H	1,166	1,207	1,194	1,252	1,274	1,216	1,214	1,271	1,216	1,212	1,244	1,248	1,266	1,274	1,228	1,246	1,232	1,241	1,147	0,2	1,23	1,223	0,049	0,049
I	1,198	1,196	1,271	1,246	1,212	1,215	1,219	1,276	1,174	1,217	1,209	1,218	1,268	1,265	1,261	1,252	1,249	1,24	1,17	1,155	1,194	1,19	0,051	0,051
J	1,181	1,198	1,206	1,231	1,24	1,198	1,21	1,269	1,216	1,202	1,231	1,26	1,269	1,252	1,25	1,202	1,216	1,209	1,135	1,165	1,227	1,224	0,051	0,051
K	1,175	1,2	1,25	1,25	1,212	1,217	1,22	1,272	1,173	1,233	1,232	1,181	1,266	1,255	1,242	1,23	1,242	1,232	1,187	1,176	1,197	1,191	0,05	0,05
L	1,19	1,204	1,206	1,247	1,275	1,198	1,219	1,274	1,204	1,202	1,198	1,266	1,26	1,253	1,241	1,217	1,24	1,23	1,174	1,144	1,23	1,233	0,05	0,05
M	1,193	1,216	1,265	1,263	1,218	1,233	1,243	1,316	1,18	1,255	1,224	1,183	1,273	1,272	1,256	1,24	1,245	1,233	1,233	1,238	1,219	1,208	1,21	1,194
N	1,203	1,216	1,229	1,244	1,254	1,218	1,215	1,276	1,191	1,184	1,202	1,246	1,247	1,233	1,241	1,226	1,21	1,23	1,215	1,218	1,208	1,172	0,809	1,185
O	1,179	1,203	1,246	1,252	1,205	1,19	1,228	1,262	1,15	1,185	1,188	1,167	1,239	1,247	1,225	1,234	1,236	1,206	1,23	1,225	1,22	1,202	1,21	1,192
P	1,191	1,196	1,193	1,202	1,225	1,19	1,202	1,246	1,172	1,179	1,188	1,197	1,223	1,212	1,208	1,206	1,198	1,203	1,208	1,182	1,194	1,189	1,203	1,198

E. coli ΔTolC

Layout N.1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	1,208	1,088	0,906	1,183	0,863	0,893	0,879	1,076	1,035	0,918	1,077	0,928	1,314	1,307	1,303	1,28	1,322	1,315	0,051	0,05	1,302	1,325	0,052	0,053
B	1,099	0,975	1,245	0,948	1,043	1,202	0,9	1,264	0,865	0,861	0,983	0,878	1,347	1,366	1,309	1,302	1,362	1,335	0,05	0,051	1,424	1,354	0,051	0,052
C	1,132	1,047	0,942	1,152	0,876	0,94	1,127	1,071	1,079	1,143	1,1	1,06	1,32	1,359	1,357	1,362	1,356	1,401	0,053	0,051	1,353	1,399	0,051	0,052
D	1,067	0,972	1,261	0,886	0,962	1,244	1,192	1,016	1,014	1,115	1,099	1,049	1,325	1,319	1,317	1,317	1,385	1,36	0,051	0,051	1,341	1,308	0,051	0,053
E	1,051	1,077	1,057	1,096	1,038	1,106	1,18	1,178	1,219	1,248	1,177	1,198	1,337	1,349	1,373	1,41	1,366	1,382	0,051	0,052	1,363	1,364	0,051	0,052
F	1,026	1,084	1,146	1,137	1,09	1,156	1,225	1,239	1,194	1,169	1,196	1,169	1,366	1,347	1,387	1,348	1,376	1,361	0,051	0,051	1,422	1,395	0,051	0,051
G	1,218	1,213	1,221	1,391	1,187	1,236	1,321	1,305	1,35	1,322	1,323	1,323	1,357	1,367	1,361	1,409	1,359	1,349	0,06	0,133	1,393	1,395	0,051	0,052
H	1,214	1,217	1,284	1,232	1,24	1,236	1,301	1,304	1,314	1,349	1,328	1,326	1,386	1,381	1,383	1,347	1,348	1,341	0,052	0,167	1,392	1,387	0,05	0,05
I	1,351	1,34	1,307	1,368	1,339	1,322	1,34	1,342	1,354	1,365	1,345	1,357	1,392	1,401	1,381	1,364	1,373	1,372	1,28	1,384	1,345	1,384	0,052	0,053
J	1,337	1,299	1,383	1,333	1,321	1,349	1,333	1,35	1,313	1,301	1,335	1,332	1,368	1,347	1,373	1,34	1,358	1,337	1,24	1,205	1,39	1,39	0,051	0,051
K	1,384	1,379	1,366	1,372	1,348	1,367	1,367	1,349	1,339	1,347	1,373	1,364	1,367	1,359	1,361	1,357	1,384	1,384	1,354	1,321	1,336	1,416	0,051	0,051
L	1,337	1,417	1,38	1,386	1,36	1,347	1,358	1,297	1,361	1,348	1,372	1,368	1,369	1,367	1,345	1,35	1,357	1,355	1,322	1,314	1,411	1,384	0,051	0,051
M	1,365	1,399	1,408	1,413	1,387	1,387	1,397	1,346	1,379	1,359	1,371	1,35	1,35	1,361	1,366	1,344	1,379	1,36	1,335	1,351	1,337	1,377	1,322	1,278
N	1,338	1,334	1,388	1,388	1,367	1,389	1,388	1,319	1,354	1,342	1,361	1,337	1,368	1,364	1,344	1,366	1,333	1,358	1,324	1,349	1,434	1,386	1,299	1,277
O	1,399	1,385	1,363	1,374	1,359	1,383	1,384	1,371	1,376	1,347	1,392	1,368	1,351	1,349	1,346	1,335	1,373	1,36	1,368	1,417	1,308	1,374	1,321	1,292
P	1,329	1,329	1,358	1,329	1,36	1,328	1,262	1,365	1,316	1,362	1,339	1,327	1,331	1,308	1,319	1,333	1,288	1,294	1,306	1,315	1,341	1,341	1,274	1,285

E. coli ΔTolC

Layout N.2	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	1,137	1,152	1,247	1,232	1,308	1,309	1,328	1,304	1,307	1,28	1,298	1,275	1,306	1,315	1,347	1,344	1,346	1,319	0,051	0,05	1,362	1,351	0,051	0,052
B	1,16	1,177	1,235	1,237	1,306	1,334	1,365	1,373	1,321	1,359	1,279	1,305	1,354	1,381	1,412	1,42	1,371	1,393	0,051	0,05	1,432	1,449	0,051	0,052
C	1,156	1,171	1,314	1,229	1,316	1,321	1,344	1,364	1,28	1,266	1,257	1,306	1,333	1,338	1,387	1,387	1,392	1,435	0,054	0,051	1,453	1,476	0,05	0,052
D	1,141	1,141	1,224	1,219	1,329	1,361	1,363	1,382	1,311	1,322	1,25	1,313	1,326	1,334	1,396	1,406	1,383	1,411	0,051	0,051	1,421	1,433	0,051	0,052
E	1,218	1,191	1,323	1,281	1,347	1,32	1,372	1,389	1,29	1,318	1,304	1,267	1,342	1,357	1,399	1,383	1,392	1,384	0,053	0,051	1,422	1,454	0,051	0,052
F	1,237	1,188	1,304	1,282	1,338	1,36	1,399	1,397	1,344	1,342	1,311	1,326	1,347	1,351	1,38	1,359	1,391	1,414	0,053	0,053	1,448	1,442	0,051	0,051
G	1,2	1,153	1,35	1,365	1,362	1,383	1,376	1,386	1,32	1,323	1,308	1,278	1,227	1,338	1,383	1,385	1,426	1,422	1,063	1,244	1,447	1,516	0,05	0,051
H	1,185	1,173	1,366	1,359	1,378	1,375	1,387	1,368	1,325	1,335	1,31	1,307	1,359	1,363	1,382	1,377	1,379	1,366	1,181	0,882	1,373	1,483	0,05	0,05
I	1,351	1,347	1,389	1,417	1,41	1,417	1,372	1,386	1,318	1,287	1,303	1,3	1,234	1,366	1,415	1,378	1,365	1,435	1,411	1,396	1,413	1,456	0,052	0,052
J	1,324	1,335	1,386	1,397	1,387	1,355	1,397	1,399	1,321	1,34	1,288	1,303	1,347	1,354	1,411	1,33	1,397	1,423	1,417	1,472	1,425	1,417	0,051	0,051
K	1,313	1,345	1,389	1,389	1,393	1,408	1,394	1,396	1,302	1,293	1,302	1,303	1,354	1,35	1,424	1,423	1,38	1,382	1,39	1,338	1,449	1,463	0,051	0,052
L	1,331	1,366	1,408	1,401	1,394	1,379	1,393	1,417	1,339	1,347	1,328	1,327	1,32	1,362	1,406	1,368	1,397	1,412	1,384	1,341	1,446	1,431	0,05	0,05
M	1,312	1,349	1,387	1,39	1,403	1,411	1,408	1,399	1,301	1,314	1,333	1,318	1,352	1,351	1,411	1,39	1,372	1,398	1,444	1,389	1,402	1,426	1,368	1,322
N	1,265	1,361	1,401	1,4	1,405	1,389	1,363	1,381	1,321	1,329	1,305	1,161	1,335	1,339	1,405	1,594	1,294	1,42	1,357	1,406	1,377	1,392	1,327	1,314
O	1,309	1,33	1,369	1,399	1,39	1,39	1,397	1,372	1,321	1,32	1,277	1,28	1,3	1,355	1,421	1,416	1,4	1,385	1,443	1,436	1,395	1,4	1,357	1,305
P	1,32	1,343	1,361	1,357	1,36	1,345	1,349	1,329	1,302	1,312	1,252	1,263	1,259	1,331	1,357	1,487	1,251	1,362	1,411	1,384	1,364	1,329	1,303	1,298

S. aureus

Layout N.1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	0,56	0,544	0,562	0,53	0,54	0,545	0,549	0,539	0,541	0,564	0,545	0,555	0,617	0,597	0,593	0,589	0,602	0,601	0,052	0,053	0,542	0,545	0,052	0,053
B	0,581	0,516	0,552	0,487	0,531	0,539	0,521	0,519	0,52	0,551	0,538	0,501	0,566	0,589	0,587	0,577	0,586	0,627	0,052	0,053	0,551	0,527	0,052	0,054
C	0,589	0,568	0,551	0,524	0,532	0,534	0,519	0,52	0,51	0,53	0,533	0,532	0,536	0,53	0,532	0,552	0,574	0,564	0,054	0,053	0,521	0,555	0,052	0,054
D	0,593	0,605	0,543	0,551	0,549	0,548	0,499	0,533	0,53	0,529	0,524	0,493	0,547	0,543	0,532	0,57	0,543	0,558	0,054	0,054	0,538	0,519	0,052	0,053
E	0,565	0,543	0,536	0,501	0,502	0,527	0,547	0,518	0,515	0,534	0,529	0,521	0,533	0,536	0,535	0,538	0,539	0,553	0,061	0,061	0,541	0,554	0,052	0,056
F	0,558	0,538	0,524	0,496	0,517	0,51	0,518	0,518	0,522	0,518	0,514	0,52	0,538	0,54	0,534	0,54	0,529	0,558	0,059	0,061	0,547	0,544	0,053	0,053
G	0,558	0,531	0,533	0,511	0,503	0,521	0,539	0,514	0,519	0,529	0,523	0,541	0,538	0,537	0,532	0,525	0,546	0,567	0,185	0,063	0,537	0,556	0,052	0,053
H	0,571	0,539	0,52	0,503	0,507	0,499	0,519	0,519	0,51	0,515	0,505	0,509	0,526	0,552	0,517	0,522	0,518	0,533	0,136	0,481	0,527	0,541	0,052	0,052
I	0,547	0,529	0,531	0,503	0,515	0,522	0,535	0,519	0,516	0,539	0,523	0,528	0,523	0,522	0,521	0,527	0,525	0,526	0,573	0,581	0,519	0,551	0,062	0,061
J	0,574	0,544	0,536	0,51	0,53	0,517	0,516	0,531	0,514	0,531	0,517	0,515	0,525	0,535	0,506	0,537	0,526	0,541	0,571	0,574	0,54	0,558	0,054	0,056
K	0,554	0,544	0,545	0,515	0,503	0,524	0,54	0,517	0,504	0,523	0,505	0,526	0,523	0,52	0,512	0,518	0,521	0,527	0,564	0,542	0,507	0,532	0,053	0,054
L	0,577	0,56	0,545	0,5	0,53	0,521	0,528	0,522	0,507	0,532	0,525	0,507	0,512	0,515	0,506	0,539	0,51	0,522	0,526	0,532	0,547	0,537	0,053	0,052
M	0,555	0,565	0,555	0,547	0,556	0,544	0,555	0,522	0,531	0,528	0,518	0,492	0,53	0,526	0,532	0,526	0,545	0,542	0,525	0,543	0,53	0,545	0,543	0,533
N	0,551	0,541	0,551	0,53	0,523	0,524	0,545	0,544	0,529	0,535	0,524	0,523	0,505	0,535	0,51	0,544	0,533	0,546	0,512	0,527	0,554	0,553	0,547	0,497
O	0,577	0,539	0,561	0,531	0,525	0,547	0,557	0,527	0,544	0,549	0,549	0,507	0,525	0,535	0,523	0,558	0,551	0,542	0,557	0,559	0,54	0,537	0,748	0,81
P	0,564	0,568	0,574	0,537	0,565	0,547	0,542	0,575	0,578	0,559	0,566	0,588	0,536	0,56	0,529	0,549	0,542	0,557	0,527	0,533	0,544	0,527	0,526	0,524

S. aureus

Layout N.2	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	0,625	0,608	0,632	0,595	0,56	0,561	0,583	0,586	0,578	0,555	0,566	0,586	0,592	0,592	0,586	0,575	0,583	0,587	0,052	0,051	0,581	0,543	0,05	0,052
B	0,62	0,606	0,625	0,602	0,597	0,559	0,564	0,552	0,526	0,557	0,557	0,569	0,562	0,549	0,58	0,574	0,578	0,544	0,052	0,051	0,537	0,553	0,052	0,051
C	0,596	0,584	0,594	0,563	0,536	0,53	0,555	0,546	0,544	0,531	0,534	0,563	0,552	0,559	0,55	0,529	0,558	0,55	0,052	0,052	0,523	0,514	0,051	0,053
D	0,621	0,575	0,639	0,601	0,586	0,536	0,547	0,527	0,536	0,544	0,55	0,571	0,555	0,546	0,569	0,548	0,558	0,56	0,051	0,052	0,534	0,537	0,052	0,052
E	0,59	0,576	0,612	0,57	0,536	0,518	0,531	0,536	0,529	0,533	0,526	0,527	0,54	0,538	0,538	0,536	0,533	0,541	0,051	0,051	0,544	0,528	0,051	0,053
F	0,597	0,592	0,655	0,613	0,612	0,542	0,527	0,54	0,545	0,544	0,541	0,535	0,554	0,53	0,542	0,536	0,552	0,554	0,052	0,052	0,542	0,537	0,057	0,065
G	0,578	0,598	0,616	0,547	0,536	0,533	0,523	0,536	0,536	0,532	0,53	0,54	0,537	0,542	0,534	0,526	0,525	0,541	0,122	0,103	0,545	0,514	0,051	0,051
H	0,588	0,585	0,623	0,626	0,581	0,527	0,532	0,53	0,528	0,531	0,543	0,54	0,535	0,542	0,529	0,519	0,548	0,544	0,361	0,497	0,522	0,524	0,05	0,05
I	0,594	0,558	0,626	0,549	0,525	0,531	0,512	0,522	0,525	0,539	0,534	0,533	0,537	0,54	0,527	0,533	0,534	0,543	0,55	0,553	0,536	0,514	0,052	0,053
J	0,589	0,567	0,647	0,633	0,607	0,528	0,518	0,527	0,527	0,531	0,534	0,554	0,54	0,526	0,528	0,505	0,538	0,532	0,538	0,529	0,511	0,527	0,053	0,052
K	0,598	0,561	0,613	0,554	0,539	0,529	0,517	0,538	0,53	0,525	0,526	0,538	0,561	0,541	0,539	0,531	0,531	0,536	0,55	0,543	0,529	0,508	0,051	0,051
L	0,584	0,571	0,652	0,629	0,613	0,531	0,529	0,534	0,532	0,527	0,546	0,555	0,53	0,53	0,529	0,527	0,543	0,544	0,543	0,553	0,527	0,543	0,051	0,051
M	0,594	0,543	0,603	0,564	0,538	0,541	0,524	0,559	0,539	0,549	0,526	0,549	0,534	0,544	0,545	0,544	0,537	0,552	0,524	0,536	0,544	0,535	0,525	0,526
N	0,595	0,566	0,644	0,629	0,627	0,536	0,537	0,53	0,55	0,535	0,549	0,56	0,527	0,536	0,531	0,55	0,544	0,532	0,52	0,546	0,499	0,54	0,496	0,511
O	0,597	0,564	0,632	0,575	0,566	0,536	0,547	0,562	0,552	0,561	0,55	0,565	0,547	0,556	0,562	0,556	0,562	0,563	0,536	0,534	0,538	0,519	0,503	0,547
P	0,593	0,567	0,664	0,637	0,649	0,568	0,578	0,572	0,583	0,565	0,577	0,562	0,576	0,551	0,546	0,543	0,587	0,58	0,539	0,54	0,503	0,551	0,532	0,585

K. pneumoniae

Layout N.1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	0,776	0,769	0,746	0,844	0,754	0,751	0,729	0,734	0,752	0,734	0,744	0,764	0,807	0,855	0,859	0,859	0,821	0,813	0,051	0,05	0,863	1,165	0,051	0,053
B	0,722	0,671	0,677	0,69	0,668	0,684	0,636	0,636	0,629	0,641	0,632	0,627	0,735	0,755	0,699	0,61	0,753	0,804	0,053	0,053	0,839	0,782	0,05	0,058
C	0,769	0,716	0,704	0,795	0,708	0,71	0,681	0,691	0,698	0,668	0,673	0,686	0,752	0,787	0,777	0,804	0,762	0,79	0,052	0,051	0,84	1,102	0,053	0,054
D	0,742	0,687	0,685	0,674	0,701	0,69	0,666	0,657	0,667	0,663	0,632	0,683	0,68	0,728	0,702	0,724	0,788	0,784	0,054	0,053	0,686	0,796	0,052	0,052
E	0,818	0,765	0,738	0,975	0,728	0,735	0,724	0,732	0,732	0,684	0,744	0,703	0,716	0,723	0,748	0,798	0,75	0,782	0,174	0,062	0,791	1,084	0,053	0,055
F	0,799	0,739	0,776	0,749	0,763	0,735	0,712	0,718	0,742	0,671	0,678	0,727	0,695	0,783	0,721	0,76	0,808	0,808	0,554	0,18	0,862	0,81	0,051	0,053
G	0,82	0,829	0,801	1,043	0,771	0,757	0,727	0,794	0,754	0,749	0,774	0,746	0,764	0,741	0,801	0,757	0,769	0,778	0,992	0,967	0,802	1,097	0,054	0,055
H	0,82	0,826	0,809	0,784	0,751	0,768	0,72	0,723	0,763	0,721	0,765	0,762	0,701	0,787	0,747	0,74	0,737	0,734	0,85	0,811	0,81	0,783	0,053	0,051
I	0,87	0,834	0,82	1,033	0,778	0,757	0,726	0,763	0,769	0,78	0,753	0,802	0,804	0,754	0,77	0,628	0,757	0,782	0,896	0,845	0,822	1,082	0,053	0,054
J	0,79	0,793	0,772	0,743	0,779	0,748	0,746	0,736	0,75	0,717	0,688	0,747	0,686	0,769	0,742	0,715	0,749	0,703	0,825	0,791	0,693	0,755	0,052	0,053
K	0,861	0,812	0,817	1,039	0,75	0,761	0,757	0,774	0,79	0,727	0,792	0,771	0,788	0,762	0,797	0,792	0,777	0,767	0,863	0,806	0,776	1,109	0,052	0,054
L	0,85	0,826	0,797	0,842	0,768	0,8	0,751	0,762	0,743	0,713	0,758	0,763	0,724	0,761	0,75	0,72	0,78	0,82	0,839	0,785	0,821	0,823	0,053	0,051
M	0,868	0,824	0,838	1,031	0,776	0,784	0,761	0,771	0,783	0,735	0,781	0,813	0,782	0,796	0,78	0,8	0,782	0,788	0,836	0,83	0,822	1,096	0,882	0,743
N	0,855	0,829	0,798	0,829	0,753	0,771	0,729	0,742	0,737	0,718	0,734	0,758	0,733	0,75	0,75	0,731	0,774	0,771	0,813	0,786	0,768	0,785	0,816	0,881
O	0,853	0,781	0,813	0,988	0,75	0,758	0,734	0,766	0,746	0,718	0,793	0,8	0,758	0,768	0,789	0,824	0,781	0,774	0,819	0,799	0,808	0,86	0,822	0,742
P	0,84	0,834	0,879	0,82	0,846	0,709	0,805	0,824	0,807	0,8	0,816	0,803	0,815	0,794	0,782	0,806	0,822	0,792	0,86	0,848	0,681	0,85	0,886	0,87

K. pneumoniae

Layout N.2	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	1,238	1,183	1,341	1,354	1,296	1,284	1,236	1,206	1,025	0,927	0,931	0,891	0,874	0,847	0,905	0,865	0,88	1,101	0,051	0,051	0,929	1,096	0,051	0,051
B	1,233	1,458	1,333	1,423	1,26	1,238	0,829	1,104	0,915	0,903	1,124	1,201	0,86	0,831	0,879	0,858	1,162	1,093	0,052	0,051	0,898	1,139	0,051	0,052
C	1,357	1,363	1,387	1,407	1,355	1,336	1,336	1,252	0,966	0,945	0,921	0,954	0,928	0,871	0,905	0,89	0,913	1,136	0,052	0,052	0,951	1,17	0,051	0,052
D	1,345	1,417	1,362	1,404	1,306	1,348	1,128	1,215	1,023	0,899	1,107	1,166	0,891	0,86	0,879	0,837	1,087	1,133	0,057	0,052	0,932	1,109	0,051	0,052
E	1,314	1,202	1,375	1,134	1,062	1,148	1,045	1,189	1,085	0,957	0,929	0,942	0,904	0,884	0,922	0,905	0,893	1,145	0,821	1,079	0,931	1,18	0,051	0,052
F	1,325	1,442	1,379	1,434	1,325	1,337	1,05	1,14	1,111	1,094	1,133	1,303	0,898	0,886	0,865	0,884	1,077	1,121	1,165	1,045	0,91	1,169	0,051	0,052
G	1,386	1,424	1,362	1,362	1,364	1,353	1,295	1,327	1,279	1,275	1,141	0,94	1,017	0,899	0,9	0,916	0,9	1,126	1,205	1,366	0,92	1,22	0,053	0,052
H	1,355	1,395	1,355	1,414	1,304	1,324	1,3	1,309	1,23	1,248	1,332	1,384	0,915	1,021	0,879	0,907	1,117	1,164	1,25	1,312	0,908	1,106	0,052	0,051
I	1,3	1,375	1,399	1,376	1,364	1,342	1,154	1,04	1,162	1,036	0,945	0,872	0,907	0,843	0,916	0,865	0,897	1,108	1,121	1,176	0,939	1,21	0,053	0,053
J	1,184	1,362	1,224	1,444	1,11	1,058	1,137	1,108	0,923	0,945	1,113	1,18	0,892	0,935	0,901	0,889	1,11	1,108	1,088	1,24	0,924	1,146	0,052	0,052
K	0,748	0,893	1,028	1,157	1,133	1,214	0,98	0,928	0,923	0,874	0,906	0,902	0,892	0,837	0,874	0,889	0,888	1,093	1,077	1,137	0,922	1,191	0,052	0,052
L	0,857	1,241	0,969	1,22	0,922	0,898	0,878	0,884	0,924	0,932	1,12	1,2	0,855	0,863	0,887	0,867	1,091	1,138	1,084	1,167	0,942	1,123	0,052	0,051
M	0,879	0,906	0,97	0,973	0,942	0,901	0,932	0,925	0,916	0,87	0,894	0,87	0,89	0,841	0,849	0,877	0,87	1,15	0,996	1,136	0,904	1,039	0,904	0,829
N	0,924	1,242	1,003	1,257	0,879	0,893	0,878	0,913	0,928	0,938	1,15	1,184	0,865	0,907	0,832	0,915	1,123	1,11	1,162	1,16	0,793	1,136	0,85	0,913
O	0,675	0,918	0,957	0,946	0,919	0,851	0,901	0,899	0,894	0,86	0,887	0,913	0,898	0,816	0,872	0,856	0,872	1,173	1,01	1,109	0,842	1,154	0,85	0,866
P	0,928	1,162	0,954	1,234	0,849	0,845	0,886	0,915	0,891	0,975	1,141	1,143	0,667	0,905	0,841	0,9	1,119	1,116	1,079	1,008	0,676	1,13	0,917	0,931

P. aeruginosa

Layout N.1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	1,005	0,995	1,022	0,959	1,094	1,111	1,137	1,148	1,123	1,084	1,138	1,119	1,064	1,071	1,077	1,122	1,064	1,079	0,058	0,058	1,051	1,058	1,314	1,291
B	0,984	0,982	0,987	0,955	1,124	1,113	1,157	1,145	1,13	1,082	1,087	1,075	1,121	1,145	1,101	1,099	1,073	1,068	0,062	0,059	1,072	1,072	1,341	1,294
C	1,008	0,996	1,061	1,037	1,127	1,134	1,137	1,139	1,115	1,08	1,123	1,112	1,078	1,175	1,11	1,136	1,094	1,137	0,158	0,379	1,102	1,087	1,341	1,145
D	0,995	1,005	1,061	1,078	1,133	1,116	1,158	1,142	1,125	1,106	1,144	1,13	1,117	1,132	1,112	1,139	1,131	1,144	0,556	0,654	1,197	1,102	1,248	0,06
E	1,009	1,001	1,121	1,106	1,139	1,133	1,147	1,142	1,154	1,115	1,138	1,147	1,086	1,154	1,149	1,115	1,119	1,099	1,107	1,099	1,087	1,098	1,329	0,06
F	0,923	0,941	0,999	1,008	1,059	1,137	1,166	1,133	1,146	1,144	1,153	1,127	1,131	1,154	1,155	1,126	1,119	1,141	1,13	1,131	1,106	1,115	0,059	0,06
G	1,016	1,03	1,049	1,068	1,075	1,048	1,117	1,102	1,104	1,105	1,16	1,126	1,147	1,155	1,154	1,148	1,115	1,104	1,115	1,11	1,097	1,068	0,049	0,061
H	1,024	1,03	1,044	1,055	1,031	1,069	1,107	1,104	1,106	1,093	1,119	1,125	1,141	1,139	1,143	1,159	1,134	1,142	1,12	1,111	1,1	1,16	0,08	0,059
I	1,045	1,062	1,132	1,116	1,111	1,114	1,161	1,087	1,141	1,137	1,152	1,141	1,131	1,126	1,132	1,111	1,114	1,114	1,114	1,143	1,123	1,136	0,594	0,061
J	1,055	1,095	1,123	1,115	1,117	1,147	1,115	1,147	1,148	1,156	1,133	1,145	1,146	1,129	1,138	1,14	1,124	1,139	1,137	1,138	1,105	1,151	0,722	1,143
K	1,083	1,045	1,106	1,101	1,106	1,116	1,139	1,133	1,163	1,129	1,148	1,122	1,119	1,132	1,131	1,129	1,101	1,126	1,117	1,109	1,099	1,104	0,061	0,061
L	1,051	1,096	1,111	1,109	1,12	1,139	1,155	1,149	1,126	1,163	1,115	1,147	1,116	1,118	1,108	1,115	1,119	1,143	1,12	1,119	1,134	1,14	0,331	0,061
M	1,043	1,047	1,095	1,108	1,119	1,114	1,171	1,131	1,153	1,163	1,143	1,137	1,129	1,126	1,124	1,131	1,099	1,159	1,107	1,098	1,114	1,065	1,091	1,044
N	1,045	1,067	1,101	1,115	1,108	1,144	1,157	1,141	1,143	1,127	1,143	1,121	1,125	1,121	1,111	1,115	1,139	1,139	1,113	1,127	1,157	1,118	1,072	1,054
O	1,039	1,04	1,073	1,085	1,113	1,103	1,125	1,123	1,138	1,126	1,12	1,141	1,107	1,113	1,115	1,127	1,094	1,142	1,116	1,105	1,127	1,064	1,089	1,063
P	1,03	1,04	1,091	1,09	1,085	1,097	1,138	1,128	1,133	1,133	1,149	1,13	1,114	1,111	1,107	1,117	1,116	1,121	1,108	1,108	1,086	1,087	1,045	1,027

P. aeruginosa

Layout N.2	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	1,119	1,111	1,121	1,111	1,126	1,144	1,05	1,07	1,056	1,043	1,075	1,089	1,065	1,066	1,075	1,061	1,069	1,079	0,06	0,059	1,188	1,127	0,058	0,058
B	1,124	1,122	1,124	1,139	1,162	1,195	1,07	1,076	1,081	1,063	1,087	1,104	1,079	1,084	1,09	1,122	1,11	1,1	0,063	0,109	1,135	1,126	0,059	0,059
C	1,06	1,078	1,083	1,11	1,122	1,094	1,104	1,151	1,095	1,099	1,107	1,125	1,11	1,15	1,106	1,126	1,121	1,105	0,895	0,768	1,103	1,146	0,06	0,06
D	1,105	1,082	1,094	1,114	1,128	1,135	1,153	1,138	1,139	1,139	1,138	1,128	1,105	1,114	1,117	1,121	1,111	1,095	1,034	0,634	1,149	1,095	0,057	0,06
E	1,166	1,166	1,146	1,155	1,145	1,128	1,178	1,233	1,184	1,167	1,147	1,173	1,136	1,113	1,105	1,113	1,111	1,103	1,134	1,152	1,105	1,14	0,156	0,061
F	1,165	1,161	1,109	1,151	1,172	1,236	1,166	1,183	1,172	1,138	1,157	1,161	1,107	1,116	1,107	1,123	1,105	1,11	1,152	1,128	1,147	1,135	0,059	0,062
G	1,143	1,143	1,174	1,141	1,159	1,187	1,181	1,185	1,157	1,19	1,157	1,217	1,114	1,108	1,116	1,126	1,115	1,1	1,128	1,124	1,127	1,174	0,071	0,052
H	1,153	1,131	1,185	1,168	1,148	1,209	1,137	1,136	1,141	1,118	1,167	1,151	1,105	1,111	1,105	1,112	1,115	1,095	1,149	1,129	1,129	1,11	0,048	0,059
I	1,079	1,102	1,113	1,14	1,121	1,166	1,176	1,16	1,122	1,143	1,16	1,157	1,127	1,135	1,129	1,13	1,108	1,089	1,156	1,156	1,112	1,133	0,807	0,061
J	1,122	1,132	1,122	1,142	1,174	1,169	1,102	1,145	1,143	1,149	1,147	1,143	1,105	1,129	1,13	1,115	1,125	1,115	1,148	1,109	1,11	1,108	0,413	0,052
K	1,057	1,135	1,114	1,115	1,126	1,172	1,135	1,117	1,159	1,159	1,146	1,153	1,147	1,123	1,107	1,104	1,132	1,117	1,147	1,141	1,133	1,107	0,152	0,062
L	1,139	1,142	1,13	1,148	1,16	1,163	1,153	1,129	1,163	1,149	1,153	1,197	1,116	1,145	1,143	1,117	1,121	1,128	1,173	1,154	1,17	1,107	1,248	1,187
M	1,076	1,119	1,149	1,108	1,121	1,105	1,15	1,143	1,151	1,154	1,149	1,141	1,126	1,123	1,105	1,154	1,107	1,117	1,137	1,167	1,152	1,097	1,298	1,086
N	1,1	1,142	1,149	1,119	1,132	1,166	1,135	1,151	1,147	1,145	1,159	1,124	1,117	1,146	1,163	1,12	1,134	1,147	1,119	1,147	1,161	1,101	1,116	1,013
O	1,074	1,08	1,095	1,129	1,081	1,071	1,129	1,107	1,143	1,153	1,161	1,14	1,149	1,159	1,14	1,122	1,145	1,095	1,13	1,145	1,141	1,095	1,09	1,083
P	1,092	1,131	1,138	1,114	1,204	1,16	1,133	1,143	1,146	1,146	1,15	1,143	1,147	1,145	1,139	1,125	1,137	1,141	1,119	1,141	1,167	1,122	1,072	1,045

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