

Supporting Information

Characteristic guaiane sesquiterpenes from *Daphne penicillate* and ECD/NMR-based assignment of C-1 configuration

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Experimental section

General experimental procedures

HRESIMS measurements were tested on a Micro Q-TOF spectrometer (Bruker Daltonics, Billerica, USA). Optical rotations and ECD spectra were recorded on JASCO DIP-370 digital polarimeter (JASCO Corp., Japan) at 20 °C and Bio-Logic Science MOS-450 spectrometer (Bio-Logic Science Instruments, Seyssinet-Pariset, France). IR and UV spectra were obtained on Bruker IFS-55 spectrometer (Bruker Corp., Karlsruhe, Germany) and Shimadzu UV-1700 spectrometer (Shimadzu, Tokyo, Japan), respectively. NMR spectra were performed on Bruker AVIII-600 spectrometers (Bruker Corp., Bremen, Germany) and TMS was employed as internal standard. Column chromatography was used with silica gel (200-300 mesh, Marine Chemical Inc., China). CHP20 (25–100 µm, Green Herbs Science and Technology Development Corp., Beijing, China). Preparative HPLC separations were carried out by Shimadzu LC-20AR liquid chromatography system with an SPD-20A UV detector (Shimadzu, Kyoto, Japan), and a YMC Pack ODS column (C₁₈, 250 × 10 mm, 5 µm, YMC Corp, Kyoto, Japan) were used. The melting point was obtained on an X-6 melting point apparatus (Beijing TECH Instrument Corp., China).

Plant material

The aerial parts of *Daphne penicillata* were collected from Wenchuan County, Aba Prefecture, Sichuan Province, China, in July 2019 (N31°29'51.52", E103°38'14.35"). and authenticated by Prof. Jincai Lu (School of Traditional Chinese Materia Medica, Shenyang Pharmaceutical University). The voucher sample (No. MJ20190701) was deposited in the herbarium of Shenyang Pharmaceutical University.

Extraction and isolation

The dried herbs of *Daphne penicillata* (48.0 kg) were extracted under reflux conditions using 75% aqueous EtOH (50 L × 3 times × 4 hours). The percolates were combined and evaporated under reduced pressure to afford a crude extract. The extract was suspended in water and successively partitioned with EtOAc and *n*-BuOH. The EtOAc extract (600 g) and *n*-BuOH (1200 g) were subjected

to silica gel column using CH₂Cl₂-MeOH (100:1-1:1, v/v) as gradient eluents to afford four fractions (Fr.A-D). Fr.A (200 g) was separated by polyamide chromatography eluted with 20% and 70% EtOH to obtain two fractions (Fr.A1 to Fr.A2), then Fr.A1 (90 g) was subjected to column chromatography on HP20 resin with H₂O, 20%, 50% and 90% EtOH to give two fractions (Fr.A1-1 and Fr.A1-2). Fr.A1-2 (35 g) were separated by ODS column chromatography, eluted with a gradient of MeOH-H₂O from 10:90 to 60:40, respectively. and then redistributed in five fractions (Fr.1-5) based on HPLC analysis. Among them, Fr.3 (15 g) was subjected to silica gel CC eluting with petroleum ether/EtOAc (v/v, 100:1 to 5:1) to yield five fractions (Fr.3.1–Fr.3.4). Fr.3.1 (2.4 g) was separated by RP-C18 preparative HPLC using MeOH/H₂O (55:45) to obtain three fractions (Fr.3.1.1–Fr.3.1.4). **1** (5.0 mg, t_R = 10.3 min), **2** (3.0 mg, t_R = 12.5 min) **5** (3.0 mg, t_R = 20.4 min) and **6** (10.0 mg, t_R = 28.3 min) was obtained from Fr.3.1.1 (91.5 mg) by semipreparative HPLC eluted with CH₃CN-H₂O (20:80, 2.5 mL/min). **3** (2.0 mg, t_R = 15.8 min), **4** (5.0 mg, t_R = 21.2 min), **7** (2.0 mg, t_R = 22.9 min) and **9** (1.5 mg, t_R = 30.5 min) was isolated from Fr.3.1.3 (52.6 mg) and Fr.3.1.4 (80.5 mg) by semipreparative HPLC eluted with CH₃CN-H₂O (25:75, 2.5 mL/min).

Fr.3.2 (3.9 g) and Fr.3.3 (2.9 g) were separated by preparative HPLC using MeOH/H₂O (50:50) to obtain the following fractions (Fr.3.2.1–Fr.3.2.8 and Fr.3.3.1–Fr.3.3.5). **8** (6.5 mg, *t*_R = 20.1 min), **10** (3.0 mg, *t*_R = 20.9 min), **12** (4.0 mg, *t*_R = 32.3 min), **13** (4.5 mg, *t*_R = 33.5 min) and **15** (1.5 mg, *t*_R = 38.3 min) was obtained from Fr.3.2.2 (81.5 mg) and Fr.3.2.3 (87.3 mg) by semipreparative HPLC (CH₃CN-H₂O, 26:74, 2.5 mL/min). Fr.3.2.5 (101.5 mg) and Fr.3.2.7 (79.2 mg) were separated by semipreparative HPLC with CH₃CN-H₂O (22:78, 2.5 mL/min) to afford **11** (2.5 mg, *t*_R = 16.7 min), **14** (3.5 mg, *t*_R = 19.3 min), **16** (2.5 mg, *t*_R = 20.2 min), **17** (2.5 mg, *t*_R = 24.3 min) and **20** (6.7 mg, *t*_R = 34.2 min). Similarly, **18** (3.5 mg, *t*_R = 21.3 min), **19** (4.0 mg, *t*_R = 23.5 min), **21** (4.5 mg, *t*_R = 26.2 min), **22** (2.5 mg, *t*_R = 29.6 min), **24** (1.5 mg, *t*_R = 32.8 min) and **25** (1.5 mg, *t*_R = 39.1 min) was obtained from Fr.3.3.1 (79.2 mg) and Fr.3.3.3 (64.3mg) by semipreparative HPLC with CH₃CN-H₂O (20:80, 2.5 mL/min).

Fr.4 (3.9 g) and Fr.5 (4.2 g) was separated by RP-C18 preparative HPLC using MeOH/H₂O (42:58) to obtain the following fractions (Fr.4.1.1–Fr.4.2.4 and Fr.5.1.1–Fr.5.2.4). Among them, Fr.4.1.2 (78.3 mg) and Fr 4.1.3 (64.5 mg) were separated by semipreparative HPLC with CH₃CN-H₂O (33:67, 2.5 mL/min) to afford **23** (3.0 mg, *t*_R = 12.8 min), **26** (3.0 mg, *t*_R = 13.5 min), **27** (1.5 mg, *t*_R = 16.1 min), **29** (2.0 mg, *t*_R = 17.4 min) **33** (4.5 mg, *t*_R = 19.2 min) and **34** (5.0 mg, *t*_R = 22.5 min). Fr.5.2.3 (110.8 mg) was separated by semipreparative HPLC eluting with CH₃CN/H₂O (28:72, 2.5 mL/min) to give **28** (1.5 mg, *t*_R = 7.8 min), **30** (2.0 mg, *t*_R = 12.1 min), **31** (3.5 mg, *t*_R = 13.9 min), **32** (2.0 mg, *t*_R = 15.4 min), **35** (5.5 mg, *t*_R = 19.2 min). Fr.5.2.4 (94.7 mg) was purified by HPLC eluting with CH₃CN/H₂O (25:75, 2.5 mL/min) to give **36** (1.5 mg, *t*_R = 17.3 min), **37** (2.5 mg, *t*_R = 22.6 min), **38** (1.5 mg, *t*_R = 24.3 min), **39** (2.5 mg, *t*_R = 25.7 min) and **40** (1.5 mg, *t*_R = 32.4 min).

Daphnenicillata A (1): colorless oil $[\alpha]_D^{20}$ +28.0 (c 0.10, MeOH); UV (MeOH) λ_{max} ($\log \epsilon$): 240 nm (1.43), 287 nm (0.56); ECD (MeOH) λ_{max} ($\Delta \epsilon$) 193 (-9.22), 209 (-5.75), 240 (+2.13), 290 (-4.75) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S1; HRMS (ESI) *m/z*: [M+Na]⁺ calcd

for C₁₈H₂₂O₂Na, 309.1461; Found 309.1471.

Daphnenicillata B (5): colorless oil; $[\alpha]_D^{20} +40.2$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 241 nm (0.84), 292 nm (0.01); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 260 (+15.13), 313 (-213.75) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S1; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₂O₃Na, 273.1461; Found 273.1472.

Daphnenicillata C (6): colorless oil; $[\alpha]_D^{20} +46.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 240 nm (3.50), 299 nm (0.06); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 267 (+15.65), 317 (-195.85) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S2; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₂O₄Na, 289.1410; Found 289.1411.

Daphnenicillata D (7): colorless oil; $[\alpha]_D^{20} +53.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 238 nm (0.31), 298 nm (0.01); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 193 (-5.13), 226 (+6.34), 247 (-11.87), 315 (+1.98) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S2; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₆H₂₄O₃Na, 287.1618; Found 287.1609.

Daphnenicillata E (8): colorless oil; $[\alpha]_D^{20} +27.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 239 nm (1.01), 297 nm (0.06); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 225 (-7.21), 247 (+11.87), 315 (-1.98) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S2; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₆H₂₄O₃Na, 287.1618; Found 287.1609.

Daphnenicillata F (9): colorless oil; $[\alpha]_D^{20} +47.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 236 nm (0.46); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 195 (-3.27), 214 (+13.76), 247 (-35.65), 321 (+7.95) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S2; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₆H₂₄O₄Na, 303.1567; Found 303.1570.

Daphnenicillata G (10): colorless crystal; m.p.: 180–182 °C; $[\alpha]_D^{20} +29.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 236 nm (0.46); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 215 (+3.27), 251 (-35.47), 323 (+13.63) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S2; HRMS (ESI) *m/z*: [M+Na]⁺ calcd

for C₁₄H₂₀O₃Na, 259.1305; Found 259.1307.

Daphnenicillata H (11): colorless oil; $[\alpha]_D^{20} +64.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 237 nm (1.13); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 261 (+38.88), 317 (-150.32) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S3; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₄H₁₈O₃Na, 257.1148; Found 257.1182.

Daphnenicillata I (12): colorless oil; $[\alpha]_D^{20} +32.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 239 nm (2.00), 295 nm (0.05); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 263 (-37.38), 317 (-59.76) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S3; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₀O₂Na, 255.1356; Found 255.1351.

Daphnenicillata J (13): colorless oil; $[\alpha]_D^{20} +48.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 237 nm (3.14), 303 nm (0.04); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 197 (-7.35), 213 (-11.42), 247 (+27.89), 315 (-6.06) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S3; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₀O₃Na, 271.1305; Found 271.1295.

Daphnenicillata K (14): colorless oil; $[\alpha]_D^{20} +40.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 279 nm (0.03); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 195 (-2.99), 245 (+13.89), 315 (-6.57) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S3; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₀O₃Na, 271.1305; Found 271.1307.

Daphnenicillata L (15): colorless oil; $[\alpha]_D^{20} +41.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 279 nm (0.07); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 195 (-9.87), 243 (-17.96), 313 (+7.65) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S3; HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₁₅H₂₁O₃, 249.1485; Found 249.1486.

Daphnenicillata M (16): colorless oil; $[\alpha]_D^{20} +21.5$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 275 nm (1.52); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 209 (-22.44), 245 (+37.73), 321 (-10.84) nm. The ¹H NMR (CDCl₃, 600 MHz) and ¹³C NMR data (CDCl₃, 150 MHz), see Table S4; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₀O₃Na, 273.1305;

Found 271.1294.

Daphnenicillata N (17): colorless oil; $[\alpha]_D^{20} +58.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ϵ): 236 nm (1.22); ECD (MeOH) λ_{\max} ($\Delta\epsilon$) 195 (-7.26), 214 (-4.96), 247 (+31.65), 314 (-10.85) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S4; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₀O₄Na, 287.1254; Found 287.1232.

Daphnenicillata O (18): colorless oil; $[\alpha]_D^{20} +56.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ϵ): 242 nm (0.98); ECD (MeOH) λ_{\max} ($\Delta\epsilon$) 193 (-15.95), 221 (+20.96), 310 (-6.75) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S4; HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₁₅H₂₃O₂, 235.1693; Found 235.1692.

Daphnenicillata P (23): colorless oil; $[\alpha]_D^{20} +50.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ϵ): 244 nm (1.95), 288 nm (0.02); ECD (MeOH) λ_{\max} ($\Delta\epsilon$) 193 (-8.95), 247 (+25.64), 313 (-3.75) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S5; HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₁₅H₂₃O₂, 235.1693; Found 235.1697.

Daphnenicillata Q (24): colorless oil; $[\alpha]_D^{20} +62.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ϵ): 242 nm (1.35), 286 nm (0.09); ECD (MeOH) λ_{\max} ($\Delta\epsilon$) 220 (+35.32), 264 (+17.84) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S5; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₂O₂Na, 257.1512; Found 257.1509.

Daphnenicillata R (25): colorless oil; $[\alpha]_D^{20} +38.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ϵ): 239 nm (0.65); ECD (MeOH) λ_{\max} ($\Delta\epsilon$) 208 (-11.37), 245 (+31.34) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S5; HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₁₅H₂₅O₂, 237.1849; Found 237.1846.

Daphnenicillata S (26): colorless oil; $[\alpha]_D^{20} +30.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ϵ): 240 nm (2.03); ECD (MeOH) λ_{\max} ($\Delta\epsilon$) 203 (-27.84), 245 (-8.32), 265 (+20.34), 310 (-14.25) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S6; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₄O₂Na, 259.1669; Found 259.1668.

Daphnenicillata T (27): colorless crystal; m.p.: 192–194 °C; $[\alpha]_D^{20} +32.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 233 nm (0.29), 287 nm (0.02); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 195 (−42.94), 252 (+4.15) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S6; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₂O₃Na, 273.1461; Found 273.1462.

Daphnenicillata U (28): colorless crystal; m.p.: 185–187 °C; $[\alpha]_D^{20} +24.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 243 nm (1.11), 287 nm (0.04); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 216 (+53.65), 251 (−107.95) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S6; HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₁₅H₂₃O₂, 235.1693; Found 235.1739.

Daphnenicillata V (29): colorless crystal; m.p.: 200–202 °C; $[\alpha]_D^{20} +44.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 226 nm (1.31); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 220 (+12.65), 248 (−9.85) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S6; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₂O₃Na, 273.1461; Found 273.1466.

Daphnenicillata W (30): colorless oil; $[\alpha]_D^{20} +29.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 240 nm (0.38), 299 nm (0.17); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 192 (−16.13), 214 (−14.85), 251 (+22.64), 313 (−8.75) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S6; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₅H₂₀O₂Na, 255.1356; Found 255.1353.

Daphnenicillata X (33): colorless oil; $[\alpha]_D^{20} +65.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 241 nm (1.49); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 213 (−22.43), 230 (+5.34), 265 (+37.34), 312 (−43.37) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S7; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₆H₂₃O₂Na, 247.1693; Found 247.1697.

Daphnenicillata Y (34): colorless oil; $[\alpha]_D^{20} +29.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 243 nm (0.28), 293 nm (0.09); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 210 (−16.76), 247 (+31.45), 314 (−15.13) nm. The ^1H NMR (CDCl₃, 600 MHz) and ^{13}C NMR data (CDCl₃, 150 MHz), see Table S7; HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₆H₂₂O₃Na, 285.1461; Found 285.1469.

Daphnenicillata Z (35): colorless oil; $[\alpha]_D^{20} +53.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 236 nm (0.66), 293 nm (0.35); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 191 (-6.53), 206 (-7.76), 225 (+8.34), 247 (-11.34), 285 (-8.13) nm. The ^1H NMR (CDCl_3 , 600 MHz) and ^{13}C NMR data (CDCl_3 , 150 MHz), see Table S7; HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{23}\text{O}_3$, 263.1642; Found 263.1619.

Minjiangpenicillata A (36): colorless oil; $[\alpha]_D^{20} +58.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 233 nm (0.29), 287 nm (0.02); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 195 (-42.94), 252 (+4.15) nm. The ^1H NMR (CDCl_3 , 600 MHz) and ^{13}C NMR data (CDCl_3 , 150 MHz), see Table S8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{16}\text{H}_{26}\text{O}_4\text{Na}$, 305.1723; Found 305.1722.

Minjiangpenicillata B (37): colorless oil; $[\alpha]_D^{20} +39.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 206 nm (1.91); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 183 (+23.65), 195 (-8.25), 210 (+4.93), 251 (+51.93), 309 (-5.34) nm. The ^1H NMR (CDCl_3 , 600 MHz) and ^{13}C NMR data (CDCl_3 , 150 MHz), see Table S8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{16}\text{H}_{26}\text{O}_4\text{Na}$, 305.1723; Found 305.1737.

Minjiangpenicillata C (38): colorless oil; $[\alpha]_D^{20} +27.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 243 nm (0.43); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 193 (-8.73), 210 (+14.72), 258 (+5.34) nm. The ^1H NMR (CDCl_3 , 600 MHz) and ^{13}C NMR data (CDCl_3 , 150 MHz), see Table S8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{16}\text{H}_{26}\text{O}_3\text{Na}$, 289.1774; Found 289.1743.

Minjiangpenicillata D (39): colorless oil; $[\alpha]_D^{20} +65.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 234 nm (0.22); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 212 (+9.15), 237 (-21.15) nm. The ^1H NMR (CDCl_3 , 600 MHz) and ^{13}C NMR data (CDCl_3 , 150 MHz), see Table S8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{16}\text{H}_{22}\text{O}_4\text{Na}$, 301.1410; Found 301.1420.

Minjiangpenicillata E (40): colorless oil; $[\alpha]_D^{20} +59.0$ (c 0.10, MeOH); UV (MeOH) λ_{\max} (log ε): 234 nm (0.68); ECD (MeOH) λ_{\max} ($\Delta\varepsilon$) 227 (-29.94) nm. The ^1H NMR (CDCl_3 , 600 MHz) and ^{13}C NMR data (CDCl_3 , 150 MHz), see Table S8; HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{16}\text{H}_{22}\text{O}_4\text{Na}$, 301.1410; Found 301.1432.

Crystal data for 3:

orthorhombic, C₁₅H₂₂O₃, P 21 21 21, a = 5.9836(2) Å, b = 12.5695(4) Å, c = 17.9850(6) Å, V = 1352.67(8)

Å³, Z = 4, T = 153(2) K, $\mu(\text{Cu K}\alpha)$ = 0.673 mm⁻¹, Dcalc = 1.229 g/cm³, 8192 reflections measured ($4.29^\circ \leq \theta \leq 68.28^\circ$), 2458 unique (Rint = 0.0260), which were used in all calculations. The final R1 was 0.0289 ($I > 2\sigma(I)$), and wR2 was 0.0698 (all data). Flack parameter = -0.04(5). CCDC No: 2195139.

Crystal data for 4:

monoclinic, C₁₅H₂₂O₃, P 1 21 1, a = 5.3597(3) Å, b = 8.4494(4) Å, c = 8.4494(4) Å, V = 678.39(6) Å³, Z = 2, T = 164(2) K, $\mu(\text{Cu K}\alpha)$ = 0.671 mm⁻¹, Dcalc = 1.225 g/cm³, 3899 reflections measured ($2.95^\circ \leq \theta \leq 68.40^\circ$), 2107 unique (Rint = 0.0317), which were used in all calculations. The final R1 was 0.0648 ($I > 2\sigma(I)$), and wR2 was 0.1962 (all data). Flack parameter = -0.20(3). CCDC No: 2195138.

Crystal data for 10:

orthorhombic, C₁₄H₂₀O₃, P 21 21 21, a = 5.1817(2) Å, b = 9.2698(4) Å, c = 27.2715(13) Å, V = 1309.94(10) Å³, Z = 4, T = 153(2) K, $\mu(\text{Cu K}\alpha)$ = 0.667 mm⁻¹, Dcalc = 1.198 g/cm³, 6483 reflections measured ($3.24^\circ \leq \theta \leq 53.74^\circ$), 1574 unique (Rint = 0.0463), which were used in all calculations. The final R1 was 0.0297 ($I > 2\sigma(I)$), and wR2 was 0.0634 (all data). Flack parameter = -0.01(5). CCDC No: 2195140.

Crystal data for 20:

orthorhombic, C₁₅H₂₂O₂, P 21 21 21, a = 6.9215(2) Å, b = 12.7299(3) Å, c = 15.0170(4) Å, V = 1323.15(6) Å³, Z = 4, T = 155(2) K, $\mu(\text{Cu K}\alpha)$ = 0.596 mm⁻¹, Dcalc = 1.176 g/cm³, 8405 reflections measured ($4.29^\circ \leq \theta \leq 68.28^\circ$), 2389 unique (Rint = 0.0459), which were used in all calculations. The final R1 was 0.0405 ($I > 2\sigma(I)$), and wR2 was 0.0823 (all data). Flack parameter = -0.12(15). CCDC No: 2195142.

Crystal data for 21:

orthorhombic, C₁₅H₂₂O₃, P 21 21 21, a = 8.1320(2) Å, b = 11.3145(2) Å, c = 14.8559(3) Å, V = 1366.88(5) Å³, Z = 4, T = 193(2) K, $\mu(\text{Cu K}\alpha)$ = 0.577 mm⁻¹, Dcalc = 1.139 g/cm³, 8183 reflections measured ($4.91^\circ \leq \theta \leq 68.32^\circ$), 2492 unique (Rint = 0.0225), which were used in all calculations. The final R1 was 0.0343 ($I > 2\sigma(I)$), and wR2 was 0.0873 (all data). Flack parameter = -0.03(6). CCDC No: 2195143.

Crystal data for 27:

orthorhombic, C₁₅H₂₀O₃, P 21 21 21, a = 20.4454(19) Å, b = 8.2080(6) Å, c = 8.1965(5) Å, V = 1375.50(18) Å³, Z = 4, T = 150(10) K, $\mu(\text{Cu K}\alpha)$ = 0.661 mm⁻¹, D_{calc} = 1.199 g/cm³, 5028 reflections measured ($8.65^\circ \leq \theta \leq 148.55^\circ$), 2681 unique (R_{int} = 0.0512), which were used in all calculations. The final R1 was 0.0826 (I > 2σ(I)), and wR2 was 1976 (all data). Flack parameter = -0.10(4). CCDC No: 2195144.

Crystal data for 28:

monoclinic, C₁₅H₂₂O₂, I2, a = 8.7052(8) Å, b = 10.0397(7) Å, c = 16.0048(12) Å, V = 1351.41(19) Å, Z = 4, T = 100(10) K, $\mu(\text{Cu K}\alpha)$ = 0.583 mm⁻¹, D_{calc} = 1.152 g/cm³, 3623 reflections measured ($10.51^\circ \leq \theta \leq 147.49^\circ$), 2115 unique (R_{int} = 0.0302), which were used in all calculations. The final R1 was 0.0492 (I > 2σ(I)), and wR2 was 0.1333 (all data). Flack parameter = 0.10(3). CCDC No: 2195145.

Crystal data for 29:

monoclinic, C₁₅H₂₂O₃, P 1 21 1, a = 8.7124(4) Å, b = 6.5713(3) Å, c = 12.0658(6) Å, V = 690.76(6) Å, Z = 2, T = 153(2) K, $\mu(\text{Cu K}\alpha)$ = 0.659 mm⁻¹, D_{calc} = 1.204 g/cm³, 3297 reflections measured ($6.24^\circ \leq \theta \leq 72.38^\circ$), 2024 unique (R_{int} = 0.0343), which were used in all calculations. The final R1 was 0.0343 (I > 2σ(I)), and wR2 was 0.0943 (all data). Flack parameter = 0.13(6). CCDC No: 2195146.

Crystal data for 31:

orthorhombic, C₁₅H₂₀O₂, C222₁, a = 8.1880(3) Å, b = 23.4706(8) Å, c = 13.8857(4) Å, V = 2668.51(16) Å, Z = 8, T = 150(10) K, $\mu(\text{Cu K}\alpha)$ = 0.590 mm⁻¹, D_{calc} = 1.156 g/cm³, 6932 reflections measured ($7.53^\circ \leq \theta \leq 146.39^\circ$), 2610 unique (R_{int} = 0.0396), which were used in all calculations. The final R1 was 0.0508 (I > 2σ(I)), and wR2 was 0.1332 (all data). Flack parameter = 0.00(2). CCDC No: 2195147.

Molecular networking

The aerial parts of *Daphne penicillate* were extracted by 75% EtOH, which was successively partitioned into ethyl acetate and *n*-butanol. The ethyl acetate extract was subjected to silica gel column chromatography, followed by polyamide chromatography to afford a series of fractions. Then, they were analyzed by HPLC-

ESI-MS/MS. MSConvert software was applied to converted from .wiff format of MS/MS data to .mzXML format. Then, these converted files were conducted by the MZmine 2. The mass detection was realized keeping the noise level at 15, and peaks without an associated MS/MS spectrum were finally filtered out. The data were submitted the online platform at the Global Natural Products Social Molecular Networking website (gnps.ucsd.edu) to generate the molecular network with edges that were filtered to have a cosine score above 0.65 and more than 6 matched peaks. The parameters include parent ion mass tolerance (0.02 Da), fragment ion mass tolerance (0.5 Da), and a minimum cluster size of 1. The resulting molecular network was visualized using the Cytoscape 3.8.2 program.

NMR calculations

The conformational analysis of isolated compounds was performed on the CONFLEX software by using MMFF94s molecular force field. All the conformers whose Boltzmann distribution is more than 1% were chosen, and then they were initially optimized at B3LYP/6-31G(d) level in chloroform using the polarizable continuum model (PCM) solvent model by Gaussian 09 program package. The gauge independent atomic orbital (GIAO) shielding constants of these conformers were calculated at the mPW1PW91/6-311+G(d,p) level after geometry optimization. Boltzmann-weighted averages of the chemical shifts were calculated to scale them against the experimental values. The ¹H NMR and ¹³C NMR chemical shift of tetramethylsilane were calculated at the same level and used as reference. The shielding constants obtained were converted into chemical shifts by referencing to TMS at 0 ppm ($\delta_{\text{cal}} = \sigma_{\text{TMS}} - \sigma_{\text{cal}}$). The MAE _{$\Delta\Delta\delta$} values, DP4+ and CP3 probability were calculated for evaluation of the deviations between the experimental and calculated results.

ECD calculations

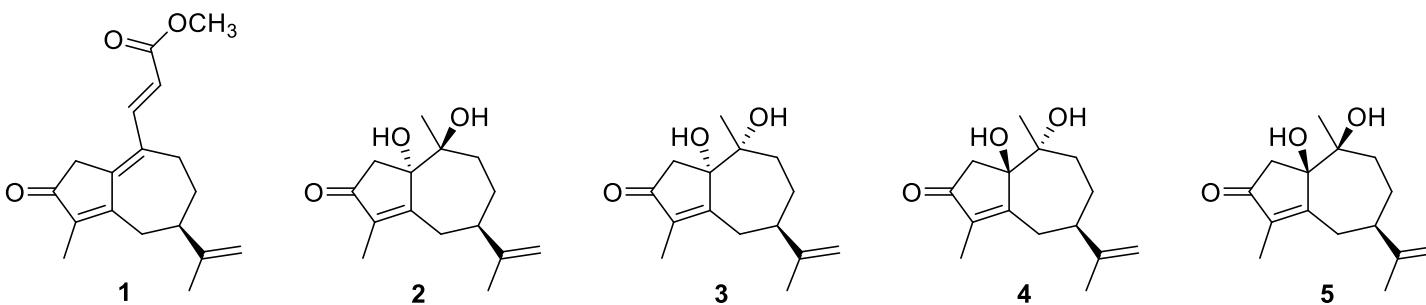
Conformational analysis of all the possible conformers of isolated compounds were performed by using the MMFF94 force field in CONFLEX software. All the conformers obtained were screened based on the energy of optimized structures at the B3LYP/6-31G(d) level in an energy window of 3 kcal/mol in the Gaussian 09 software. Then, the ECD data of all the selected conformers were calculated with the time-dependent

density functional theory (TDDFT) method at the B3LYP/6-311++G(2d, p) levels with the CPCM model in methanol solution. Finally, the Boltzmann-averaged ECD curve was generated using SpecDis 1.51.

Inflammatory mediator and cytokine assay

BV2 cells were cultured in DMEM medium containing contained 10% heat-inactivated FBS with 100 U/ml penicillin and 100 μ g/mL streptomycin at 37 °C with 5% CO₂. BV2 cells were seeded in 96 well plates at a density of 5×10^3 cells/well for 24 h. Then, the isolated compounds were added and the cells were further cultured for 1 h. After that, 10 μ g/ml of LPS were added to each well and the cells were incubated for an additional 24 h. Then, the supernatants were collected. The nitrite concentration in the medium, which is an indicator of NO production, was measured using the Griess reaction. The concentration of NO was measured using a commercially available NO assay kit according to the manufacturer's instructions.

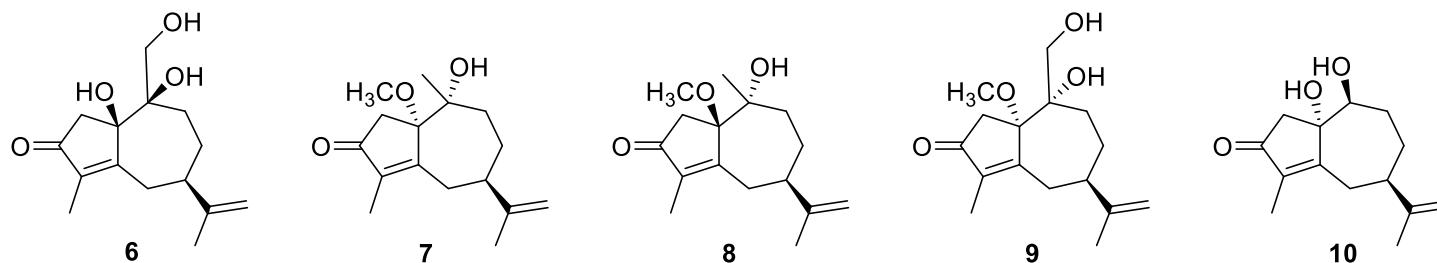
Table S1. ^1H (600 MHz) and ^{13}C (150 MHz) NMR data of **1–5** in CDCl_3 .



No.	1		2		3		4		5	
	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}
1		143.2		84.9		85.6		83.0		81.7
2	3.19, d, (20.5) 3.15, d, (20.5)	39.7	3.03, d, (17.7) 2.26, d, (17.7)	48.8	3.09, d, (18.6) 2.29, d, (18.6)	49.0	3.02, d, (17.7) 2.21, d, (17.7)	47.0	2.56, d, (18.0) 2.39, d, (18.0)	46.7
3		203.0		205.2		205.7		205.9		206.9
4		143.4		140.2		139.7		139.1		137.8
5		166.2		169.9		169.9		170.4		173.2
6	2.84, dd, (15.3, 4.7) 2.79, dd, (15.3, 8.7)	32.8	2.77, m 2.63, dd, (17.6, 10.7)	35.4	2.75, m 2.50, dd, (19.4, 12.0)	36.0	2.70, dd, (12.9, 11.5) 2.53, dd, (12.9, 4.4)	28.7	2.74, dd, (12.0, 11.5) 2.49, dd, (12.0, 2.6)	30.6
7	2.52, overlapped	42.8	2.70, m	43.0	2.87, m	42.3	2.43, m	42.1	2.06, overlapped	47.1
8	2.00, dddd, (14.3, 9.8, 7.0, 3.0) 1.82, dt, (14.2, 8.1, 3.1)	31.8	1.68, m	29.2	1.79, m	30.8	1.85, m	25.2	1.92, m	27.5
9	2.65, ddd, (16.7, 9.8, 3.1) 2.55, overlapped	25.6	2.21, m	39.7	2.25, m	40.6	2.28, ddd, (15.2, 12.1, 3.1) 1.52, ddd, (15.2, 6.2, 3.1)	33.1	2.04, overlapped	35.3
10		133.5		75.3		77.1		74.7		74.3
11		148.9		150.5		150.6		149.9		149.8
12	4.76, d, (1.5)	110.1	4.77, d, (1.6)	109.5	4.75, d, (1.6)	109.4	4.79, d, (1.6)	109.8	4.76, d, (1.6)	109.8

	4.75, d, (1.5)	4.72, d, (1.6)	4.72, d, (1.6)	4.76, d, (1.6)	4.72, d, (1.6)		
13	1.77, s	20.8	1.77, s	20.3	1.75, s	20.5	1.78, s
14	7.56, d, (15.6)	143.8	1.39, s	27.6	1.02, s	22.4	1.37, s
15	1.85, s	118.4	1.71, s	8.5	1.67, s	8.2	1.74, s
16	6.04, d, (15.6)	167.7					
17		9.1					
-OCH ₃	3.78, s	51.9					

Table S2. ^1H (600 MHz) and ^{13}C (150 MHz) NMR data of **6-10** in CDCl_3 .



No.	6		7		8		9		10	
	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}
1		80.9		90.3		88.4		90.2		82.6
2	2.50, d, (17.7) 2.42, d, (17.7)	45.3	2.76, d, (18.3)	41.3	2.37, d (18.2)	38.4	2.92, d, (18.1)	40.2	2.87, d (17.6)	50.9
			2.39, d, (18.3)		2.70, d (18.2)		2.37, d, (18.1)		2.40, d (17.6)	
3		206.1		205.3		205.9		204.9		204.8
4		137.9		143.0		141.7		143.4		140.8
5		172.4		167.9		169.3		167.0		168.6
6	2.72, dd, (11.6, 11.4) 2.59, brd, (11.6)	31.7	2.66, m 2.58, overlapped	36.8	2.41, overlapped 2.46, overlapped	28.8	2.68, m 2.60, overlapped	35.2	2.72, ddd (18.7, 3.1) 2.61, ddd (18.5, 11.3)	35.0
7	1.94, m	49.4	2.58, overlapped	42.5	2.40, overlapped	41.7	2.56, overlapped	42.9	2.78, m	43.2
8	2.09, m 1.59, m	27.5	1.65, m 1.51, m	29.5	1.52, m 1.85, m	25.1	1.70, m 1.58, m	28.0	1.65, m 1.57, m	27.9
9	1.83, ddd, (14.8, 6.0, 2.4) 1.22, ddd, (14.8, 12.6, 2.2)	30.2	2.24, m 1.65, m	39.8	1.47, m 2.37, overlapped	32.8	2.20, ddd, (15.2, 12.8, 2.6) 1.87, ddd, (15.2, 6.1, 2.6)	34.3	2.20, m 1.87, m	32.4
10		74.1		75.8		74.8		76.0	4.09, brs	74.1
11		149.6		150.7		150.0		150.3		150.6
12	4.80, d, (1.6) 4.76, d, (1.6)	109.9	4.76, d, (1.7) 4.72, d, (1.7)	109.3	4.77, d (1.5) 4.73, d (1.5)	109.4	4.78, d, (1.5) 4.75, d, (1.5)	109.6	4.77, d, (1.6) 4.72, d, (1.6)	109.5
13	1.79, s	20.3	1.77, s	20.4	1.77, s	20.1	1.79, s	20.7	1.77, s	20.3
14	3.79, d, (10.5) 3.48, d, (10.5)	68.4	1.33, s	28.1	1.29, s	27.8	3.70, d, (11.0) 3.63, d, (11.0)	69.2	1.71, s	
15	1.72, s	7.7	1.75, s	8.4	1.78, s	8.05	1.75, s	8.6		8.4

-OCH₃

3.05, s

50.7

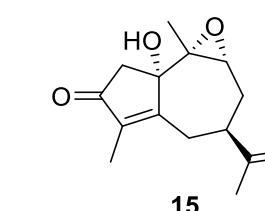
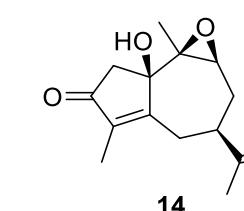
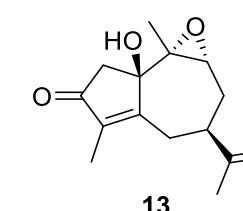
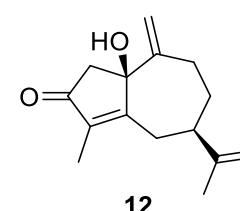
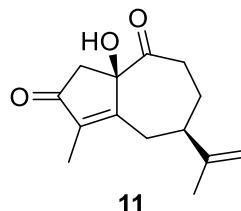
3.05, s

50.8

3.05, s

50.6

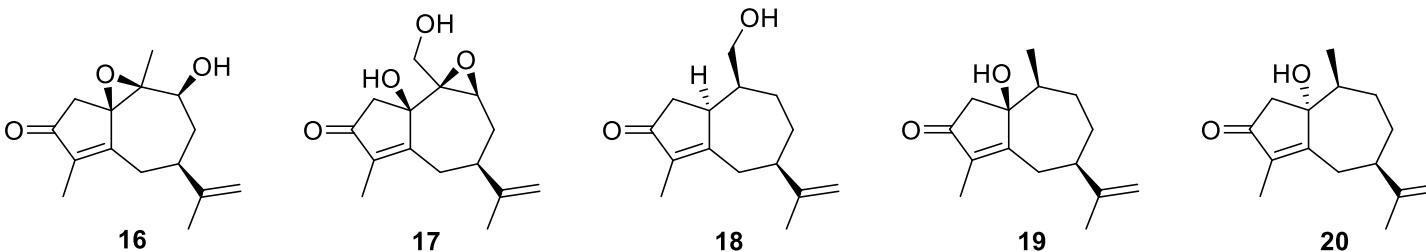
Table S3. ¹H (600 MHz) and ¹³C (150 MHz) NMR data of **11–15** in CDCl₃.



No.	11		12		13		14		15	
	δ_{H} , multi, <i>J</i> (Hz)	δ_{C}								
1		82.9		80.4		81.4		77.5		78.1
2	2.52, overlapped	45.5	2.63, d, (18.5)	49.7	2.98, d (18.4)	48.2	2.99, d (17.4)	49.0	2.94, d (17.9)	48.4
	2.52, overlapped		2.48, d, (18.5)		2.48, d (18.4)		2.48, d (17.4)		2.49, d (17.9)	
3		205.1		207.0		205.6		204.7		204.9
4		141.2		137.8		138.6		138.2		138.8
5		167.7		172.2		170.6		169.6		169.9
6	2.77, m	32.3	2.69, brd, (12.1)	32.2	2.58, brd (12.5)	32.3	2.73, dd (13.6, 3.2)	32.9	2.87, overlapped	30.9
					2.26, m					
	2.17, overlapped		2.23, dd, (12.1, 11.9)				2.64, dd (13.6, 12.1)		2.78, dd (14.4, 6.9)	
7	2.16, overlapped	48.9	2.44, m	48.9	2.09, m	40.2	2.27, overlapped	42.6	2.71, m	40.3
8	2.07, m	33.1	2.03, overlapped	37.7	2.20,ddd (15.4, 12.2, 0.9)	33.8	2.24, overlapped	33.7	2.41,ddd, (14.1, 6.9, 5.5)	29.3
	1.60, m		1.44, m		2.35, m		2.03,ddd, (13.7, 11.6, 8.1)		2.16,ddd, (14.1, 8.2, 2.8)	
9	2.54, overlapped(2H)	37.8	2.05, overlapped 1.68, m	33.4	3.12, dd (5.6, 0.9)	65.7	3.04, dd (8.1, 7.2)	64.0	2.89, overlapped	63.7
10		211.9		153.1		63.7		61.3		61.4
11		148.1		149.3		148.7		148.7		147.6
12	4.80, d (1.5) 4.78, d (1.3)	111.0	4.78, overlapped 4.77, overlapped	110.1	4.78, d (1.5) 4.77, d (1.5)	110.4	4.81, d (1.5) 4.78, d (1.5)	110.5	4.78, d (1.5) 4.61, d (1.5)	110.5

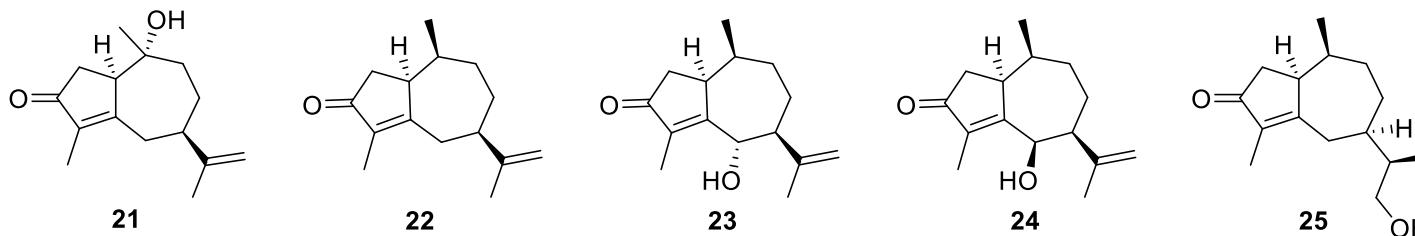
13	1.75, s	20.4	1.77, s	20.5	1.77, s	20.3	1.77, s	19.9	1.80, s	22.7
14	1.84, s		5.44, d, (1.1)	112.5	1.50, s	21.4	1.19, s	18.4	1.19, s	19.0
			5.15, d, (1.1)							
15	4.21, s	8.1	1.77, s	7.9	1.65, s	8.0	1.76, s	8.4	1.78, s	8.8

Table S4. ^1H (600 MHz) and ^{13}C (150 MHz) NMR data of **16–20** in CDCl_3 .



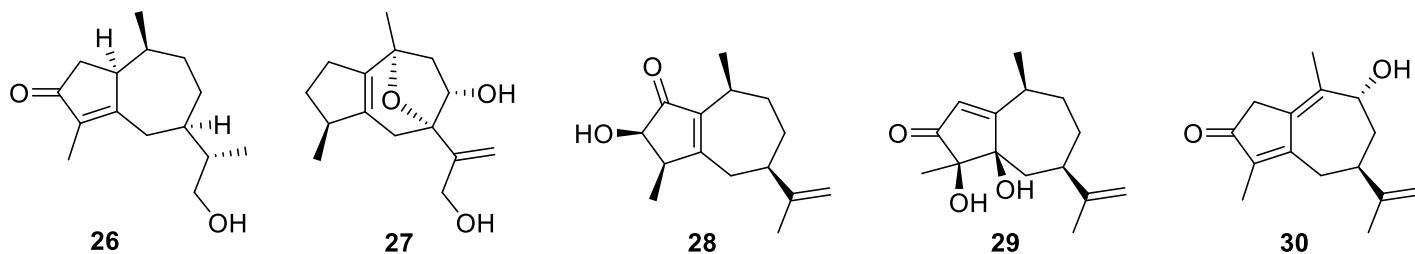
No.	16		17		18		19		20	
	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}
1		70.4		81.4	3.19, m	44.3		79.7		82.9
2	2.72, d, (18.7) 2.50, d, (18.7)	40.8	3.04, d, (18.2) 2.61, d, (18.2)	48.3	2.64, dd, (18.8, 6.8) 2.29, brd, (18.8)	41.5	2.58, d, (18.1) 2.43, d, (18.1)	51.0	2.55, d, (18.2) 2.40, d, (18.2)	51.2
3		203.8		204.8		208.0		205.8		205.7
4		142.1		139.4		137.7		137.5		138.4
5		167.1		168.8		174.4		173.8		172.1
6	2.76, dd, (11.9, 2.3) 2.30, overlapped	34.5	2.64, overlapped 2.35, dd, (12.1, 11.9)	32.1	2.79, brd, (19.4) 2.49, dd, (19.4, 12.1)	37.8	2.70, dd, (12.6, 12.2) 2.52, dd, (12.6, 5.0)	28.0	2.68, brd, (19.1) 2.46, dd, (19.1, 11.6)	35.8
7	2.31, overlapped	36.5	2.13, m	40.4	2.38, m	44.4	2.43, overlapped	41.7	2.82, m	42.8
8	2.00, m 1.88, m	38.3	2.41, m 2.26,ddd, (15.5, 11.9, 1.2)	33.6	1.82, m 1.57, overlapped	31.6	1.81, overlapped 1.51, m	30.9	1.63, m 1.43, m	30.0
9	4.41, brd, (5.7)	74.4	3.38, dd, (5.4, 1.2)	63.6	2.21, overlapped 1.61, overlapped	31.4	1.80, overlapped 1.38, m	27.4	2.15, m 1.48, overlapped	30.8
10		67.7		63.8	2.19, overlapped	43.0	1.43, m	45.9	2.23, m	40.0
11		149.7		148.5		150.7		149.7		151.0
12	4.79, d, (1.5) 4.76, d, (1.5)	110.1	4.82, d, (1.5) 4.80, d, (1.5)	110.6	4.76, d, (1.6) 4.71, d, (1.6)	109.3	4.78, d, (1.5) 4.75, d, (1.5)	109.5	4.70, d, (1.7) 4.65, d, (1.7)	109.1
13	1.76, s	20.3	1.80, s	20.4	1.77, s	20.4	1.78, s	20.7	1.71, s	20.4
14	1.57, s	23.0	4.25, d, (11.6) 3.59, d, (11.6)	67.0	3.41, dd, (10.8, 4.9) 3.47, dd, (10.8, 8.7)	60.9	1.09, d, (6.9)	17.6	0.71, d, (7.1)	14.5
15	1.80, s	8.8	1.72, s	8.1	1.64, s	8.2	1.72, s	7.8	1.59, s	7.9

Table S5. ^1H (600 MHz) and ^{13}C (150 MHz) NMR data of **21–25** in CDCl_3 .



No.	21		22		23		24		25	
	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}
1	3.19, m	52.1	3.12, m	46.1	3.24, m	43.5	3.06, m	46.0	3.11, ddd, (5.9, 3.8, 1.9)	46.0
2	2.57, dd, (19.3, 2.1) 2.46, dd, (19.3, 6.5)	37.6	2.03, dd (18.8, 1.5) 2.57, ddd (18.8, 6.6, 1.5)	41.3	2.61, dd, (18.6, 6.6) 2.08, brd, (18.6)	42.5	2.60, dd (19.1, 6.7) 2.10, dd (19.1, 1.8)	41.5	2.55, dd, (18.8, 6.6) 2.03, brd, (18.8)	41.5
3		208.2		208.4		209.1		209.1		208.5
4		138.4		137.8		143.3		143.1		137.9
5		172.1		175.4		171.3		172.3		175.9
6	2.79, brd, (19.3) 2.44, overlapped	37.8	2.76, brd (19.5) 2.45, dd, (19.5, 12.2)	38.1	4.41, d, (10.5) 2.45, ddd, (11.1, 10.0, 1.0)	69.9	4.60, brs 2.31, dd (11.2, 1.5)	68.1	2.67, brd, (18.8) 2.27, m	33.8
7	2.38, m	44.0	2.32, m	44.7	1.57, m	53.5	1.52, m	50.0	1.90, m	37.5
8	1.89, ddd, (14.2, 4.5, 3.4) 1.41, ddd, (14.2, 13.2, 10.4)	32.0	1.74, m 1.57, m	31.5	1.48, m 1.76, overlapped	25.6	2.21, m 1.71, m	22.5	1.62, m 1.47, m	30.5
9	2.02, ddd, (13.3, 4.5, 3.4) 1.82, m	46.7	1.83, m 1.71, m	36.9	1.78, overlapped 2.15, m	36.4	1.82, m 2.09, overlapped	36.9	1.83, overlapped 1.72, m	37.0
10		74.8	2.11, m	35.5		36.1		35.9	2.10, m	35.6
11		150.3		151.0		147.2		149.2	1.78, overlapped	42.6
12	4.76, d, (1.5) 4.73, d, (1.5)	109.5	1.76, s 4.74, d (1.6)	109.1	4.95, d, (1.7) 4.92, d, (1.7)	113.0	4.98, d (1.6) 4.87, d (1.6)	112.2	3.60, dd, (10.7, 7.3) 3.53, dd, (10.7, 6.6)	65.9
13	1.77, s	20.4	4.69, d (1.6)	20.3	1.78, s	18.5	1.85, s	23.6	0.92, d, (7.0)	12.6
14	0.94, s	21.0	0.64, d (7.1)	12.2	0.58, d, (7.1)	12.7	0.75, d (7.1)	12.2	0.62, d, (7.1)	12.3
15	1.66, s	8.3	1.65, s	8.1	1.87, s	8.9	1.85, s	9.0	1.66, s	8.2

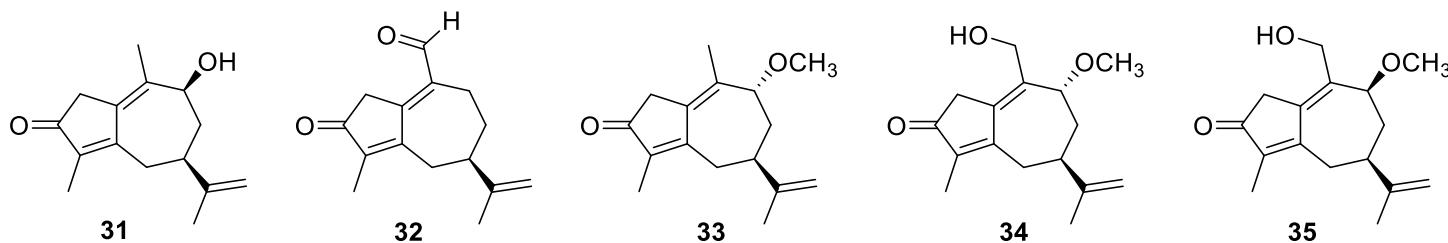
Table S6. ^1H (600 MHz) and ^{13}C (150 MHz) NMR data of **26–30** in CDCl_3 .



No.	26		27		28		29		30	
	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}
1	3.13, m	46.0		141.4		142.0		184.6		132.6
2	2.56, dd, (18.8, 6.6) 2.03, brd, (18.8)	41.5	2.33, overlapped 2.27, overlapped	30.0		208.3	6.00, s	127.3	2.98, d, (20.6) 2.93, d, (20.6)	41.2
3		208.5	2.12, m	32.0	4.22, d (6.5)	74.3		209.1		204.0
4		137.7	1.37, m	41.0	2.90, overlapped	44.2		80.3		140.5
5		176.0	2.58, m	135.3		176.2		80.7		165.2
6	2.42, dd, (19.6, 12.4) 1.93, dd, (19.6, 10.2)	37.3		35.4	2.61, dd (16.3, 12.1) 2.33, brd, (16.3)	38.2	2.20, brd (15.0) 1.98, dd (15.0, 10.7)	40.5	2.93, overlapped 2.59, dd, (17.1, 11.4)	36.5
7	2.64, m	37.5	2.28, overlapped	87.2	2.07, m	46.2	1.84, overlapped	44.8	2.69, m	37.6
8	1.65, overlapped	26.7		80.6	1.85, overlapped	30.7	1.80, overlapped	32.0	2.15, ddd, (14.4, 6.2, 3.2)	41.5
		1.30, m		4.19, dd (7.4, 5.3)		1.82, overlapped		1.70, m		2.02, ddd, (14.4, 9.3, 3.0)
9	1.83, m 1.67, overlapped	36.9	2.62, dd (12.3, 7.4) 1.61, dd (12.3, 5.2)	52.5	1.78, overlapped 1.56, m	32.7	2.04, m 1.62, m	34.9	4.49, m	72.5
10	2.11, m	35.6		79.2	2.93, m	27.9	3.19, m	38.2		134.9
11	1.74, m	42.3		148.2		150.8		150.1		149.5
12	3.60, dd, (10.6, 7.4) 3.54, dd, (10.6, 6.4)	66.1	5.38, d (1.4) 5.29, d (1.4)	113.9	4.75, d (1.6) 4.72, d (1.6)	109.4	4.65, d (1.6) 4.64, d (1.6)	109.3	4.80, d, (1.5) 4.78, d, (1.5)	110.0
13	0.90, d, (7.0)	12.3	4.32, dd (12.2, 1.2) 4.29, dd (12.2, 0.9)	65.1	1.77, s	20.4	1.73, s	19.7	1.80, s	20.5

14	0.62, d, (7.1)	12.1	1.43, s	21.6	1.02, d (7.2)	17.7	1.35, d, (7.2)	18.7	1.97, s	21.0
15	1.67, s	8.2	0.97, d (6.9)	19.5	1.03, d (7.2)	14.6	1.30, s	21.6	1.77, s	8.7

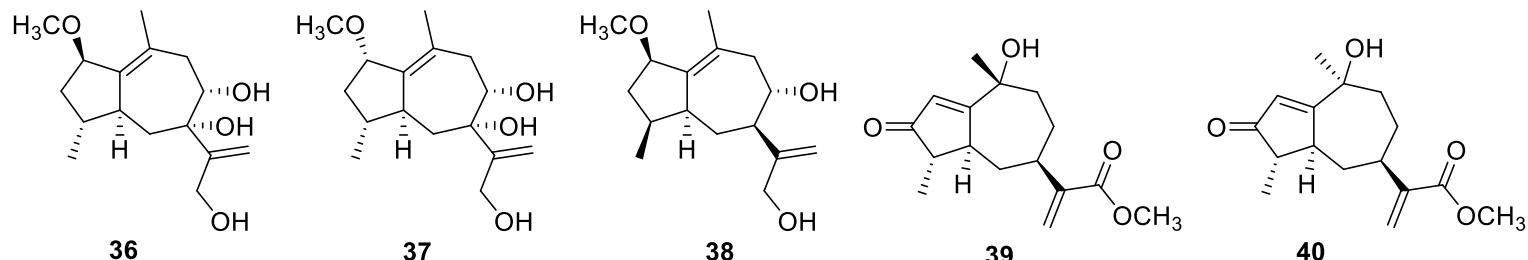
Table S7. ^1H (600 MHz) and ^{13}C (150 MHz) NMR data of **31–35** in CDCl_3 .



No.	31		32		33		34		35	
	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}
1		132.1		152.7		133.3		135.6		136.2
2	3.00, d, (20.6) 2.93, d, (20.6)	41.2	3.40, d, (20.5) 3.40, d, (20.5)	37.5	2.97, d, (20.6) 2.90, d, (20.6)	41.1	3.12, d, (20.5) 3.00, d, (20.5)	39.6	3.10, d, (20.5) 3.07, d, (20.5)	39.6
3		204.0		202.8		204.1		203.5		203.6
4		140.5		144.4		140.4		142.4		142.4
5		165.4		166.3		165.3		165.0		165.3
6	2.81, dd, (16.7, 10.2) 2.75, brd, (16.7)	35.5	2.86, overlapped 2.84, overlapped	32.5	2.93, overlapped 2.59, m	36.2	2.93, dd, (15.9, 2.6) 2.61, dd, (15.9, 11.2)	35.3	2.91, m 2.71, dd, (16.5, 3.4)	34.3
7	2.40, m	40.3	2.55, m	42.9	2.70, m	37.5	2.68, m	37.8	2.41, m	40.7
8	2.25, ddd, (13.8, 5.0, 3.5) 1.88, ddd, (13.8, 9.6, 8.8)	42.1	1.95, m	31.6	2.26, ddd, (14.6, 6.1, 3.3) 1.78, overlapped	35.8	2.26, ddd, (14.6, 7.0, 4.2) 1.82, ddd, (14.6, 9.4, 2.4)	35.9	2.24, ddd, (14.0, 4.6, 1.3) 1.91, ddd, (14.0, 9.8, 8.6, 2.8)	37.2
9	4.33, m	73.9	2.68, m	21.5	3.88, dd, (6.2, 2.3)	81.8	4.28, overlapped	80.1	4.16, dd, (8.0, 4.6)	81.4
10		136.0		135.4		134.2		135.3		135.5
11		149.3		148.7		149.7		149.2		149.0
12	4.78, d, (1.5) 4.75, d, (1.5)	110.1	4.75, d, (1.5) 4.73, d, (1.5)	110.2	4.78, d, (1.5) 4.75, d, (1.5)	109.8	4.80, d, (1.5) 4.79, d, (1.5)	110.1	4.78, d, (1.5) 4.76, d, (1.5)	110.3
13	1.79, s	20.1	1.76, s	20.8	1.78, s	20.4	1.80, s	20.5	1.78, s	20.1

14	1.97, s	20.7	9.94, s	191.4	1.92, s	21.5	4.28, d, (12.5) 4.25, d, (12.5)	64.7	4.25, d, (12.5) 4.23, d, (12.5)	64.6
15 -OCH ₃	1.77, s	8.7	1.89, s	9.1	1.75, s 3.41, s	8.7 57.8	1.79, s 3.44, s	8.8 57.4	1.79, s 3.42, s	8.8 57.0

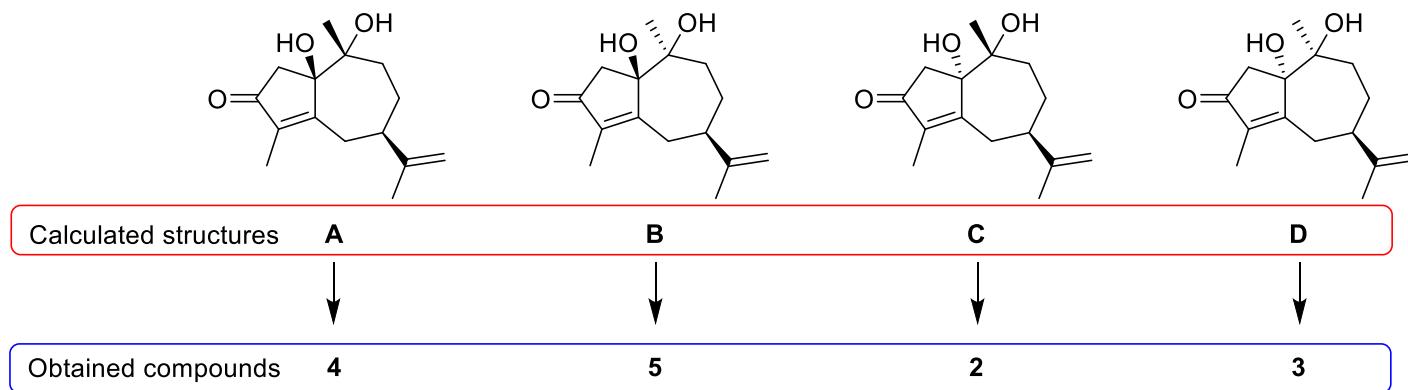
Table S8. ^1H (600 MHz) and ^{13}C (150 MHz) NMR data of **36–40** in CDCl_3 .



No.	36		37		38		39		40	
	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}	δ_{H} , multi, J (Hz)	δ_{C}
1		146.5			144.6			144.0		187.8
2	4.21, brd, (4.7) 1.95, dd, (13.4, 5.7)	82.2	4.30, t, (6.0) 2.00, m	83.2	4.22, dd, (5.6, 4.8) 1.88, overlapped	82.4	6.22, d, (1.7)	128.8	6.22, s	128.1
3	1.27, overlapped	38.8	1.51, overlapped	39.4	1.58, ddd, (12.5, 7.2, 4.8)	38.0		210.3		211.3
4	2.35, m	35.7	2.09, m	35.7	2.13, m	35.3	2.02, overlapped	50.1	2.52, m	50.7
5	2.97, m	39.4	2.92, m	40.2	2.46, m	45.5	2.70, m	50.8	2.06, qd, (7.4, 1.3)	51.4
6	1.56, dd, (13.9, 1.6) 1.32, dd, (13.9, 12.7)	39.3	1.60, dd, (13.9, 2.2) 1.55, dd, (13.9, 11.9)	40.1	1.66, m 1.31, m	33.6	2.07, overlapped 1.91, ddd, (14.0, 7.7, 1.5)	40.4	2.21, m 1.28, m	43.2
7		80.5			80.4	2.23, overlapped	55.6	2.80, m	43.2	2.77, m
8	3.56, dd, (11.1, 1.9) 3.13, dd, (13.6, 11.1)	72.5	3.62, dd, (11.0, 2.0) 3.10, dd, (14.0, 11.0)	72.8	3.55, m	71.0	1.96, m 1.51, overlapped	30.6	1.77, m 1.63, overlapped	29.0
9	1.81, dd, (13.6, 1.9)	39.3	1.79, dd, (14.0, 2.0)	39.6	2.54, dd, (14.0, 11.4) 2.25, dd, (14.0, 2.2)	44.5	2.04, overlapped 1.46, m	39.2	2.01, ddd, (15.2, 8.4, 1.3) 1.91, ddd, (15.2, 10.9, 1.3)	40.8
10		134.3			133.2		131.4		73.7	74.5
11		157.0			157.1		152.0		145.4	145.4
12	5.25, d, (1.5) 5.20, d, (1.5)	111.1	5.28, d, (1.4) 5.21, d, (1.4)	111.0	5.20, brs 5.05, brs	112.7	6.18, d, (0.8) 5.54, d, (0.8)	123.7	6.17, d, (0.7) 5.53, d, (0.7)	123.7
13	1.84, s	63.7	1.81, s	63.6	1.85, s	65.4		167.4		167.5

14	4.15, d, (15.5) 4.12, d, (15.5)	22.1	4.18, d, (14.9) 4.15, d, (14.9)	21.7	4.14, d, (23.4) 4.11, d, (23.4)	22.2	1.55, s	30.1	1.43, s	32.2
15 -OCH ₃	0.94, d, (7.0) 3.30, s	15.7 56.1	0.96, d, (7.1) 3.32, s	16.7 55.8	0.98, d, (7.2) 3.30, s	16.6 55.8	1.19, d, (7.4) 3.78, s	14.3 52.1	1.18, d, (7.4) 3.77, s	16.9 52.2

Table S9. Calculated chemical shifts of ^1H NMR and ^{13}C NMR for **A–D** corresponds to **2–5**.

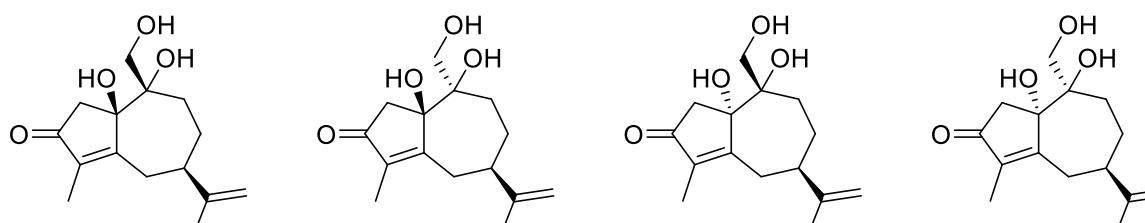


No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$	$\delta_{\text{calcd}}\text{-C}^{\text{a}}$	$\delta_{\text{calcd}}\text{-D}^{\text{a}}$
9-C	31.6	37.3	33.7	39.5
8-C	21.4	29.4	25.1	30.4
7-C	41.9	42.4	44.4	41.5
6-C	26.4	37.9	26.9	36.5
5-C	82.7	84.1	81.3	85.4
4-C	174.8	179.6	177.9	177.8
3-C	142.6	141.6	142.4	142.7
2-C	208.3	208.3	208.7	206.9
1-C	47.3	48.2	47.5	49.0
17-C	23.6	24.1	18.0	18.8
15-C	110.3	109.8	110.6	110.0
14-C	18.6	17.1	15.9	18.0
13-C	157.8	159.9	157.5	159.7
12-C	6.5	4.3	6.0	4.0
10-C	73.1	74.3	75.7	75.7
39-H	1.33	1.36	1.04	0.92
38-H	1.33	1.36	1.04	0.92
37-H	1.33	1.36	1.04	0.92
35-H	5.17	5.08	5.10	5.13
34-H	5.19	5.15	5.10	5.17

33-H	1.98	1.93	1.91	1.93
32-H	1.98	1.93	1.91	1.93
31-H	1.98	1.93	1.91	1.93
30-H	1.86	1.76	1.81	1.75
29-H	1.86	1.76	1.81	1.75
28-H	1.86	1.76	1.81	1.75
27-H	1.35	1.61	1.29	1.64
26-H	2.36	2.46	2.87	2.36
25-H	1.80	1.90	1.66	1.47
24-H	1.50	1.65	1.66	1.72
23-H	2.69	3.06	2.43	3.33
22-H	2.67	2.80	2.51	2.80
21-H	2.82	2.89	3.00	2.76
20-H	3.14	3.04	3.07	3.41
19-H	2.03	2.25	2.24	2.18

^a Calculated in CDCl₃

Table S10. Calculated chemical shifts of ^1H NMR and ^{13}C NMR for **A–D** corresponds to **6**.



Calculated structures **A** **B** **C** **D**

↓

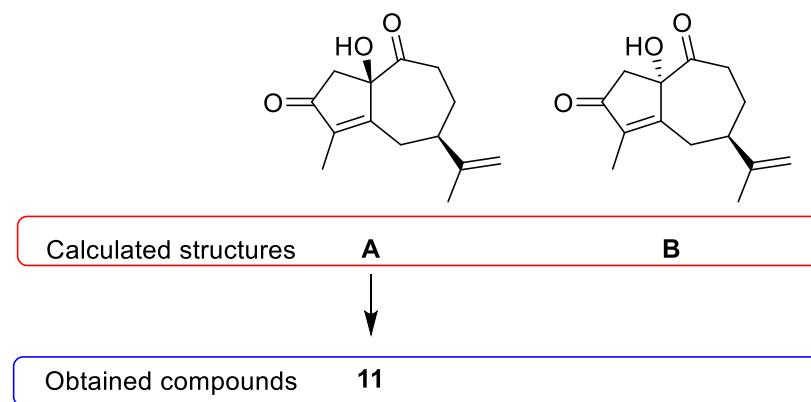
Obtained compounds **6**

No	$\delta_{\text{calcd-}\mathbf{A}}^{\text{a}}$	$\delta_{\text{calcd-}\mathbf{B}}^{\text{a}}$	$\delta_{\text{calcd-}\mathbf{C}}^{\text{a}}$	$\delta_{\text{calcd-}\mathbf{D}}^{\text{a}}$
1-C	87.1	87.3	81.5	86.9
2-C	180.9	180.6	186.0	184.1
3-C	30.8	39.8	35.5	39.3
4-C	46.2	45.2	53.5	46.0
5-C	26.5	32.5	31.6	32.0
6-C	29.5	36.5	31.9	34.3
7-C	75.9	79.9	76.5	77.6
8-C	162.5	163.4	162.8	163.4
9-C	22.6	22.7	22.7	22.6
10-C	114.5	114.7	114.8	114.3
11-C	70.6	63.9	66.5	69.6
12-C	50.4	54.0	47.4	51.4
14-C	147.5	147.4	144.1	145.4
15-C	212.3	210.3	213.3	212.2
17-C	10.1	8.6	8.5	9.1
20-H	2.68	2.68	2.91	2.69
21-H	2.68	2.71	2.54	2.89
22-H	2.54	3.24	1.98	2.72
23-H	1.97	1.55	1.50	1.52

24-H	1.39	1.24	2.18	1.97
25-H	1.70	1.92	1.33	2.04
26-H	2.22	1.98	1.93	1.94
27-H	1.87	1.88	1.94	1.93
28-H	1.95	1.75	1.92	1.86
29-H	1.80	1.85	1.73	1.77
30-H	5.06	5.08	5.06	4.99
31-H	5.09	5.06	5.06	5.03
32-H	3.85	2.93	3.38	3.81
33-H	3.73	3.28	3.75	3.59
34-H	1.96	3.07	2.09	3.17
35-H	3.11	2.26	2.13	1.95
37-H	1.68	1.38	1.39	1.46
38-H	1.77	2.21	1.57	1.41
39-H	1.83	1.28	2.10	2.04

^a Calculated in CDCl₃

Table S11. Calculated chemical shifts of ¹H NMR and ¹³C NMR for **A–B** corresponds to **11**.

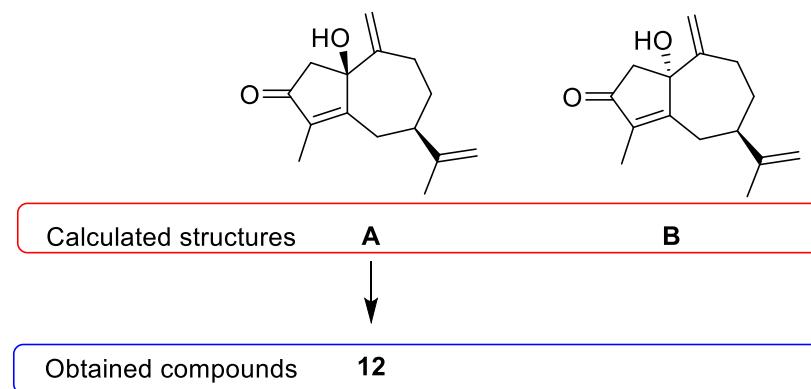


No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$	No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$
9-C	17.88	18.43	35-H	2.00	1.98
8-C	158.10	157.38	34-H	2.00	1.98

7-C	222.83	222.79	33-H	2.00	1.98
6-C	37.94	36.03	31-H	2.62	2.53
5-C	34.15	29.32	30-H	2.52	2.68
4-C	50.61	42.17	29-H	5.28	5.27
3-C	31.74	33.51	28-H	5.31	5.32
2-C	176.69	176.77	27-H	1.95	1.99
1-C	84.57	85.43	26-H	1.95	1.99
17-C	6.97	6.28	25-H	1.95	1.99
15-C	212.05	210.31	24-H	2.82	2.69
14-C	146.10	146.22	23-H	2.66	2.87
12-C	46.65	47.12	22-H	2.10	1.97
10-C	113.32	113.94	21-H	1.81	2.09
			20-H	2.47	2.95
			19-H	2.80	2.91
			18-H	2.56	3.03

^a Calculated in CDCl₃

Table S12. Calculated chemical shifts of ¹H NMR and ¹³C NMR for **A–B** corresponds to **12**.

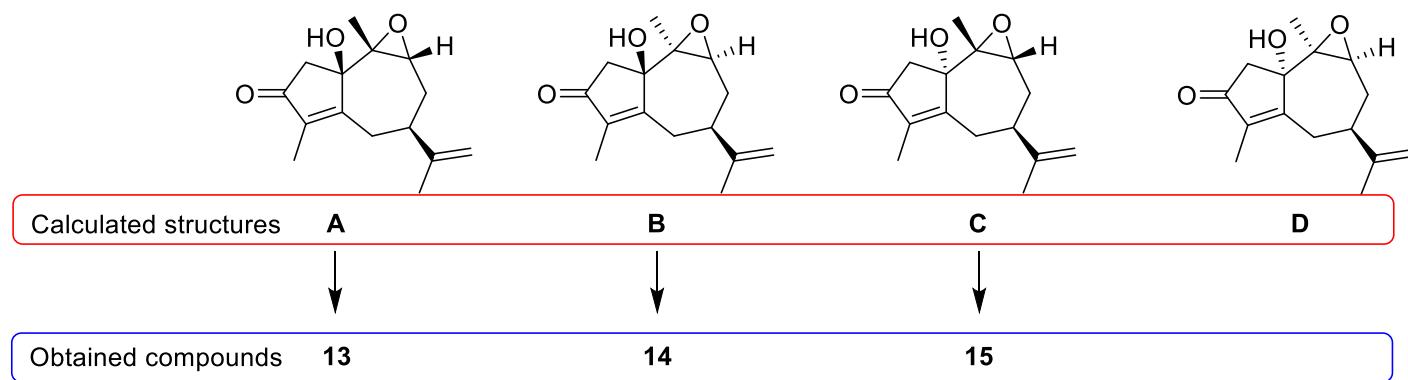


No	$\delta_{\text{calcd-A}}^{\text{a}}$	$\delta_{\text{calcd-B}}^{\text{a}}$	No	$\delta_{\text{calcd-A}}^{\text{a}}$	$\delta_{\text{calcd-B}}^{\text{a}}$
9-C	17.5	18.8	37-H	1.92	1.81
8-C	158.4	158.9	36-H	1.92	1.81

7-C	161.3	161.0	35-H	1.92	1.81
6-C	33.0	32.5	33-H	2.58	2.74
5-C	37.7	35.2	32-H	2.65	2.87
4-C	51.2	42.4	31-H	5.97	5.52
3-C	32.3	34.2	30-H	5.66	5.67
2-C	181.4	182.3	29-H	5.27	5.27
1-C	82.4	83.3	28-H	5.24	5.23
17-C	6.4	5.0	27-H	1.98	2.00
15-C	213.3	210.7	26-H	1.98	2.00
14-C	141.9	140.4	25-H	1.98	2.00
12-C	50.3	51.8	24-H	1.93	2.78
11-C	115.2	114.2	23-H	2.59	2.29
			22-H	1.95	1.89
			21-H	1.82	1.93
			20-H	2.37	3.29
			19-H	2.77	2.77
			18-H	2.42	2.93

^a Calculated in CDCl₃

Table S13. Calculated chemical shifts of ¹H NMR and ¹³C NMR for **A–D** corresponds to **13–15**.



No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$	$\delta_{\text{calcd}}\text{-C}^{\text{a}}$	$\delta_{\text{calcd}}\text{-D}^{\text{a}}$
----	---	---	---	---

1-C	51.6	52.7	52.5	53.2
2-C	212.2	211.4	210.9	211.3
3-C	145.7	145.8	149.2	145.7
4-C	182.3	182.5	178.3	181.7
5-C	84.6	81.0	85.8	80.7
6-C	36.2	35.3	36.7	36.4
7-C	43.5	45.2	44.4	46.5
8-C	37.6	32.8	34.8	36.6
9-C	67.9	66.2	67.1	66.9
10-C	66.0	63.9	64.8	63.9
12-C	8.7	10.1	9.4	9.9
14-C	161.6	159.8	161.1	161.7
15-C	115.5	117.0	115.5	115.5
16-C	22.1	25.6	22.1	21.7
17-C	22.9	19.3	21.9	18.63
19-H	2.36	2.38	2.18	2.36
20-H	2.86	2.84	2.94	2.83
21-H	2.31	2.91	2.70	2.64
22-H	2.52	3.01	2.70	2.90
23-H	2.08	2.63	2.86	2.19
24-H	2.14	2.25	1.38	2.14
25-H	2.24	2.42	1.92	2.05
26-H	2.99	2.71	2.93	2.85
27-H	1.67	1.83	1.70	1.74
28-H	1.67	1.83	1.70	1.74
29-H	1.67	1.83	1.70	1.74
31-H	5.08	5.09	5.07	5.05
32-H	5.05	4.99	5.07	5.08
33-H	1.83	1.85	1.81	1.84
34-H	1.83	1.85	1.81	1.84
35-H	1.83	1.85	1.81	1.84
36-H	1.36	0.99	1.33	0.99
37-H	1.36	0.99	1.33	0.99

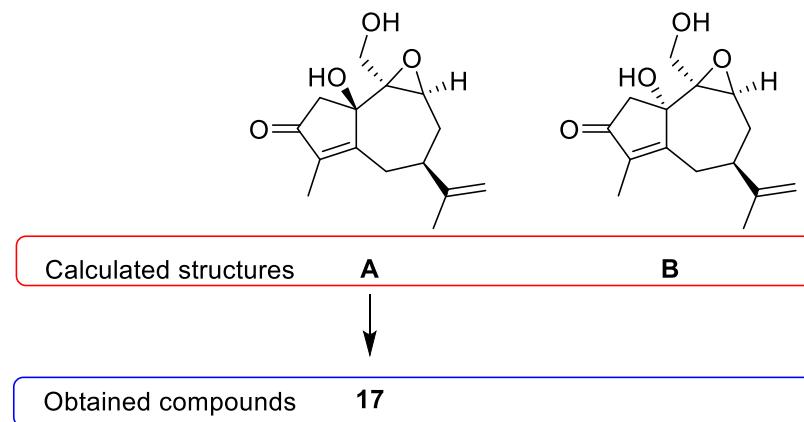
38-H

1.36

0.99

1.33

0.99

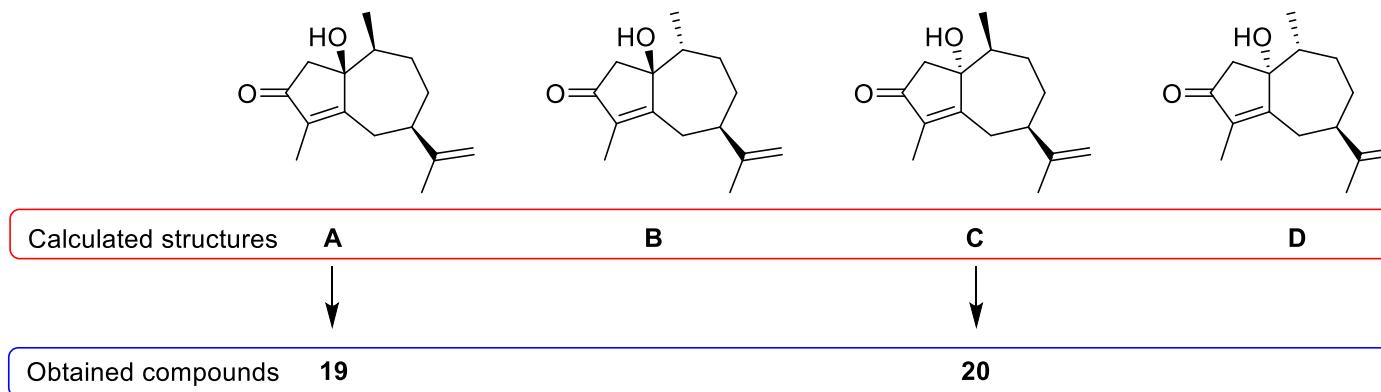
^aCalculated in CDCl₃**Table S14.** Calculated chemical shifts of ¹H NMR and ¹³C NMR for **A–B** corresponds to **17**.

No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$	No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$
9-C	64.2	62.4	38-H	3.45	3.40
8-C	30.5	32.8	37-H	4.45	3.78
7-C	41.6	44.2	36-H	2.03	2.00
6-C	33.0	33.5	35-H	2.03	2.00
5-C	84.9	78.5	34-H	2.03	2.00
4-C	174.8	179.0	33-H	5.23	5.28
3-C	145.9	143.1	32-H	5.30	5.25
2-C	209.6	210.2	30-H	1.89	1.91
1-C	49.7	48.7	29-H	1.89	1.91
17-C	68.0	60.1	28-H	1.89	1.91
16-C	18.7	17.4	27-H	1.64	2.27
15-C	112.7	112.8	26-H	2.16	2.37
14-C	157.9	158.2	25-H	3.14	2.44
12-C	6.8	7.1	24-H	3.01	2.90
10-C	63.5	65.2	23-H	2.86	3.03
			22-H	3.12	3.49

	21-H	2.52	2.58
	19-H	3.38	3.49

^a Calculated in CDCl₃

Table S15. Calculated chemical shifts of ¹H NMR and ¹³C NMR for **A–D** corresponds to **19–20**.

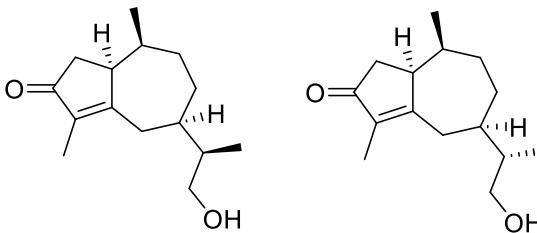


No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$	$\delta_{\text{calcd}}\text{-C}^{\text{a}}$	$\delta_{\text{calcd}}\text{-D}^{\text{a}}$
9-C	17.9	17.8	18.2	17.2
8-C	158.1	160.1	157.0	160.4
7-C	46.7	42.3	39.3	40.1
6-C	25.9	33.2	25.5	29.4
5-C	29.1	33.3	27.1	29.4
4-C	42.5	43.0	42.1	42.4
3-C	27.0	37.2	31.5	37.0
2-C	180.1	182.1	179.5	180.2
1-C	79.2	81.7	81.1	82.6
17-C	6.3	4.9	4.6	3.8
15-C	208.4	208.0	208.4	206.5
14-C	140.4	139.2	140.4	141.3
12-C	51.0	51.3	49.6	52.1
11-C	14.4	15.9	13.5	11.8
10-C	110.7	109.8	111.8	109.8

39-H	1.82	1.75	1.79	1.74
38-H	1.82	1.75	1.79	1.74
37-H	1.82	1.75	1.79	1.74
35-H	2.64	2.78	2.54	2.64
34-H	2.29	2.40	2.49	2.44
33-H	1.12	1.13	0.82	0.73
32-H	1.12	1.13	0.82	0.73
31-H	1.12	1.13	0.82	0.73
30-H	5.17	5.11	5.30	5.09
29-H	5.14	5.15	5.28	5.18
28-H	1.98	1.93	1.92	1.91
27-H	1.98	1.93	1.92	1.91
26-H	1.98	1.93	1.92	1.91
25-H	1.19	1.59	2.19	2.20
24-H	1.40	1.67	1.53	1.53
23-H	1.93	1.86	2.17	2.45
22-H	1.39	1.59	1.81	1.80
21-H	1.90	1.79	2.13	1.58
20-H	2.73	3.06	2.59	3.38
19-H	2.66	2.83	2.71	2.71
18-H	2.96	2.92	2.89	2.77

^a Calculated in CDCl₃

Table S16. Calculated chemical shifts of ¹H NMR and ¹³C NMR for **A–B** corresponds to **25–26**.



Calculated structures

A**B**

Obtained compounds

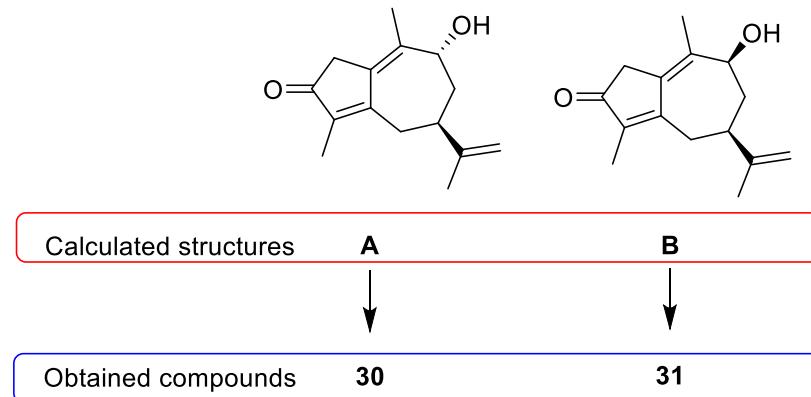
25**26**

No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$	No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$
1-C	214.5	214.8	18-H	3.20	3.23
2-C	144.9	145.1	19-H	1.91	1.89
3-C	189.5	188.8	20-H	2.55	2.53
4-C	50.8	50.8	21-H	2.76	2.69
5-C	46.4	46.4	22-H	2.39	2.56
6-C	37.2	41.2	23-H	2.00	2.06
7-C	39.8	39.9	24-H	1.49	1.52
8-C	34.3	30.2	25-H	1.57	1.36
9-C	40.1	40.2	26-H	1.82	1.78
10-C	41.2	41.4	27-H	1.77	1.69
11-C	9.0	9.5	28-H	1.93	1.97
13-C	47.0	46.9	29-H	1.46	1.54
14-C	12.6	12.8	30-H	1.64	1.77
15-C	69.4	68.8	31-H	1.90	1.73
17-C	14.2	14.1	32-H	1.66	1.60
			33-H	0.85	0.98
			34-H	0.99	0.96
			35-H	0.69	0.67
			36-H	3.59	3.62
			37-H	3.60	3.52

	39-H	0.37	0.41
	40-H	0.57	0.53
	41-H	0.66	0.61

^a Calculated in CDCl₃

Table S17. Calculated chemical shifts of ¹H NMR and ¹³C NMR for A–B corresponds to 30–31.

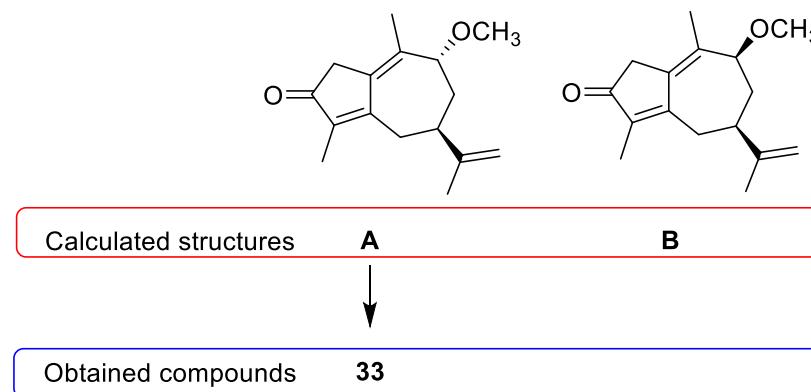


No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$	No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$
9-C	17.4	17.2	36-H	1.76	2.12
8-C	158.0	158.8	35-H	2.34	2.06
7-C	145.7	144.6	34-H	1.62	1.61
6-C	72.1	75.2	33-H	3.19	3.23
5-C	40.3	39.9	32-H	3.13	3.11
4-C	39.8	42.4	31-H	2.03	2.02
3-C	35.8	35.6	30-H	2.12	2.08
2-C	173.7	174.2	29-H	2.10	2.38
1-C	136.0	137.0	28-H	5.24	5.22
16-C	5.2	5.2	27-H	5.24	5.21
14-C	206.9	206.6	26-H	2.06	2.04
13-C	142.6	142.8	25-H	1.96	2.14
12-C	41.4	41.5	24-H	2.20	1.94
11-C	18.8	20.5	23-H	4.69	4.46

10-C	112.6	112.5	22-H	2.49	2.13
			21-H	2.20	2.18
			20-H	2.84	2.56
			19-H	2.99	2.83
			18-H	2.78	3.38

^a Calculated in CDCl₃

Table S18. Calculated chemical shifts of ¹H NMR and ¹³C NMR for **A–B** corresponds to **33**.

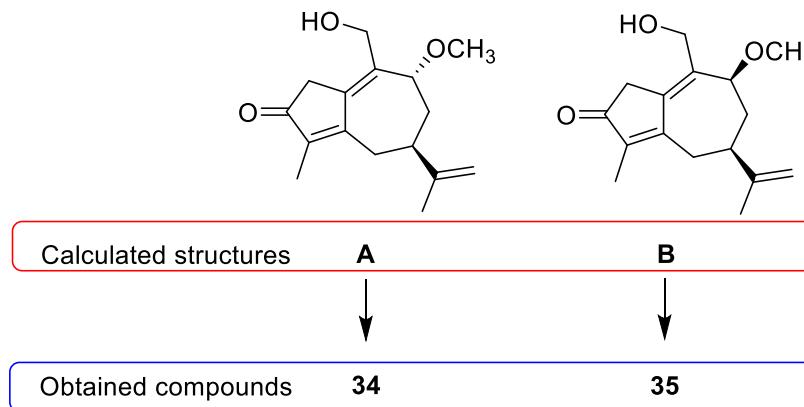


No	$\delta_{\text{calcd-A}}^{\text{a}}$	$\delta_{\text{calcd-B}}^{\text{a}}$	No	$\delta_{\text{calcd-A}}^{\text{a}}$	$\delta_{\text{calcd-B}}^{\text{a}}$
9-C	82.8	80.7	40-H	3.35	3.75
8-C	37.5	33.5	39-H	3.40	3.24
7-C	40.5	39.7	38-H	3.61	3.62
6-C	34.7	34.9	37-H	2.00	1.96
5-C	143.0	142.7	36-H	1.92	2.05
4-C	207.3	207.2	35-H	2.18	2.04
3-C	41.1	41.2	34-H	2.24	2.27
2-C	137.6	137.9	33-H	1.83	1.84
1-C	173.8	173.9	32-H	1.74	1.60
18-C	53.6	54.8	31-H	1.95	2.02
15-C	20.7	18.2	30-H	2.10	2.33
14-C	6.3	5.1	29-H	2.29	2.08

13-C	21.2	20.0	28-H	5.25	5.23
12-C	110.5	112.2	27-H	5.29	5.23
11-C	160.0	157.9	26-H	3.87	4.02
10-C	143.6	144.9	25-H	2.45	2.26
			24-H	1.90	1.97
			23-H	2.27	3.01
			22-H	2.98	3.15
			21-H	3.32	2.89
			20-H	3.22	3.19
			19-H	3.11	3.10

^a Calculated in CDCl₃

Table S19. Calculated chemical shifts of ¹H NMR and ¹³C NMR for **A–B** corresponds to **34–35**.

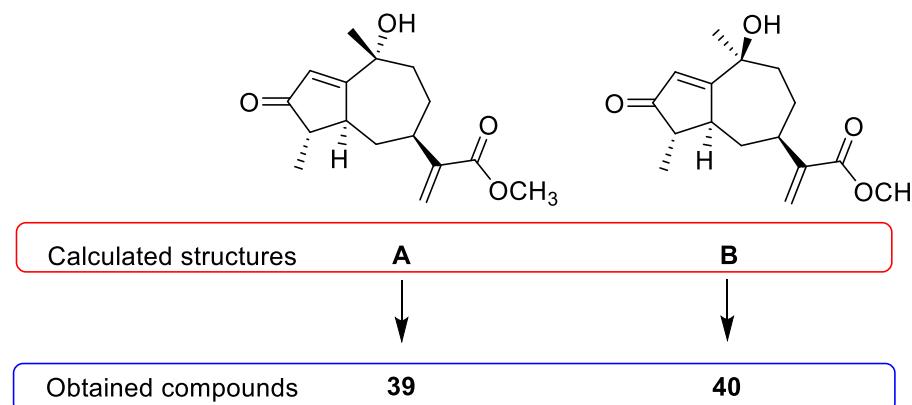


No	$\delta_{\text{calcd-A}}^{\text{a}}$	$\delta_{\text{calcd-B}}^{\text{a}}$	No	$\delta_{\text{calcd-A}}^{\text{a}}$	$\delta_{\text{calcd-B}}^{\text{a}}$
9-C	81.9	84.2	41-H	3.77	3.74
8-C	34.6	36.9	40-H	3.28	3.60
7-C	40.2	40.5	39-H	3.67	3.48
6-C	33.3	36.2	37-H	2.00	1.97
5-C	144.4	146.3	36-H	2.05	1.99
4-C	207.4	206.5	35-H	2.11	2.16
3-C	39.8	40.3	34-H	2.27	2.56

2-C	138.8	140.2	33-H	1.70	1.68
1-C	173.7	172.4	32-H	1.91	1.65
19-C	54.1	54.5	31-H	4.42	4.23
15-C	18.3	17.7	30-H	4.36	4.31
14-C	5.4	5.7	29-H	5.24	5.26
13-C	64.0	64.9	28-H	5.29	5.24
12-C	112.6	111.8	27-H	4.46	4.15
11-C	156.8	158.4	26-H	2.08	2.35
10-C	145.04	142.87	25-H	2.28	1.92
			24-H	2.77	2.39
			23-H	2.91	2.88
			22-H	2.88	3.21
			21-H	3.29	3.25
			20-H	3.17	3.33

^a Calculated in CDCl₃

Table S20. Calculated chemical shifts of ¹H NMR and ¹³C NMR for A–B corresponds to 39–40.



No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$	No	$\delta_{\text{calcd}}\text{-A}^{\text{a}}$	$\delta_{\text{calcd}}\text{-B}^{\text{a}}$
1-C	198.49	200.11	21-H	2.84	2.63
2-C	53.87	52.05	22-H	1.61	1.68
3-C	38.10	38.42	23-H	2.20	1.81

4-C	39.18	40.08	24-H	2.32	2.32
5-C	34.75	35.01	25-H	1.83	1.64
6-C	46.13	46.55	26-H	1.51	1.67
7-C	77.05	78.25	27-H	1.95	1.96
8-C	155.27	154.59	28-H	1.52	1.65
9-C	173.49	173.28	29-H	6.83	6.78
10-C	132.87	132.86	30-H	5.92	5.92
11-C	134.01	134.17	31-H	5.95	6.38
12-C	52.76	53.89	32-H	2.36	2.41
13-C	216.91	215.61	33-H	1.62	1.62
14-C	13.86	13.89	34-H	1.10	1.09
16-C	30.96	26.15	35-H	0.46	0.45
20-C	53.08	53.20	36-H	1.81	1.81
			37-H	1.32	1.20
			38-H	1.24	1.27
			40-H	3.64	3.59
			41-H	3.64	3.66
			42-H	3.58	3.66

^a Calculated in CDCl₃

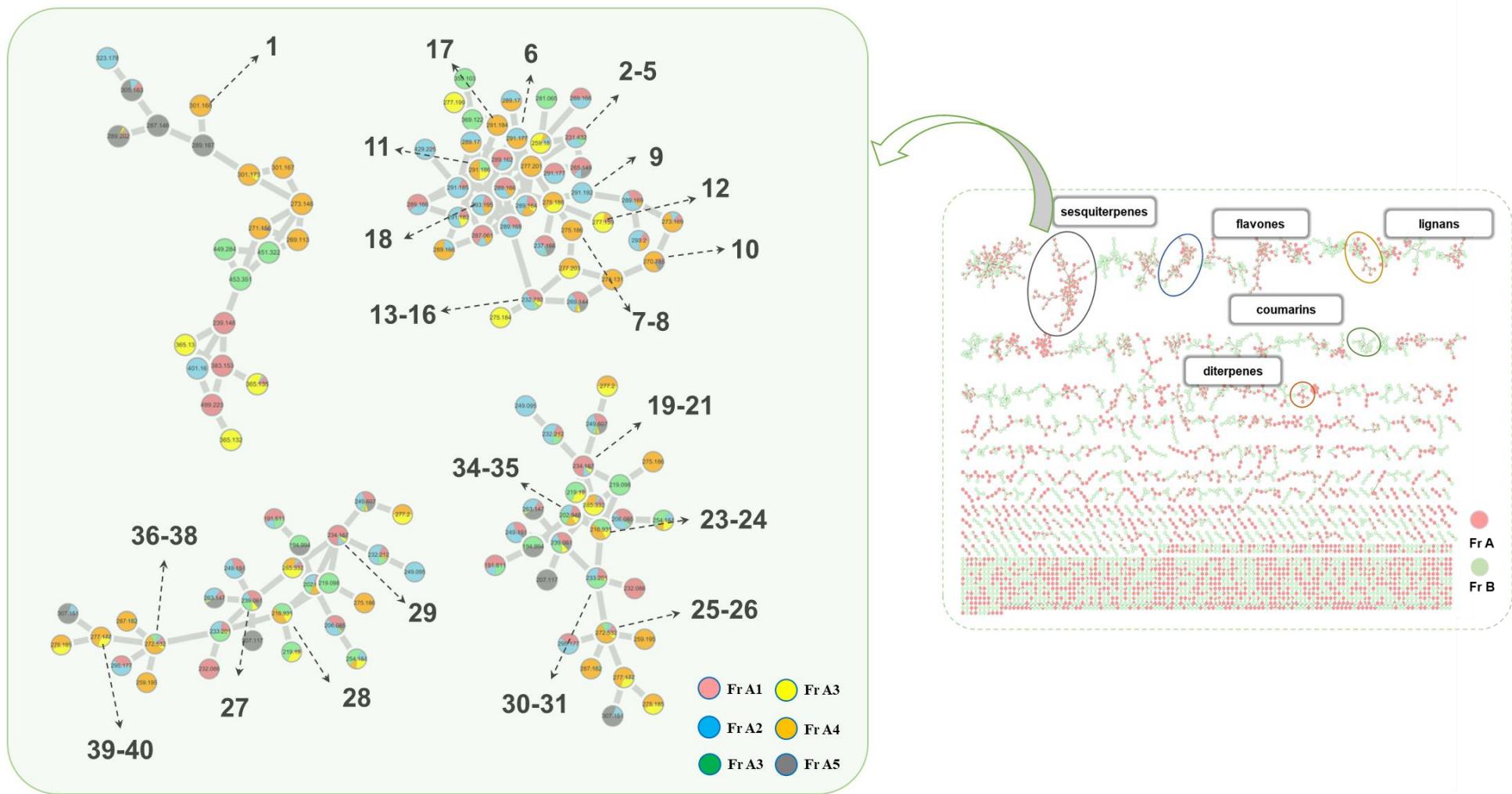
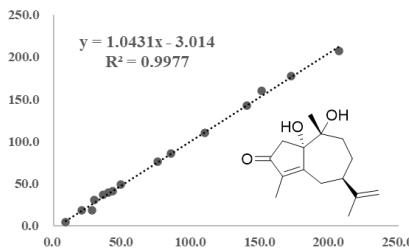
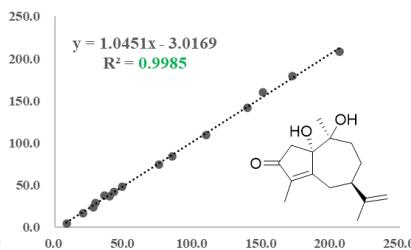
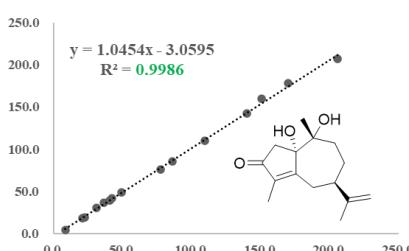
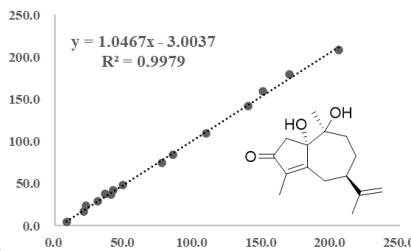


Figure S1. The molecular network was built by HPLC-MS/MS analyses of fractions in *Daphne penicillata*. The molecule cluster including the novel sesquiterpenes is highlighted. The parent m/z of nodes are displayed; The pie charts of nodes represent the source of the compounds.

2/1*S*,7*R*,10*R*-C******2/1*S*,7*R*,**10*S*-D******3/1*S*,7*R*,**10*R*-C******3/1*S*,7*R*,**10*S*-D******CP3 calculation Probabilities:**

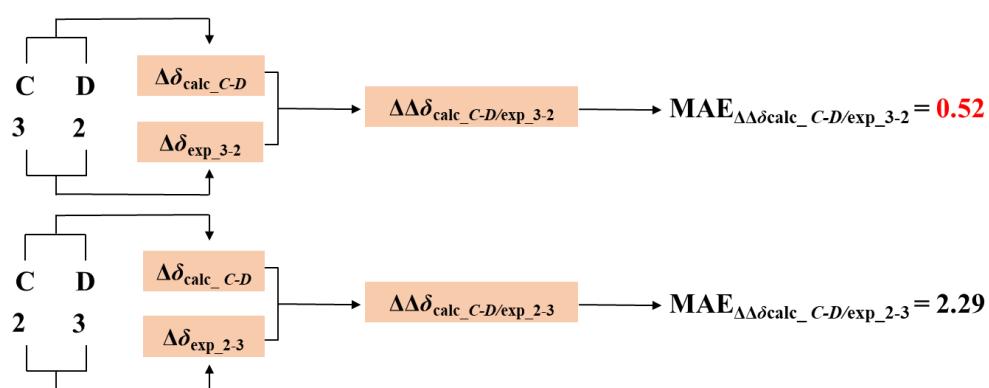
C data H data All data

Exp_3-Cal_C & Exp_2-Cal_D

100.0% **100.0%** **100.0%**

Exp_3-Cal_D & Exp_2-Cal_C

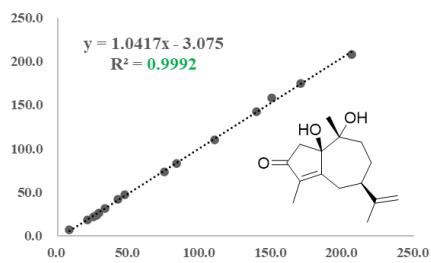
0.0% 0.1% 0.0%

MAE_{ΔΔδ} parameter:**DP4+ calculation Probabilities:**

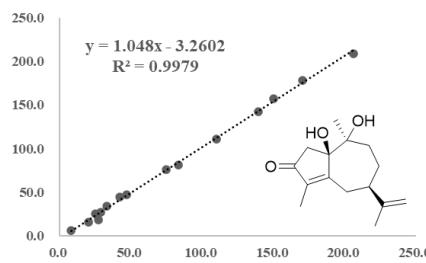
Number/isomers	C	D
2	0.0%	100.0%
3	100.0%	0.0%

Figure S2. Linear correlation (R^2), DP4+, CP3 and $MAE_{\Delta\Delta\delta}$ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **2–3** and **A–D**.

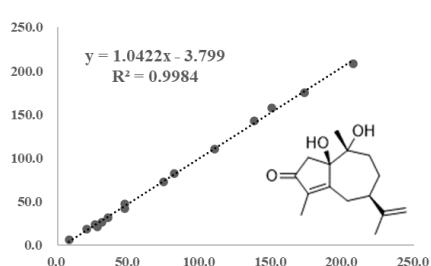
4/1*R*,7*R*,10*R*-A



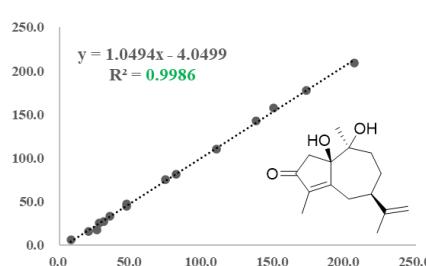
4/1*R*,7*R*,10*S*-B



5/1*R*,7*R*,10*R*-A



5/1*R*,7*R*,10*S*-B



CP3 calculation Probabilities:

C data H data All data

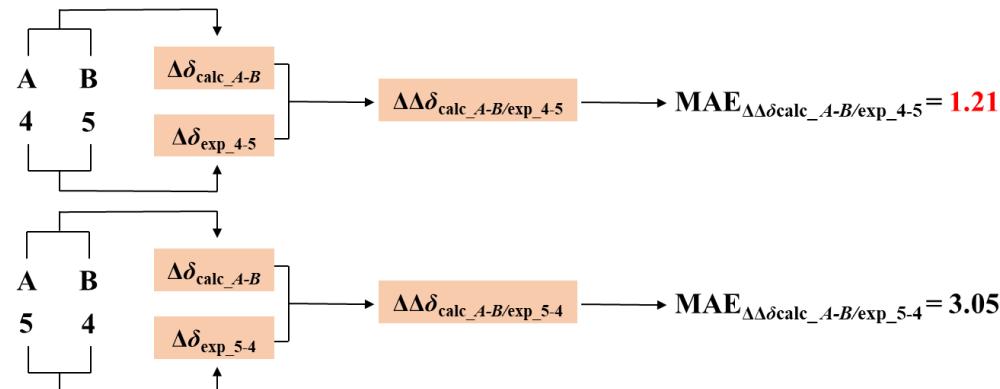
Exp_4-Cal_A & Exp_5-Cal_B

100.0% **100.0%** **100.0%**

Exp_4-Cal_B & Exp_5-Cal_A

0.0% 0.1% 0.0%

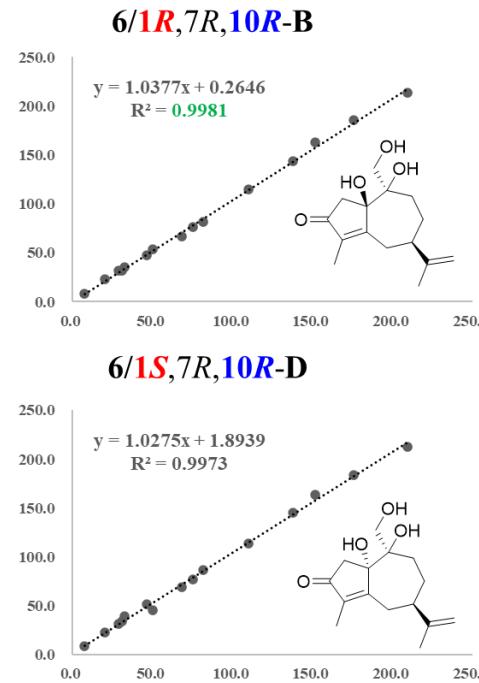
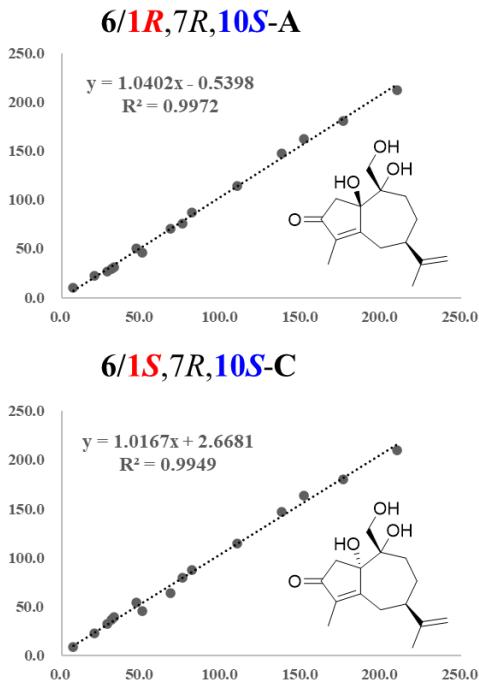
MAE_{ΔΔδ} parameter:



DP4+ calculation Probabilities:

Number/isomers	A	B
4	100.0%	0.0%
5	1.2%	98.8%

Figure S3. Linear correlation (R^2), DP4+, CP3 and $\text{MAE}_{\Delta\Delta\delta}$ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **4–5** and **A–D**.

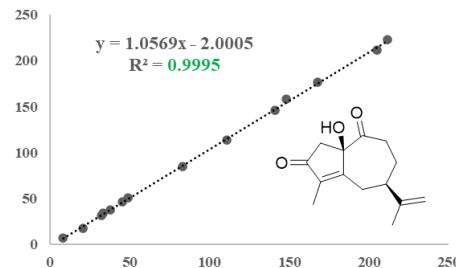


DP4+ calculation Probabilities:

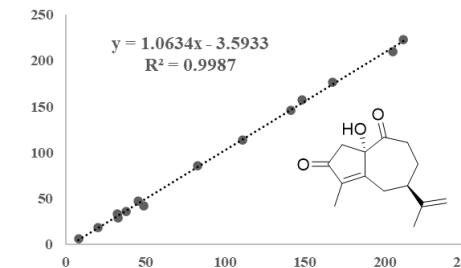
Number/isomers	A	B	C	D
6	0.0%	100.0%	0.0%	0.0%

Figure S4. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **6** and **A–D**.

11/1*R*,7*R*-A



11/1*S*,7*R*-B

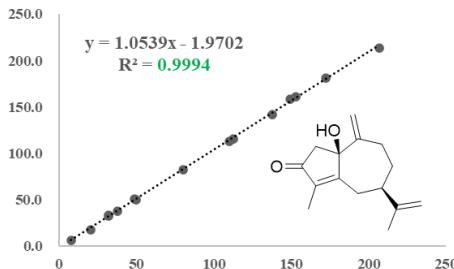


DP4+ calculation Probabilities:

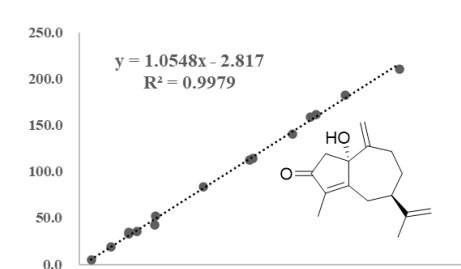
Number/isomers	A	B
11	100.0%	0.0%

Figure S5. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **11** and **A–B**.

12/1*S*,7*R*-A



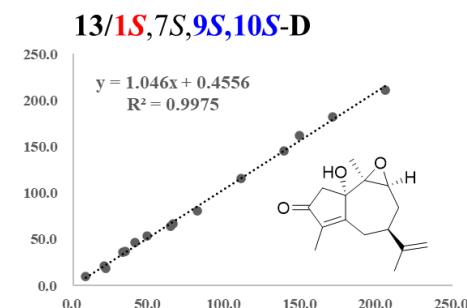
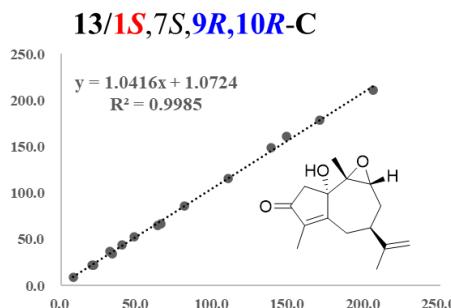
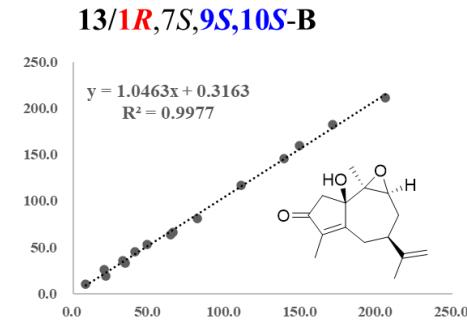
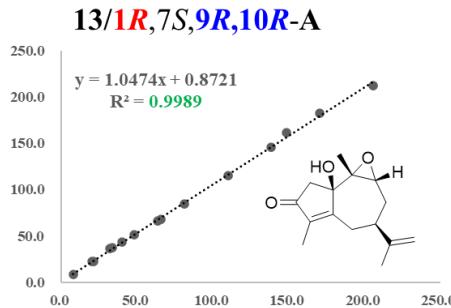
12/1*R*,7*R*-B



DP4+ calculation Probabilities:

Number/isomers	A	B
12	100.0%	0.0%

Figure S6. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **12** and **A–B**.

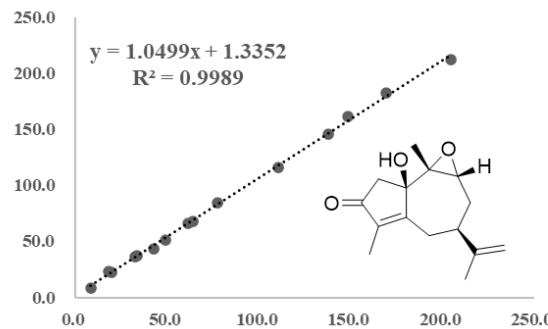


DP4+ calculation Probabilities:

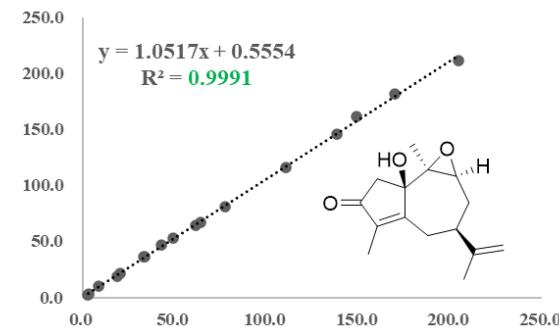
Number/isomers	A	B	C	D
13	100.0%	0.0%	0.0%	0.0%

Figure S7. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **13** and **A–D**.

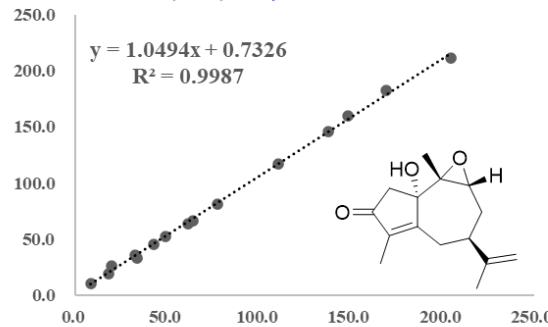
14/1*R*,7*S*,9*R*,10*R*-A



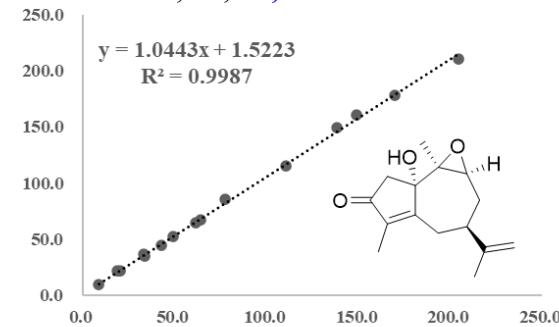
14/1*R*,7*S*,9*S*,10*S*-B



14/1*S*,7*S*,9*R*,10*R*-C



14/1*S*,7*S*,9*S*,10*S*-D

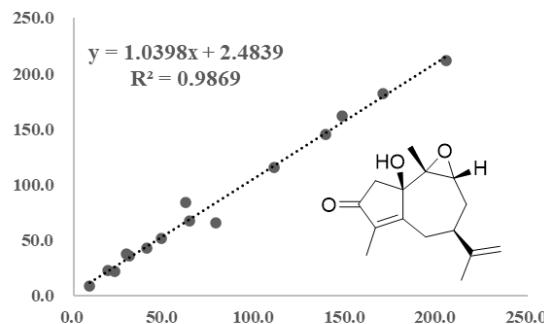


DP4+ calculation Probabilities:

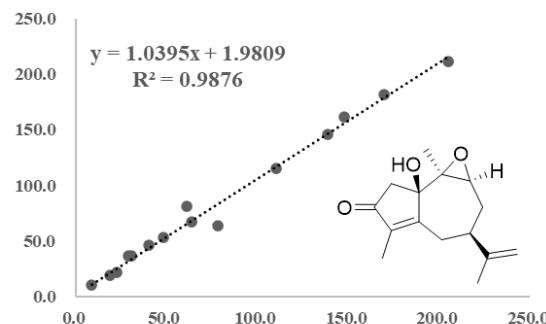
Number/isomers	A	B	C	D
14	0.0%	100.0%	0.0%	0.0%

Figure S8. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **14** and **A–D**.

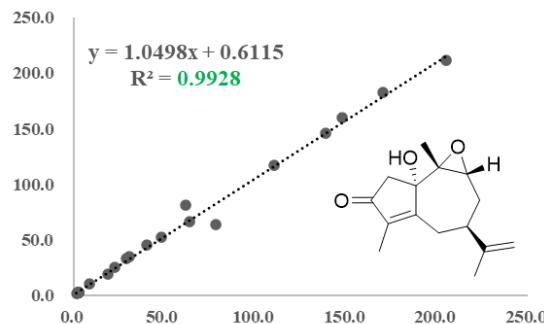
15/1*R*,7*S*,9*R*,10*R*-A



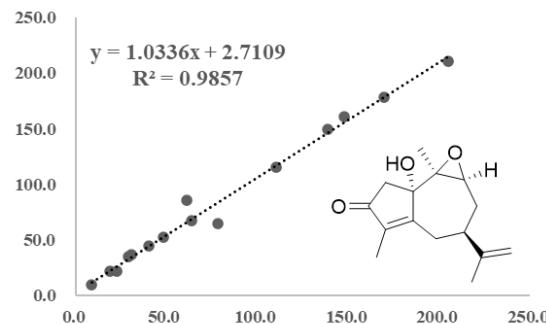
15/1*R*,7*S*,9*S*,10*S*-B



15/1*S*,7*S*,9*R*,10*R*-C



15/1*S*,7*S*,9*S*,10*S*-D

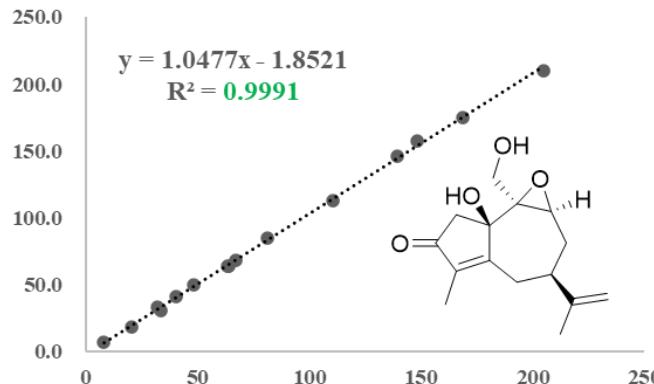


DP4+ calculation Probabilities:

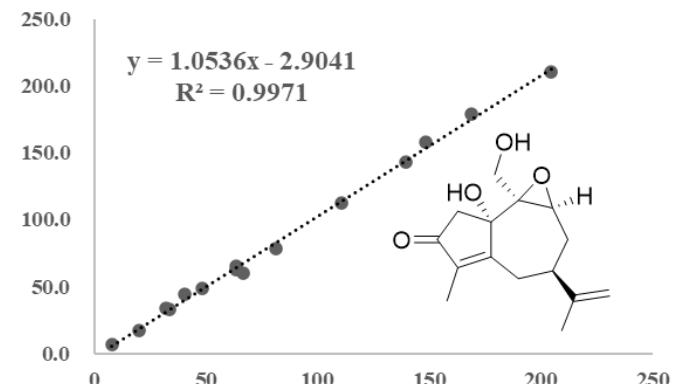
Number/isomers	A	B	C	D
15	0.0%	0.0%	100.0%	0.0%

Figure S9. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **15** and A–D.

17/*1R*,*7S*,*9S*,*10S*-A



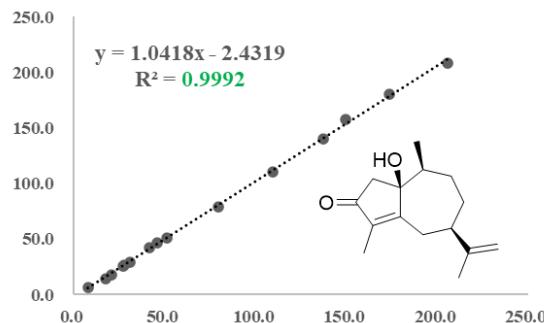
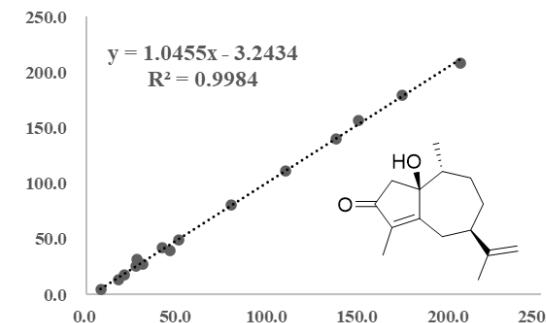
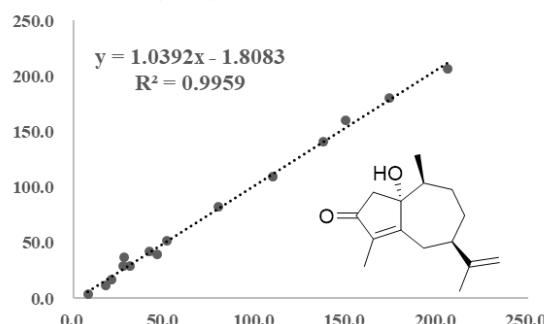
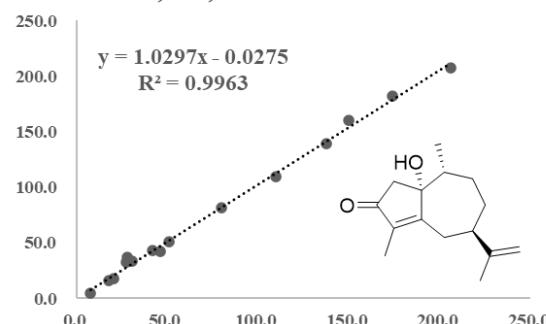
17/*1S*,*7S*,*9S*,*10S*-B



DP4+ calculation Probabilities:

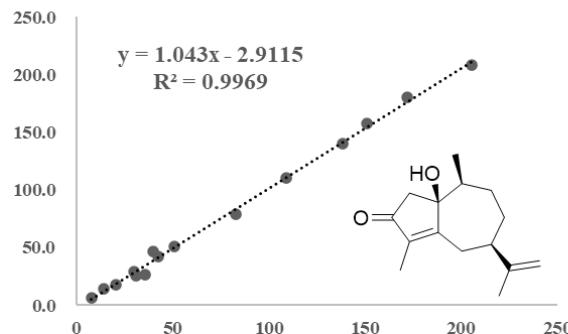
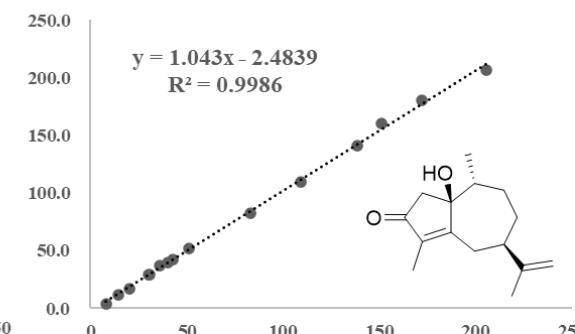
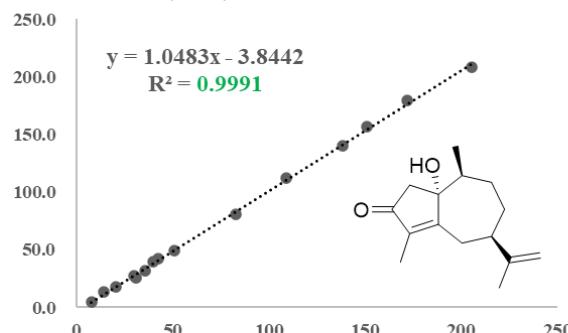
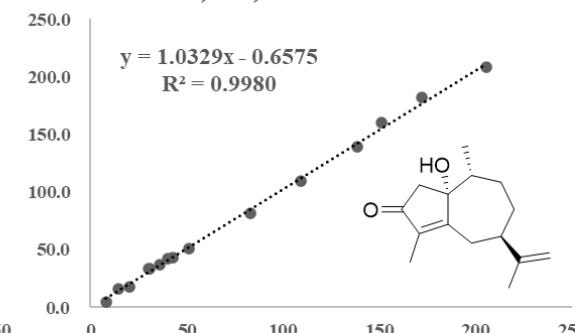
Number/isomers	A	B
17	0.0%	100.0%

Figure S10. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ¹³C NMR chemical shifts between **17** and **A–B**.

19/1*S*,7*R*,10*S*-A**19/1*S*,7*R*,10*R*-B****19/1*R*,7*R*,10*S*-C****19/1*R*,7*R*,10*R*-D****DP4+ calculation Probabilities:**

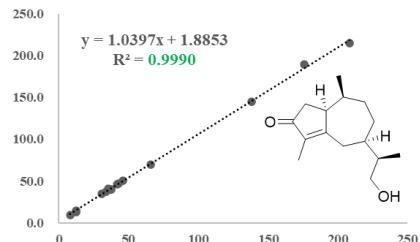
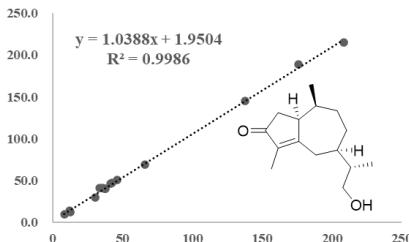
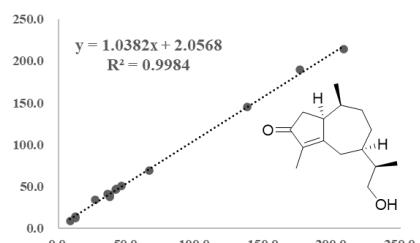
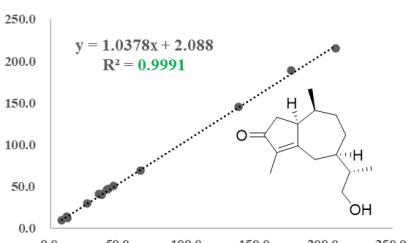
Number/isomers	A	B	C	D
19	100.0%	0.0%	0.0%	0.0%

Figure S11. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **19** and **A–D**.

20/1*S*,7*R*,10*S*-A**20/1*S*,7*R*,10*R*-B****20/1*R*,7*R*,10*S*-C****20/1*R*,7*R*,10*R*-D****DP4+ calculation Probabilities:**

Number/isomers	A	B	C	D
20	0.0%	0.0%	100.0%	0.0%

Figure S12. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **20** and A–D.

25/1S,7R,10S,11R-A**25/1S,7R,10S,11S-B****26/1S,7R,10S,11R-A****26/1S,7R,10S,11S-B****DP4+ calculation Probabilities:**

Number/isomers	A	B
25	99.9%	0.1%
26	0.0%	100%

CP3 calculation Probabilities:

C data H data All data

Exp_25-Cal_A & Exp_26-Cal_B **100.0%** **100.0%** **100.0%**

Exp_25-Cal_B & Exp_26-Cal_A 0.0% 0.0% 0.0%

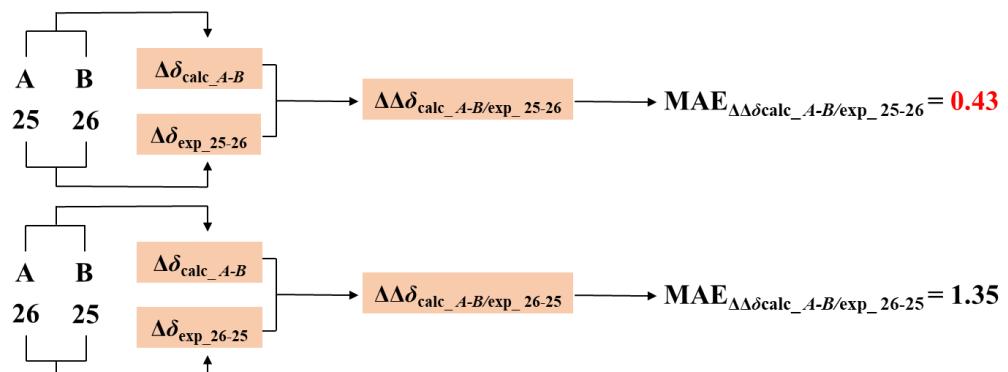
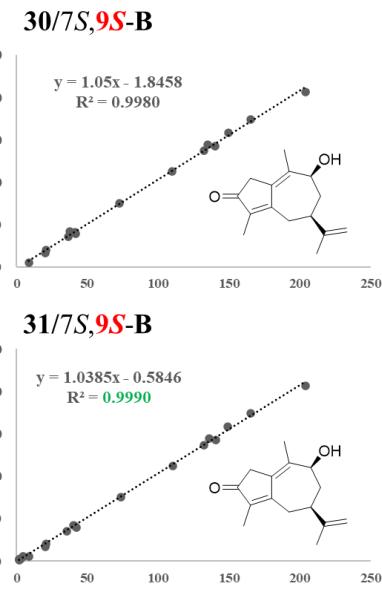
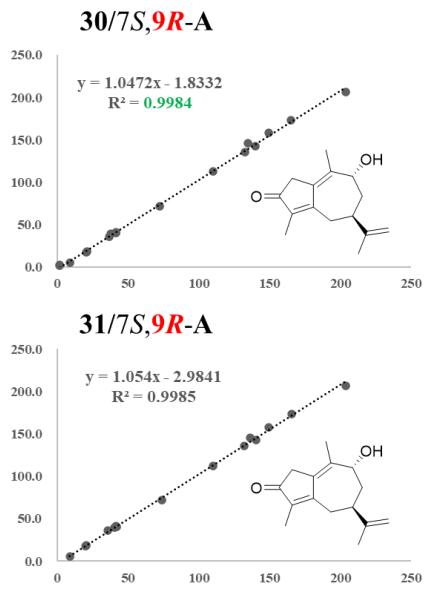
MAE_{ΔΔδ} parameter:

Figure S13. Linear correlation (R^2), DP4+, CP3 and $\text{MAE}_{\Delta\Delta\delta}$ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **25–26** and **A–D**.



DP4+ calculation Probabilities:

Number/isomers	A	B
30	99.9%	0.1%
31	3.7%	96.3%

CP3 calculation Probabilities:

	C data	H data	All data
Exp_30-Cal_A & Exp_31-Cal_B	100.0%	100.0%	100.0%
Exp_30-Cal_B & Exp_31-Cal_A	0.0%	0.1%	0.0%

MAE_{ΔΔδ} parameter:

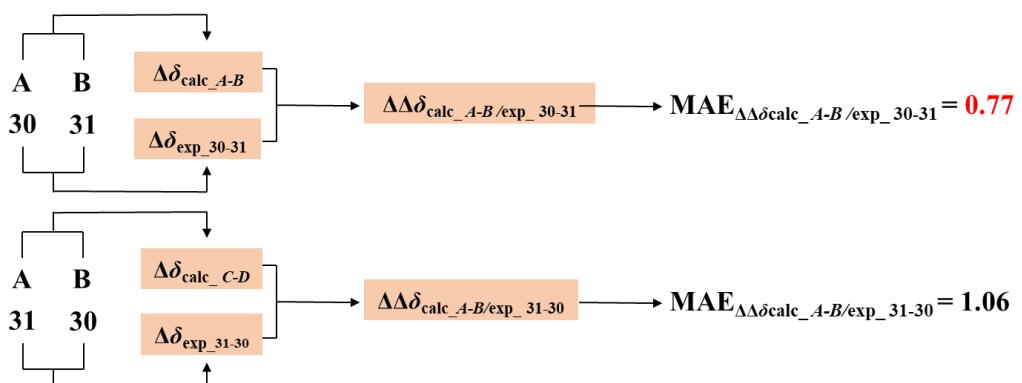
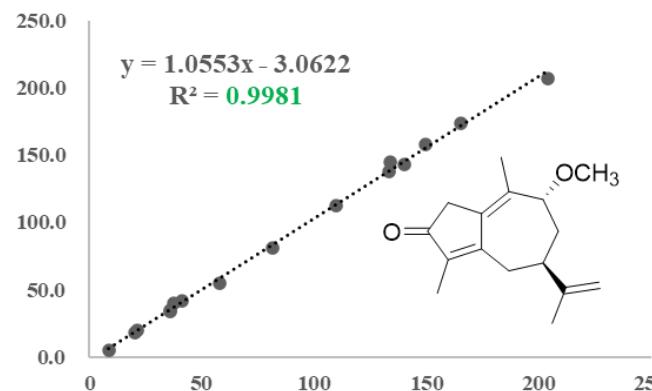
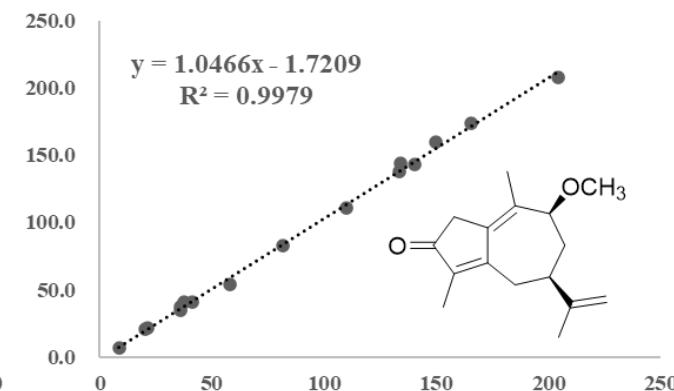


Figure S14. Linear correlation (R^2), DP4+, CP3 and $\text{MAE}_{\Delta\Delta\delta}$ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **30–31** and **A–B**.

33/7*S*,9*R*-A



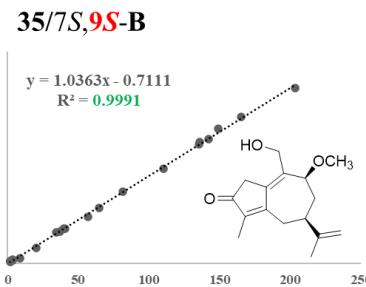
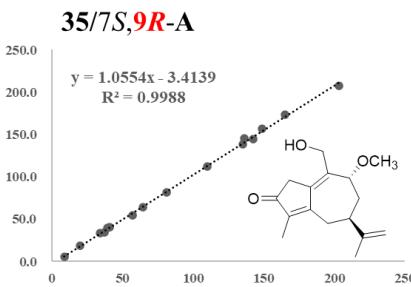
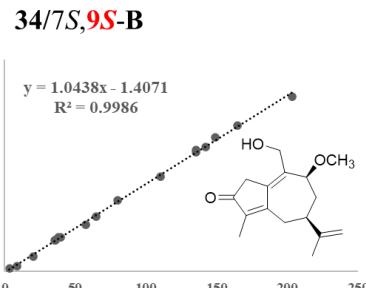
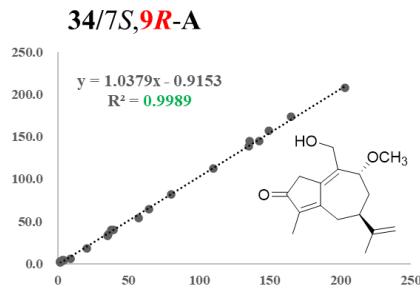
33/7*S*,9*S*-B



DP4+ calculation Probabilities:

Number/isomers	A	B
33	93.2%	0.0%

Figure S15. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **33** and **A–B**.



DP4+ calculation Probabilities:

Number/isomers	A	B
34	99.0%	1.0%
35	0.0%	100%

CP3 calculation Probabilities:

	C data	H data	All data
Exp_34-Cal_A & Exp_35-Cal_B	100.0%	100.0%	100.0%
Exp_34-Cal_B & Exp_35-Cal_A	0.0%	0.1%	0.0%

MAE_{ΔΔδ} parameter:

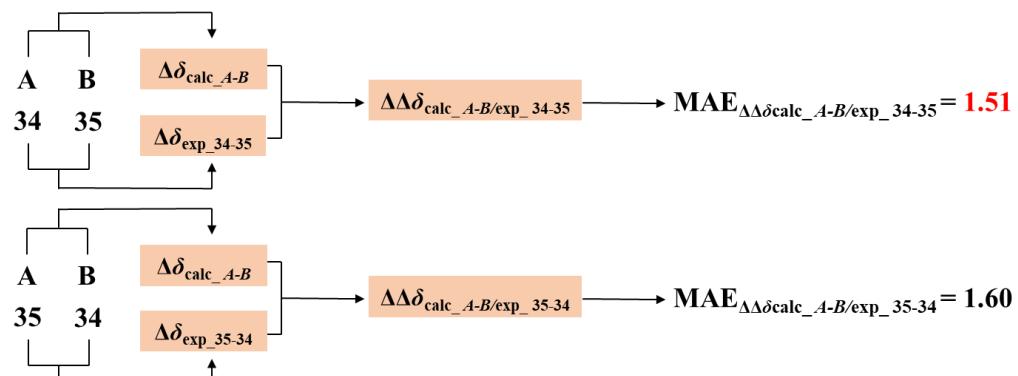
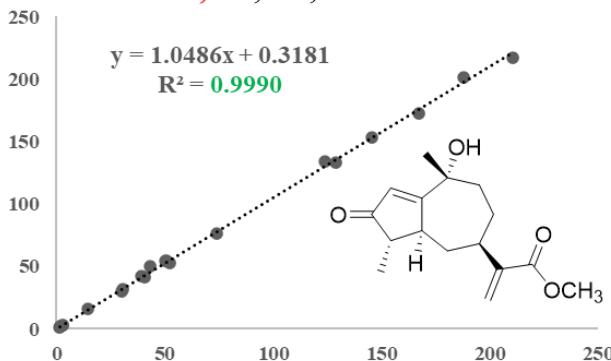
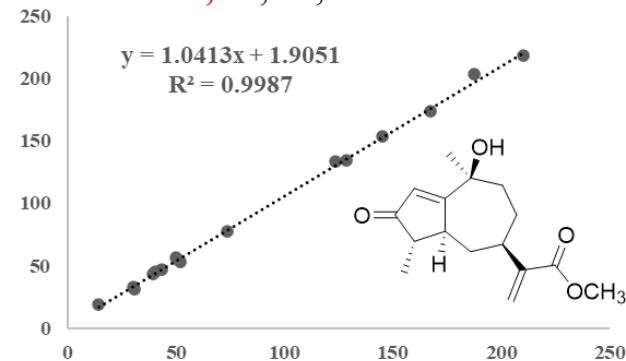


Figure S16. Linear correlation (R^2), DP4+, CP3 and MAE_{ΔΔδ} parameter between the experimental and calculated ^{13}C NMR chemical shifts between 34–35 and A–B.

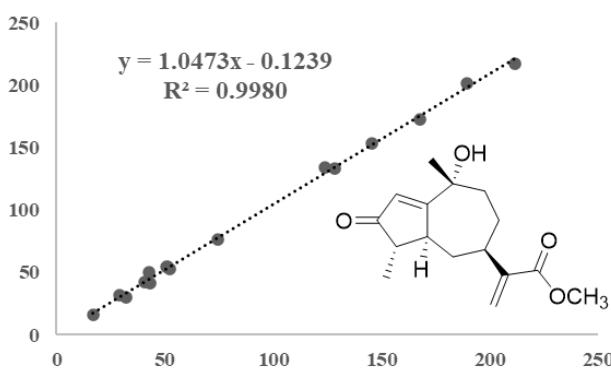
39/4S,5S,7R,10R-A



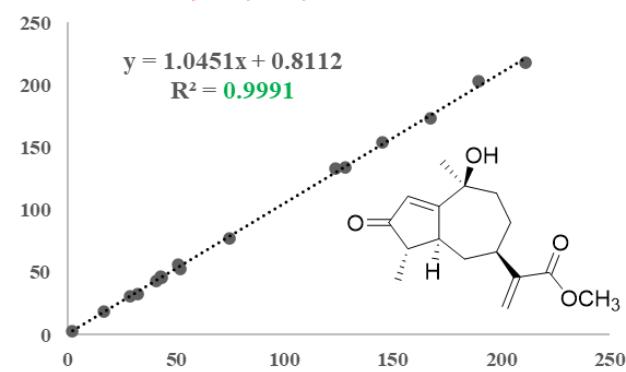
39/4S,5S,7R,10S-B



40/4S,5S,7R,10R-A



40/4S,5S,7R,10S-B



DP4+ calculation Probabilities:

Number/isomers	A	B
39	100.0%	0.0%
40	0.0%	100.0%

Figure S17. Linear correlation (R^2) and DP4+ parameter between the experimental and calculated ^{13}C NMR chemical shifts between **39–40** and **A–B**.

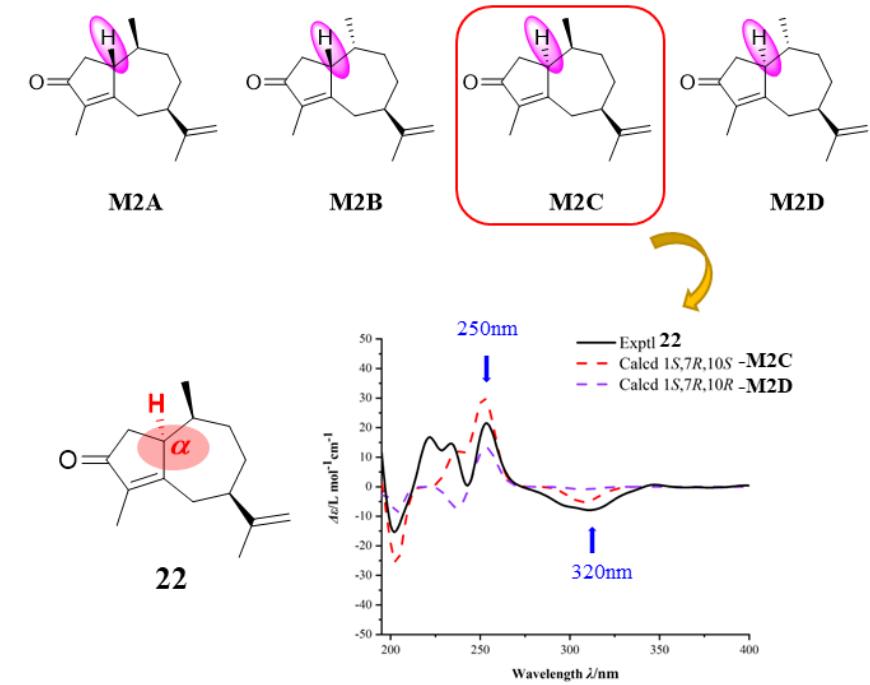
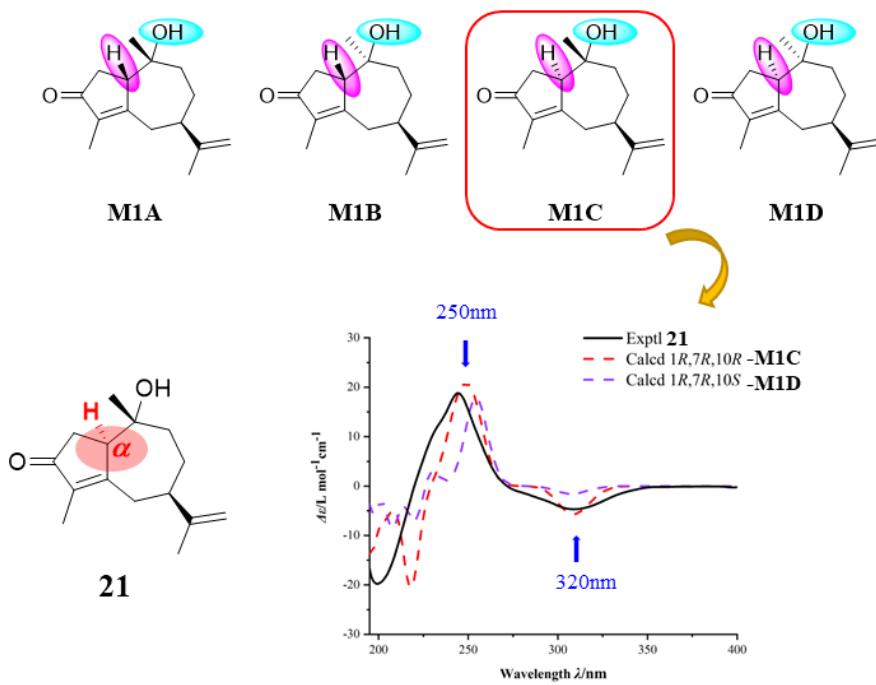


Figure S18. Calculated ECD spectra of model compounds (**M1A-M1D** and **M2A-M2D**) and experimental spectra of **21** and **22**.

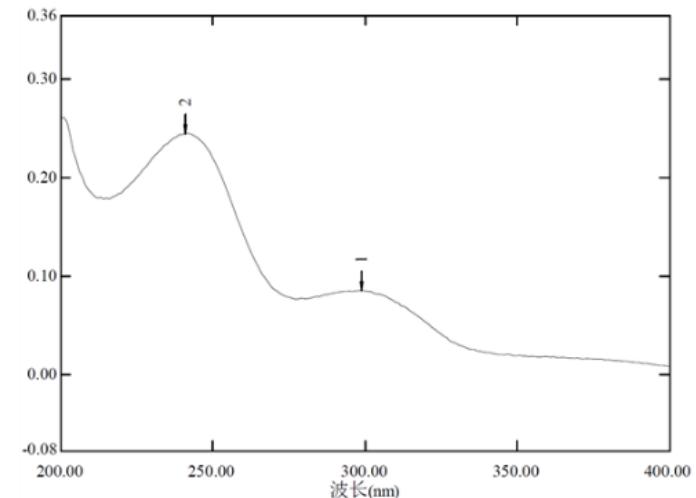
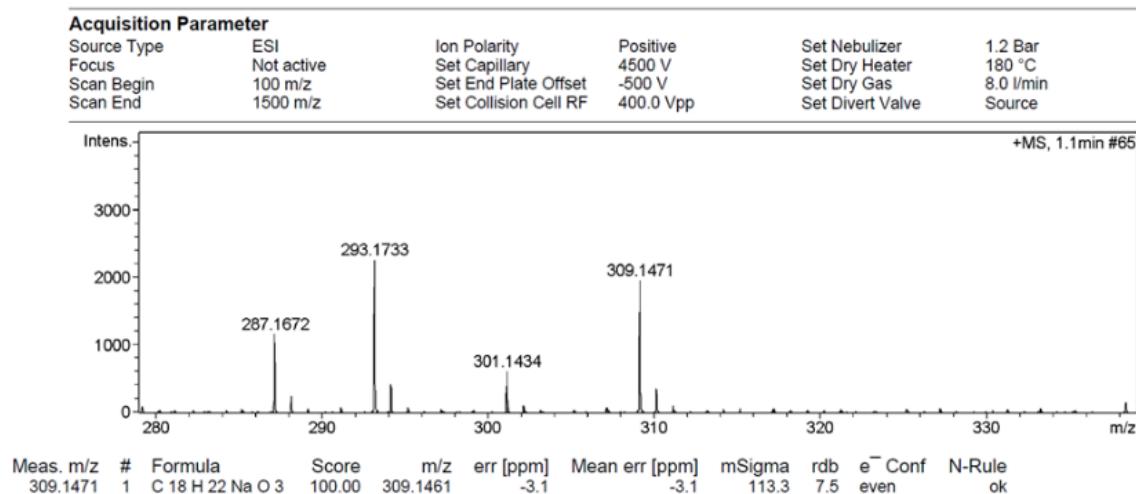


Figure S19 HRESIMS and UV spectra of compound 1

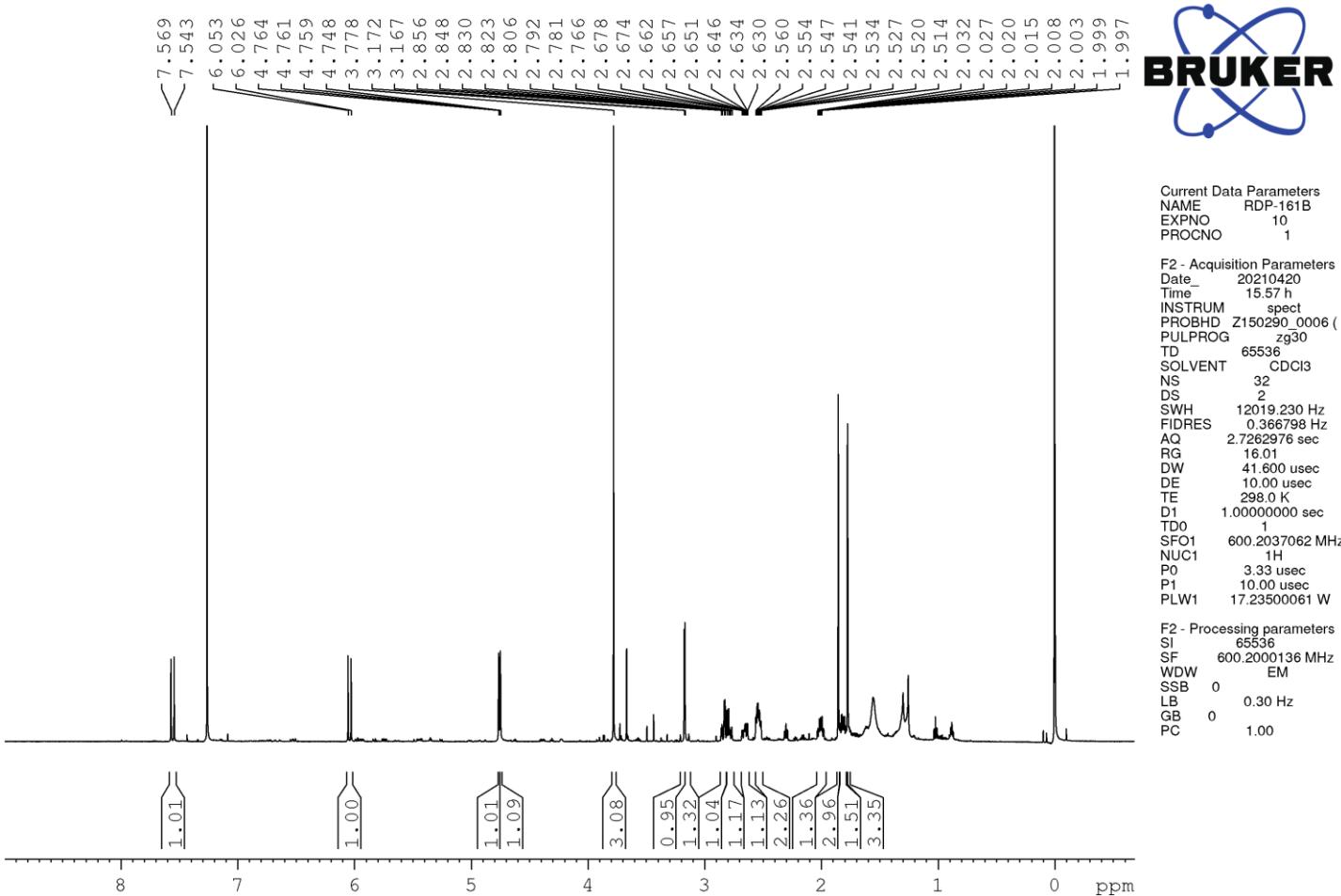


Figure S20 ¹H NMR spectrum (600 MHz, CDCl₃) of compound **1**

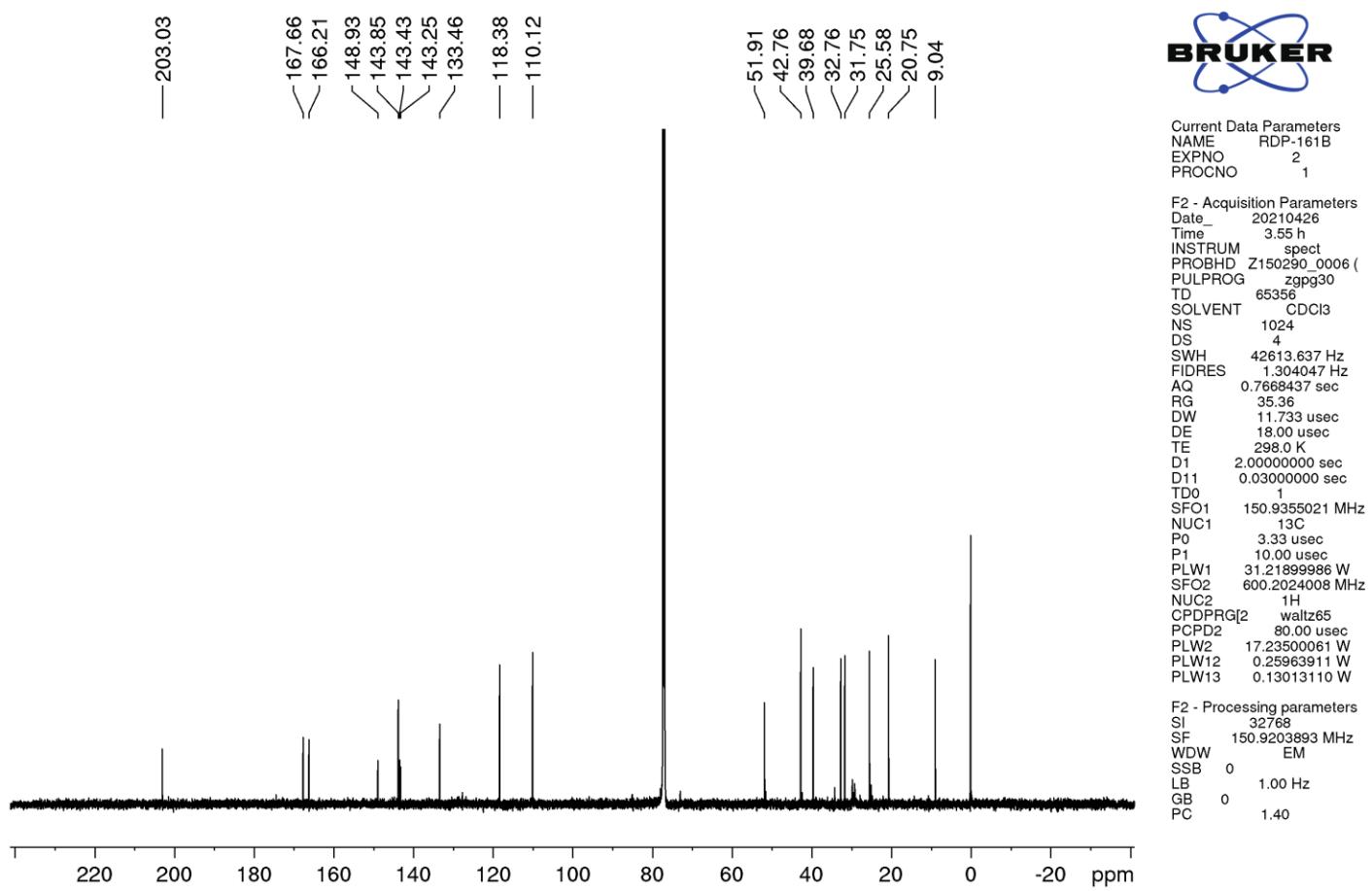


Figure S21 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 1

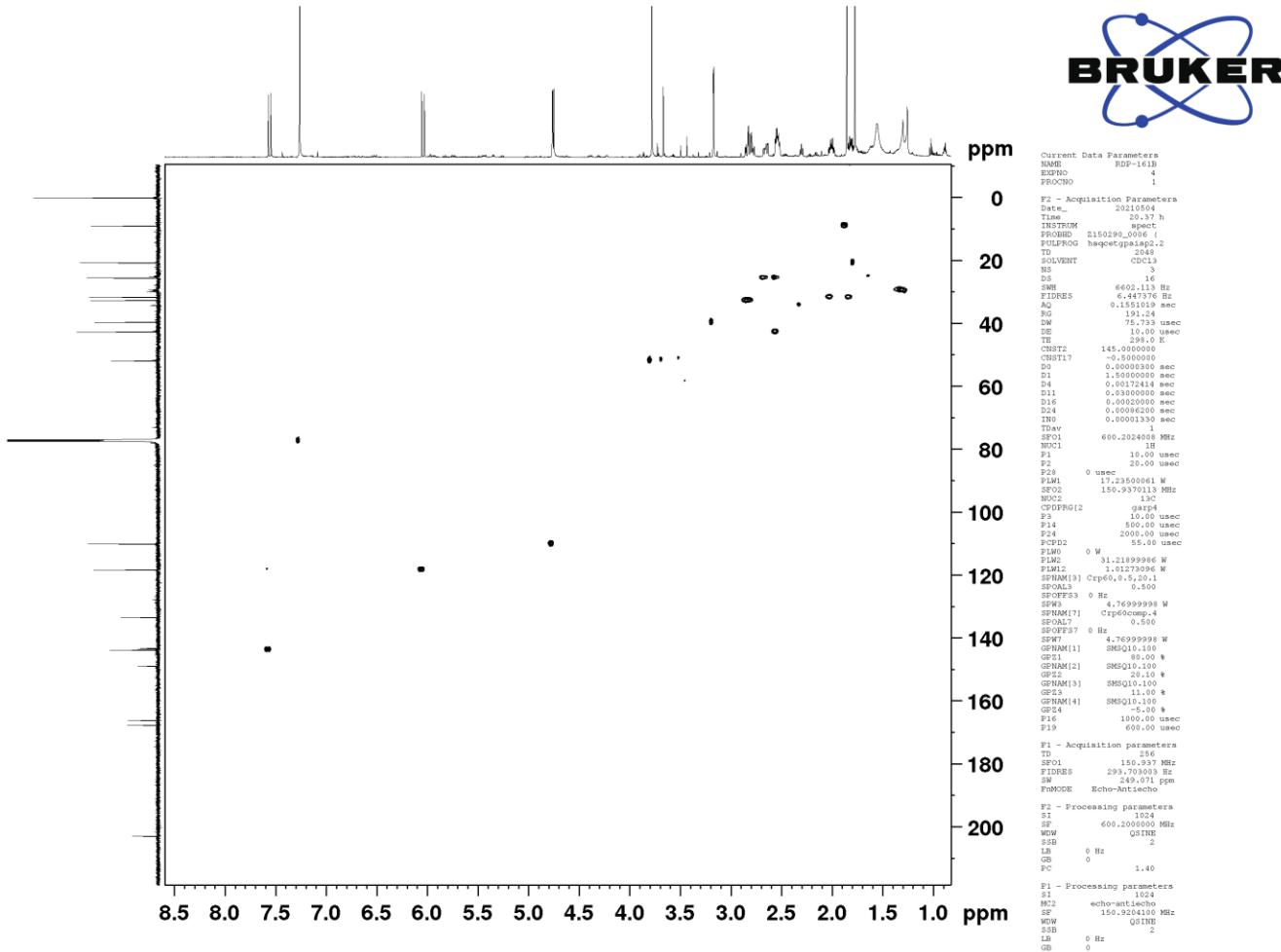


Figure S22 HSQC spectrum (600 MHz, CDCl₃) of compound 1

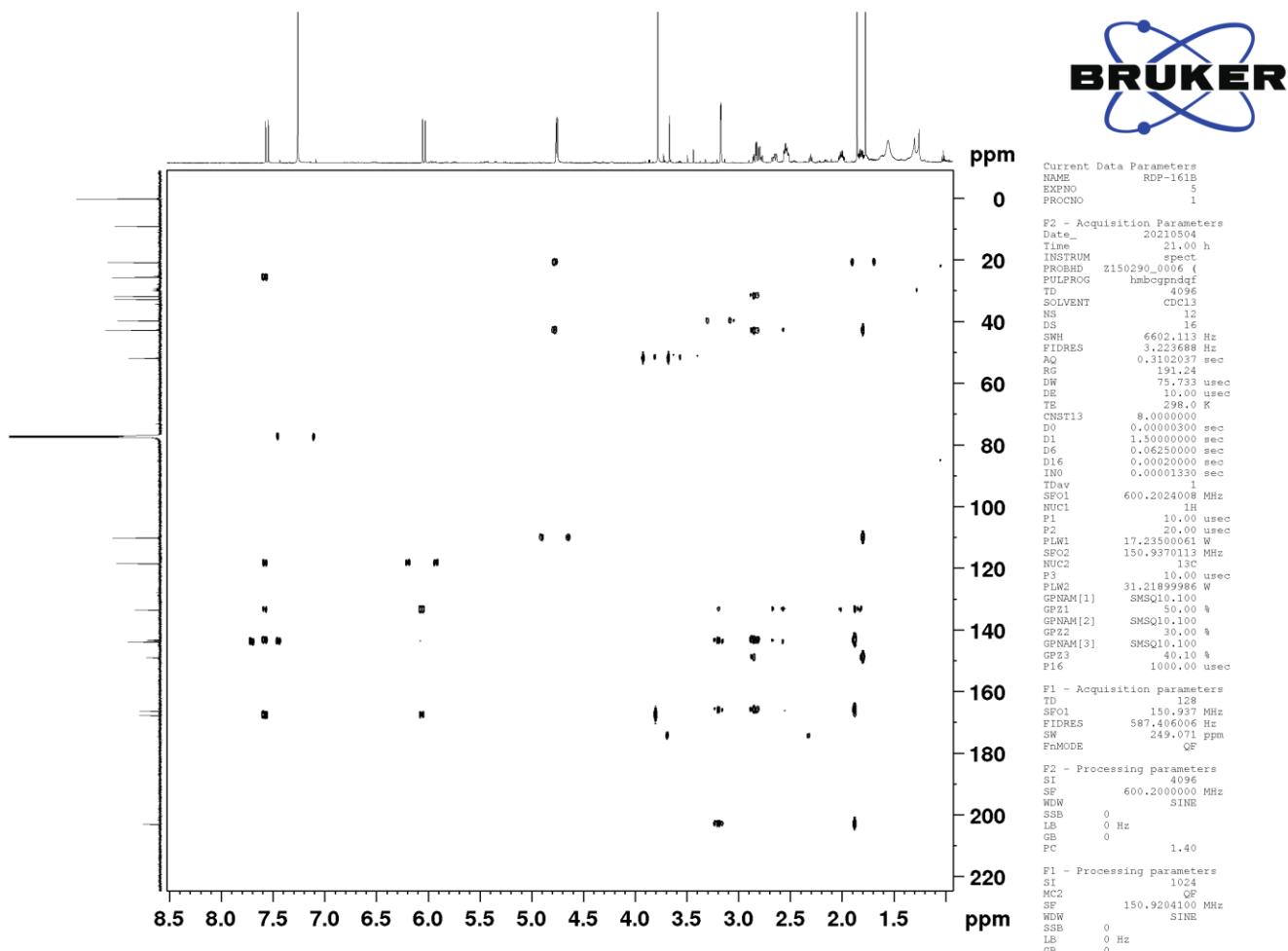


Figure S23 HMBC spectrum (600 MHz, CDCl_3) of compound **1**

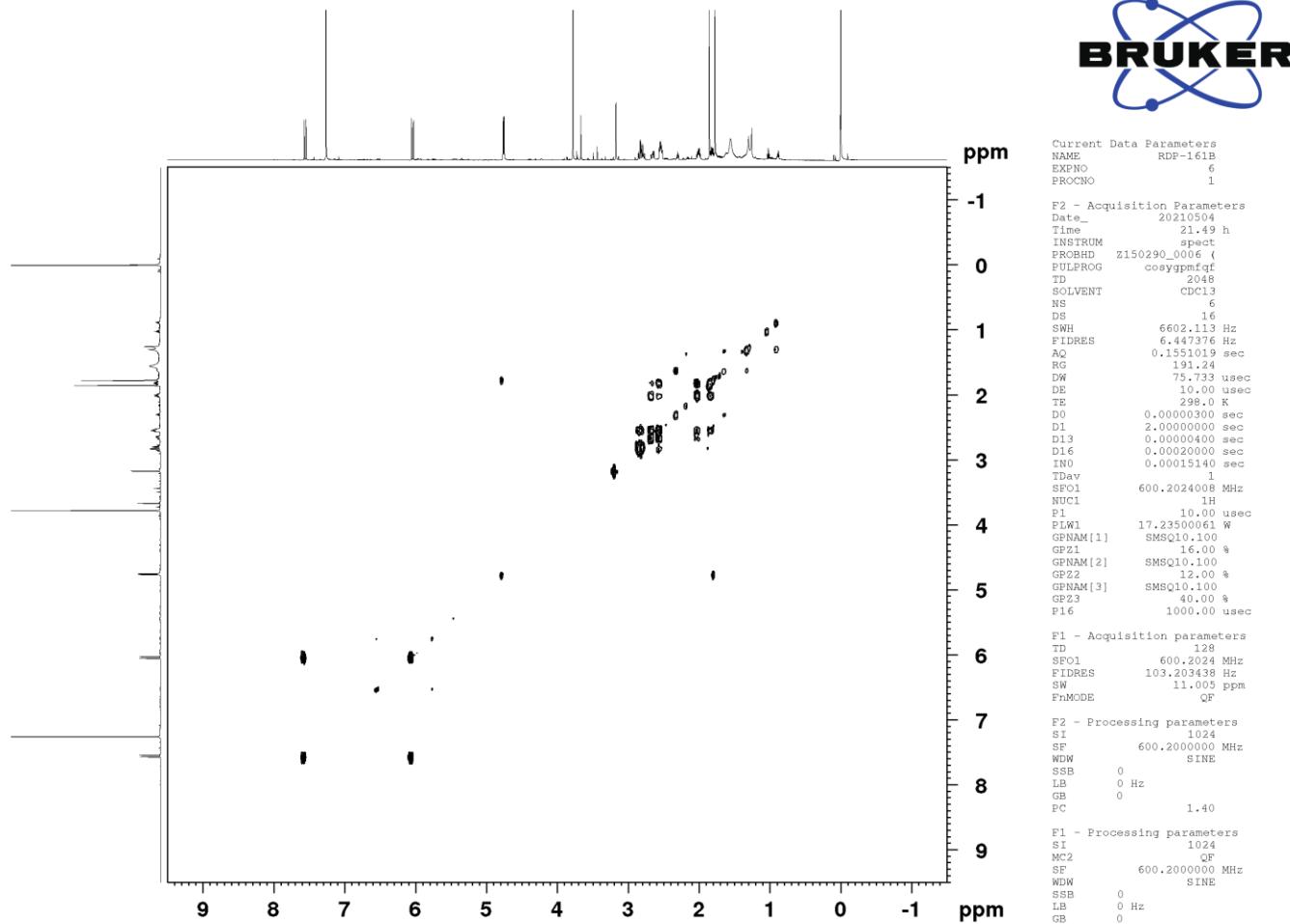


Figure S24 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **1**

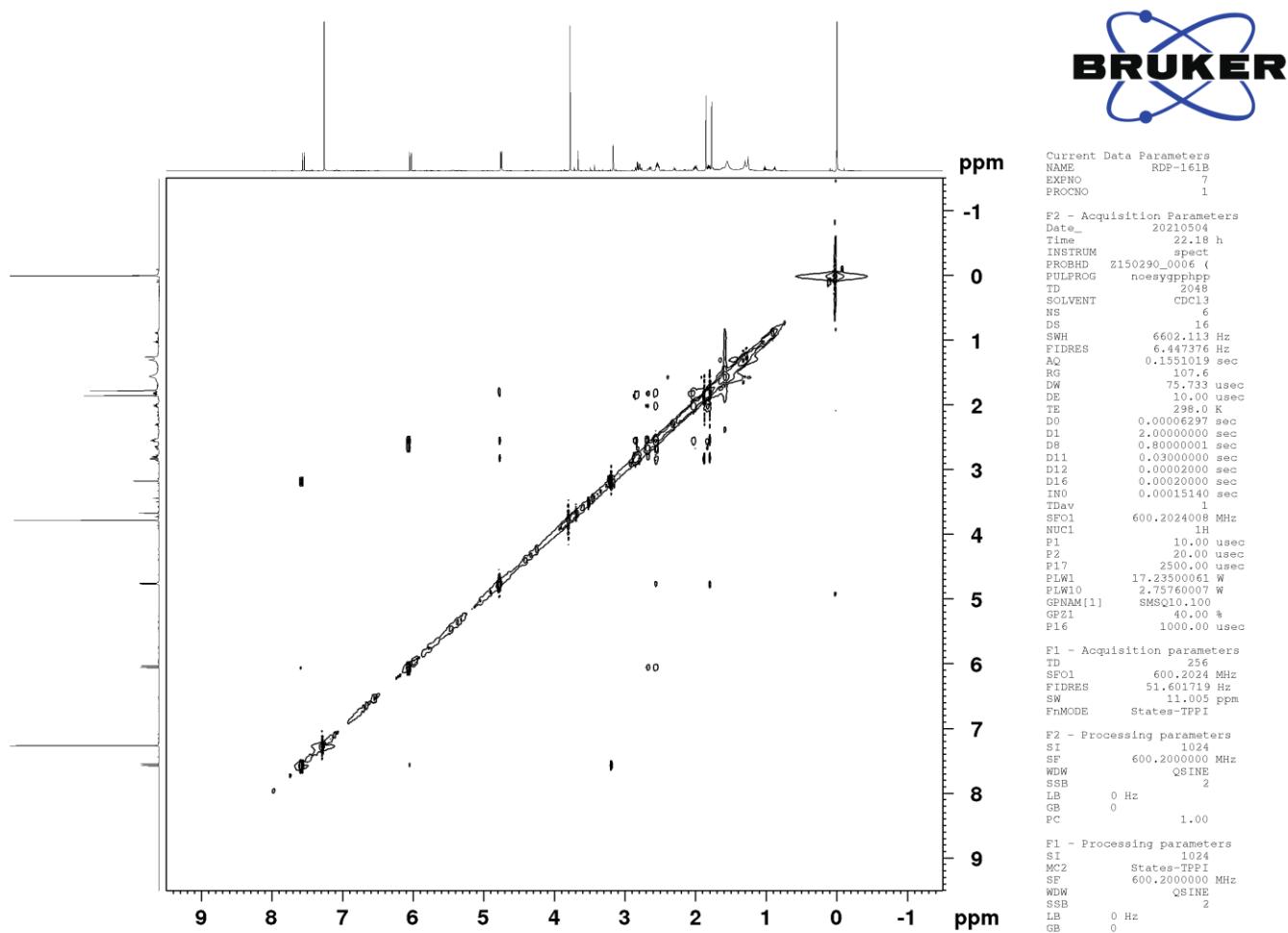


Figure S25 NOESY spectrum (600 MHz, CDCl₃) of compound **1**

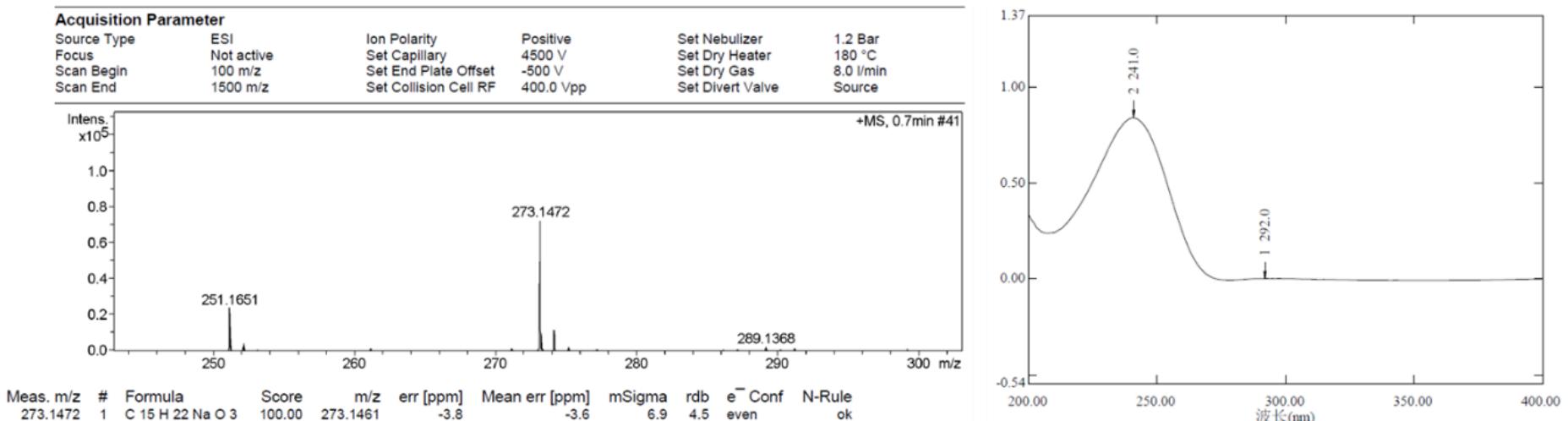


Figure S26 HRESIMS and UV spectra of compound 5

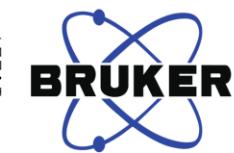
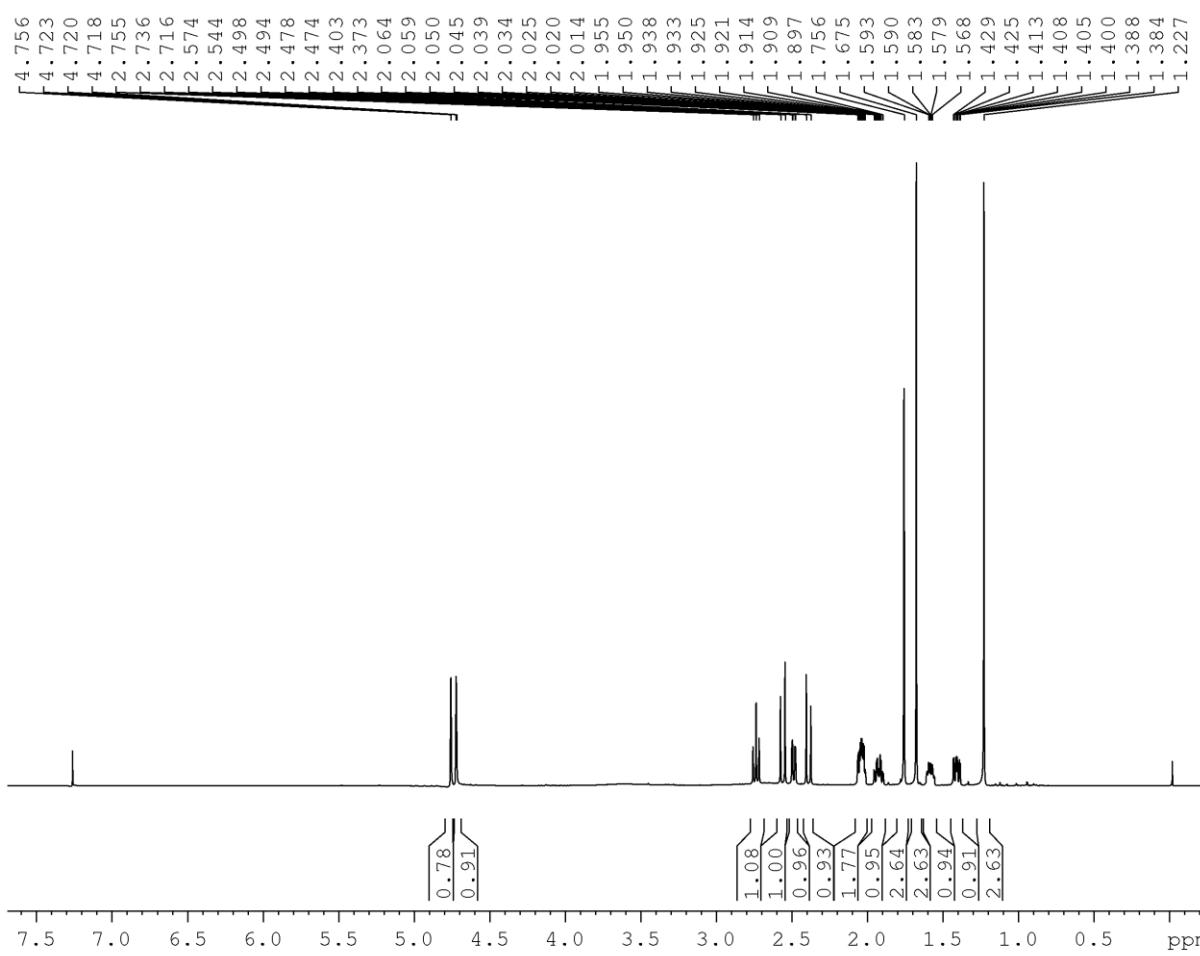


Figure S27 ^1H NMR spectrum (600 MHz, CDCl_3) of compound 5

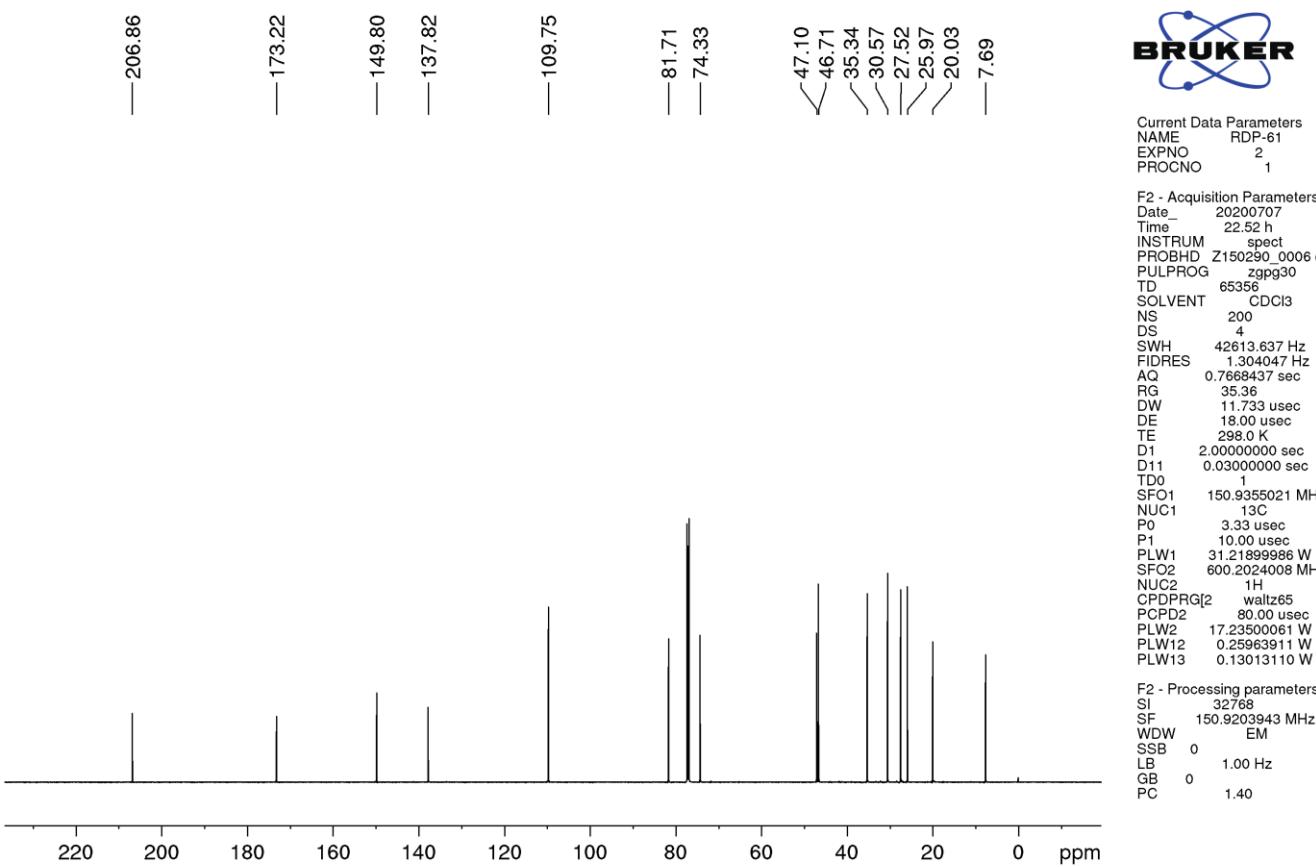


Figure S28 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **5**

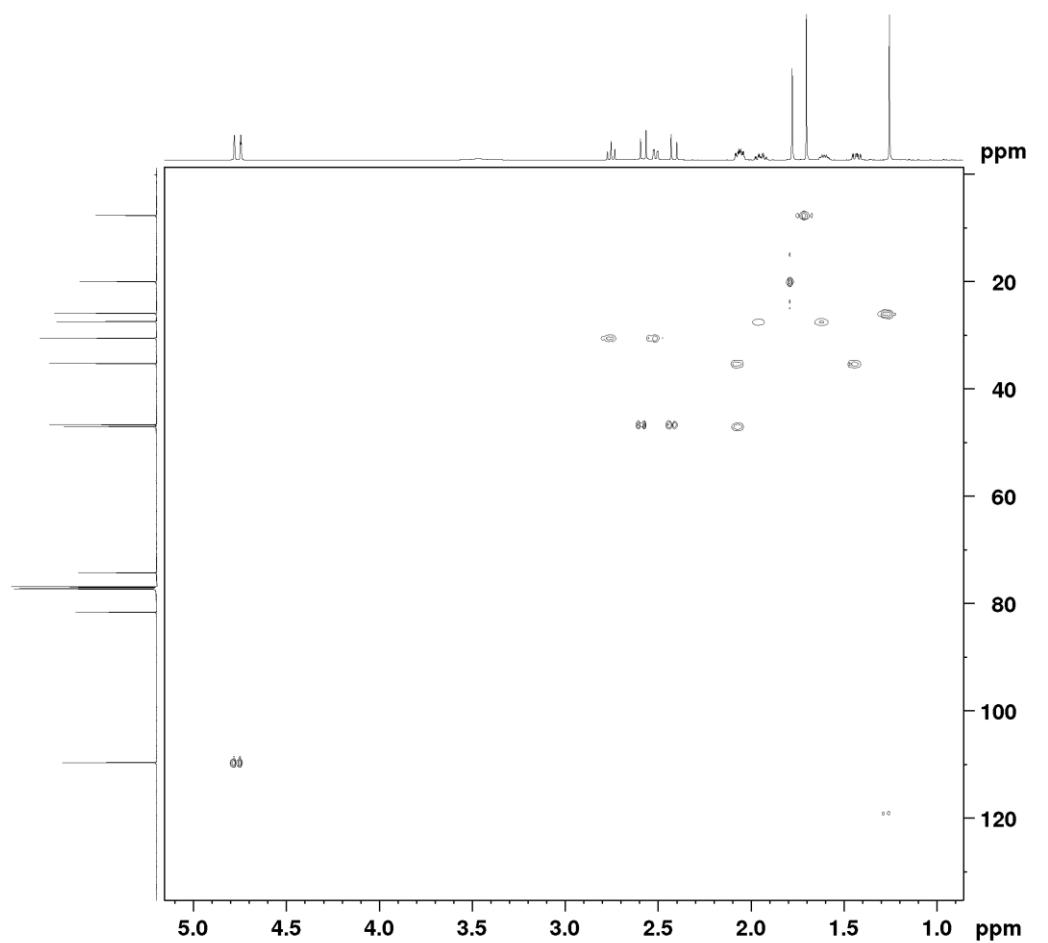
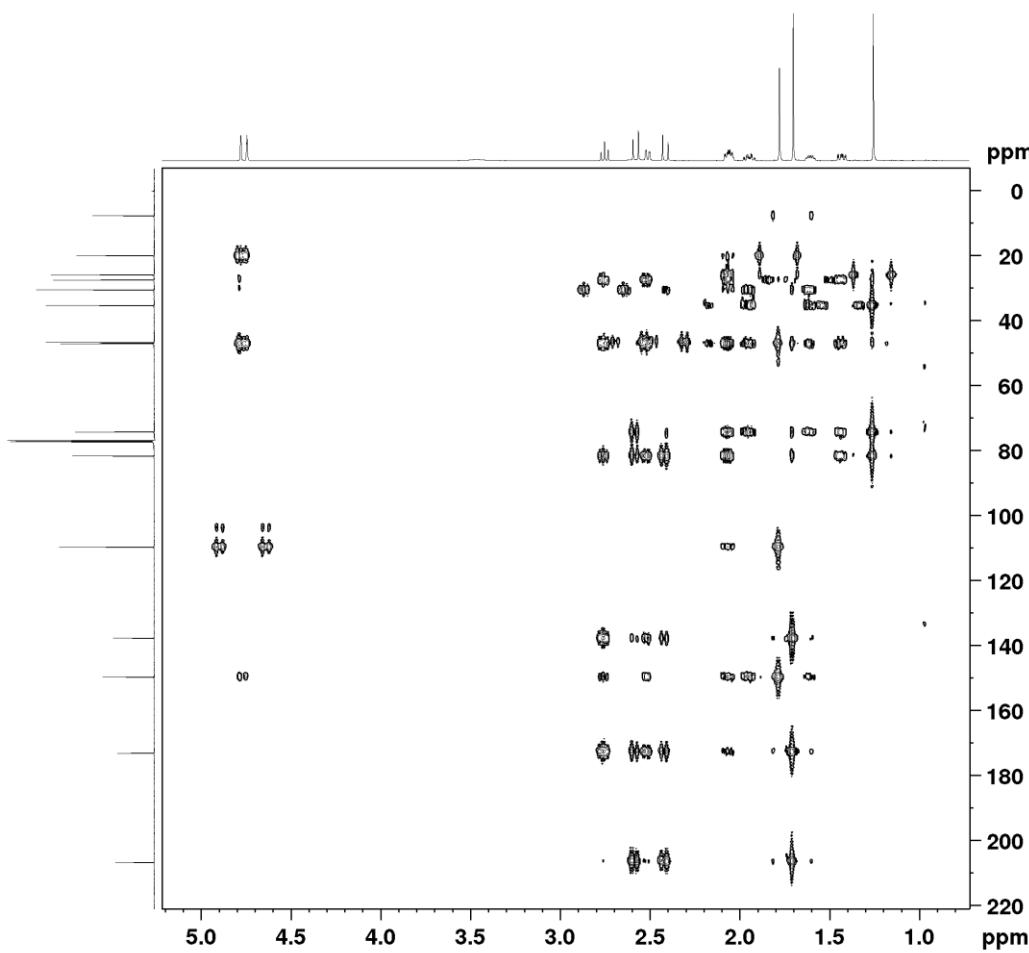


Figure S29 HSQC spectrum (600 MHz, CDCl₃) of compound 5



Current Data Parameters
NAME RDP-61
EXPNO 5
PROCNO 1

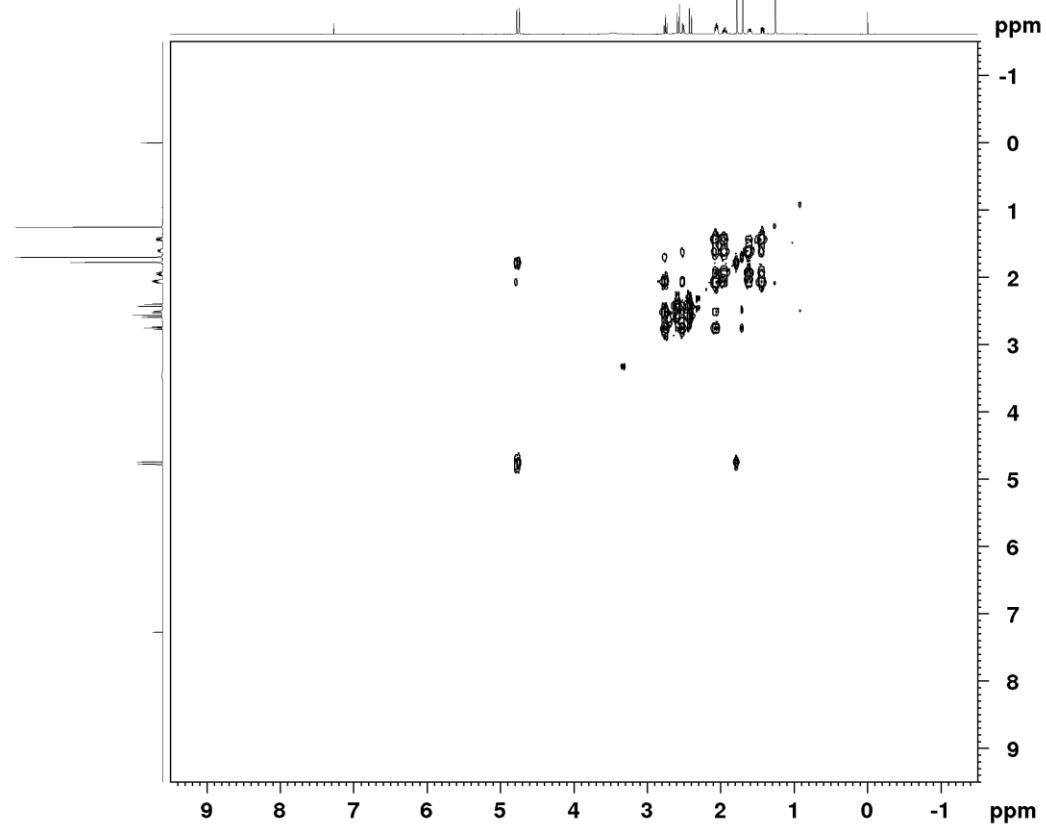
P2 - Acquisition Parameters
Date_ 20210129
Time_ 3.18 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG hmbcgrndqf
TD 4096
SOLVENT CDCl3
NS 2
DS 16
SWH 6602.113 Hz
FIDRES 3.223688 Hz
AQ 0.3102037 sec
RG 10.00
DW 75.733 usec
DE 10.00 usec
TE 298.0 K
CNS13 8.0000000
D0 0.0000000 sec
D1 1.15000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001330 sec
TDav 1
SF01 600.2024000 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLN1 17.23500061 W
SF02 150.9370113 MHz
NUC2 13C
P3 10.00 usec
PLN2 31.21899986 W
GPNAME[1] SNSQ10.100
GPZ1 50.00 %
GPNAME[2] SNSQ10.100
GPZ2 30.00 %
GPNAME[3] SNSQ10.100
GPZ3 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.937 MHz
FIDRES 587.40605 Hz
SW 249.071 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S30 HMBC spectrum (600 MHz, CDCl_3) of compound 5



Current Data Parameters
NAME RDE-61
EXPNO 6
PROCNO 1

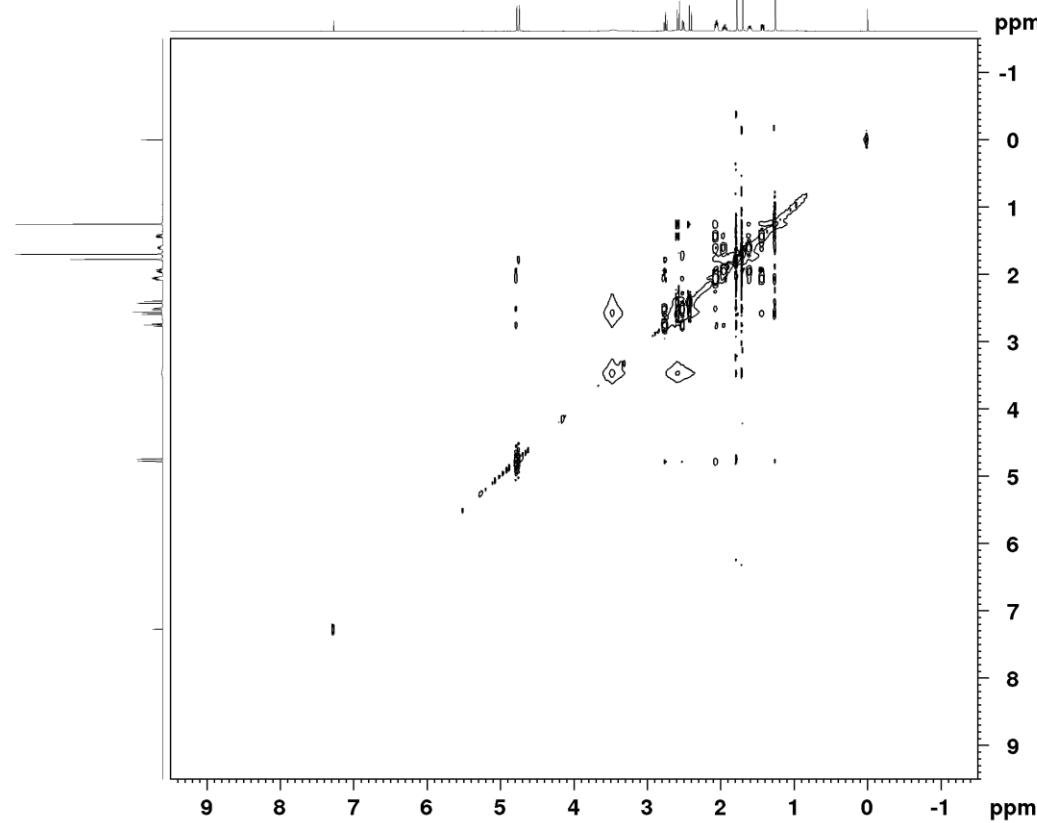
F2 - Acquisition Parameters
Date_ 20210129
Time 3.27 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG cosygppmfd
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 6602.113 Hz
FIDRES 6.447376 Hz
AQ 0.1551019 sec
RG 191.24
DW 75.733 usec
DE 10.00 usec
TE 296.76 K
DO 0.00000300 sec
D1 2.0000000 sec
D13 0.0000400 sec
D16 0.0002000 sec
IN0 0.00015140 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 103.203438 Hz
SW 11.005 ppm
PnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 64
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S31 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 5



Current Data Parameters
NAME RDP-61
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210129
Time 3.38 h
INSTRUM spect
PROBHD Z150290_0066_1
PULPROG noeipypphphp
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 6602.113 Hz
FIDRES 6.447376 Hz
AQ 0.1551019 sec
RG 60.93
DW 75.73 usec
DB 10.00 usec
TE 298.0 K
D0 0.00006297 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.0001519 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 51.601719 Hz
SW 11.005 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW QSIMEN
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
M22 States-TPPI
SF 600.2000000 MHz
WDW QSIMEN
SSB 2
LB 0 Hz
GB 0

Figure S32 NOESY spectrum (600 MHz, CDCl_3) of compound **5**

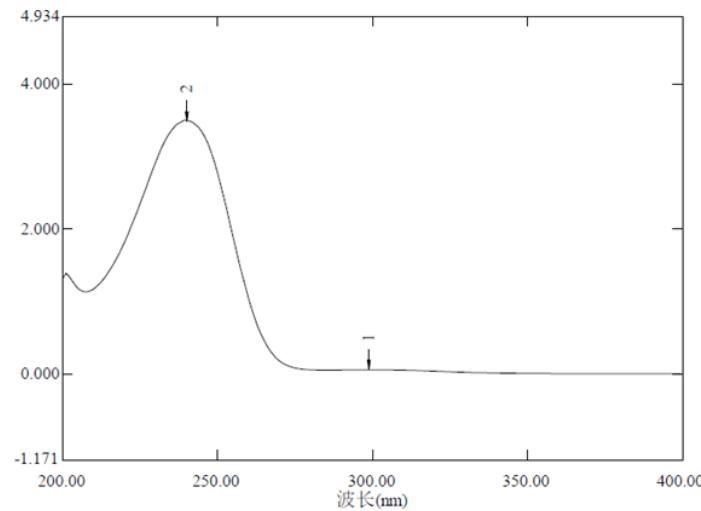
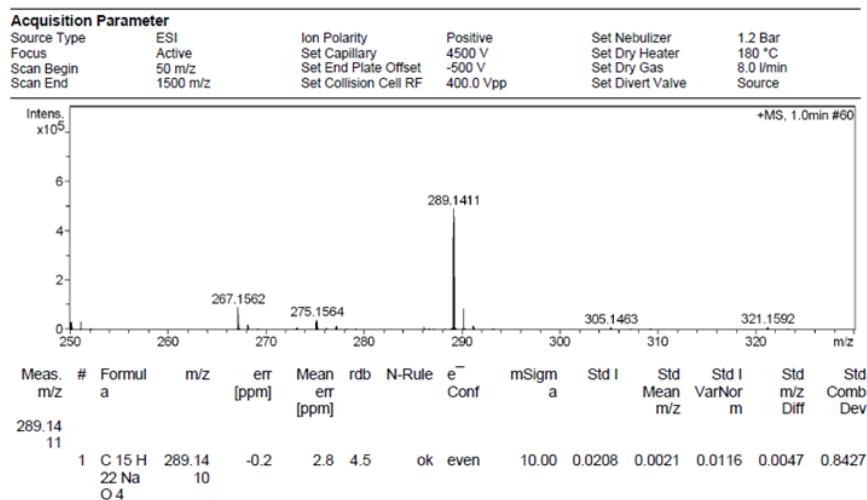


Figure S33 HRESIMS and UV spectra of compound **6**

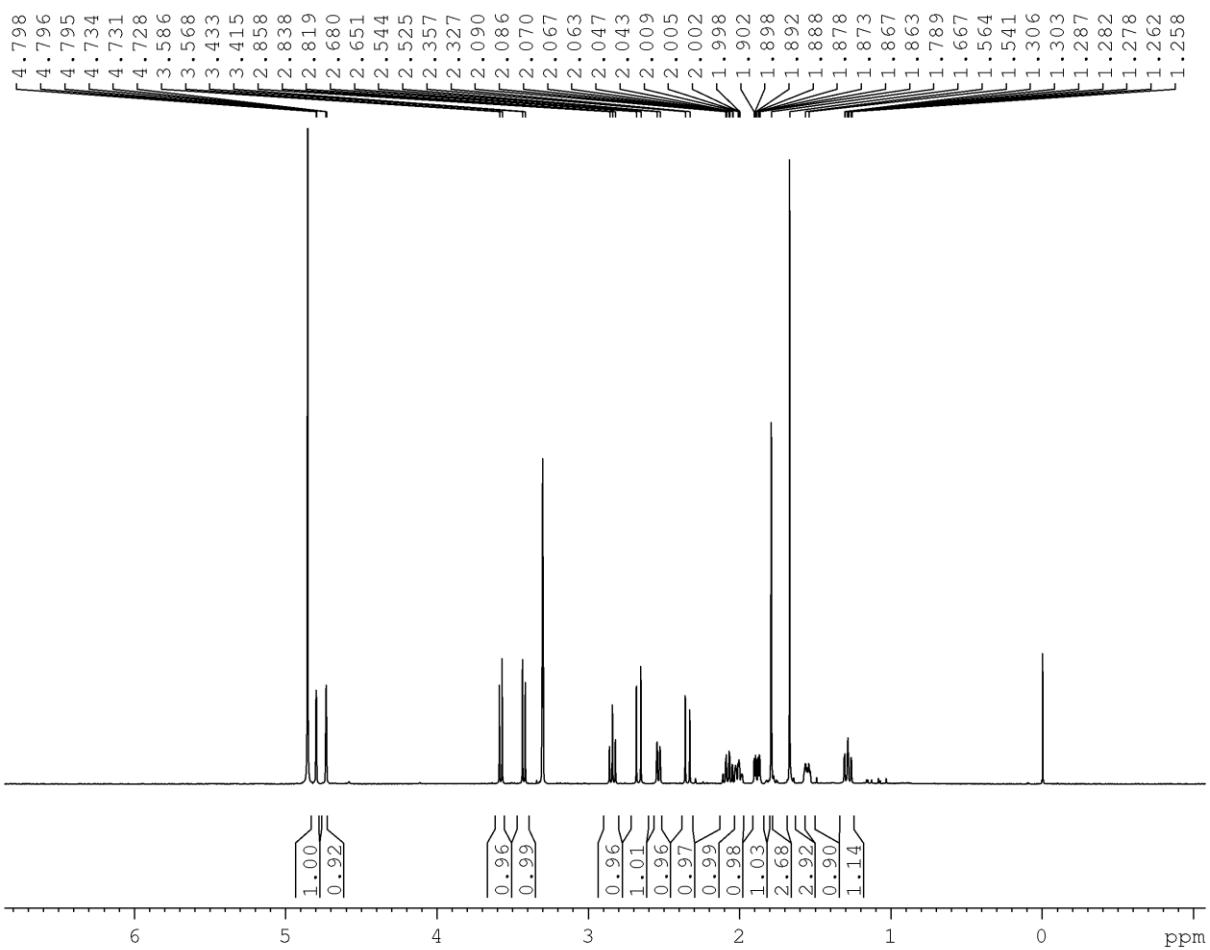


Figure S34 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **6**

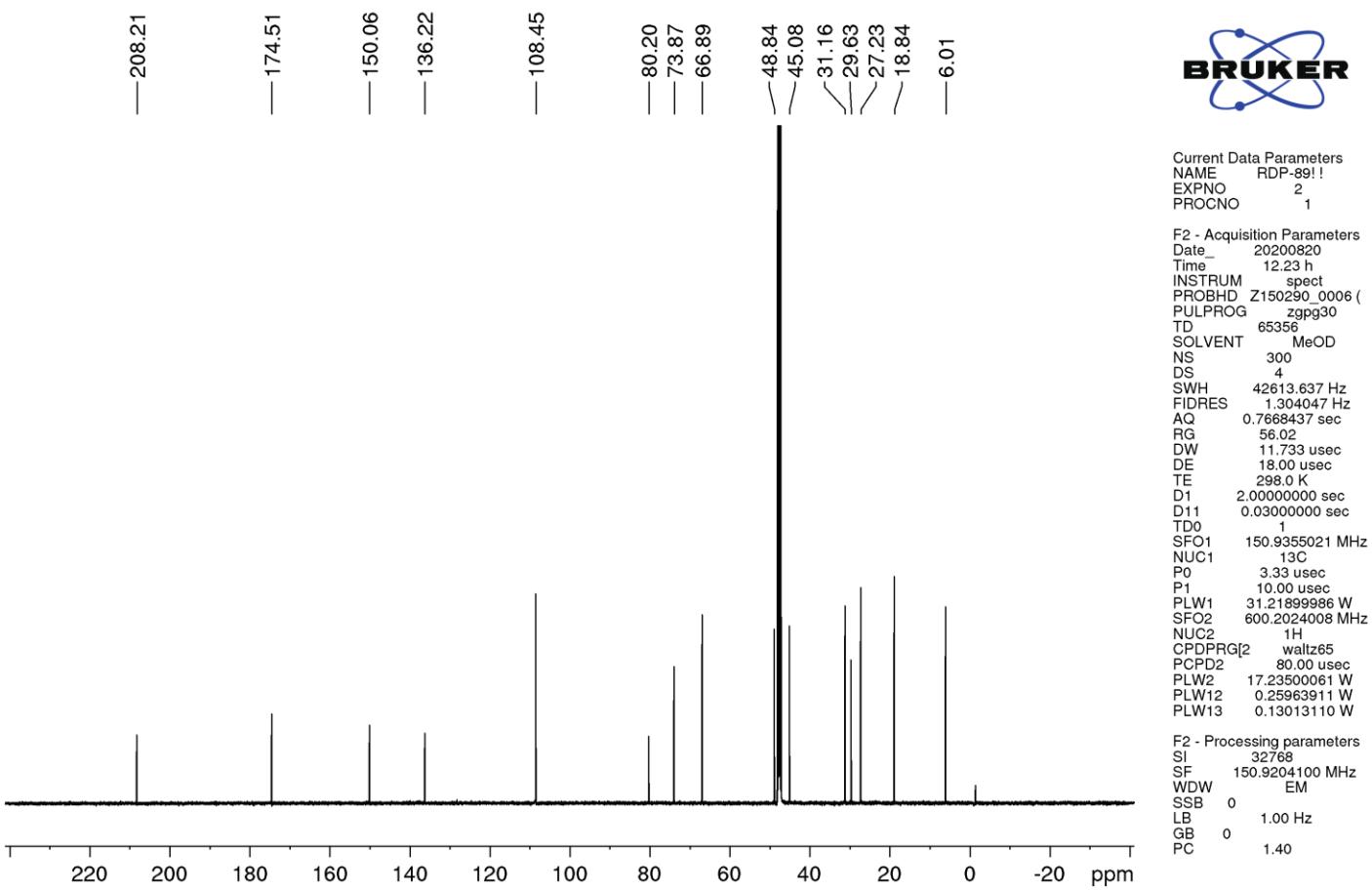


Figure S35 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **6**

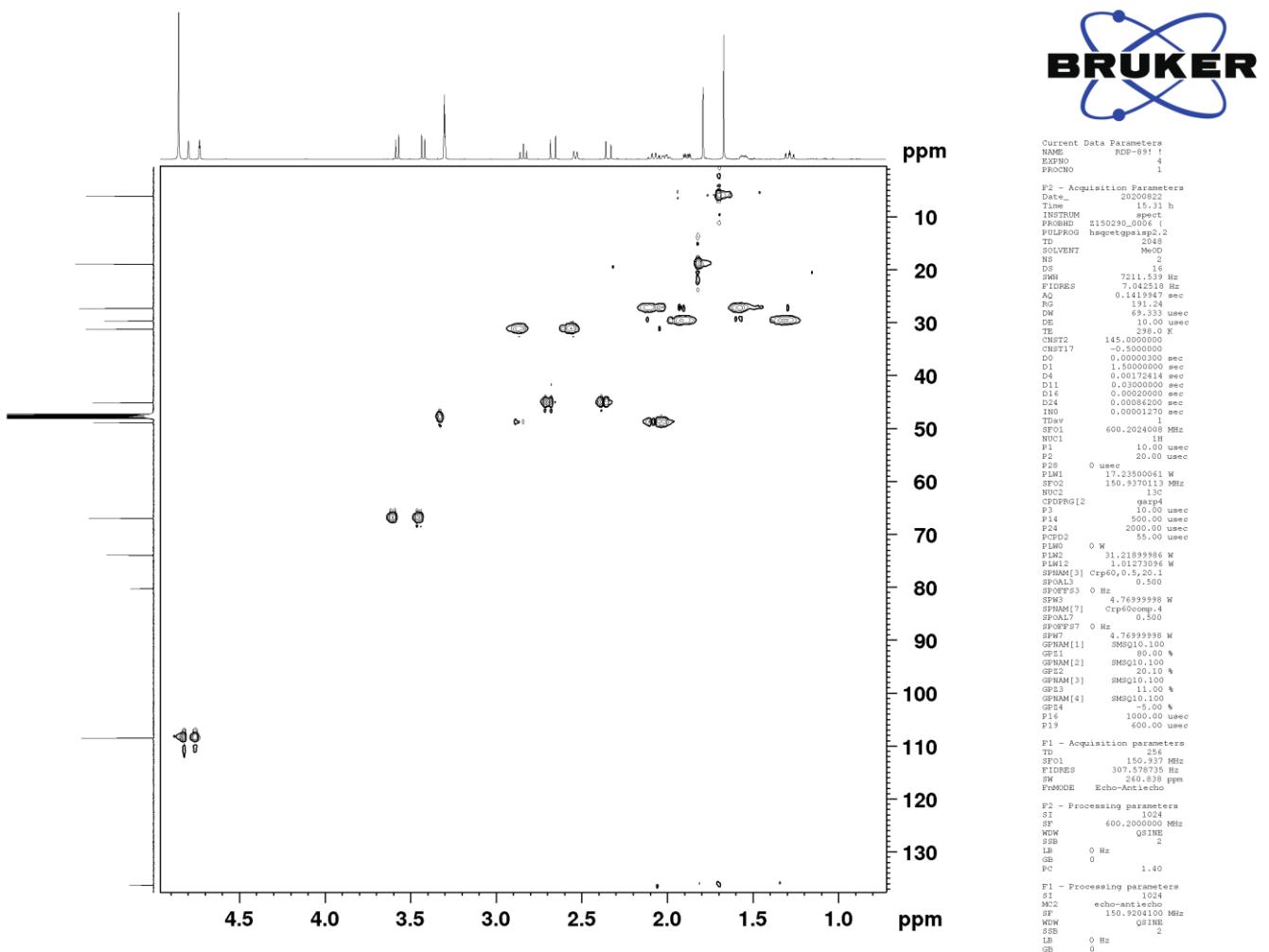
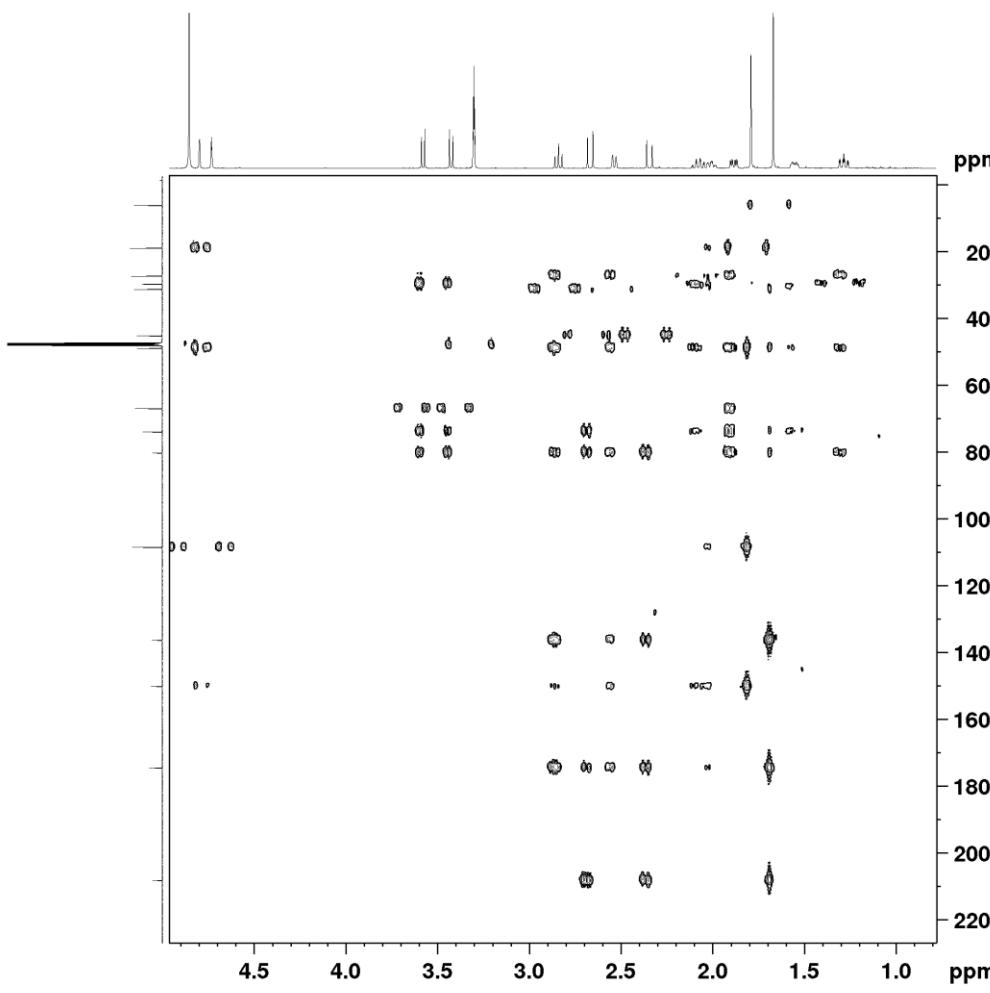


Figure S36 HSQC spectrum (600 MHz, CDCl_3) of compound 6



Current Data Parameters
NAME RDP-89! !
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200822
Time 15.46 h
INSTRUM spect
PROBID Z150290_0001
PULPROG hmbcgpndqf
TD 4096
SOLVENT MeOD
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 131.224
DW 69.433 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.000000
D0 0.00000300 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
DW0 0.00001270 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
SF02 150.9370100 MHz
NUC2 13C
P3 10.00 usec
PLW2 31.2189986 W
GPNAME[1] SMSQ10.100
GP21 50.00 °
GPNAME[2] SMSQ10.100
GP22 30.00 °
GPNAME[3] SMSQ10.100
GP23 40.10 °
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.937 MHz
FIDRES 615.157471 Hz
SW 260.838 ppm
FhMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S37 HMBC spectrum (600 MHz, CDCl_3) of compound **6**

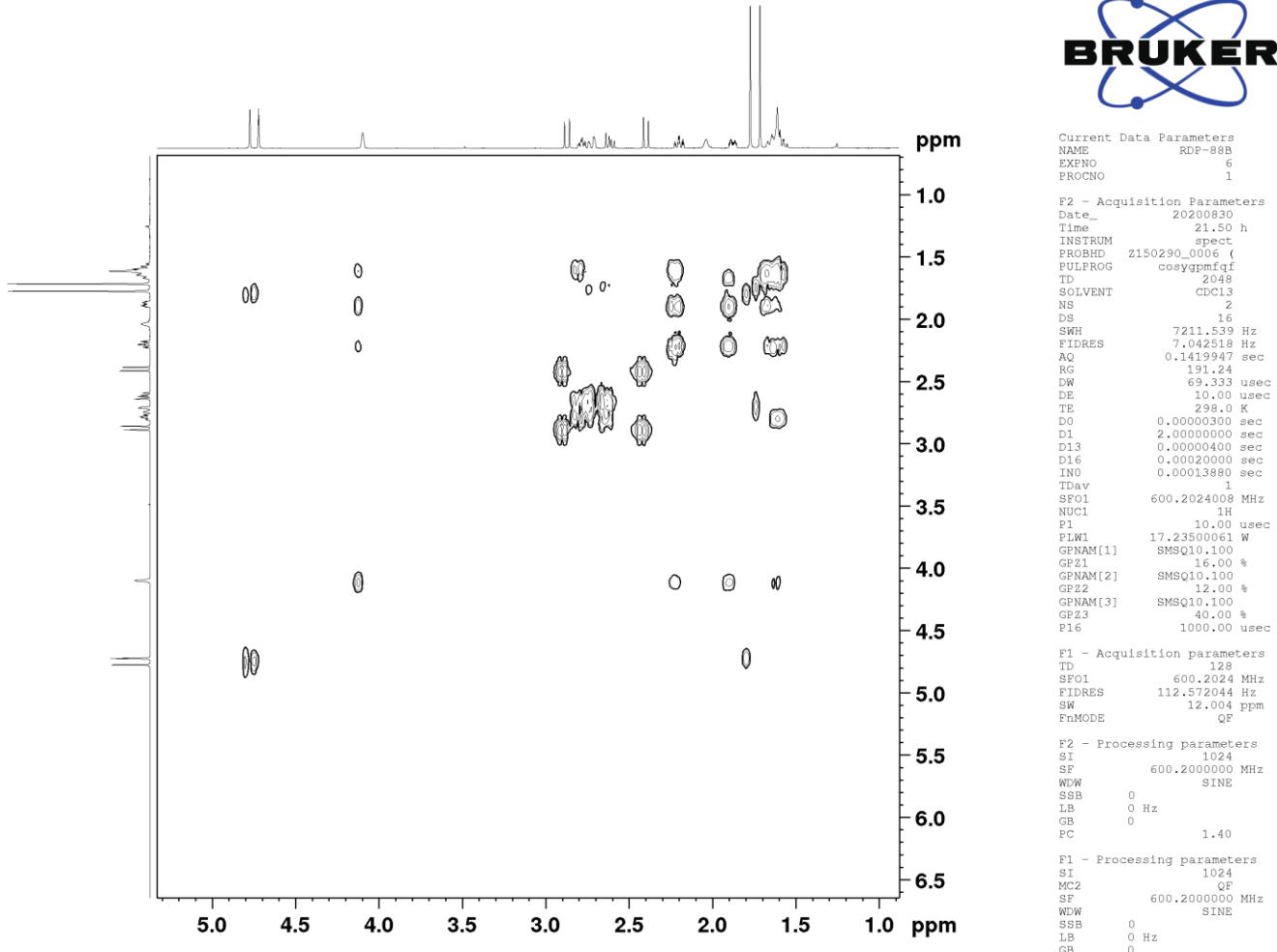
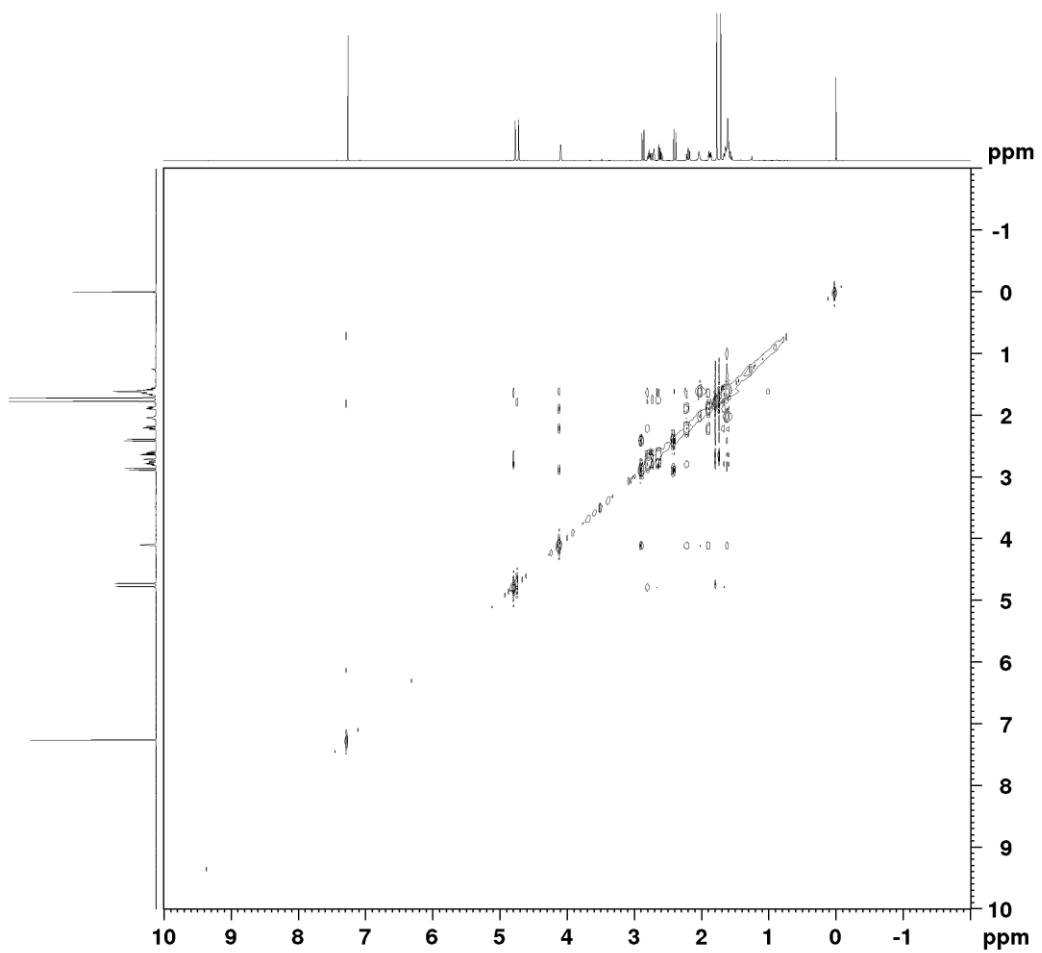


Figure S38 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **6**



Current Data Parameters
NAME RDP-66B
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200830
Time 22.00 h
INSTRUM spect
PROBHD Z150290_0064 ('
PULFRCG noeipypphph
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60
DW 69.333 usec
DB 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.0001386 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
M22 States-TPPI
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S39 NOESY spectrum (600 MHz, CDCl_3) of compound 6

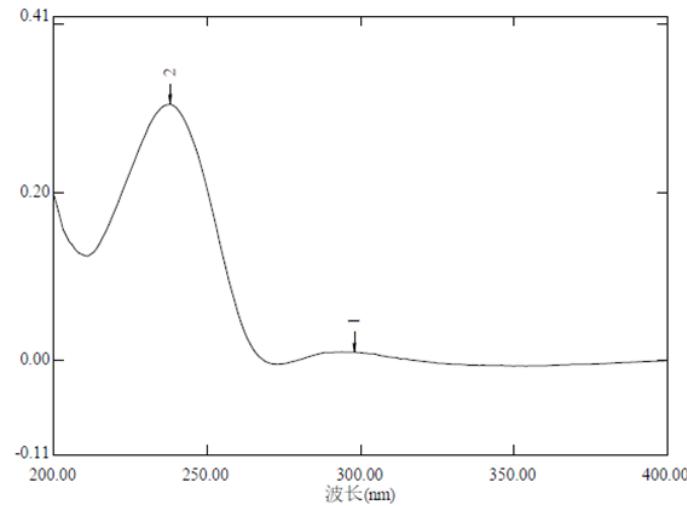
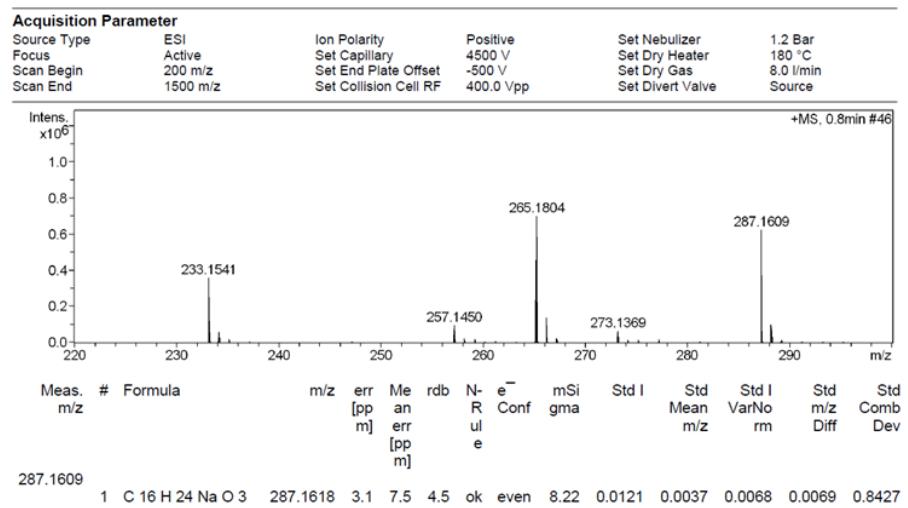


Figure S40 HRESIMS and UV spectra of compound 7

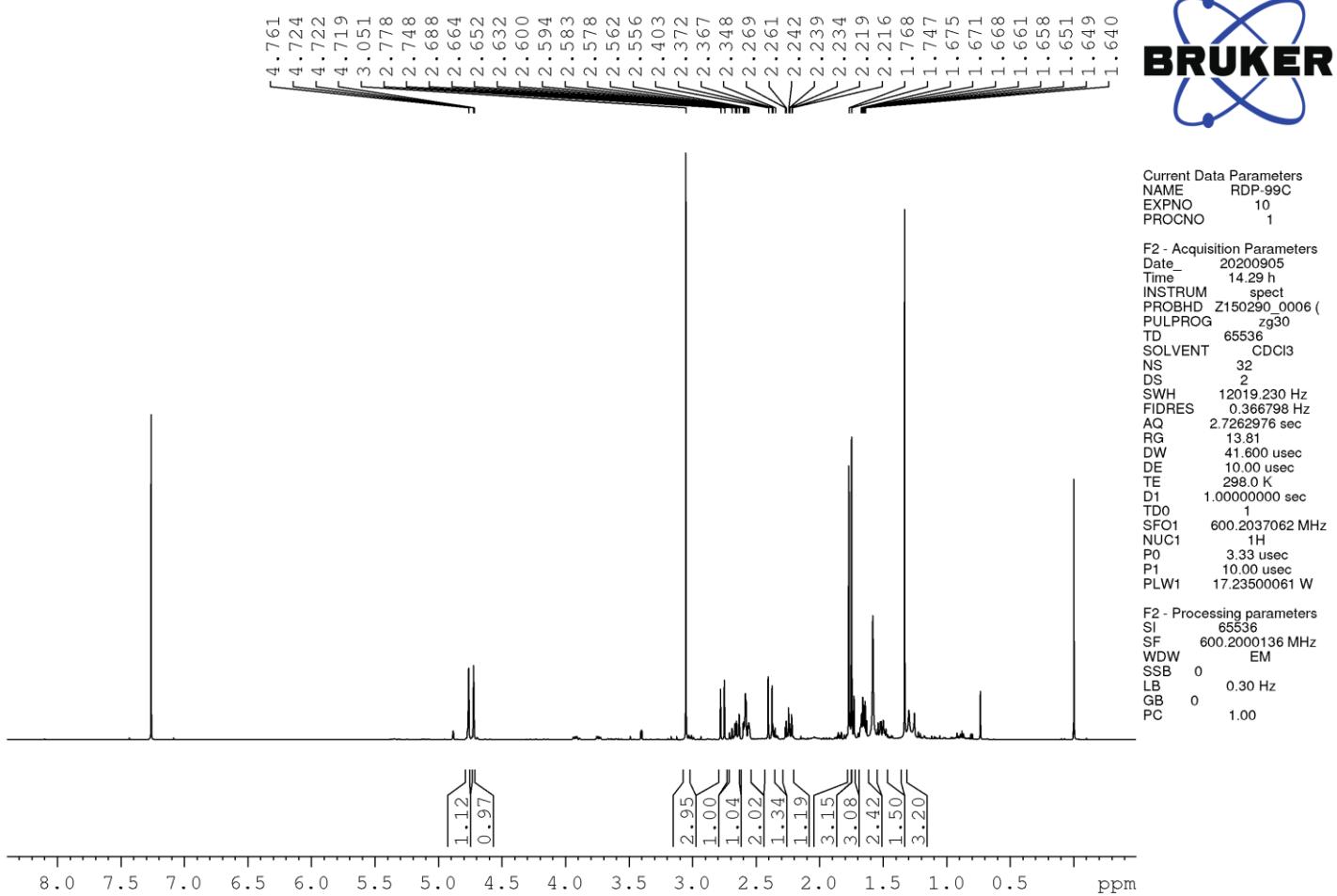


Figure S41 ^1H NMR spectrum (600 MHz, CDCl_3) of compound 7

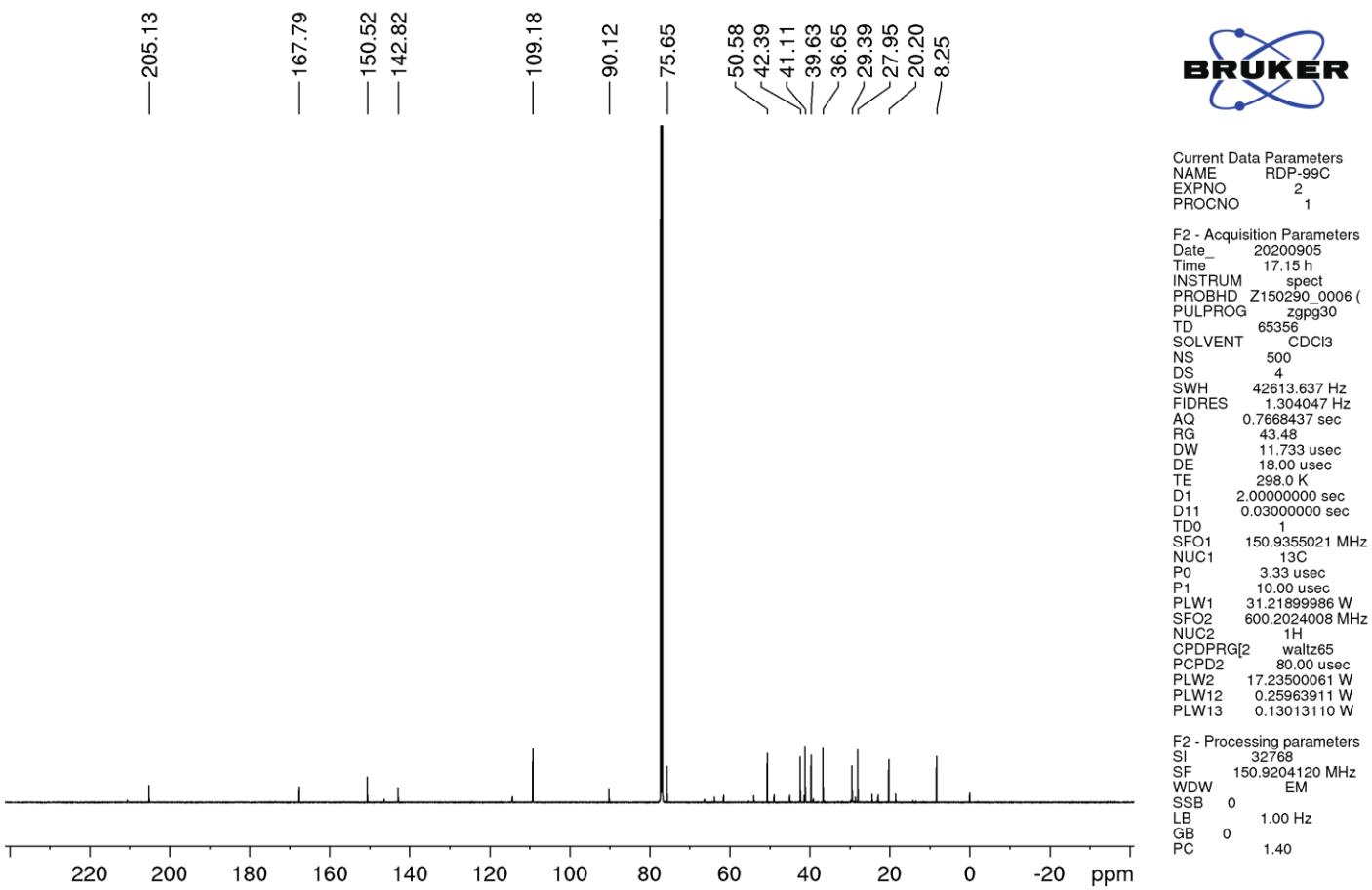


Figure S42 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound 7

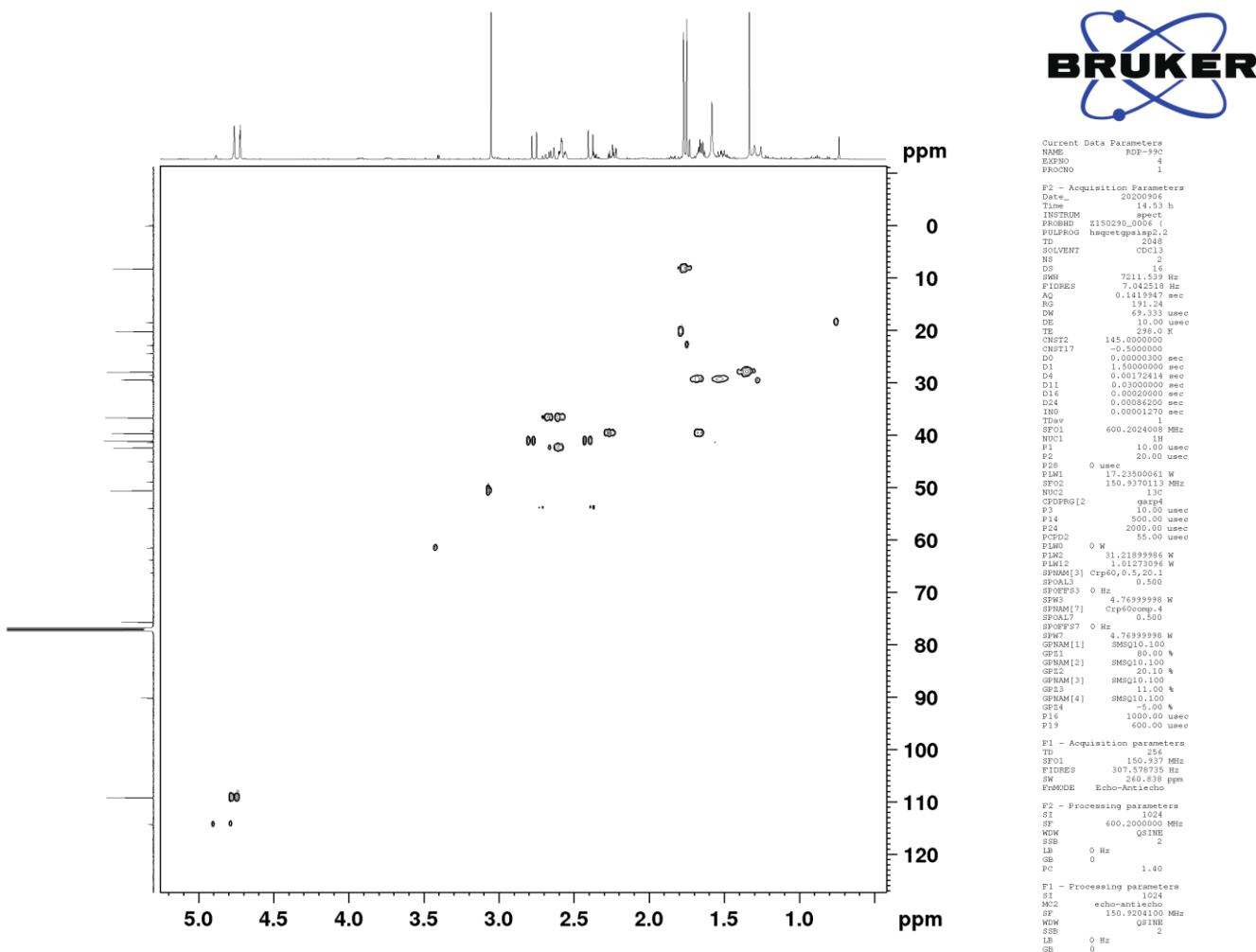


Figure S43 HSQC spectrum (600 MHz, CDCl₃) of compound 7

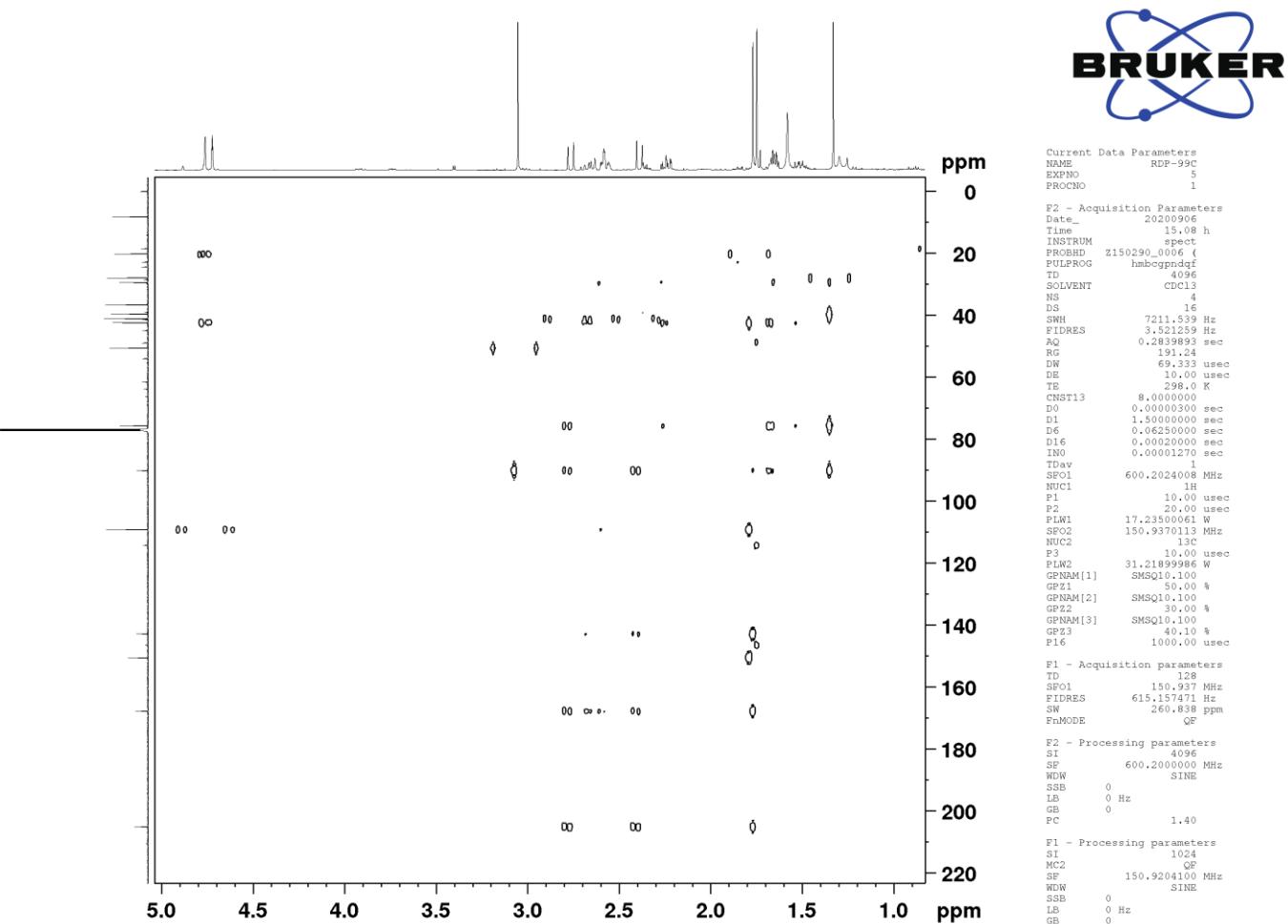


Figure S44 HMBC spectrum (600 MHz, CDCl₃) of compound 7

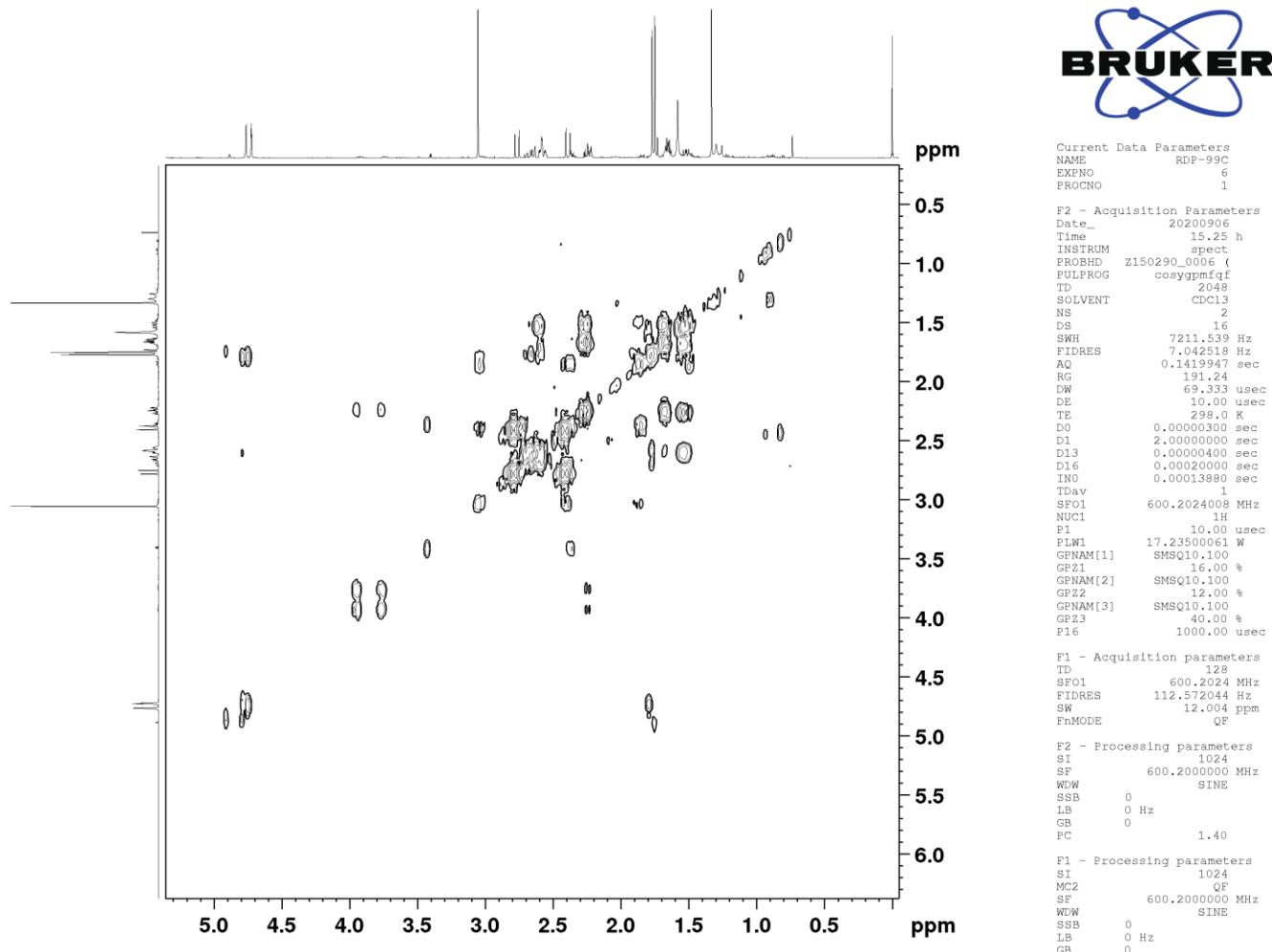
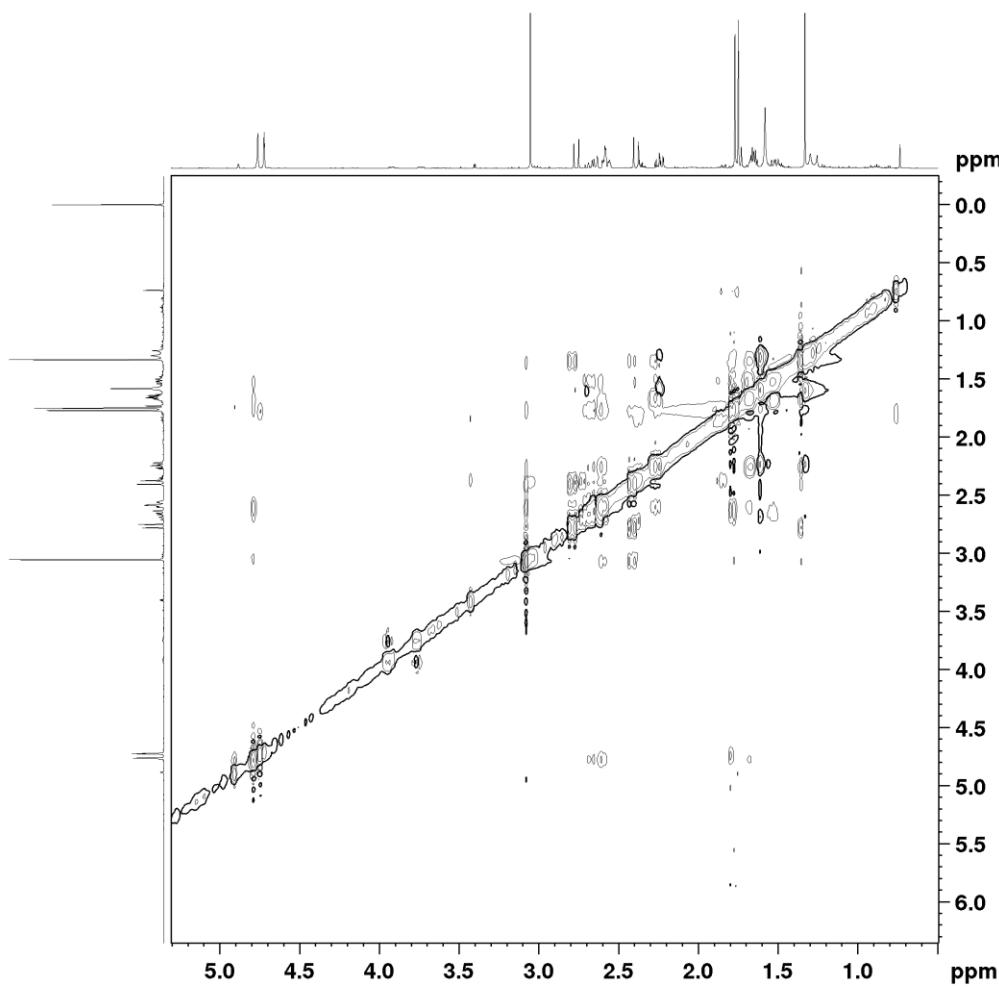


Figure S45 ^1H - ^1H COSY spectrum (600 MHz, CDCl₃) of compound 7



Current Data Parameters
NAME RDP-99C
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200906
Time 15.35 h
INSTRUM sec
PROBHD Z150290_0004 (
PULPROG noeesypphp.ppp
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60.93
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000000 sec
D11 0.0000000 sec
D12 0.00002000 sec
D16 0.00002000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

P1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12.004 ppm
PrMODE States-TPP1

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

P1 - Processing parameters
SI 1024
MC2 States-TPP1
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S46 NOESY spectrum (600 MHz, CDCl_3) of compound 7

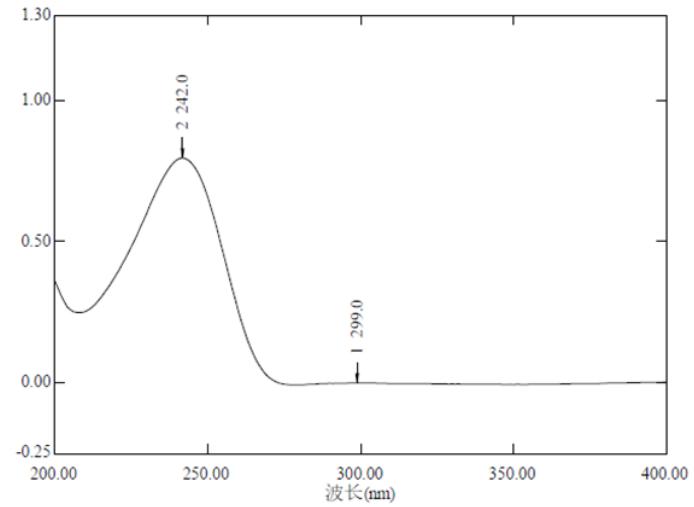
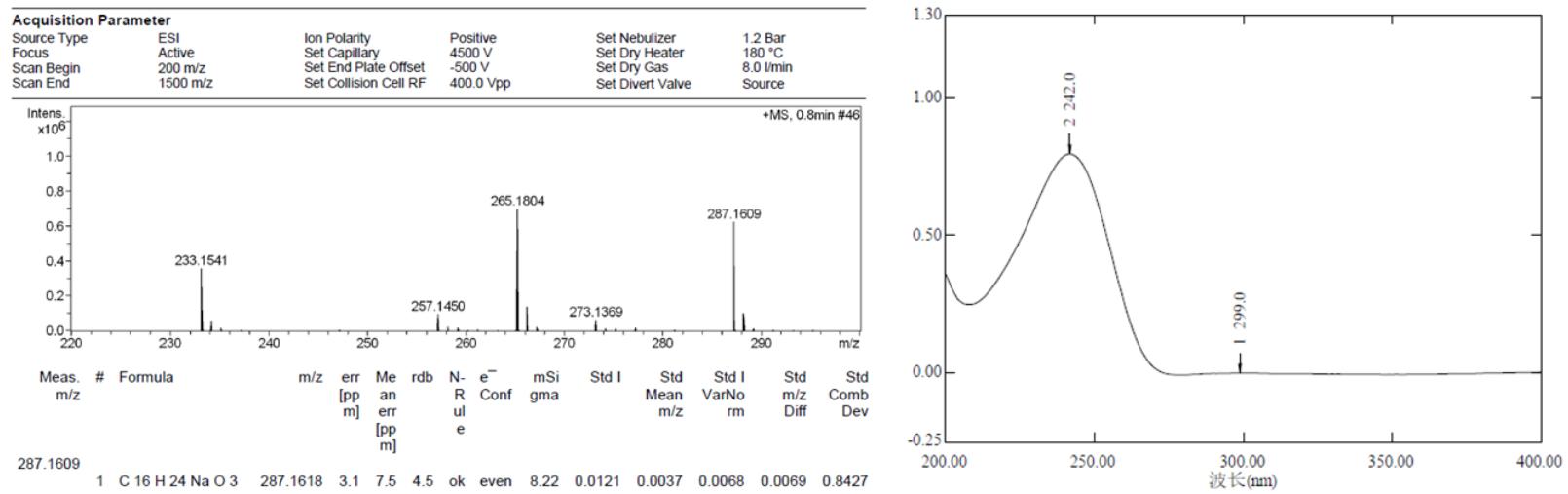
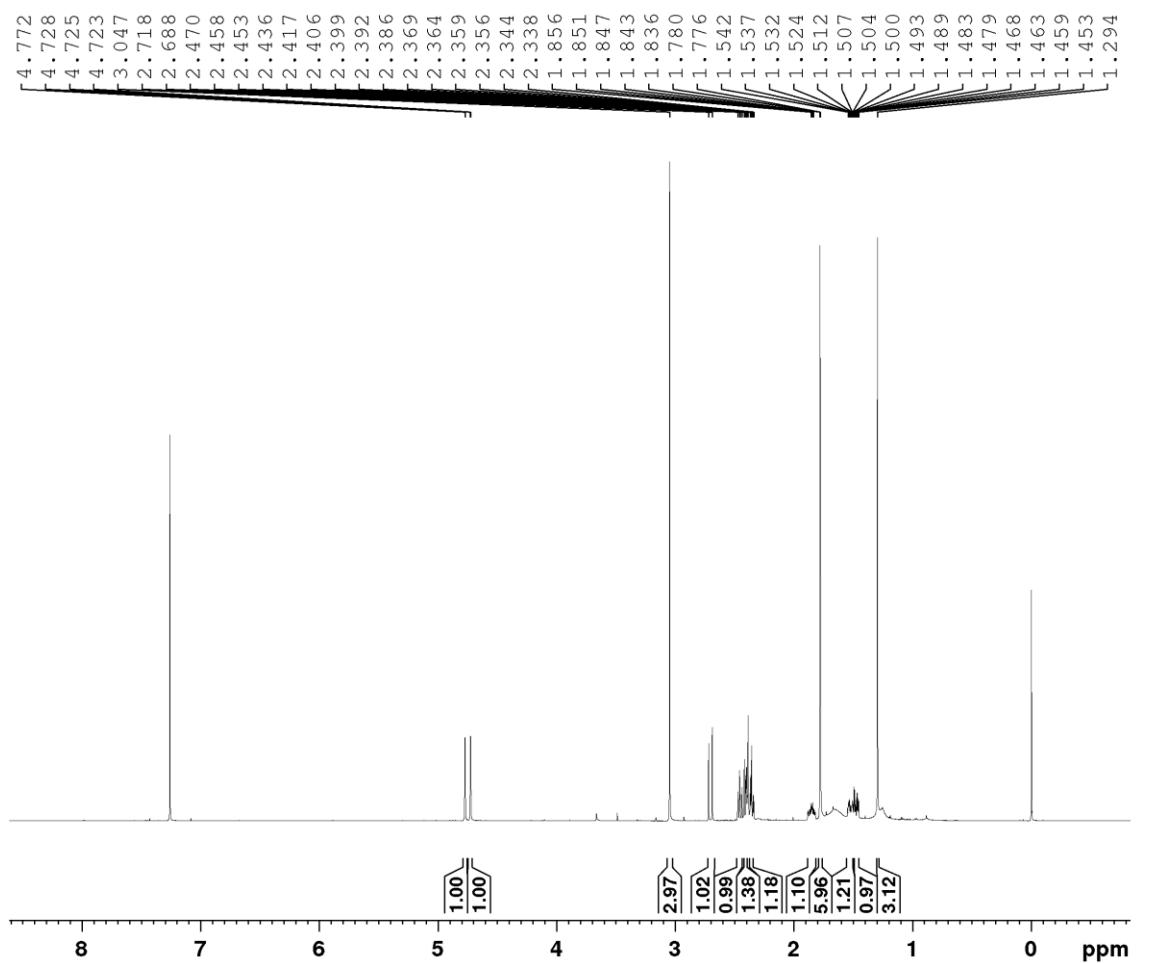


Figure S47 HRESIMS and UV spectra of compound **8**

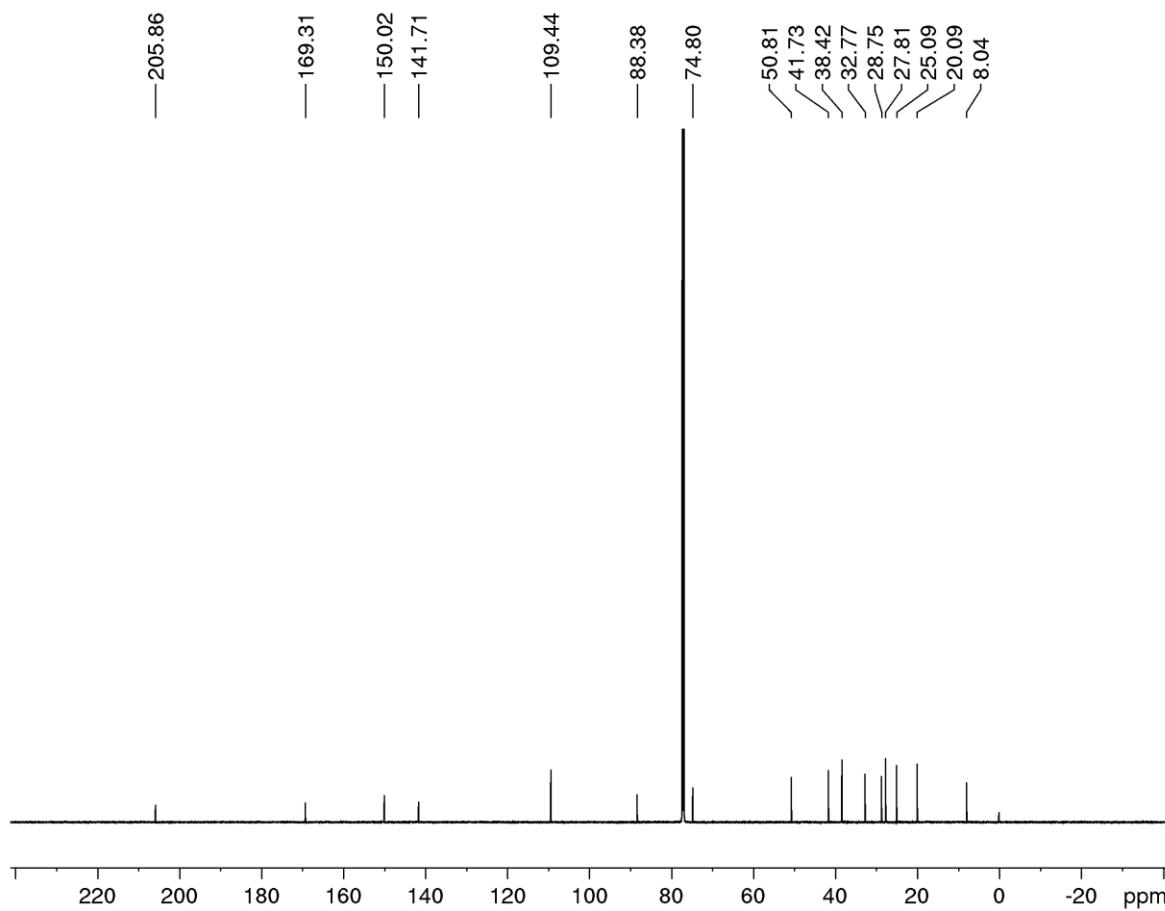


Current Data Parameters
NAME RDP-99C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201118
Time 20.43 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 13.81
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1
SF01 600.2037062 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 17.23500061 W

F2 - Processing parameters
SI 65536
SF 600.2000136 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S48 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **8**



Current Data Parameters
NAME RDP-99C-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20201122
Time 6.24 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgpg30
TD 65356
SOLVENT CDCl3
NS 200
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 35.36
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9203897 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S49 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **8**

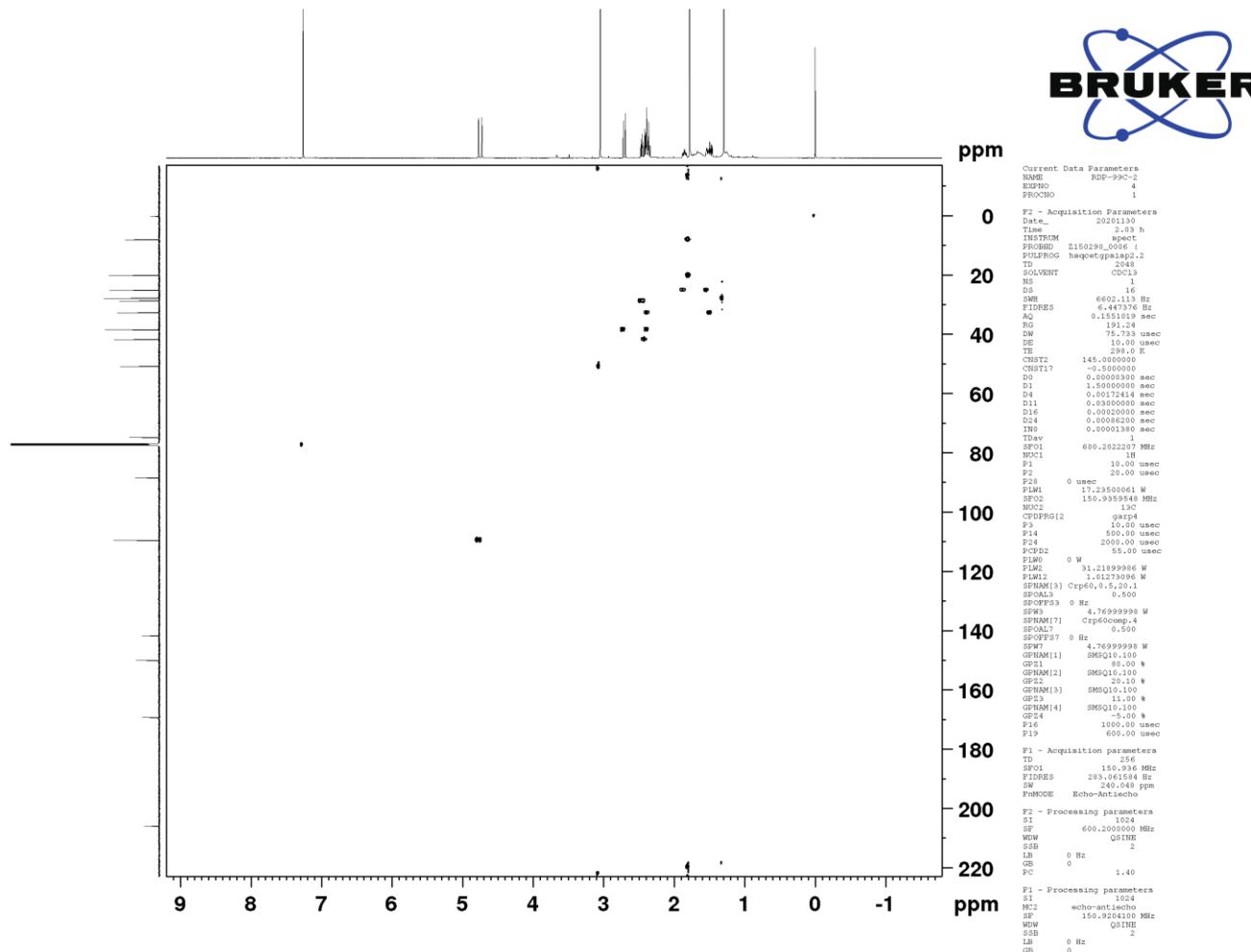


Figure S50 HSQC spectrum (600 MHz, CDCl₃) of compound 8

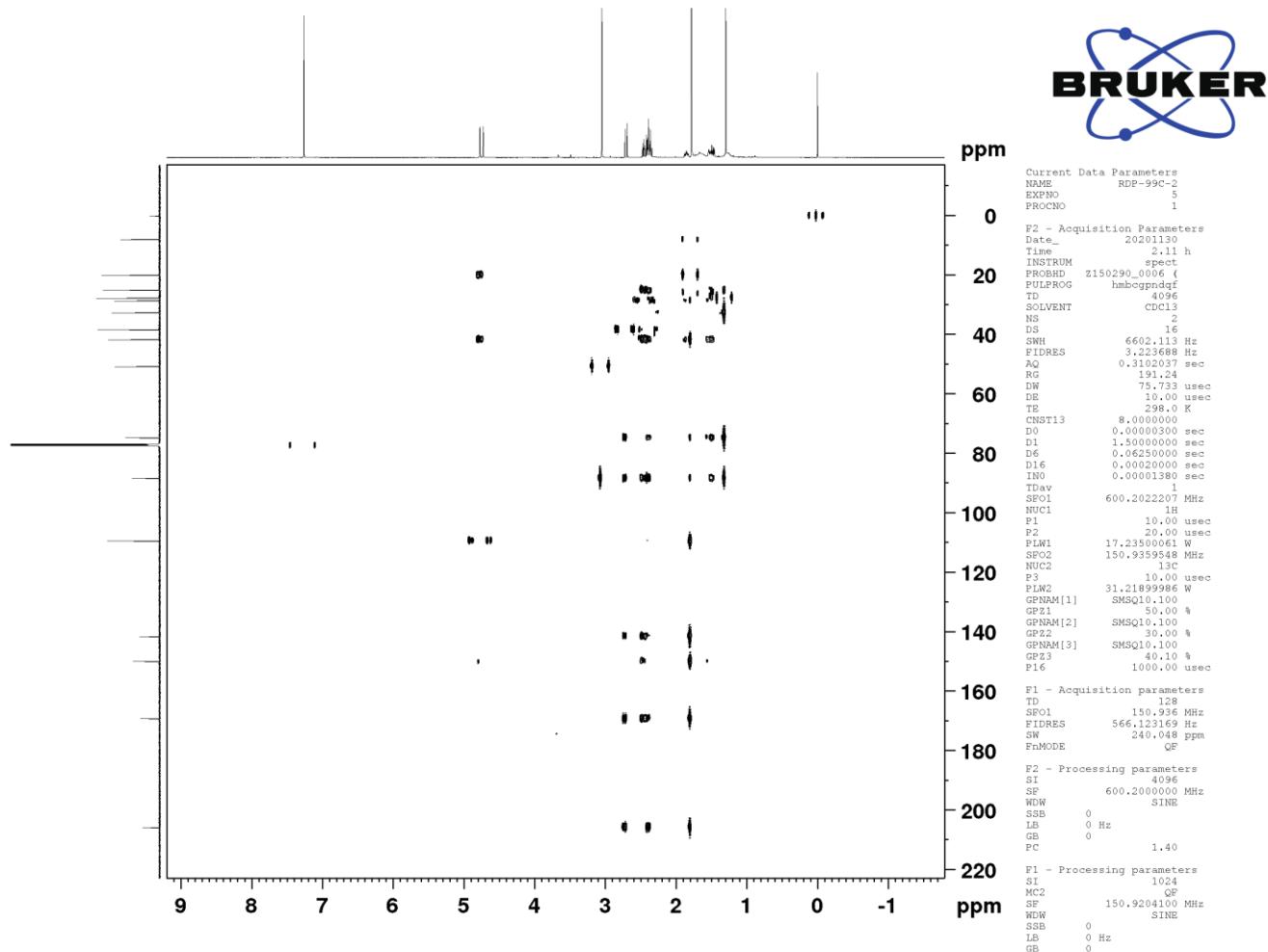


Figure S51 HMBC spectrum (600 MHz, CDCl₃) of compound **8**

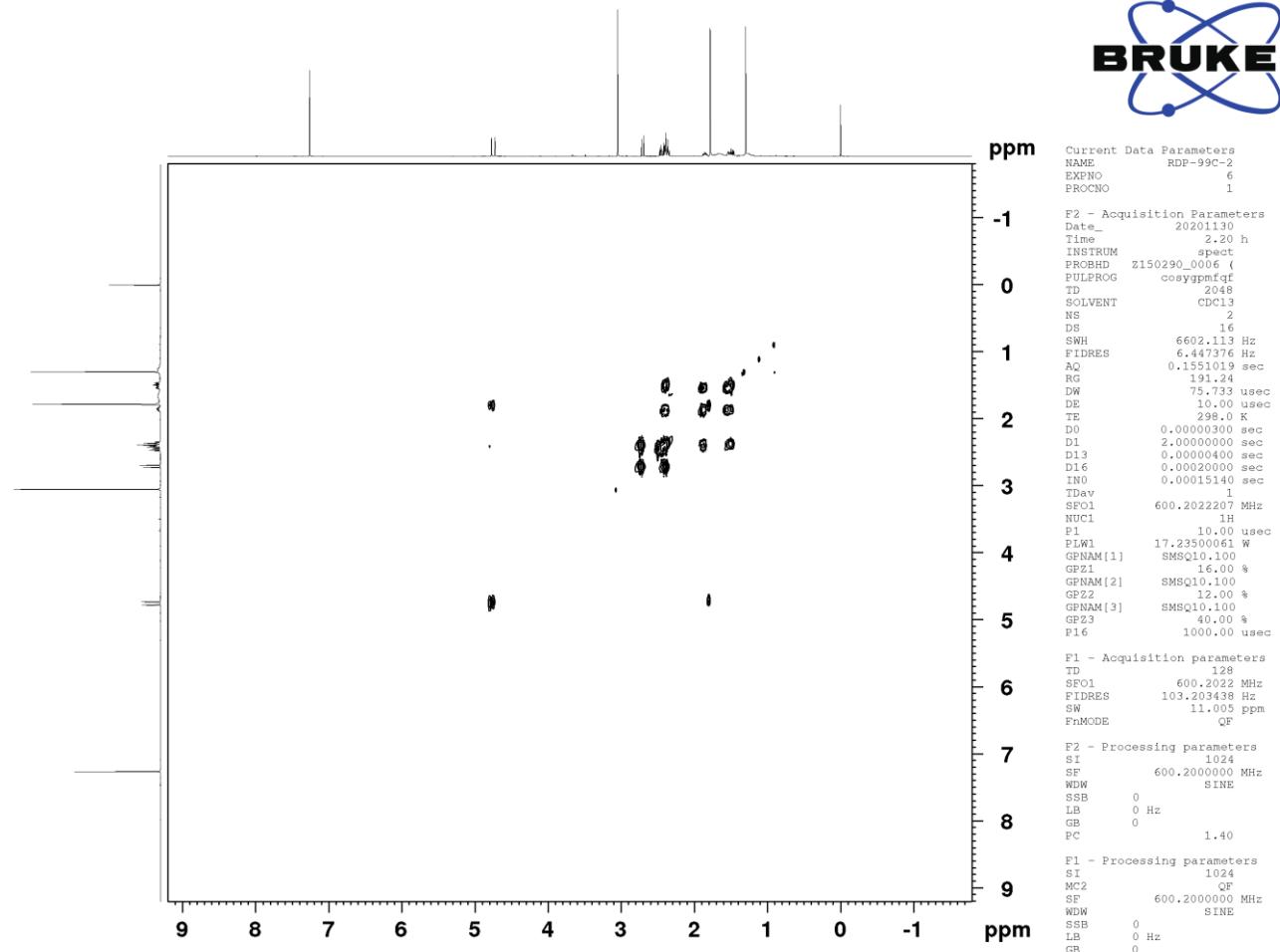


Figure S52 ¹H-¹H COSY spectrum (600 MHz, CDCl₃) of compound 8

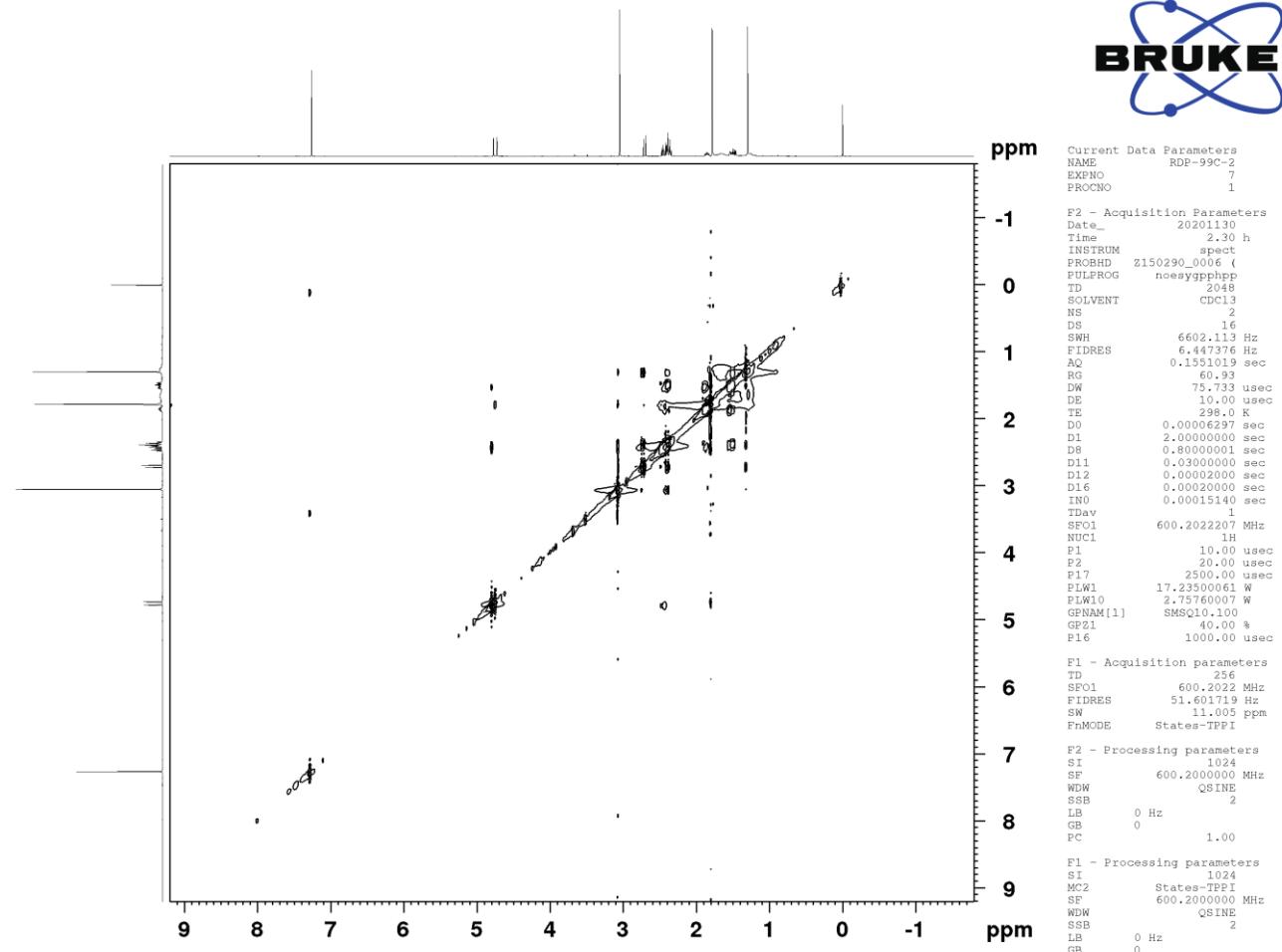


Figure S53 NOESY spectrum (600 MHz, CDCl₃) of compound 8

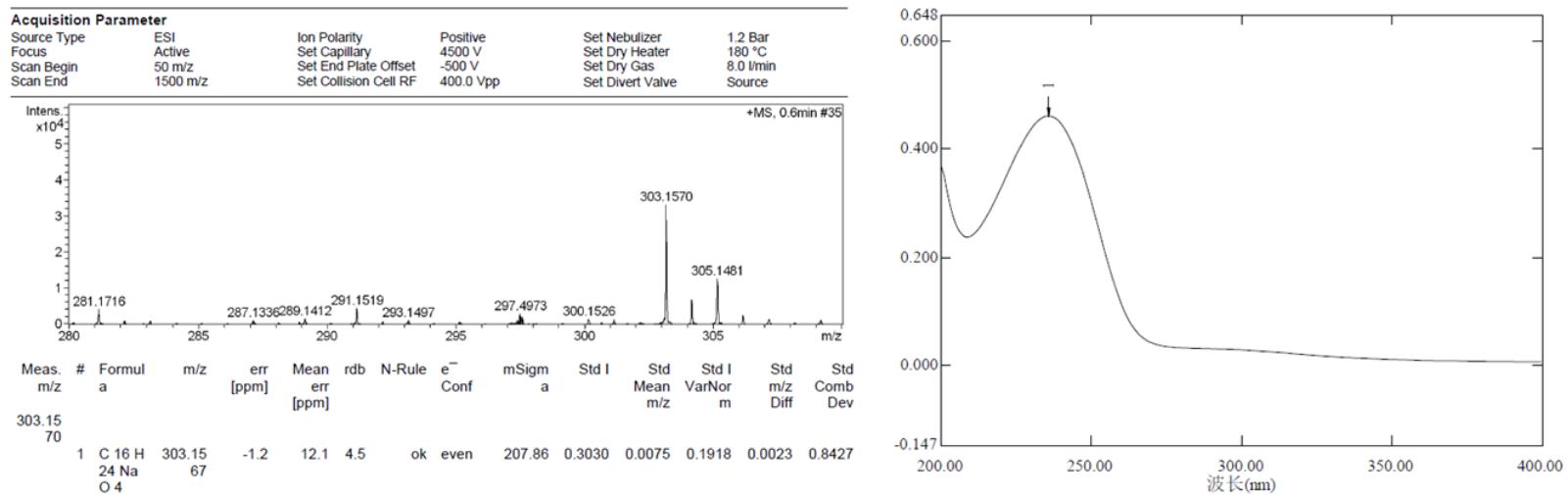


Figure S54 HRESIMS and UV spectra of compound 9

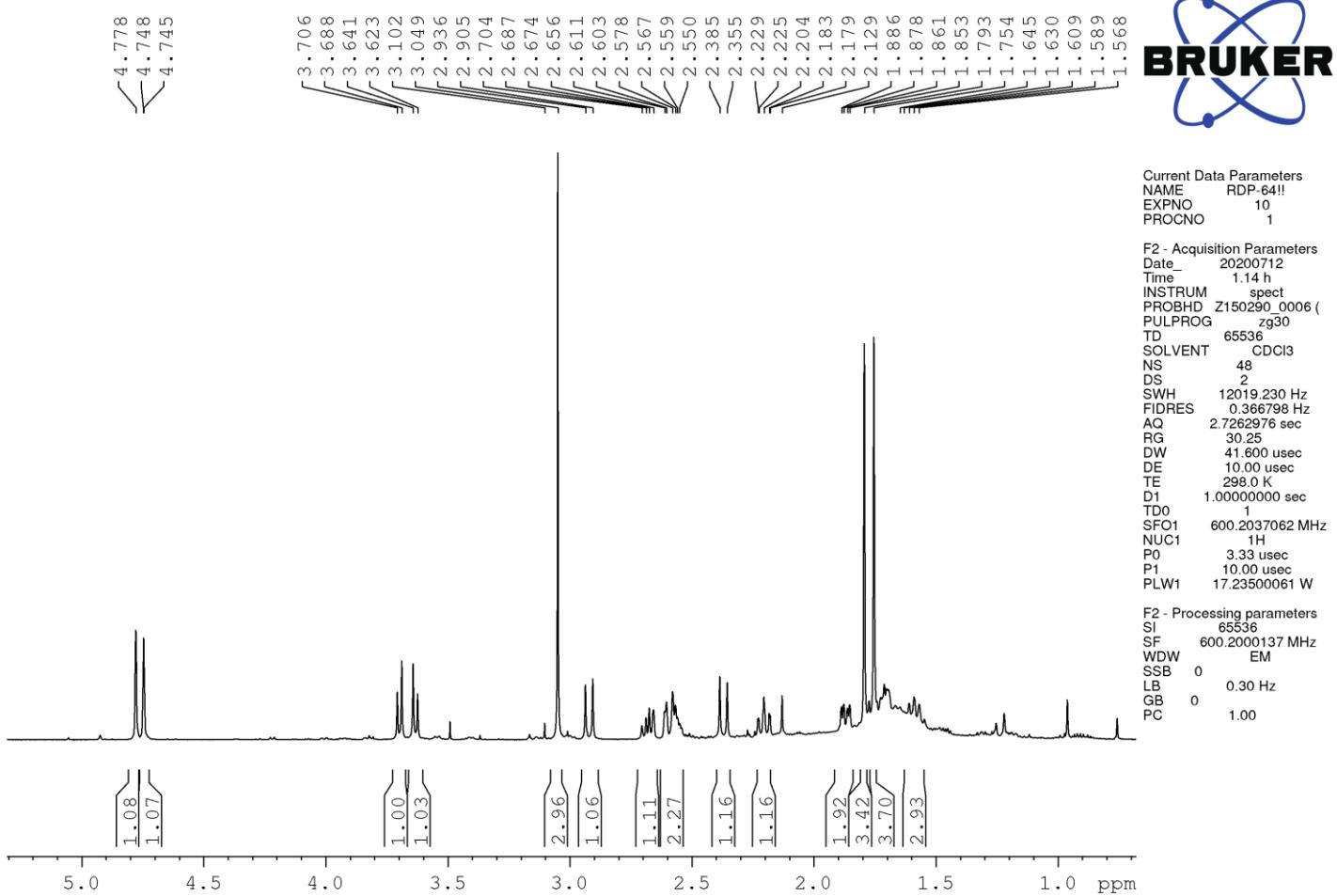
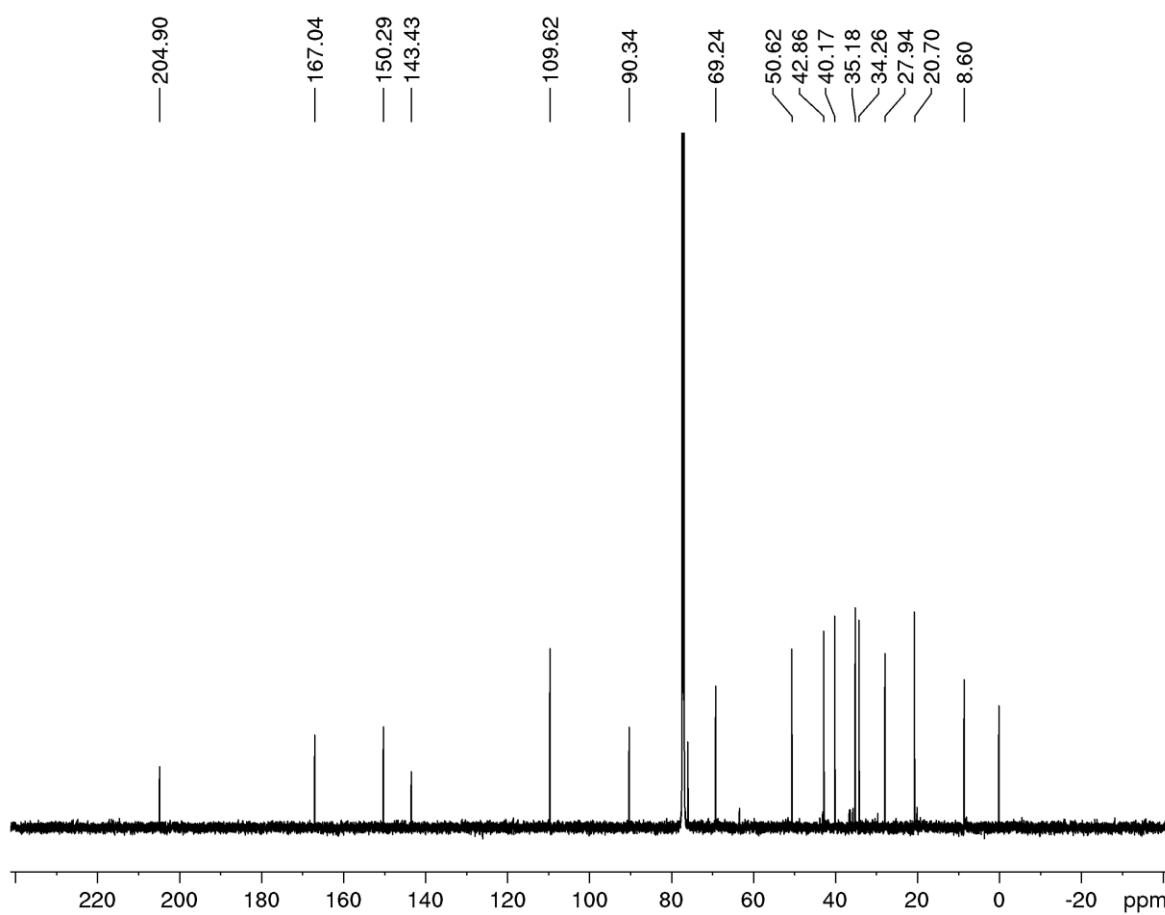


Figure S55 ¹H NMR spectrum (600 MHz, CDCl₃) of compound 9



Current Data Parameters
NAME RDP-64!!
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20200712
Time 15.15 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zpg30
TD 65356
SOLVENT CDCl3
NS 800
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 21.56
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9203906 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S56 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound 9

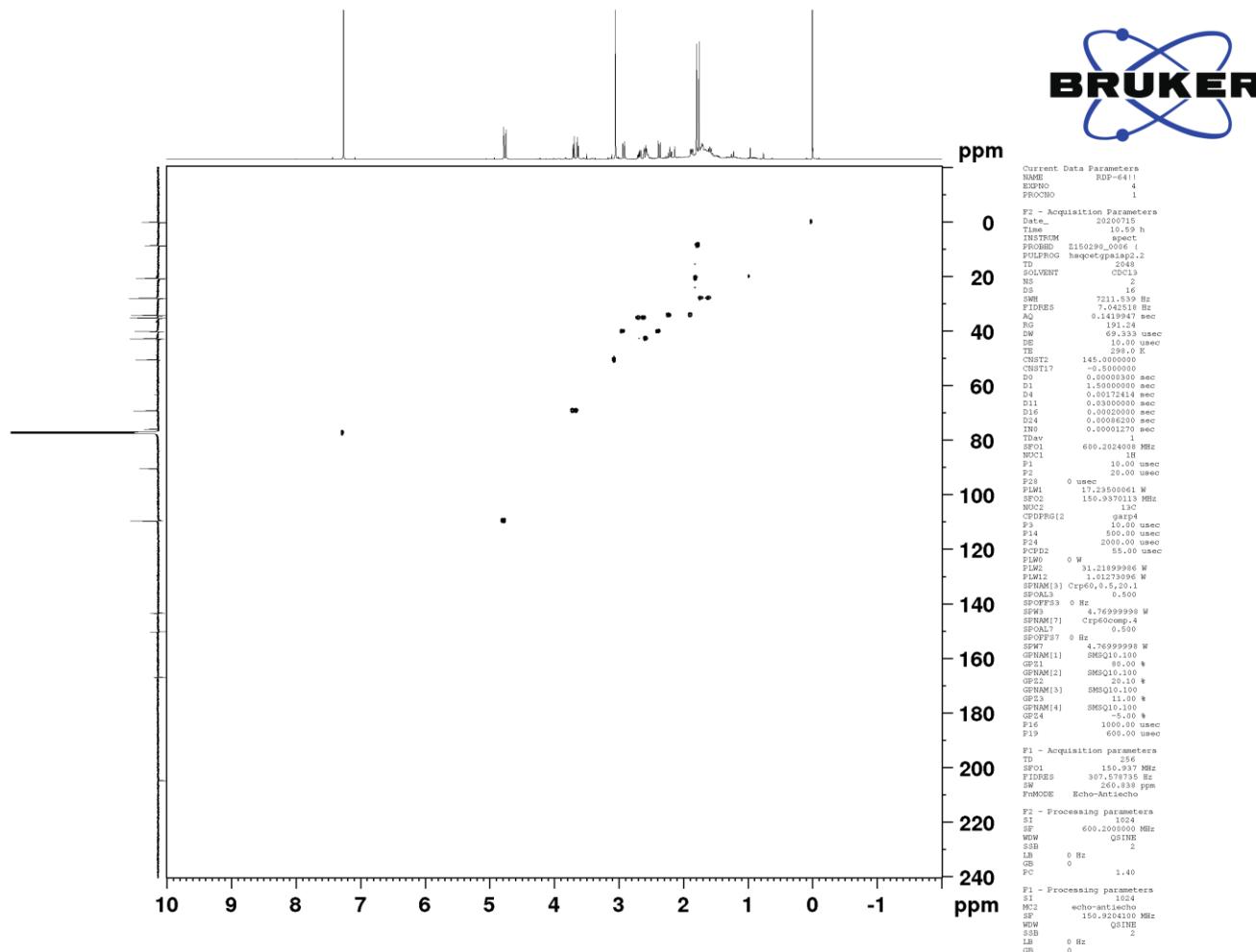
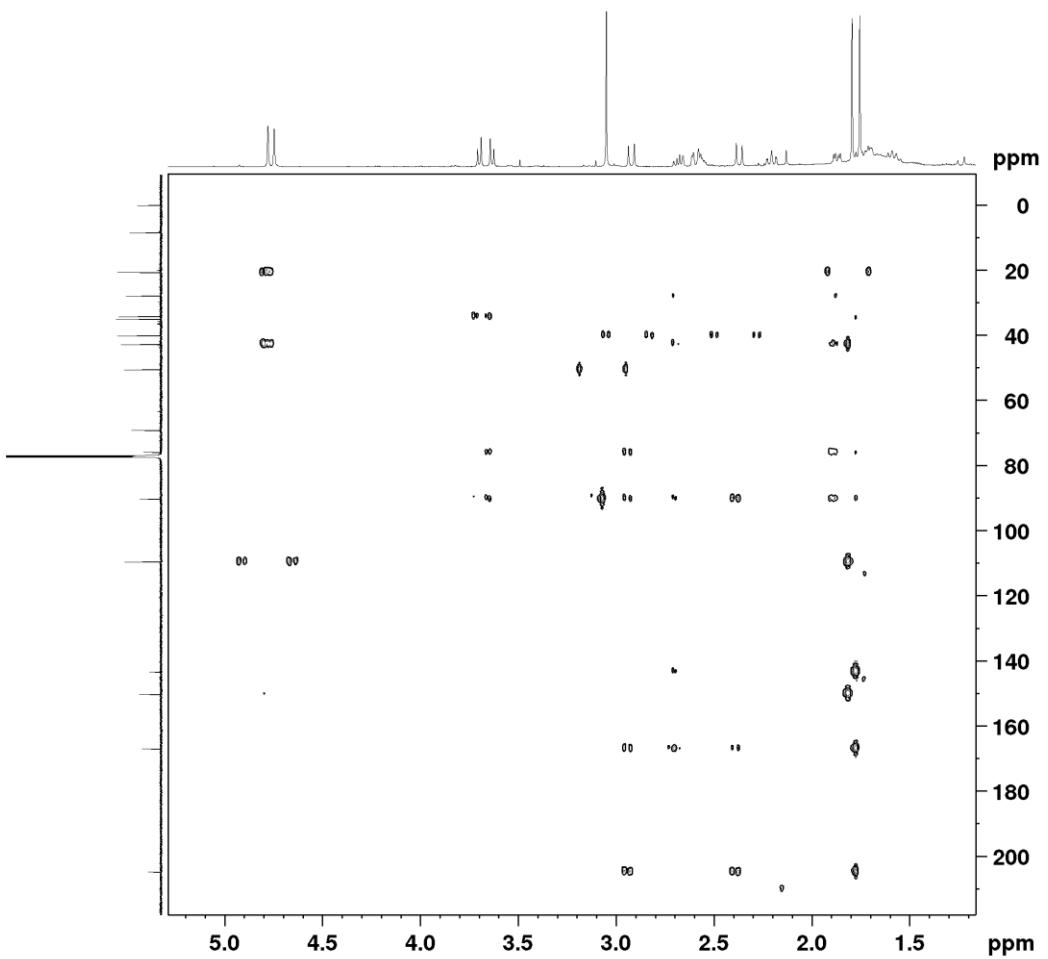


Figure S57 HSQC spectrum (600 MHz, CDCl₃) of compound 9



Current Data Parameters
NAME RDP-64!!
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200715
Time 11.14 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG hmbcgrndqf
TD 4096
SOLVENT CDCl3
NS 6
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 130.00
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.0000000
D0 0.0000300 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001270 sec
TDav 600.2024018 sec
SF01 600.2024018 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLN1 17.23500061 W
SF02 150.9370113 MHz
NUC2 13C
P3 10.00 usec
PLN2 31.21899986 W
GPNAME[1] SNSQ10.100
GPZ1 50.00 %
GPNAME[2] SNSQ10.100
GPZ2 30.00 %
GPNAME[3] SNSQ10.100
GPZ3 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.9370113 MHz
FIDRES 615.157471 Hz
SW 260.838 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S58 HMBC spectrum (600 MHz, CDCl_3) of compound 9

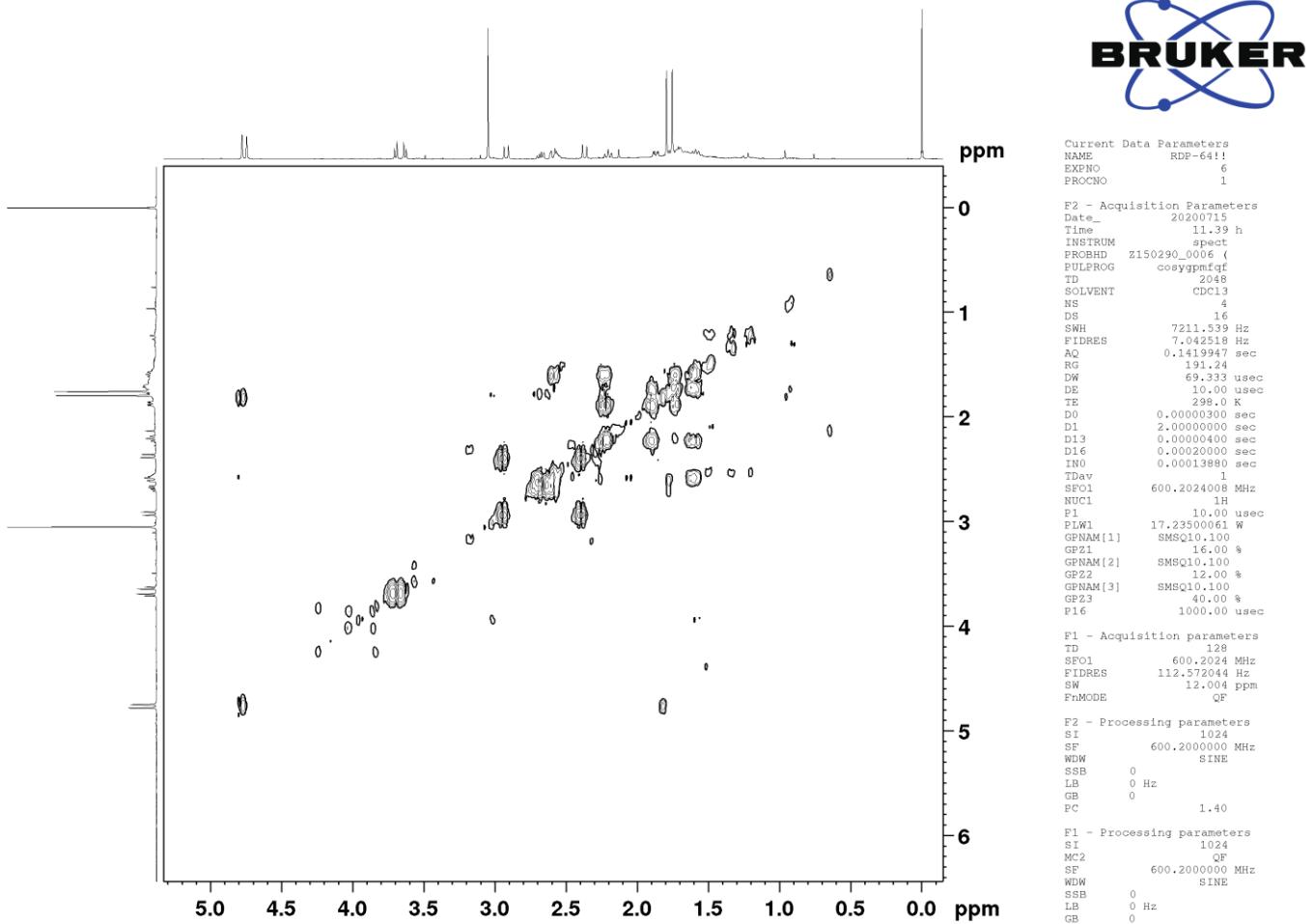
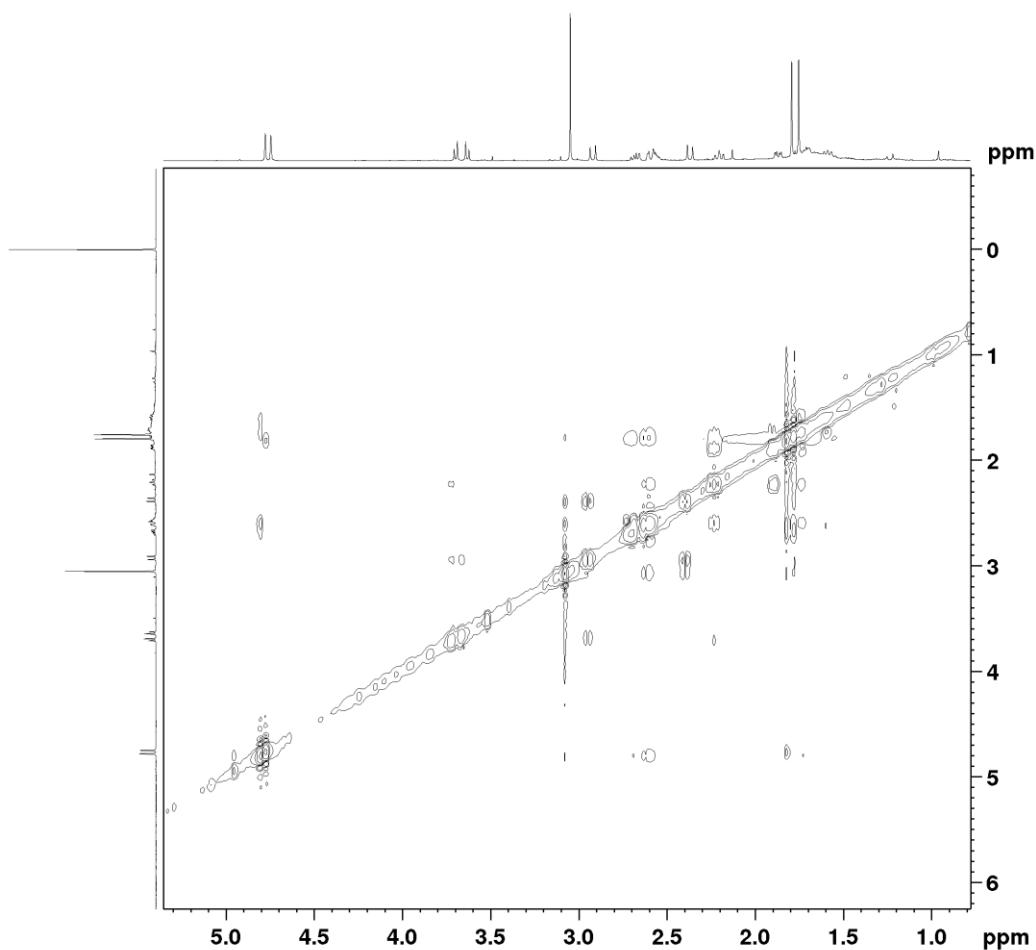


Figure S59 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 9



Current Data Parameters
NAME RDP-64!!
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200715
Time 11.59 h
INSTRUM spect
PROBHD Z150290_0066_1
PULFRQG noe3yppphpp
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.0001389 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
M22 States-TPPI
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S60 NOESY spectrum (600 MHz, CDCl_3) of compound **9**

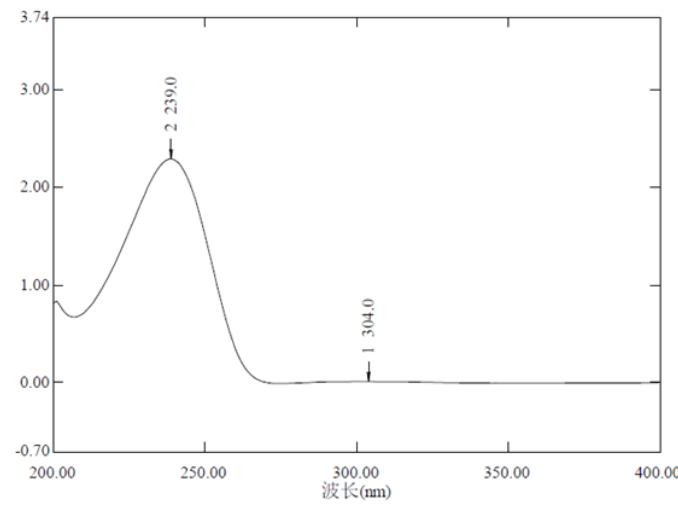
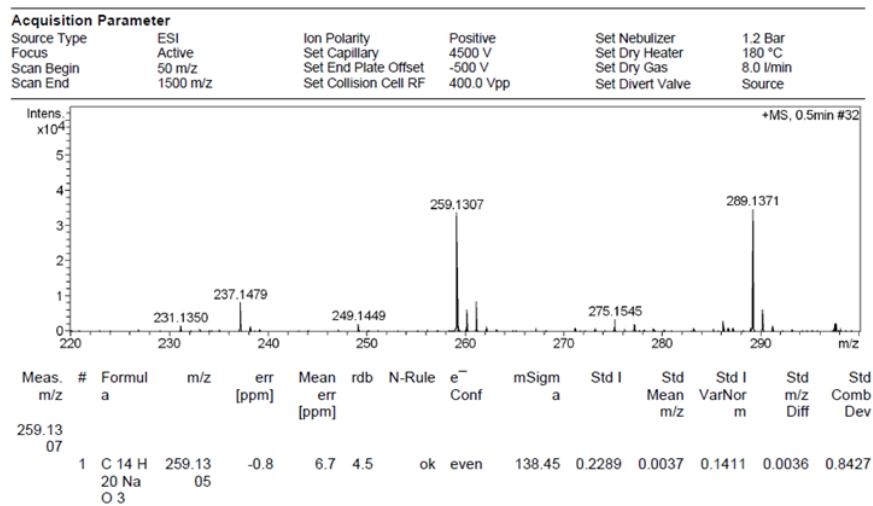


Figure S61 HRESIMS and UV spectra of compound **10**

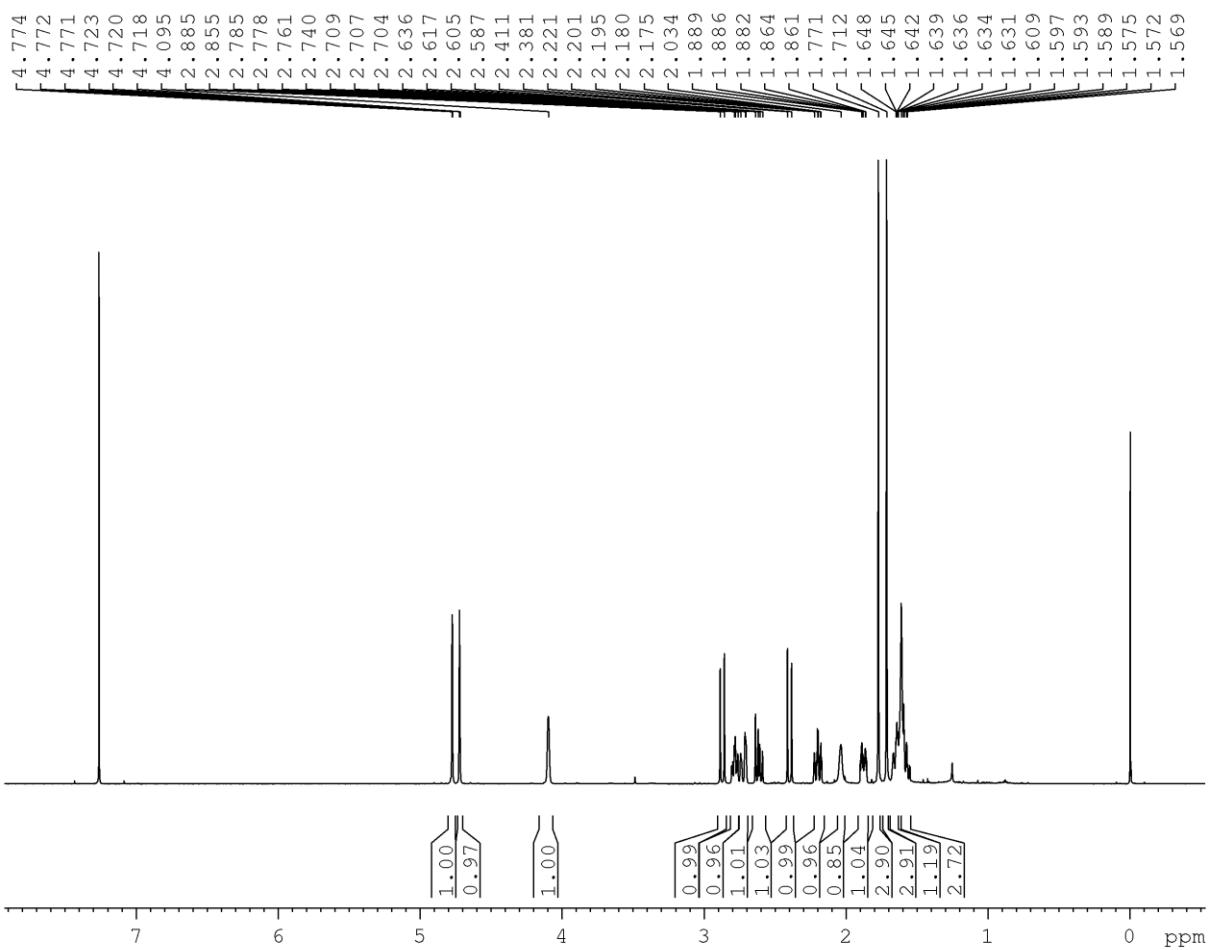
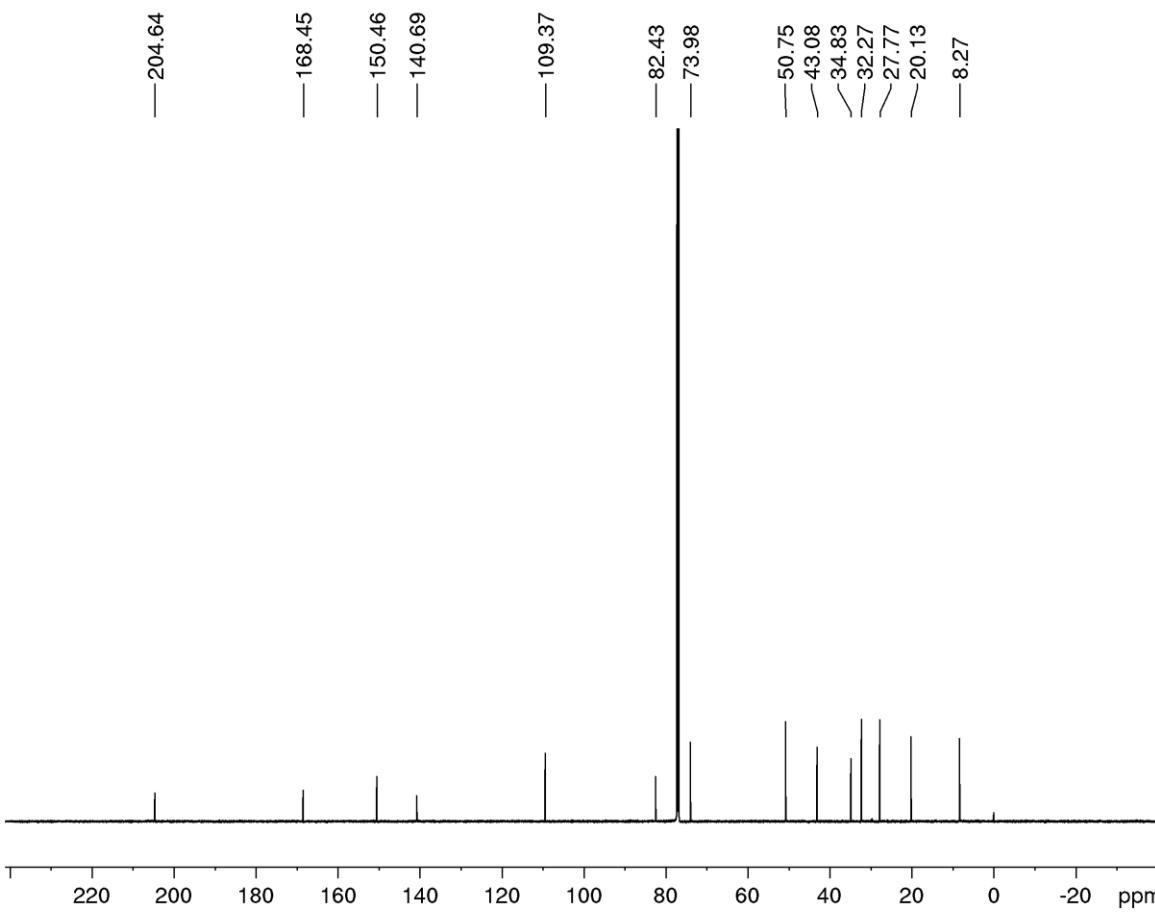


Figure S62 ¹H NMR spectrum (600 MHz, CDCl₃) of compound **10**



Current Data Parameters
NAME RDP-88B
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200823
Time_ 13.59 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgppg30
TD 65356
SOLVENT CDCl₃
NS 200
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 35.36
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 ¹³C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 ¹H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9204119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S63 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **10**

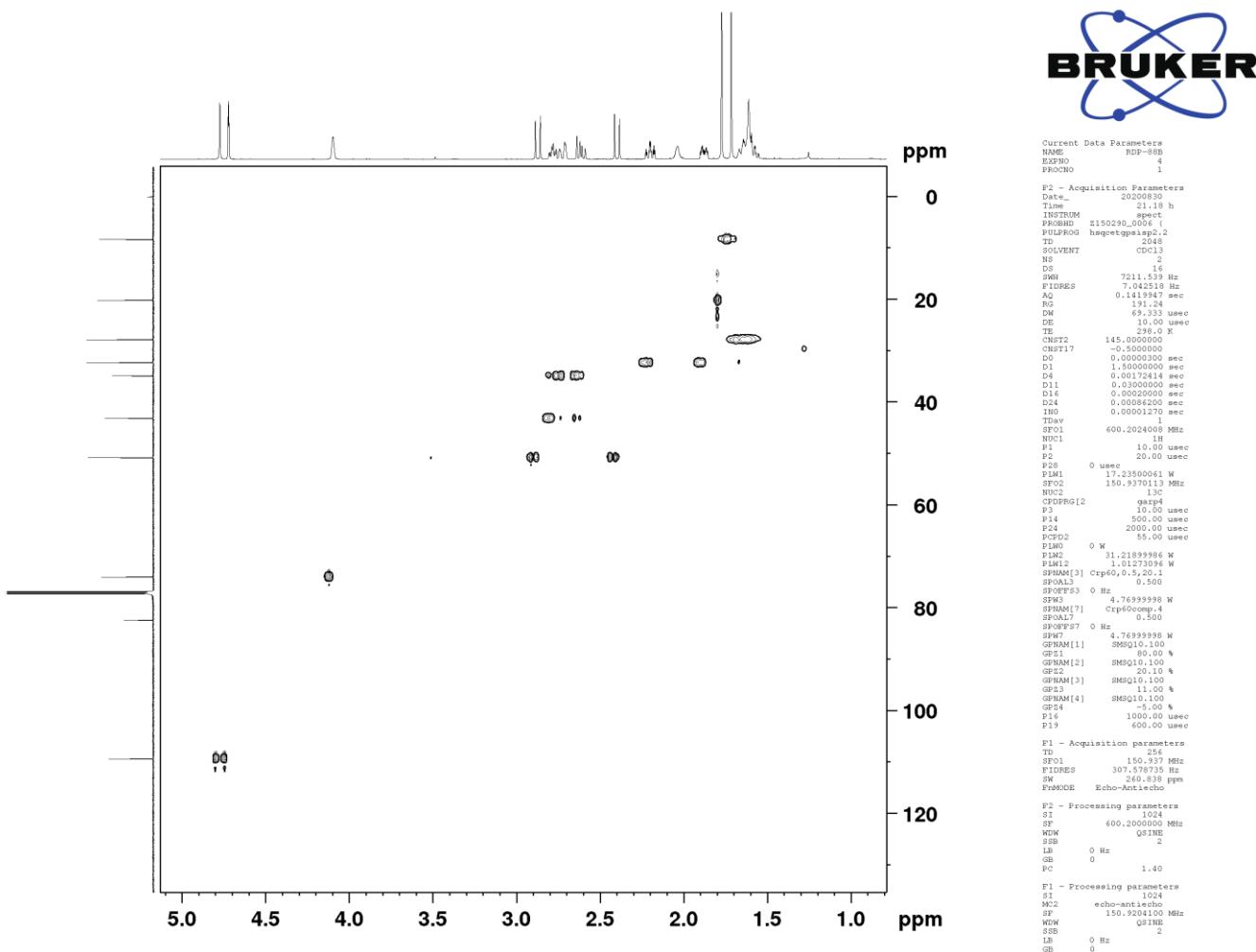
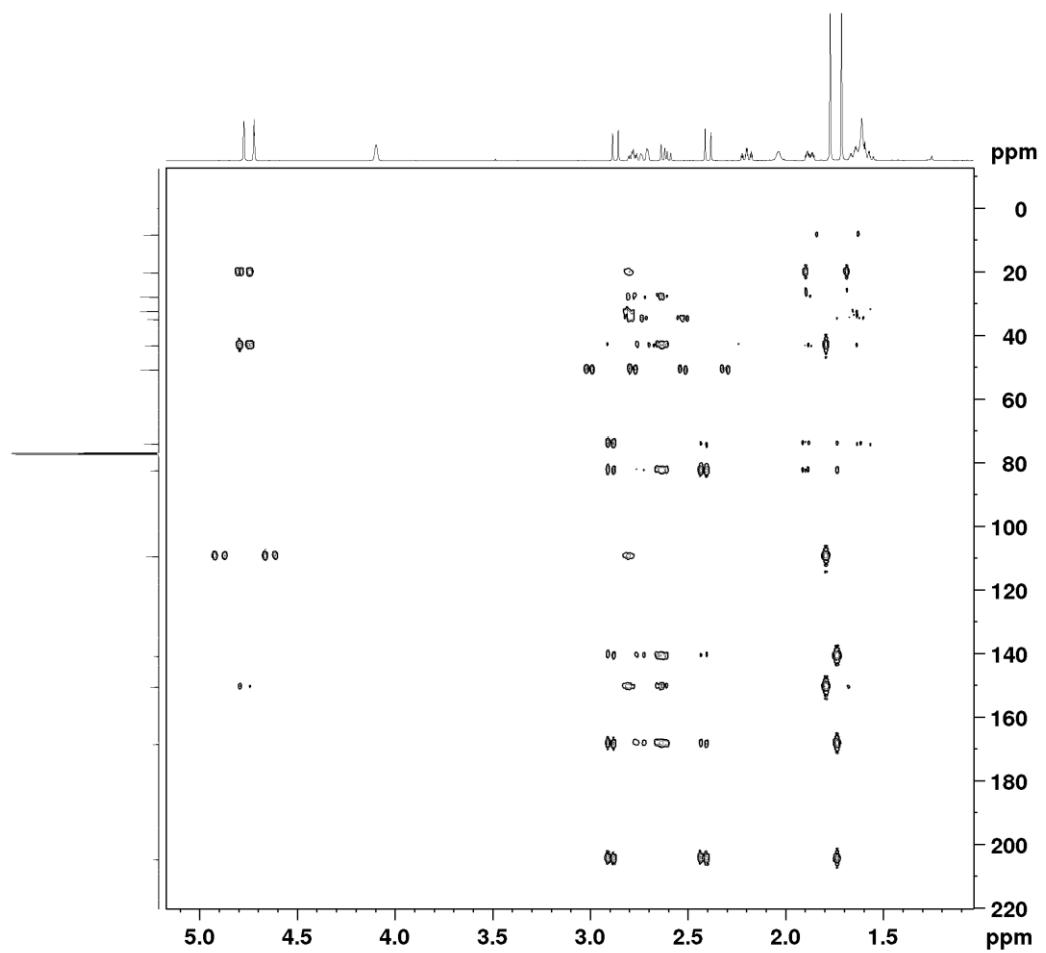


Figure S64 HSQC spectrum (600 MHz, CDCl₃) of compound **10**



Current Data Parameters
NAME RDP-88B
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200830
Time_ 21.33 h
INSTRUM spect
PROBHD Z150290_0006 (bruker)
PULPROG hmbcgrndqf
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 130
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.0000000

D0 0.0000350 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001270 sec
TDav 1
SF01 600.2024000 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLN1 17.23500061 W
SF02 150.9370113 MHz
NUC2 13C
P3 10.00 usec
PLN2 31.21899986 W
GPNAME[1] SNSQ10.100
GPZ1 50.00 %
GPNAME[2] SNSQ10.100
GPZ2 30.00 %
GPNAME[3] SNSQ10.100
GPZ3 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.9370113 MHz
FIDRES 615.157471 Hz
SW 260.838 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S65 HMBC spectrum (600 MHz, CDCl_3) of compound **10**

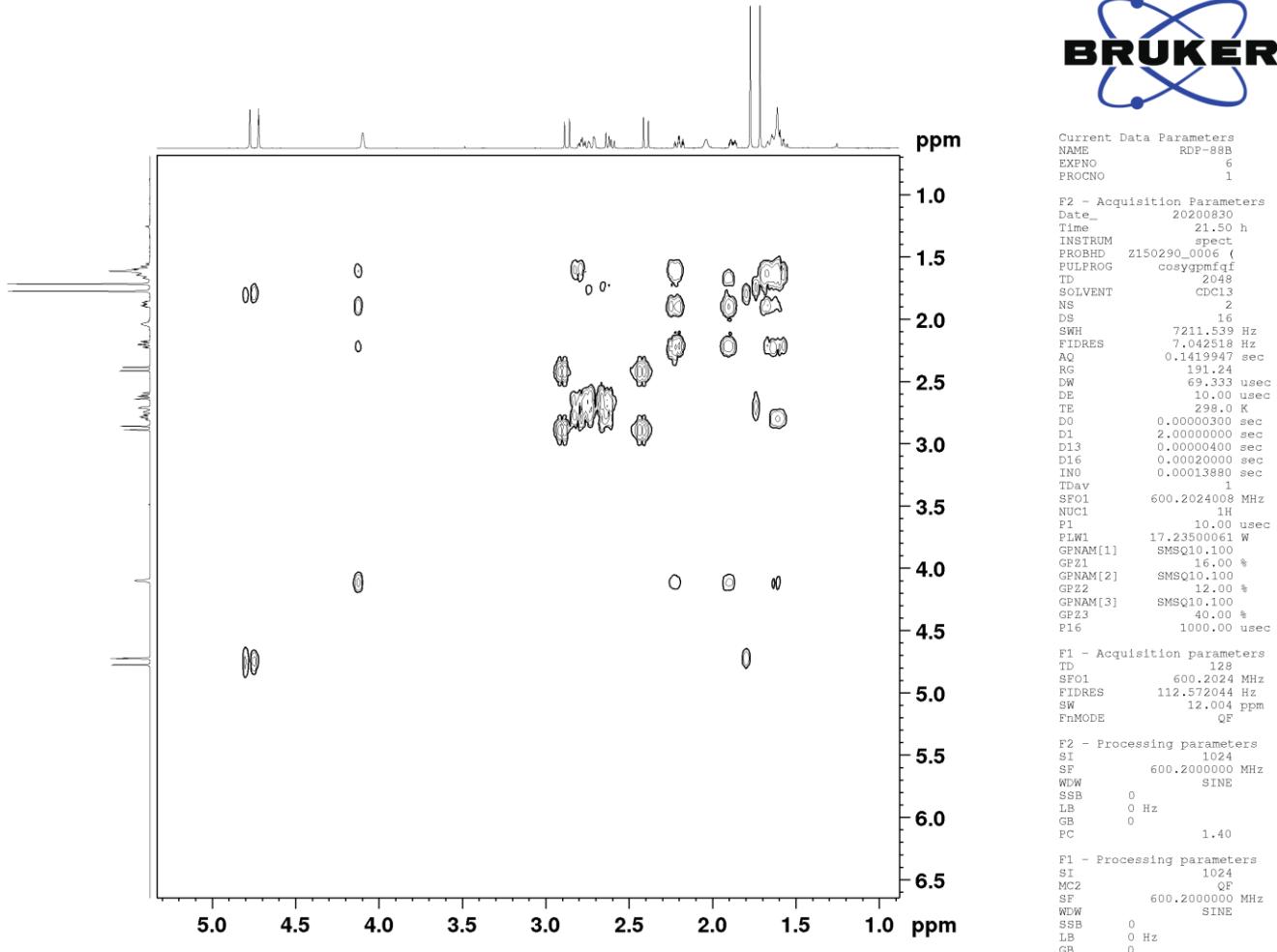
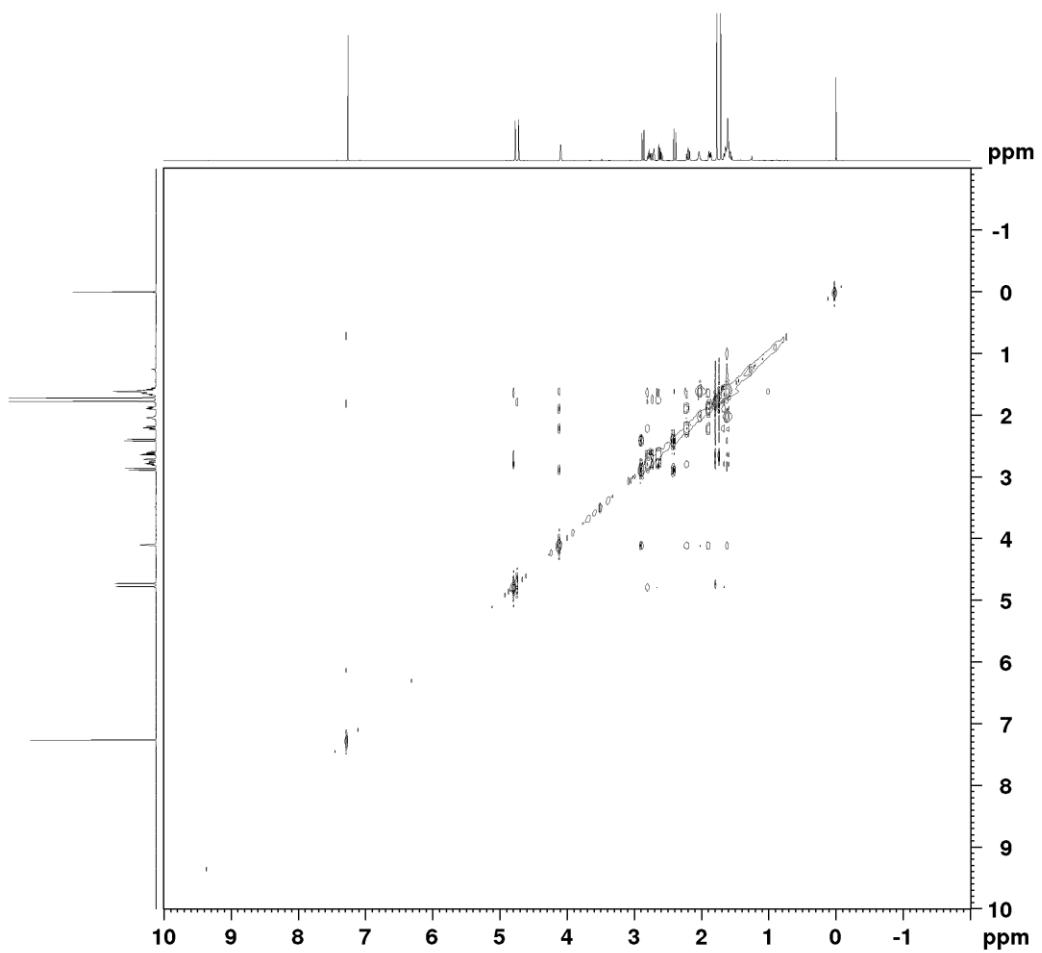


Figure S66 ¹H-¹H COSY spectrum (600 MHz, CDCl₃) of compound **10**



Current Data Parameters
NAME RDP-66B
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200830
Time 22.00 h
INSTRUM spect
PROBHD Z150290_006.i
PULFRCG noeipypphph
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60
DW 69.333 usec
DB 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.0001389 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
M22 States-TPPI
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S67 NOESY spectrum (600 MHz, CDCl₃) of compound **10**

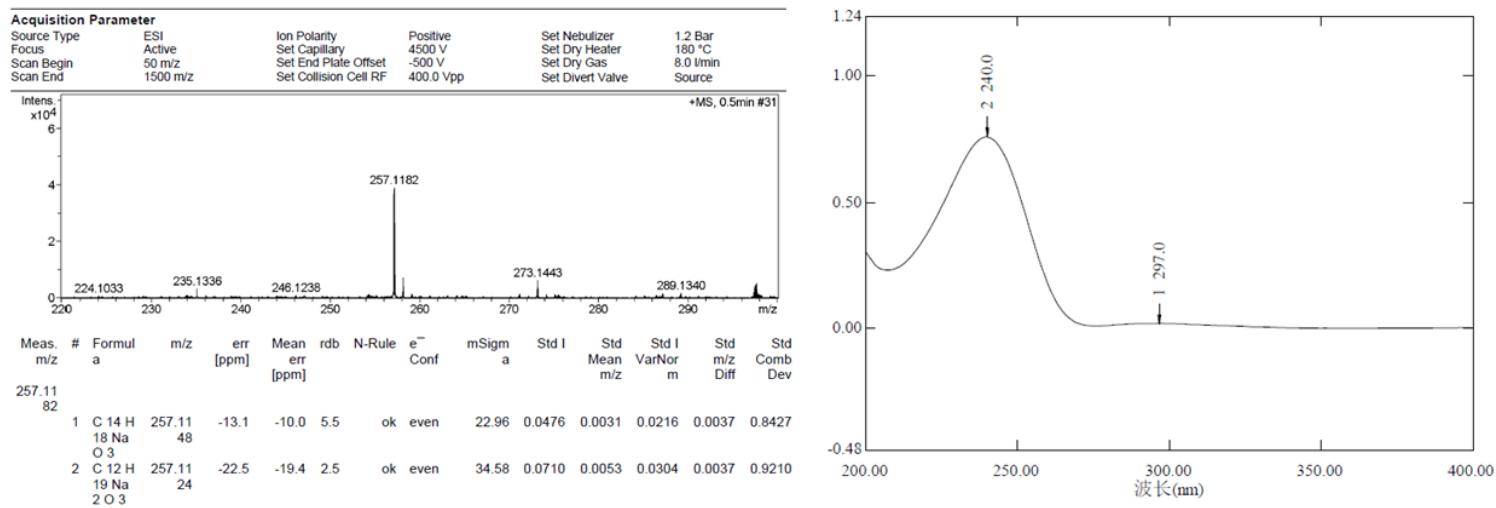


Figure S68 HRESIMS and UV spectra of compound **11**

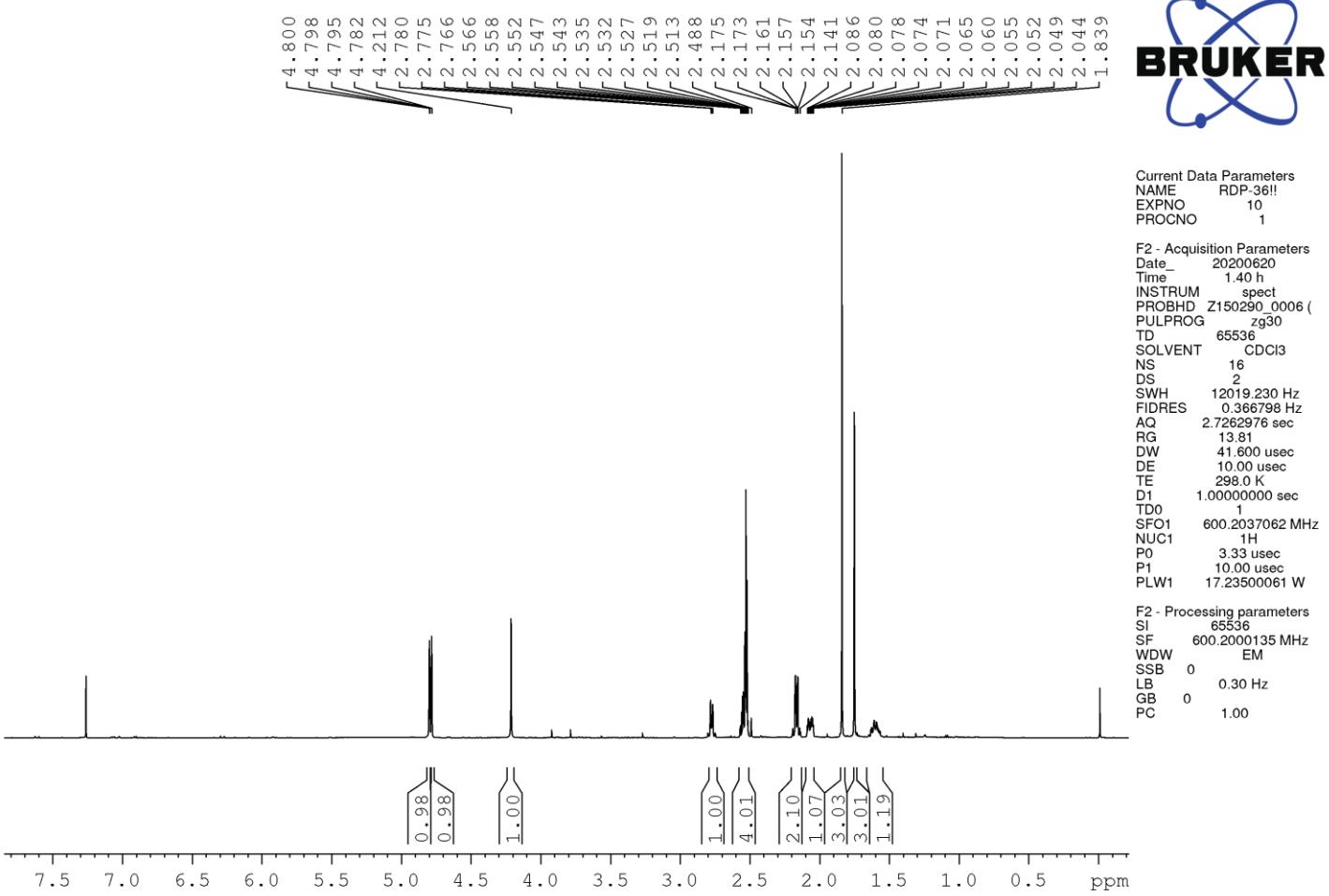
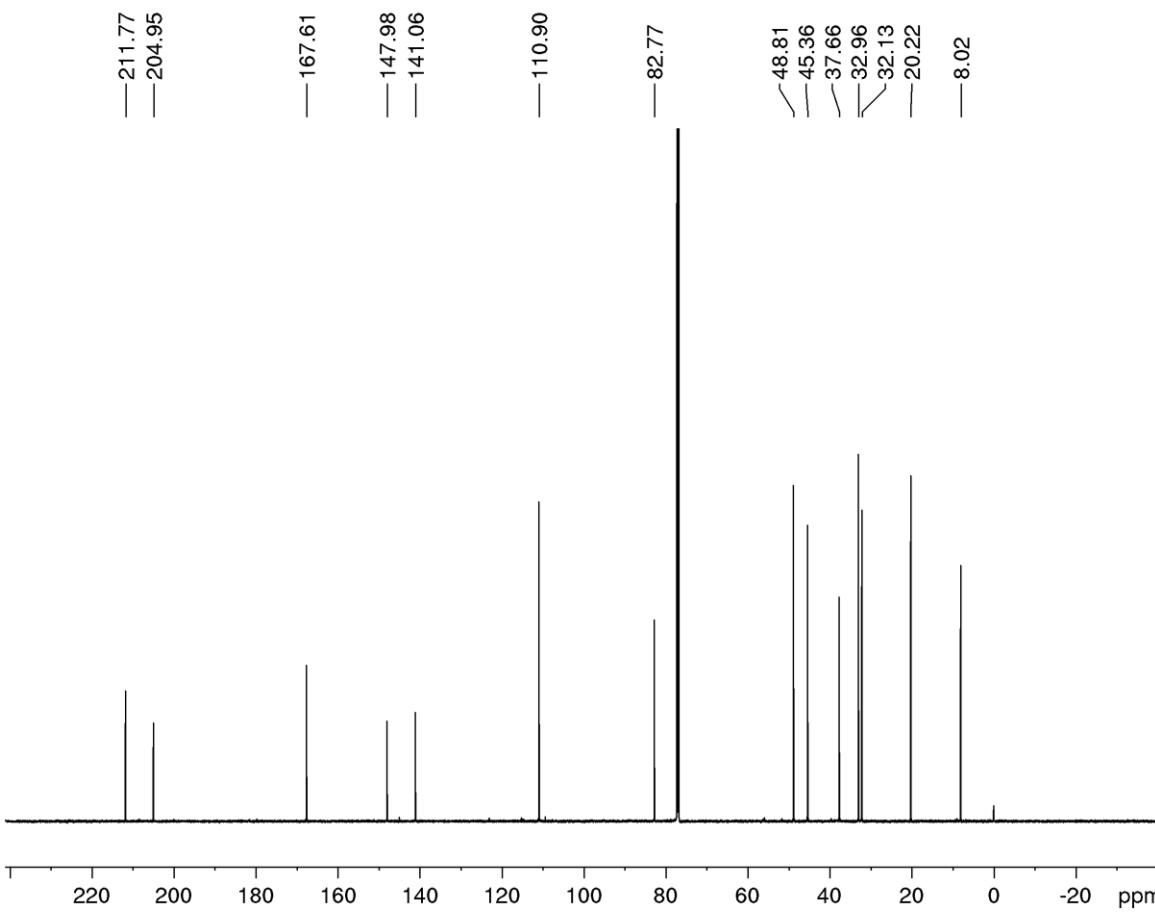


Figure S69 ¹H NMR spectrum (600 MHz, CDCl₃) of compound **11**



Current Data Parameters
NAME RDP-36!!
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200620
Time_ 1.50 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgpg30
TD 65356
SOLVENT CDCl₃
NS 200
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 17.53
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 ¹³C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 ¹H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9204100 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S70 ^{13}C NMR spectrum (150 MHz, CDCl₃) of compound 11

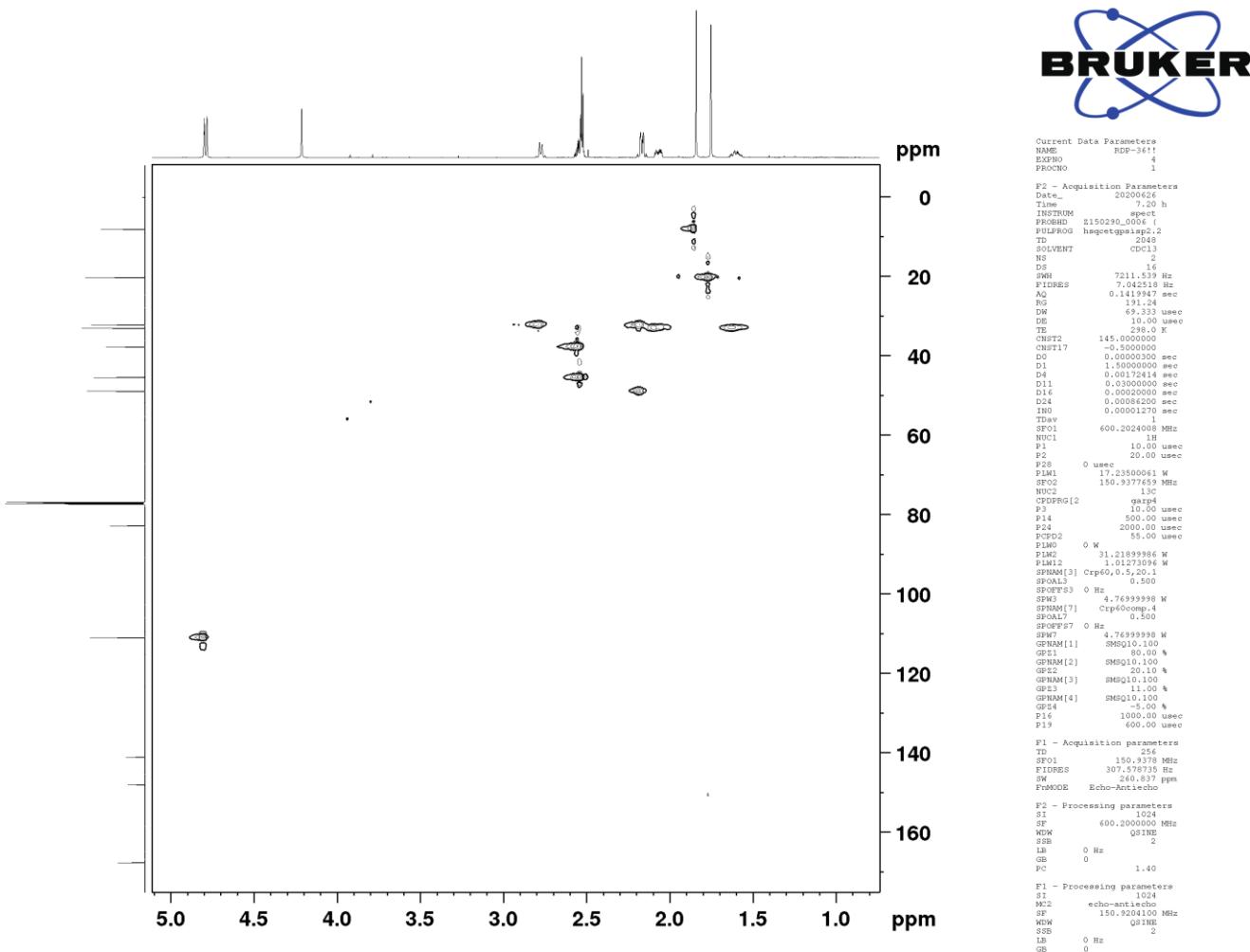
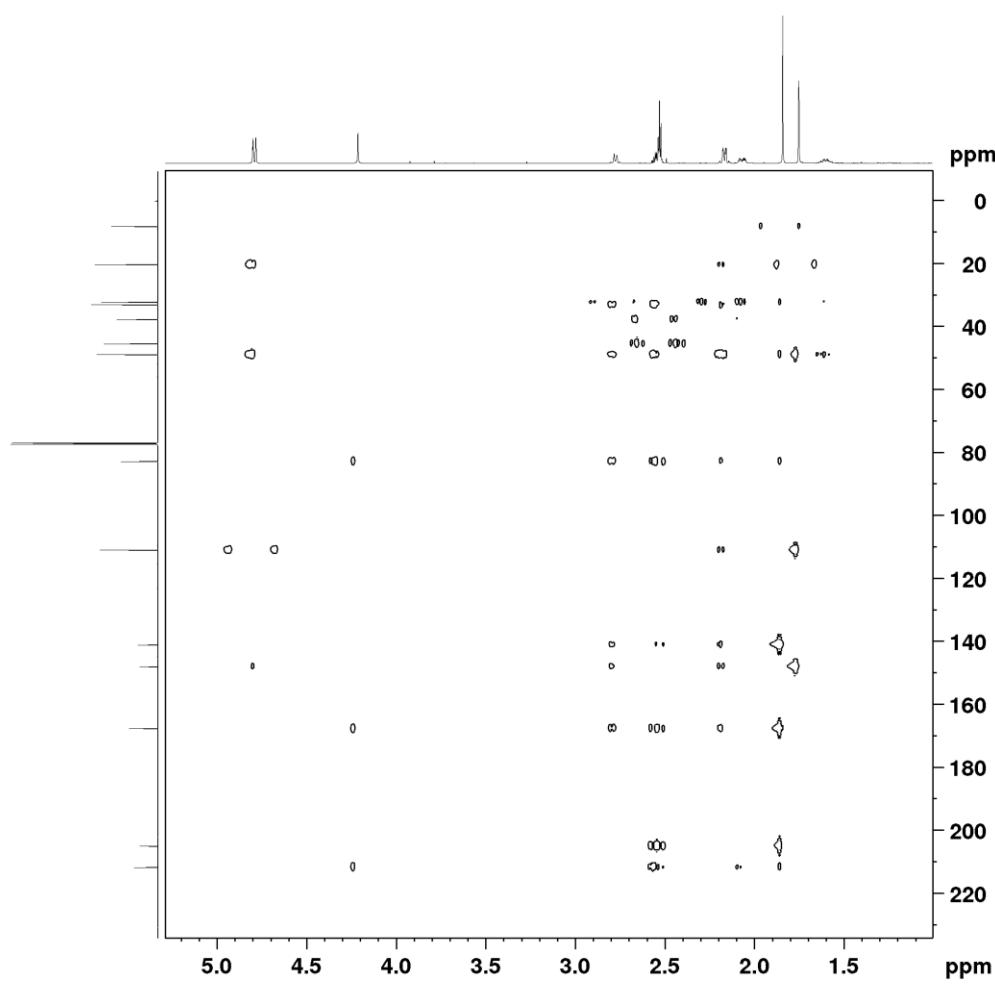


Figure S71 HSQC spectrum (600 MHz, CDCl₃) of compound 11



Current Data Parameters
NAME RDP-361
EXPNO 5
PROCNO 1

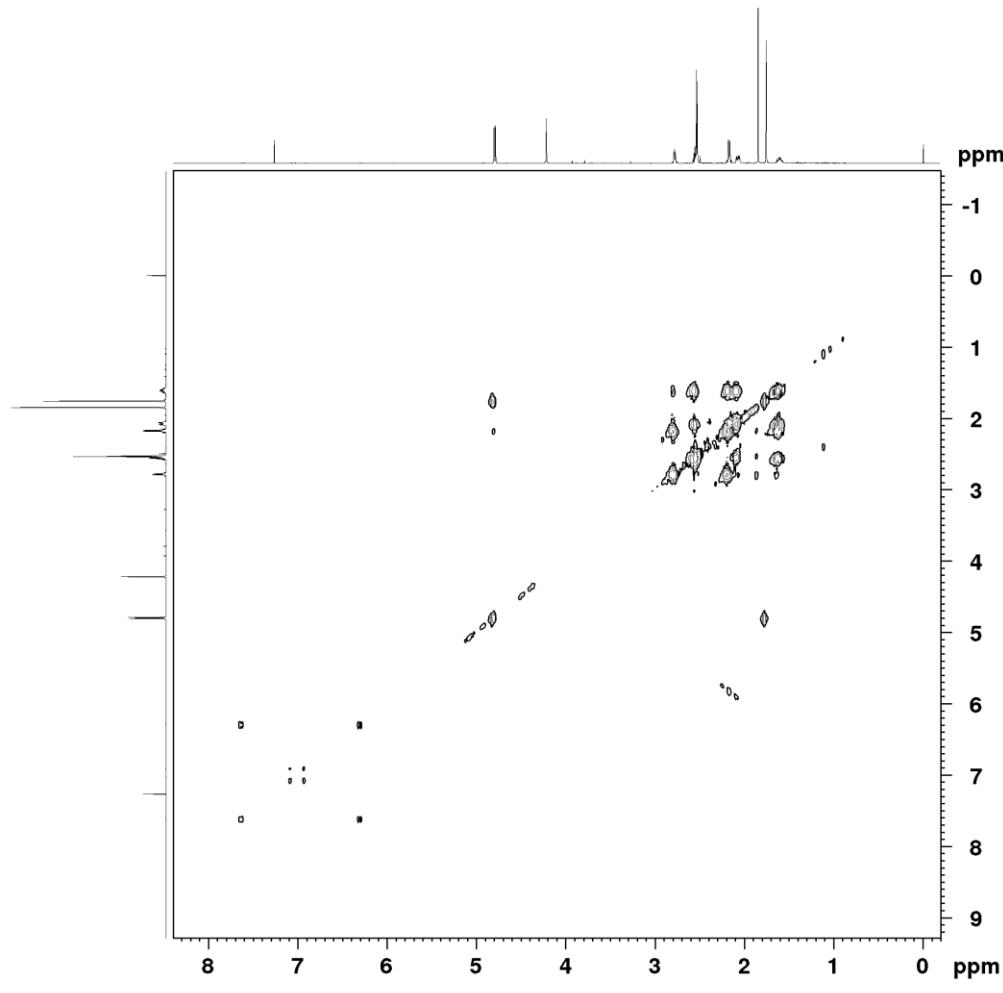
F2 - Acquisition Parameters
Date_ 20200626
Time 7.35 h
INSTRUM spect
PROBID Z150290_0001
PULPROG hmbcogn4prf
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 131.224
DW 69.433 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.000000
D0 0.00000300 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
DNO 0.00001270 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
SF02 150.9377651 MHz
NUC2 13C
P3 10.00 usec
PLW2 31.2189986 W
GPNAME[1] SMSQ10.100
GP21 50.00 %
GPNAME[2] SMSQ10.100
GP22 30.00 %
GPNAME[3] SMSQ10.100
GP23 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.9378 MHz
FIDRES 615.157471 Hz
SW 260.837 ppm
FhMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S72 HMBC spectrum (600 MHz, CDCl_3) of compound 11



BRUKER

```

Current Data Parameters
NAME RDP-36!_
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200626
Time_ 7.53 h
INSTRUM spect
PROBHD Z150290_0006 ( 
PULPROG cosygpmf
TD 2048
SOLVENT CDC13
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 0.742518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 10.00 usec
TE 299.0 K
D0 0.0000030 sec
D1 2.0000000 sec
D13 0.0000040 sec
D16 0.00002000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024000 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.00
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

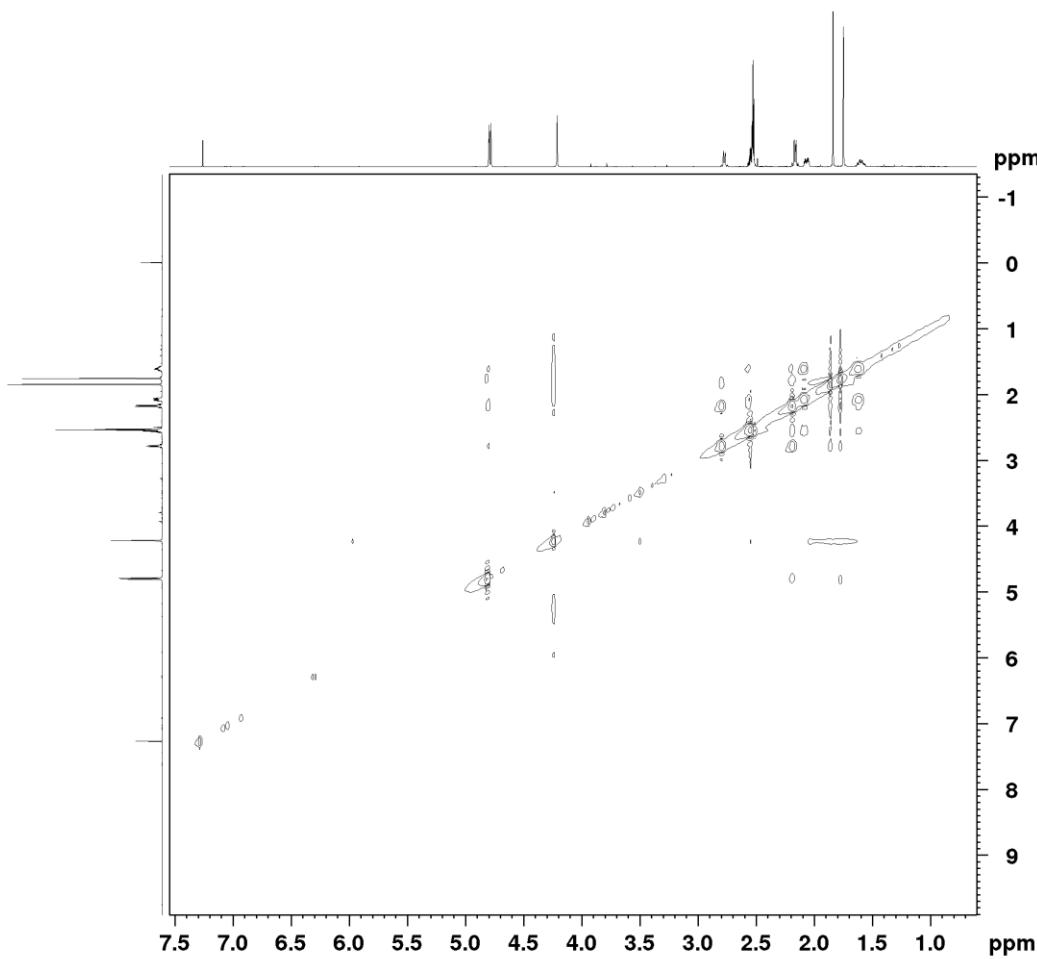
F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

```

Figure S73 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **11**



Current Data Parameters
NAME RDP-361!
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200626
Time 8.03 h
INSTRUM spect
PROBHD Z150290_0066_1
PULPROG noe3sypphp
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.0001389 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S74 NOESY spectrum (600 MHz, CDCl_3) of compound 11

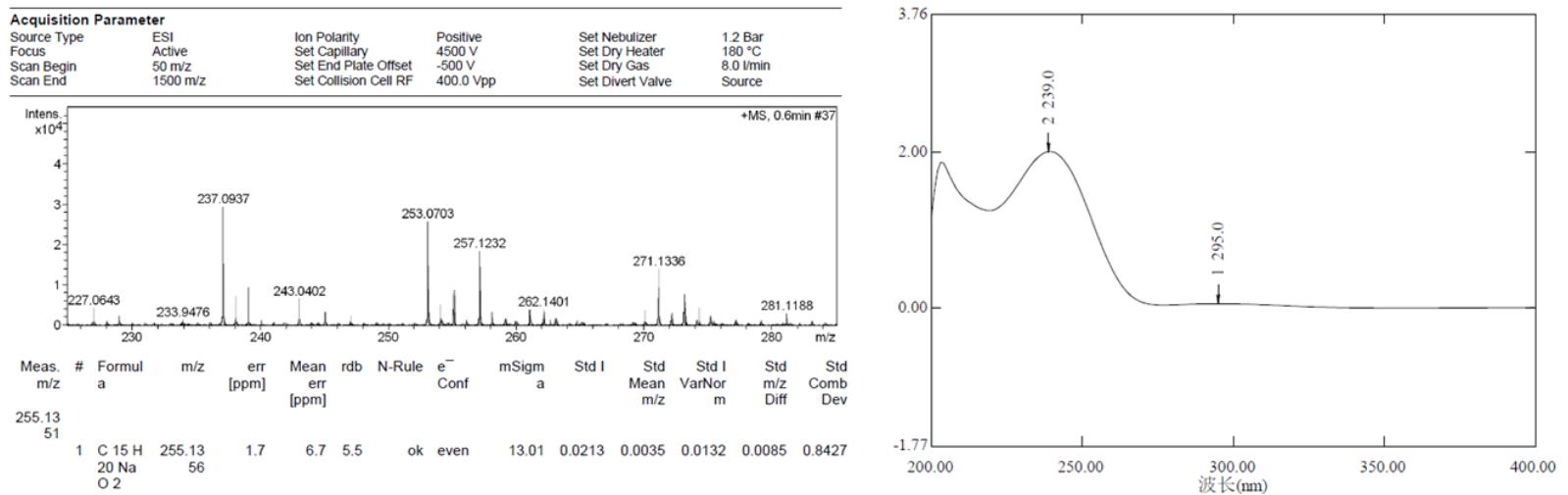


Figure S75 HRESIMS and UV spectra of compound **12**

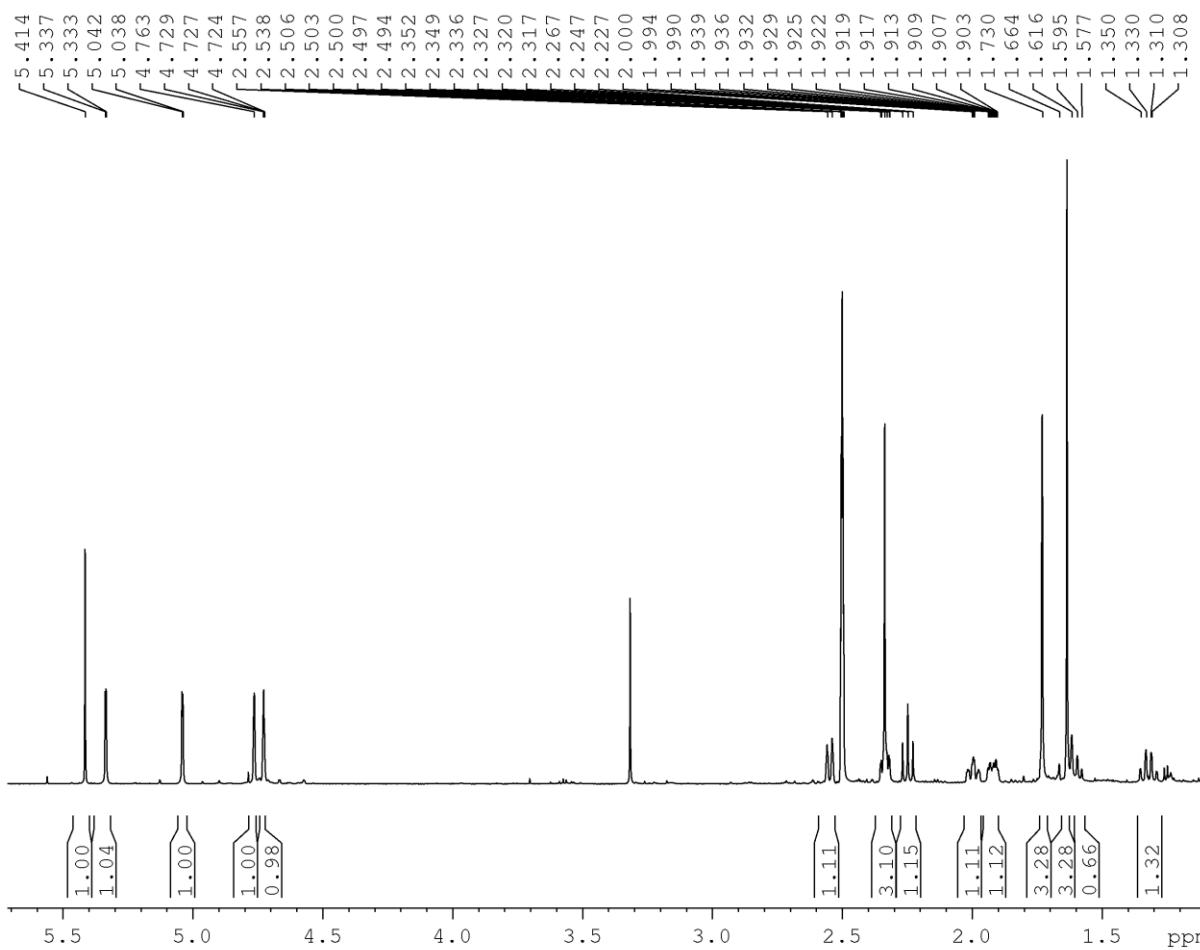
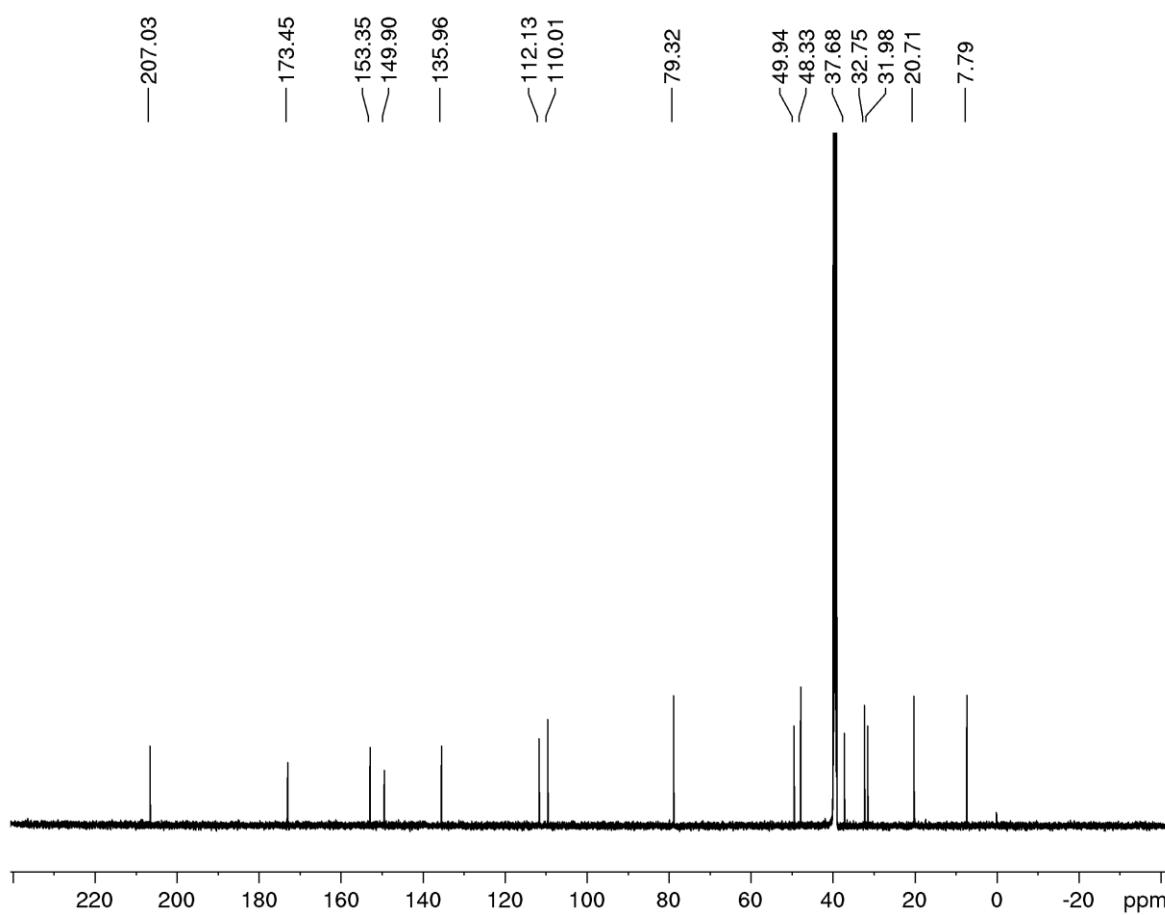


Figure S76 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **12**



Current Data Parameters
NAME RDP-16!!
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20200328
Time 6.03 h
INSTRUM spect
PROBHD Z816801_0163 (
PULPROG zgpg30
TD 65356
SOLVENT DMSO
NS 10000
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 75.38
DW 11.733 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 ¹³C
P0 4.00 usec
P1 12.00 usec
PLW1 194.77999878 W
SFO2 600.2024008 MHz
NUC2 ¹H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 5.44000006 W
PLW12 0.12240000 W
PLW13 0.08041300 W

F2 - Processing parameters
SI 32768
SF 150.9204823 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S77 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **12**

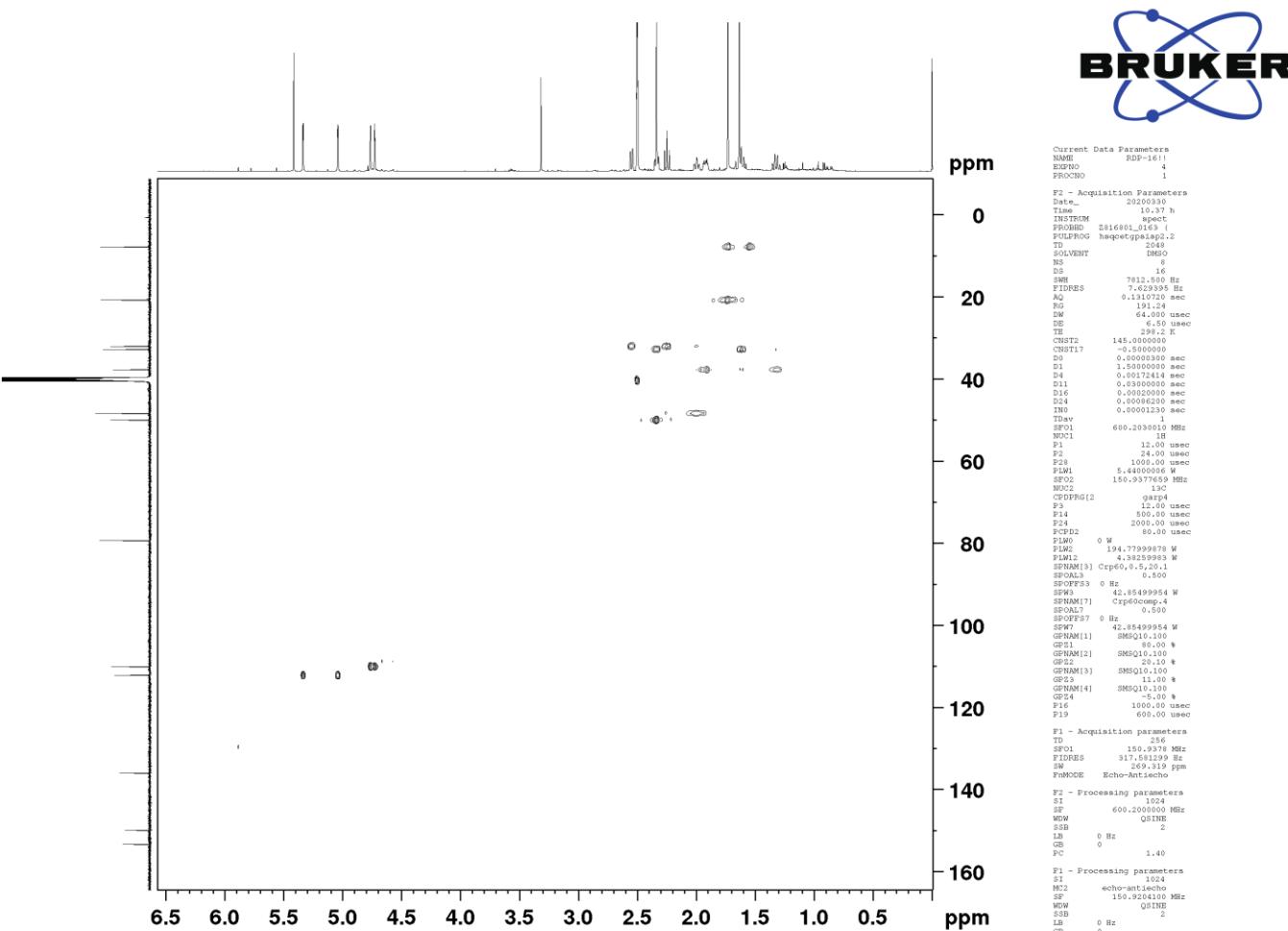


Figure S78 HSQC spectrum (600 MHz, CDCl₃) of compound 12

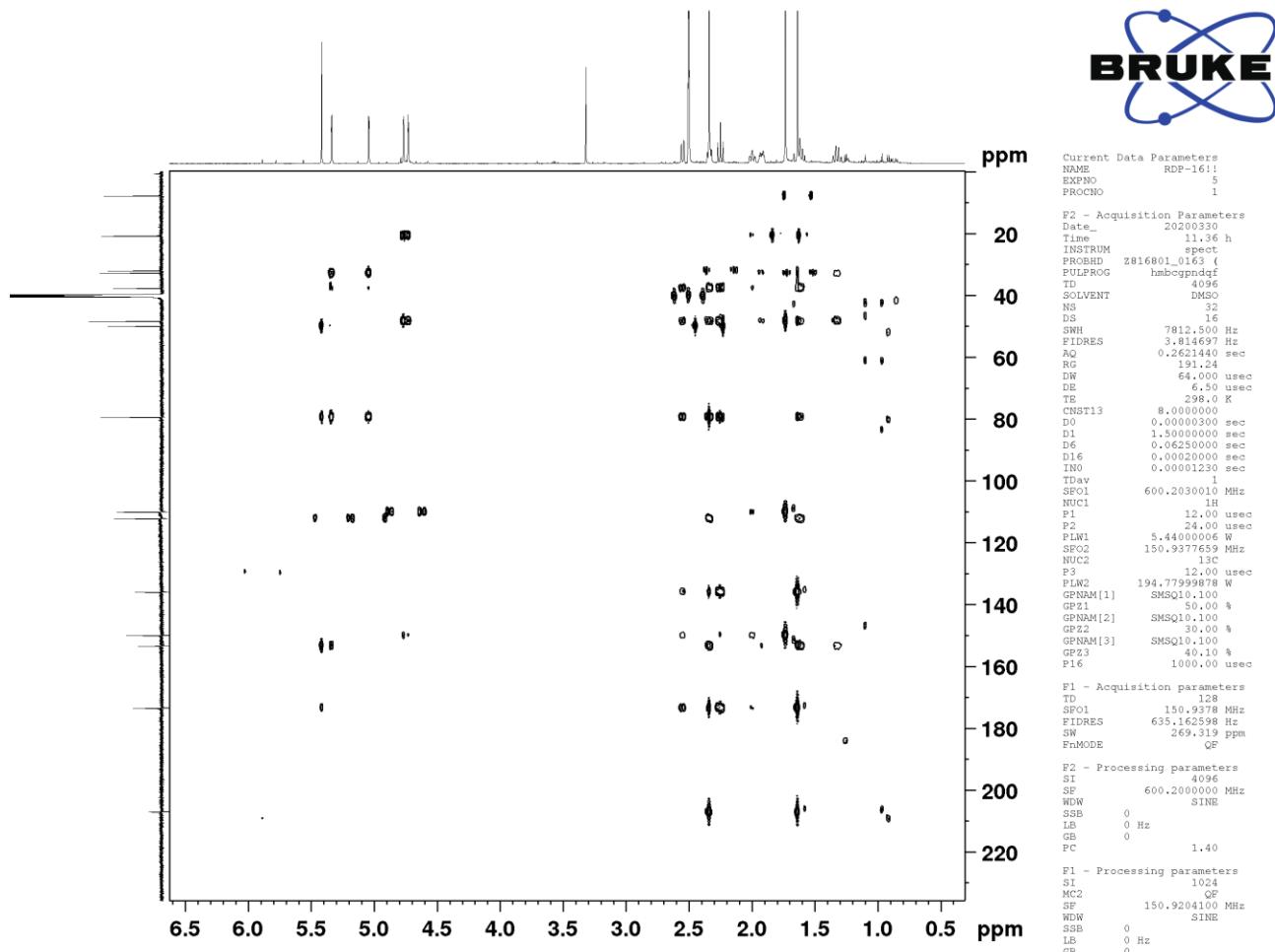
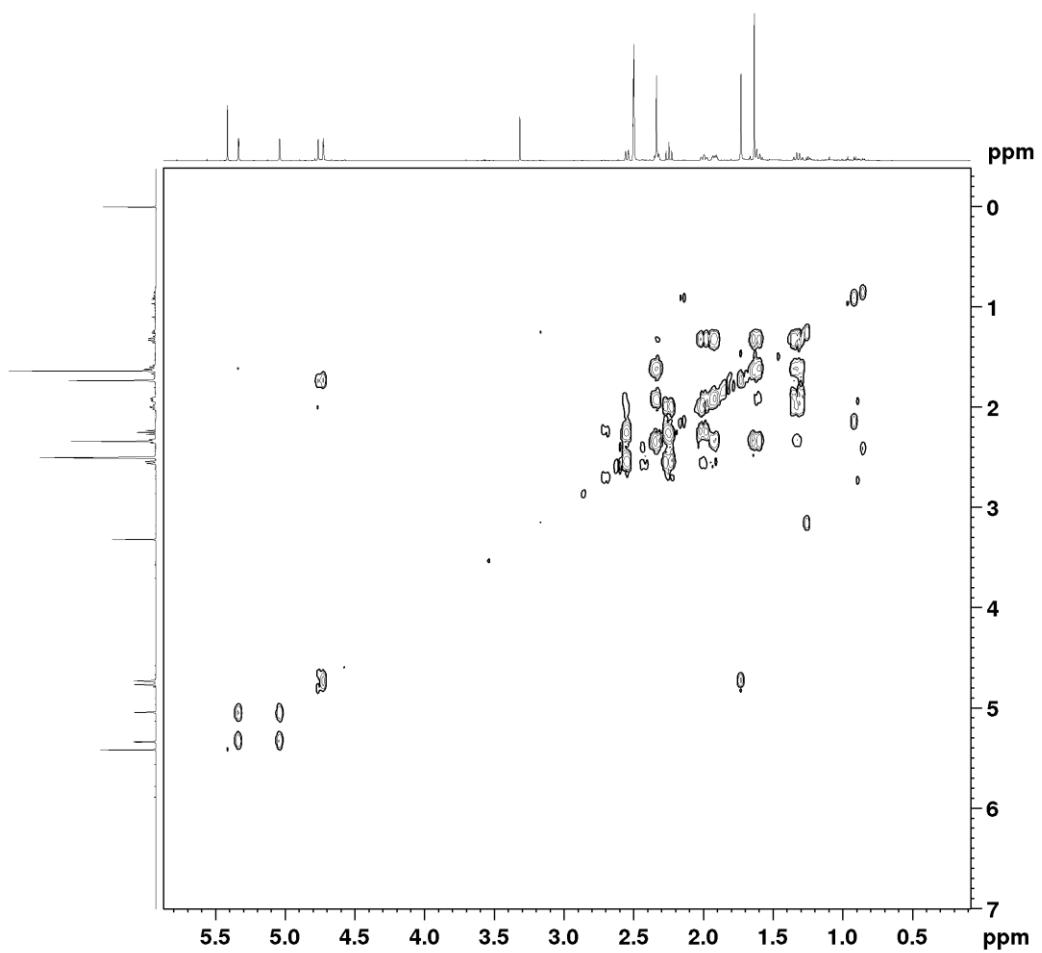


Figure S79 HMBC spectrum (600 MHz, CDCl₃) of compound **12**



Current Data Parameters
NAME RDE-161!
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200330
Time 13.42 h
INSTRUM spect
PROBHD Z816801_0163 (
PULPROG cosygppmfd
TD 2048
SOLVENT DMSO
NS 16
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 191.24
DW 64.000 usec
DE 6.50 usec
TE 296.760 K
D0 0.00000300 sec
D1 2.0000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00012800 sec
TDav 1
SF01 600.2030010 MHz
NUC1 1H
P1 12.00 usec
PLW1 5.4400006 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.203 MHz
FIDRES 122.070313 Hz
SW 13.016 ppm
PnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 64
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S80 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **12**

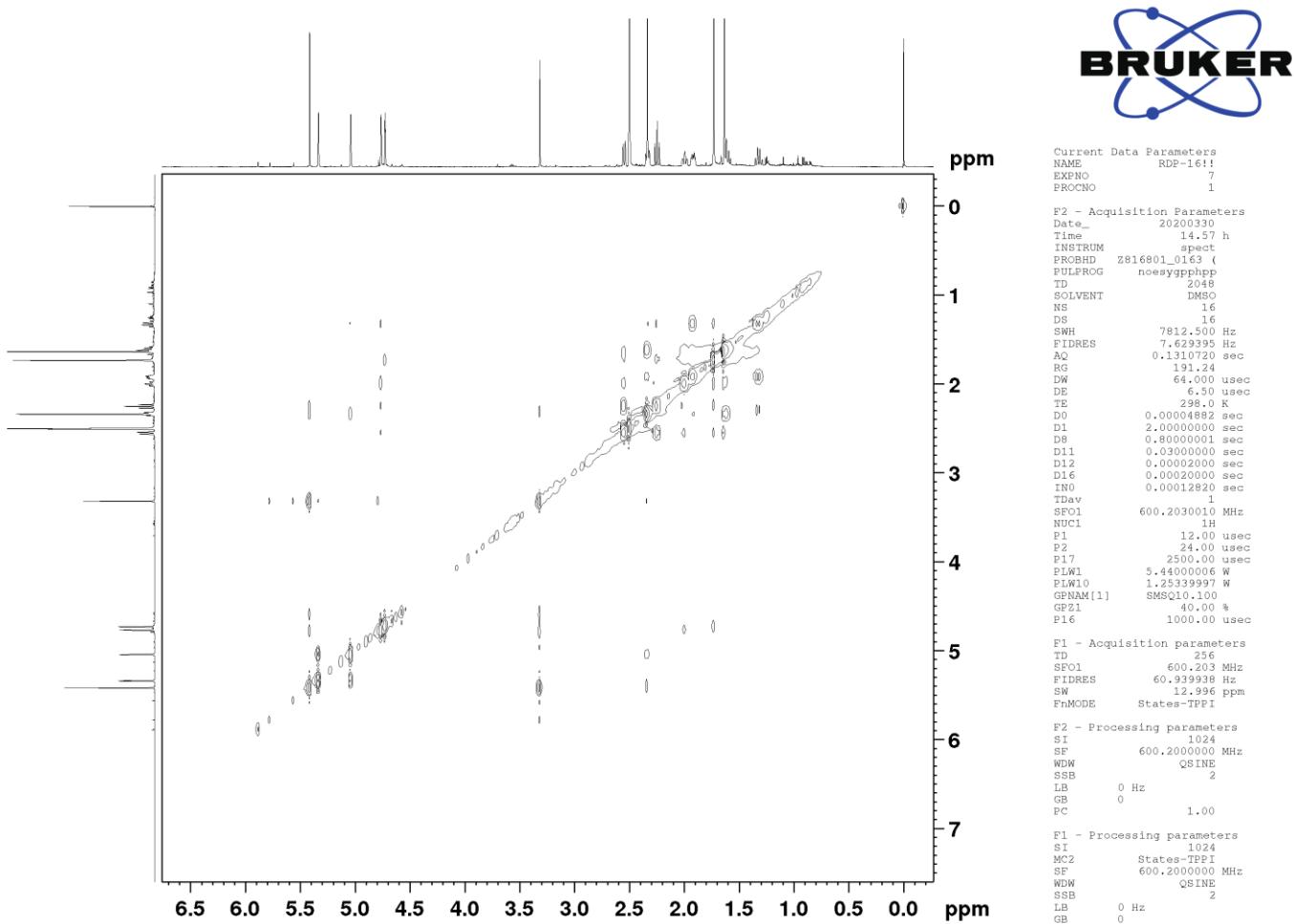


Figure S81 NOESY spectrum (600 MHz, CDCl_3) of compound **12**

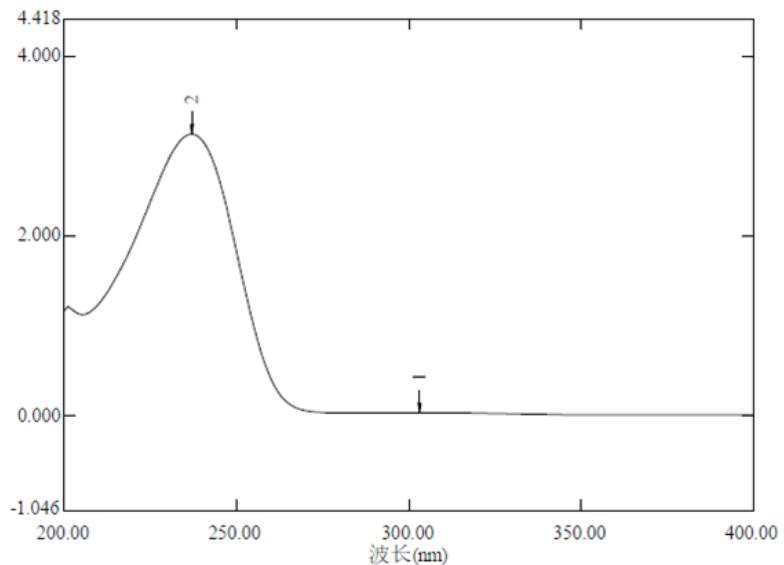
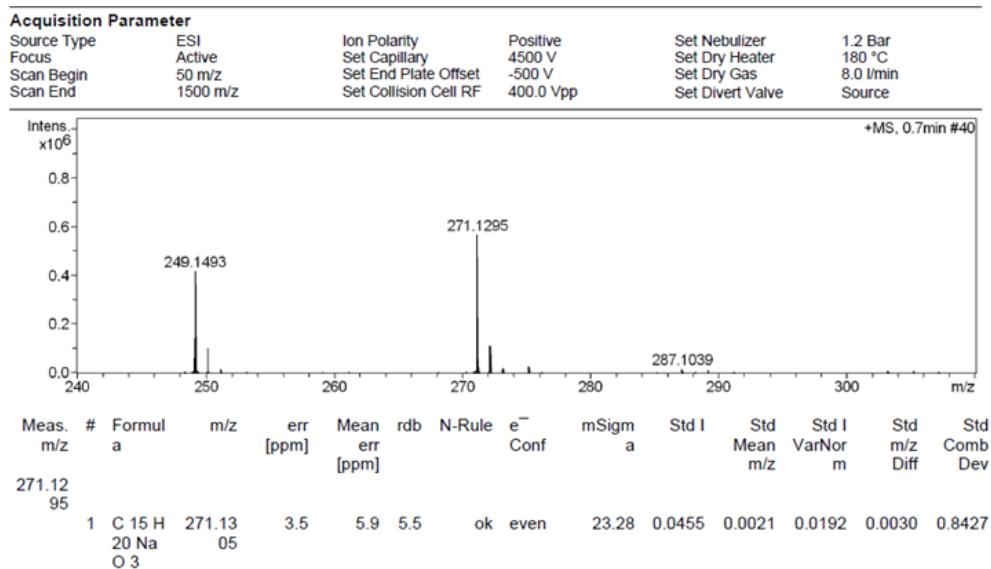


Figure S82 HRESIMS and UV spectra of compound **13**

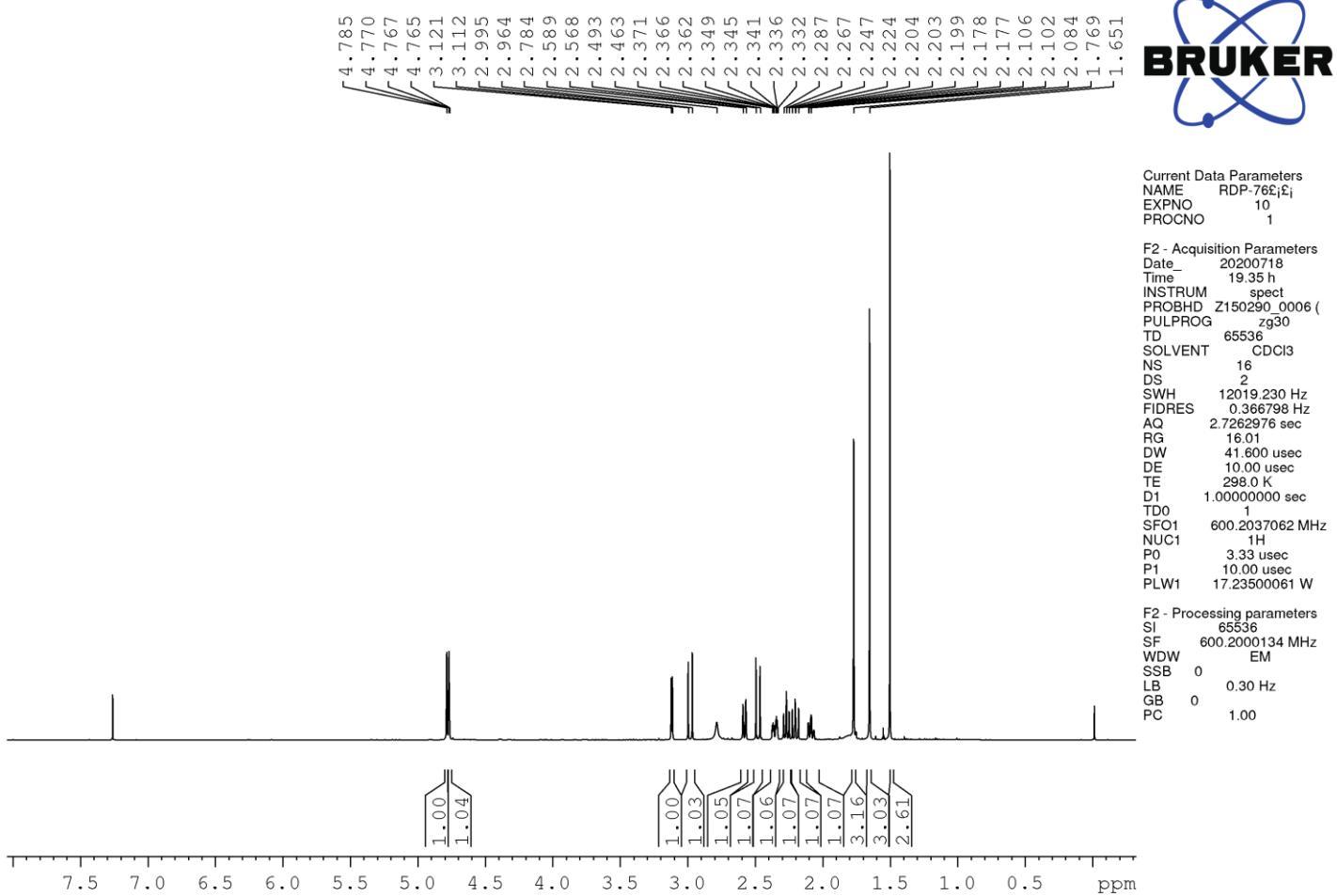
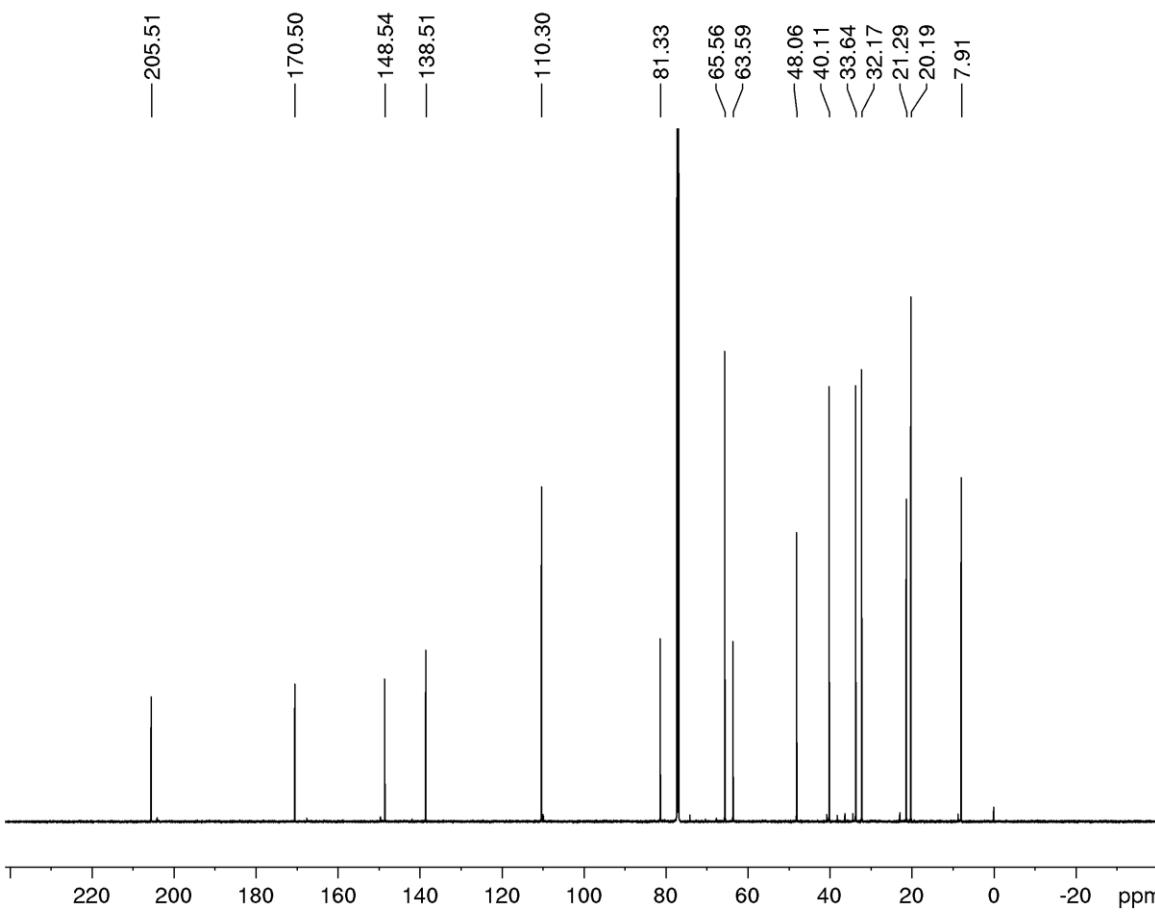


Figure S83 ¹H NMR spectrum (600 MHz, CDCl₃) of compound **13**



Current Data Parameters
NAME RDP-76 $\ddot{\Sigma}$
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200718
Time_ 23.32 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgppg30
TD 65356
SOLVENT CDCl3
NS 150
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 37.95
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9204099 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S84 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **13**

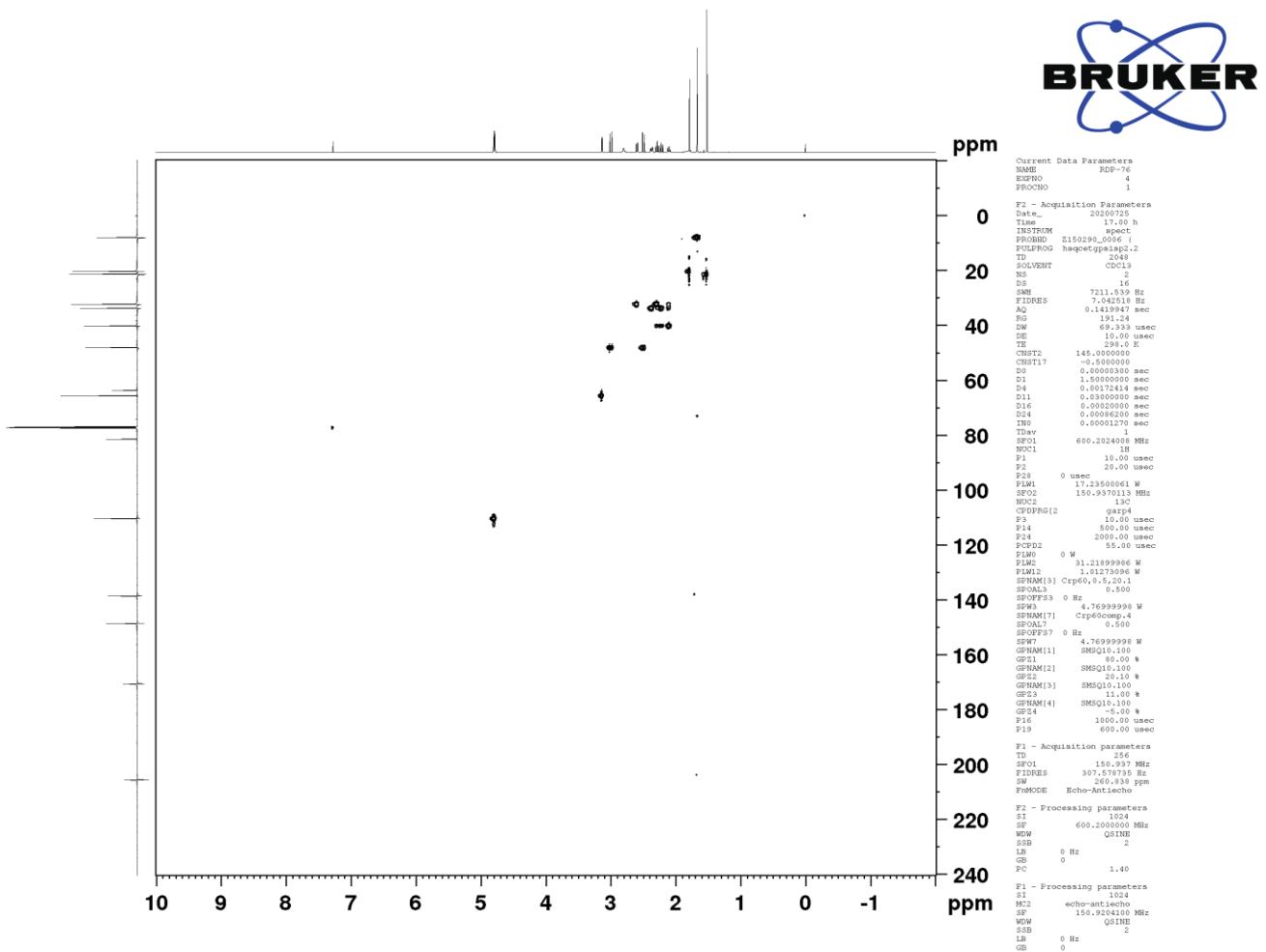


Figure S85 HSQC spectrum (600 MHz, CDCl₃) of compound 13

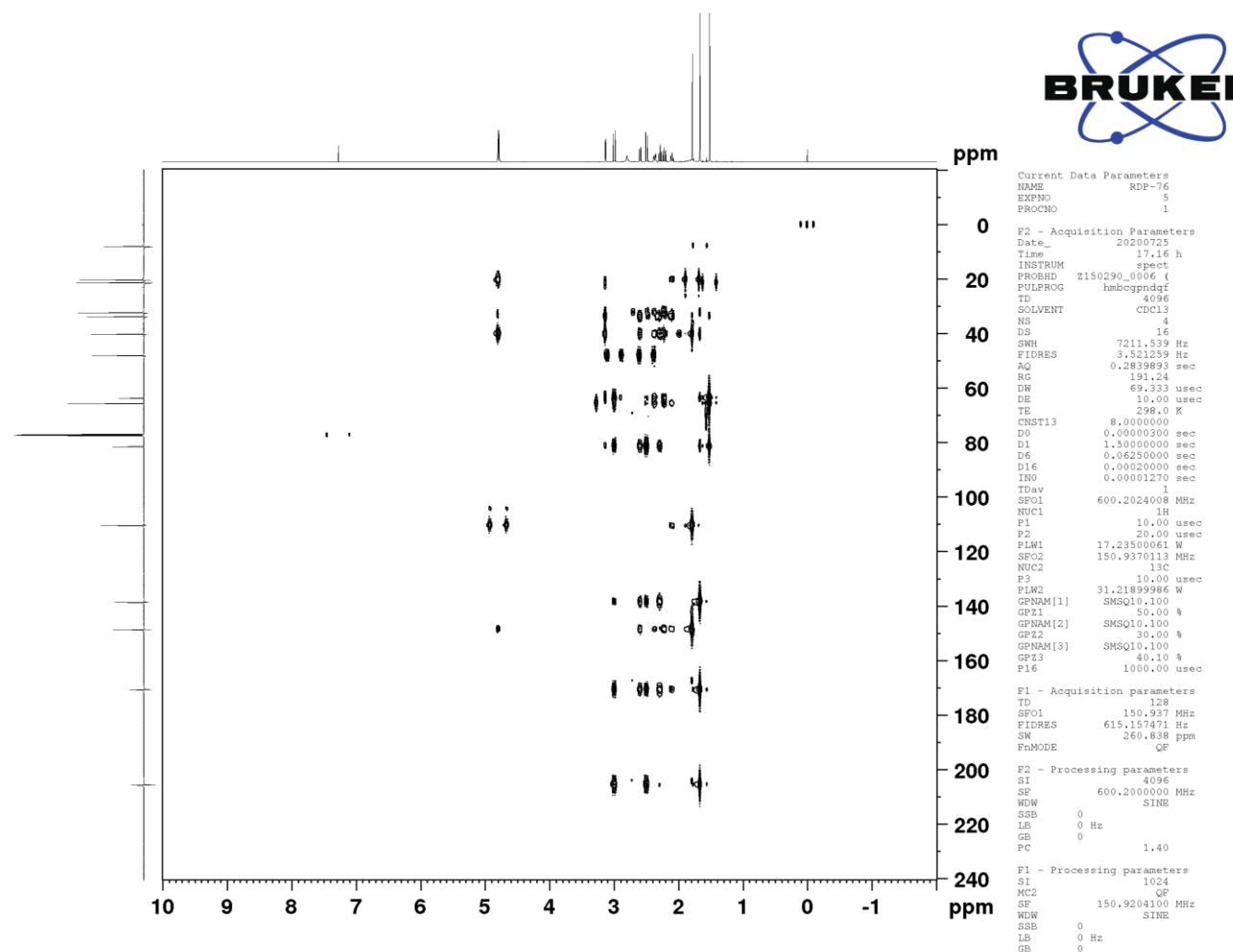


Figure S86 HMBC spectrum (600 MHz, CDCl₃) of compound 13

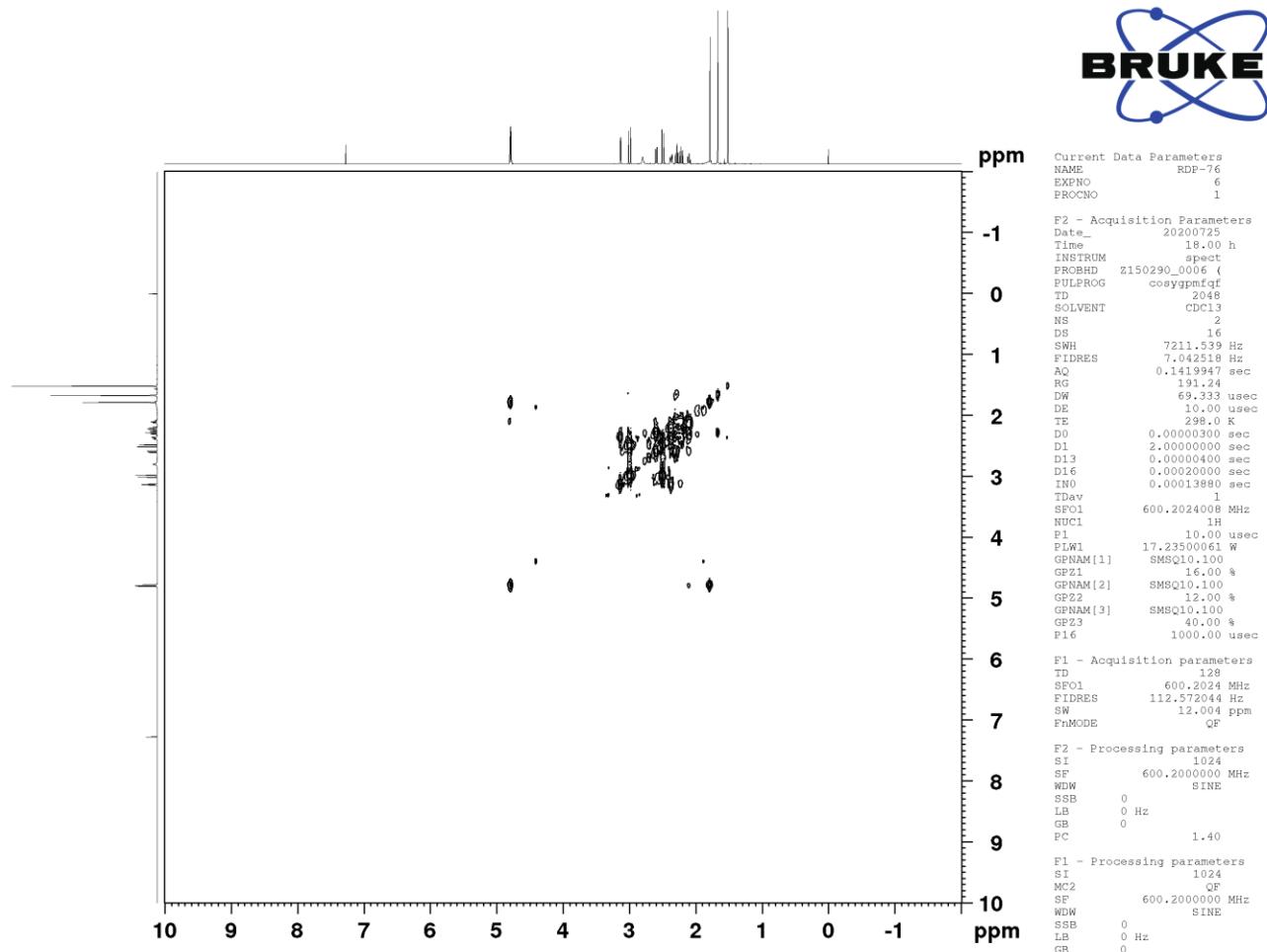


Figure S87 ¹H-¹H COSY spectrum (600 MHz, CDCl₃) of compound 13

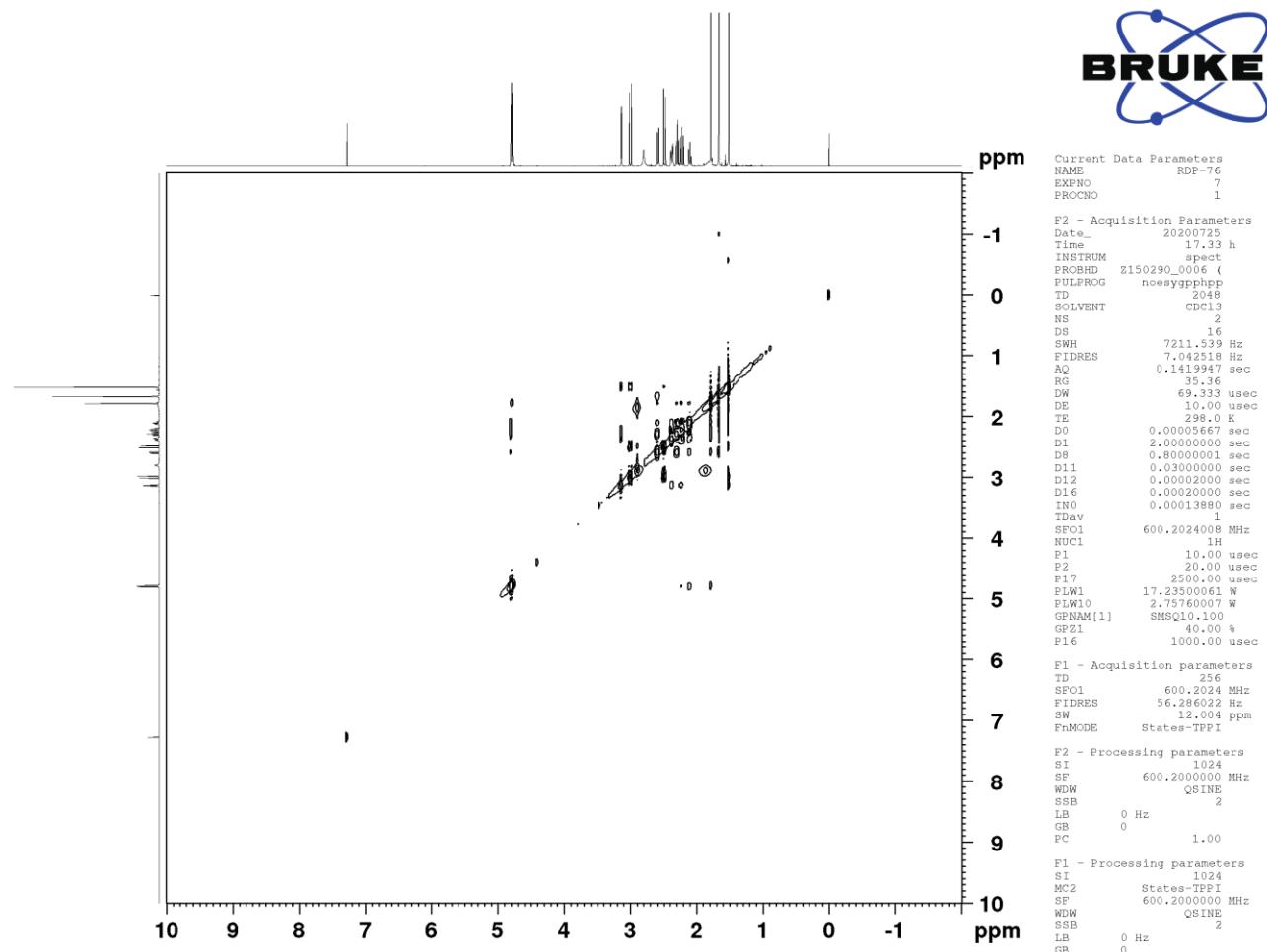


Figure S88 NOESY spectrum (600 MHz, CDCl₃) of compound 13

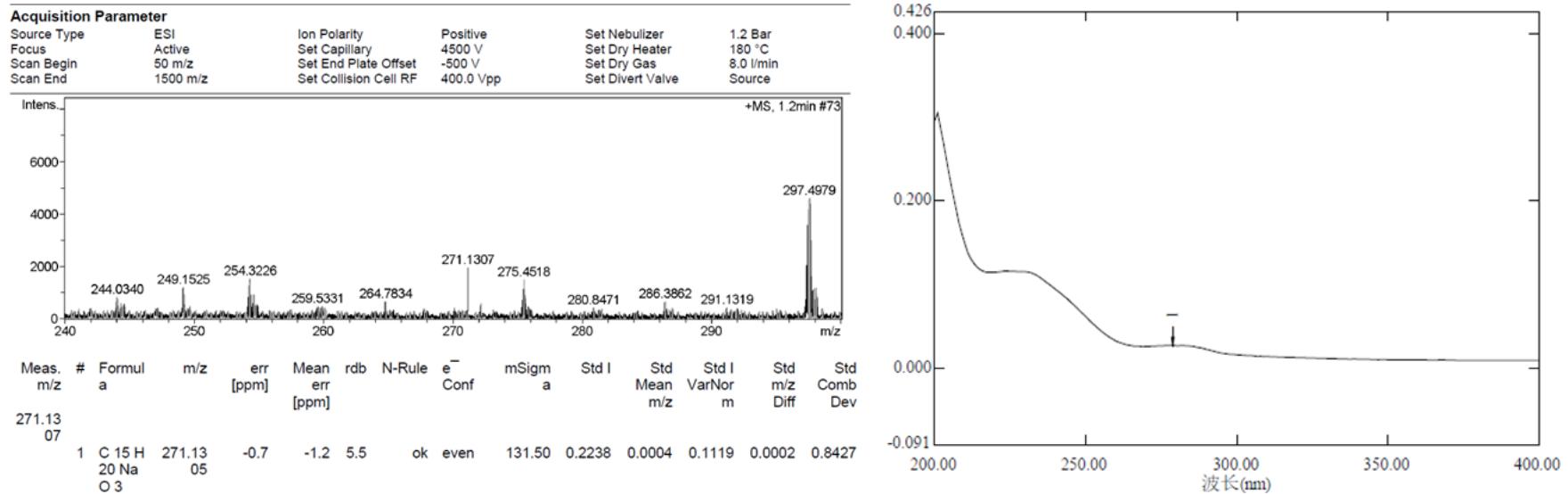


Figure S89 HRESIMS and UV spectra of compound 14

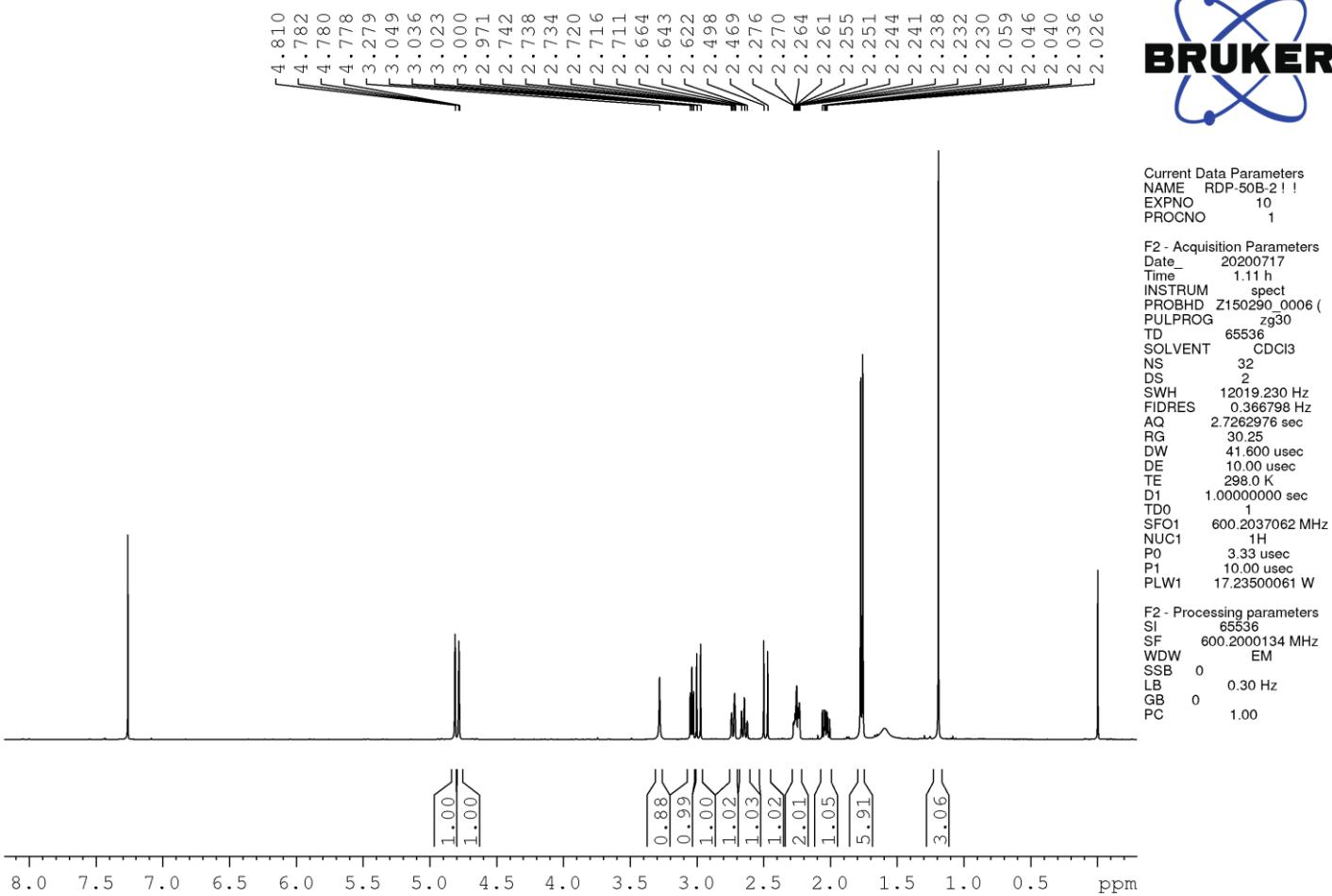


Figure S90 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **14**

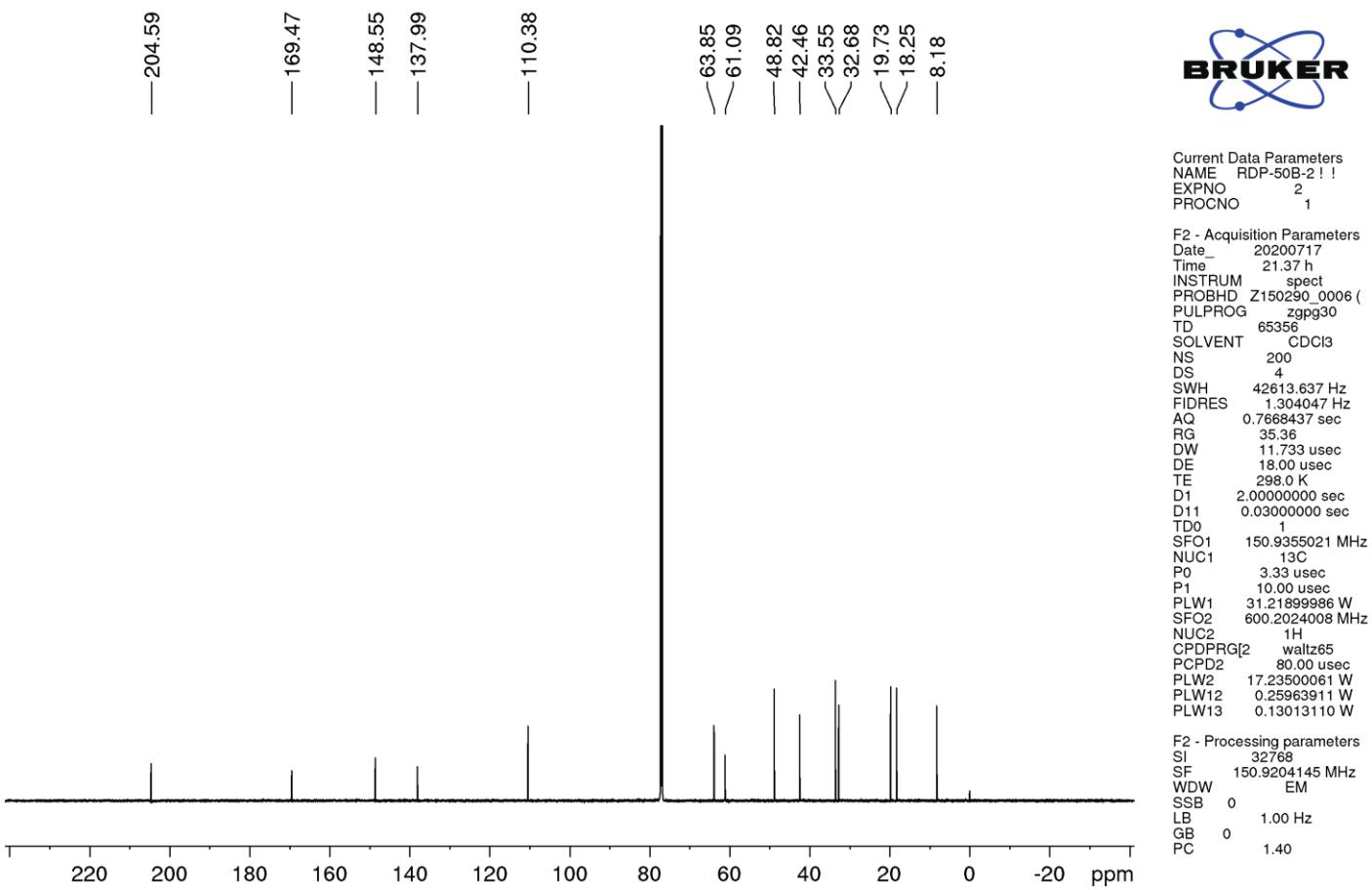
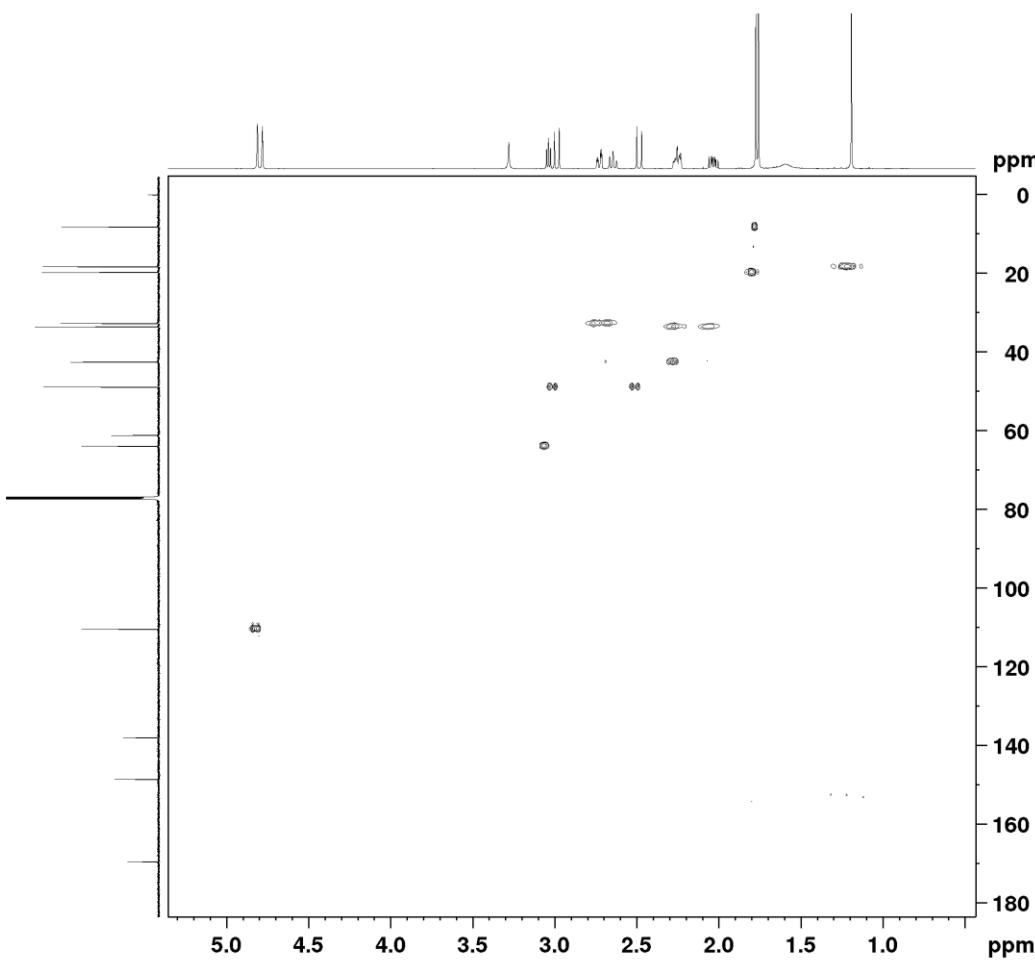


Figure S91 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 14



Current Data Parameters
NAME RDP-50B-2 1
ND 4
PFGNO 1

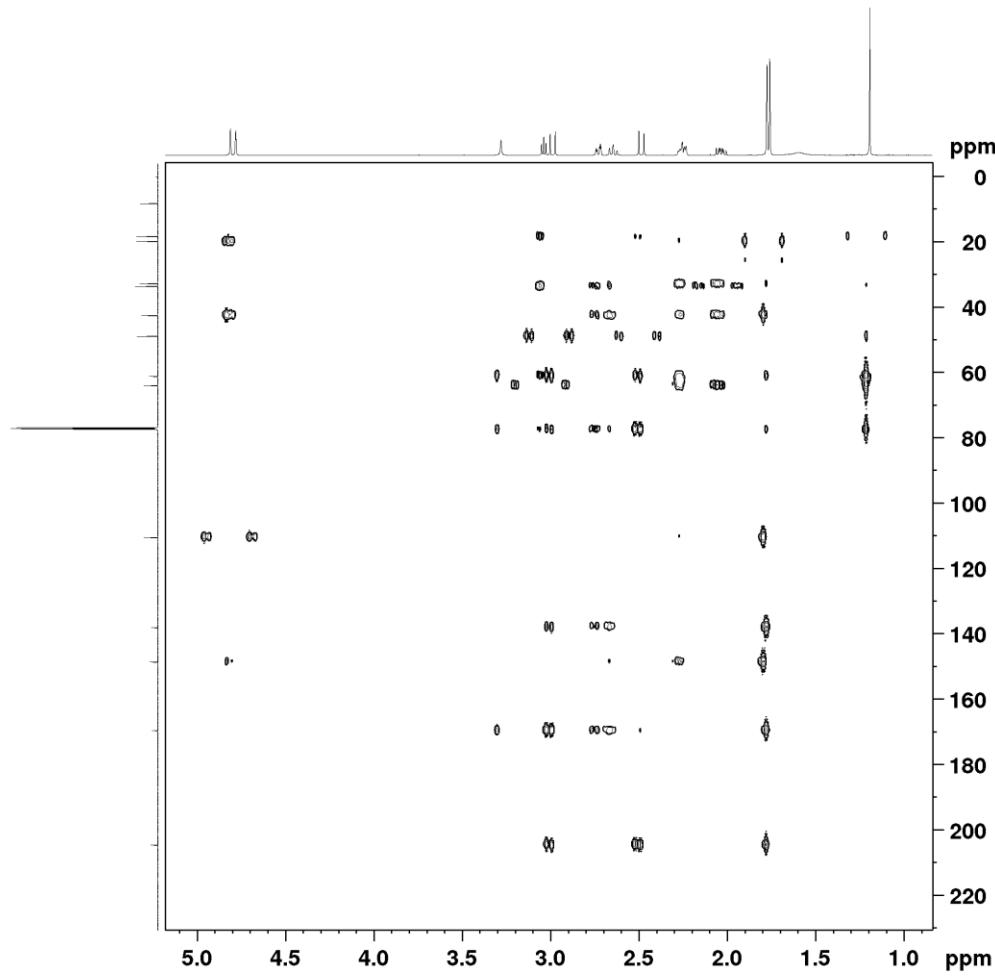
F2 - Acquisition Parameters
Date_ 20200710
Time 19:47 h
INSTRUM spect
PROBHD 1150299_0006 (PULPROG hsqcetgpsp12
TD 65536
SOLVENT CDCl₃
NS 2
DS 16
SWH 7211.539 Hz
ETRATES 7.0493 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.493 usec
DE 10.00 usec
TB 298.0 K
CNUST2 145.000000
CNST17 0.5000000
D0 0.0000300 sec
D1 0.0000000 sec
D4 0.00172414 sec
D11 0.0300000 sec
D16 0.0000000 sec
D24 0.00008200 sec
IRW 0.00001250 sec
TDav 600.2024099 MHz
SF01 150.000000 W
P1 10.00 usec
P2 20.00 usec
P2A 0 usec
PLW1 17.23505061 W
SF02 150.3377659 MHz
M02 0 W
CPDPFGS(2 garp4
P3 10.00 usec
P14 100.00 usec
P24 2000.00 usec
PCTD2 55.00 usec
PLW0 0 W
PLW2 31.21899986 W
PDPFGS(1 10.00 usec
SPNAM[3] Cmso6@4.5,20.1
SPDALS 0.500
SPDPFGS3 0 Hz
SPW1 4.76999999 W
SPNAM[7] Cgs6@comp.4
SPDALS 0.500
SPDPFGS7 0 Hz
SPW7 4.76999998 W
SPNAM[1] SMSQ10.100
GP1 80.00 *
SPNAM[2] SMSQ10.100
GP2 11.00 *
SPNAM[3] SMSQ10.100
GP2 11.00 *
SPNAM[4] SMSQ10.100
GP24 -5.00 *
P16 1000.00 usec
P13 600.00 usec

F1 - Acquisition parameters
TD 256
SF01 150.3375 MHz
ETRATES 31.21899986 Hz
DW 269.319 ppm
PFGMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.20000000 MHz
WGW 0.31333333 Hz
SSB 0 Hz
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.3204100 MHz
WGW 0.31333333 Hz
SSB 0 Hz
LB 0 Hz
GB 0

Figure S92 HSQC spectrum (600 MHz, CDCl₃) of compound 14



Current Data Parameters
NAME RDF-50B-2 !
EXPNO 5
PROCNO 1

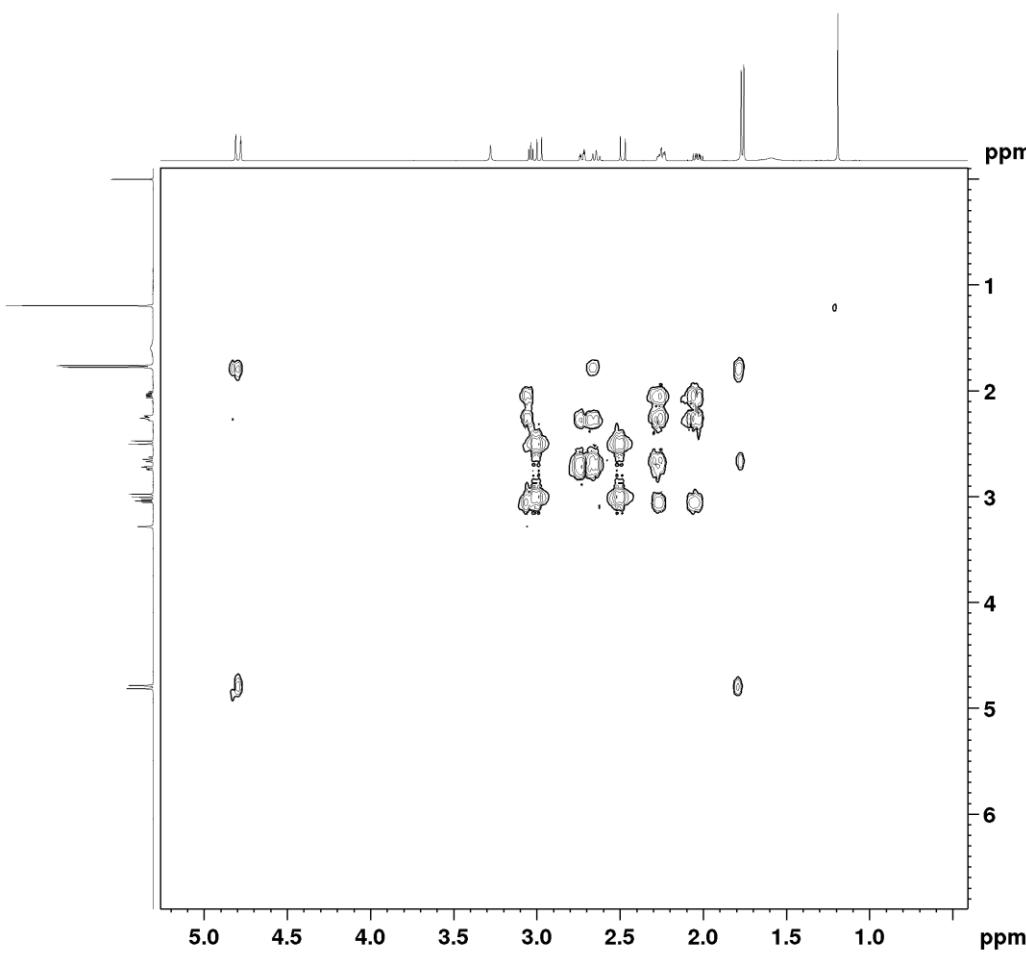
F2 - Acquisition Parameters
Date_ 20200718
Time 20.03 h
INSTRUM spect
PROBID Z150290_0001
PULPROG hmbcogn.dpr
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 131.224
DW 69.433 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.000000
D0 0.00000300 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
DW0 0.00001230 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
SF02 150.9377651 MHz
NUC2 13C
P3 10.00 usec
PLW2 31.2189986 W
GPNAME[1] SMSQ10.100
GP21 50.00 %
GPNAME[2] SMSQ10.100
GP22 30.00 %
GPNAME[3] SMSQ10.100
GP23 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.9378 MHz
FIDRES 635.162598 Hz
SW 269.319 ppm
FmMode QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S93 HMBC spectrum (600 MHz, CDCl_3) of compound 14



Current Data Parameters
NAME RDP-50B-2 !
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200718
Time 20.20 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG cosygppmfd
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 10.00 usec
TE 296.00 K
DO 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2000000 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
PnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 64
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S94 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **14**

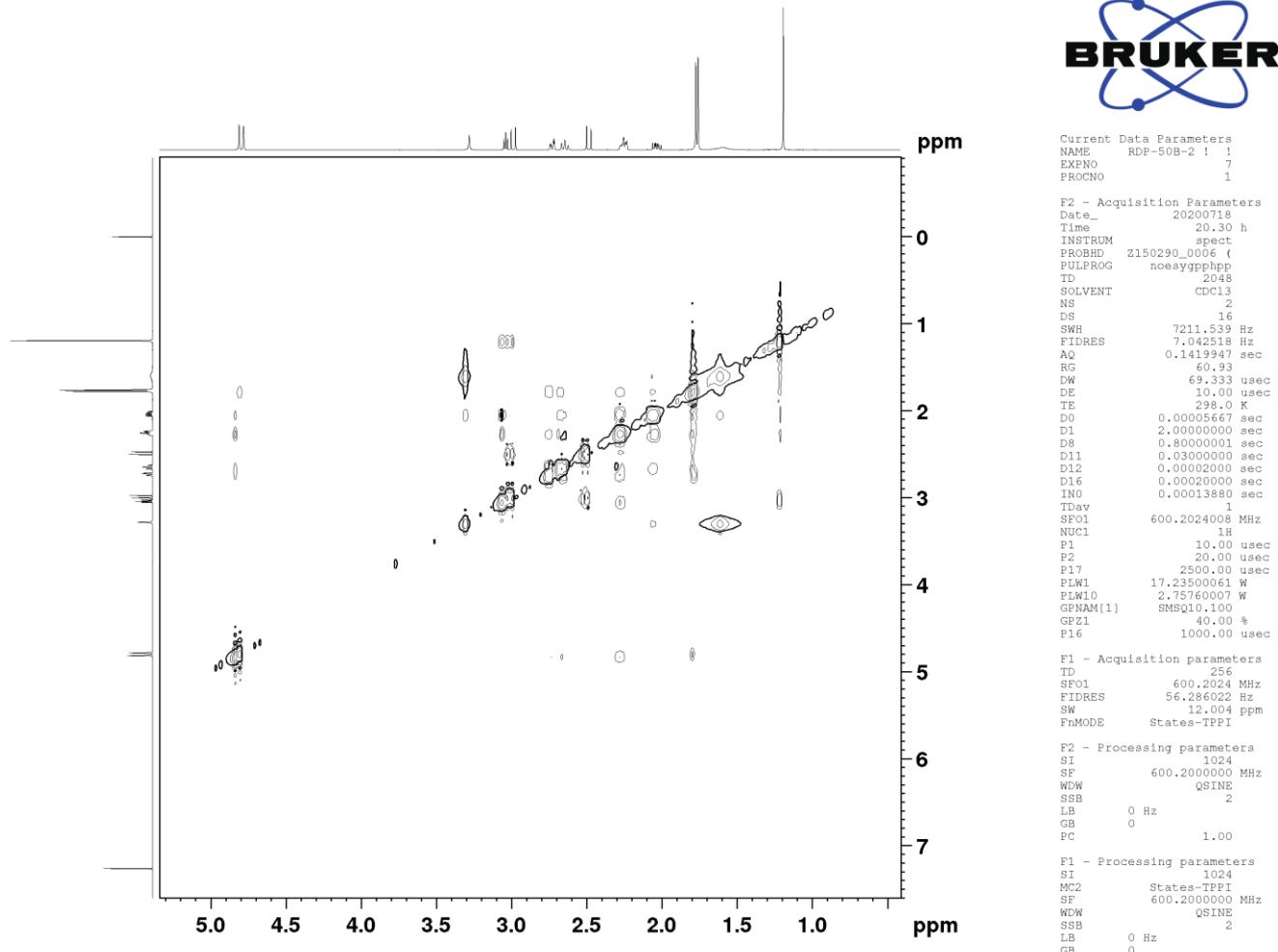


Figure S95 NOESY spectrum (600 MHz, CDCl_3) of compound **14**

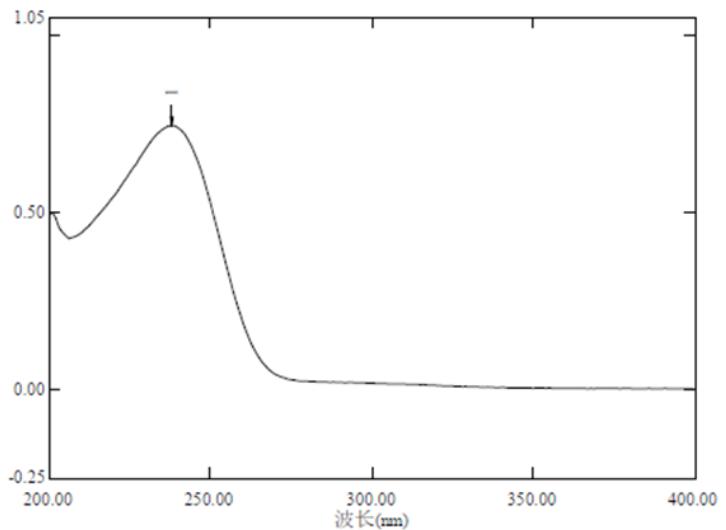
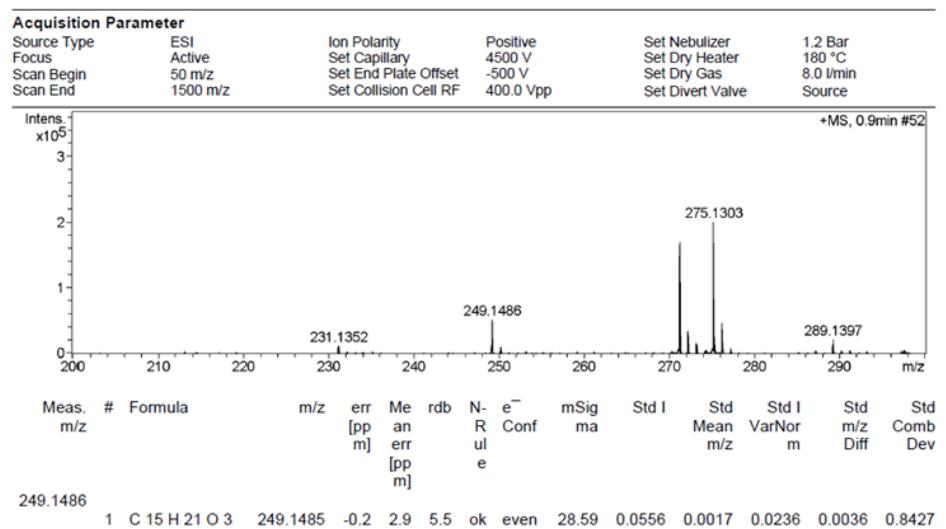
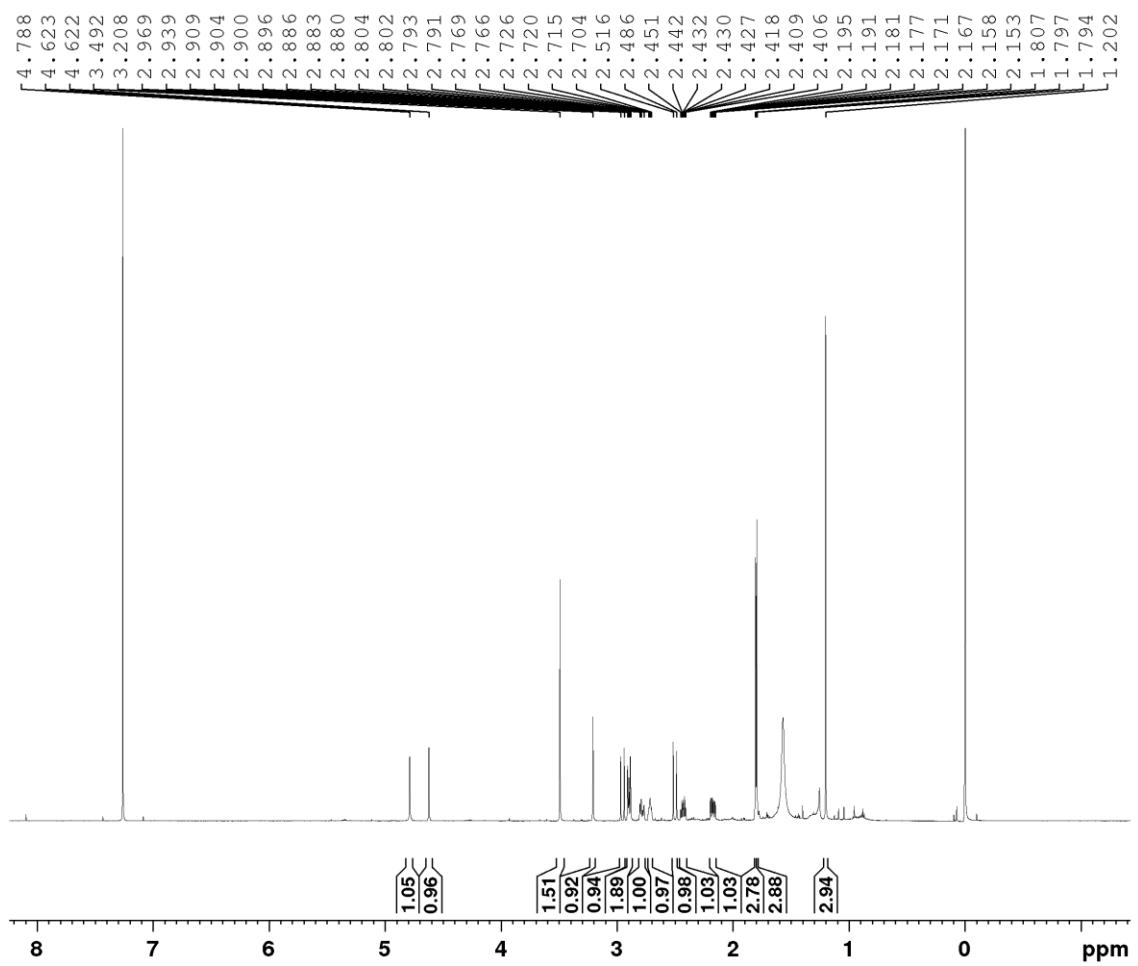


Figure S96 HRESIMS and UV spectra of compound 15



Current Data Parameters
NAME A19-2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220904
Time 16.46 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 48
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 13.81
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1
SF01 600.2037062 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 17.23500061 W

F2 - Processing parameters
SI 65536
SF 600.2000128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S97 ¹H NMR spectrum (600 MHz, CDCl₃) of compound 15

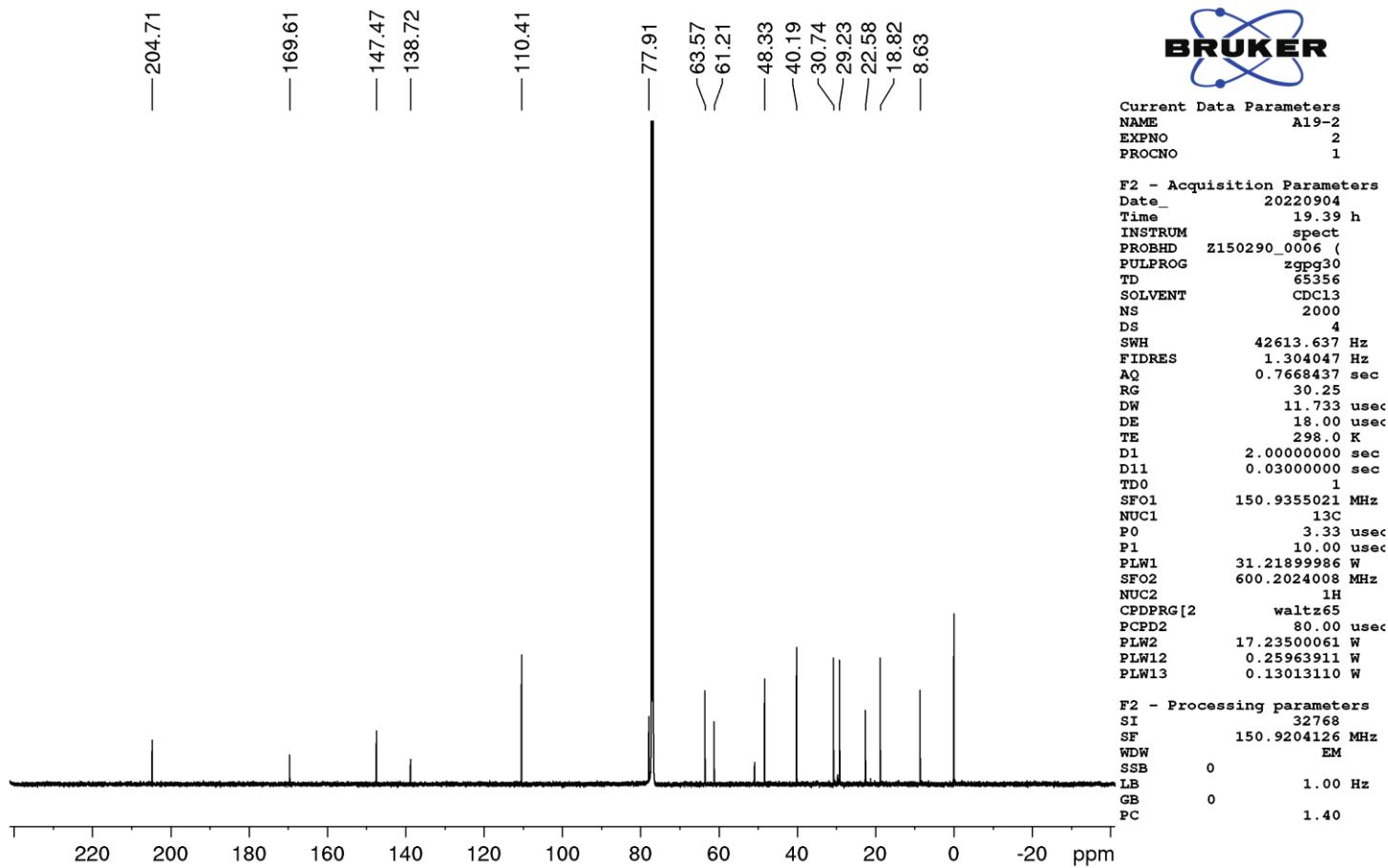
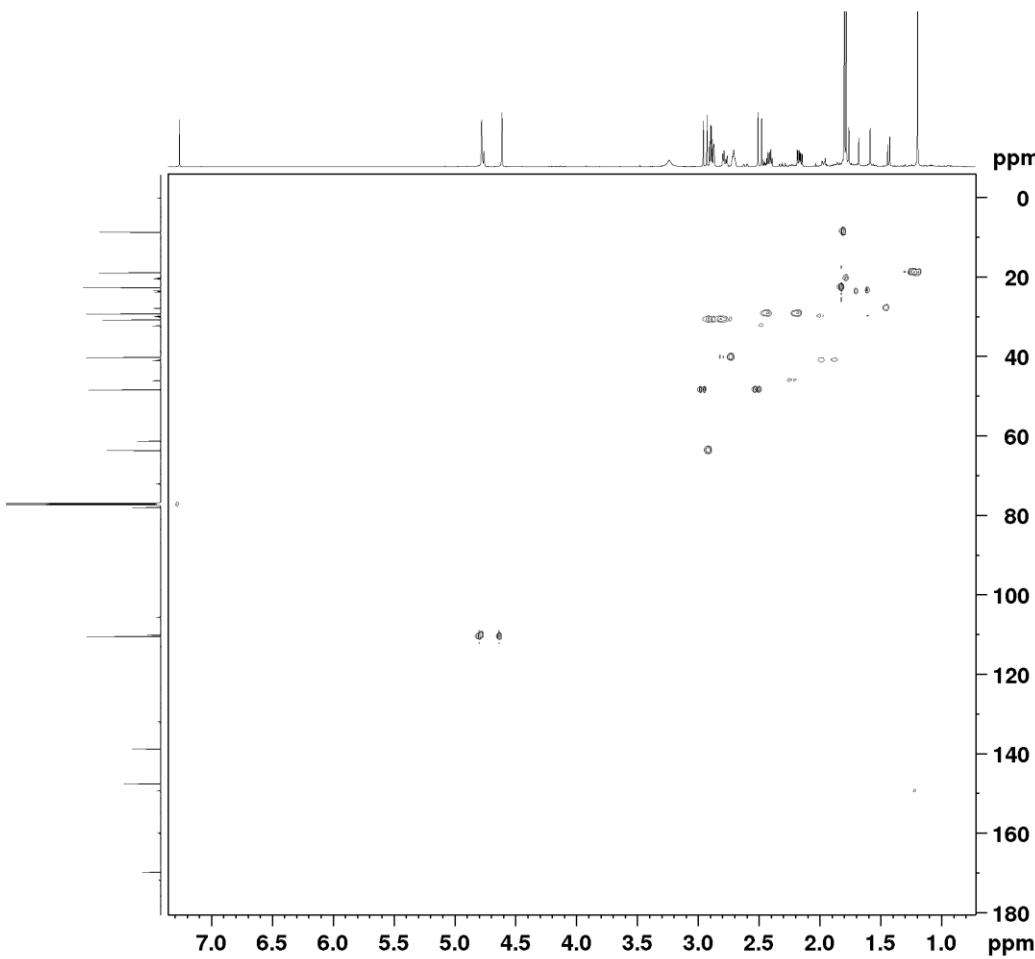


Figure S98 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **15**



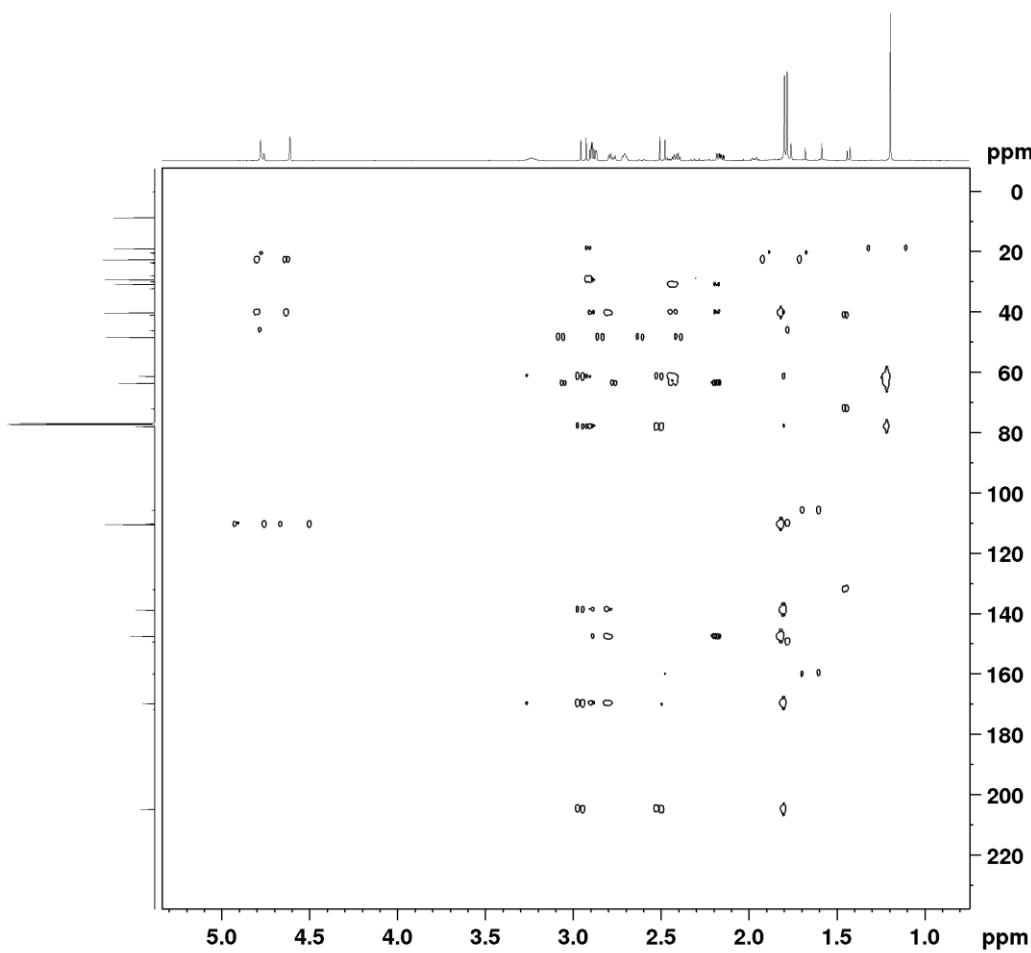
Current Data Parameters
NAME RDP-341
BPPNO 4
PRONCO 1

F2 - Acquisition Parameters
Data_ 2020623
Time 0.41 h
INSTRM spect
PROBHD 1150299_0006 (PULPROG hsqcetgpsp12.p
TD 65536
SOLVENT CDCl₃
NS 2
DS 16
SWH 7211.539 Hz
ETRATES 7.04938 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.493 usec
DE 10.00 usec
TB 298.0 K
CNUST2 145.000000
CNST17 -0.5000000
CNST16 0.0000000
D0 0.0000300 sec
D1 0.0000000 sec
D4 0.00172414 sec
D11 0.0300000 sec
D16 0.0000000 sec
D24 0.00008200 sec
INO 0.00001270 sec
TDav 600.2024098 MHz
SF01 150.000000 W
P1 10.00 usec
P2 20.00 usec
P2A 0 usec
PLW1 17.23508061 W
SF02 150.3377659 MHz
NOESY 100.000000
CPDPFGS(2 garp4
P3 10.00 sec
P14 100.00 usec
P24 2000.00 usec
PCPDZ 55.00 usec
PLW0 0 W
PLW2 31.21899986 W
P1D 10.00 usec
SPNAM[3] Cpmg60,4,5,20,1
SPDALS 0.500
SPDPFGS3 0 Hz
SPW 4.76999999 W
SPNAM[7] Cpmg60comp,4
SPDALS 0.500
SPDPFGS7 0 Hz
SPW7 4.76999999 W
GPBNM[1] SMSG10.00 *
GP21 80.00 *
GPBNM[2] SMSG10.100 *
GP22 100.00 *
GPBNM[3] SMSG10.100 *
GP23 11.00 *
GPBNM[4] SMSQ10.100 *
GP24 -5.00 *
P16 1000.00 usec
P13 600.00 usec

P1 - Acquisition parameters
TD 256
SF01 150.3377659 MHz
ETRATES 34.000000 Hz
DW 260.837 ppm
PRMode Echo-Antiecho
F2 - Processing parameters
SI 1024
SF 600.200000000 MHz
WDW QSBIN
SSB Z
LB 0 Hz
GB 0
PC 1.40

P1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.3204100 MHz
WDW QSBIN
SSB Z
LB 0 Hz
GB 0

Figure S99 HSQC spectrum (600 MHz, CDCl₃) of compound 15



Current Data Parameters
NAME RDP-34!!
EXPNO 5
PROCNO 1

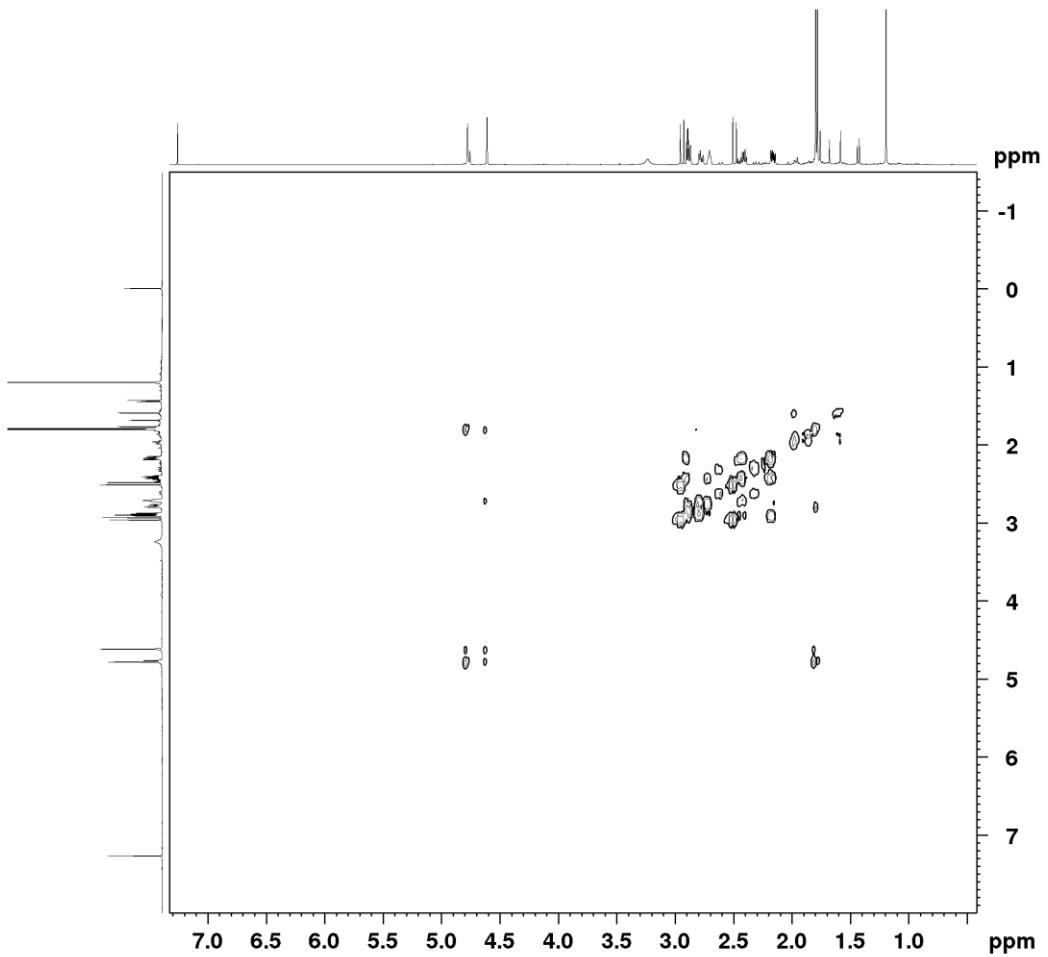
P2 - Acquisition Parameters
Date_ 20200623
Time 9.57 h
INSTRUM spect
PROBHD Z150290_0006 (4096)
PULPROG hmbcgrndqf
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 130
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
CNS13 8.0000000
D0 0.0000000 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001270 sec
TDav 1
SF01 600.2024010 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLN1 17.23500061 W
SF02 150.9377659 MHz
NUC2 13C
P3 10.00 usec
PLN2 31.21899986 W
GPNAME[1] SNSQ10.100
GPZ1 50.00 %
GPNAME[2] SNSQ10.100
GPZ2 30.00 %
GPNAME[3] SNSQ10.100
GPZ3 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.9378 MHz
FIDRES 615.15741 Hz
SW 260.837 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S100 HMBC spectrum (600 MHz, CDCl_3) of compound 15



Current Data Parameters
NAME RDE-341!
EXPNO 6
PROCNO 1

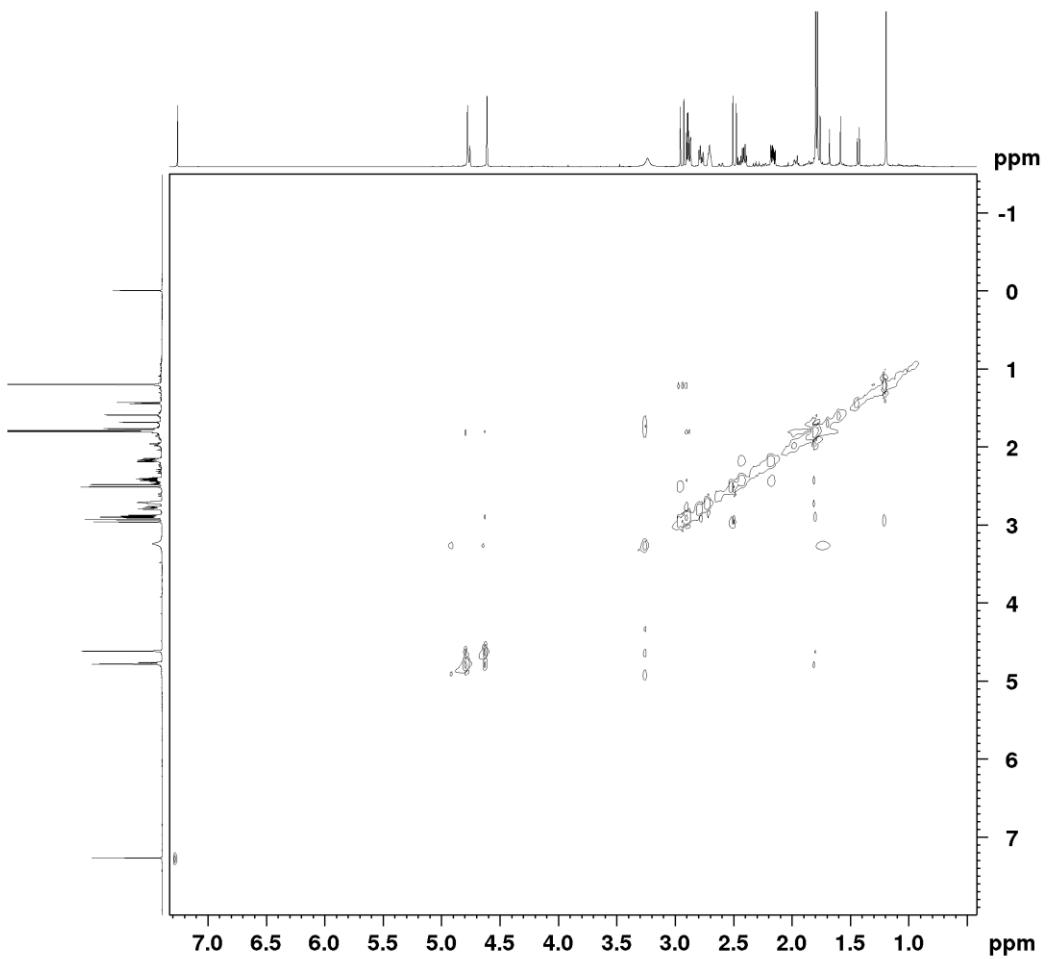
F2 - Acquisition Parameters
Date_ 20200623
Time 11.24 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG cosygppmrf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 10.00 usec
TE 290.00 K
DO 0.00000300 sec
D1 2.0000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.20024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
PnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 64
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S101 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 15



Current Data Parameters
NAME RDP-34!!
EXPNO 7
PROCNO 1

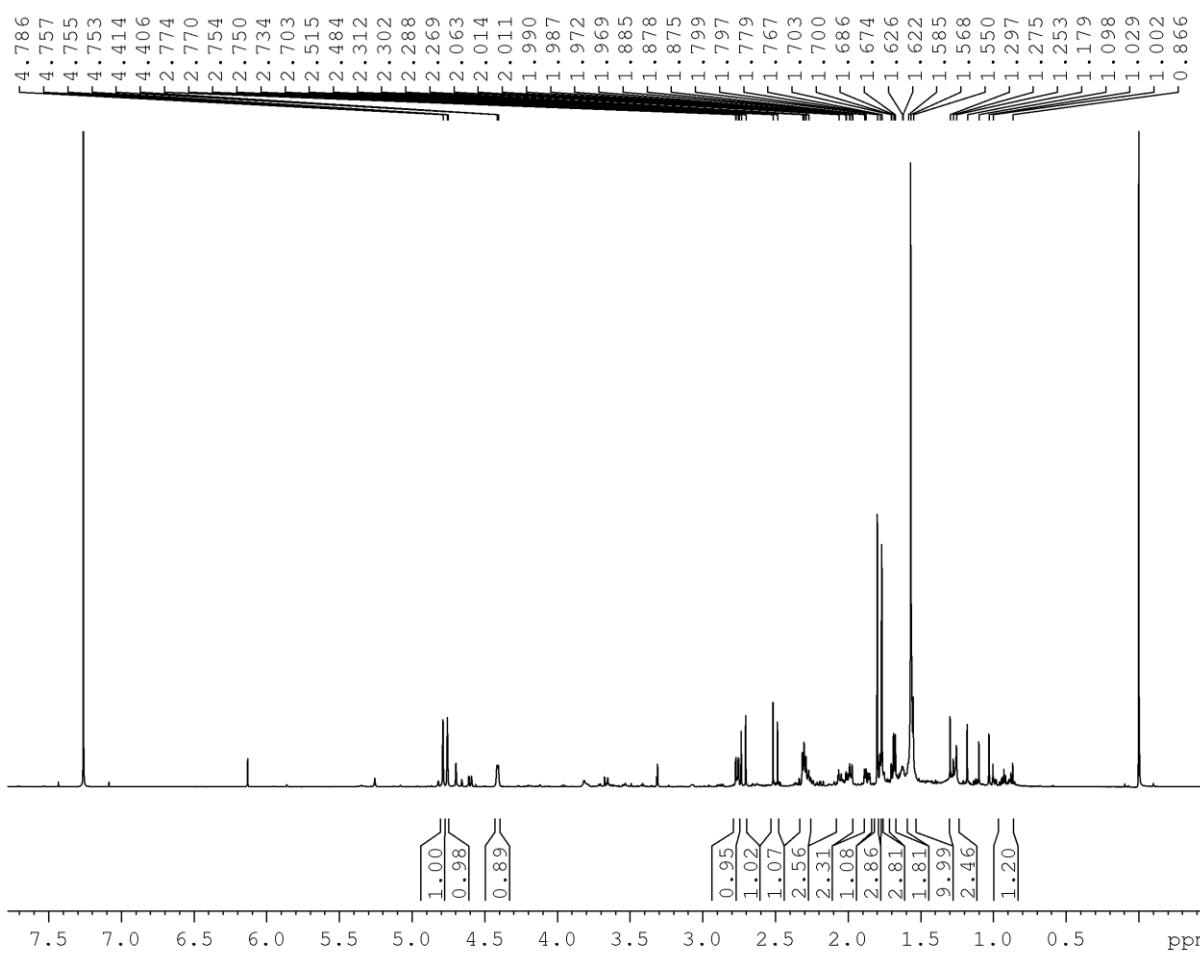
F2 - Acquisition Parameters
Date_ 20200623
Time 10:56 h
INSTRUM spect
PROBHD Z150290_0066_1
PULPROG noeipypphphh
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 107.6
DW 69.00 usec
DB 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D19 0.00013860 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
SF2 States-TPPI
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S102 NOESY spectrum (600 MHz, CDCl_3) of compound **15**



Current Data Parameters
NAME RDP-98B
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200905
Time 14.06 h
INSTRUM spect
PROBHD Z150290_0006 (Zg30
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 13.81
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1
SF01 600.2037062 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 17.23500061 W

F2 - Processing parameters
SI 65536
SF 600.2000136 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S103 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **16**

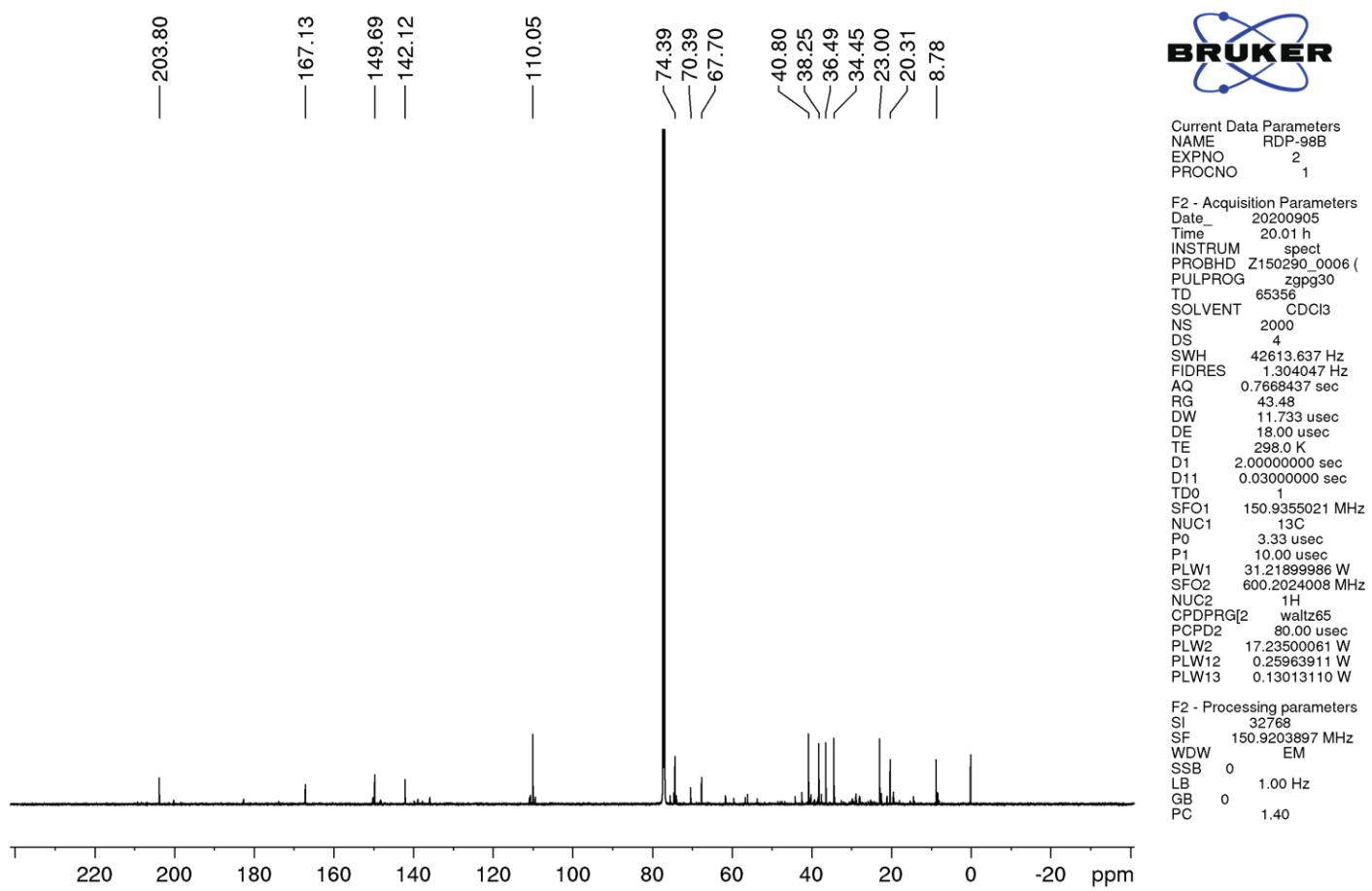


Figure S104 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **16**

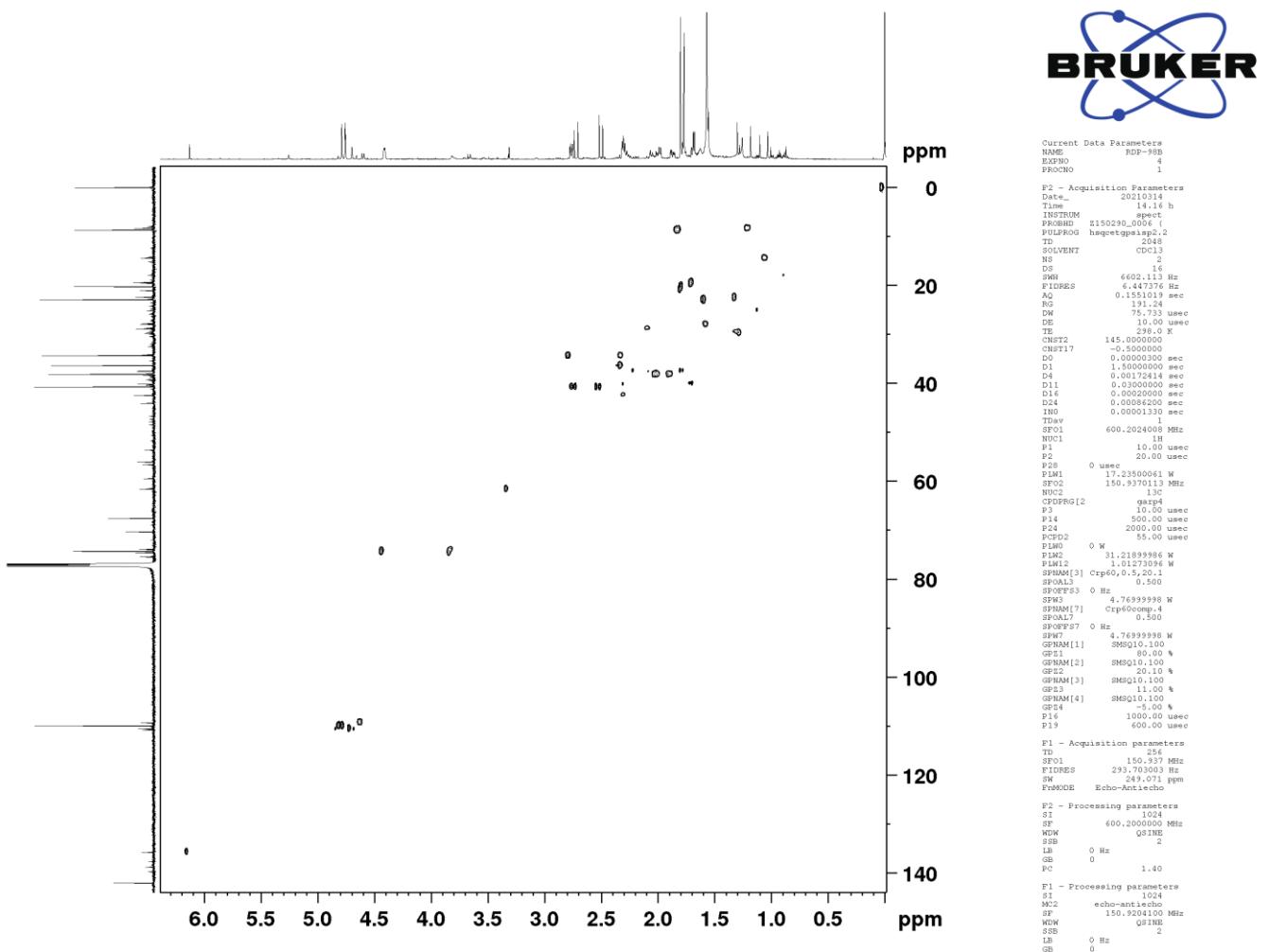
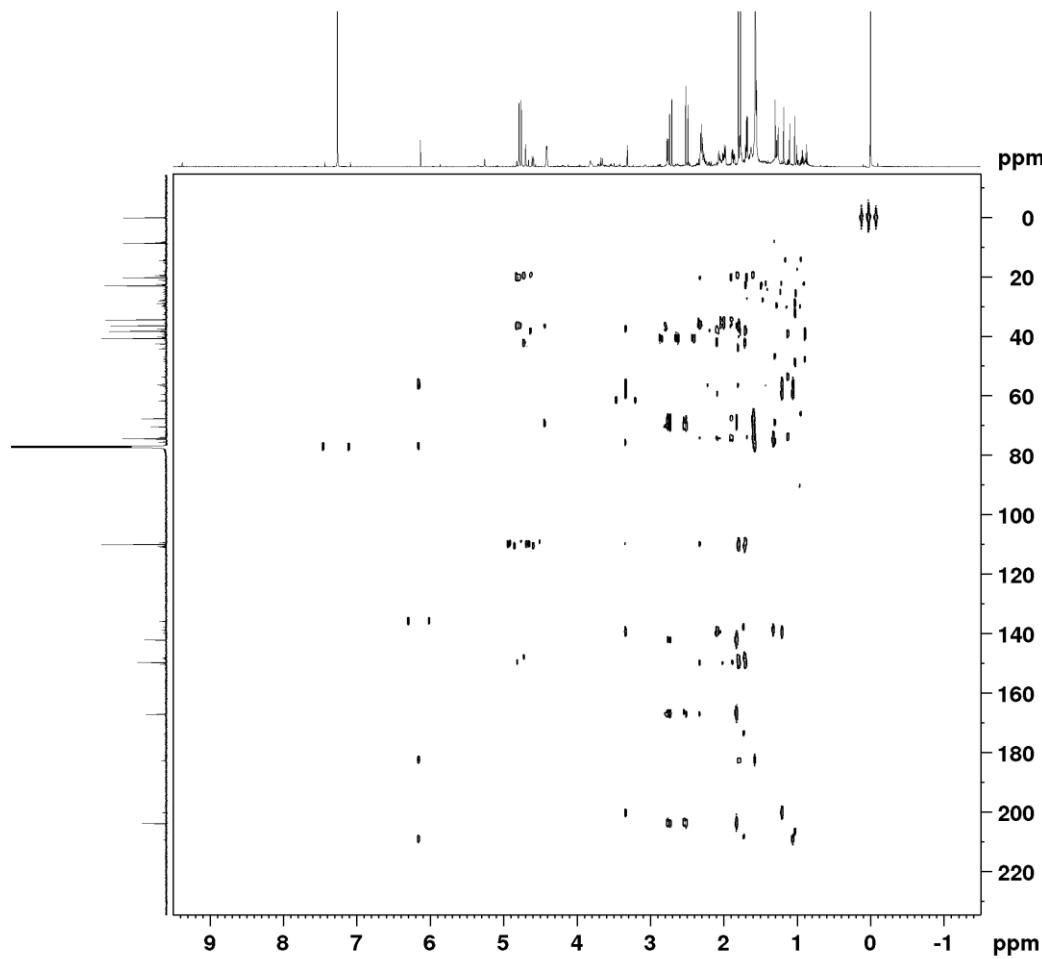


Figure S105 HSQC spectrum (600 MHz, CDCl₃) of compound 16



Current Data Parameters
NAME RDP-98B
EXPNO 5
PROCNO 1

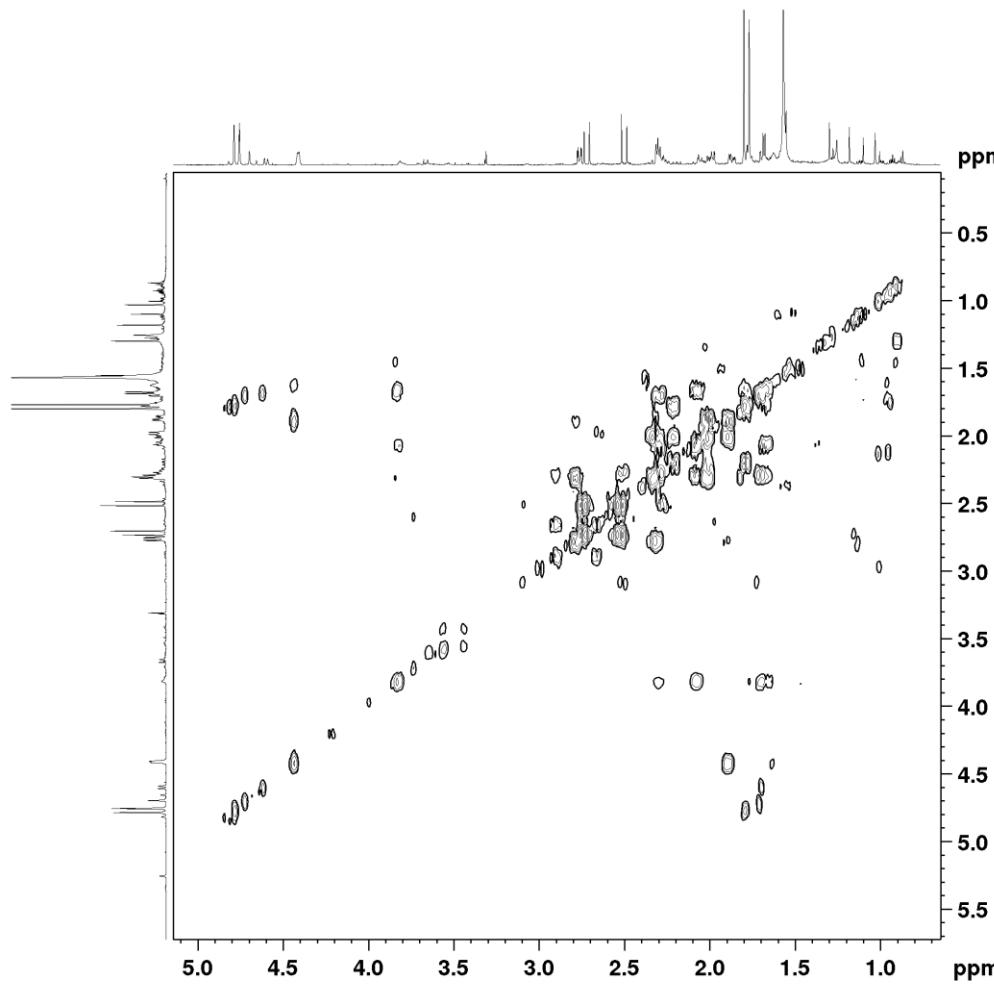
F2 - Acquisition Parameters
Date_ 20210314
Time 14:31 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG hmbcgrndf
TD 4096
SOLVENT CDCl3
NS 8
DS 16
SWH 6602.113 Hz
FIDRES 3.223688 Hz
AQ 0.3102037 sec
RG 100.00
DW 75.733 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.0000000
D0 0.0000000 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001330 sec
TDav 600.2024016 sec
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
NUC2 150.9370113 MHz
P3 10.00 usec
PLW2 31.21899986 W
GP[NAM[1] SNSQ10.100
GPZ1 50.00 %
GP[NAM[2] SNSQ10.100
GPZ2 30.00 %
GP[NAM[3] SNSQ10.100
GPZ3 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.937 MHz
FIDRES 587.40605 Hz
SW 249.071 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S106 HMBC spectrum (600 MHz, CDCl_3) of compound **16**



Current Data Parameters
NAME RDP-98B
EXPNO 6
PROCNO 1

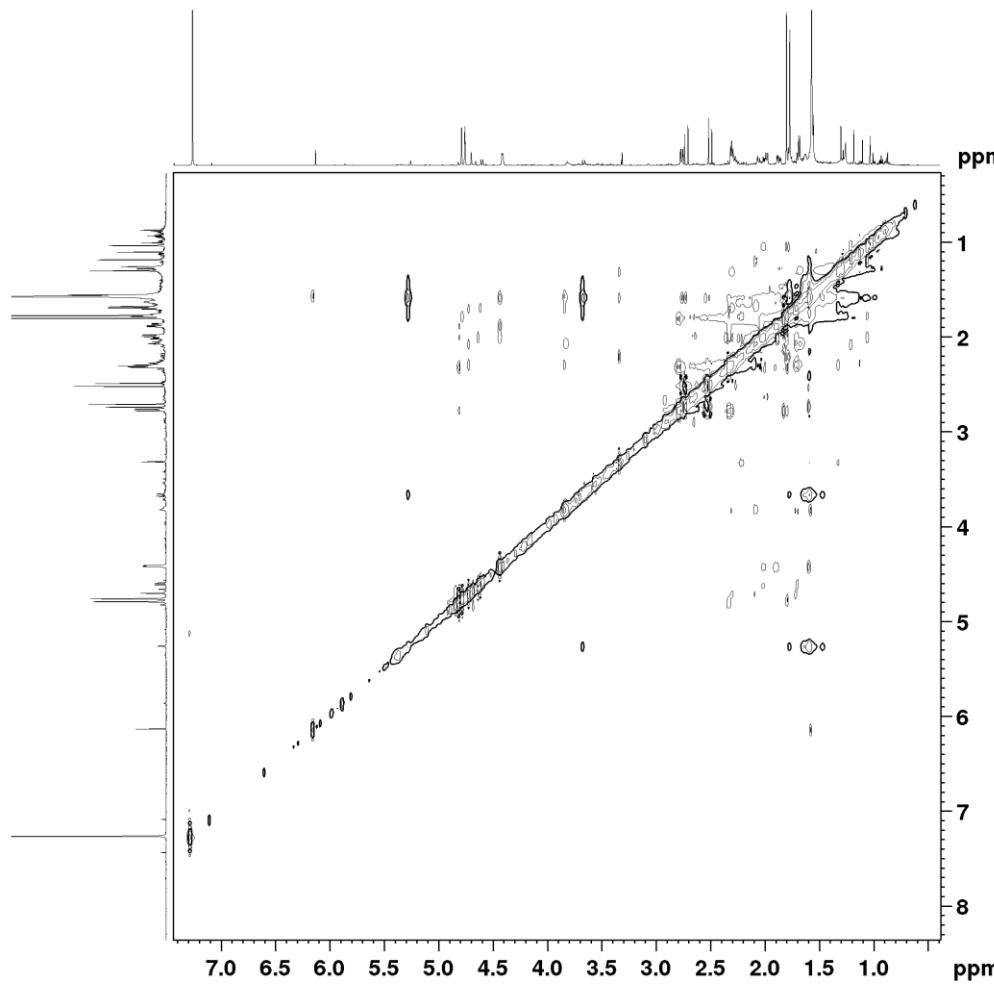
F2 - Acquisition Parameters
Date_ 20210314
Time 15.04 h
INSTRUM spect
PROBHD Z150290_0006 (cosyqppmfr)
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 6602.113 Hz
FIDRES 6.447376 Hz
AQ 0.1551019 sec
RG 191.24
DW 75.733 usec
DE 10.00 usec
TE 299.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.0000400 sec
D16 0.00020000 sec
IN0 0.00015140 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPBM1 16.00 %
GPBM2 12.00 %
GPBM3 10.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 103.203438 Hz
SW 11.005 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S107 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **16**



Current Data Parameters
NAME RDP-98B
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210314
Time 15.24 h
INSTRUM sec
PROBHD Z150290_0004 (
PULPROG noeesypphp
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 6602.113 Hz
FIDRES 6.447376 Hz
AQ 0.1551019 sec
RG 60.93
DW 75.733 usec
DE 10.00 usec
TE 298.0 K
D0 0.00006297 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0000000 sec
D12 0.00002000 sec
D16 0.00002000 sec
IN0 0.00015140 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 51.601719 Hz
SW 11.005 ppm
PrMODE States-TPP1

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPP1
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S108 NOESY spectrum (600 MHz, CDCl₃) of compound **16**

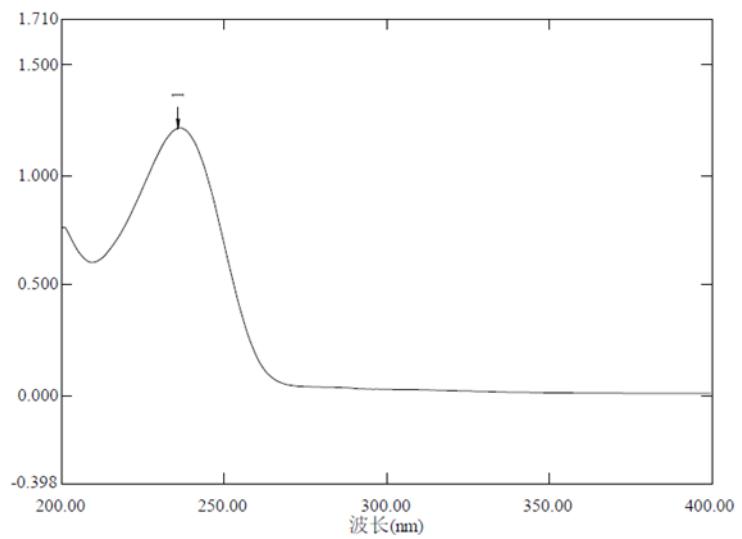
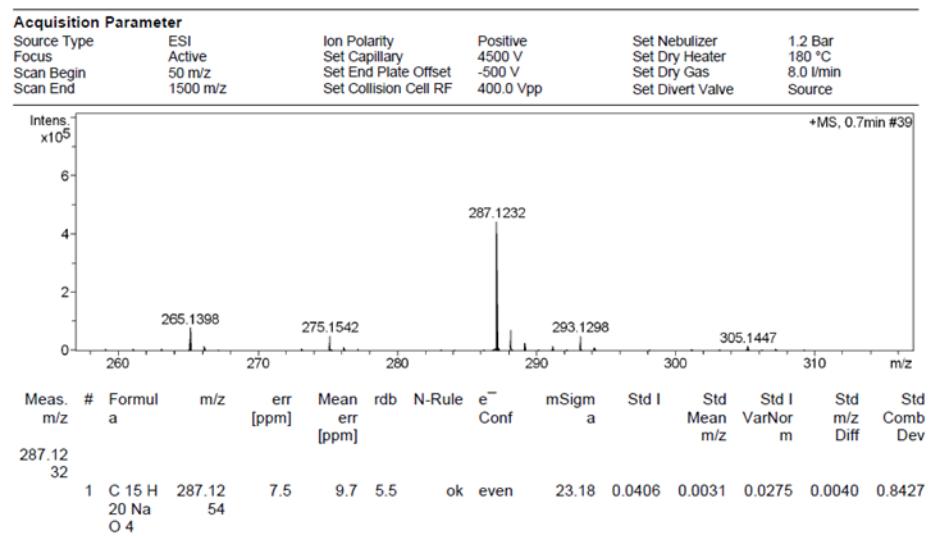


Figure S109 HRESIMS and UV spectra of compound 17

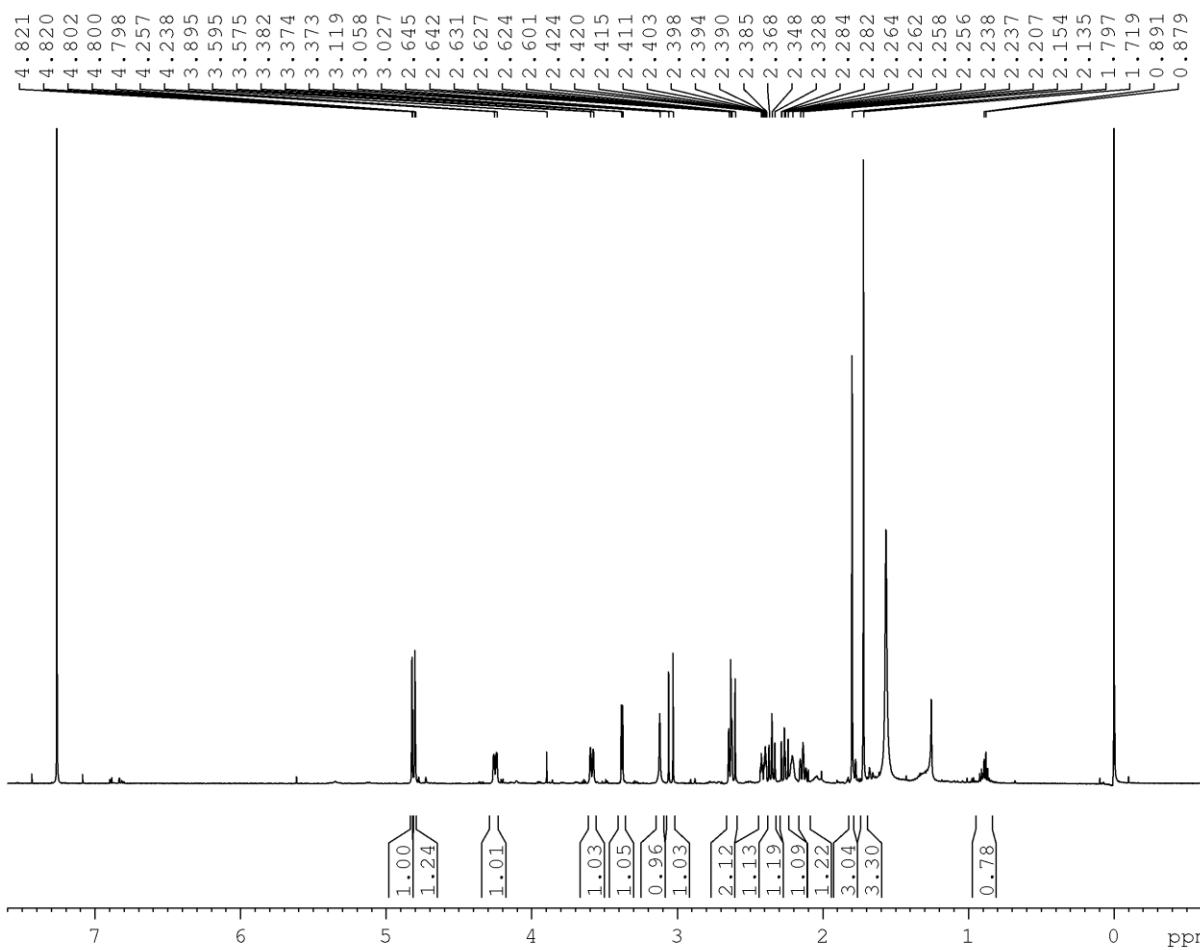


Figure S110 ^1H NMR spectrum (600 MHz, CDCl₃) of compound **17**

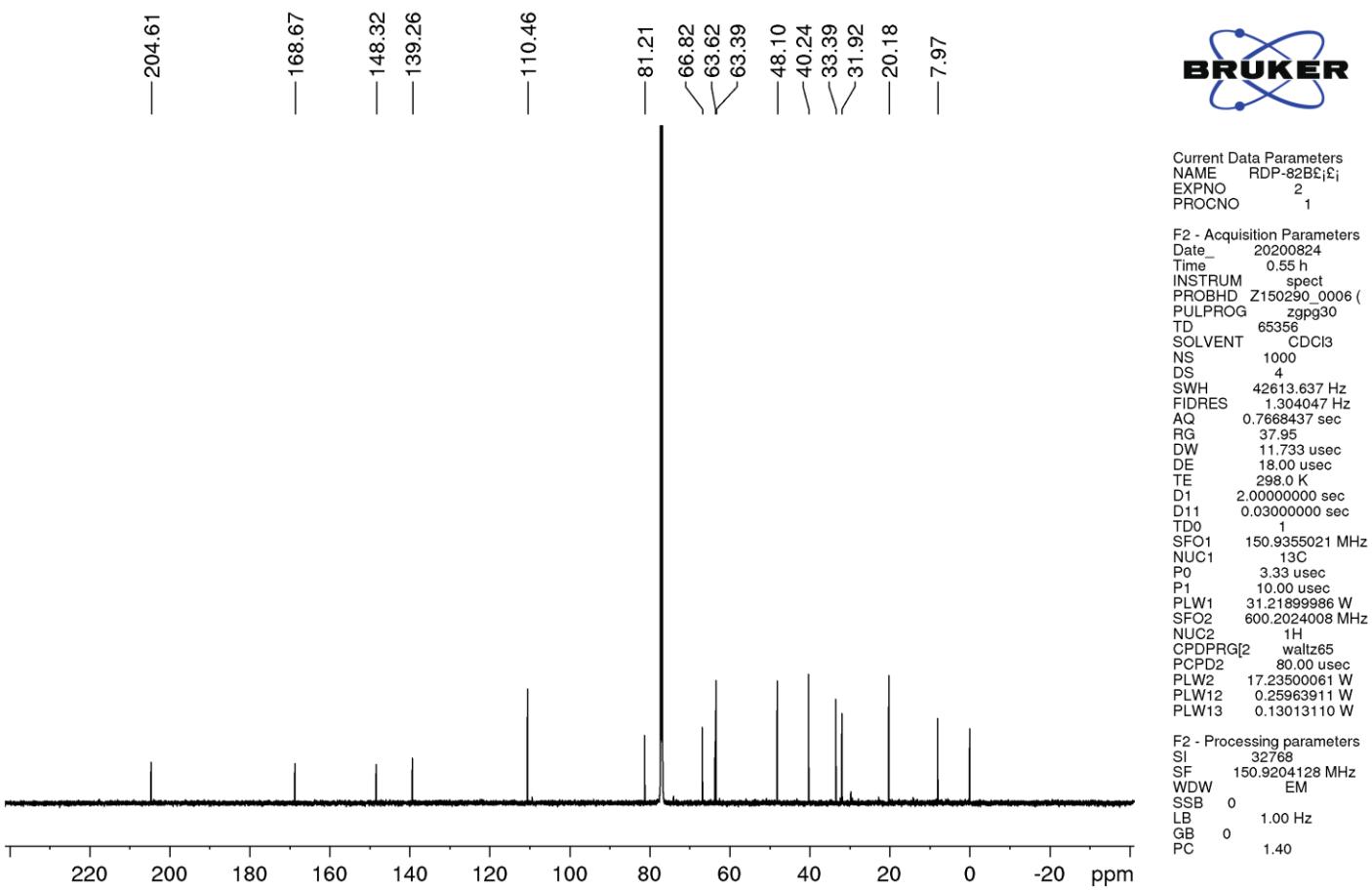


Figure S111 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **17**

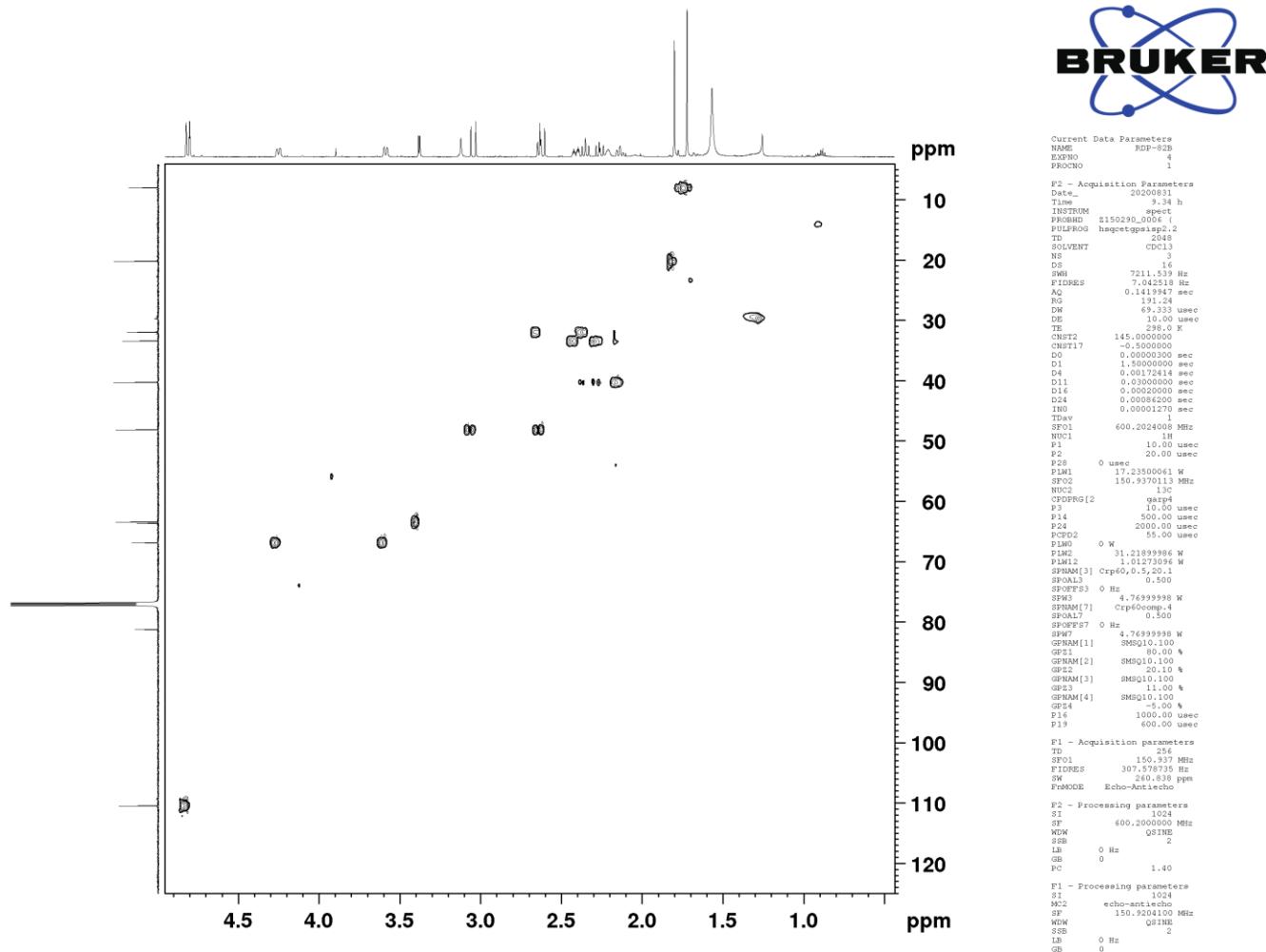
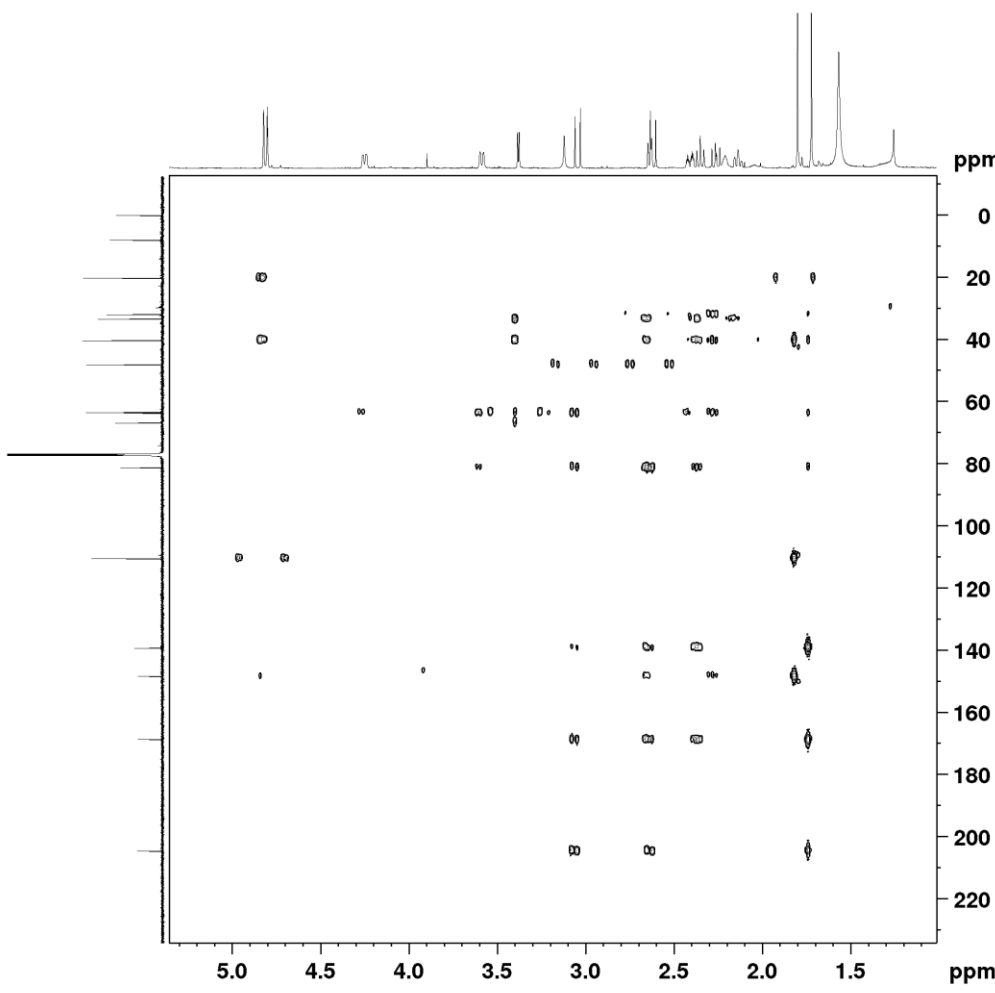


Figure S112 HSQC spectrum (600 MHz, CDCl₃) of compound 17



Current Data Parameters
NAME RDP-82B
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200831
Time 9.57 h
INSTRUM spect
PROBHD Z150290_0001 (
PULPROG hmbcogn.drf
TD 4096
SOLVENT CDCl3
NS 12
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 131.224
DW 69.433 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.000000
D0 0.00000300 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
DW0 0.00001270 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
SF02 150.9370100 MHz
NUC2 13C
P3 10.00 usec
PLW2 31.2189986 W
GPNAME[1] SMSQ10.100
GP21 50.00 °
GPNAME[2] SMSQ10.100
GP22 30.00 °
GPNAME[3] SMSQ10.100
GP23 40.10 °
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.937 MHz
FIDRES 615.157471 Hz
SW 260.838 ppm
FhMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S113 HMBC spectrum (600 MHz, CDCl_3) of compound **17**

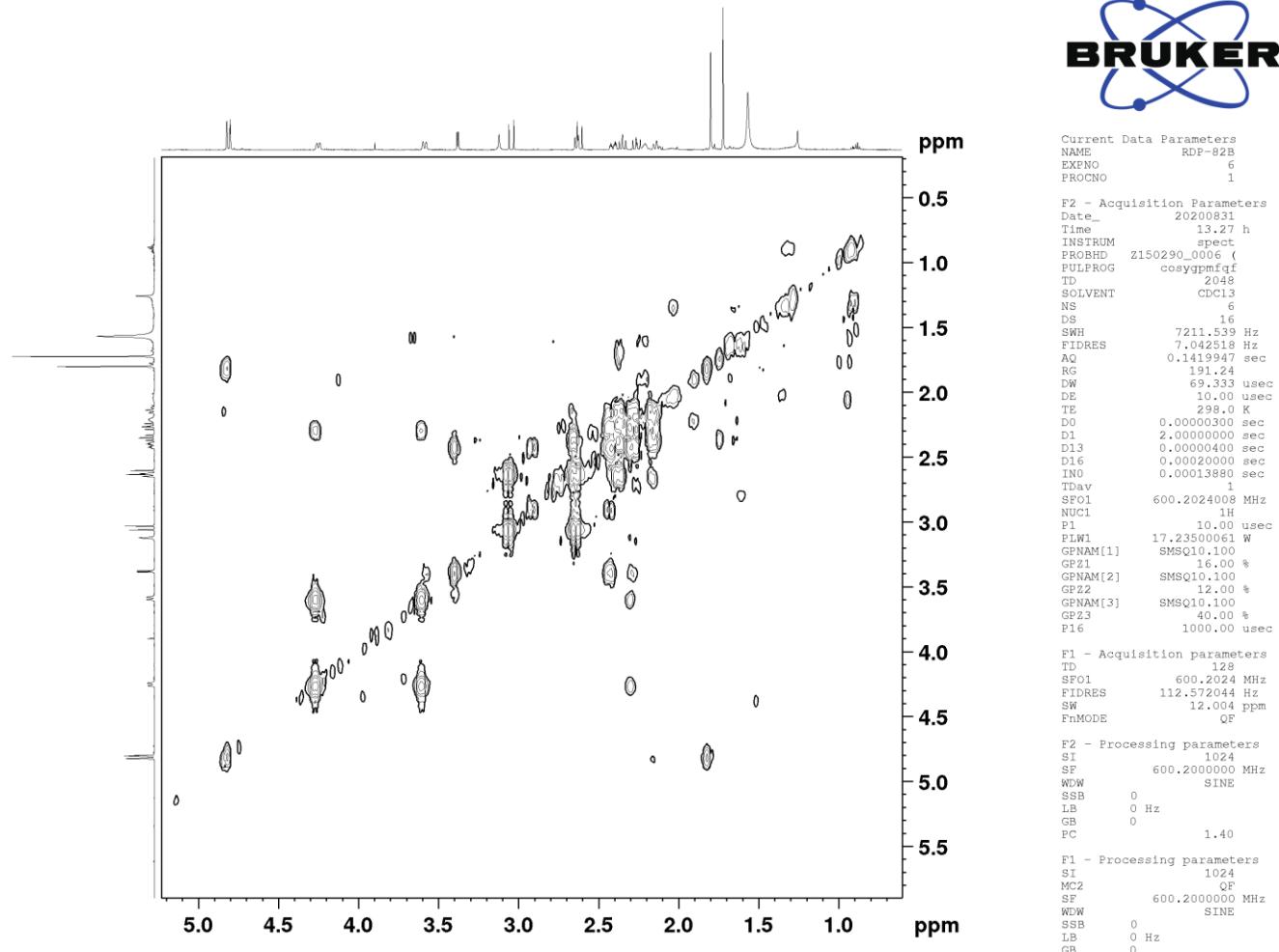


Figure S114 ^1H - ^1H COSY spectrum (600 MHz, CDCl₃) of compound **17**

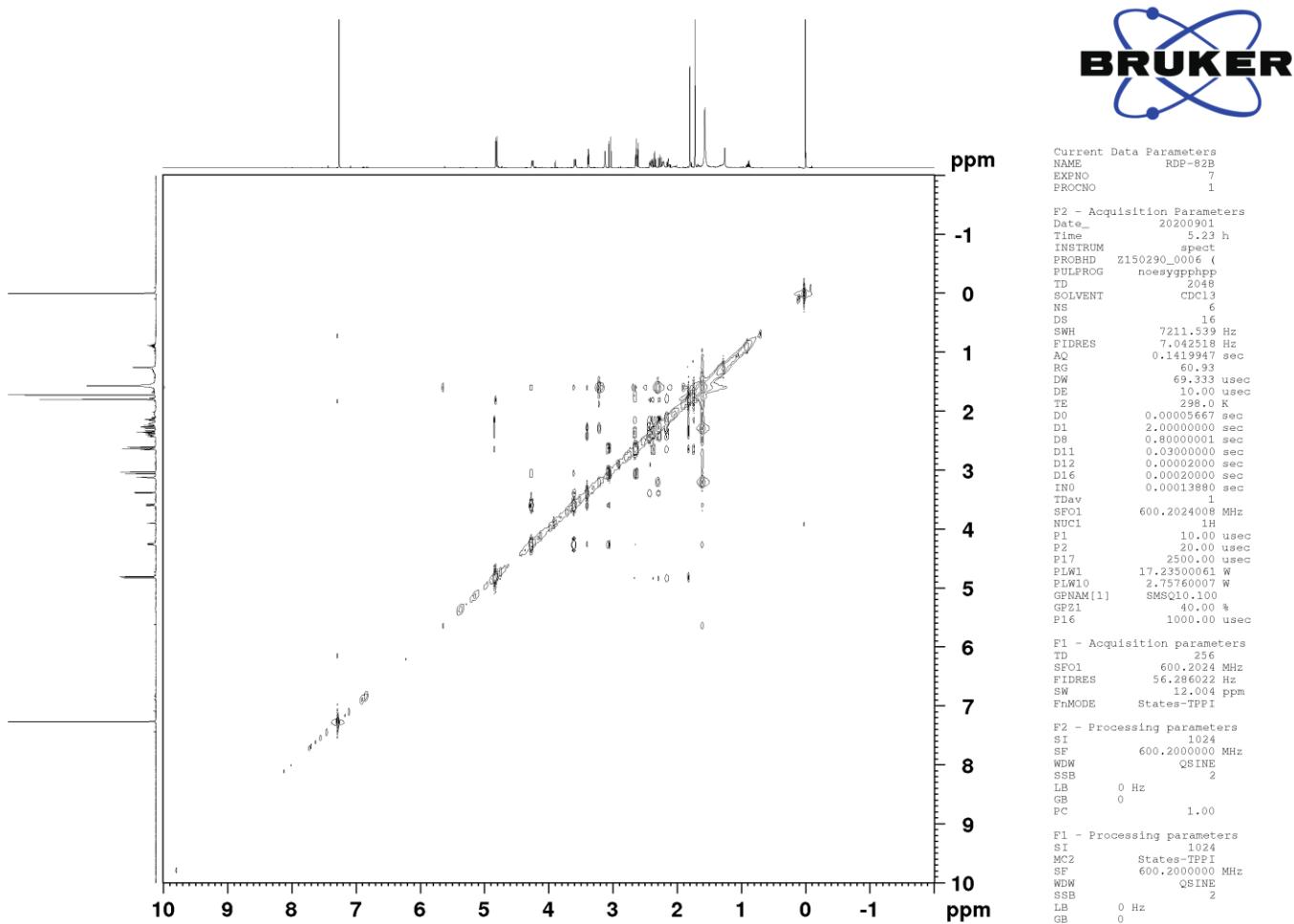


Figure S115 NOESY spectrum (600 MHz, CDCl_3) of compound **17**

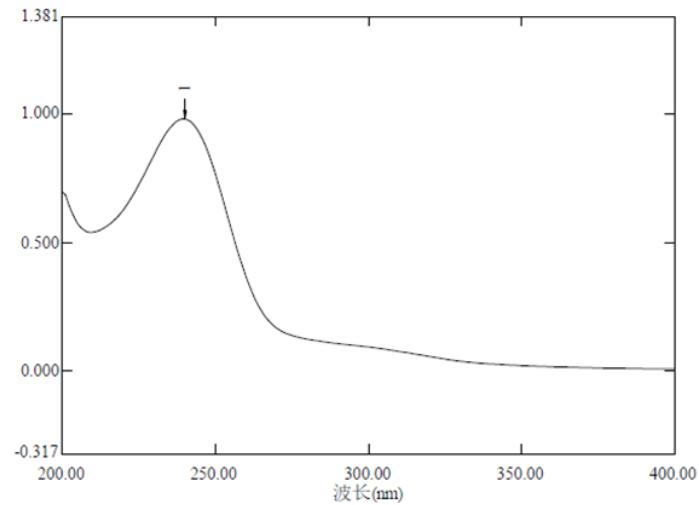
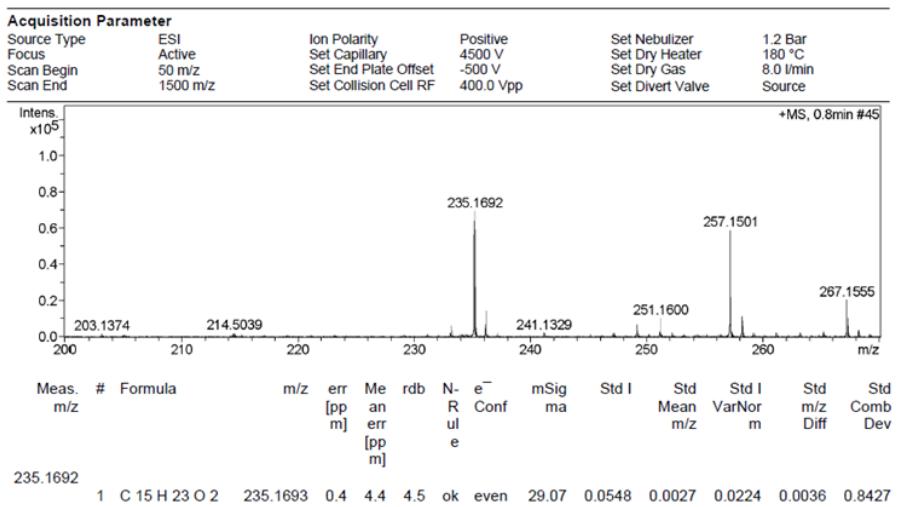


Figure S116 HRESIMS and UV spectra of compound **18**

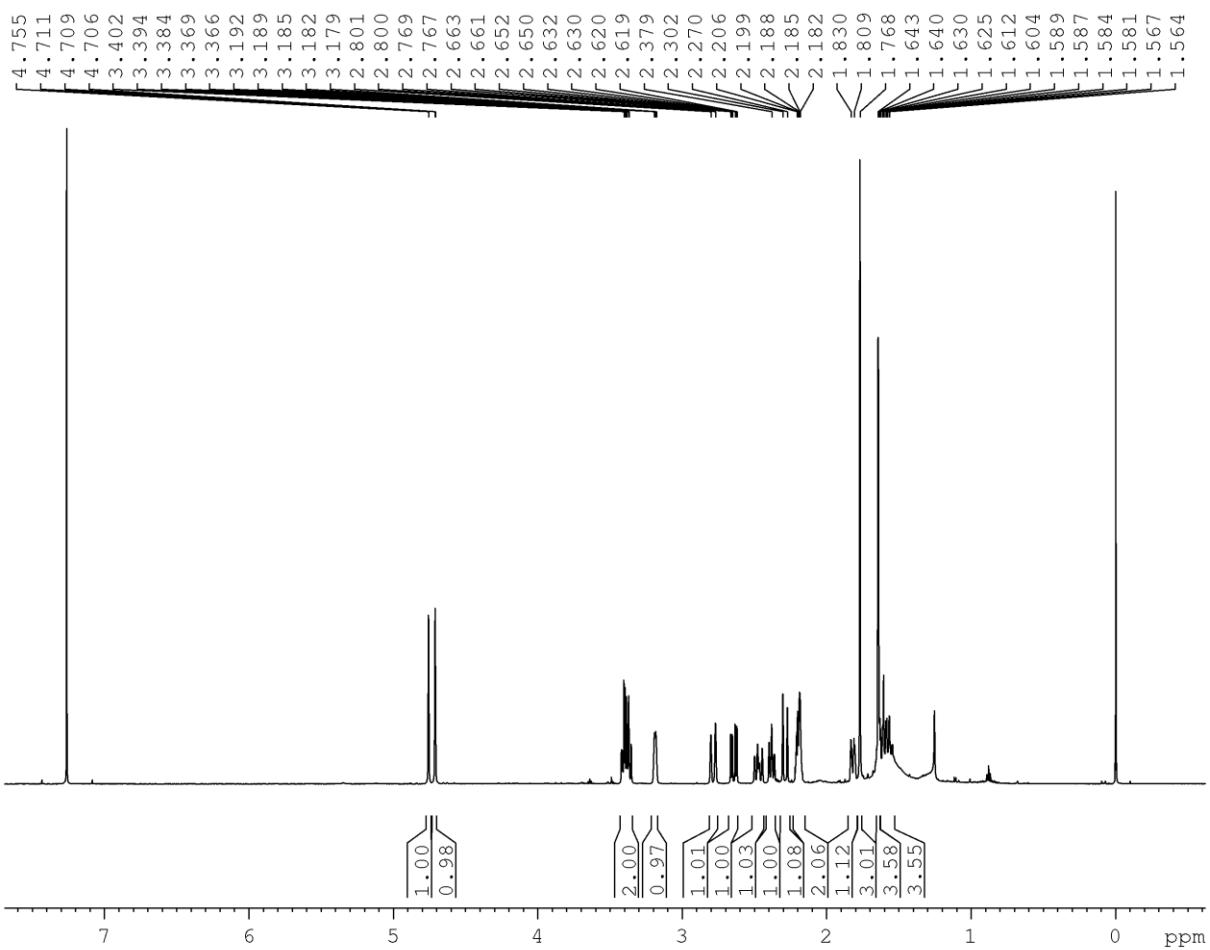
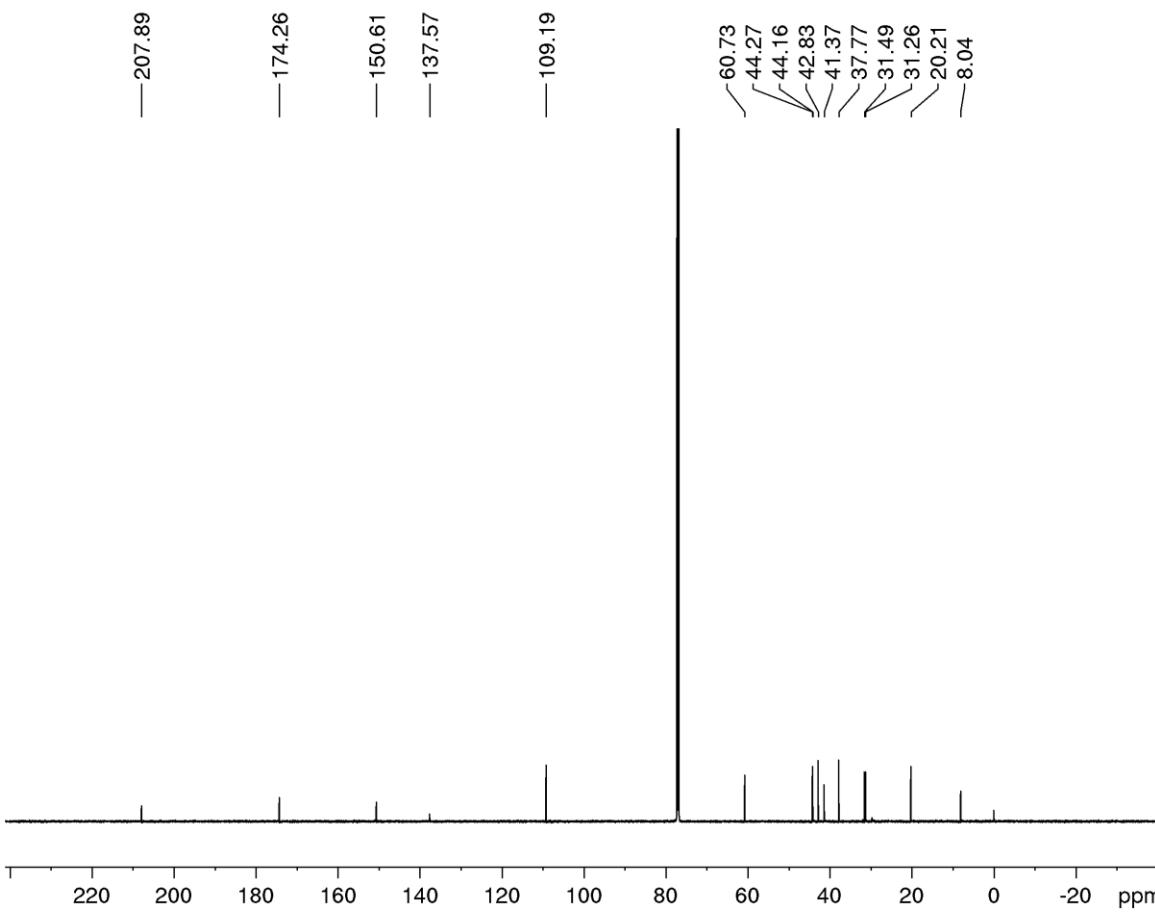


Figure S117 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **18**

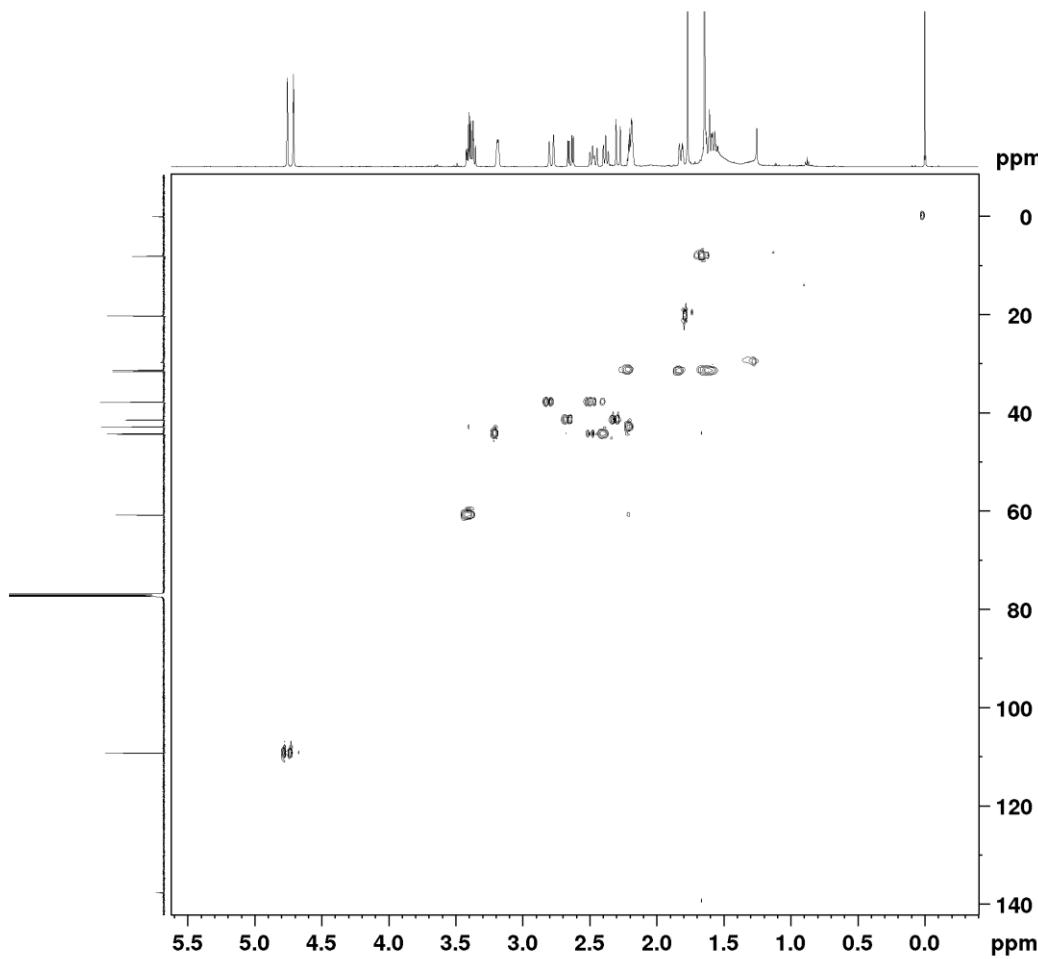


Current Data Parameters
NAME RDP-49B!!
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200712
Time_ 15.28 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgppg30
TD 65356
SOLVENT CDCl3
NS 200
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 37.95
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9204119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S118 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **18**



Current Data Parameters
NAME R0F-49B1
BPPN 1
PRONCO 1

F2 - Acquisition Parameters

Data_ 20200720

Time 20.11 h

INSTRUM spect

PROBHD 1150299_0006 (

PULPROG hsqcetgpsa2sp1.2

TD 65536

SOLVENT CDCl3

NS 4

D1 16

SWH 7211.539 Hz

EDD 7.04948 Hz

RG 0.1419947 sec

RG 191.24

DW 65.633 usec

DE 10.00 usec

TE 298.0 K

CNT12 145.000000

CNT17 -0.5000000

D0 0.00005300 sec

D1 0.000000 sec

D4 0.00172414 sec

D11 0.03300000 sec

D16 0.00000000 sec

D24 0.00008200 sec

TDav 0.00001270 sec

TDav

SI 600.2324099 MHz

SWC1 10

P1 10.00 usec

P2 20.00 usec

P2A 0 usec

PLW1 17.23508061 W

SI 150.9370113 MHz

SWC2 10

CPDPFGS(2) garp4

P3 10.00 usec

P1A 10.00 usec

P2A 2000.00 usec

CPDZ2 55.00 usec

PLW0 0 W

PLW2 31.21899986 W

SI 30.00000000 W

SPNAM[1] Cmso6@4.5,20.1

SPDALS 0.500

SPDPFGS3 0 Hz

SPW1 4.76999998 W

SPNAM[7] Cgs6@comp.4

SPDALS 0.500

SPDPFGS7 0 Hz

SPW7 4.76999998 W

SPNAM[1] SMSQ10.100

GP1 80.00 *

SPNAM[2] SMSQ10.100

GP2 80.00 *

SPNAM[3] SMSQ10.100

GP2 11.00 *

SPNAM[4] SMSQ10.100

GP2 5.00 *

GP16 1000.00 usec

P13 600.00 usec

F1 - Acquisition parameters

TD 256

SI 150.9370113 MHz

SWF 300.23000000 MHz

WDW QSBINE

SSB Z

LB 0 Hz

GB 0

PC 1.40

F1 - Processing parameters

SI 1024

SF 600.23000000 MHz

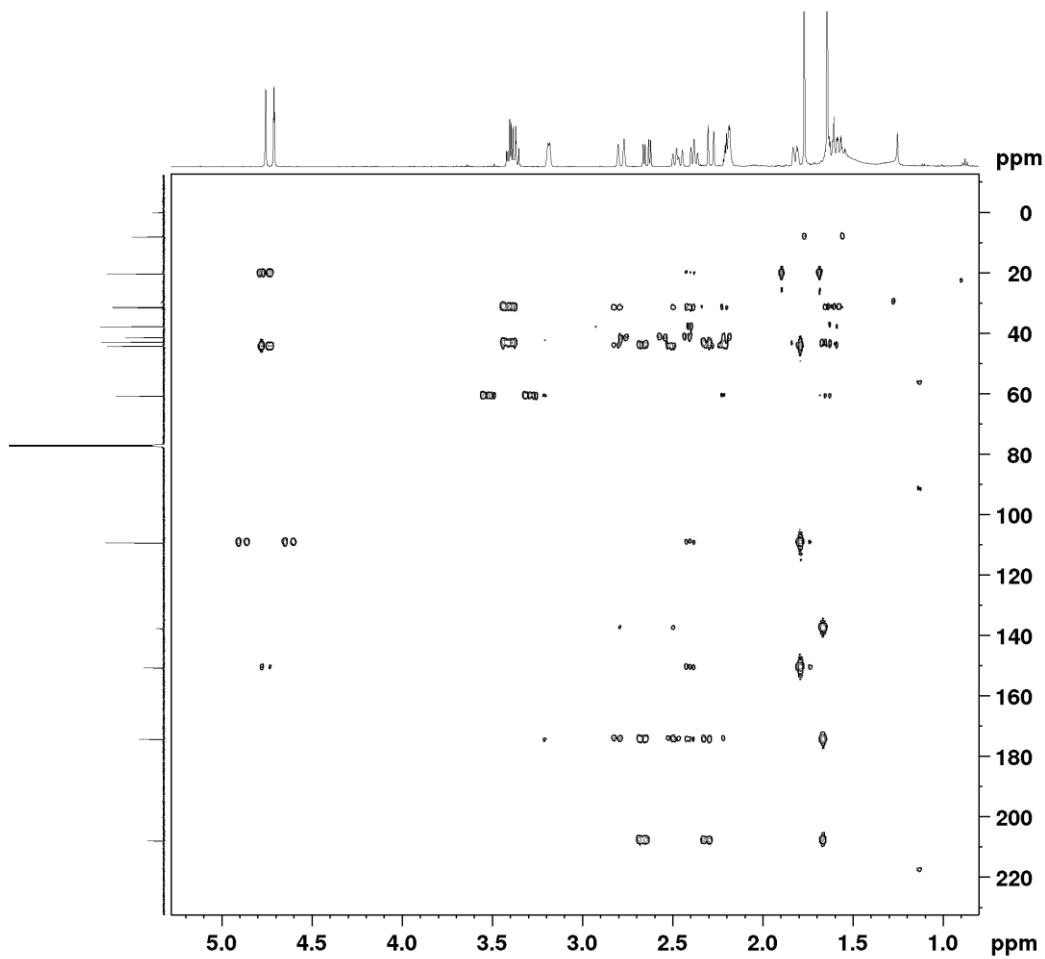
WDW QSBINE

SSB Z

LB 0 Hz

GB 0

Figure S119 HSQC spectrum (600 MHz, CDCl₃) of compound 18



Current Data Parameters
NAME RDP-49B!!
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200720
Time 20.42 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG hmbcgrndf
TD 4096
SOLVENT CDCl3
NS 16
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 130
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.0000000
D0 0.0000300 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001270 sec
TDav 1 sec
SF01 600.2024010 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
SF02 150.9370113 MHz
NUC2 13C
P3 10.00 usec
PLW2 31.21899986 W
GPNAME[1] SNSQ10.100
GPZ1 50.00 %
GPNAME[2] SNSQ10.100
GPZ2 30.00 %
GPNAME[3] SNSQ10.100
GPZ3 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.9370100 MHz
FIDRES 615.157471 Hz
SW 260.838 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S120 HMBC spectrum (600 MHz, CDCl₃) of compound 18

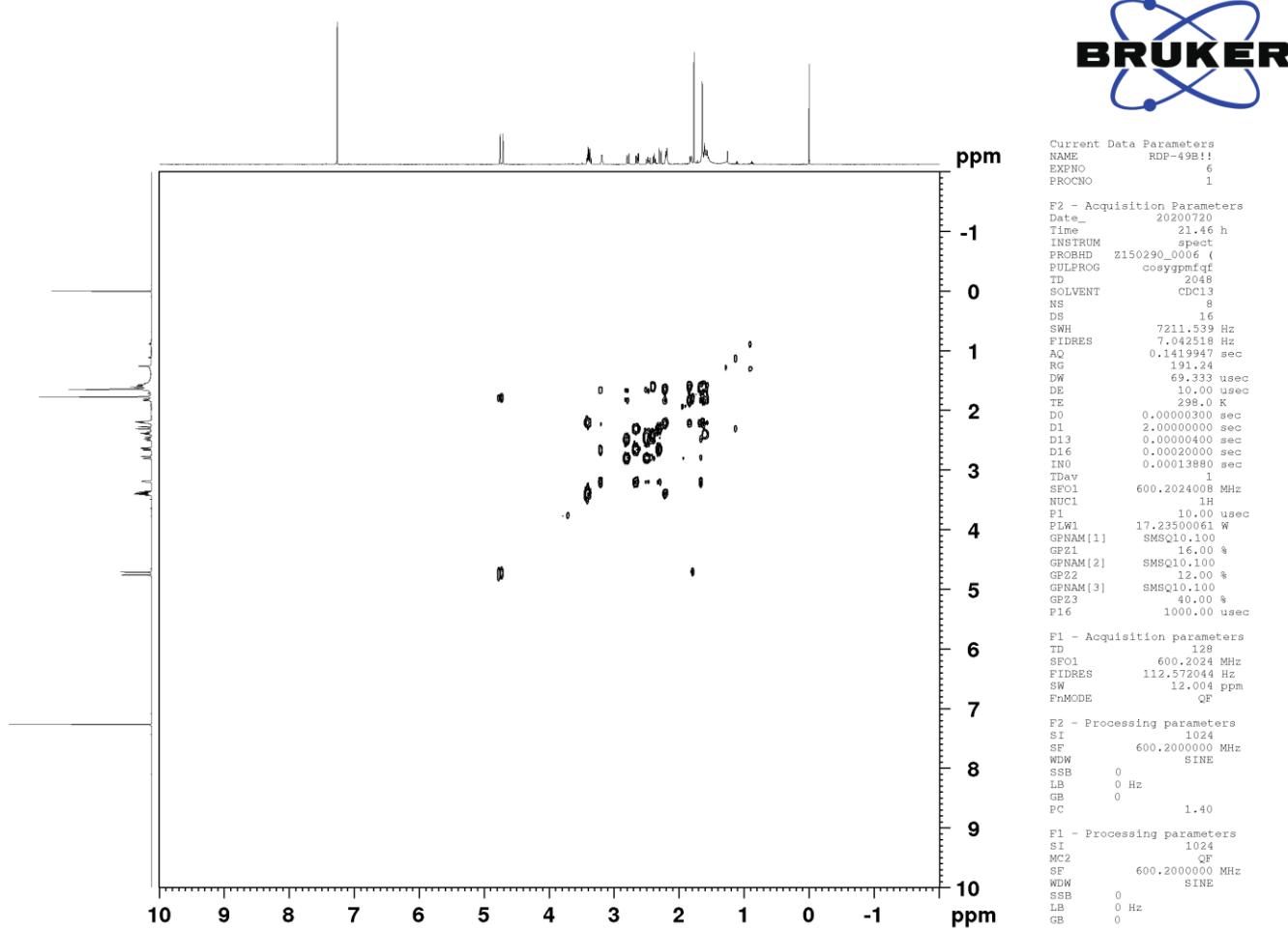


Figure S121 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **18**

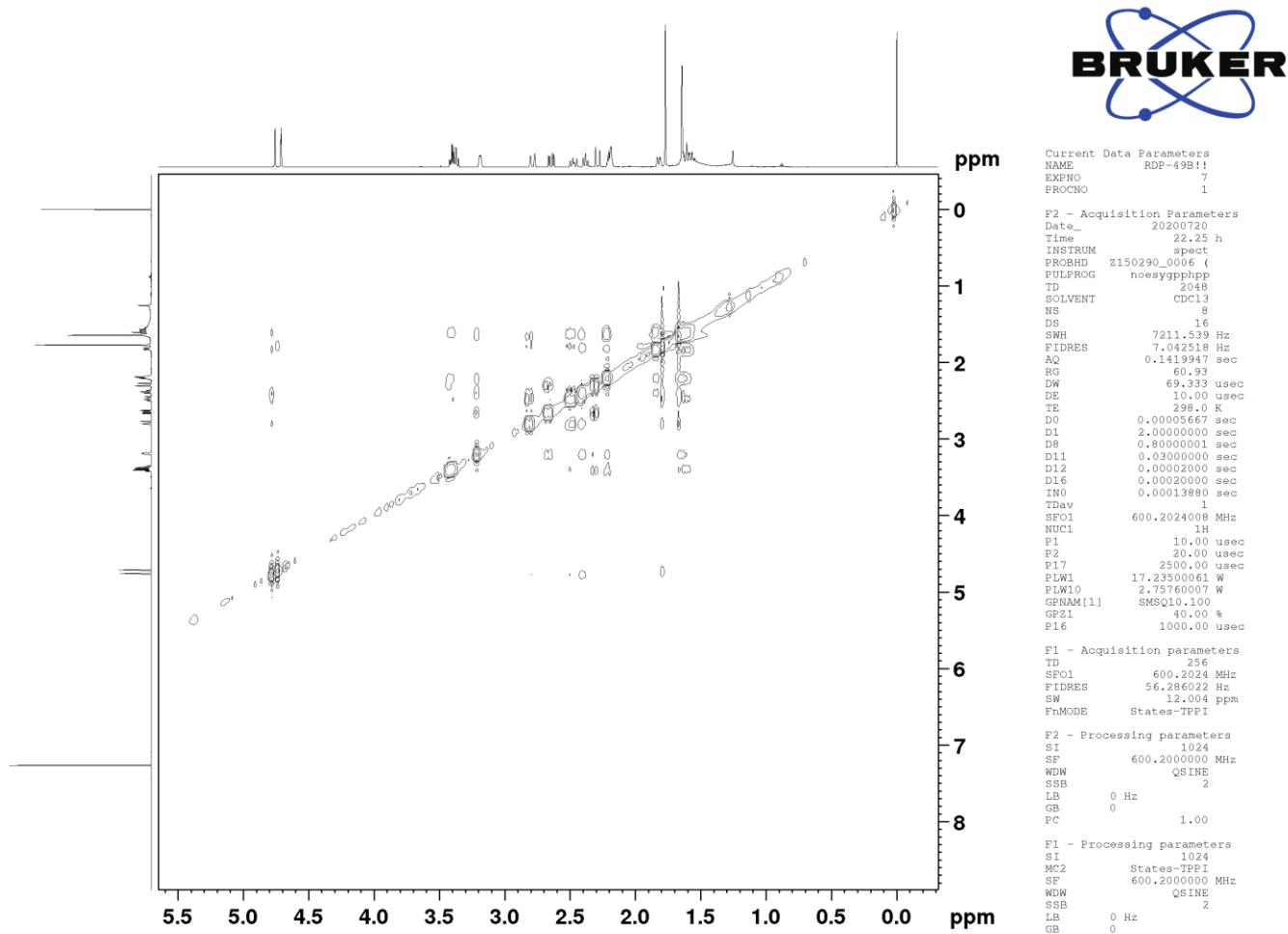


Figure S122 NOESY spectrum (600 MHz, CDCl_3) of compound **18**

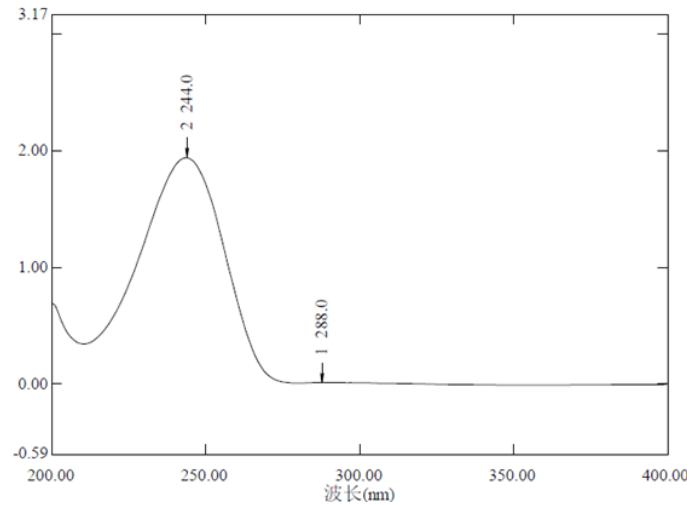
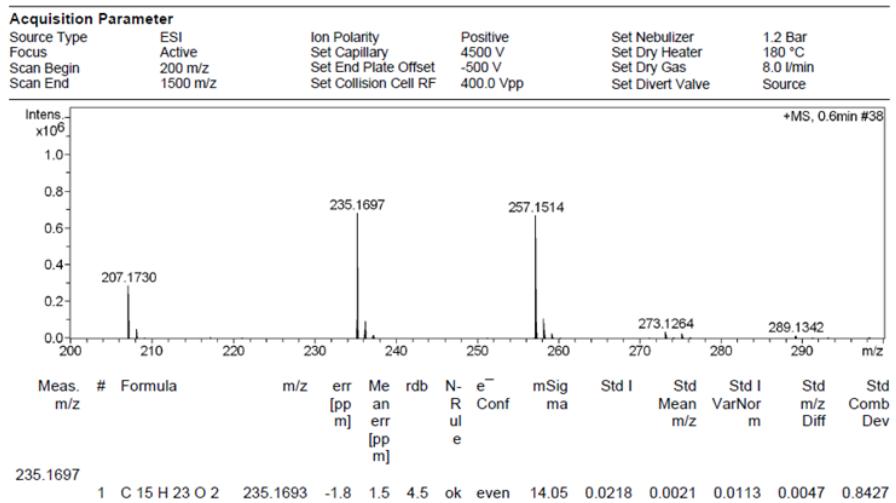


Figure S123 HRESIMS and UV spectra of compound **23**

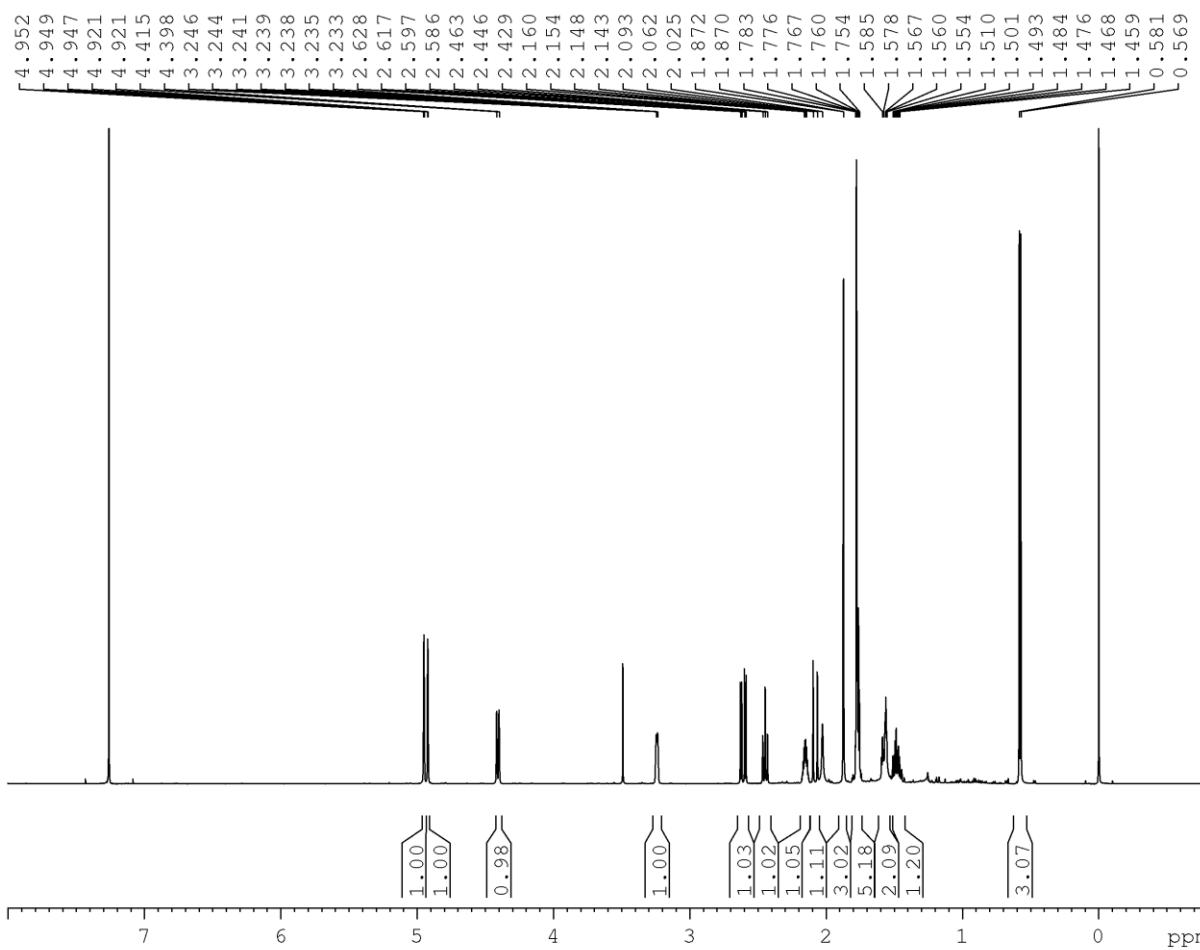
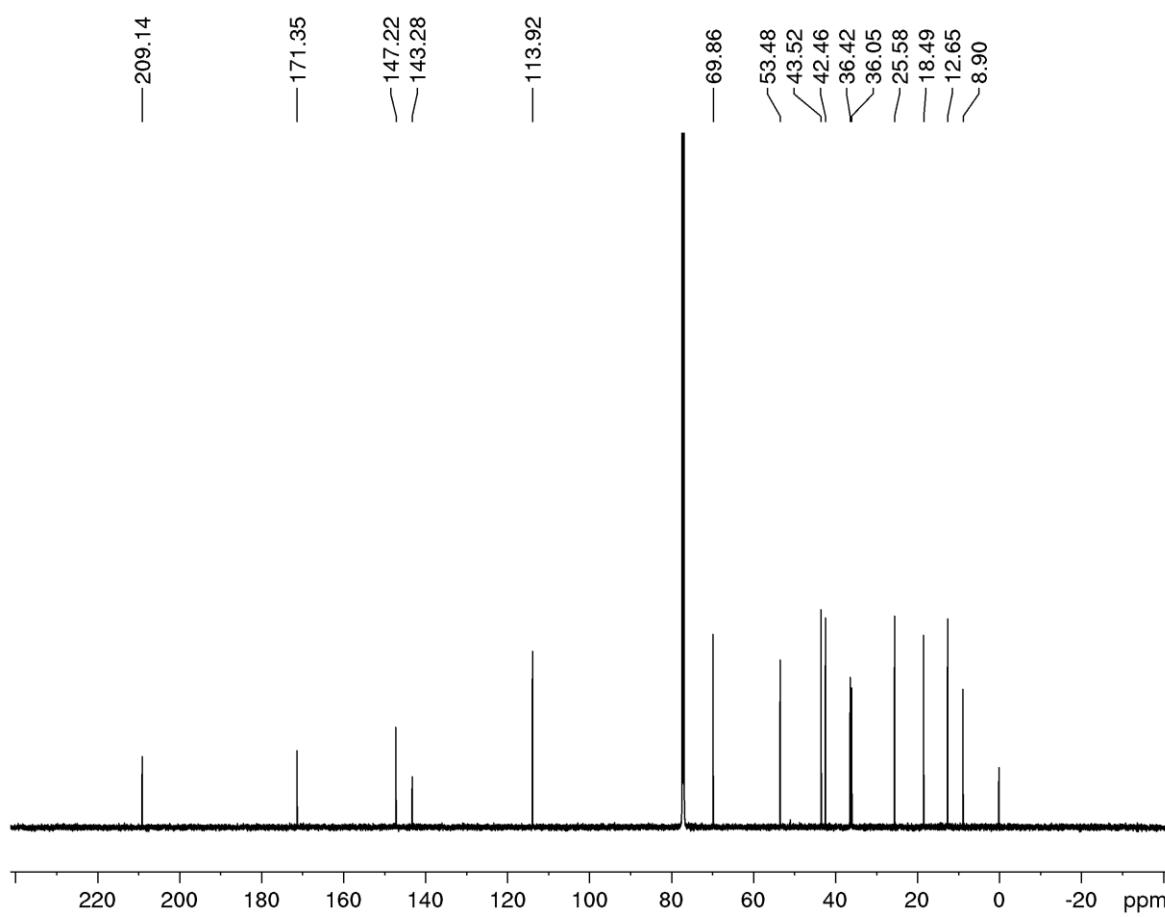


Figure S124 ¹H NMR spectrum (600 MHz, CDCl₃) of compound 23



Current Data Parameters
NAME RDP-126
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20201025
Time 4.41 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgpg30
TD 65356
SOLVENT CDCl3
NS 300
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 35.36
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9203889 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S125 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **23**

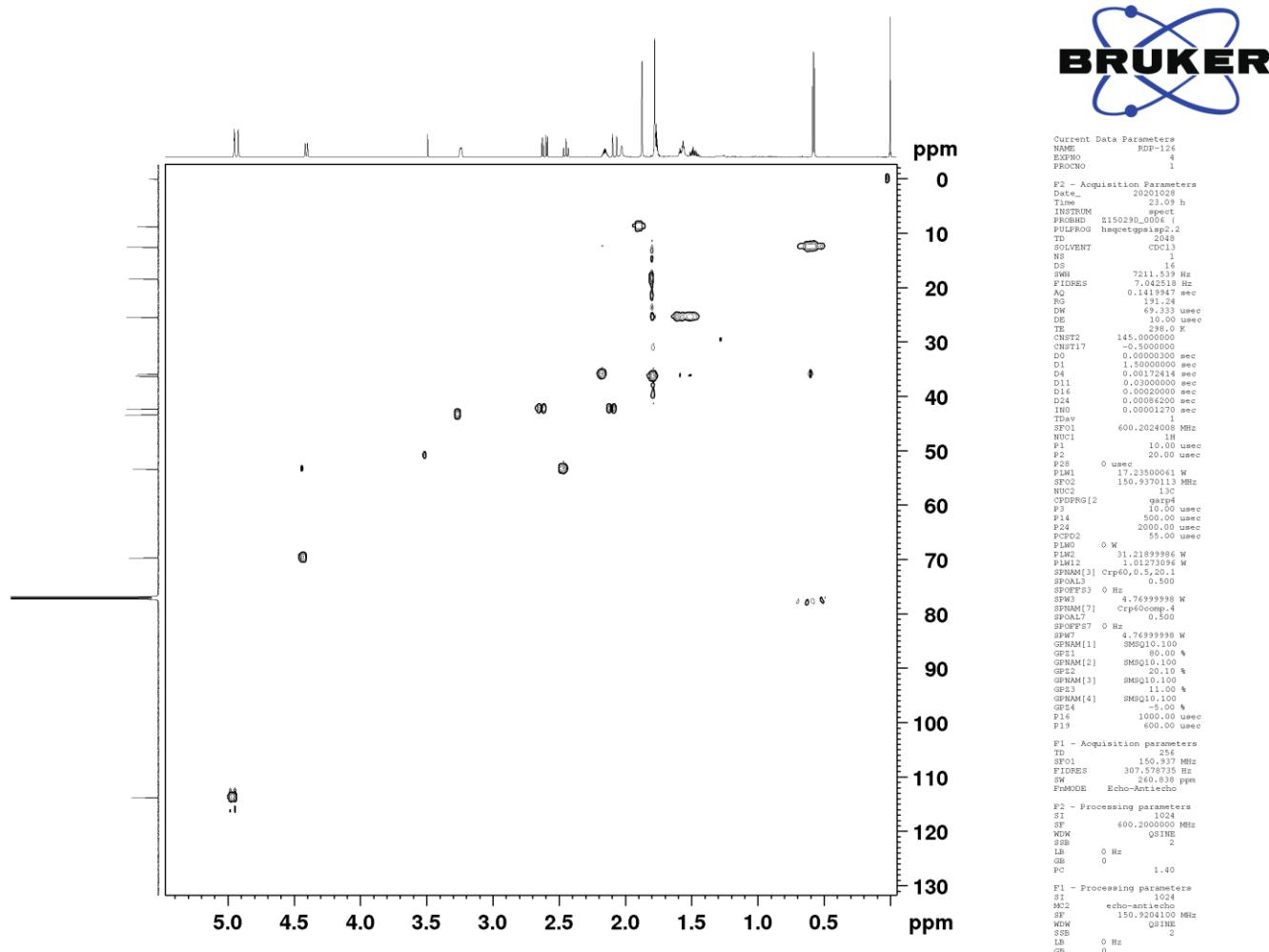


Figure S126 HSQC spectrum (600 MHz, CDCl₃) of compound 23

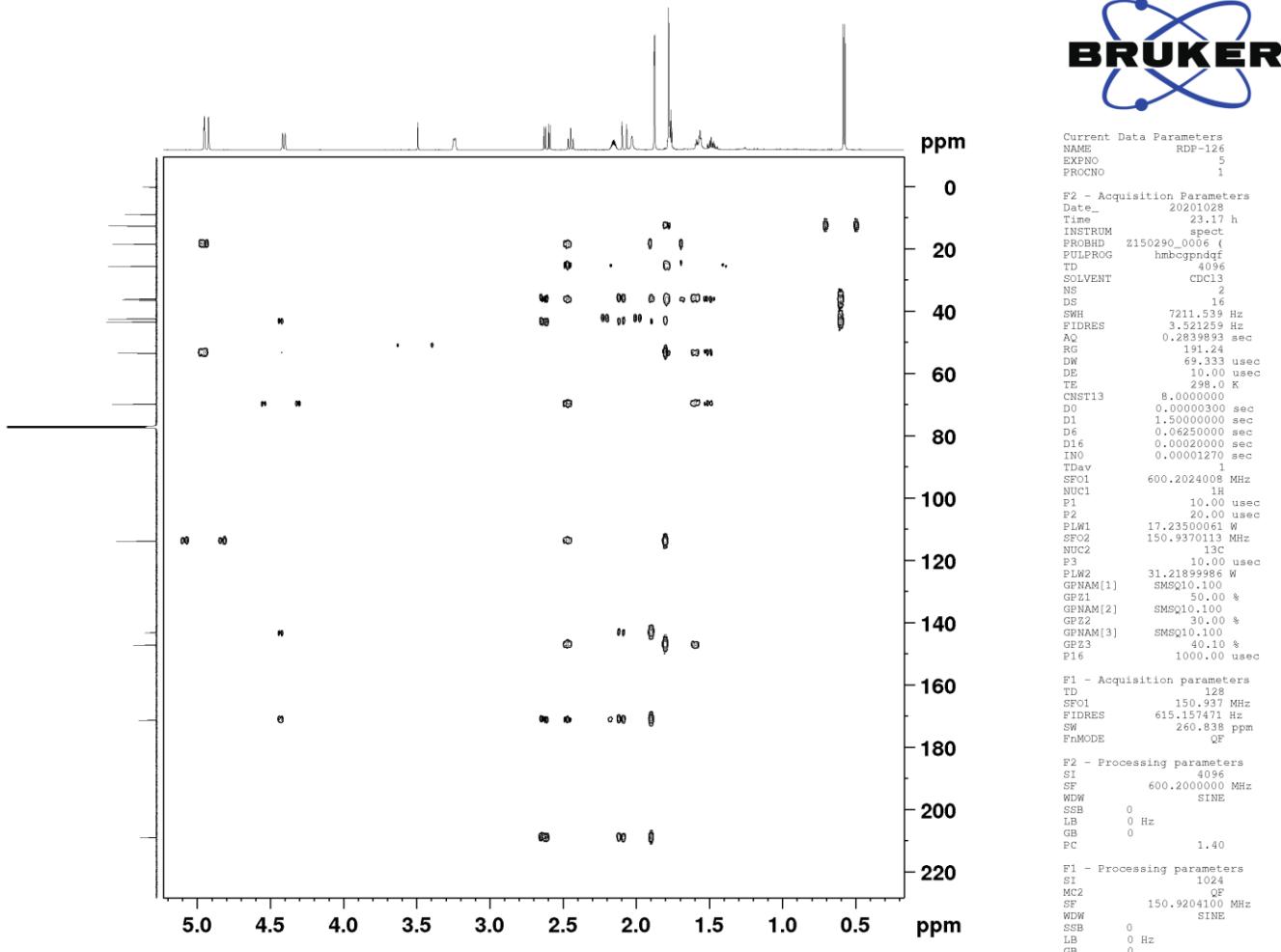


Figure S127 HMBC spectrum (600 MHz, CDCl₃) of compound **23**

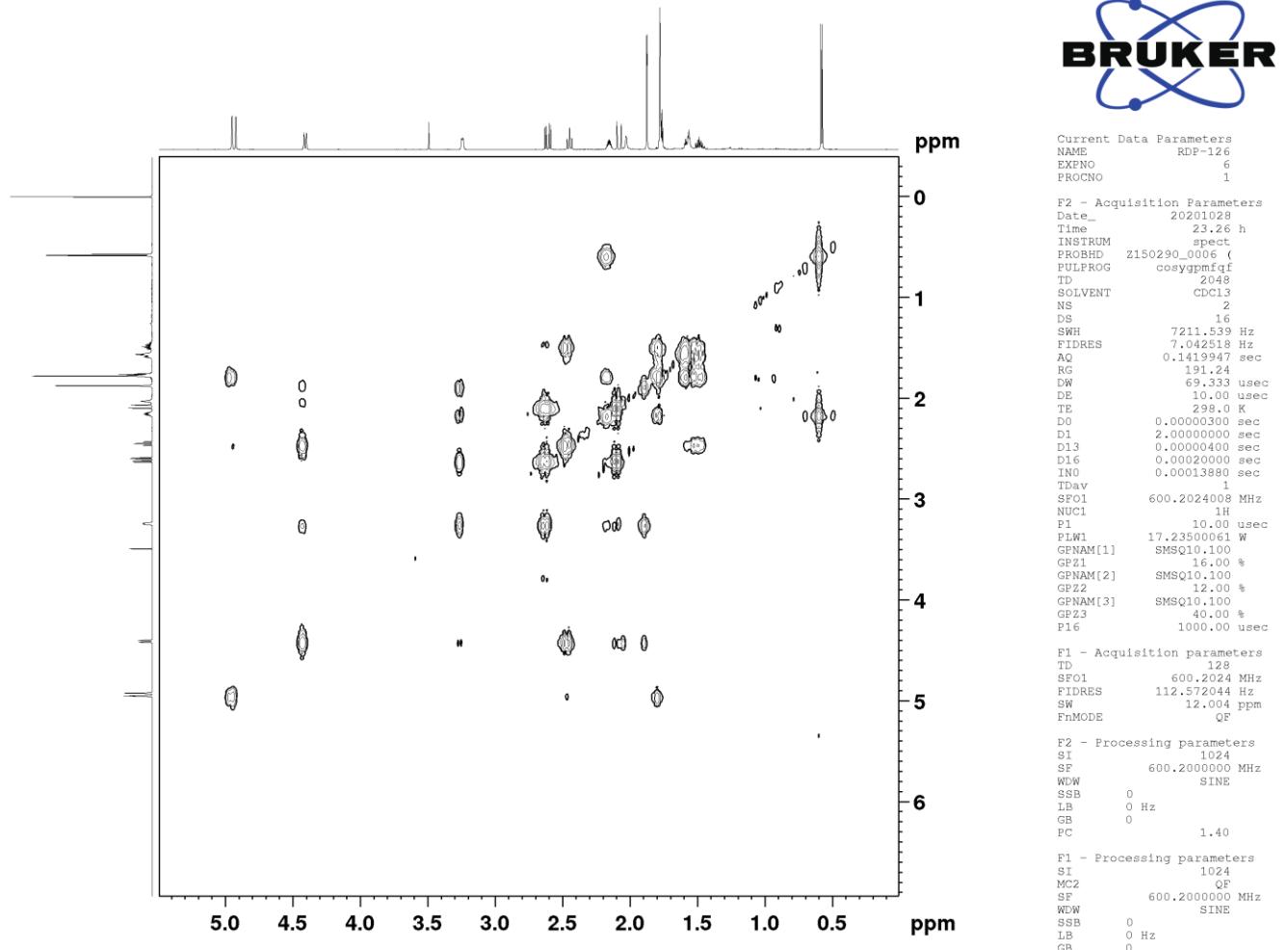
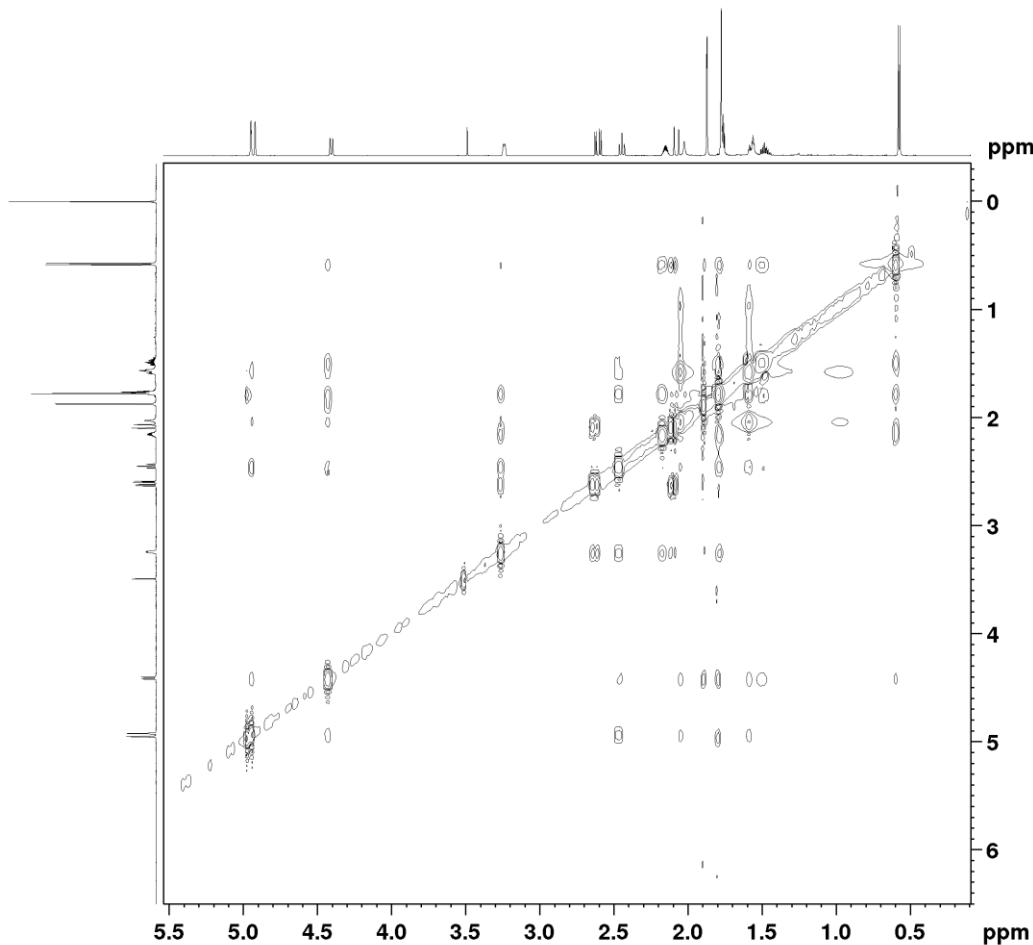


Figure S128 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **23**



Current Data Parameters
NAME RDP-126
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date 20201028
Time 23.36 h
INSTRUM spect
PROBHD Z150290_006 ('
PULFRCG ncesypphp
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60
DW 69.333 usec
DB 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D18 0.00013860 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S129 NOESY spectrum (600 MHz, CDCl₃) of compound **23**

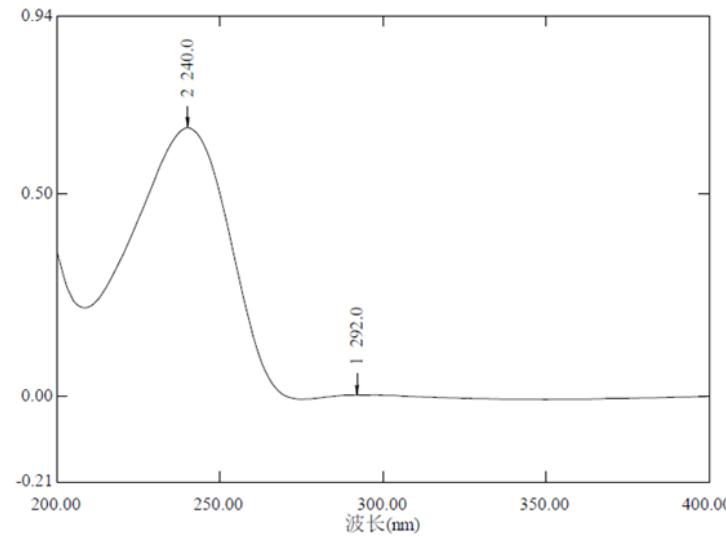
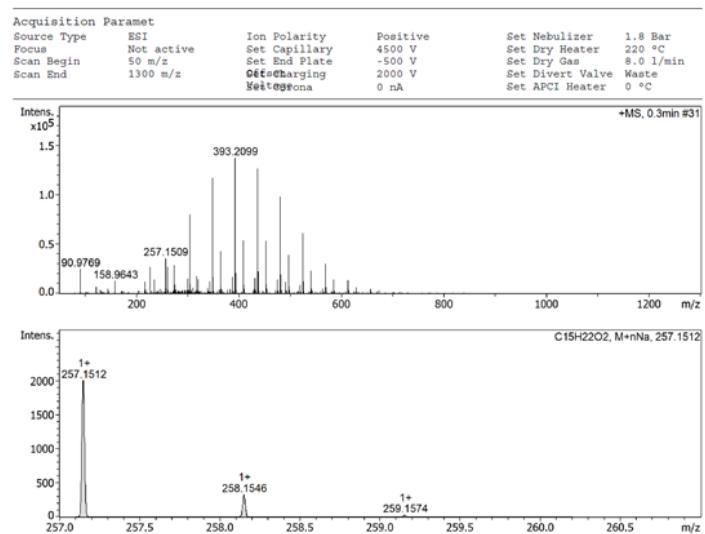
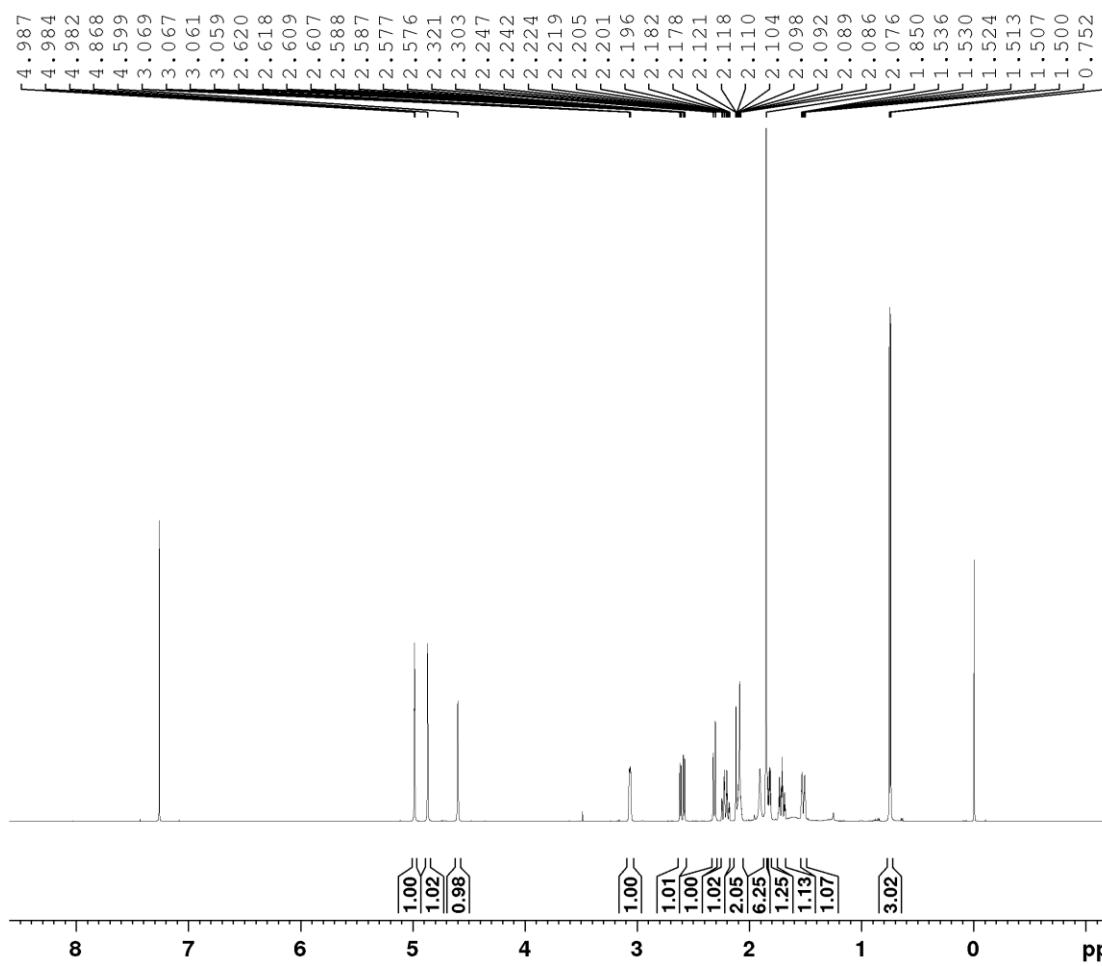


Figure S130 HRESIMS and UV spectra of compound 24

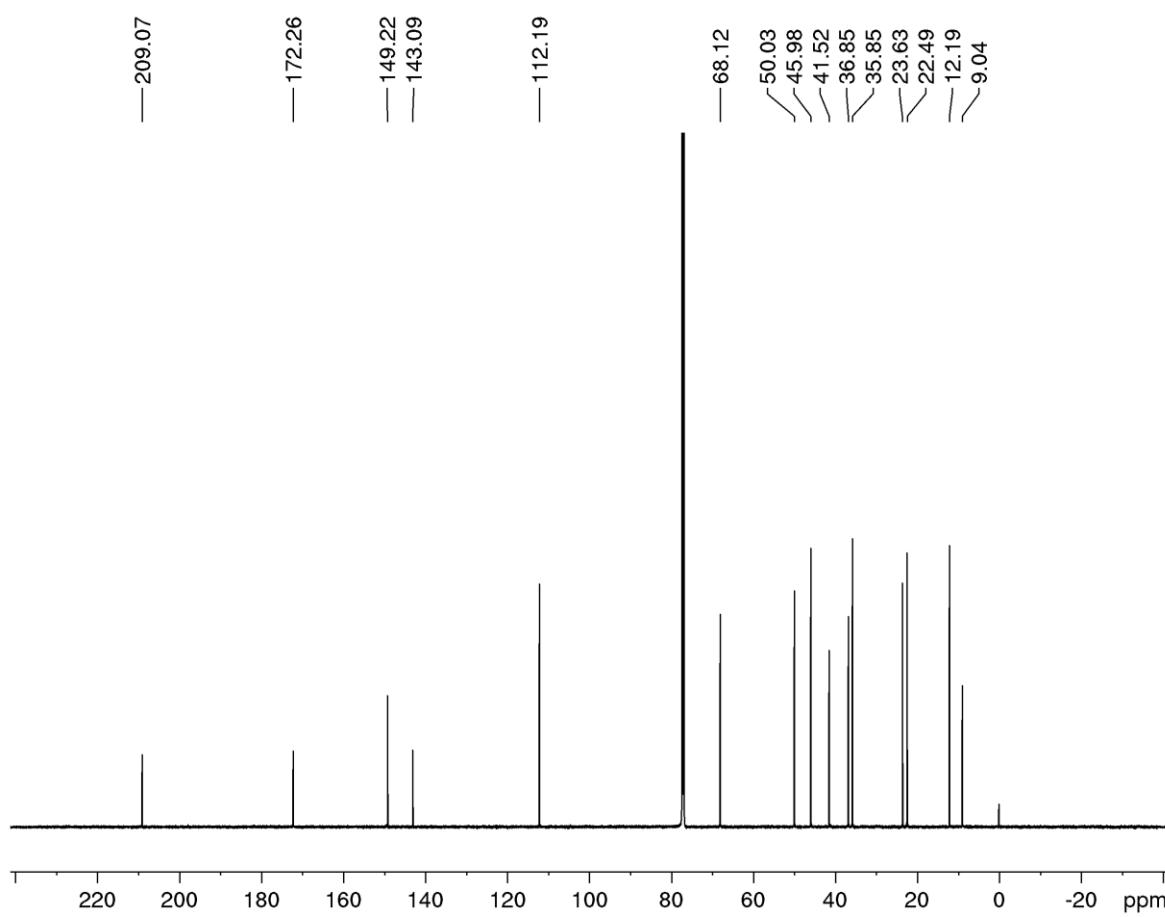


Current Data Parameters
NAME RDP-126-2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191103
Time 18.15 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 13.81
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1
SF01 600.2037062 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 23.40500069 W

F2 - Processing parameters
SI 65536
SF 600.2000141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S131 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **24**



Current Data Parameters
NAME RDP-126-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20191111
Time 1.57 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgpg30
TD 65356
SOLVENT CDCl3
NS 500
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 28.15
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 25.65299988 W
SFO2 600.2030010 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 23.40500069 W
PLW12 0.22597121 W
PLW13 0.11325680 W

F2 - Processing parameters
SI 32768
SF 150.9203908 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S132 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **24**

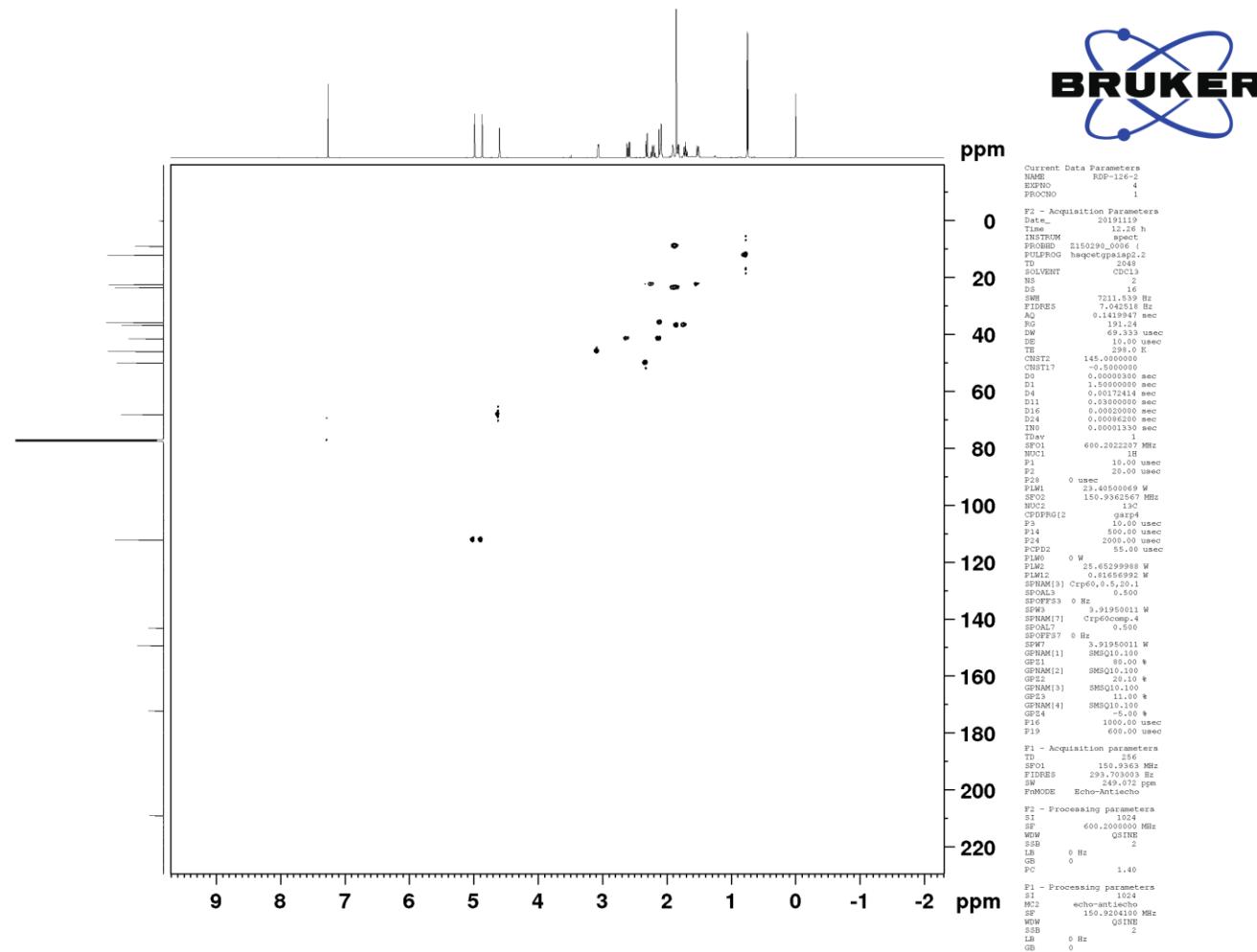


Figure S133 HSQC spectrum (600 MHz, CDCl₃) of compound 24

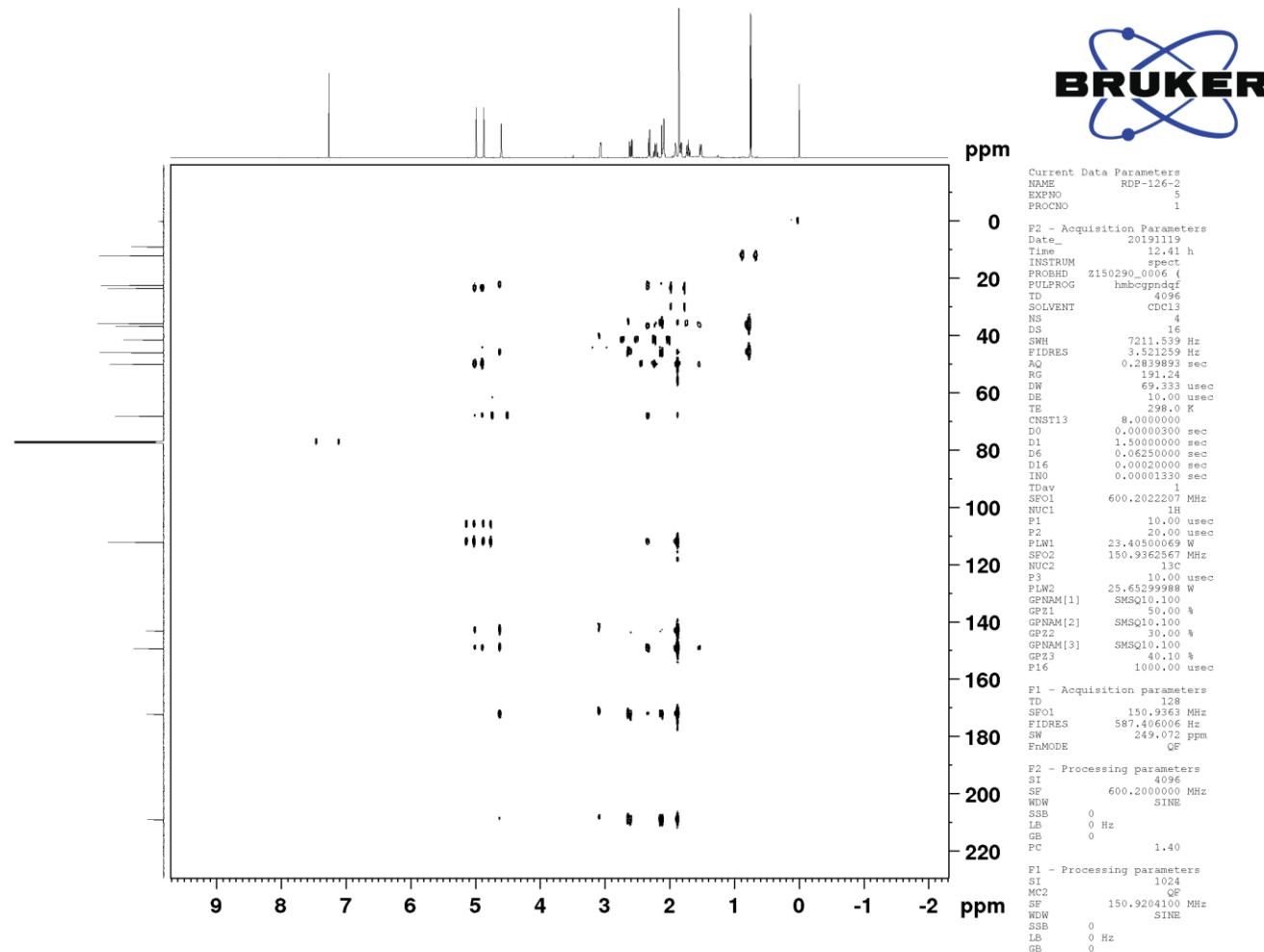


Figure S134 HMBC spectrum (600 MHz, CDCl₃) of compound **24**

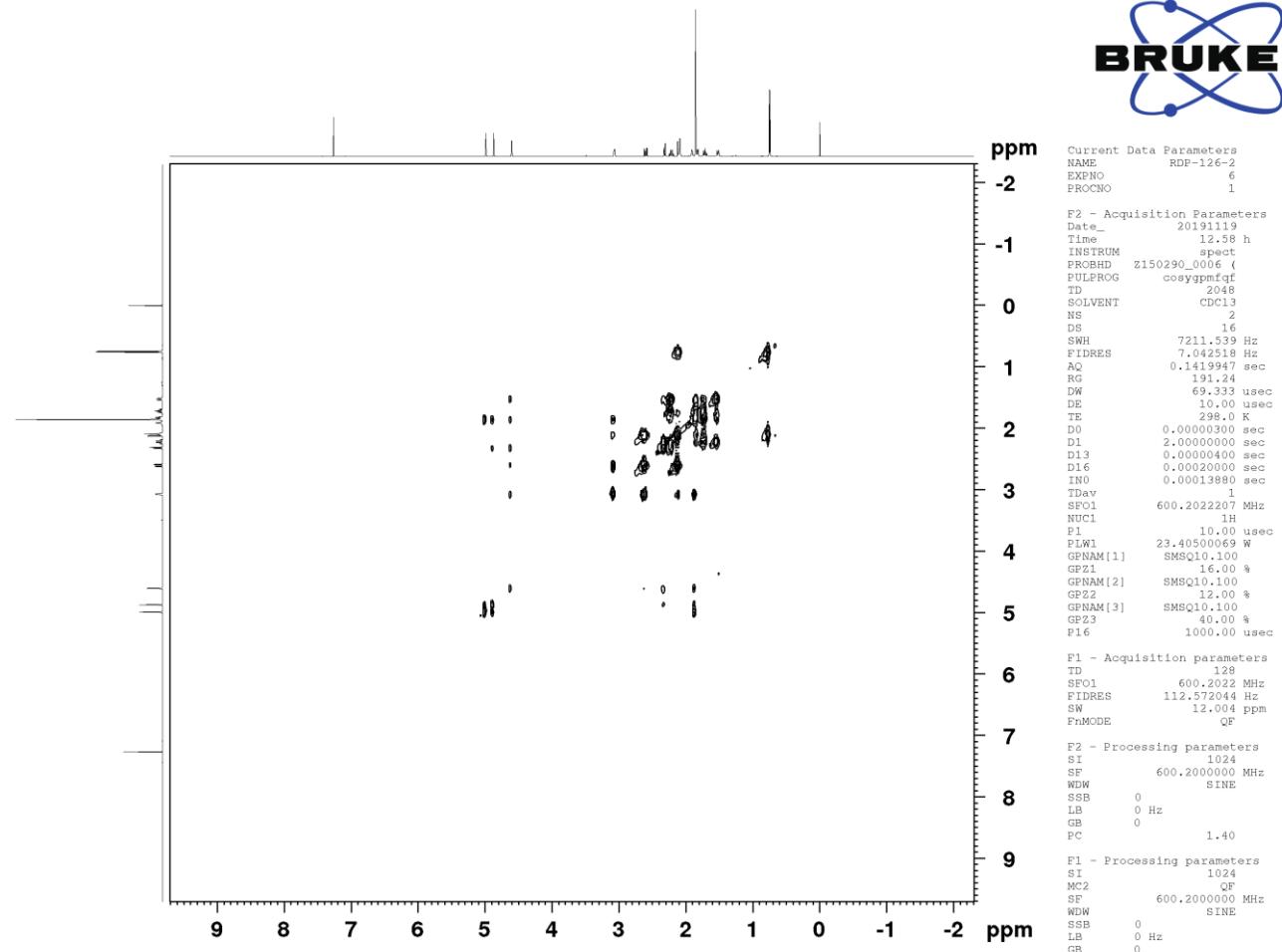


Figure S135 ¹H-¹H COSY spectrum (600 MHz, CDCl₃) of compound 24

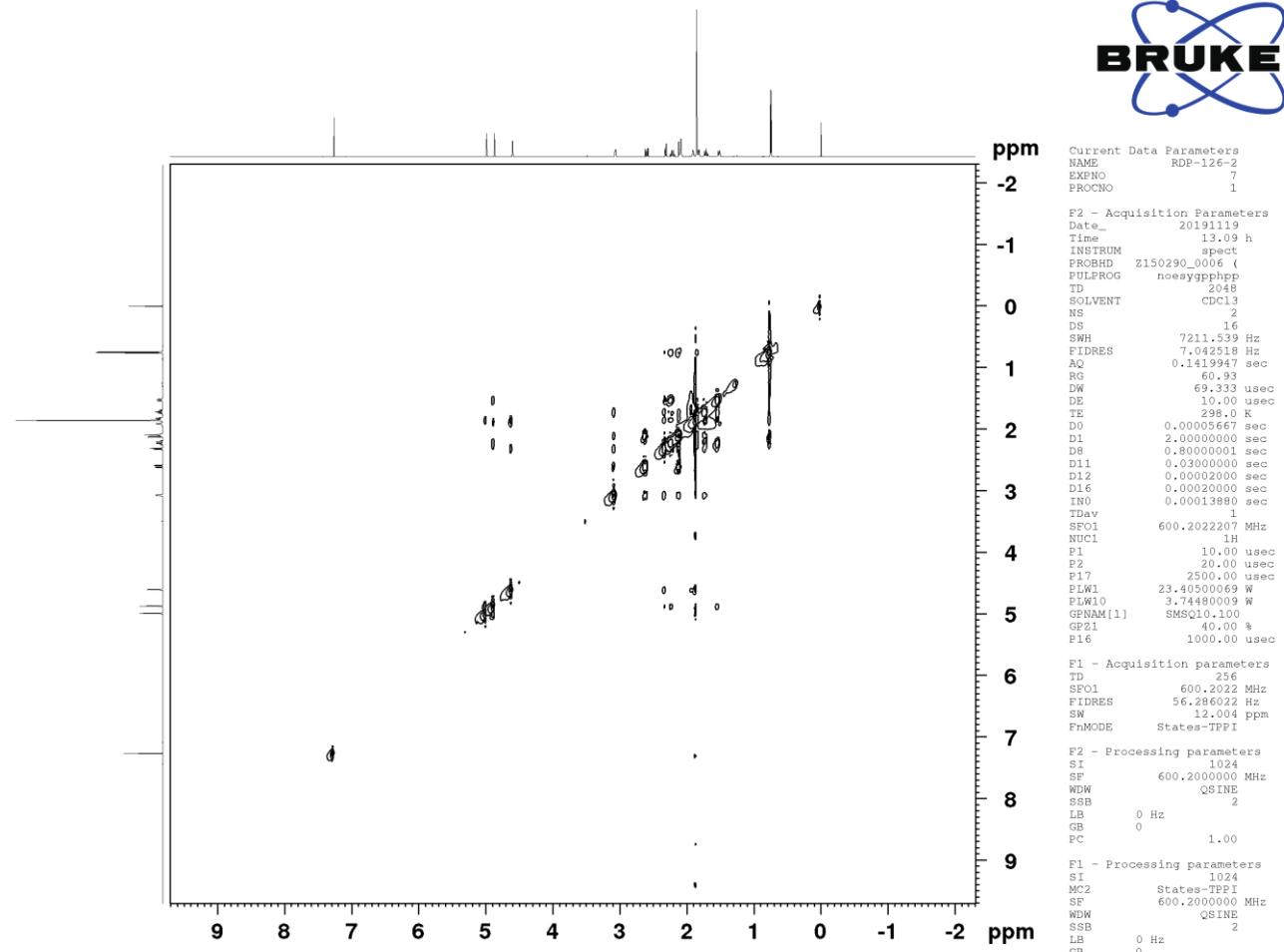


Figure S136 NOESY spectrum (600 MHz, CDCl₃) of compound 24

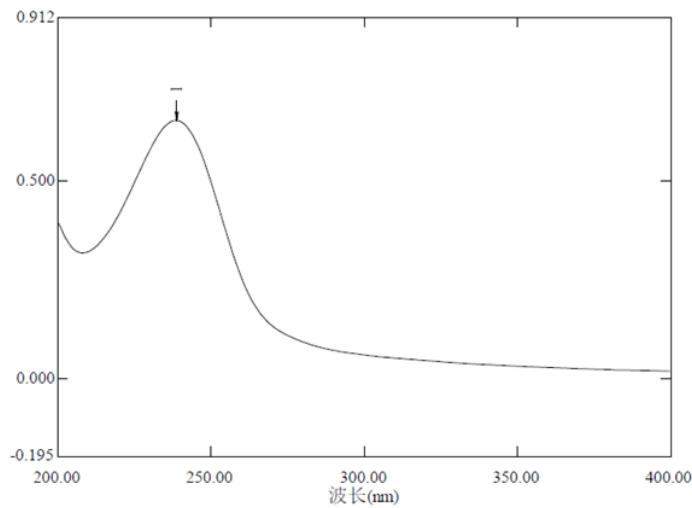
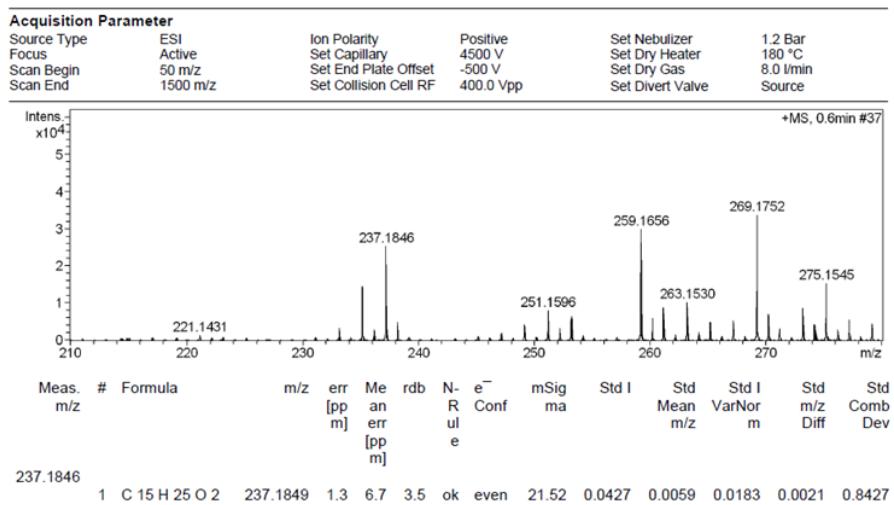


Figure S137 HRESIMS and UV spectra of compound 25

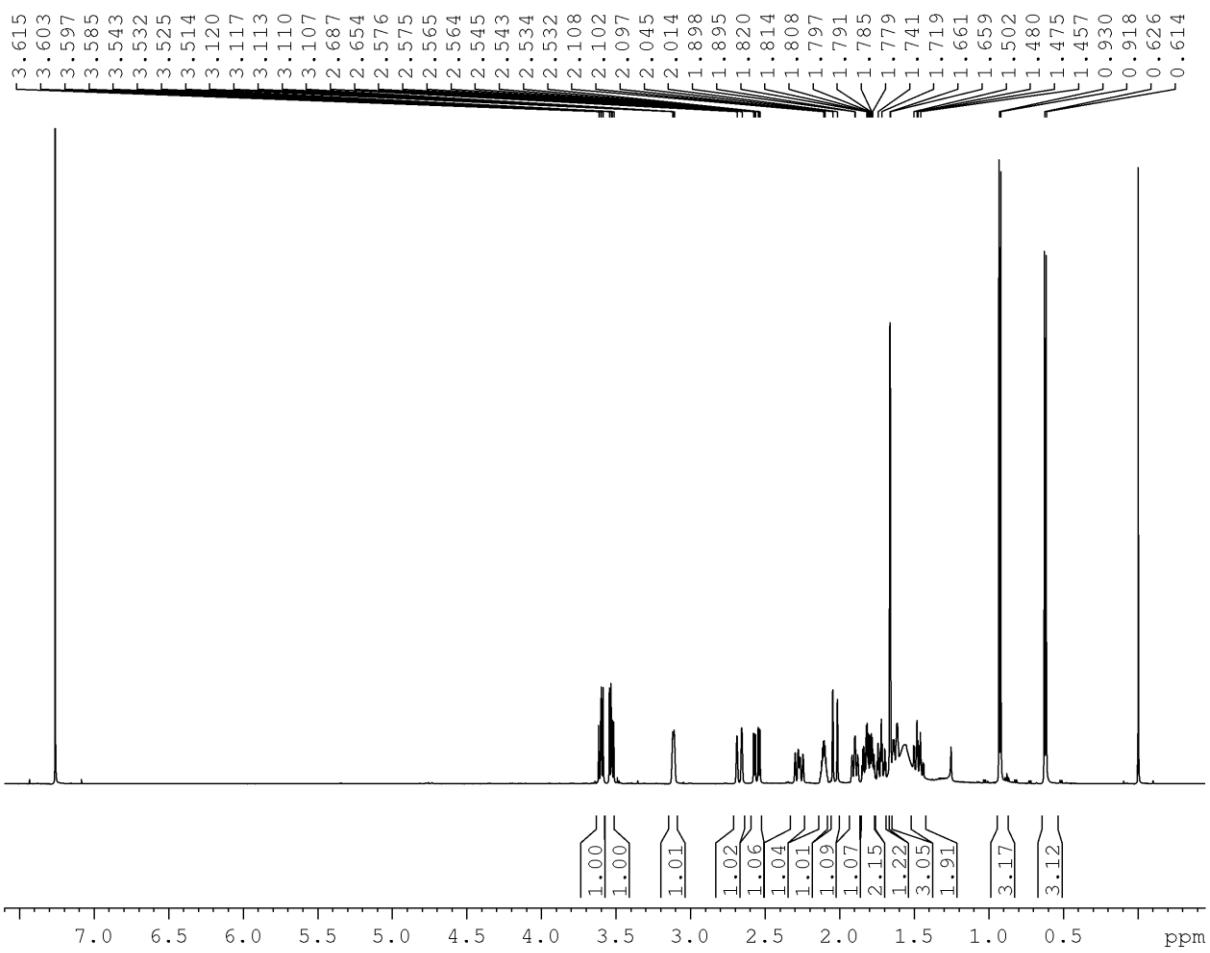
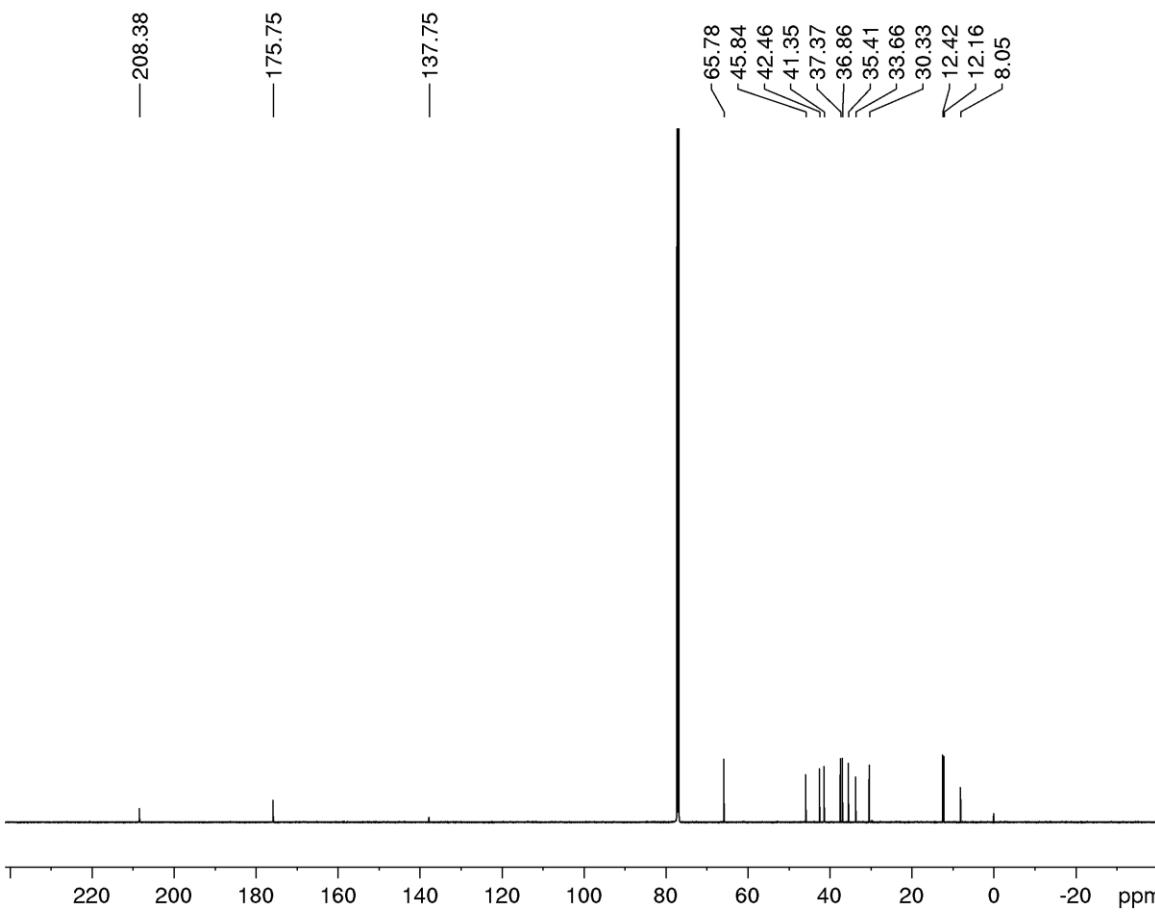


Figure S138 ¹H NMR spectrum (600 MHz, CDCl₃) of compound 25



Current Data Parameters
NAME RDP-65!!
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200712
Time_ 15.56 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgppg30
TD 65356
SOLVENT CDCl3
NS 500
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 37.95
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9204119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S139 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **25**

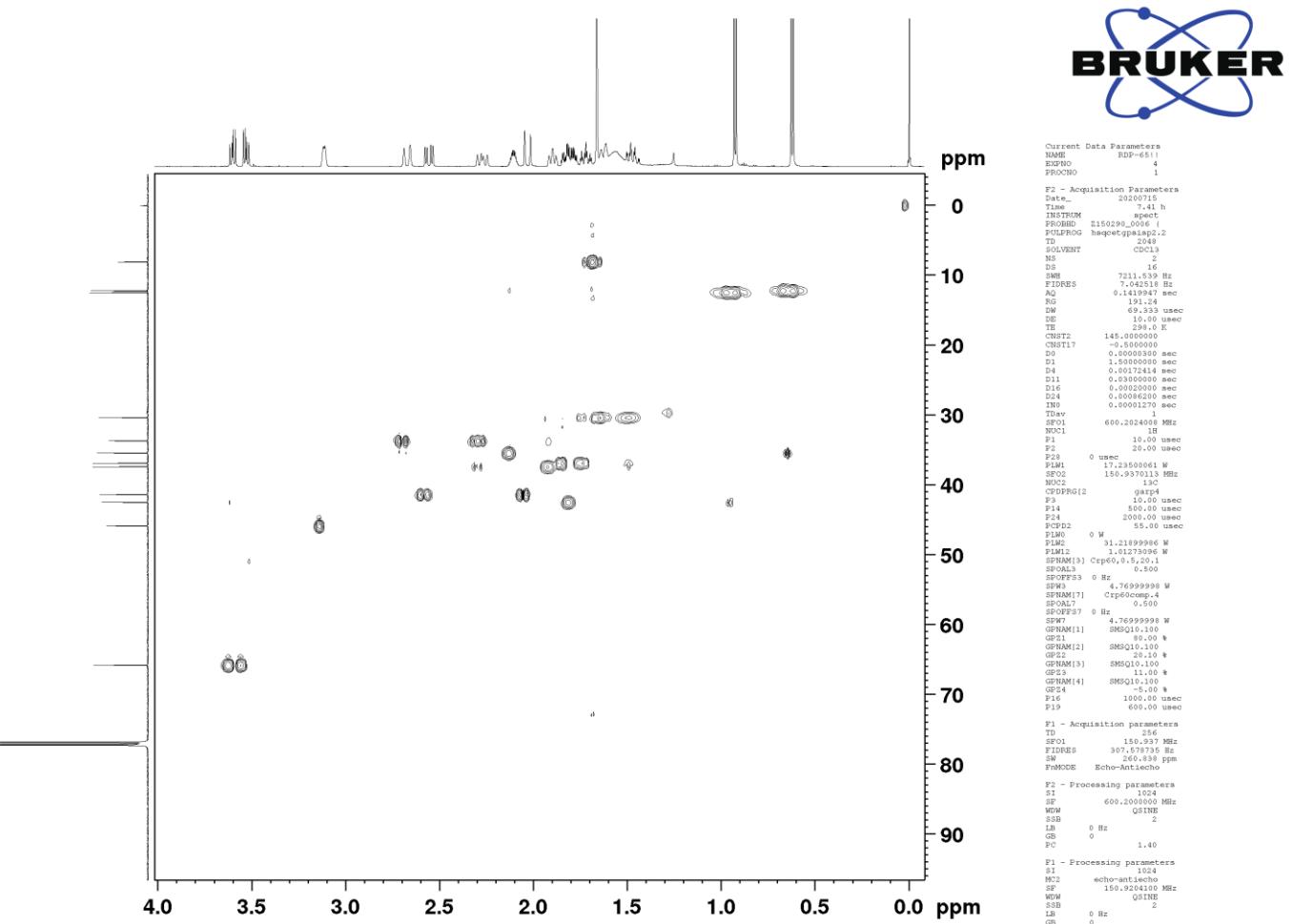
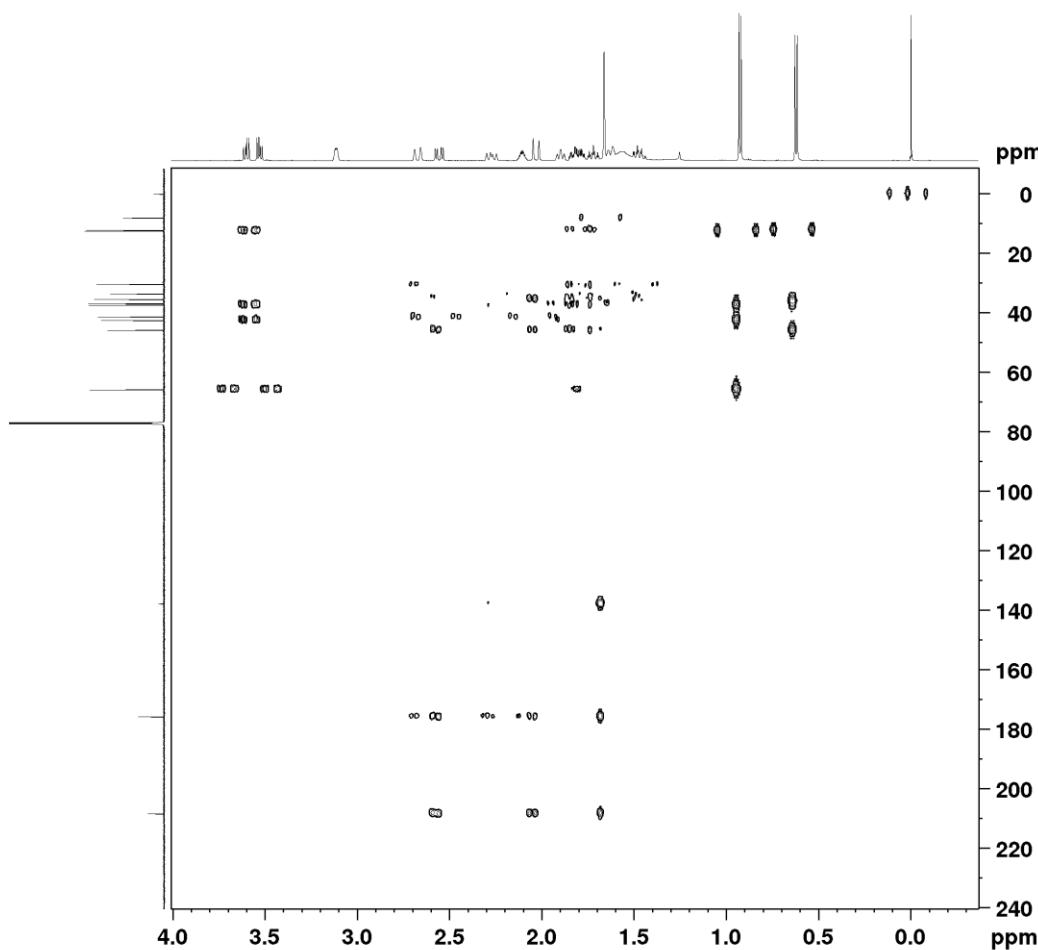


Figure S140 HSQC spectrum (600 MHz, CDCl₃) of compound 25



Current Data Parameters
NAME RDP-65!!
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200715
Time 7.57 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG hmbcgrndqf
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 130
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.0000000
D0 0.0000300 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001270 sec
TDav 1
SF01 600.2024010 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLN1 17.23500061 W
SF02 150.9370113 MHz
NUC2 13C
P3 10.00 usec
PLN2 31.21899986 W
GPNAME[1] SNSQ10.100
GPZ1 50.00 %
GPNAME[2] SNSQ10.100
GPZ2 30.00 %
GPNAME[3] SNSQ10.100
GPZ3 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.9370113 MHz
FIDRES 615.157471 Hz
SW 260.838 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S141 HMBC spectrum (600 MHz, CDCl_3) of compound 25

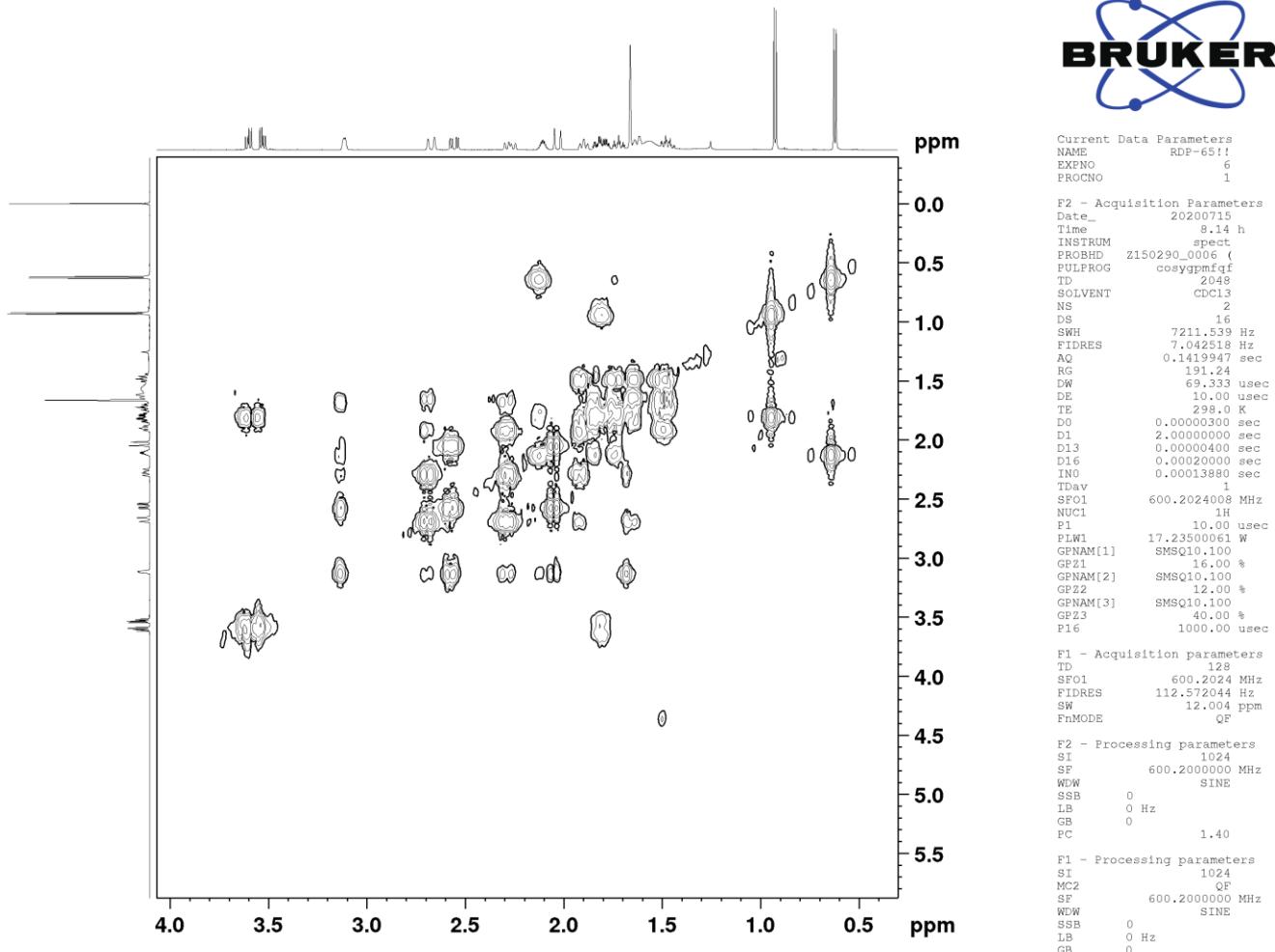
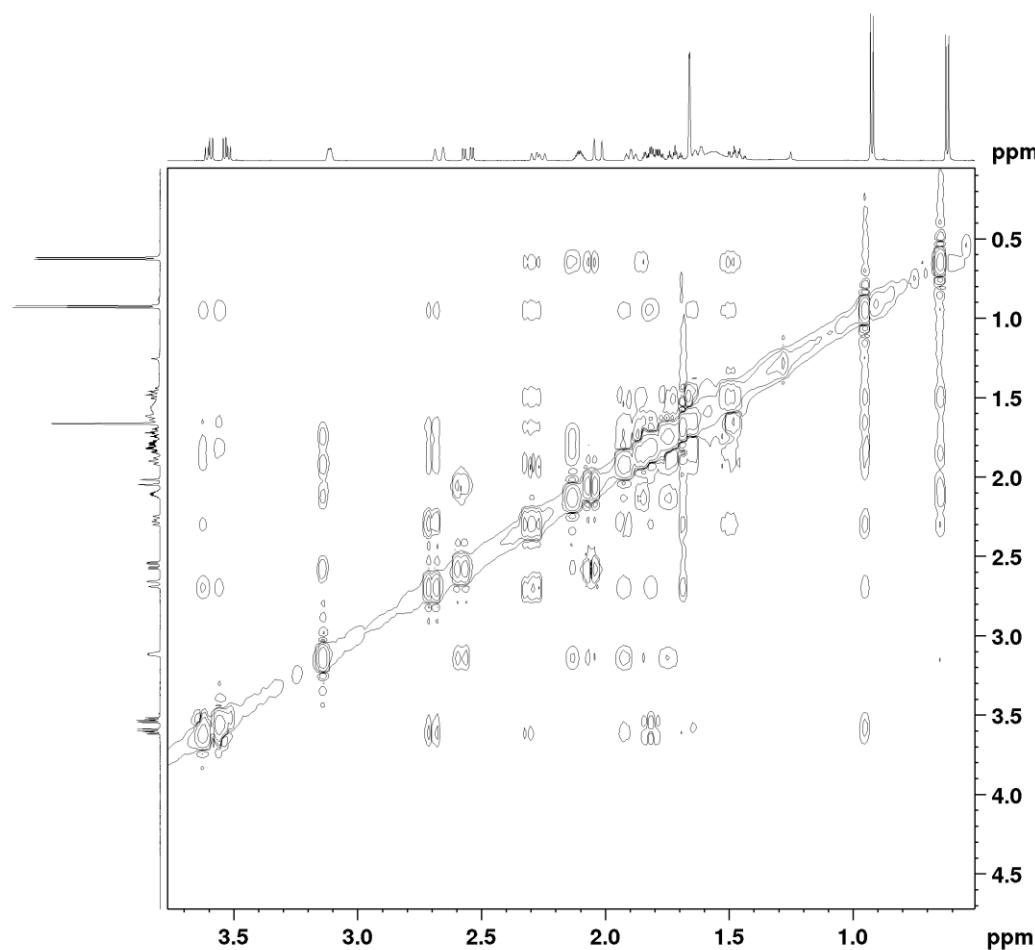


Figure S142 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **25**



Current Data Parameters
NAME RDP-651!!
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200715
Time 8.25 h
INSTRUM spect
PROBHD Z150290_0066_1
PULPROG noe3sypphp
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D18 0.00013860 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW States-TPPI
SSB 2
LB 0 Hz
GB 0

Figure S143 NOESY spectrum (600 MHz, CDCl_3) of compound **25**

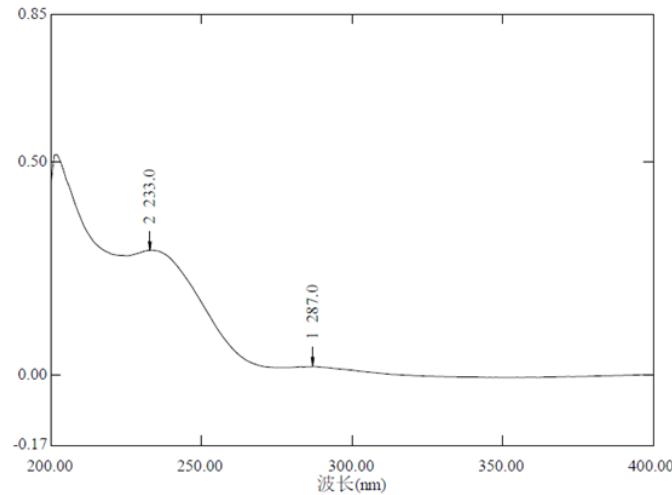
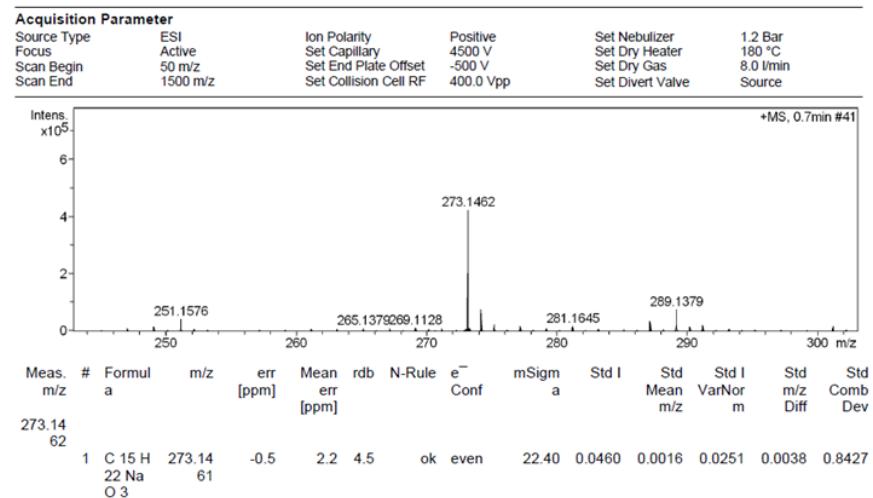


Figure S144 HRESIMS and UV spectra of compound 27

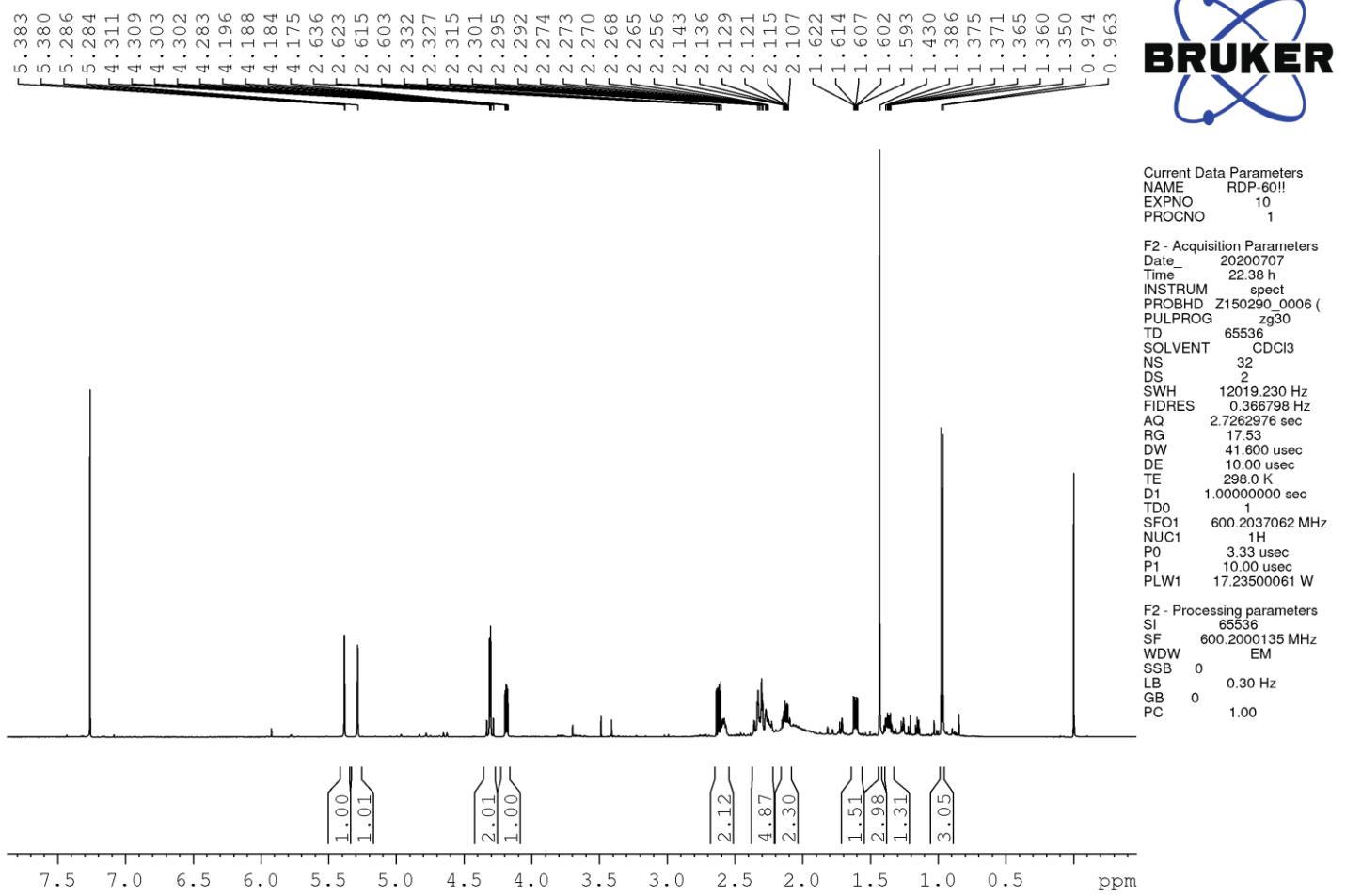


Figure S145 ^1H NMR spectrum (600 MHz, CDCl_3) of compound 27

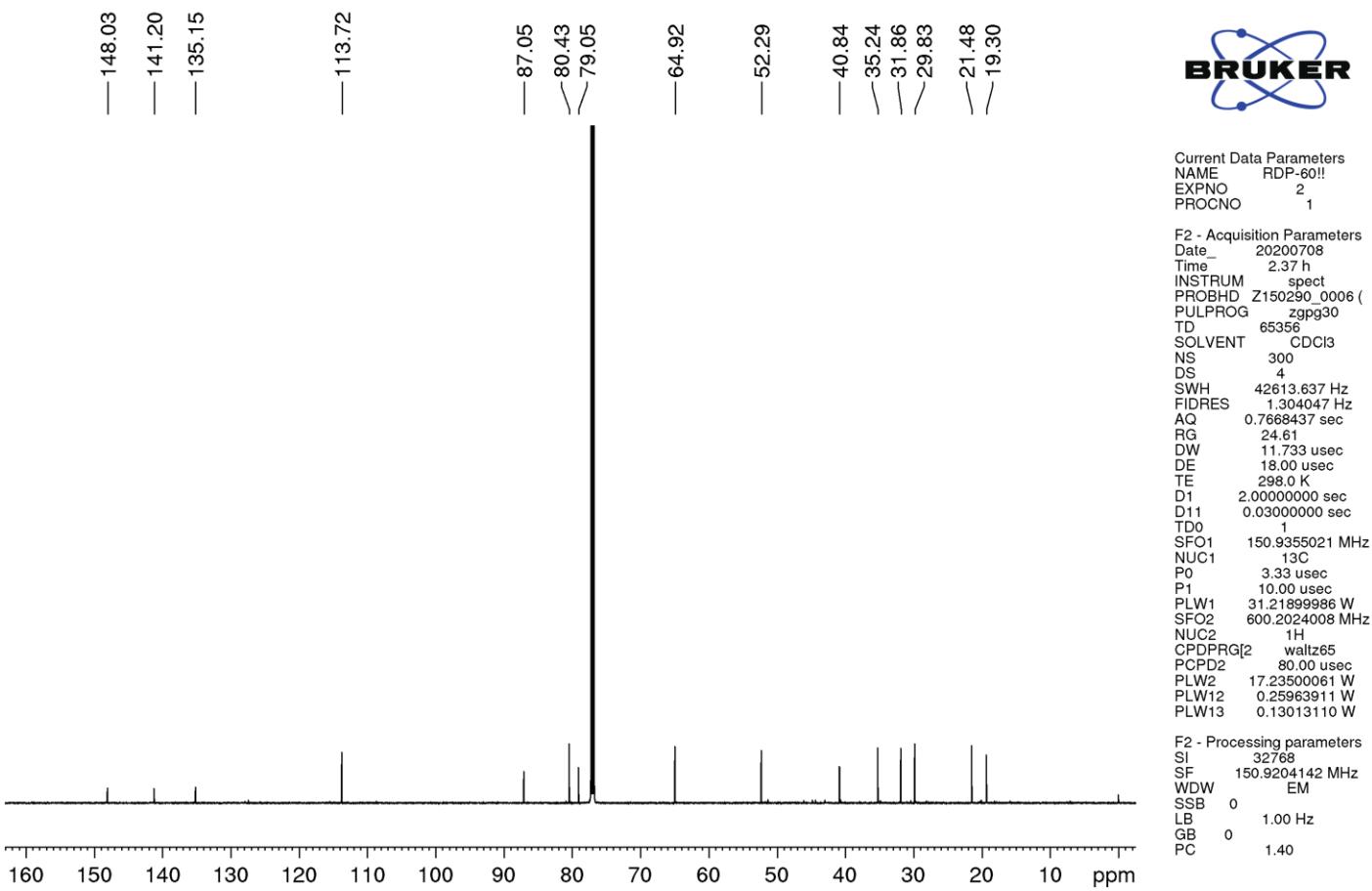


Figure S146 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **27**

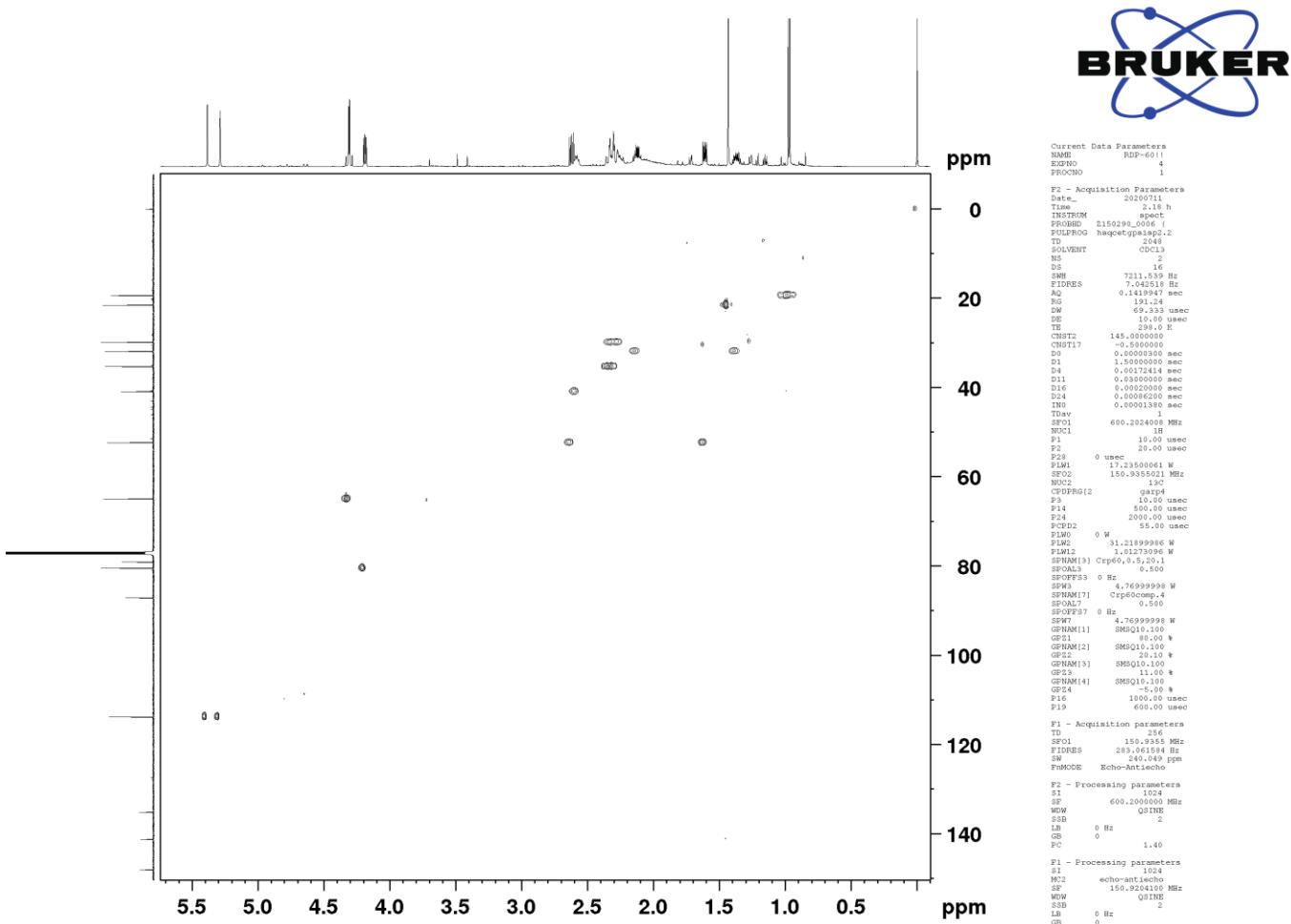
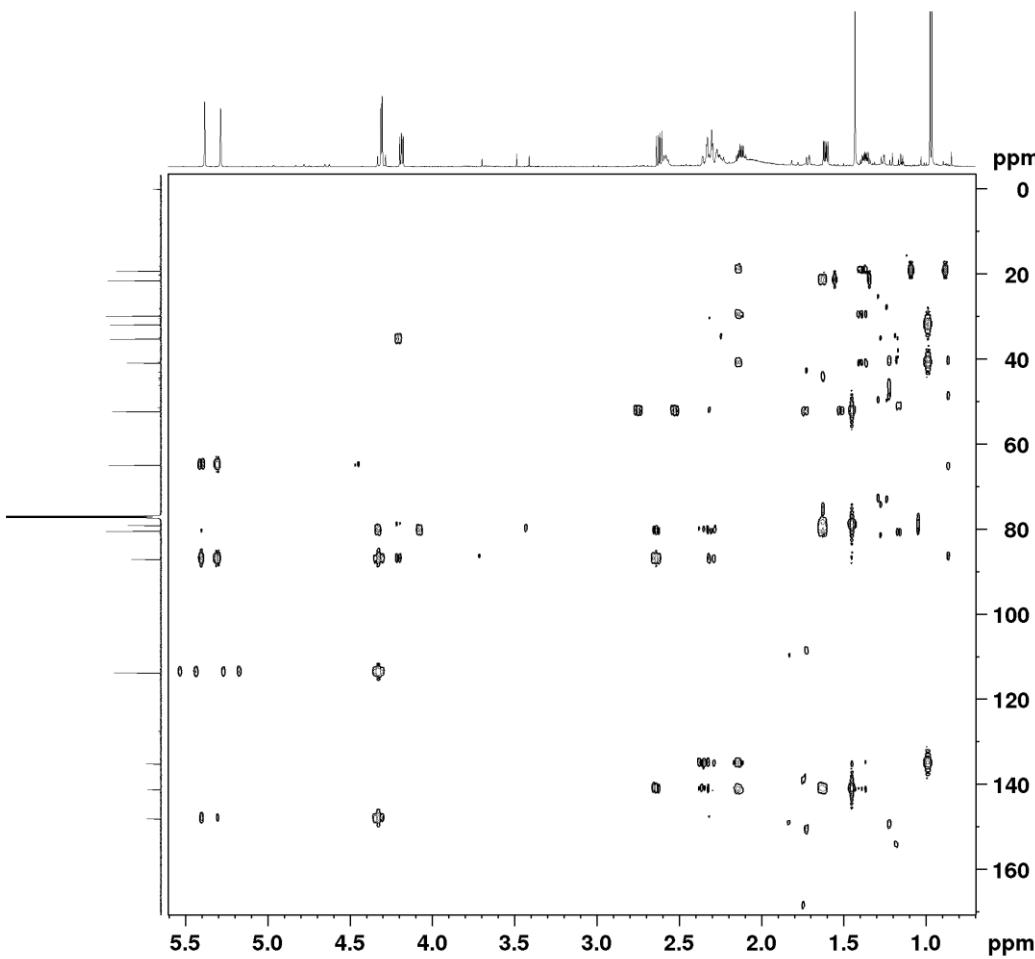


Figure S147 HSQC spectrum (600 MHz, CDCl₃) of compound 27



Current Data Parameters
NAME RDP-60!!
EXPNO 5
PROCNO 1

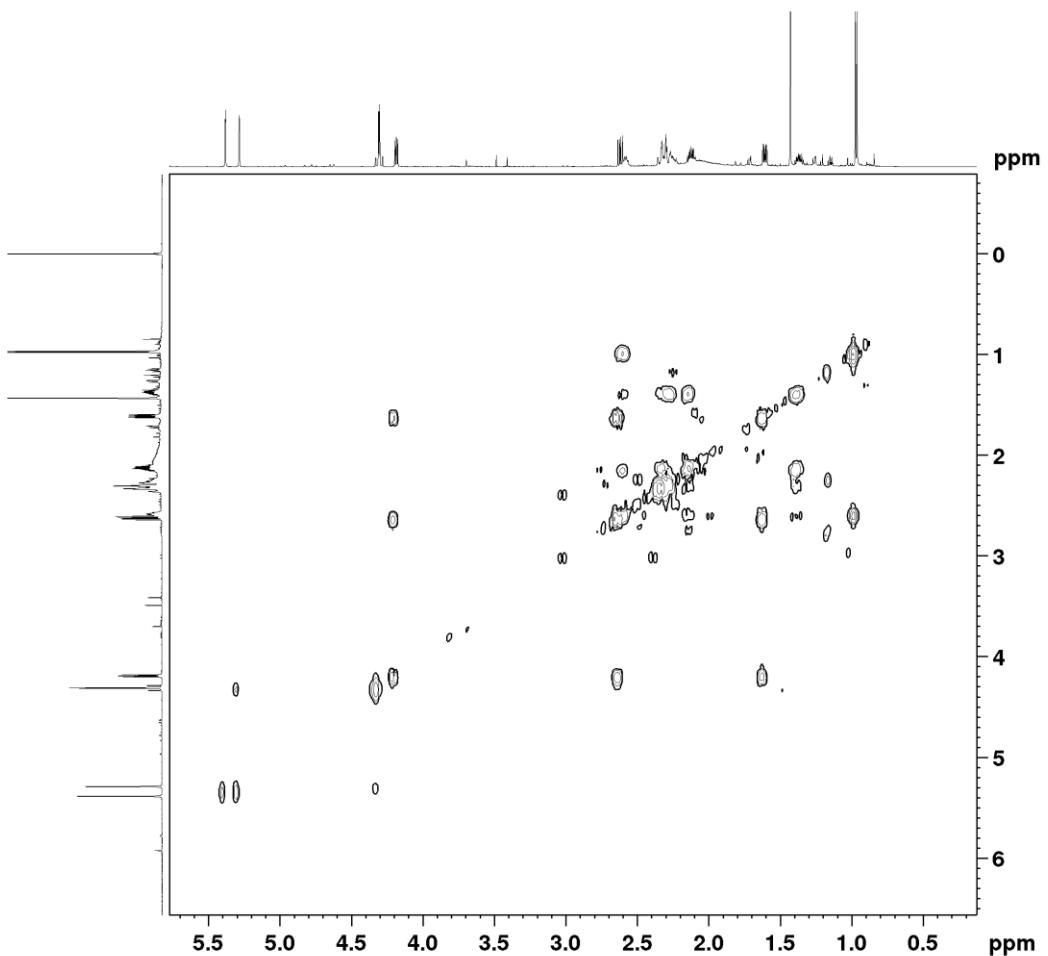
F2 - Acquisition Parameters
Date_ 20200711
Time 2.34 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG hmbcgrndqf
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 130
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.0000000
D0 0.0000000 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001380 sec
TDav 600.2024000
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
SFO1 600.2024000 MHz
NUC2 13C
P3 10.00 usec
PLW2 31.21899986 W
GPNAME[1] SNSQ10.100
GPZ1 50.00 %
GPNAME[2] SNSQ10.100
GPZ2 30.00 %
GPNAME[3] SNSQ10.100
GPZ3 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.933 MHz
FIDRES 566.123169 Hz
SW 240.049 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S148 HMBC spectrum (600 MHz, CDCl_3) of compound 27



Current Data Parameters
NAME RDP-601!
EXPNO 6
PROCNO 1

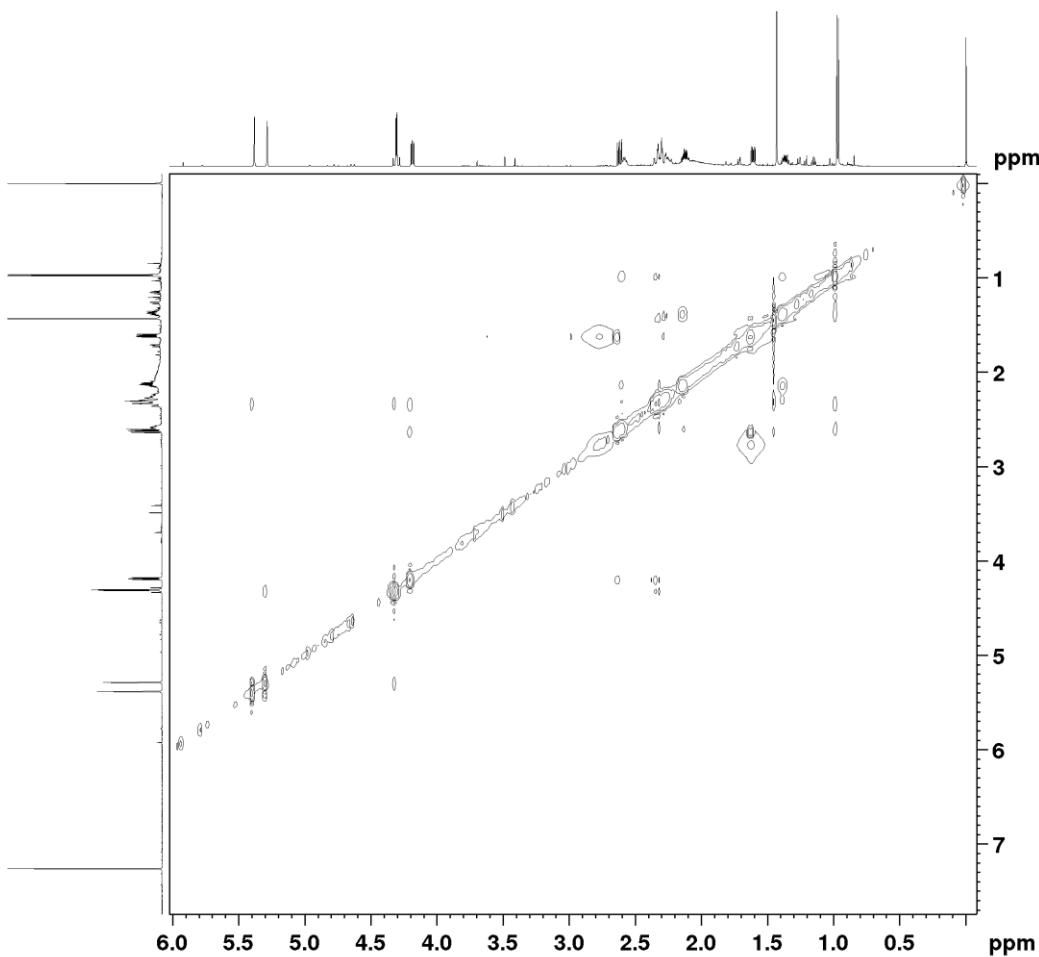
F2 - Acquisition Parameters
Date_ 20200711
Time 2.51 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG cosygppmfd
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 10.00 usec
TE 290.00 K
DO 0.00000300 sec
D1 2.0000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
PmMode QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 64
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S149 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 27



Current Data Parameters
NAME RDP-601!
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200711
Time 3.01 h
INSTRUM spect
PROBHD Z150290_0066 ('
PULPROG noeipypphph
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.0001389 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
SF2 States-TPPI
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S150 NOESY spectrum (600 MHz, CDCl_3) of compound **27**

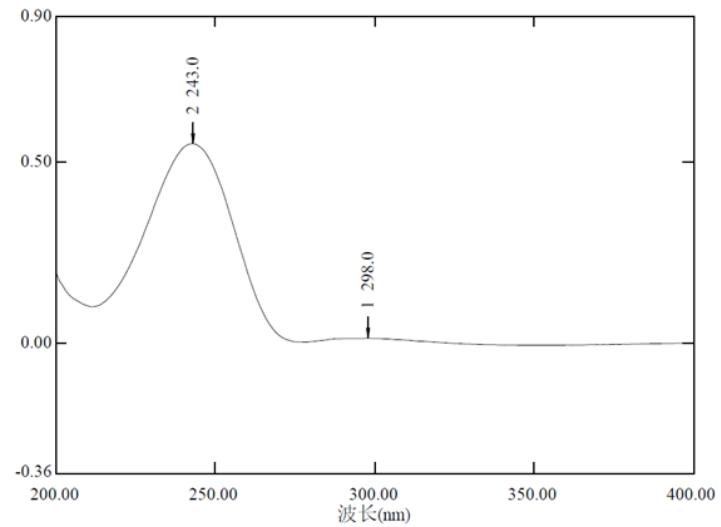
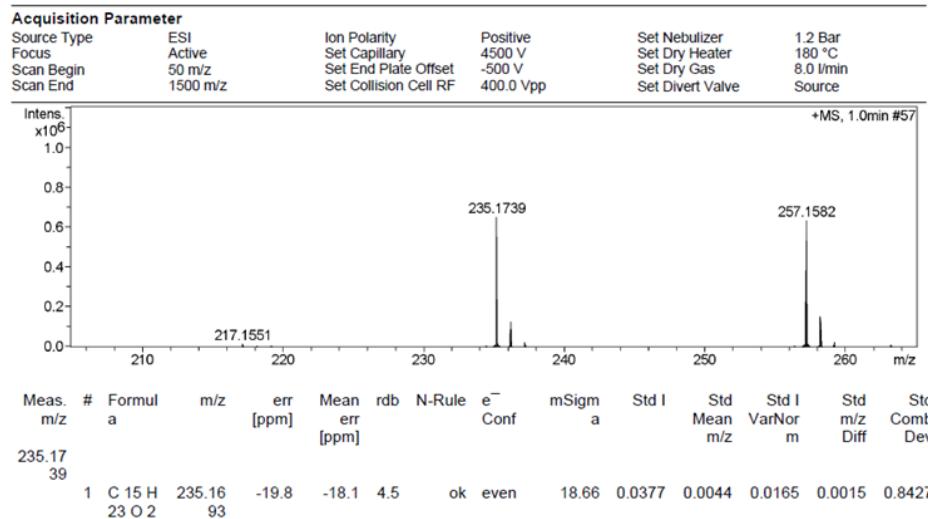


Figure S151 HRESIMS and UV spectra of compound **28**

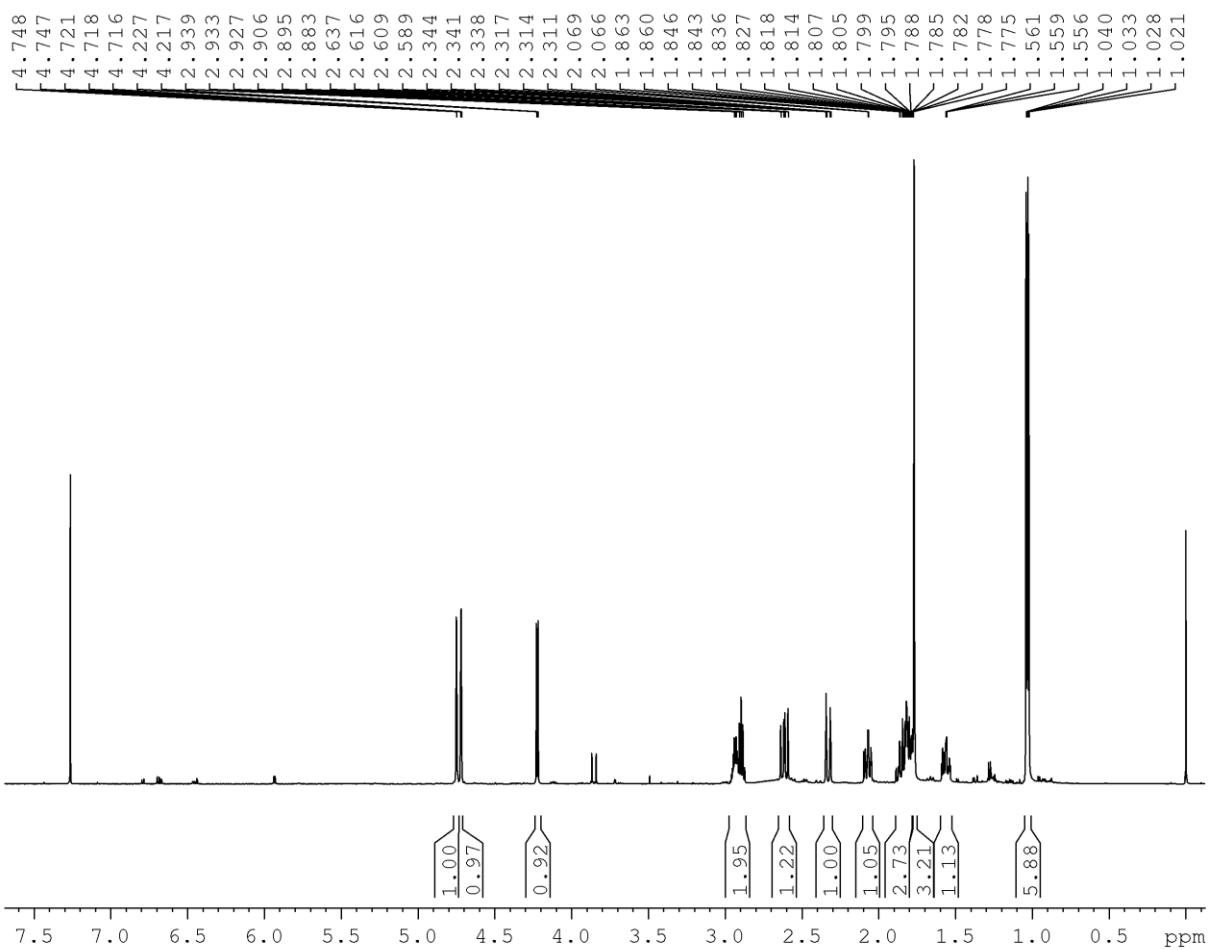
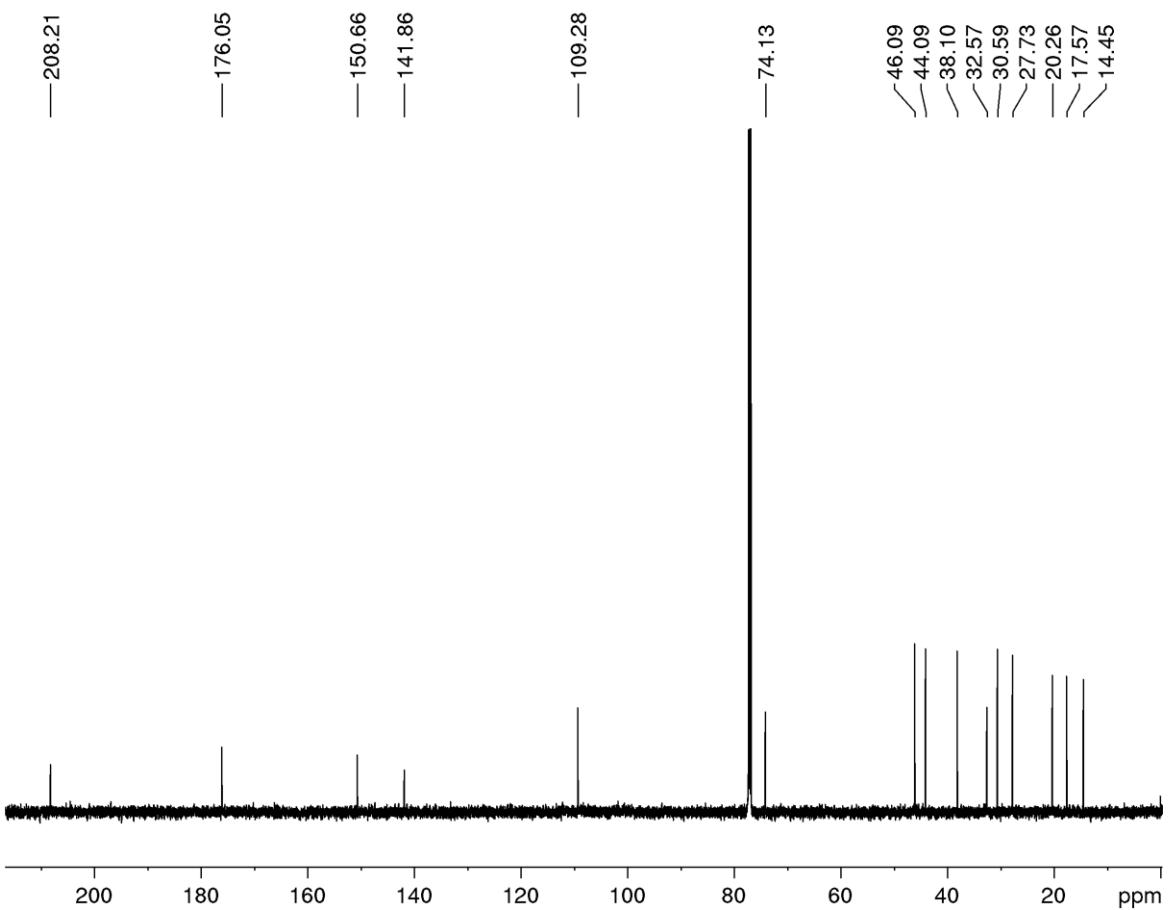


Figure S152 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **28**

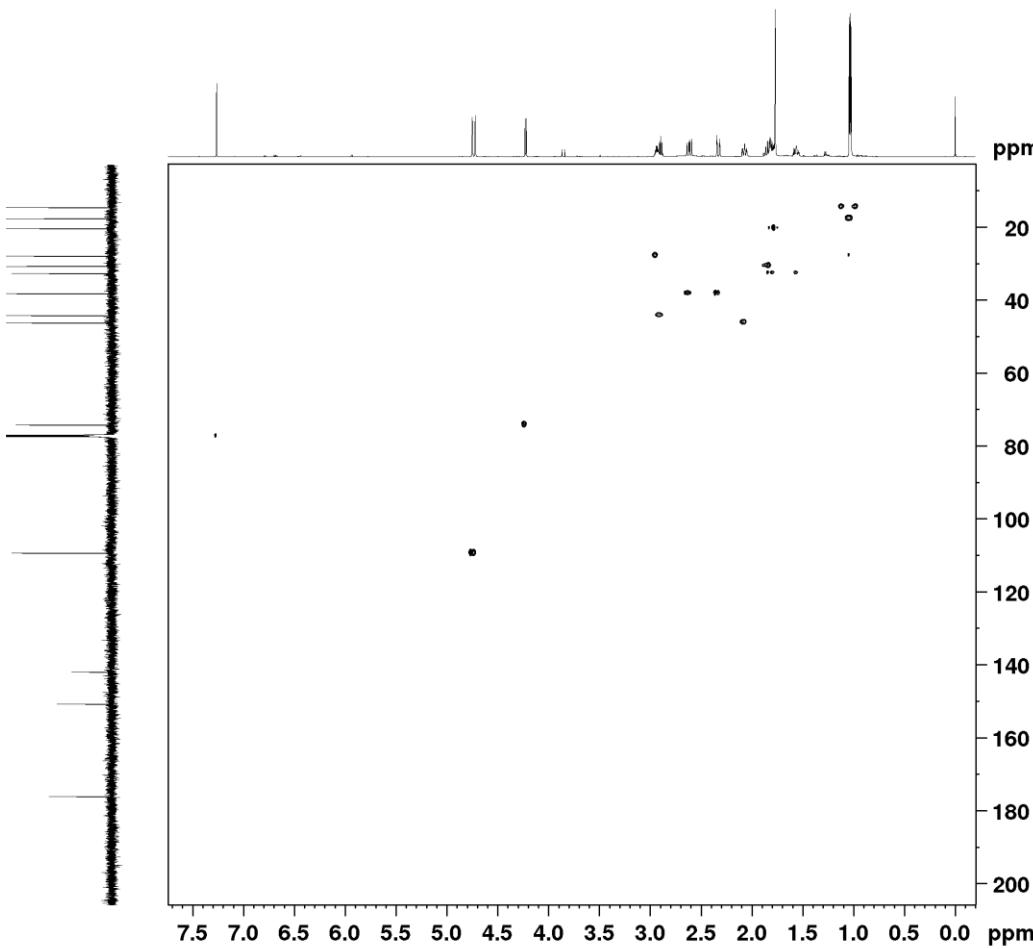


Current Data Parameters
NAME RDP-11!!
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200107
Time_ 2.38 h
INSTRUM spect
PROBHD Z816801_0163 (
PULPROG zgppg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 42613.637 Hz
FIDRES 1.300465 Hz
AQ 0.7689557 sec
RG 75.38
DW 11.733 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 194.77999878 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 5.44000006 W
PLW12 0.12240000 W
PLW13 0.08041300 W

F2 - Processing parameters
SI 32768
SF 150.9204100 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S153 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **28**



Current Data Parameters
NAME RDP-111
BPPNO 4
PRONCO 1

F2 - Acquisition Parameters
Date_ 20200112
Time 14.02 h
INSTRUM spect
PROBHD Z816801_0163 (
PULPROG hsqcetgpsa2p2
TD 65536
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
ETRSES 7.04938 sec
AQ 0.1419947 sec
RG 191.24
DW 69.93 usec
DE 6.50 usec
TE 298.3 K
CNUST2 145.000000
CNUST17 -0.5000000
D0 0.00005300 sec
D1 0.000000 sec
D4 0.00172414 sec
D11 0.03300000 sec
D16 0.00000000 sec
D24 0.00008200 sec
IRW 0.00001270 sec
TDav 600.3204098 MHz
SW01 1000.000000 Hz
P1 12.00 usec
P2 24.00 usec
P2A 144.00 usec
PLW1 5.44000000 MHz
SF02 150.9370113 MHz
M002 100.000000 Hz
CPDPRGS2 garp4
P3 12.00 sec
P1A 1000.00 usec
P2A 2000.00 usec
PCTDZ 80.00 usec
PLW0 0 Hz
PLW2 194.77999878 Hz
PDR1 1.38289889 Hz
SPNAM[1] Cpm600.1000
SPDALS 0.500
SPDPFS3 0 Hz
SPW1 42.85499954 Hz
SPNAM[7] Cpm600comp.4
SPDALS 0.500
SPDPFS7 0 Hz
SPW7 42.85499954 Hz
SPNAM[1] SMMQ10.100
GP1 80.00 *
SPNAM[2] SMMQ10.100
GP2 11.00 *
SPNAM[3] SMMQ10.100
GP2Z 11.00 *
SPNAM[4] SMMQ10.100
GP24 -5.00 *
P16 1000.00 usec
P13 600.00 usec

F1 - Acquisition parameters
TD 65536
SF01 150.937 MHz
ETRSES 340.000000 Hz
DW 260.8330 ppm
PRMode Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WGW QSBINE
SSB z
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9204100 MHz
WGW QSBINE
SSB z
LB 0 Hz
GB 0

Figure S154 HSQC spectrum (600 MHz, CDCl_3) of compound 28

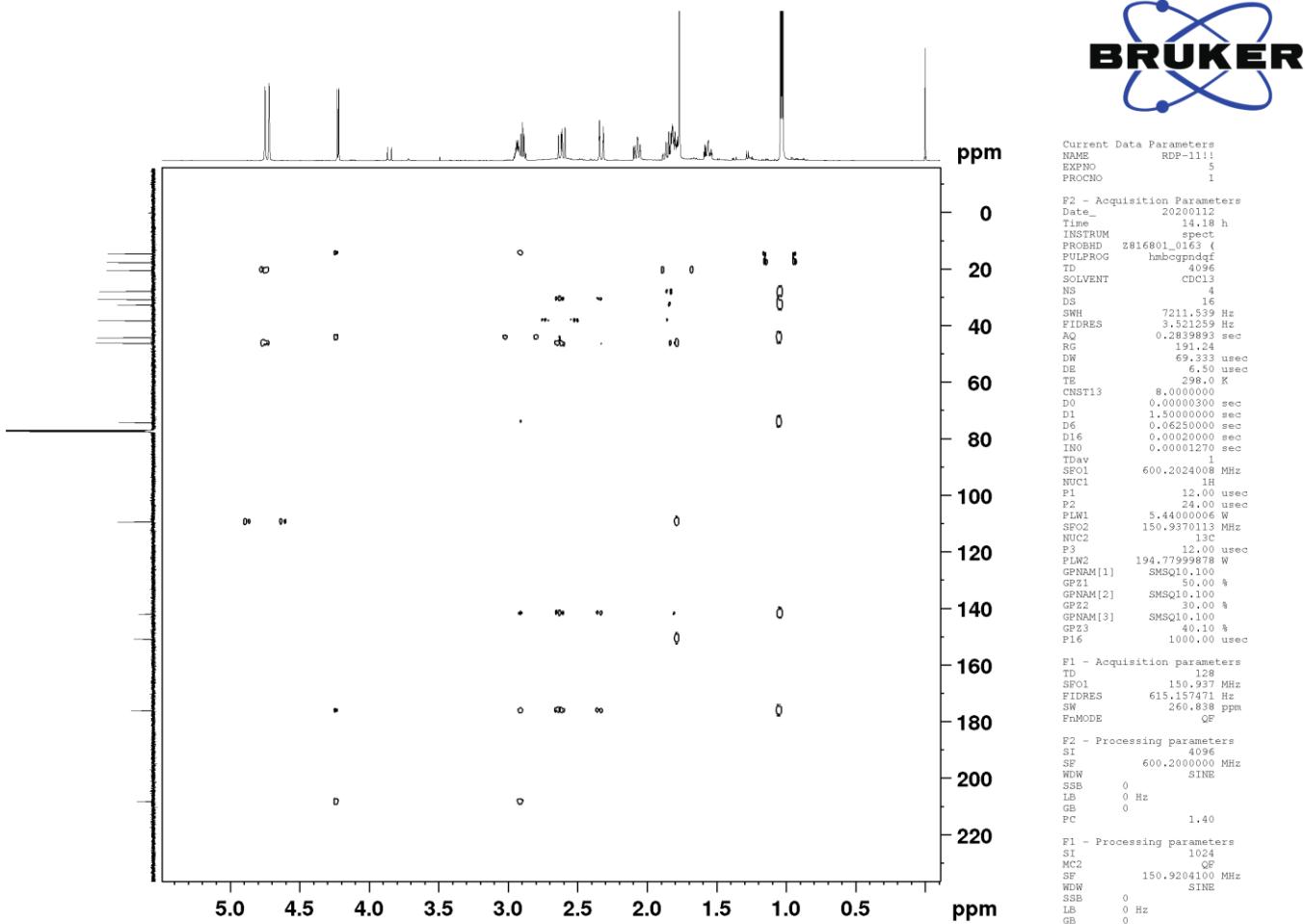
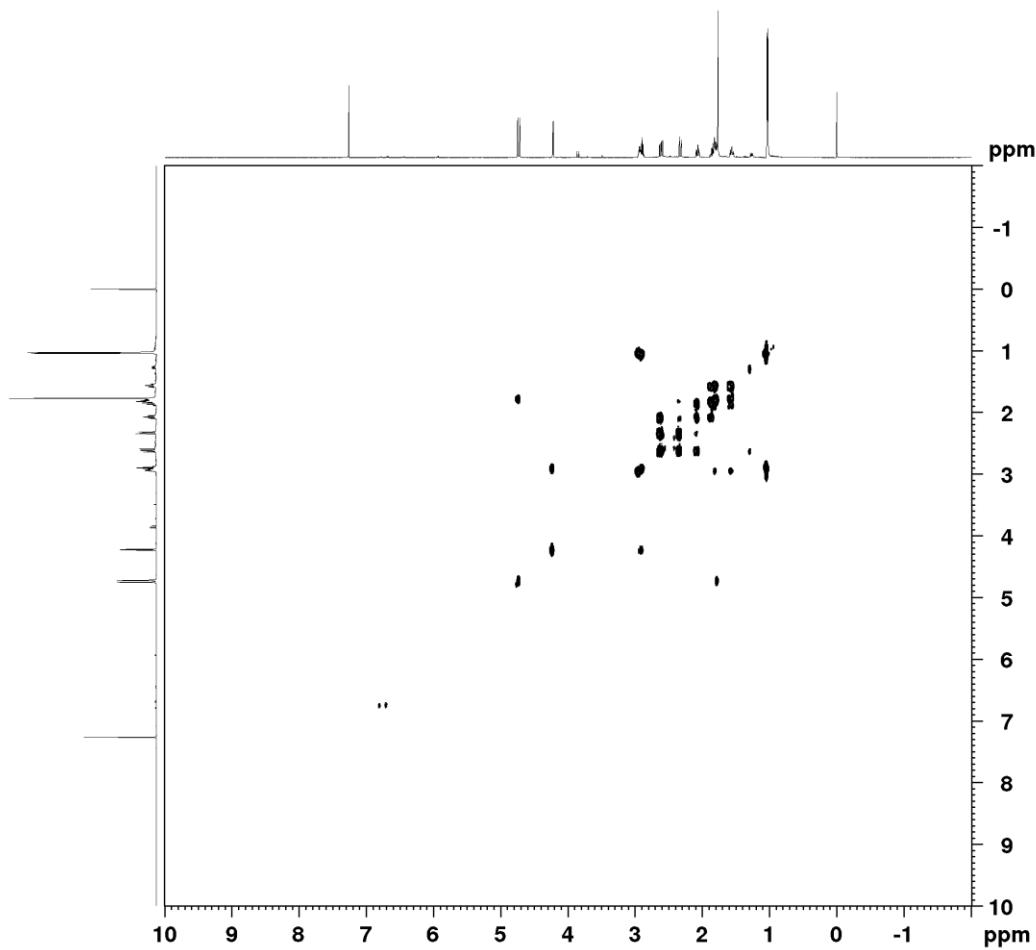


Figure S155 HMBC spectrum (600 MHz, CDCl_3) of compound **28**



Current Data Parameters
NAME RDE-11!!
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200112
Time 14:35 h
INSTRUM spect
PROBHD Z816801_0163 (
PULPROG cosygppmfd
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 6.50 usec
TE 2.65 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 12.00 usec
PLW1 5.44000006 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
PnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 0F
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S156 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 28

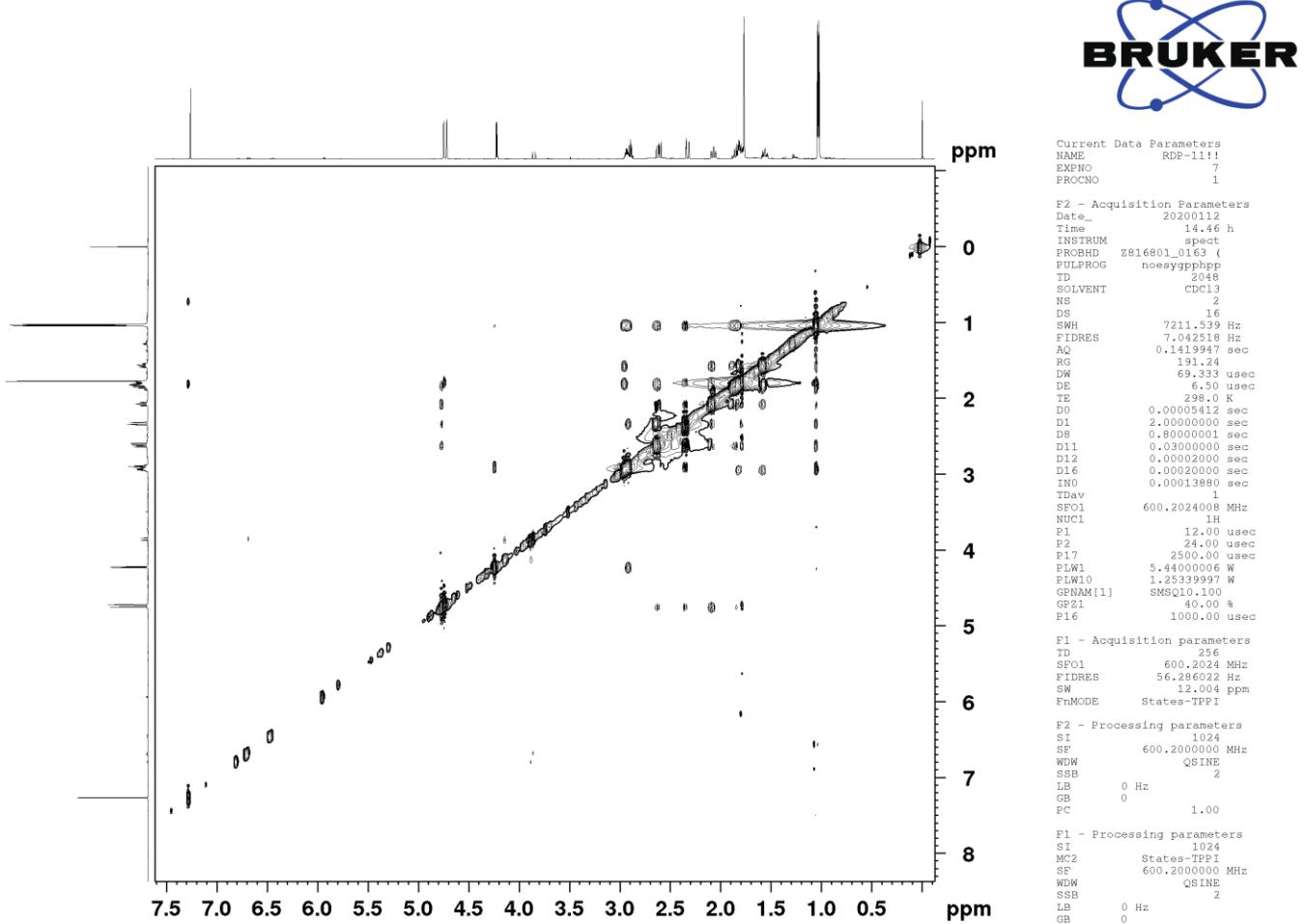


Figure S157 NOESY spectrum (600 MHz, CDCl₃) of compound **28**

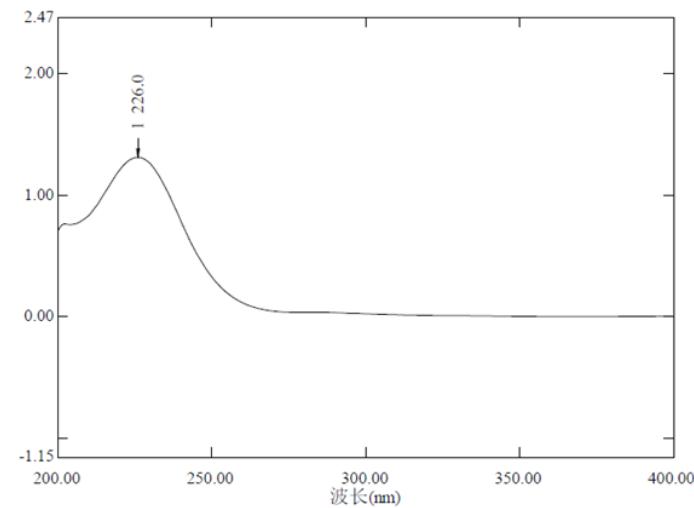
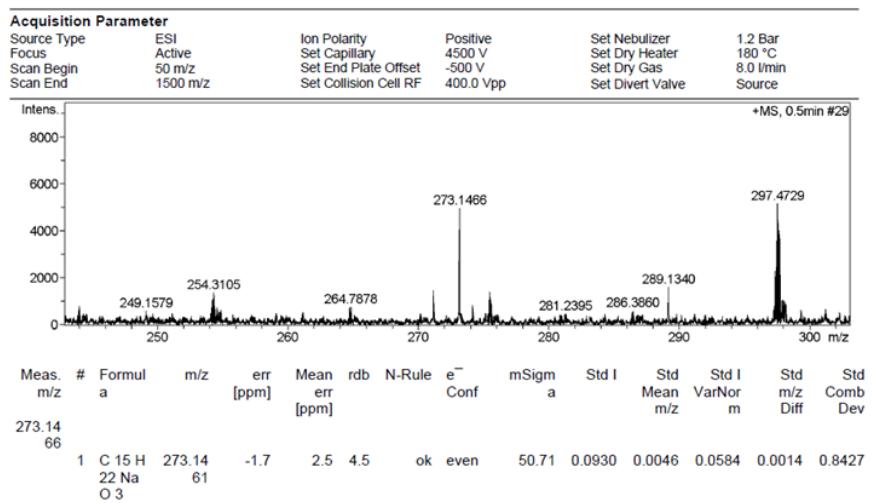


Figure S158 HRESIMS and UV spectra of compound 29

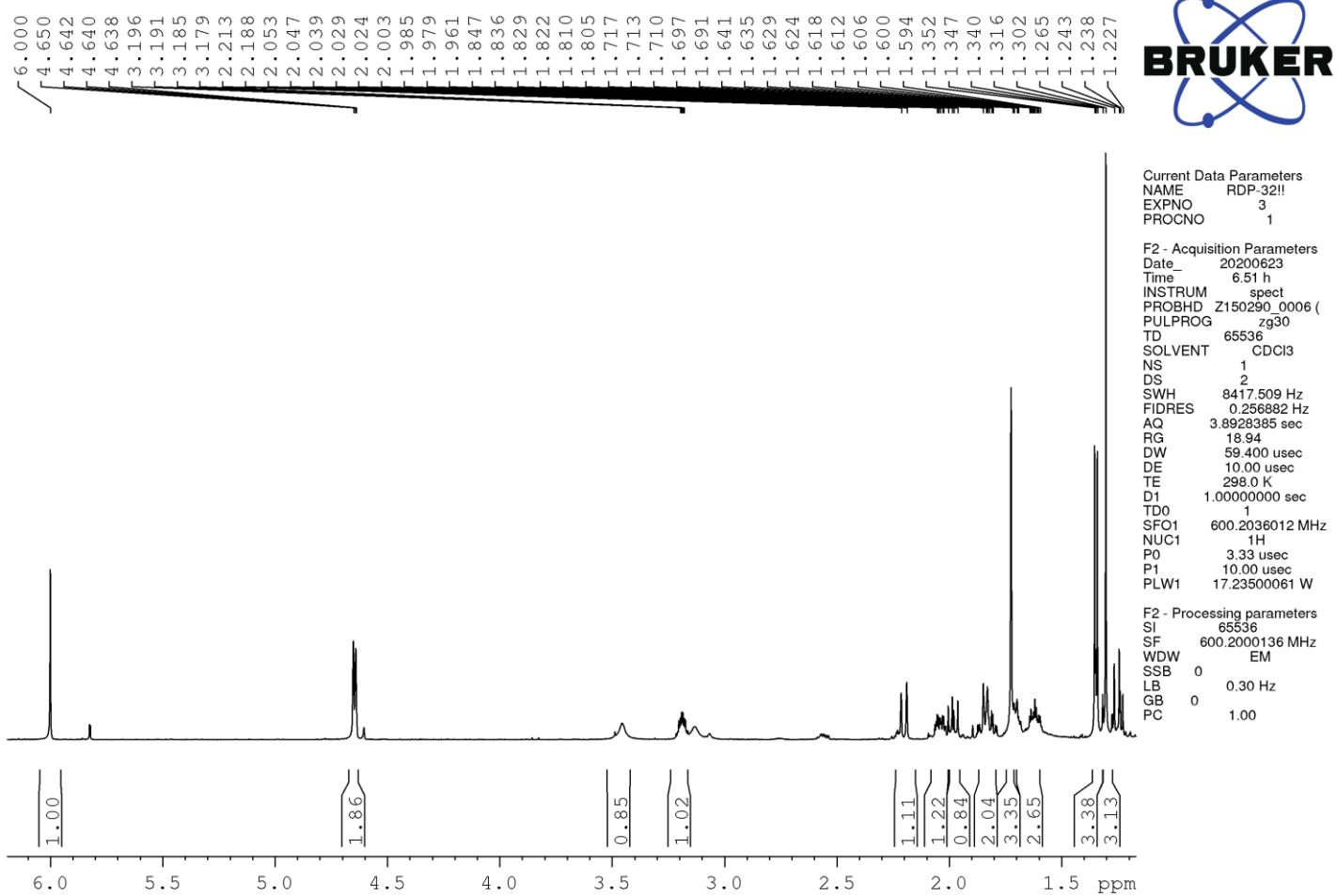


Figure S159 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **29**

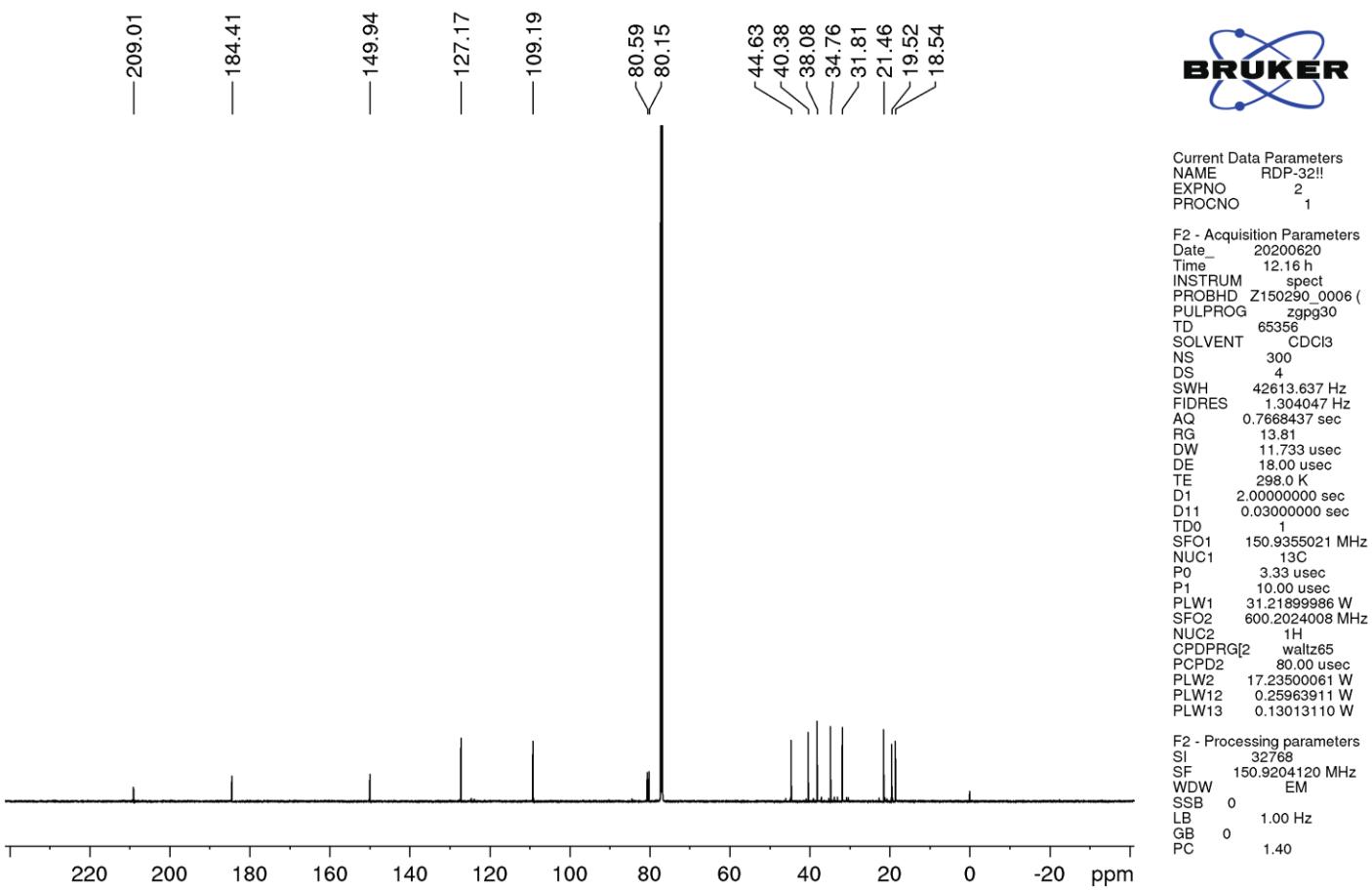
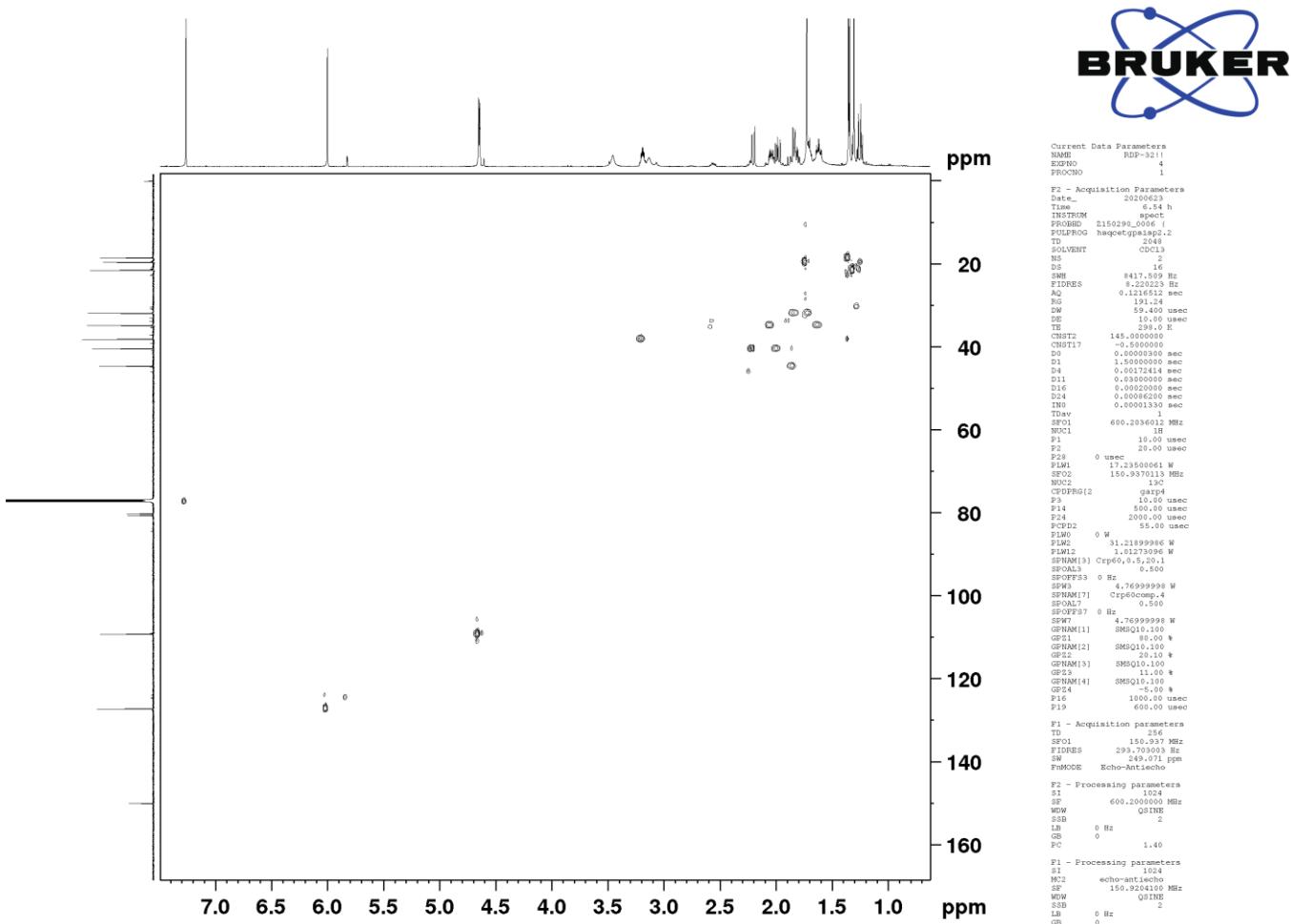


Figure S160 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **29**



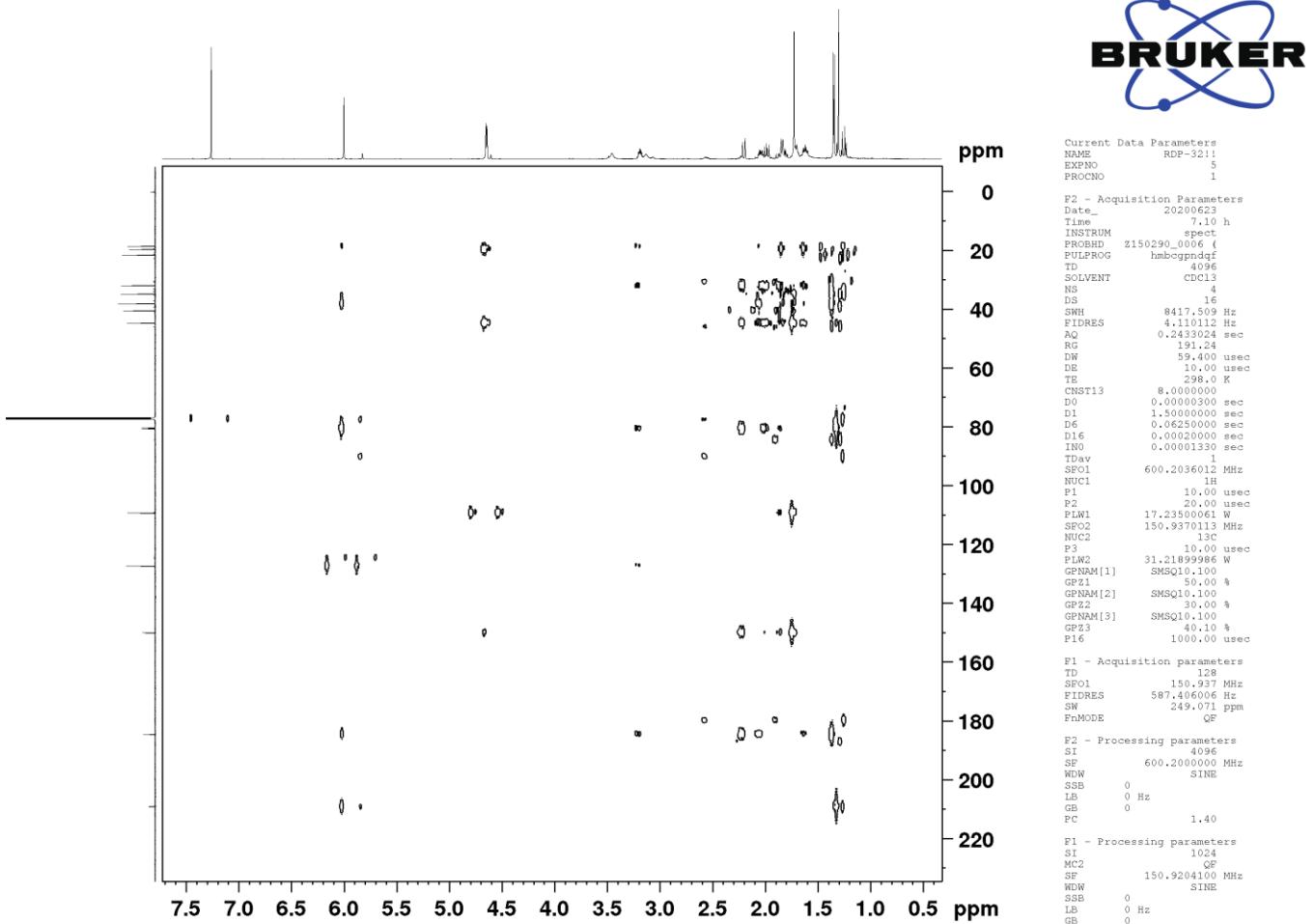
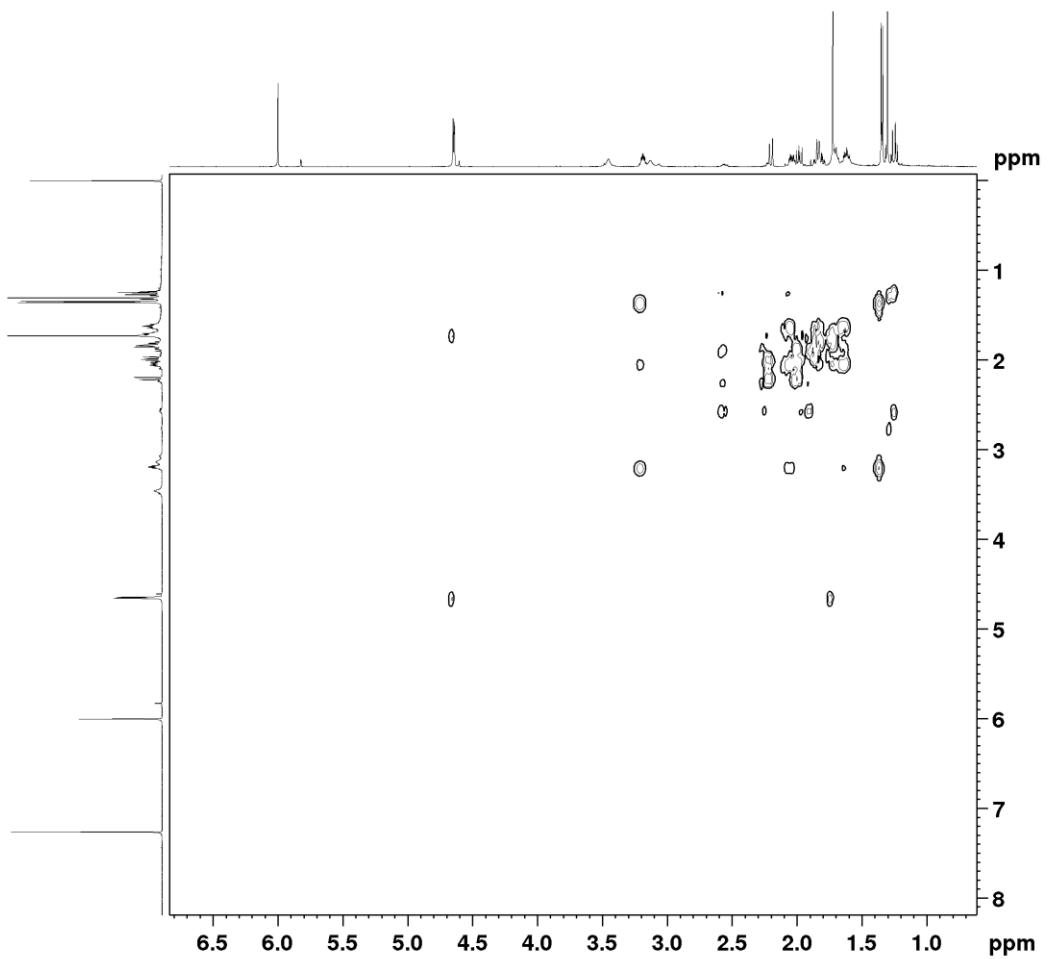


Figure S162 HMBC spectrum (600 MHz, CDCl₃) of compound **29**



Current Data Parameters
NAME RDP-3211
EXPNO 6
PROCNO 1

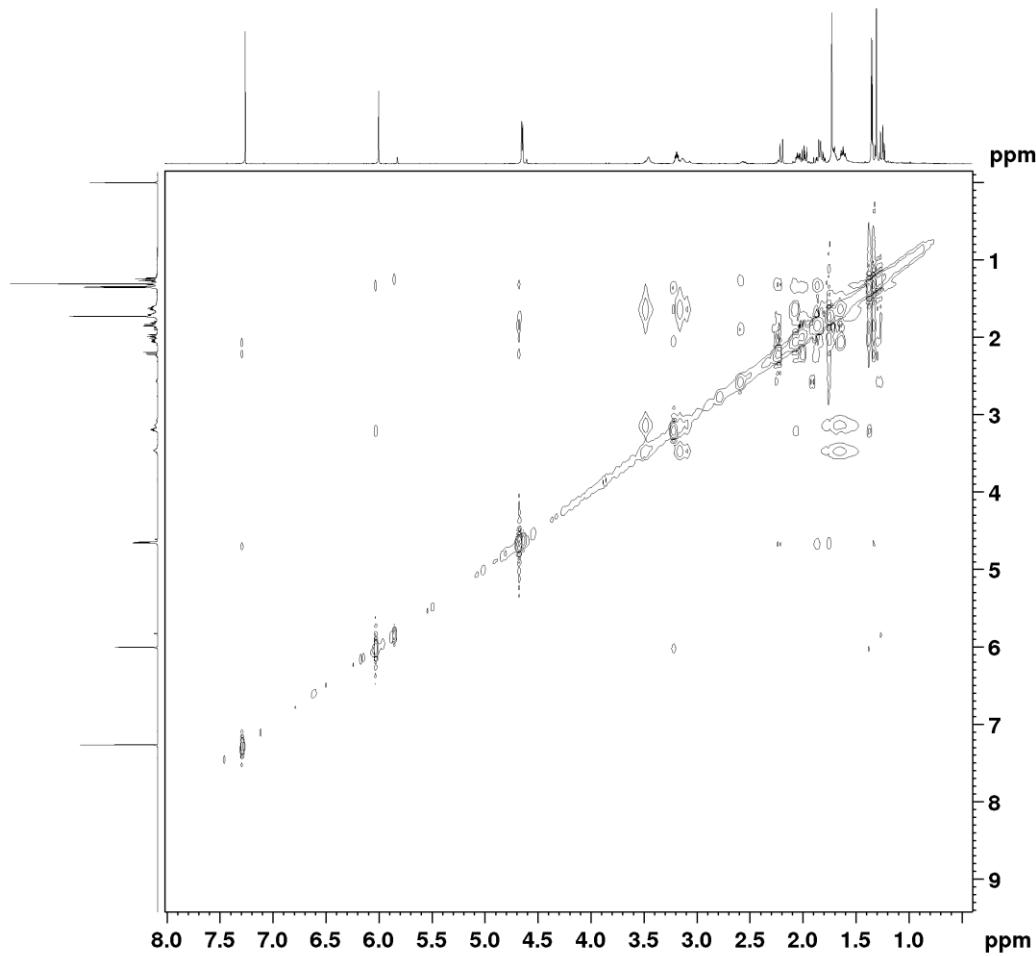
F2 - Acquisition Parameters
Date_ 20200623
Time 7.53 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG cosygppmfr
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 8417.509 Hz
FIDRES 0.220223 Hz
AQ 0.1216512 sec
RG 191.24
DW 59.400 usec
DE 10.00 usec
TE 296.00 K
D0 0.00000300 sec
D1 2.0000000 sec
D13 0.0000400 sec
D16 0.0002000 sec
IN0 0.00011900 sec
TDav 1
SF01 600.2036012 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2036 MHz
FIDRES 131.302521 Hz
SW 14.001 ppm
PnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 64
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S163 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 29



Current Data Parameters
NAME RDP-321!!
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200623
Time 7.27 h
INSTRUM spect
PROBHD Z150290_0066_1
PULPROG noe3sypphp
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 8417.509 Hz
FIDRES 8.220223 Hz
AQ 0.1216512 sec
RG 60.93
DW 59.400 usec
DE 10.00 usec
TE 298.0 K
D0 0.00004677 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.0002000 sec
IN0 0.0001190 sec
DDav 1
SF01 600.2036012 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2036 MHz
FIDRES 65.651260 Hz
SW 14.001 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S164 NOESY spectrum (600 MHz, CDCl₃) of compound **29**

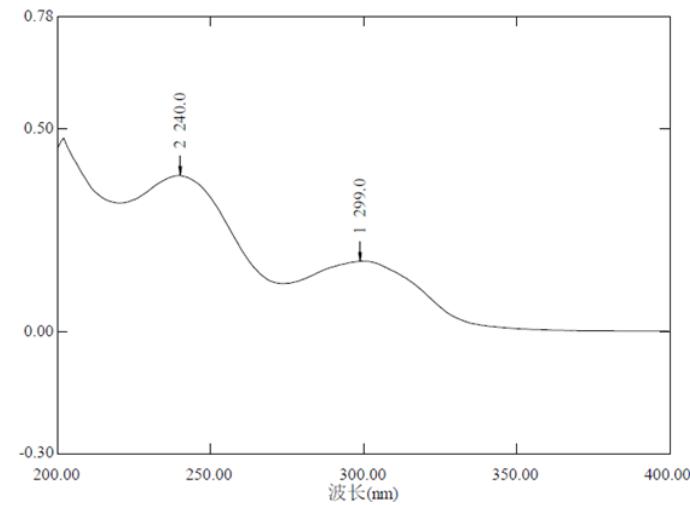
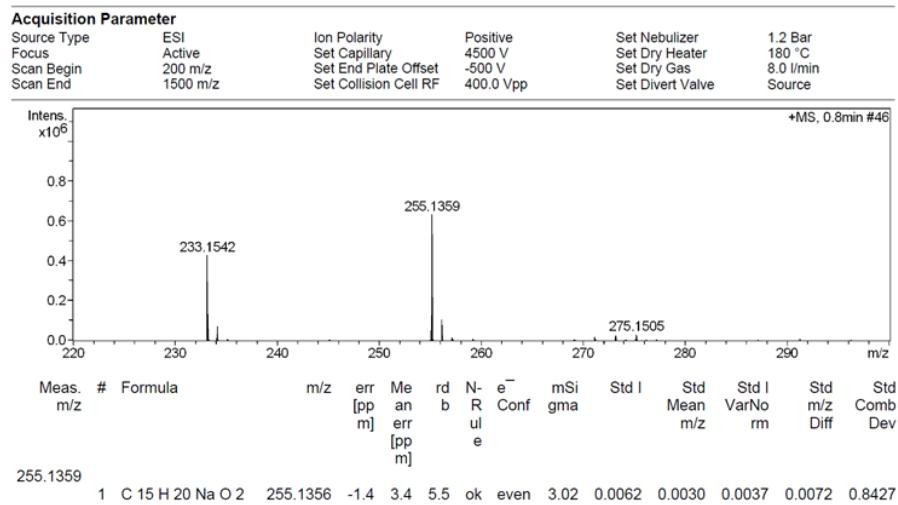


Figure S165 HRESIMS and UV spectra of compound **30**

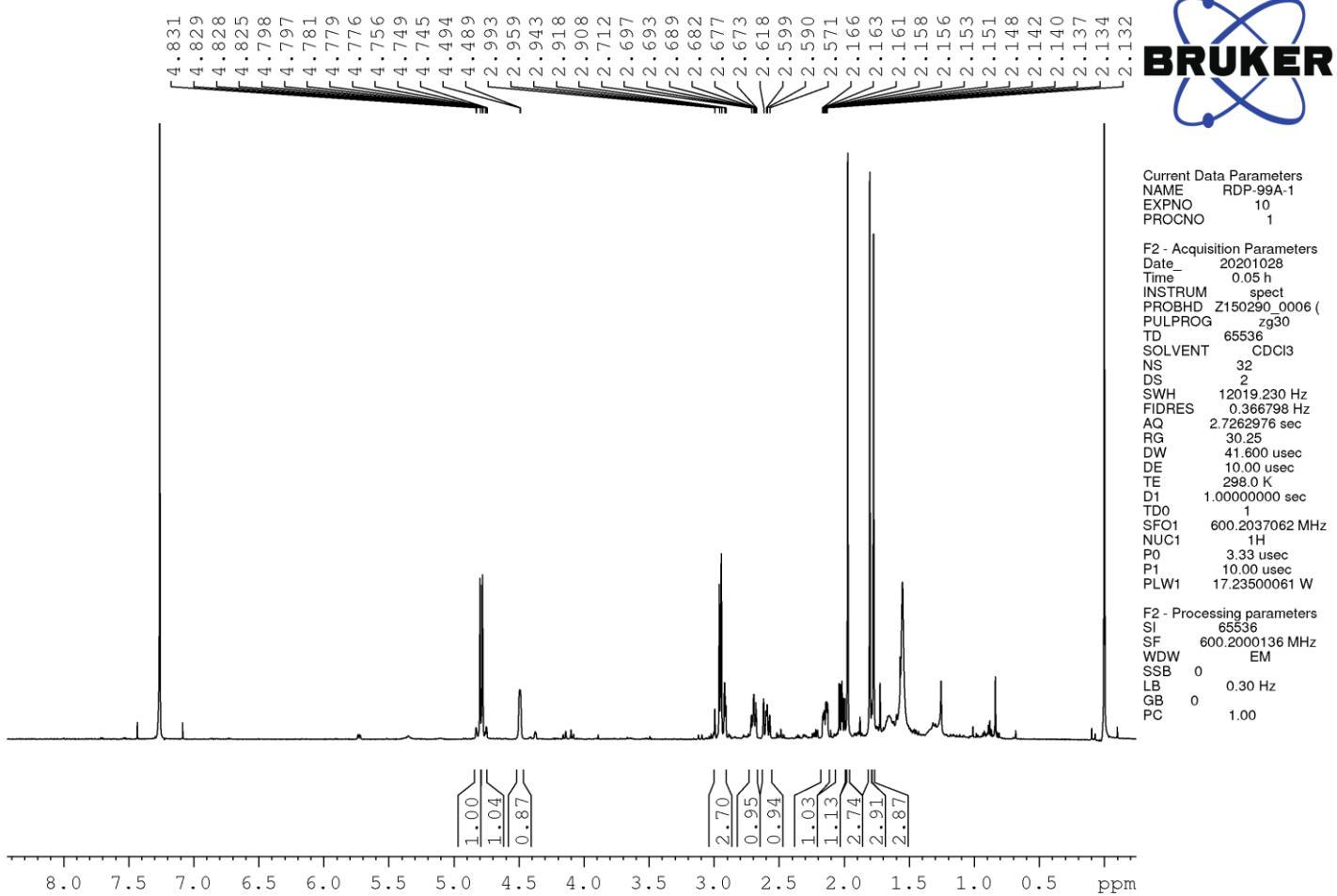


Figure S166 ¹H NMR spectrum (600 MHz, CDCl₃) of compound **30**

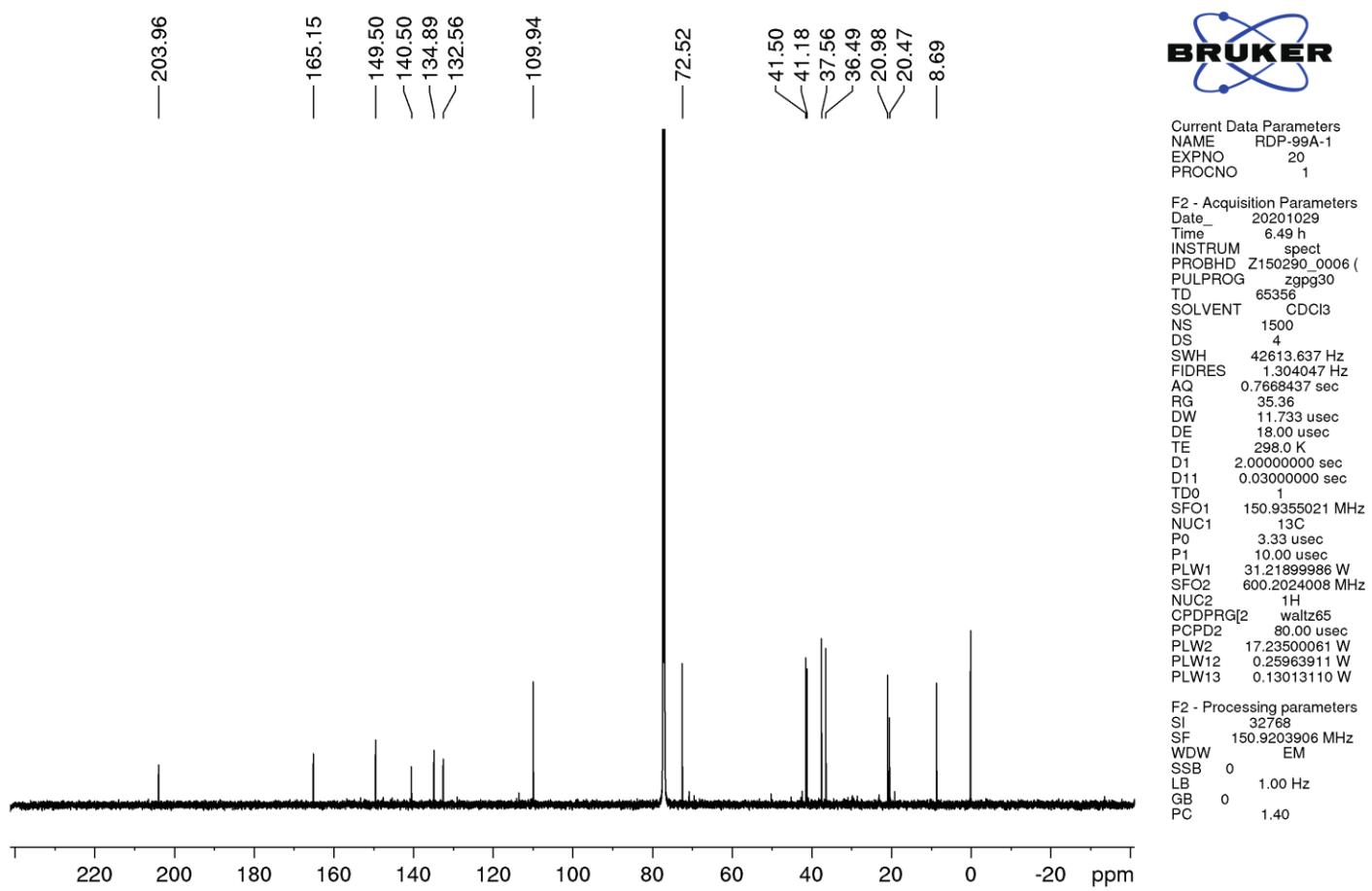


Figure S167 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **30**

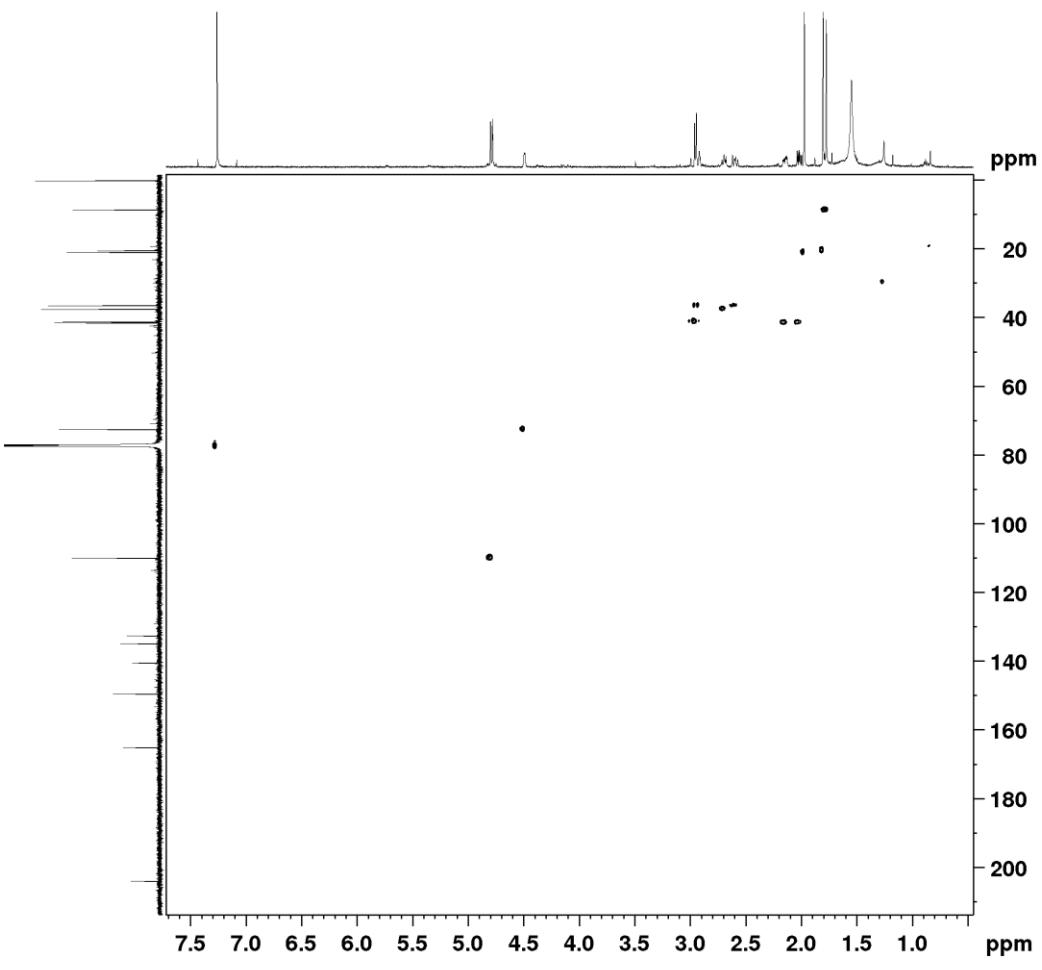
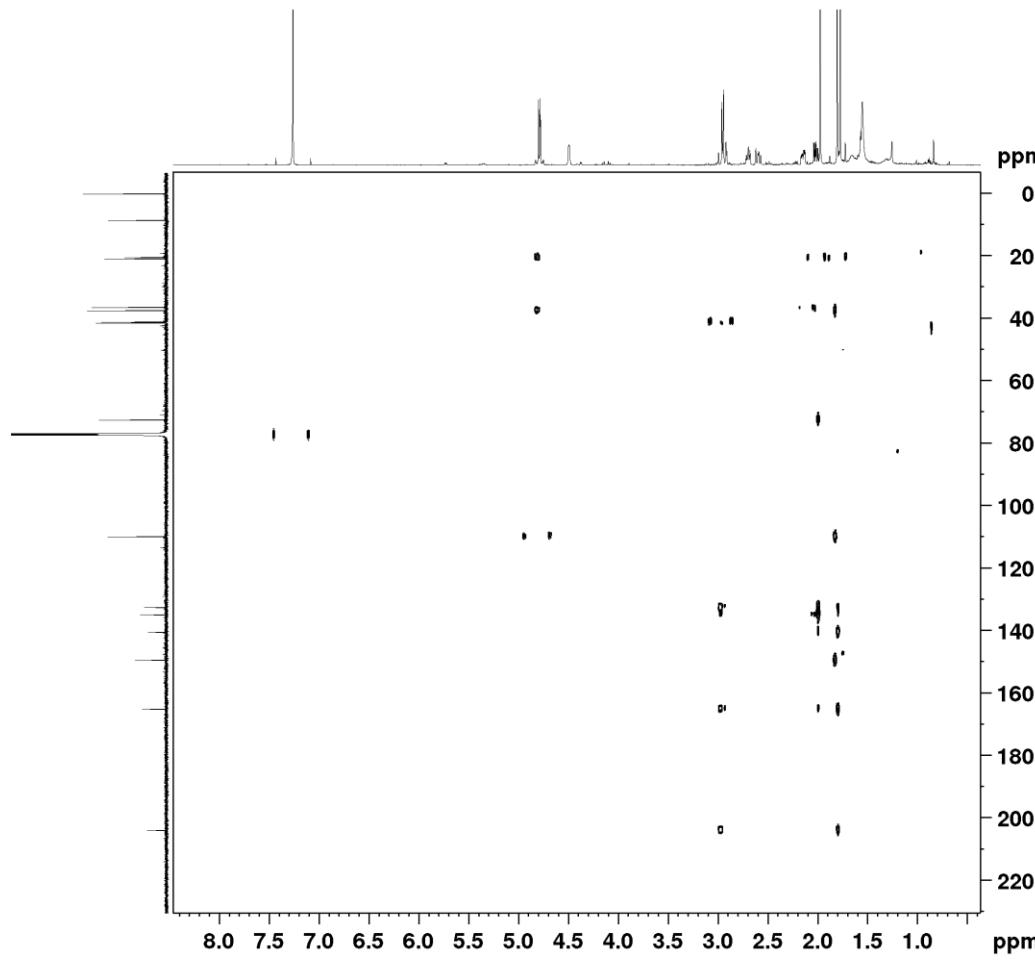


Figure S168 HSQC spectrum (600 MHz, CDCl₃) of compound 30



Current Data Parameters
NAME RDP-99A-1
EXPNO 5
PROCNO 1

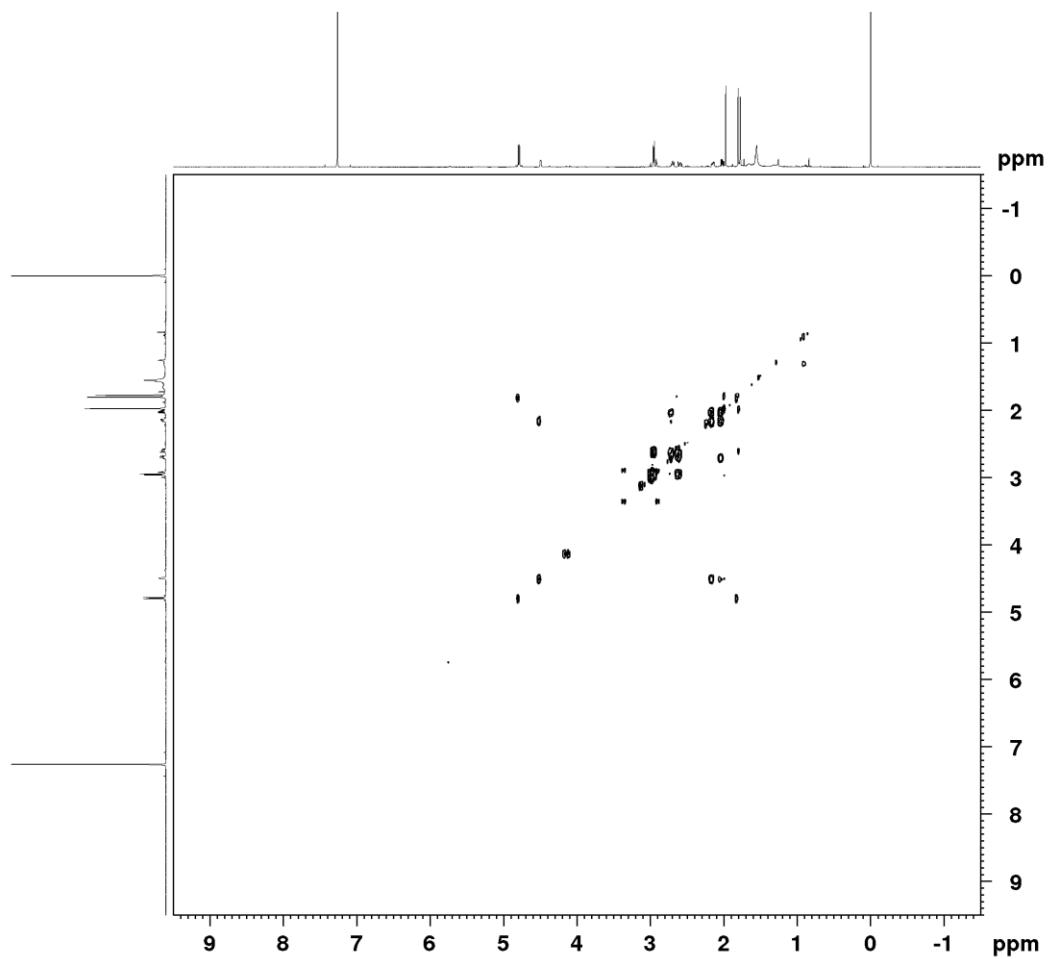
F2 - Acquisition Parameters
Date_ 20210130
Time_ 5.23 h
INSTRUM spect
PROBHD Z150290_0006 (bruker)
PULPROG hmbcgrndf
TD 4096
SOLVENT CDCl3
NS 16
DS 16
SWH 6602.113 Hz
FIDRES 3.223688 Hz
AQ 0.3102037 sec
RG 100.00
DW 75.733 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.0000000
D0 0.0000000 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001330 sec
TDav 1
SF01 600.2024010 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLN1 17.23500061 W
SF02 150.9370113 MHz
NUC2 13C
P3 10.00 usec
PLN2 31.21899986 W
GPNAME[1] SNSQ10.100
GPZ1 50.00 %
GPNAME[2] SNSQ10.100
GPZ2 30.00 %
GPNAME[3] SNSQ10.100
GPZ3 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.937 MHz
FIDRES 587.40605 Hz
SW 249.071 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S169 HMBC spectrum (600 MHz, CDCl_3) of compound 30



Current Data Parameters
NAME RDP-99A-1
EXPNO 6
PROCNO 1

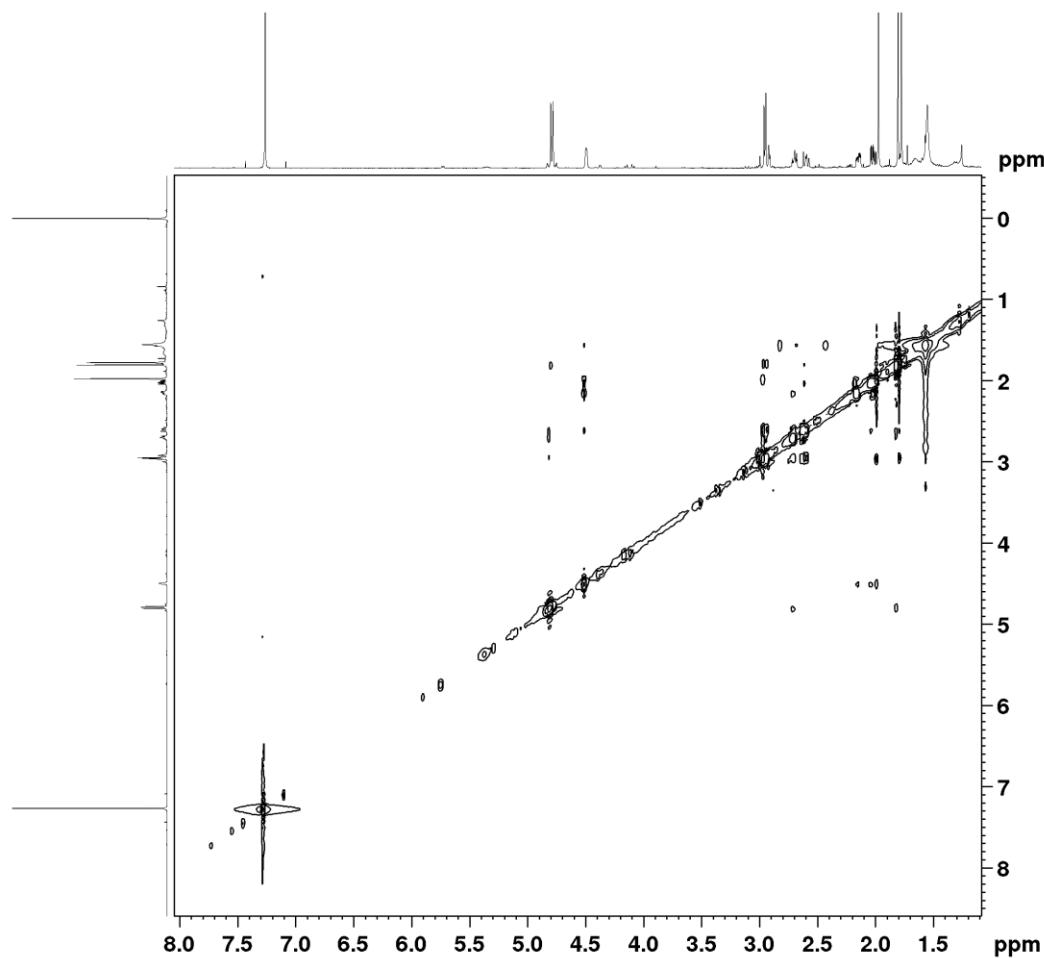
F2 - Acquisition Parameters
Date_ 20210130
Time 6.28 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG cosygppmfd
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 6602.113 Hz
FIDRES 6.447376 Hz
AQ 0.1551019 sec
RG 191.24
DW 75.733 usec
DE 10.00 usec
TE 296.00 K
DO 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00015140 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2000000 MHz
FIDRES 103.203438 Hz
SW 11.005 ppm
PnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S170 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 30



Current Data Parameters
NAME RDP-99r-1
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date 20210130
Time 7.06 h
INSTRUM spect
PROBHD Z150290_0066_1
PULPROG noeipypphph
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 6602.113 Hz
FIDRES 6.447376 Hz
AQ 0.1551019 sec
RG 60.93
DW 75.73 usec
DB 10.00 usec
TE 298.0 K
D0 0.00006297 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D18 0.00015100 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 51.601719 Hz
SW 11.005 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW States-TPPI
SSB 2
LB 0 Hz
GB 0

Figure S171 NOESY spectrum (600 MHz, CDCl_3) of compound **30**

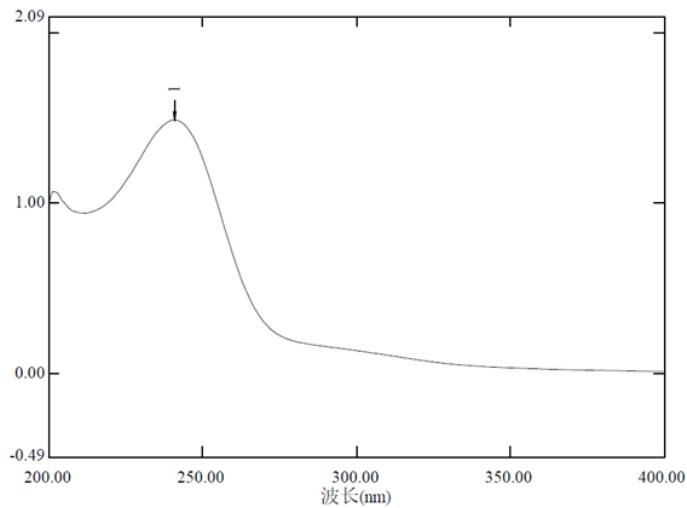
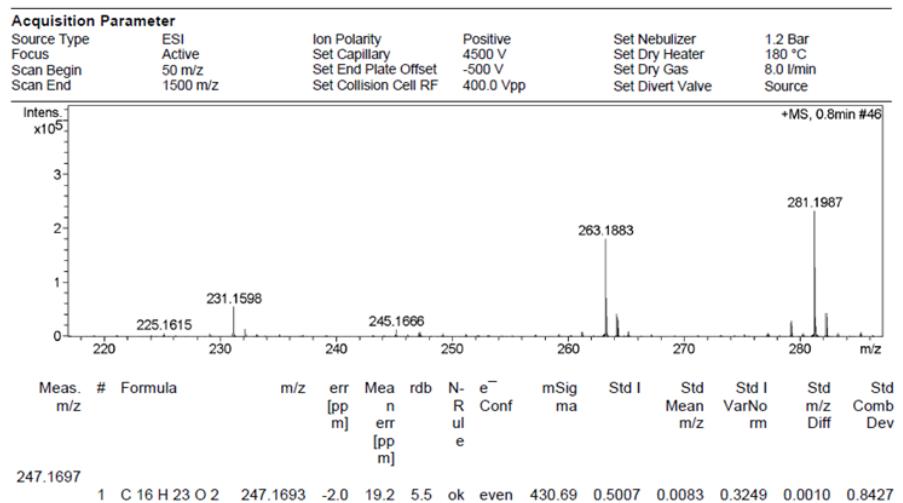


Figure S172 HRESIMS and UV spectra of compound 33

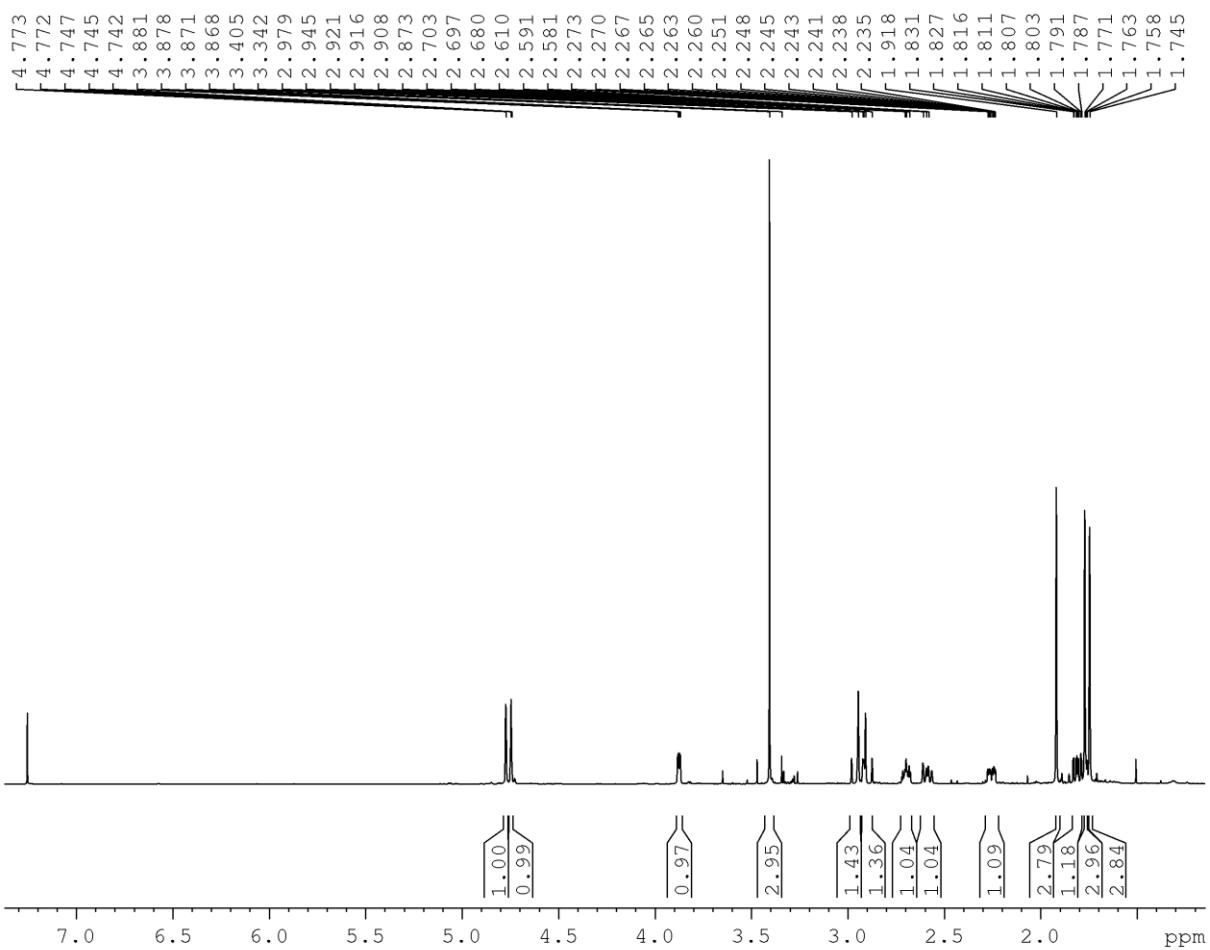
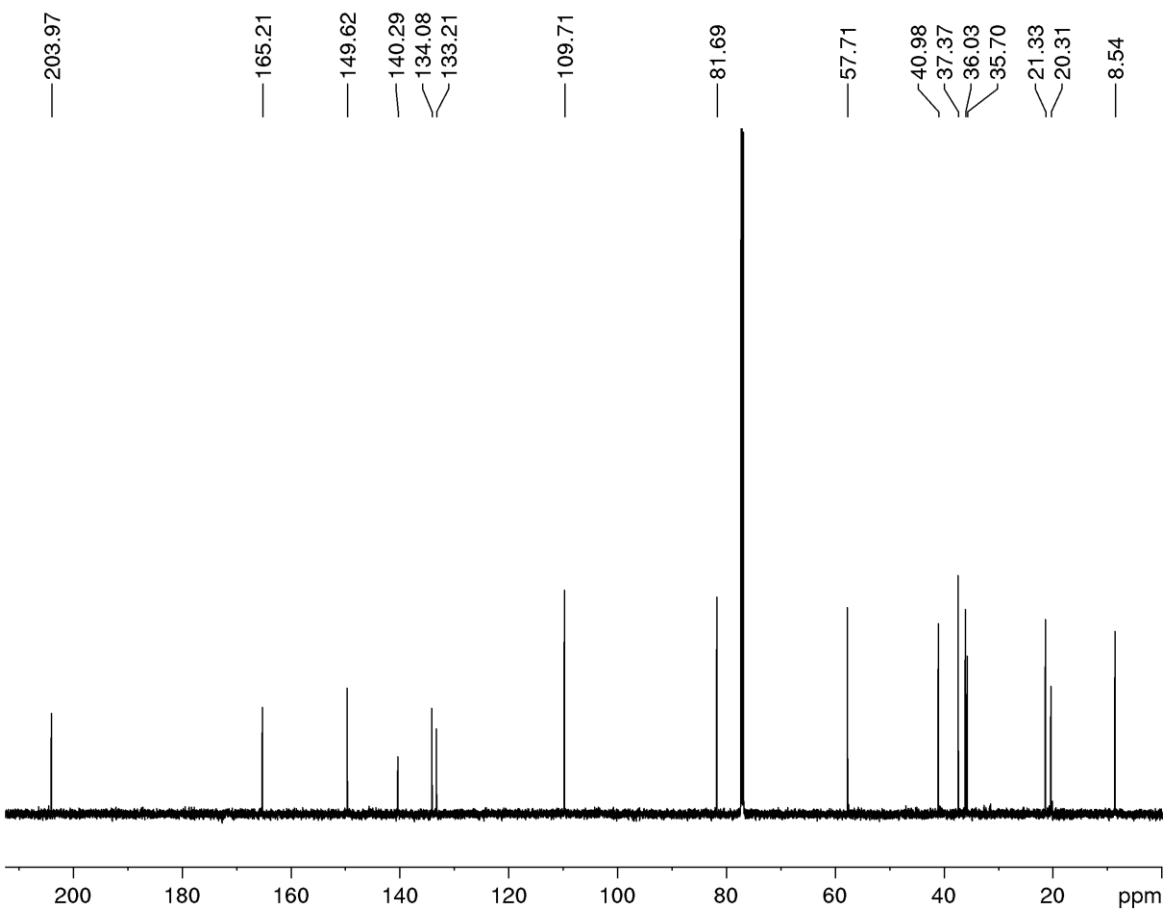


Figure S173 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **33**

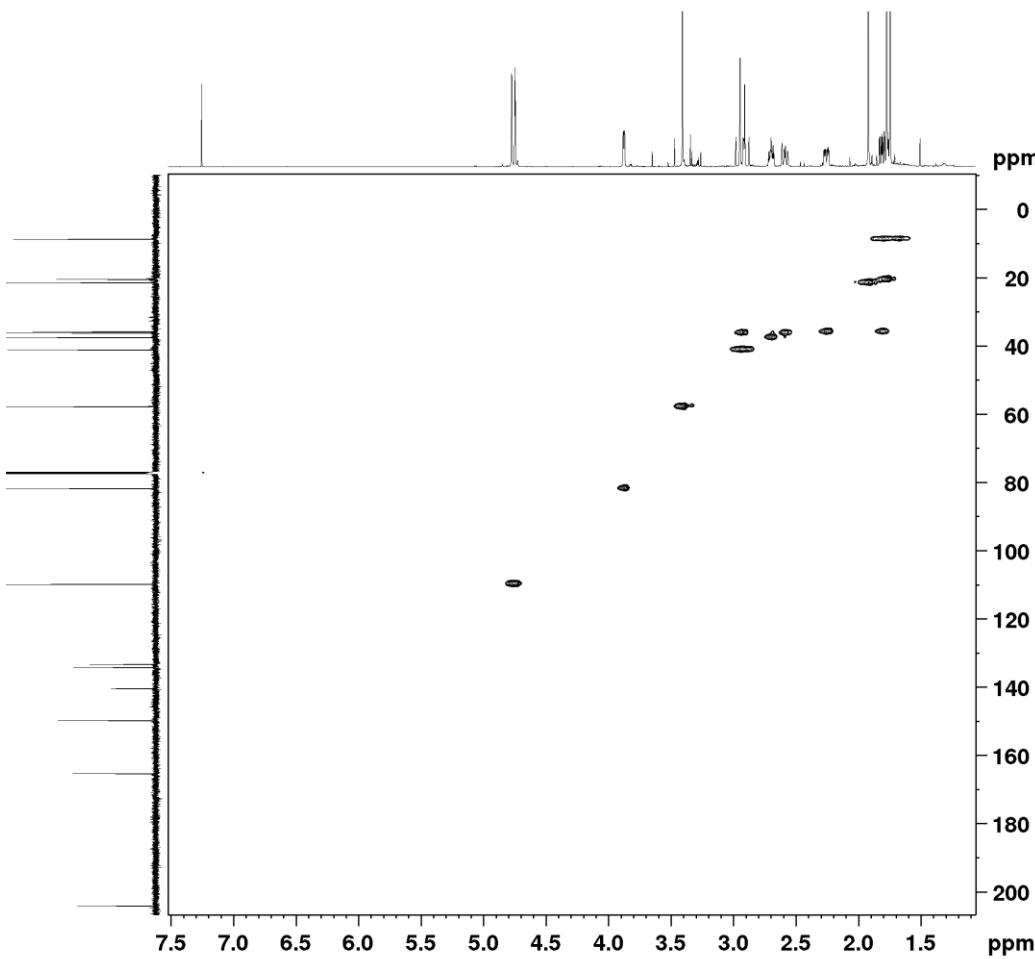


Current Data Parameters
NAME RDP-12!!
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200102
Time_ 3.41 h
INSTRUM spect
PROBHD Z816801_0163 (
PULPROG zgppg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 42613.637 Hz
FIDRES 1.300465 Hz
AQ 0.7689557 sec
RG 85.5
DW 11.733 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 194.77999878 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 5.44000006 W
PLW12 0.12240000 W
PLW13 0.08041300 W

F2 - Processing parameters
SI 32768
SF 150.9204100 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S174 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **33**



Current Data Parameters
NAME RDP-121
BPPNO 1
PRONCO 1

P2 - Acquisition Parameters
Date 20200107
Time 2.45 h
INSTRUM spect
PROBHD Z816801_0163 (PULPROG hsqcetgpsa2p2
TD 65536
SOLVENT CDCl₃
NS 2
DS 16
SWH 7211.539 Hz
ETRIM 7.04938 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.93 usec
DE 6.50 usec
TB 298.3 K
CNUST2 145.000000 Hz
CNST17 -0.5000000
CNST17 0.5000000
D0 0.00005300 sec
D1 0.000000 sec
D4 0.00172414 sec
D11 0.03300000 sec
D16 0.00000000 sec
D24 0.00008200 sec
IRW 0.00001270 sec
TDav 600.3204096 MHz
SW01 1000.000000 Hz
P1 12.00 usec
P2 24.00 usec
P2A 144.000000 sec
PLW1 5.44000000 W
SF02 150.9370113 MHz
SW02 1000.000000 Hz
CPDPRGS2 garp4
P3 12.00 sec
P14 100.00 usec
P24 2000.00 usec
CPDQZ 80.00 usec
PLW0 0 Hz
PLW2 194.77999878 W
PDP1 13.18289889 W
SPNAM[1] Cpm60.000000
SPNAM[3] Cpm60.000000
SPDFF33 0 Hz
SPW1 42.85499954 W
SPNAM[7] Cpm60comp.4
SPDFF33 0.500
SPDFF33 0 Hz
SPW7 42.85499954 W
SPNAM[1] SMDQ10.100
GP1 80.00 *
SPNAM[2] SMDG10.100
GP2 100.00 *
SPNAM[3] SMDG10.100
GP2 11.00 *
SPNAM[4] SMDQ10.100
GP24 -5.00 *
P16 1000.00 usec
P13 600.00 usec

P1 - Acquisition parameters
TD 65536
SW01 150.9370113 MHz
ETRIM 347.6888 Hz
DW 260.8330 ppm
PR1 Ech0-Antiecho

P2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW QSBIN
SSB Z
LB 0 Hz
GB 0
PC 1.40

P1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9204100 MHz
WDW QSBIN
SSB Z
LB 0 Hz
GB 0

Figure S175 HSQC spectrum (600 MHz, CDCl₃) of compound 33

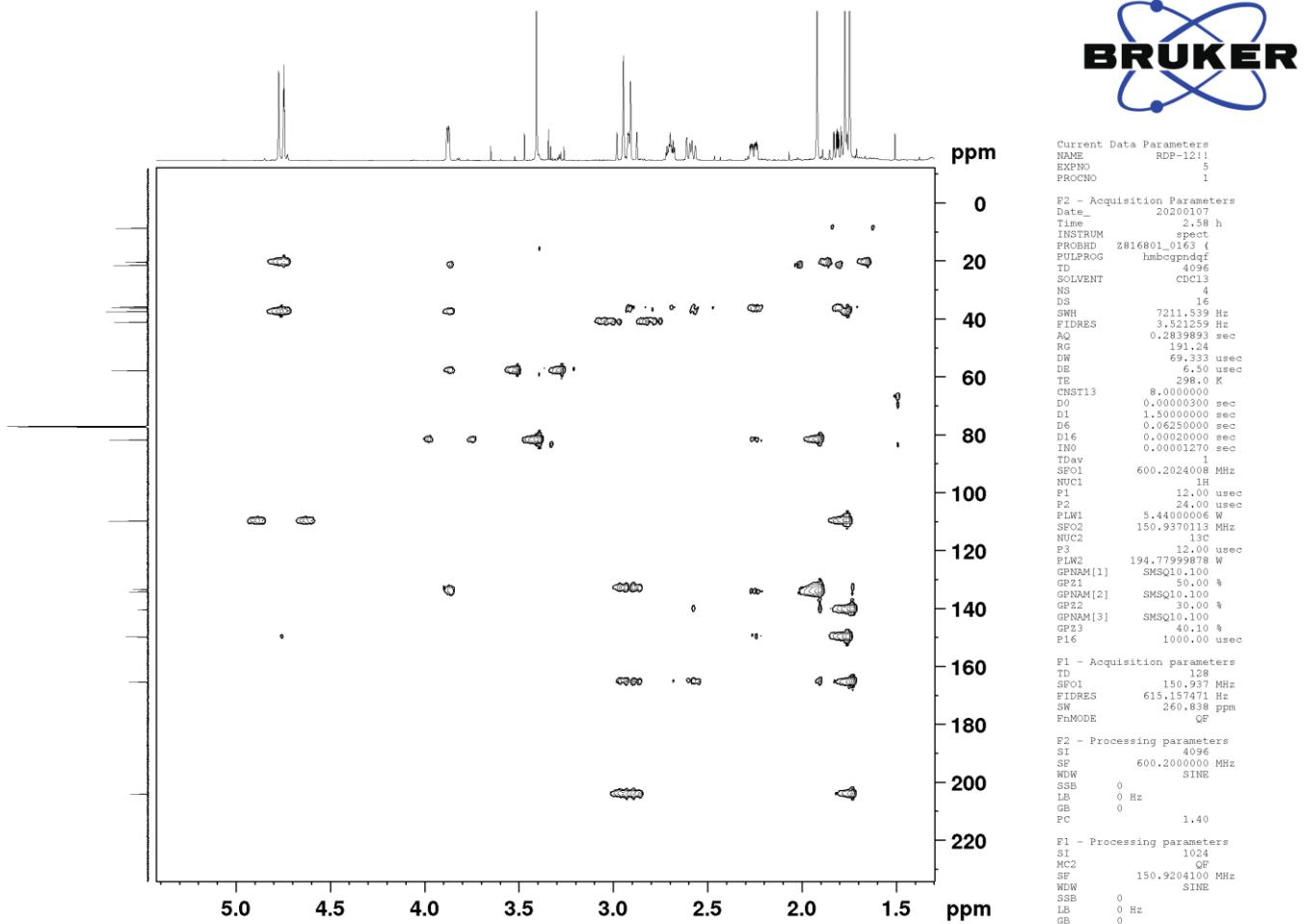
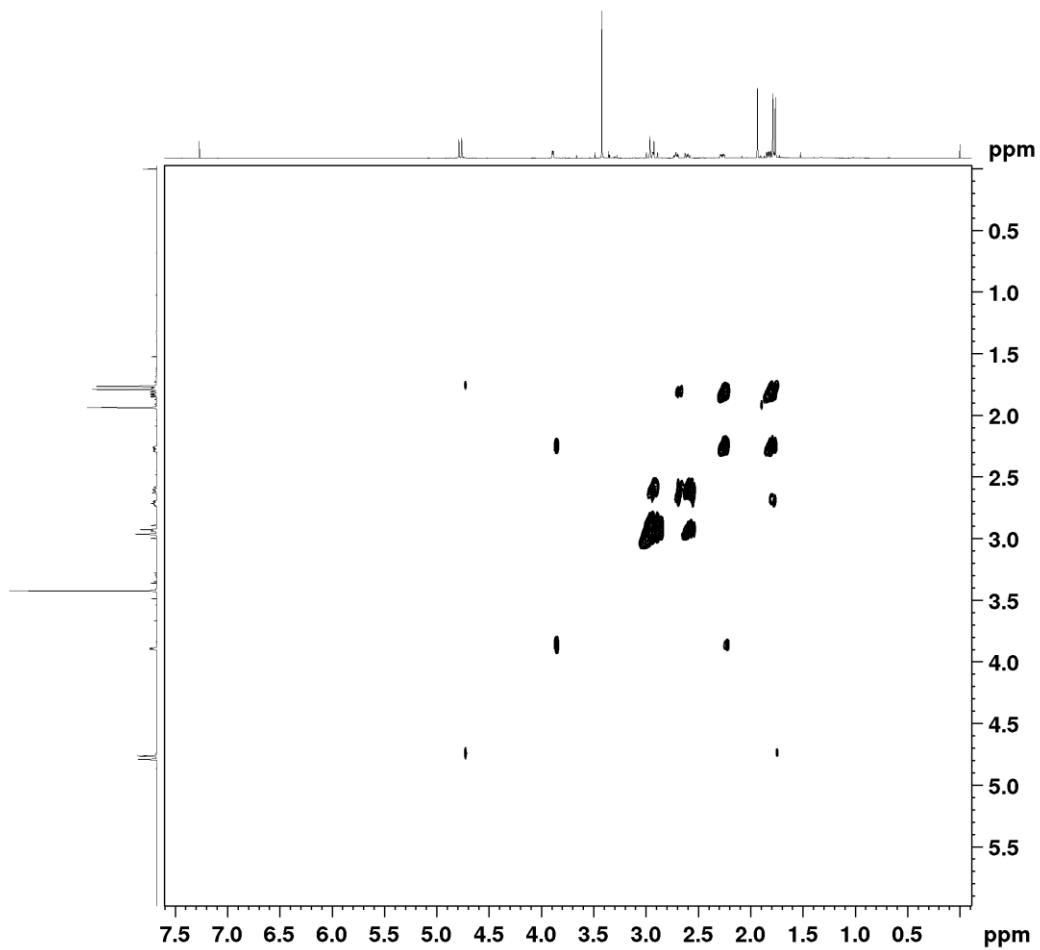


Figure S176 HMBC spectrum (600 MHz, CDCl_3) of compound **33**



Current Data Parameters
NAME RDE-121!
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200107
Time 3.16 h
INSTRUM spect
PROBHD Z816801_0163 (
PULPROG cosygppmfd
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 6.50 usec
TE 2.65 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 12.00 usec
PLW1 5.44000006 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
PmMode QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S177 ¹H-¹H COSY spectrum (600 MHz, CDCl₃) of compound 33

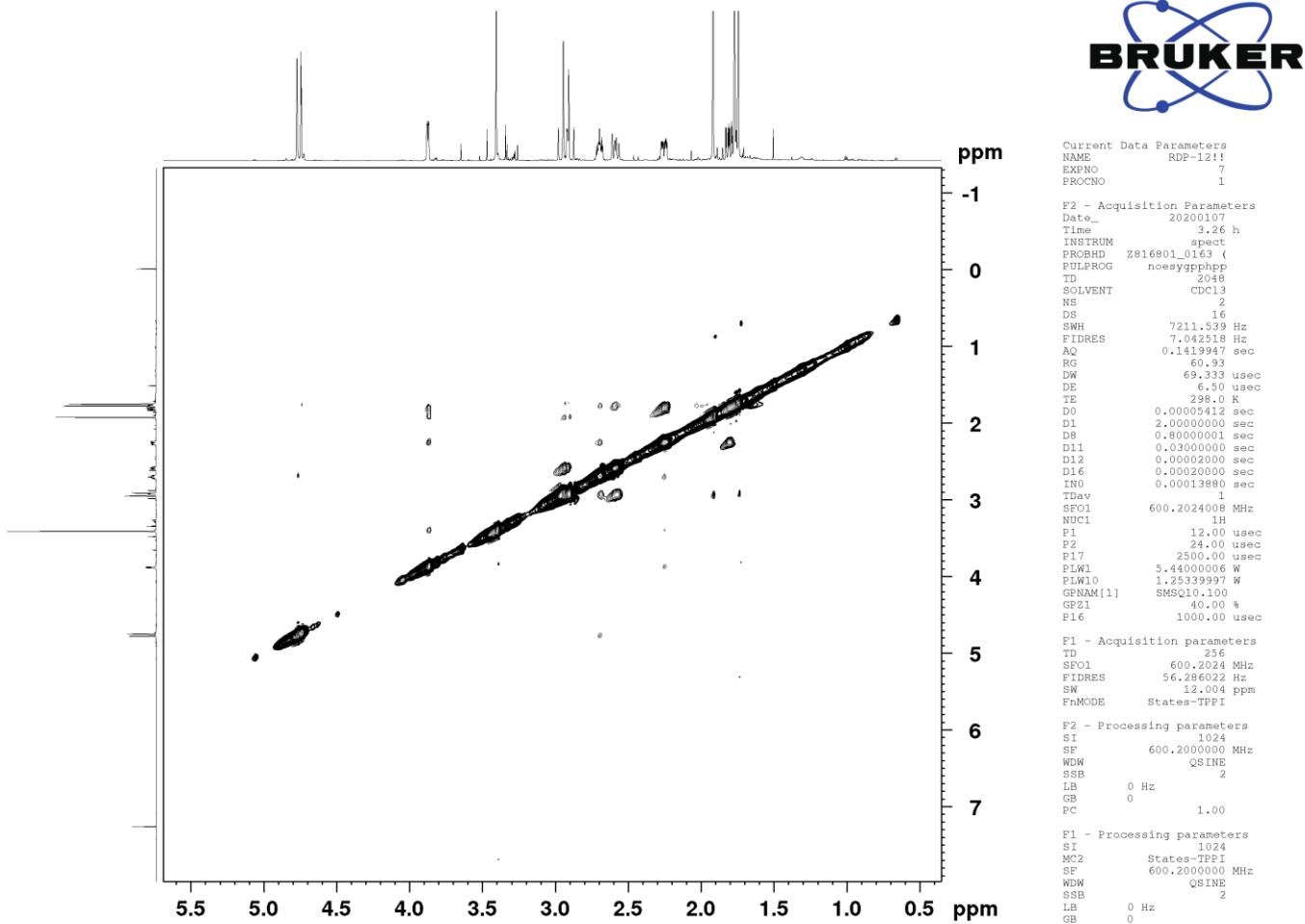


Figure S178 NOESY spectrum (600 MHz, CDCl_3) of compound **33**

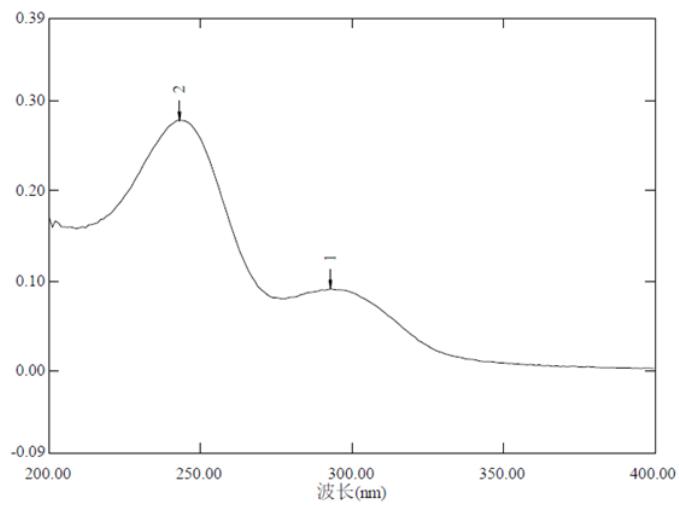
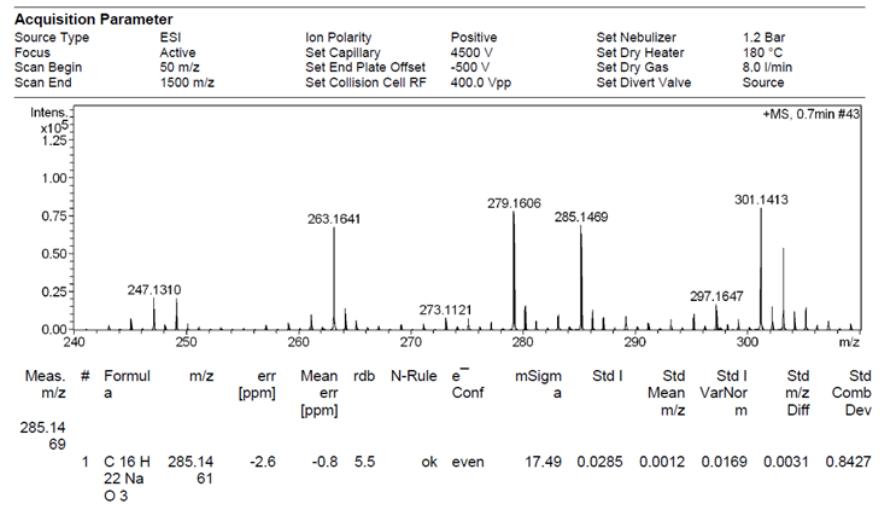


Figure S179 HRESIMS and UV spectra of compound 34

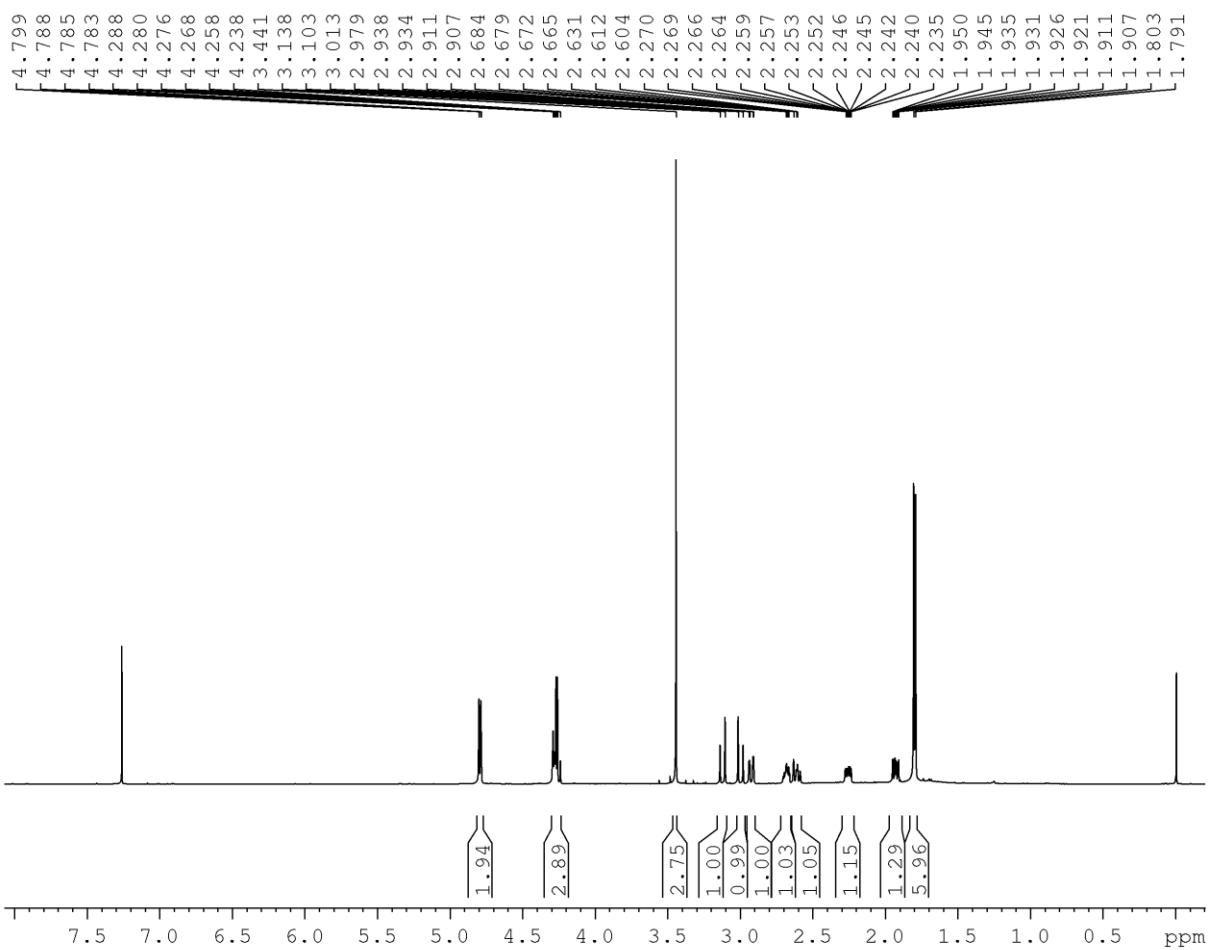


Figure S180 ¹H NMR spectrum (600 MHz, CDCl₃) of compound 34

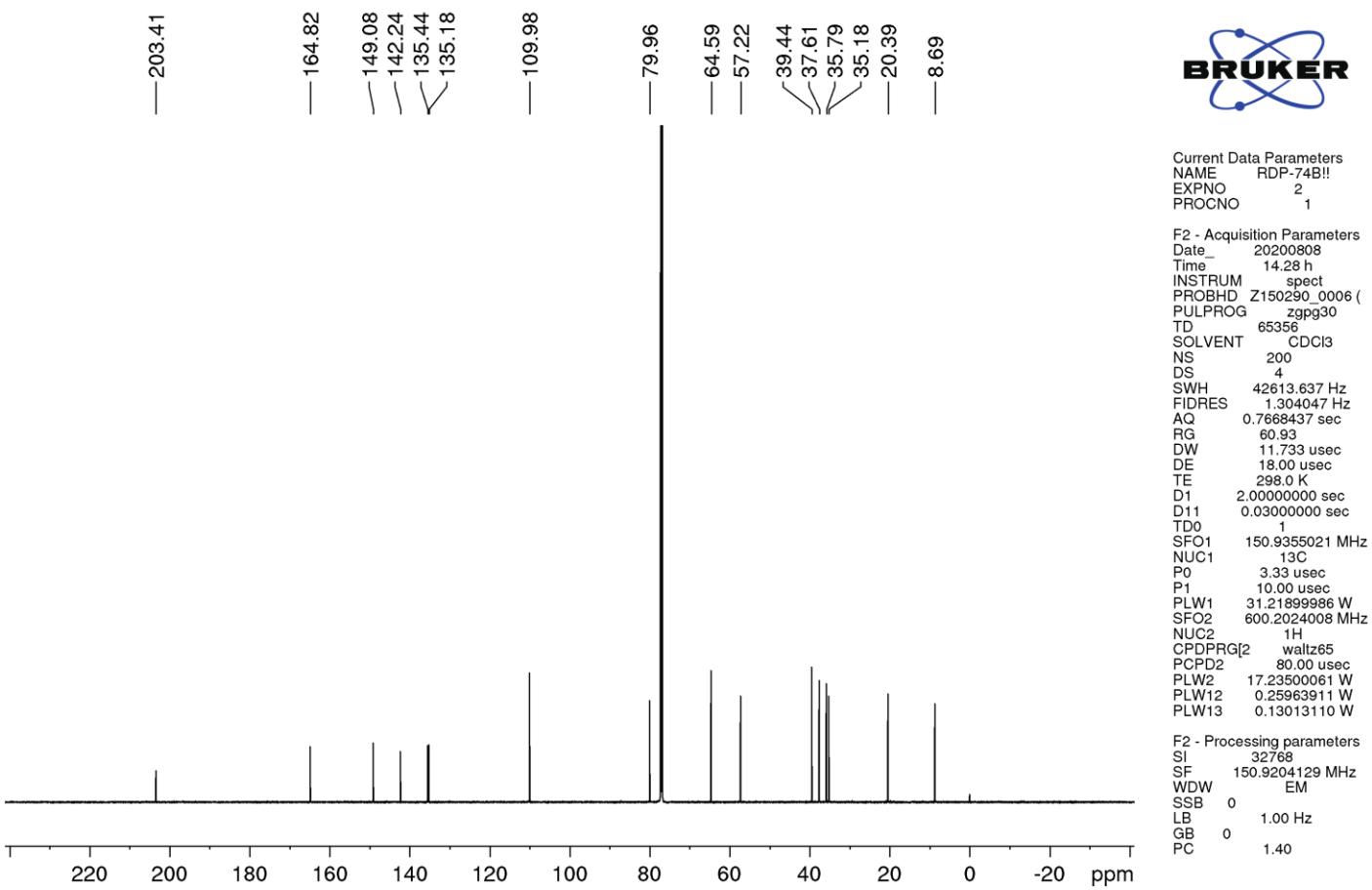


Figure S181 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **34**

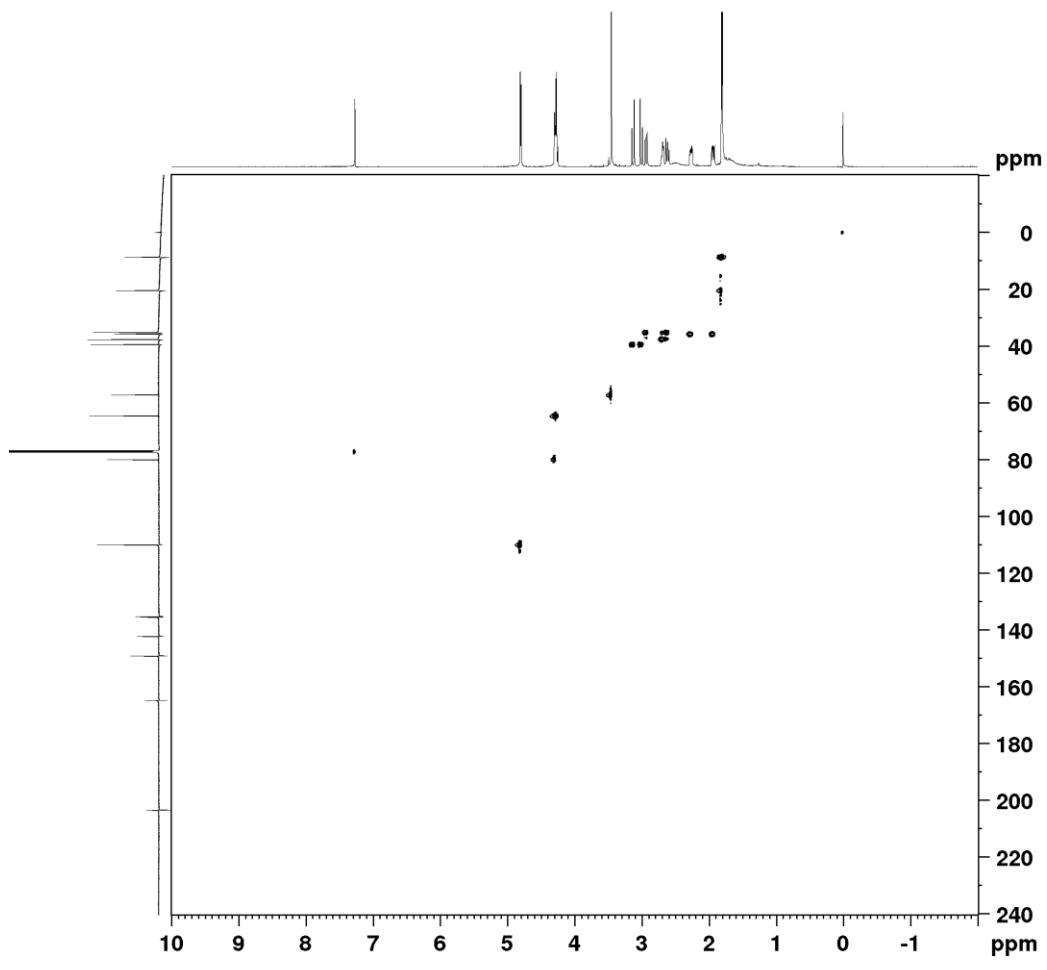
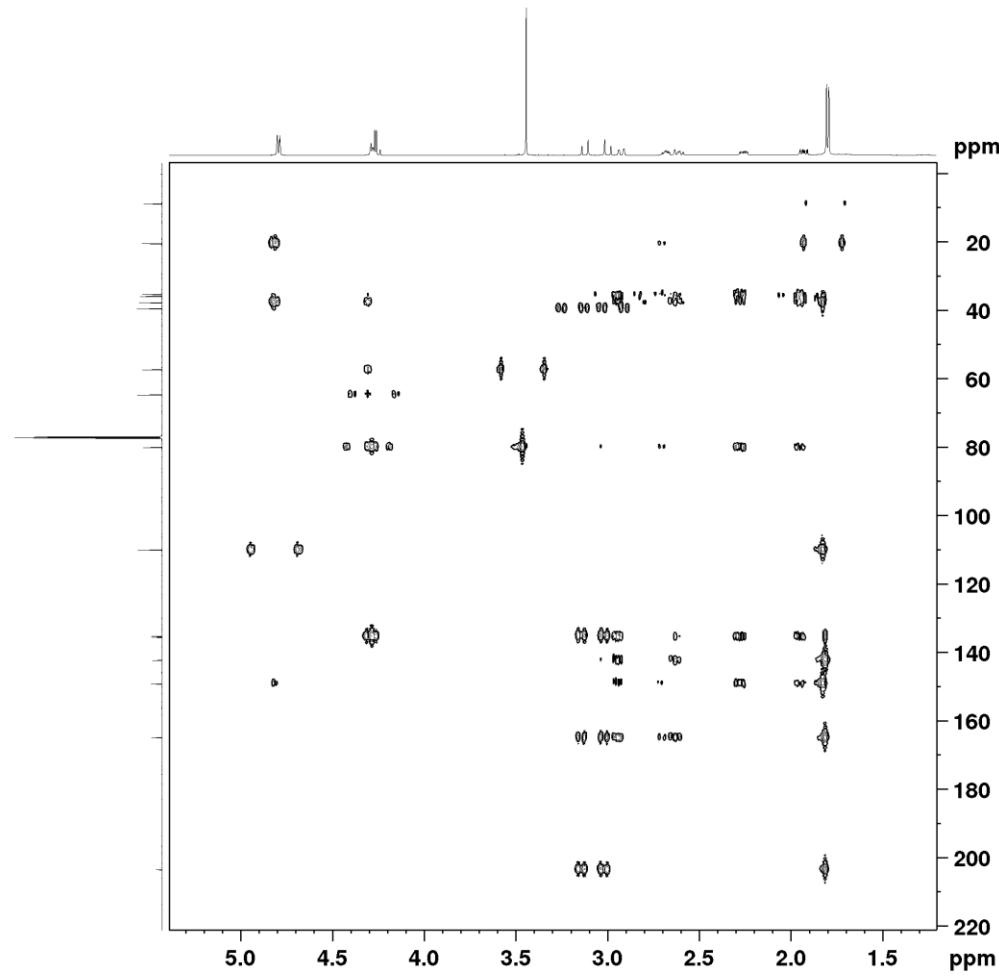


Figure S182 HSQC spectrum (600 MHz, CDCl₃) of compound 34



Current Data Parameters
NAME RDP-74B1:
EXPNO 5
PROCNO 1

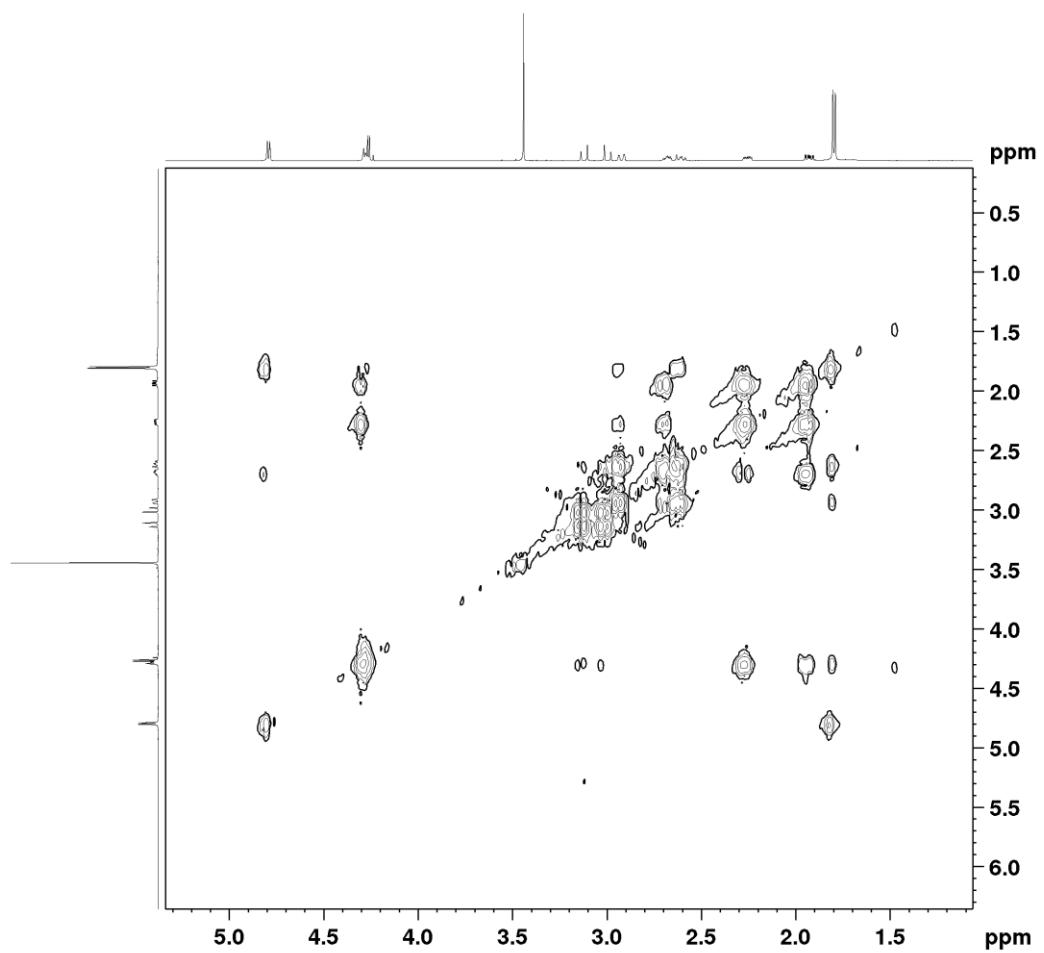
P2 - Acquisition Parameters
Date_ 20200815
Time 8.31 h
INSTRUM spect
PROBID Z150290_0001
PULPROG hmbcogn.drf
TD 4096
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 131.224
DW 69.433 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.000000
D0 0.00000300 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
DNO 0.00001270 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
SF02 150.9370100 MHz
NUC2 13C
P3 10.00 usec
PLW2 31.21899986 W
GPNAME[1] SMSQ10.100
GP21 50.00 °
GPNAME[2] SMSQ10.100
GP22 30.00 °
GPNAME[3] SMSQ10.100
GP23 40.10 °
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.937 MHz
FIDRES 615.157471 Hz
SW 260.838 ppm
FhMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S183 HMBC spectrum (600 MHz, CDCl_3) of compound 34



Current Data Parameters
NAME RDP-74B!!
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200815
Time 8.40 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG cosygppmfd
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 10.00 usec
TE 290.00 K
D0 0.00000300 sec
D1 2.0000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
PnMODE QF

F2 - Processing parameters

SI 1024

SF 600.2000000 MHz

WDW SINE

SSB 0

LB 0 Hz

GB 0

PC 1.40

F1 - Processing parameters

SI 1024

MC2 64

SF 600.2000000 MHz

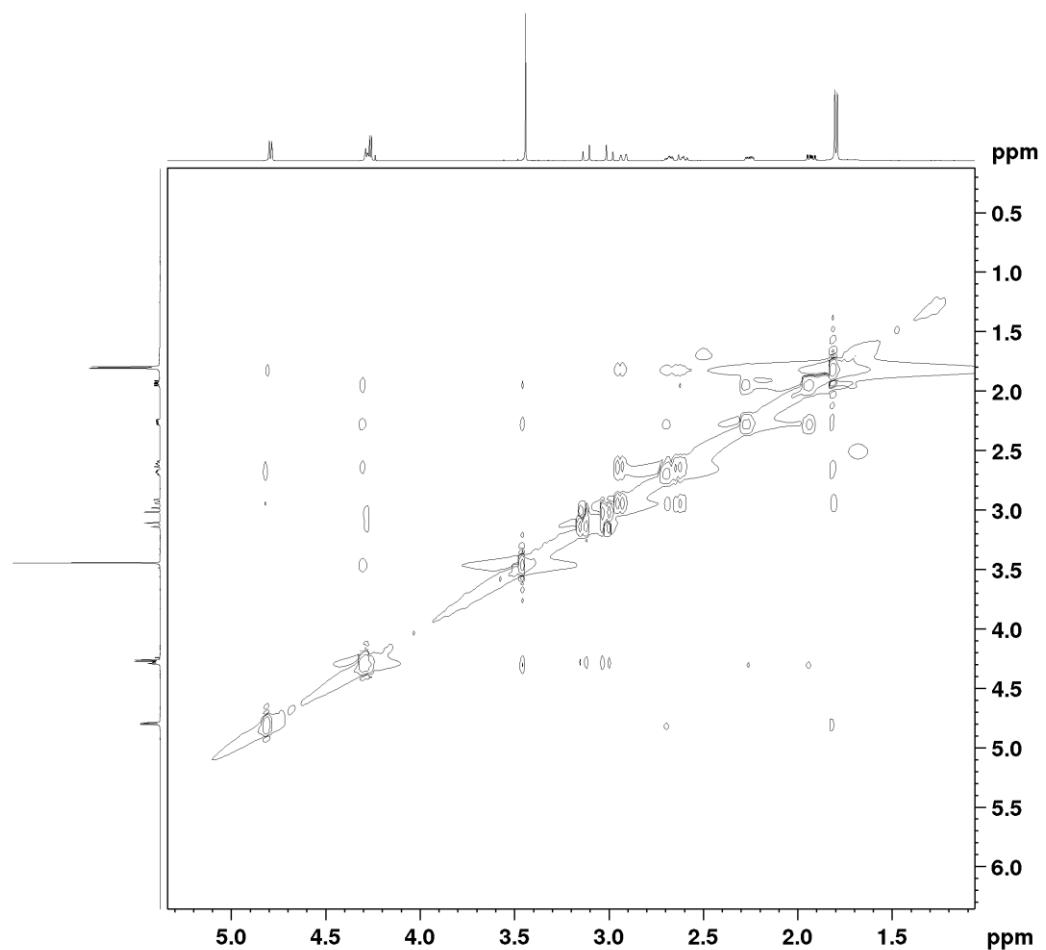
WDW SINE

SSB 0

LB 0 Hz

GB 0

Figure S184 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 34



Current Data Parameters
NAME RDP-74B!!
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200815
Time 8.50 h
INSTRUM spect
PROBHD Z150290_0066_1
PULPROG noeipypphphh
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60
DW 69.333 usec
DB 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D18 0.00013860 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S185 NOESY spectrum (600 MHz, CDCl₃) of compound 34

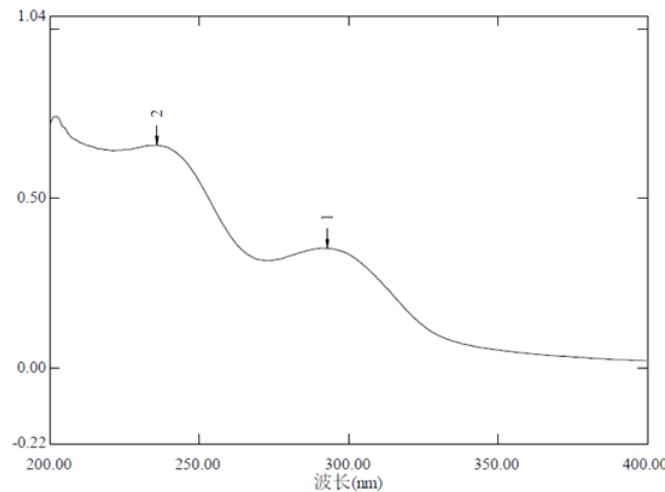
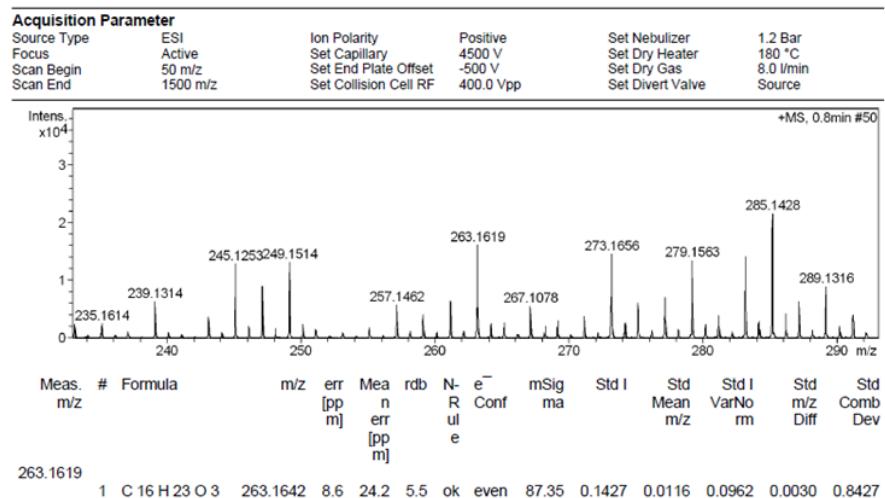


Figure S186 HRESIMS and UV spectra of compound 35

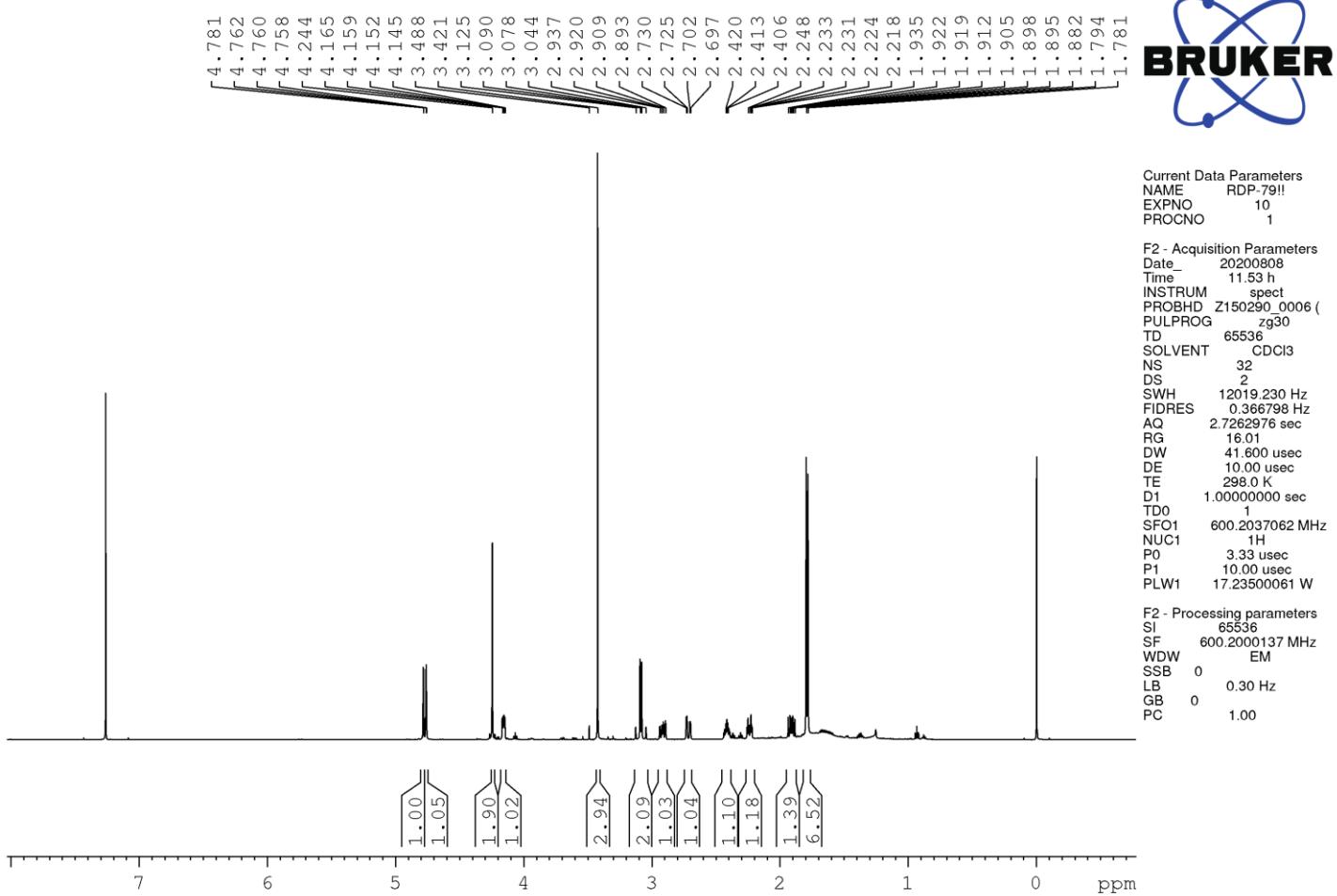
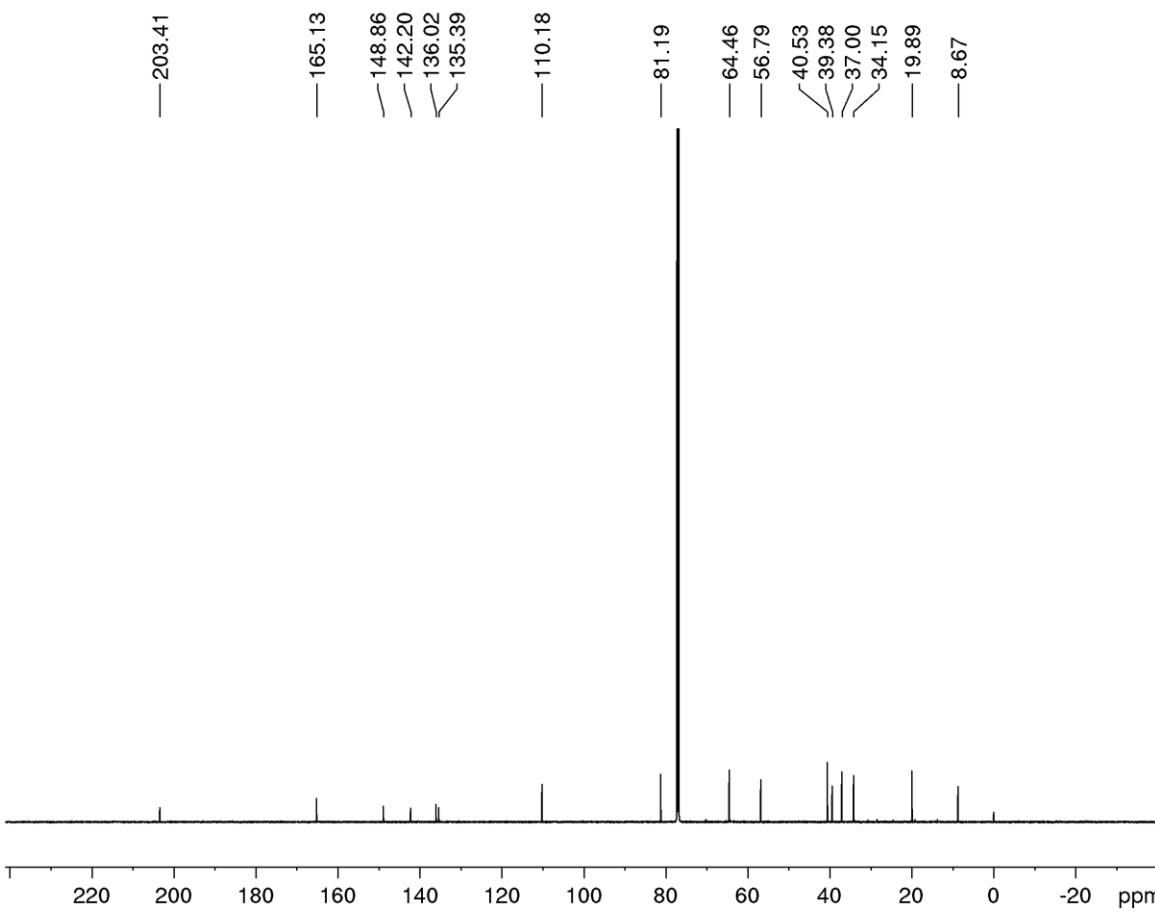


Figure S187 ¹H NMR spectrum (600 MHz, CDCl₃) of compound 35



Current Data Parameters
NAME RDP-79!!
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200808
Time_ 15.03 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgppg30
TD 65356
SOLVENT CDCl₃
NS 300
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 43.48
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 ¹³C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 ¹H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9204148 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S188 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **35**

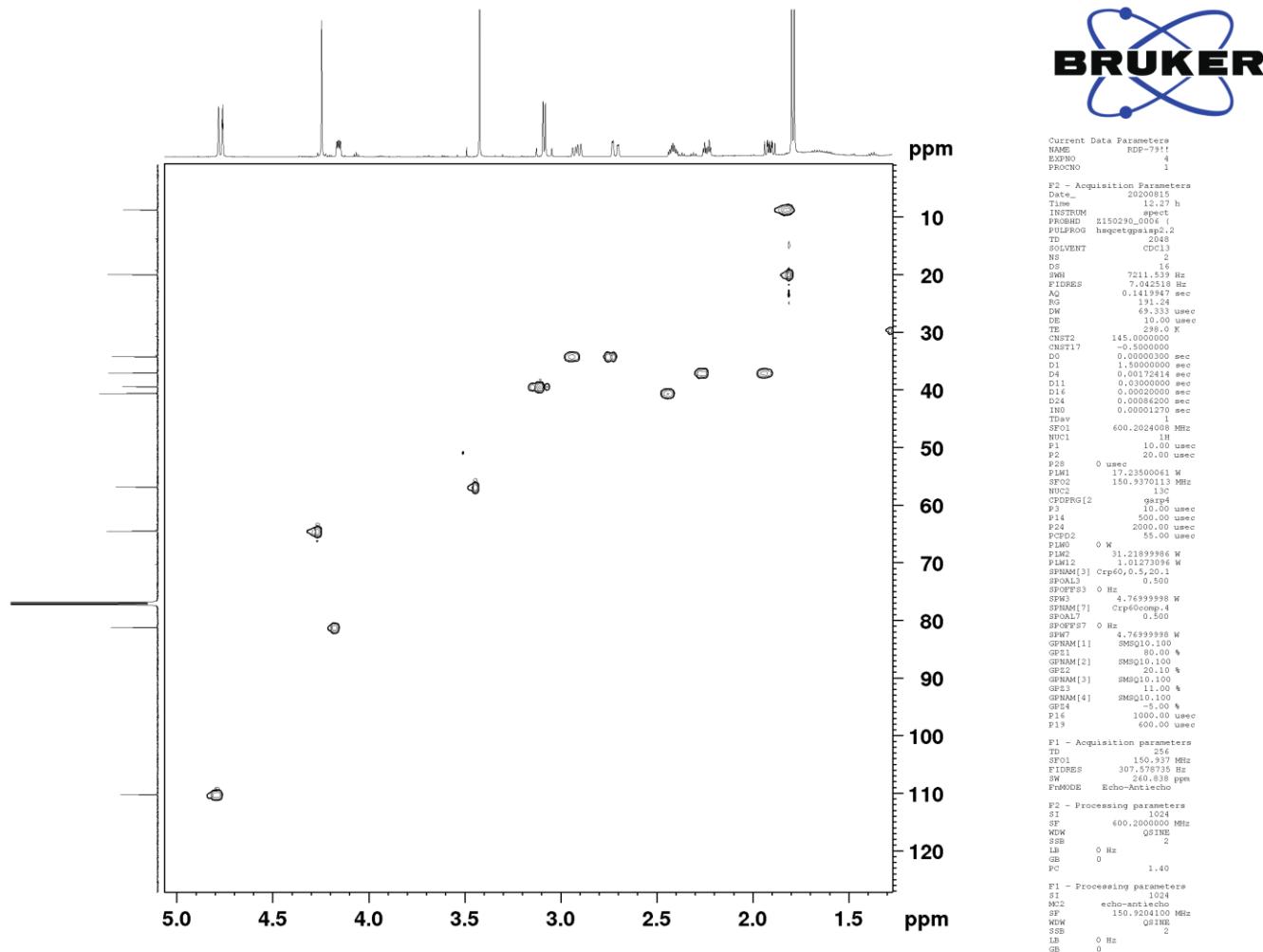
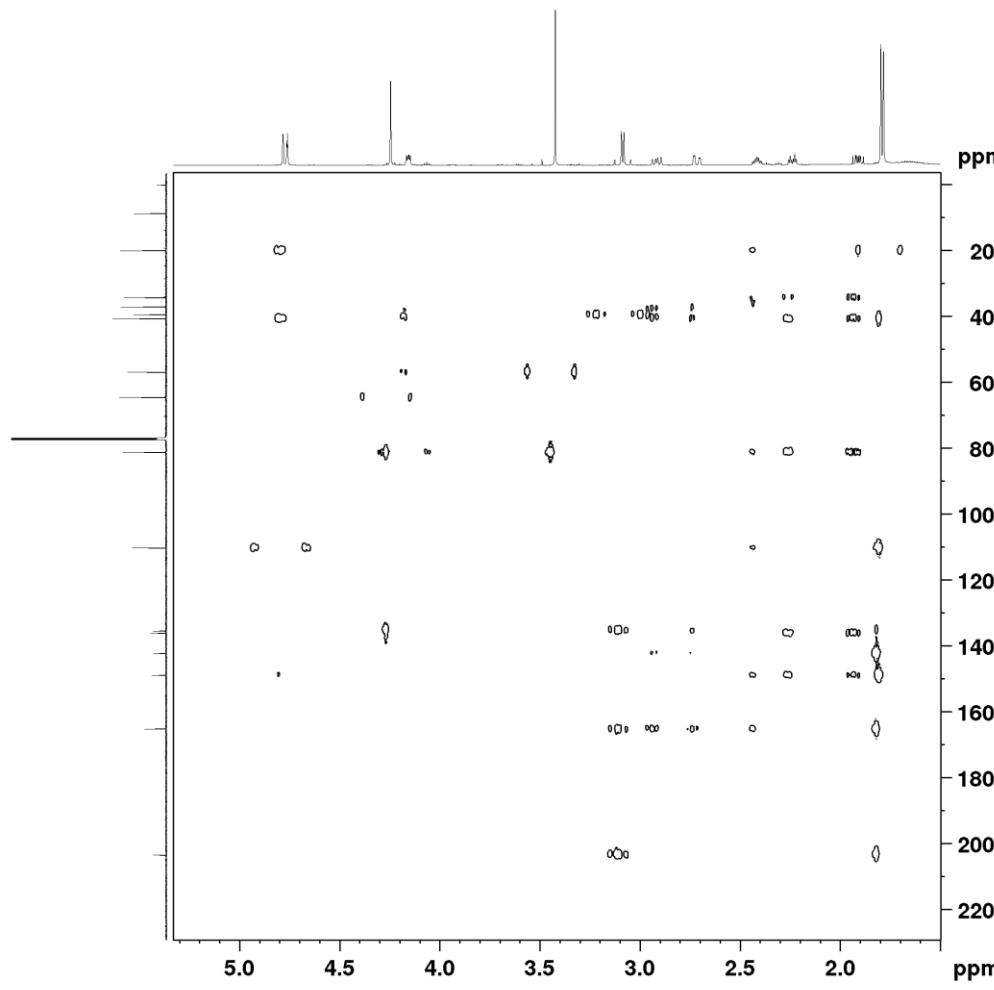


Figure S189 HSQC spectrum (600 MHz, CDCl₃) of compound 35



Current Data Parameters
NAME RDP-791
EXPNO 5
PROCNO 1

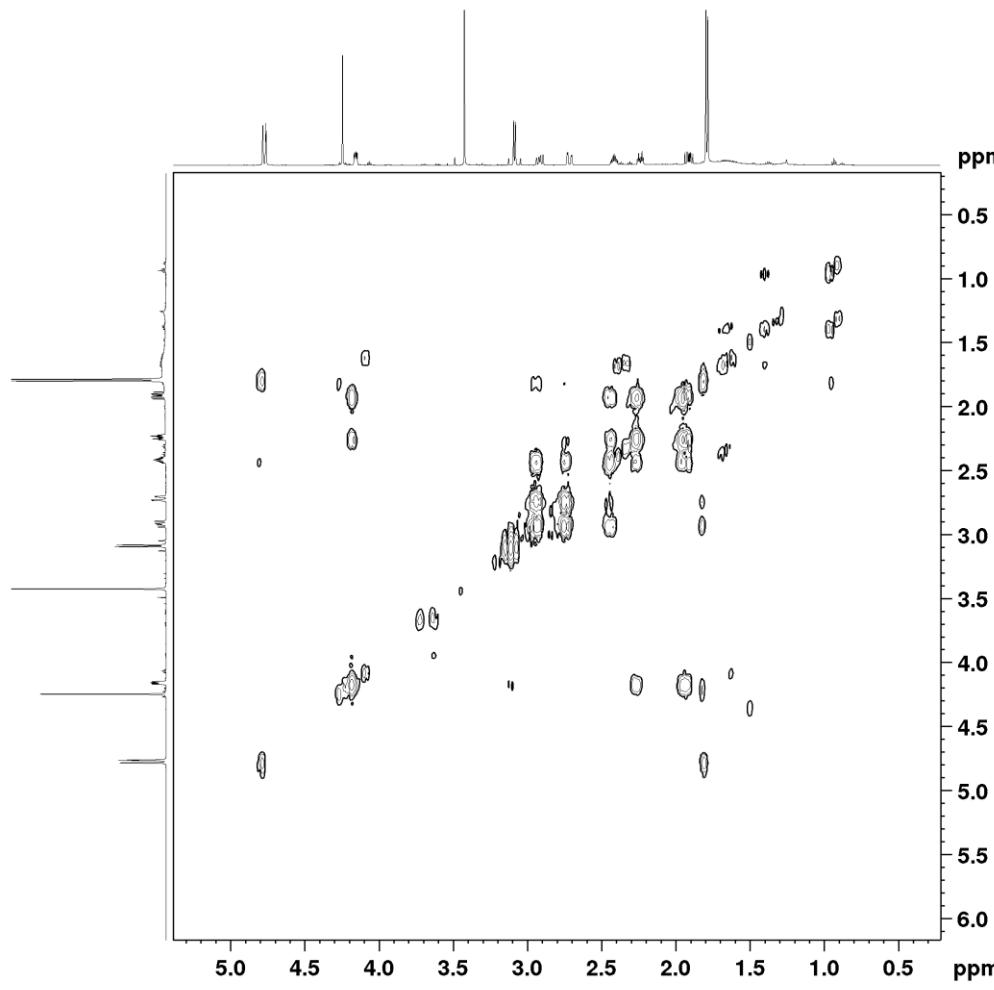
F2 - Acquisition Parameters
Date_ 20200815
Time 12.43 h
INSTRUM spect
PROBID Z150290_0001
PULPROG hmbcogn.dif
TD 4096
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 131.224
DW 69.433 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.000000
D0 0.00000300 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
DW0 0.00001270 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
SF02 150.9370100 MHz
NUC2 13C
P3 10.00 usec
PLW2 31.21899986 W
GPNAME[1] SMSQ10.100
GP21 50.00 °
GPNAME[2] SMSQ10.100
GP22 30.00 °
GPNAME[3] SMSQ10.100
GP23 40.10 °
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.937 MHz
FIDRES 615.157471 Hz
SW 260.838 ppm
FhMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S190 HMBC spectrum (600 MHz, CDCl_3) of compound **35**



Current Data Parameters
NAME RDP-79!!
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date 20200815
Time 12.52 h
INSTRUM spect
PROBHD Z150290_0006 (cosygppmfr
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 10.00 usec
TE 299.0 K
D0 0.00000300 sec
D1 2.0000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S191 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 35

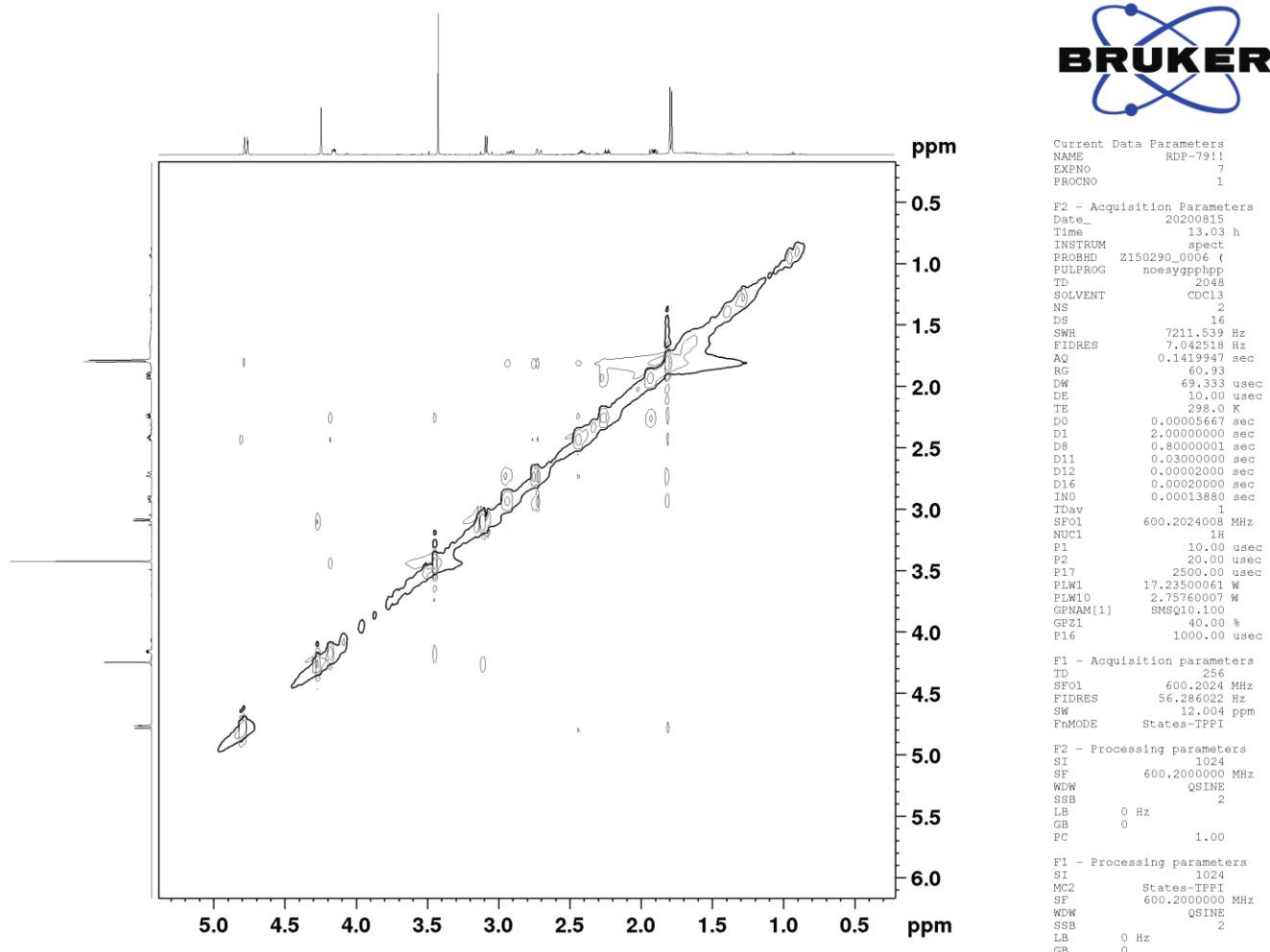


Figure S192 NOESY spectrum (600 MHz, CDCl_3) of compound **35**

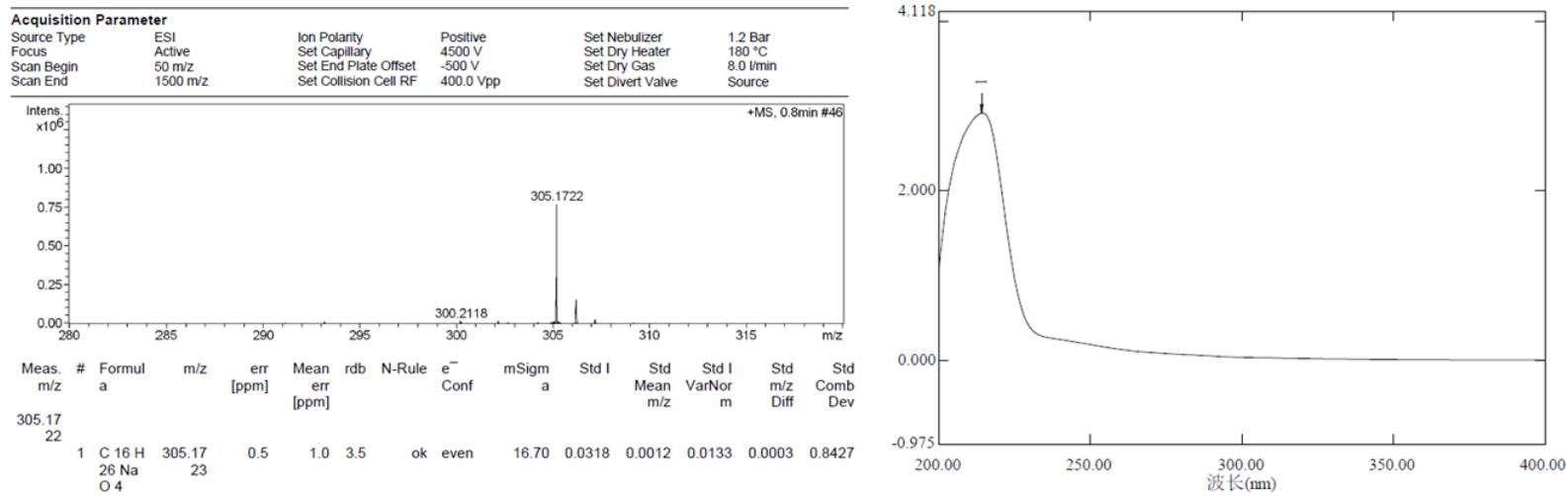
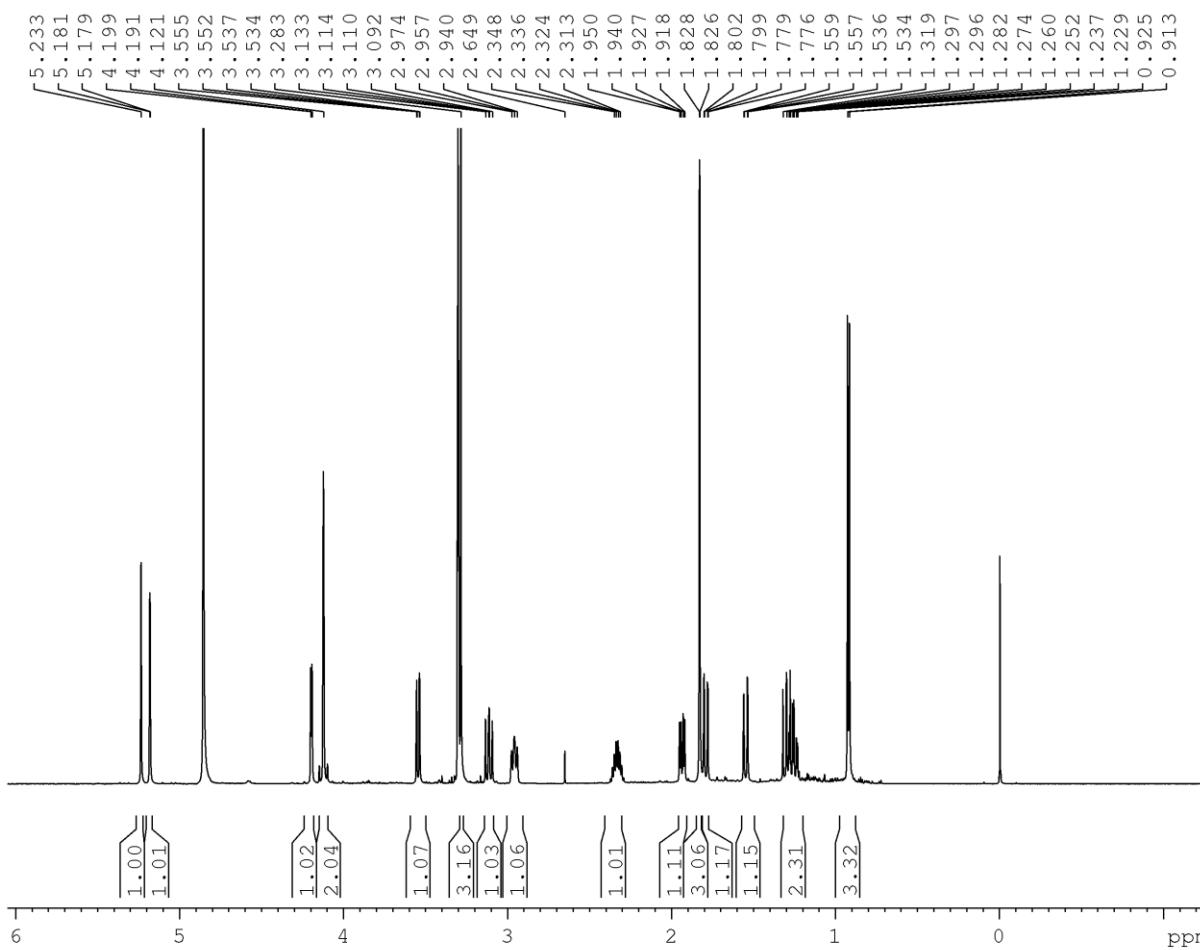


Figure S193 HRESIMS and UV spectra of compound **36**



Current Data Parameters
NAME RDP-87! !
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200815
Time 23.44 h
INSTRUM spect
PROBHD Z150290_00006 (
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 30.25
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1
SF01 600.2037062 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 17.23500061 W

F2 - Processing parameters
SI 65536
SF 600.2000166 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S194 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **36**

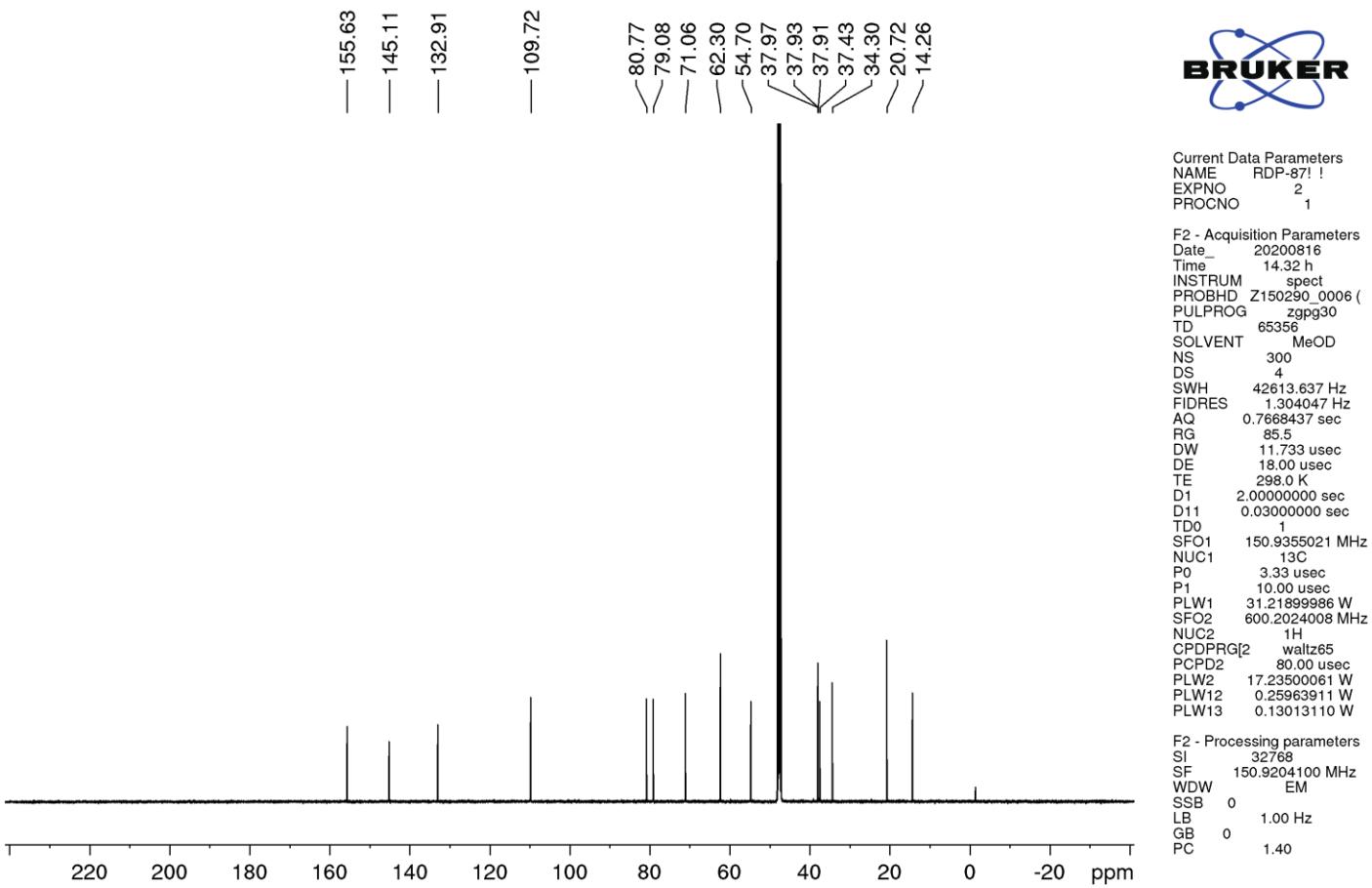
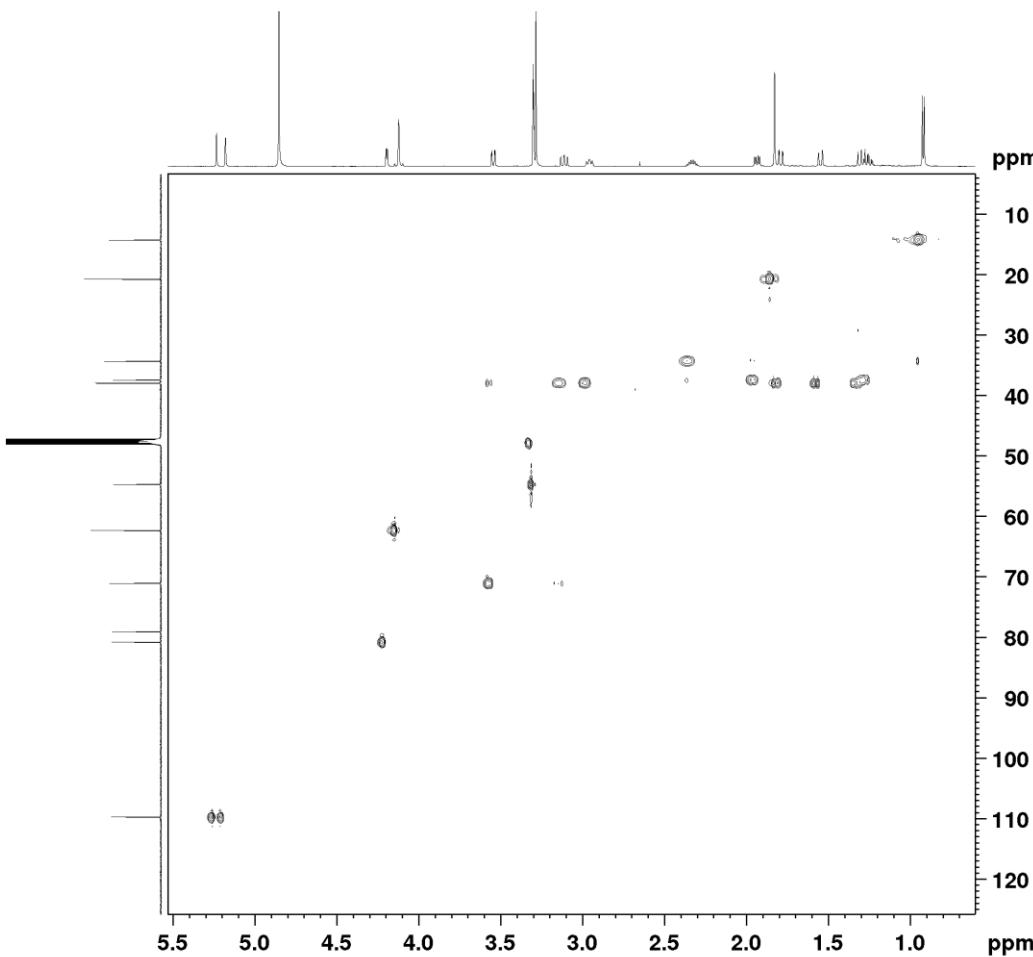


Figure S195 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **36**



Current Data Parameters
NMAM RDP-871
BPPN 4
PRCNO 1

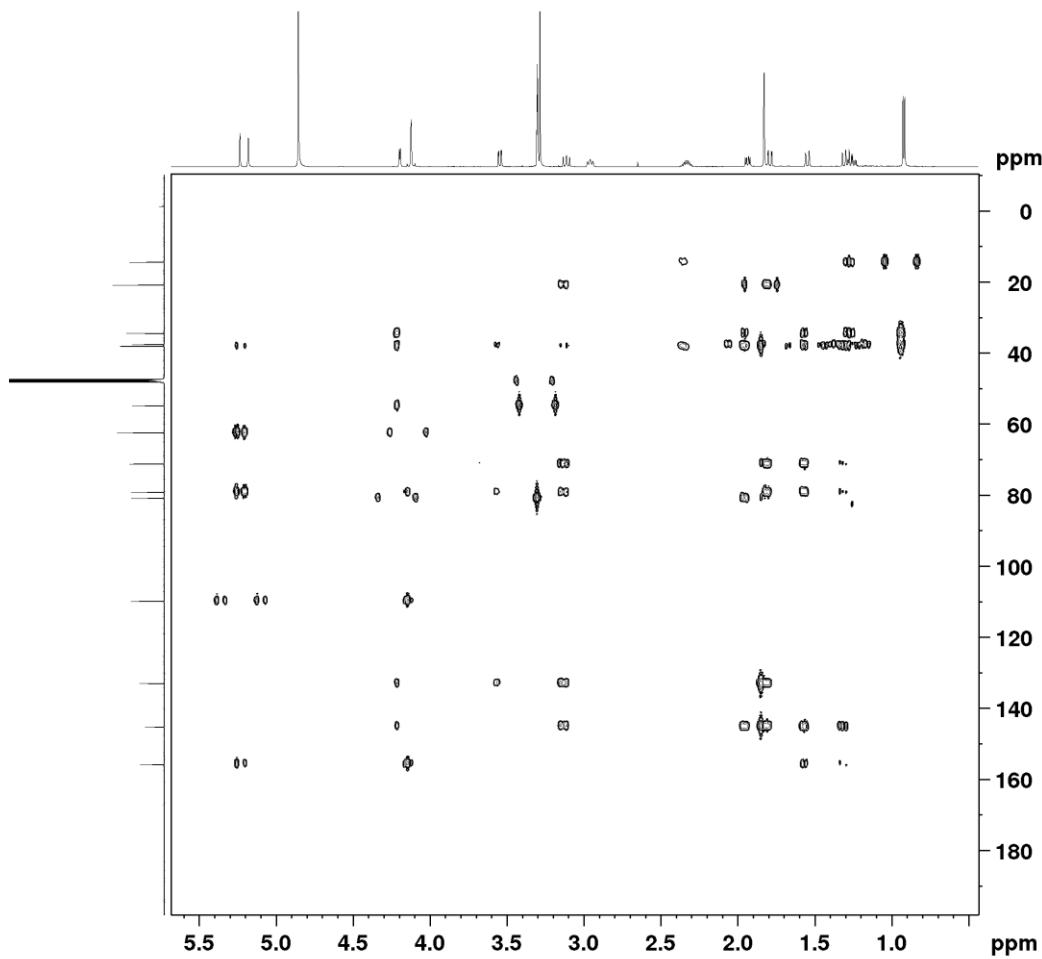
F2 - Acquisition Parameters
Data_ 20200820
Time 0.56 h
INSTRUM spect
PROBHD 1150299_0006 (PULPROG hsqcetgpsp12
TD 65536
SOLVENT MeOD
DS 2
SWH 7211.539 Hz
ETRATES 7.0493 Hz
AQ 0.1419947 sec
RG 191.24
DW 65.00 usec
DE 10.00 usec
TB 298.0 K
CNUST2 145.000000
CNUST17 -0.5000000
CNUST1 0.5000000
D0 0.0000300 sec
D1 0.0000300 sec
D4 0.00172414 sec
D11 0.0300000 sec
D16 0.0000300 sec
D24 0.00008200 sec
TDav 0.00001380 sec
TDav 600.12024099 MHz
SW01 1000.000000 Hz
P1 10.00 usec
P2 20.00 usec
P2A 0 usec
PLW1 17.23505061 W
SF02 150.9355021 MHz
SW02 1000.000000 Hz
CPDPNS(2 garp4 10.00 usec
P1A 10.00 usec
P2A 2000.00 usec
CPD2Z 55.00 usec
PLW0 0 W
PLW2 31.21899986 W
P1D 10.00 usec
GPNAME[3] Cpmg60,4,5,20,1
SPDALS 0.500
SPDPFS3 0 Hz
SPW 4.76999998 W
SPRNAME[7] Cpmg60comp,4
SPDOL 0.500
SPDPFS7 0 Hz
SPW7 4.76999998 W
GPNAME[1] SMSQ10,100
GP2 80.00 *
GPNAME[2] SMSQ10,100
GP3 100.00 *
GPNAME[3] SMSQ10,100
GP21 11.00 *
GPNAME[4] SMSQ10,100
GP24 -5.00 *
P16 1000.00 usec
P13 600.00 usec

F1 - Acquisition parameters
TD 256
SF01 150.9355 MHz
ETRATES 240.049 ppm
DW 240.049 ppm
PRMode Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WGW Q3INE
SSB Z
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9204100 MHz
WGW Q3INE
SSB Z
LB 0 Hz
GB 0

Figure S196 HSQC spectrum (600 MHz, CDCl₃) of compound 36



Current Data Parameters
NAME RDP-871_5
EXPNO 5
PROCNO 1

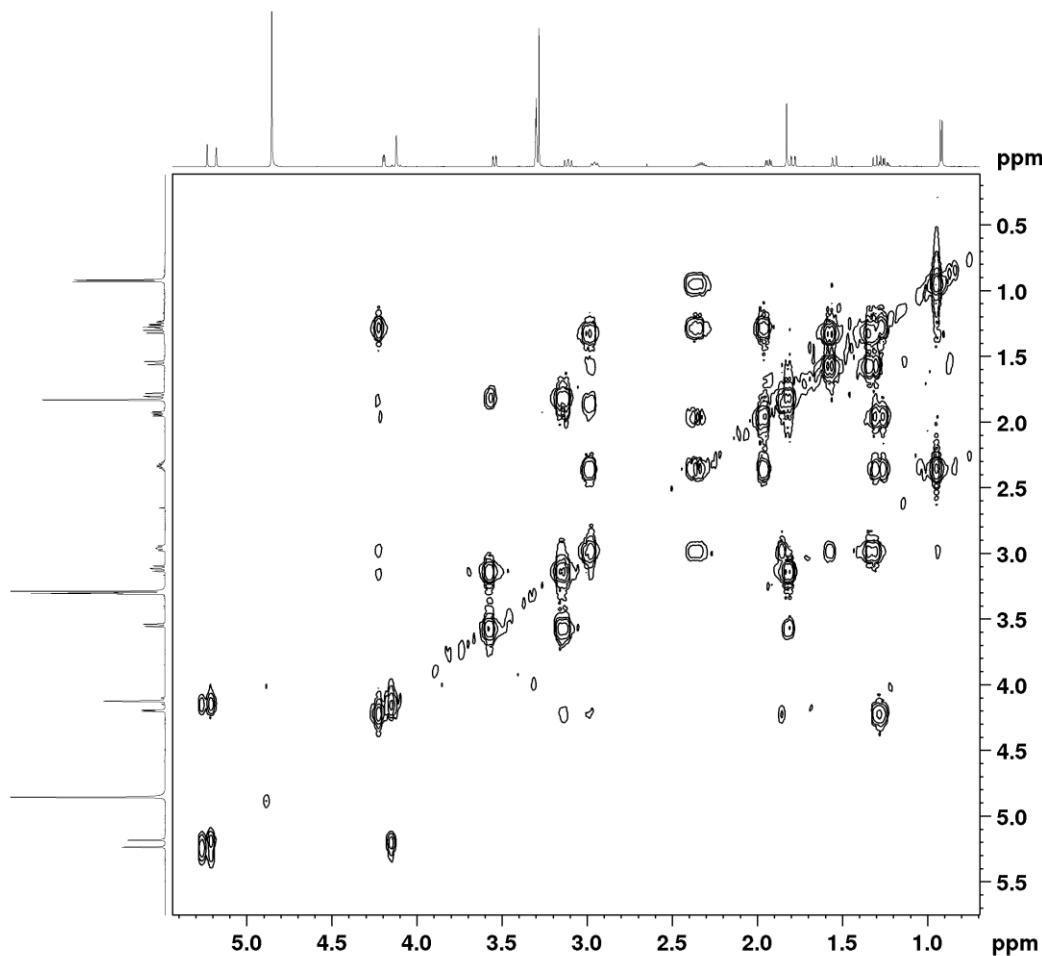
F2 - Acquisition Parameters
Date_ 20200820
Time 7.22 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG hmbcgrndqf
TD 4096
SOLVENT Me₃Si
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 3.521259 Hz
AQ 0.2839893 sec
RG 130
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
CNS13 8.0000000
D0 0.0000000 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001380 sec
TDav 600.2024000 sec
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
SFO1 600.2024000 MHz
NUC2 150.9355021 MHz
P1C 10.00 usec
P2C 31.21899986 W
GPNAME[1] SNSQ10.100
GPZ1 50.00 %
GPNAME[2] SNSQ10.100
GPZ2 30.00 %
GPNAME[3] SNSQ10.100
GPZ3 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9355021 MHz
FIDRES 566.123169 Hz
SW 240.049 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S197 HMBC spectrum (600 MHz, CDCl₃) of compound 36



Current Data Parameters
NAME RDP-671 !
EXPNO 6
PROCNO 1

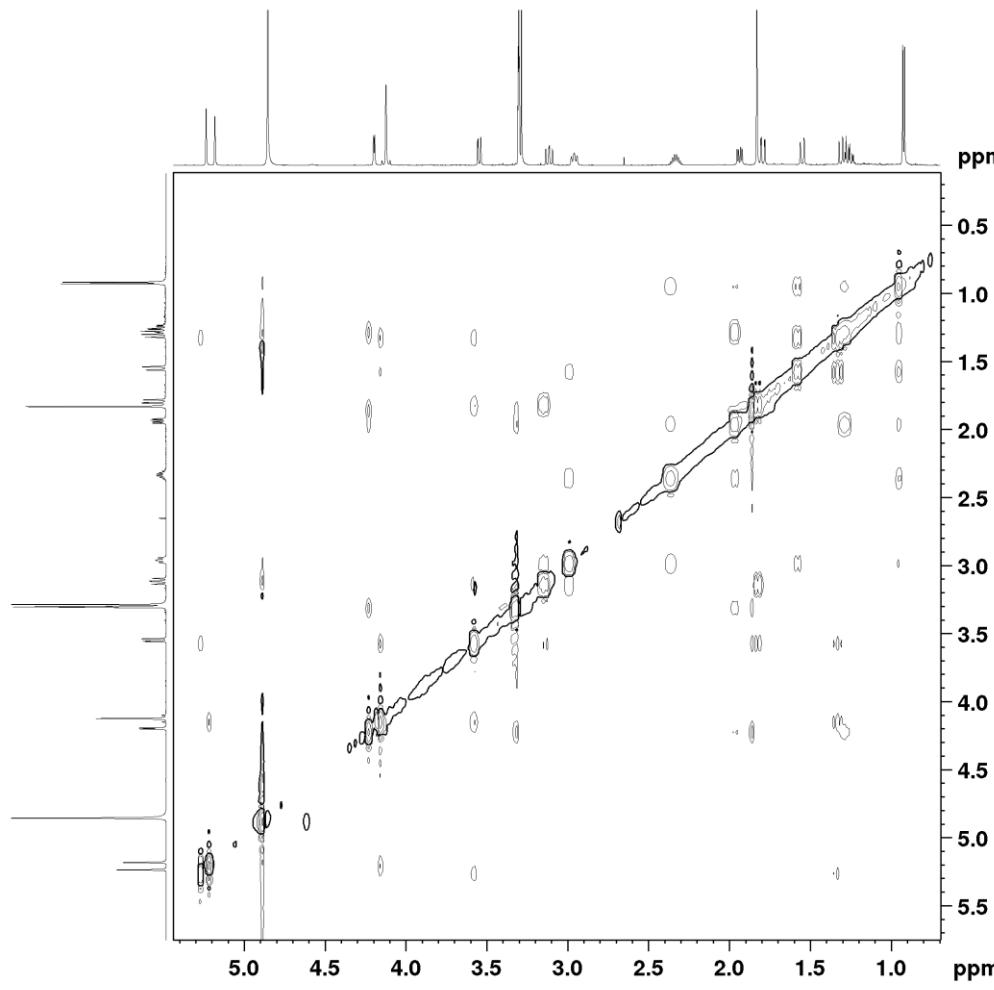
F2 - Acquisition Parameters
Date_ 20200820
Time 7.39 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG cosyppmfd
TD 2048
SOLVENT MeOD
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 10.00 usec
TE 29.64 K
DO 0.00000300 sec
D1 2.0000000 sec
D13 0.0000400 sec
D16 0.0002000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.2350061 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
PmMode QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 64
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S198 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 36



Current Data Parameters
NAME RDP-87!
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200820
Time 7.50 h
INSTRUM spect
PROBHD Z150290_0004 (
PULPROG noeugpphp
TD 2048
SOLVENT MeOD
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60.93
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000000 sec
D11 0.0000000 sec
D12 0.00002000 sec
D16 0.00002000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12.004 ppm
PrMODE States-TIPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TIPI
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S199 NOESY spectrum (600 MHz, CDCl_3) of compound **36**

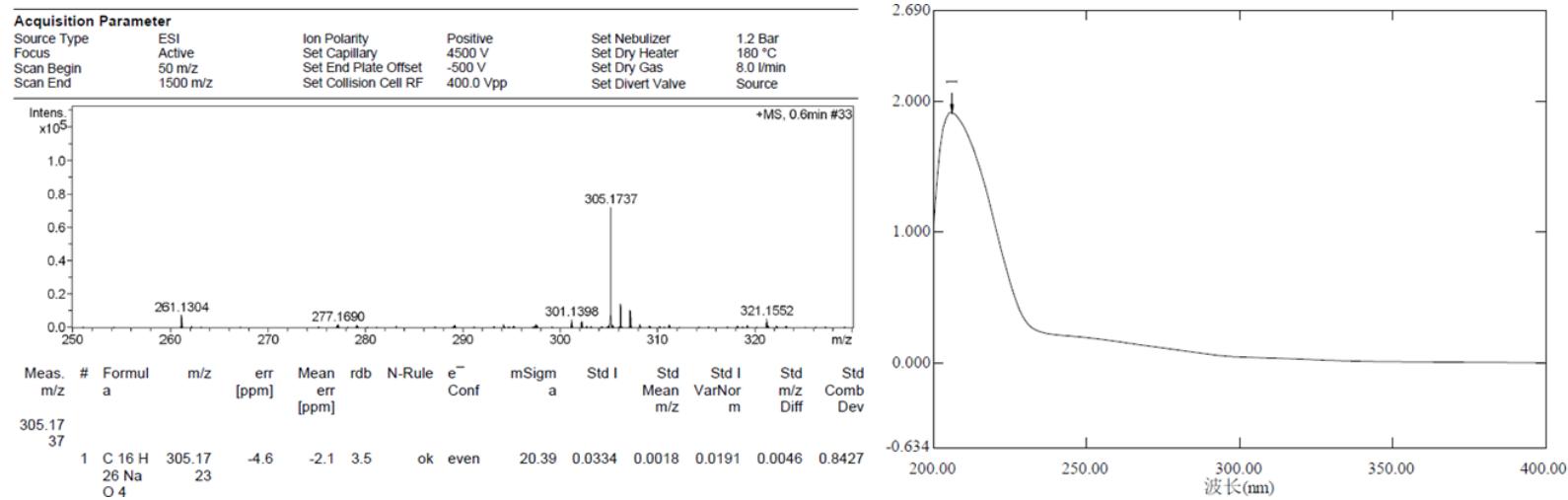


Figure S200 HRESIMS and UV spectra of compound 37

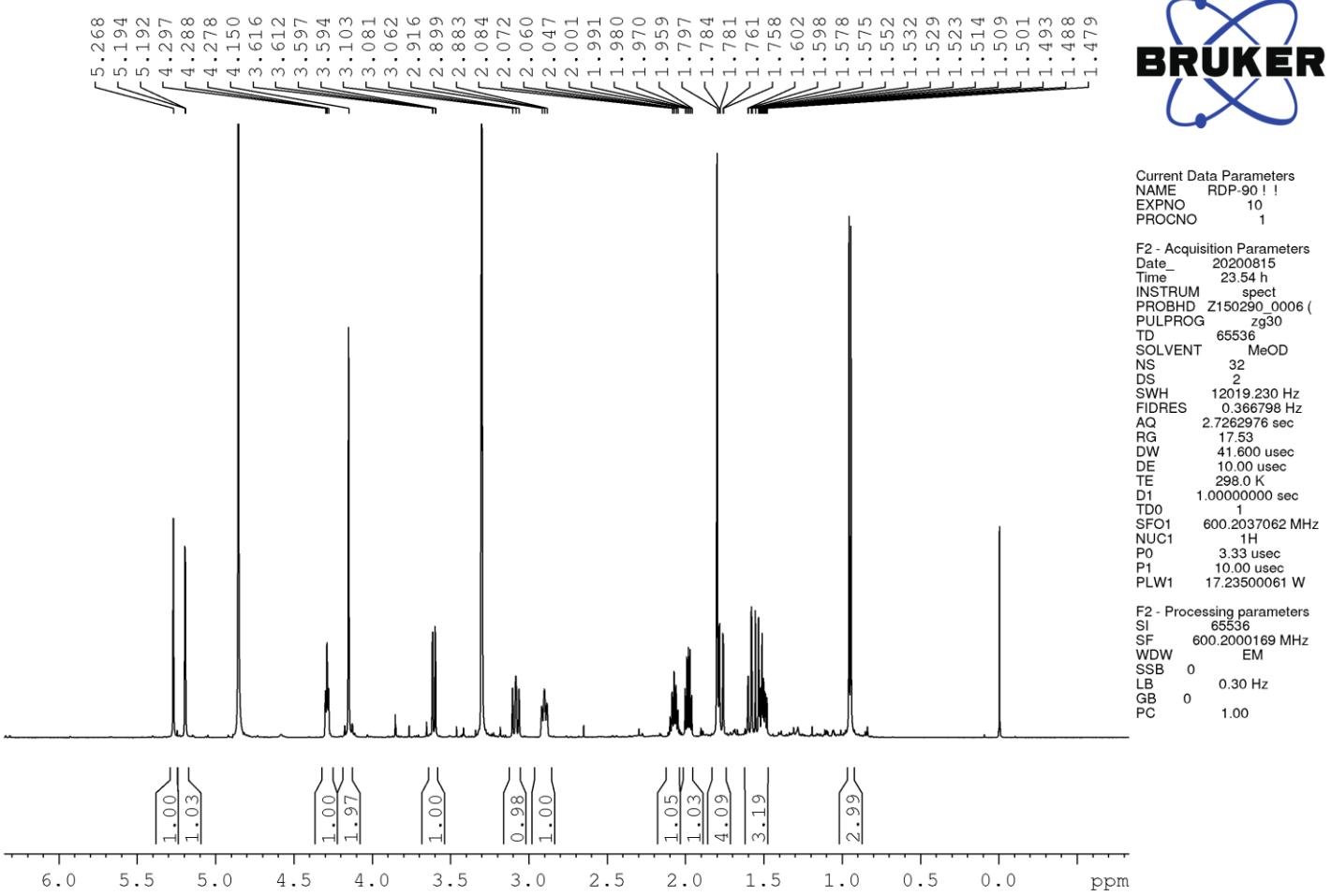


Figure S201 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **37**

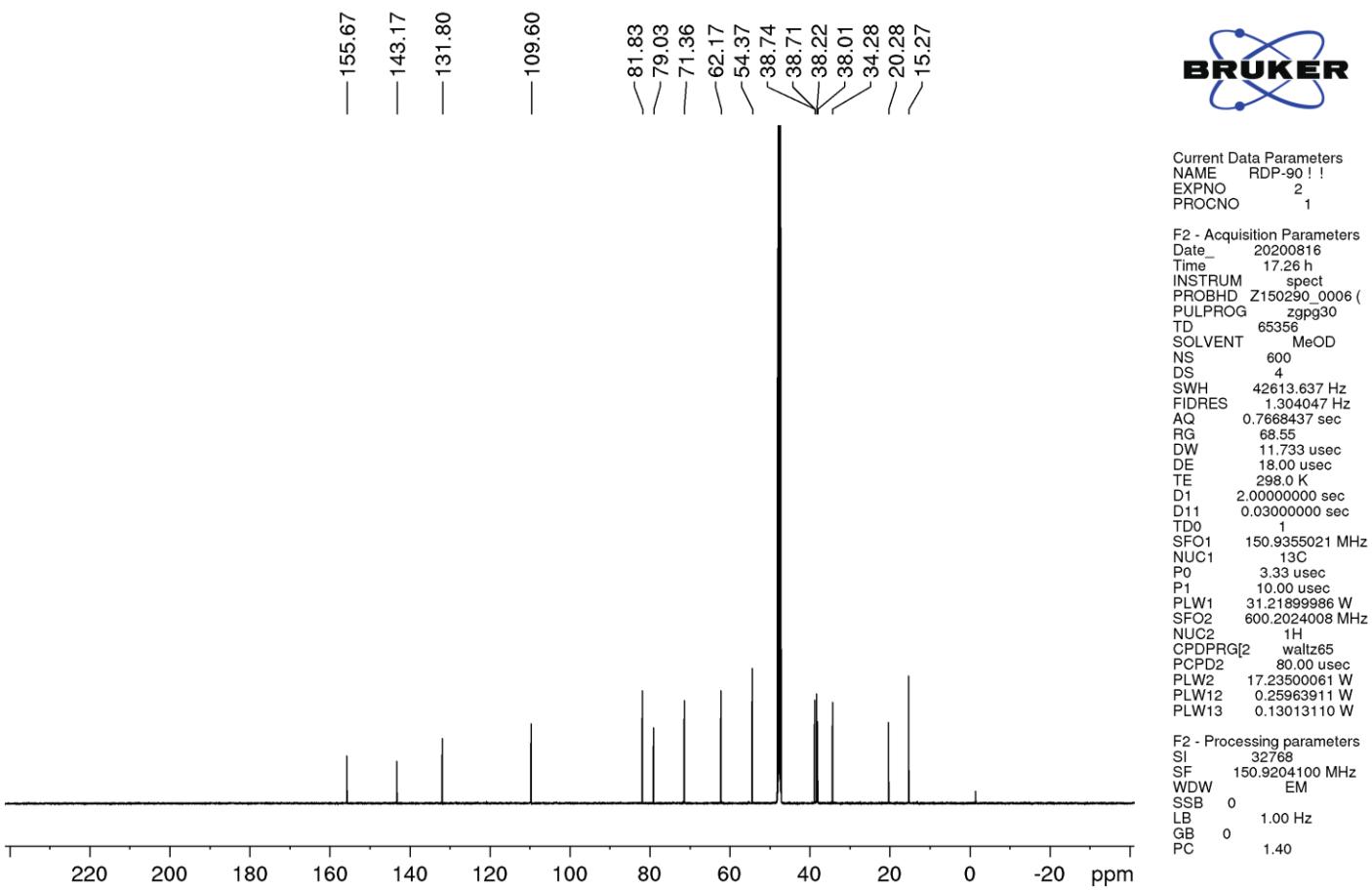


Figure S202 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **37**

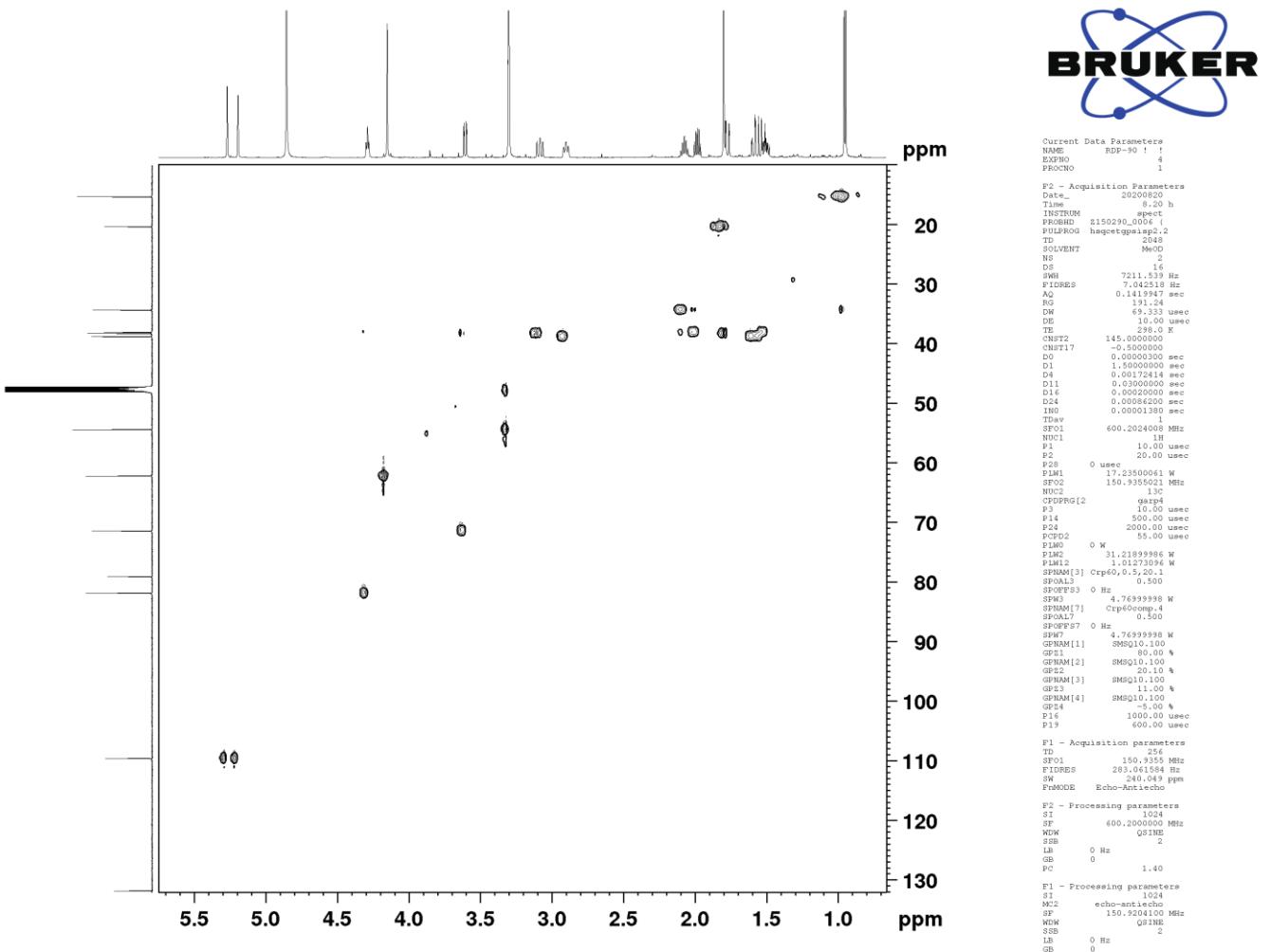


Figure S203 HSQC spectrum (600 MHz, CDCl_3) of compound **37**

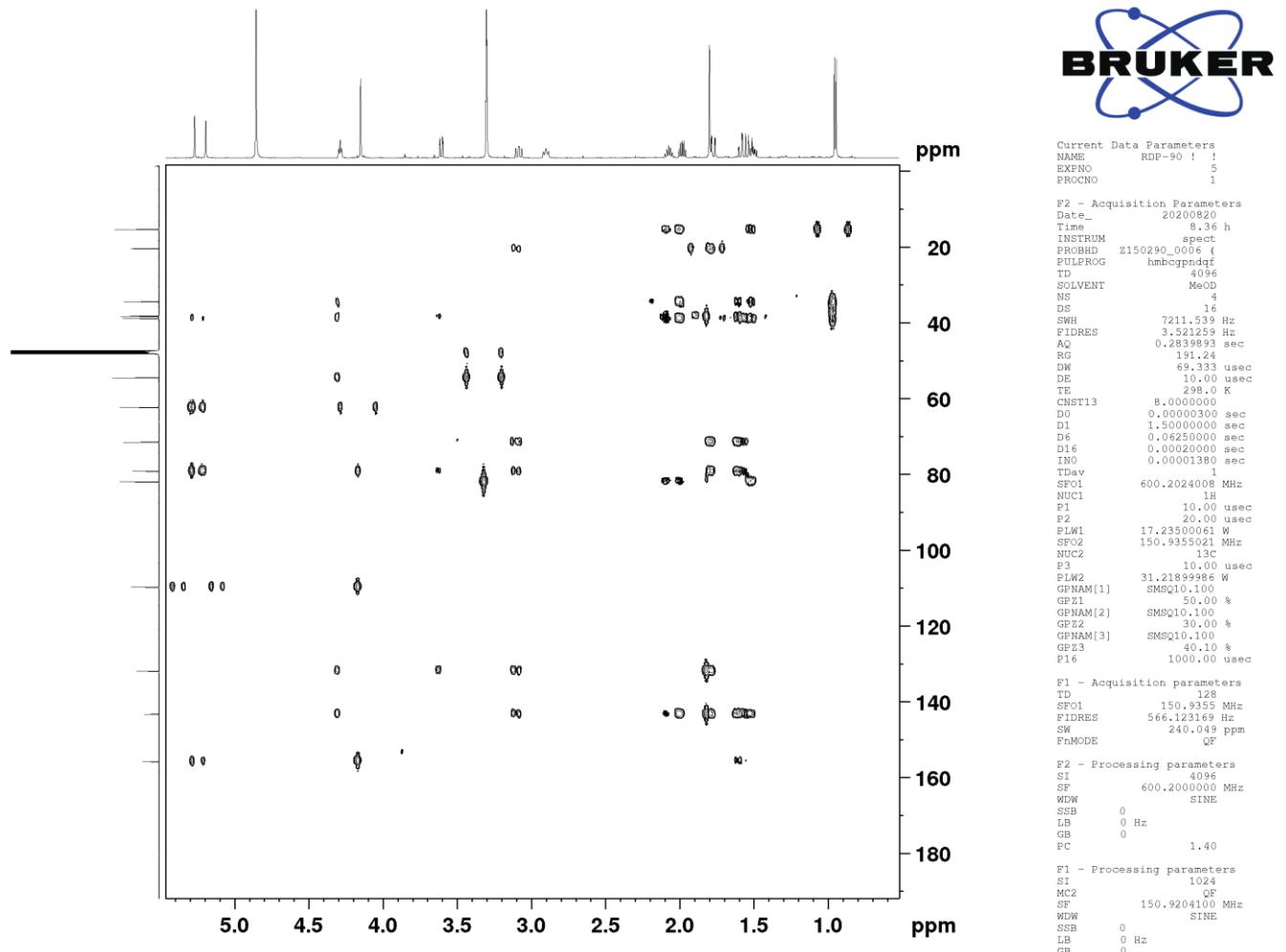
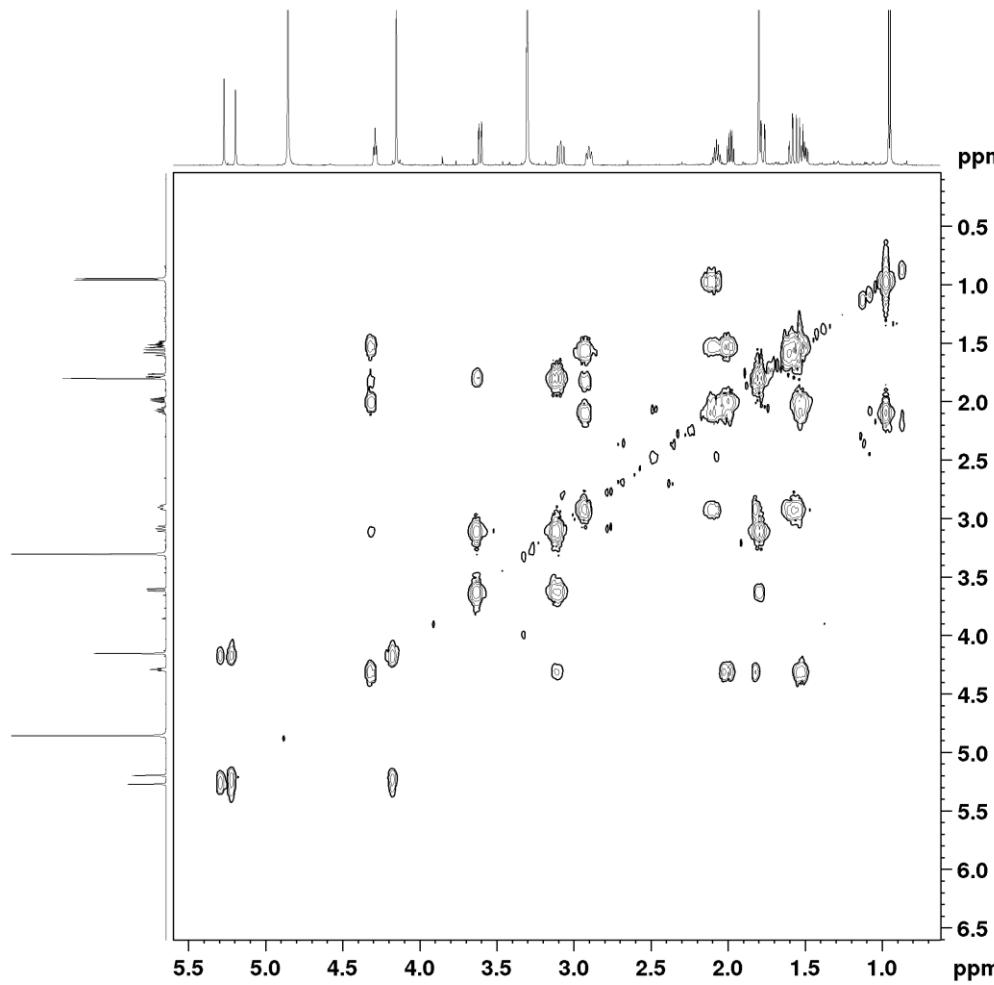


Figure S204 HMBC spectrum (600 MHz, CDCl_3) of compound **37**



Current Data Parameters
NAME RDP-90 !
EXPNO 6
PROCNO 1

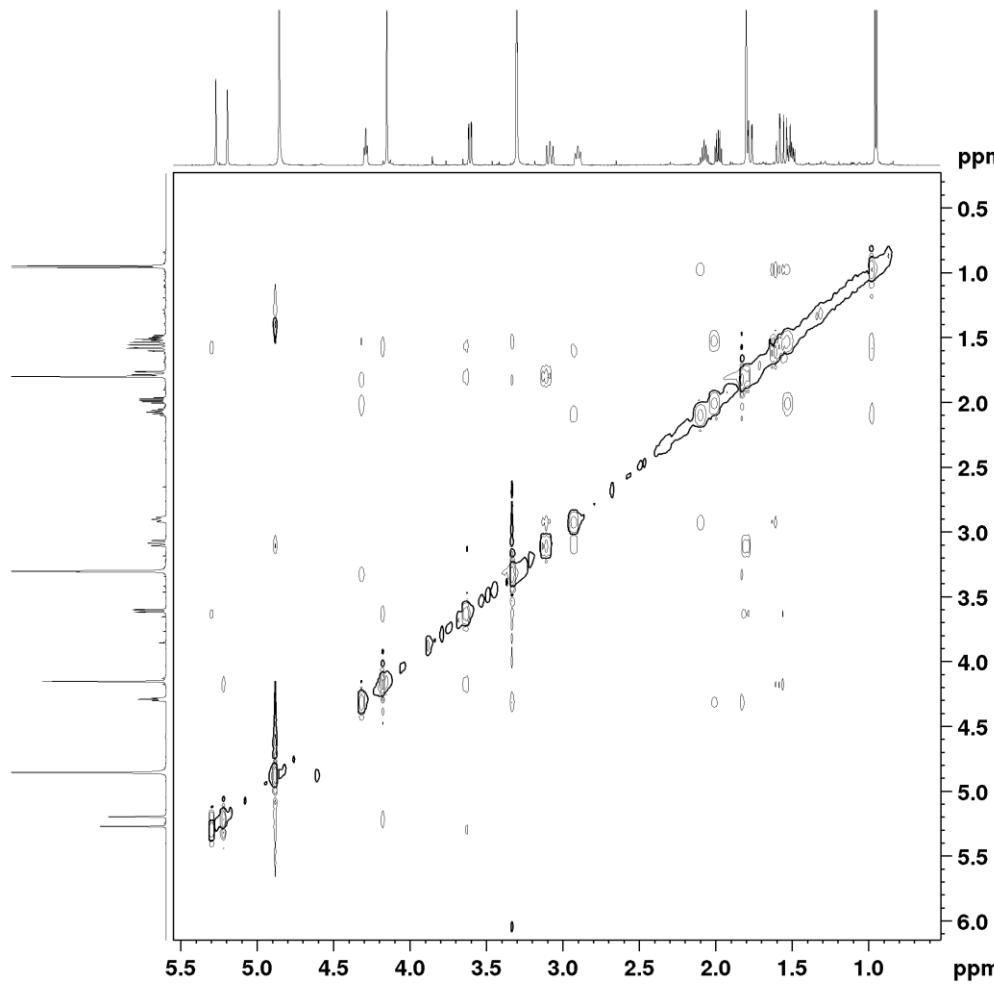
F2 - Acquisition Parameters
Date_ 20200820
Time 8.53 h
INSTRUM spect
PROBHD Z150290_0006 (cosyggppfrf
TD 2048
SOLVENT MeD
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 10.00 usec
TE 299.0 K
D0 0.00000300 sec
D1 2.0000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.100
GPNAME[2] SMSQ10.100
GPNAME[3] SMSQ10.100
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S205 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 37



Current Data Parameters
NAME RDP-90 !
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200820
Time 9.03 h
INSTRUM sec
PROBHD Z150290_0004 (
PULPROG noeasygpph.ppp
TD 2048
SOLVENT MeOD
NS 2
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60.93
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000000 sec
D11 0.0000000 sec
D12 0.00002000 sec
D16 0.00002000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

P1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12.004 ppm
PrMODE States-TPP1

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPP1
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S206 NOESY spectrum (600 MHz, CDCl_3) of compound 37

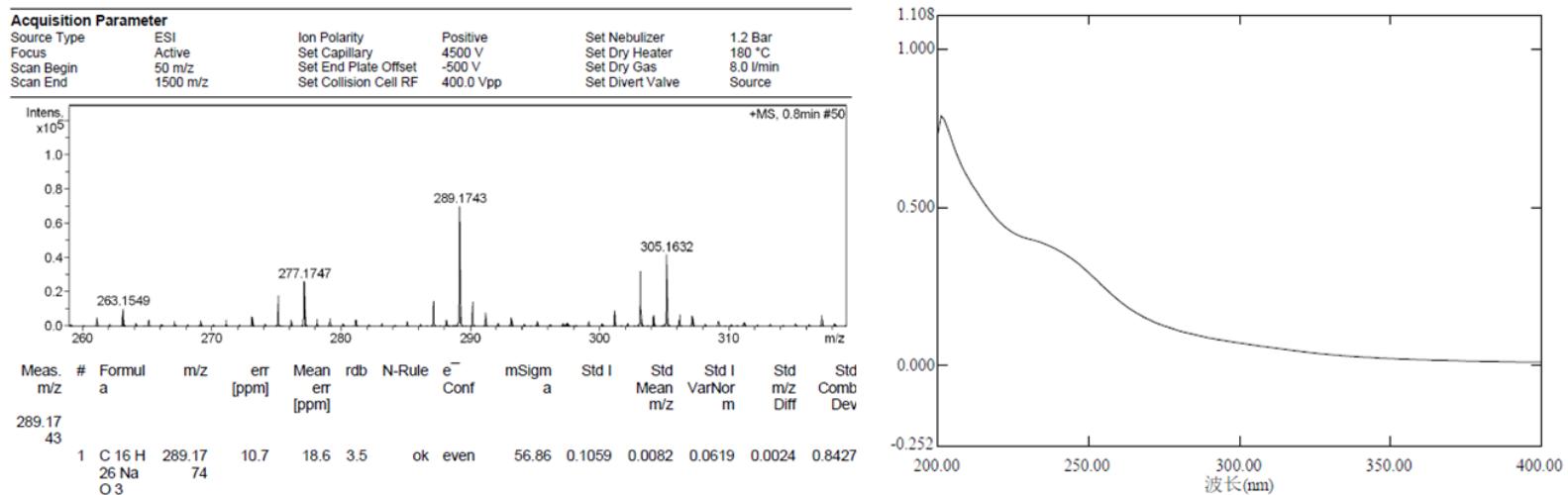


Figure S207 HRESIMS and UV spectra of compound 38

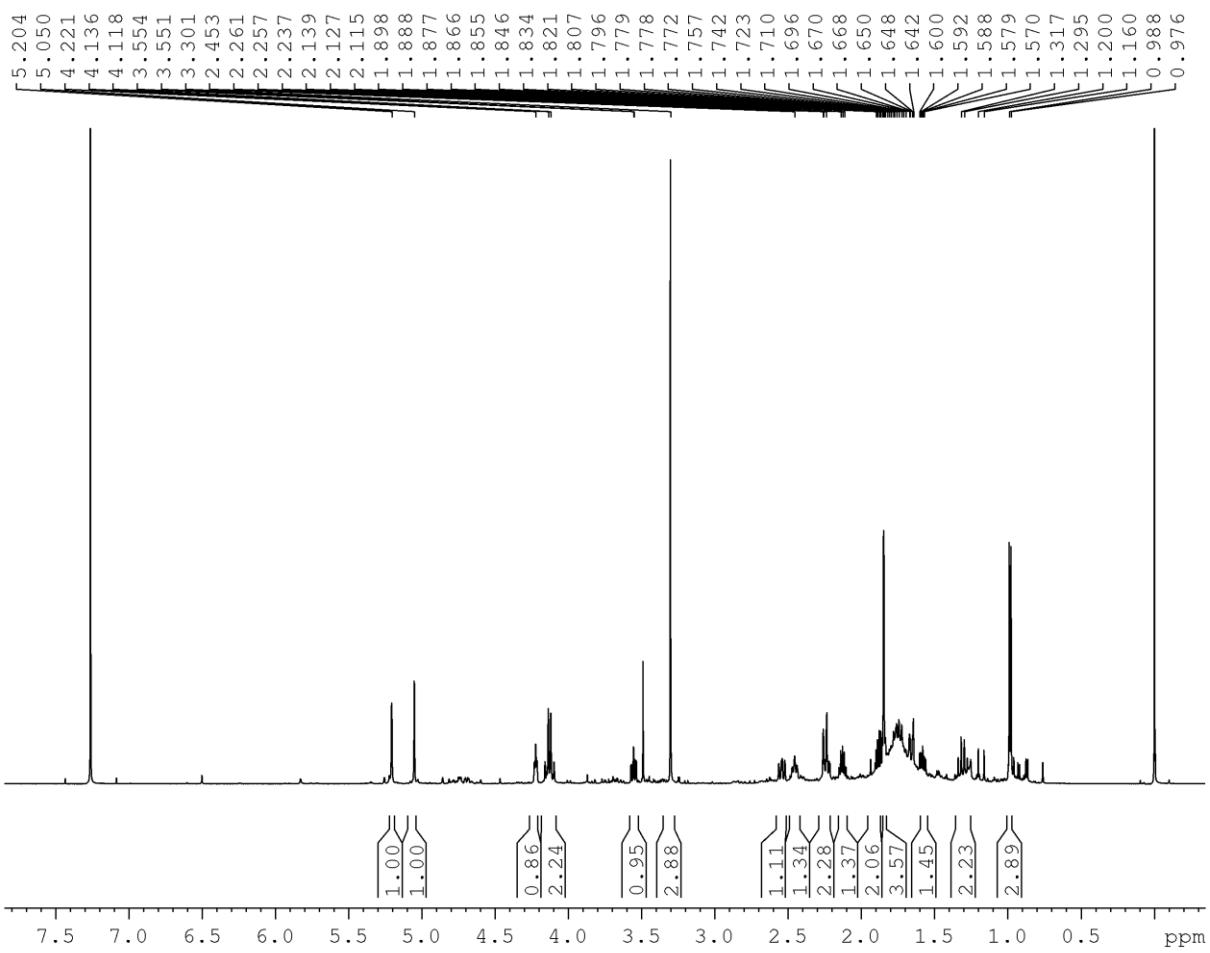
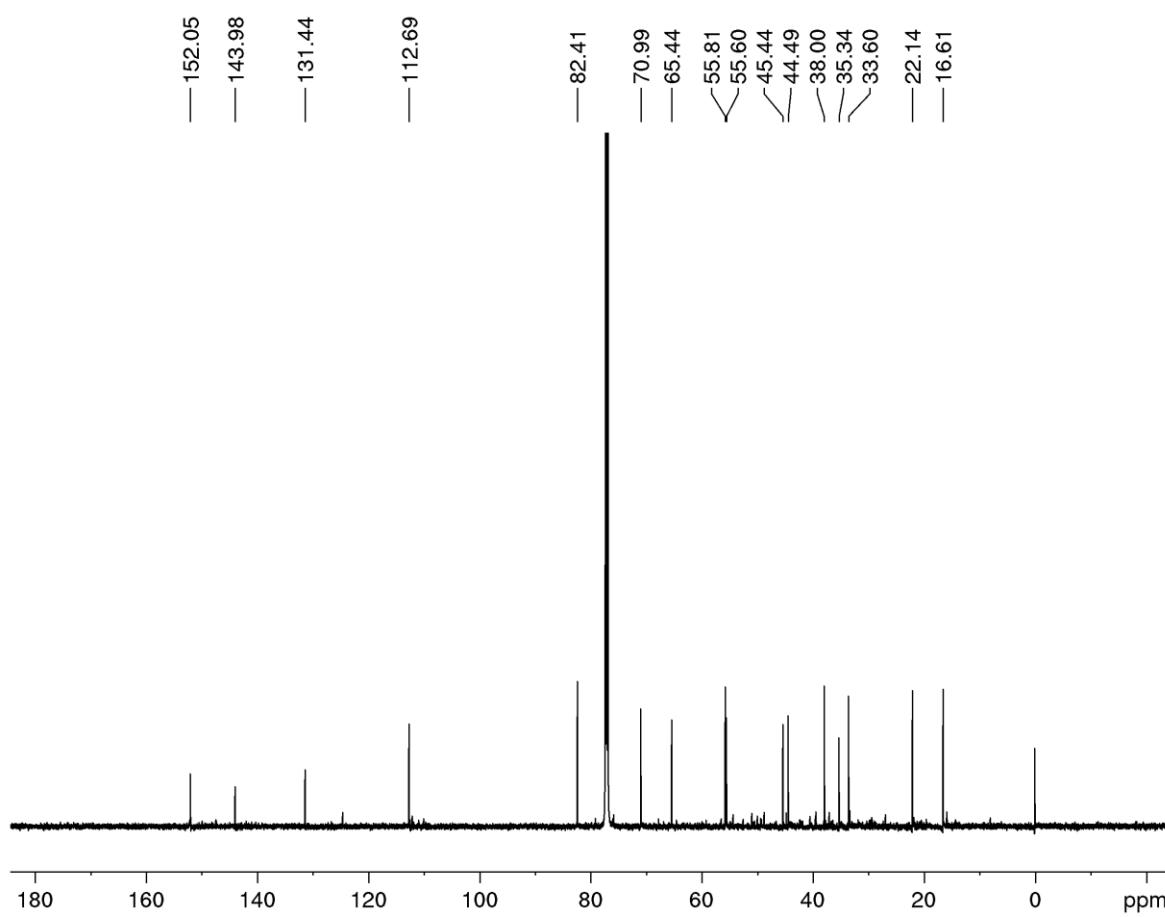


Figure S208 ¹H NMR spectrum (600 MHz, CDCl₃) of compound **38**



Current Data Parameters
NAME RDP-81 !!
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20200808
Time 20.50 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgpg30
TD 65356
SOLVENT CDCl3
NS 1024
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 43.48
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9203895 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S209 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **38**

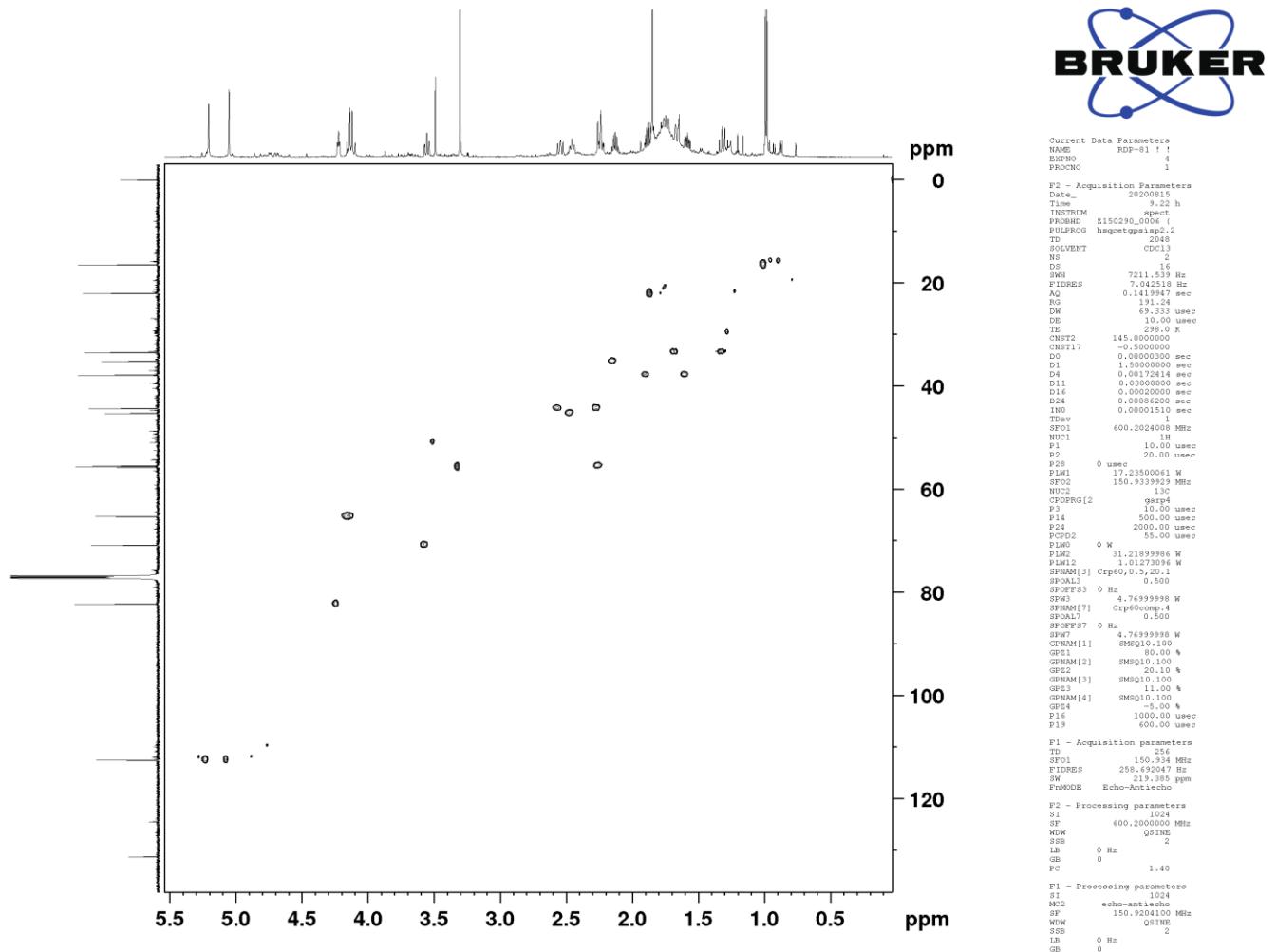


Figure S210 HSQC spectrum (600 MHz, CDCl₃) of compound **38**

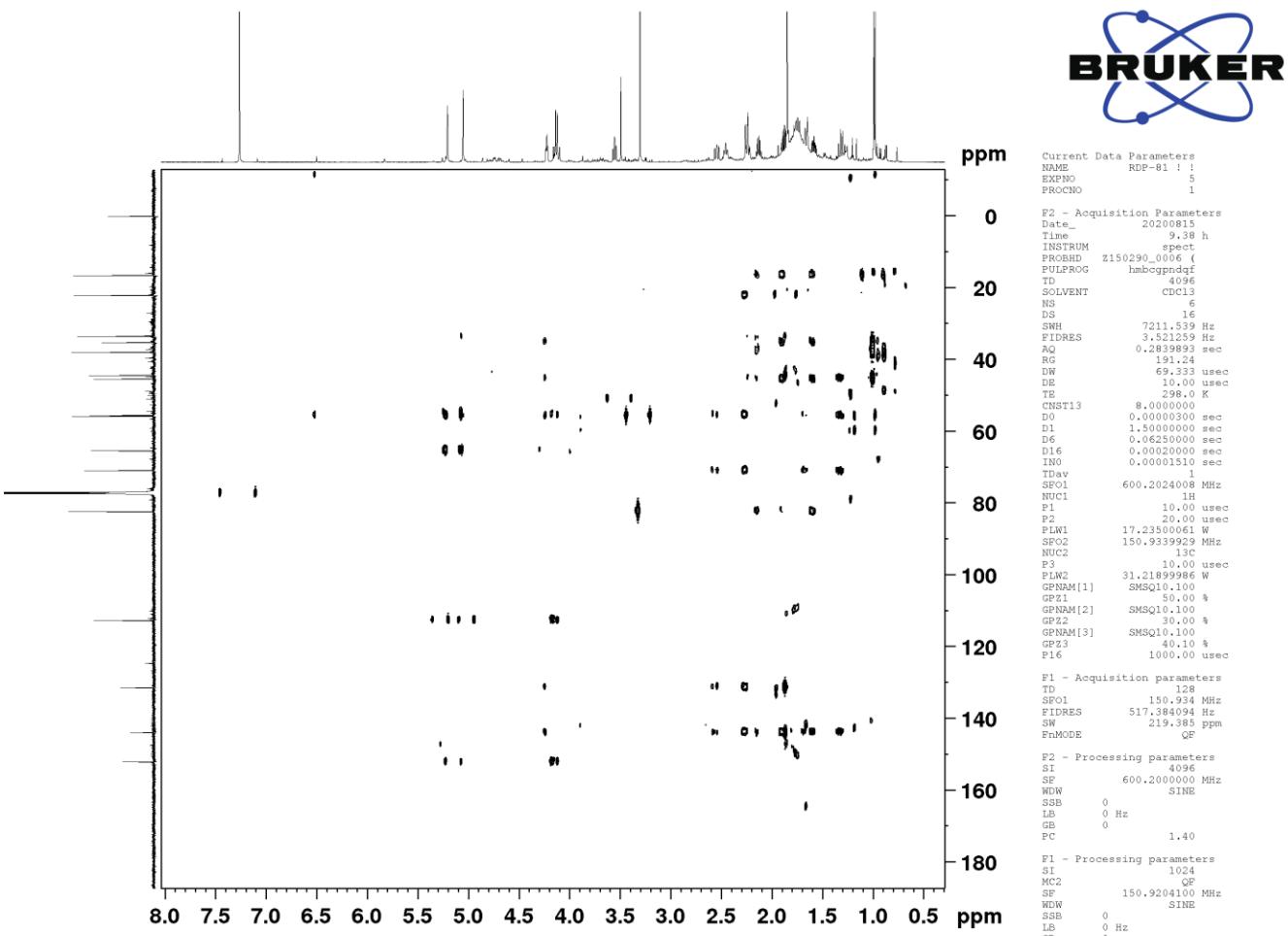
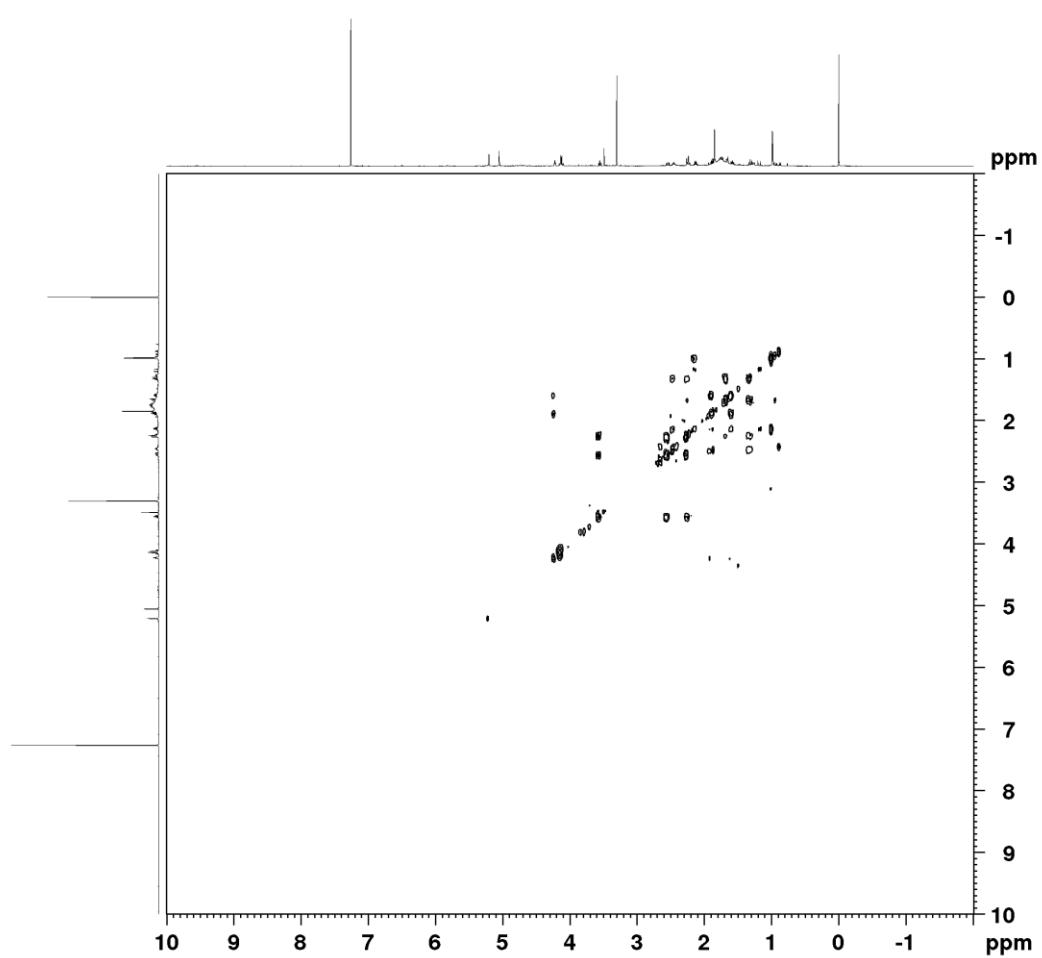


Figure S211 HMBC spectrum (600 MHz, CDCl₃) of compound **38**



Current Data Parameters
NAME RDP-61 ! !
EXPNO 6
PROCNO 1

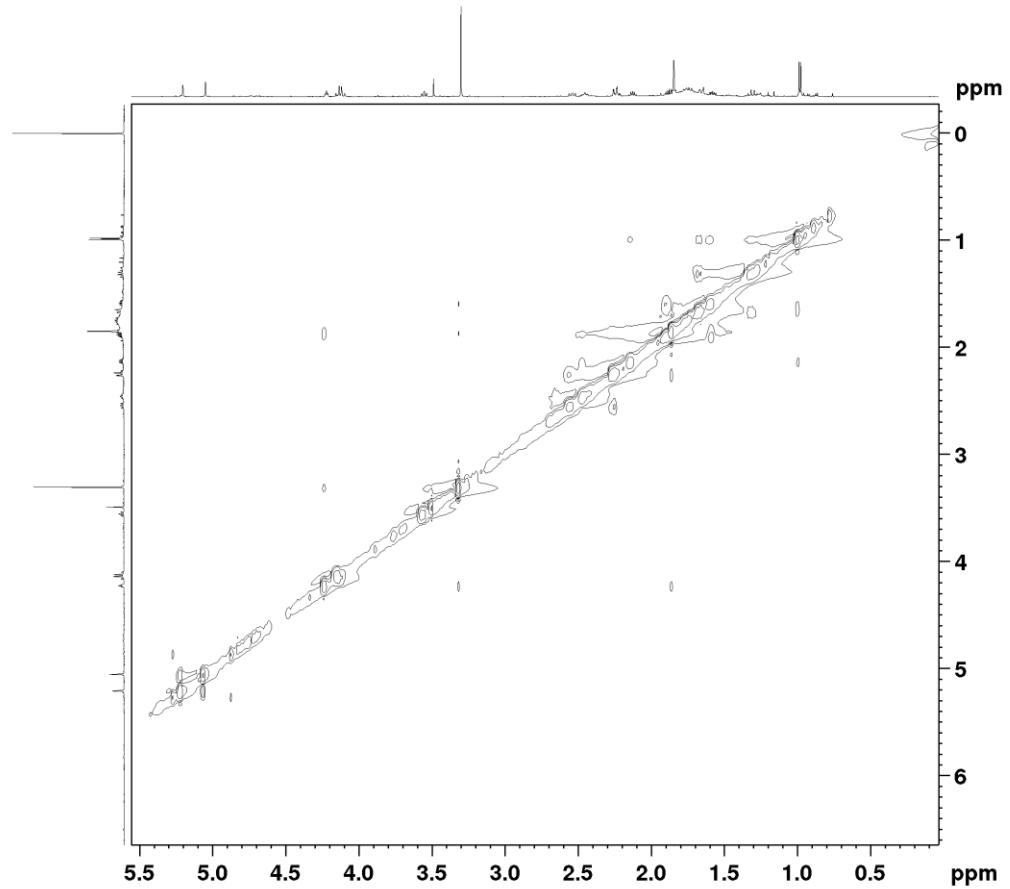
F2 - Acquisition Parameters
Date_ 20200815
Time 10.03 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG cosygppmrf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 10.00 usec
TE 290.00 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.23500061 W
GPNAME[1] SMSQ10.100
GPZ1 16.00 %
GPNAME[2] SMSQ10.100
GPZ2 12.00 %
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
PnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 64
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S212 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound 38



Current Data Parameters
NAME RDP-81 !
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200815
Time 10.23 h
INSTRUM spect
PROBHD Z150290_0066_1
PULPROG noe3sypphp
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60
DW 69.333 usec
DE 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.0001389 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
M22 States-TPPI
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S213 NOESY spectrum (600 MHz, CDCl_3) of compound **38**

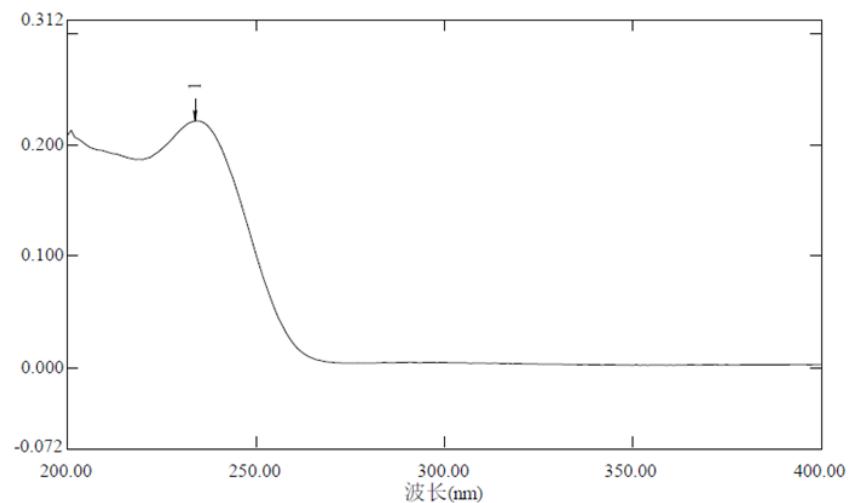
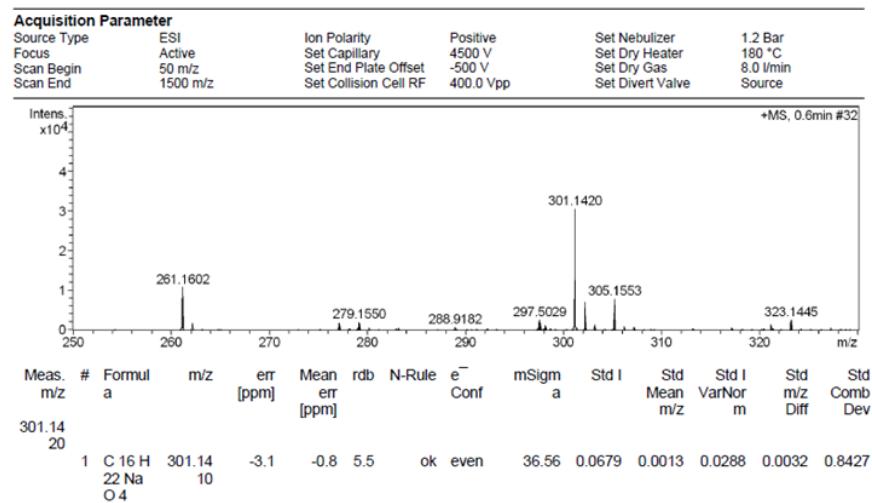


Figure S214 HRESIMS and UV spectra of compound 39

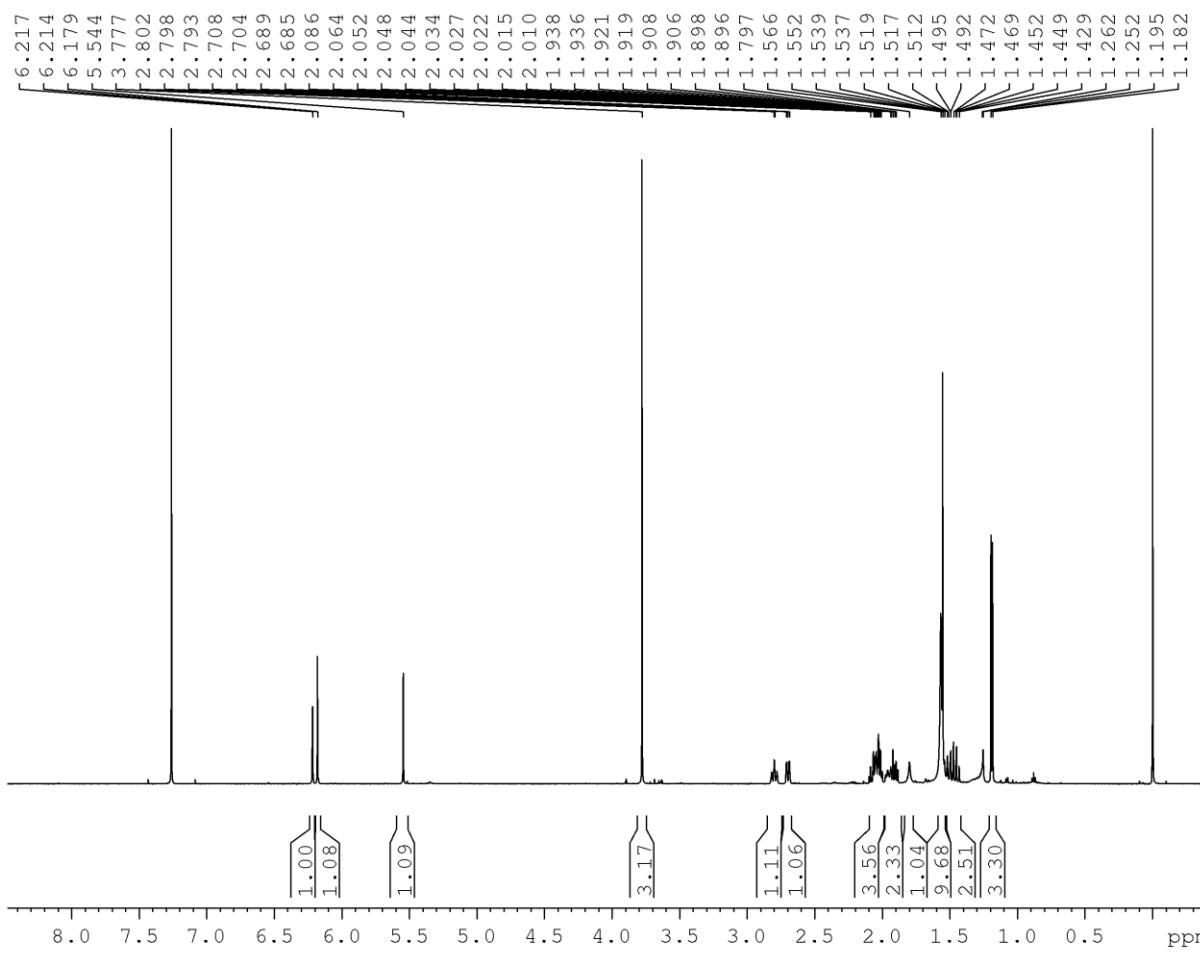


Figure S215 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **39**

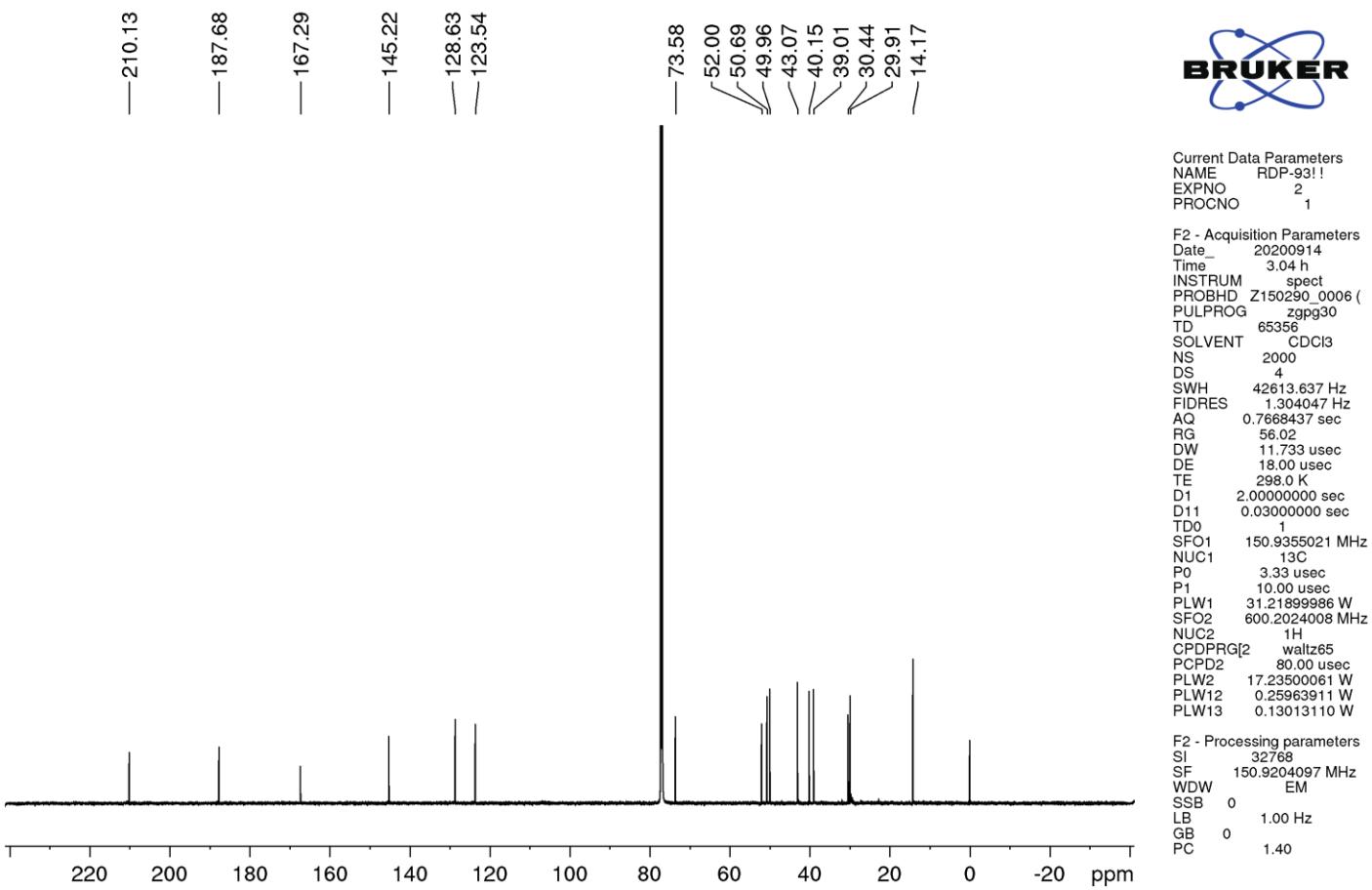


Figure S216 ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **39**

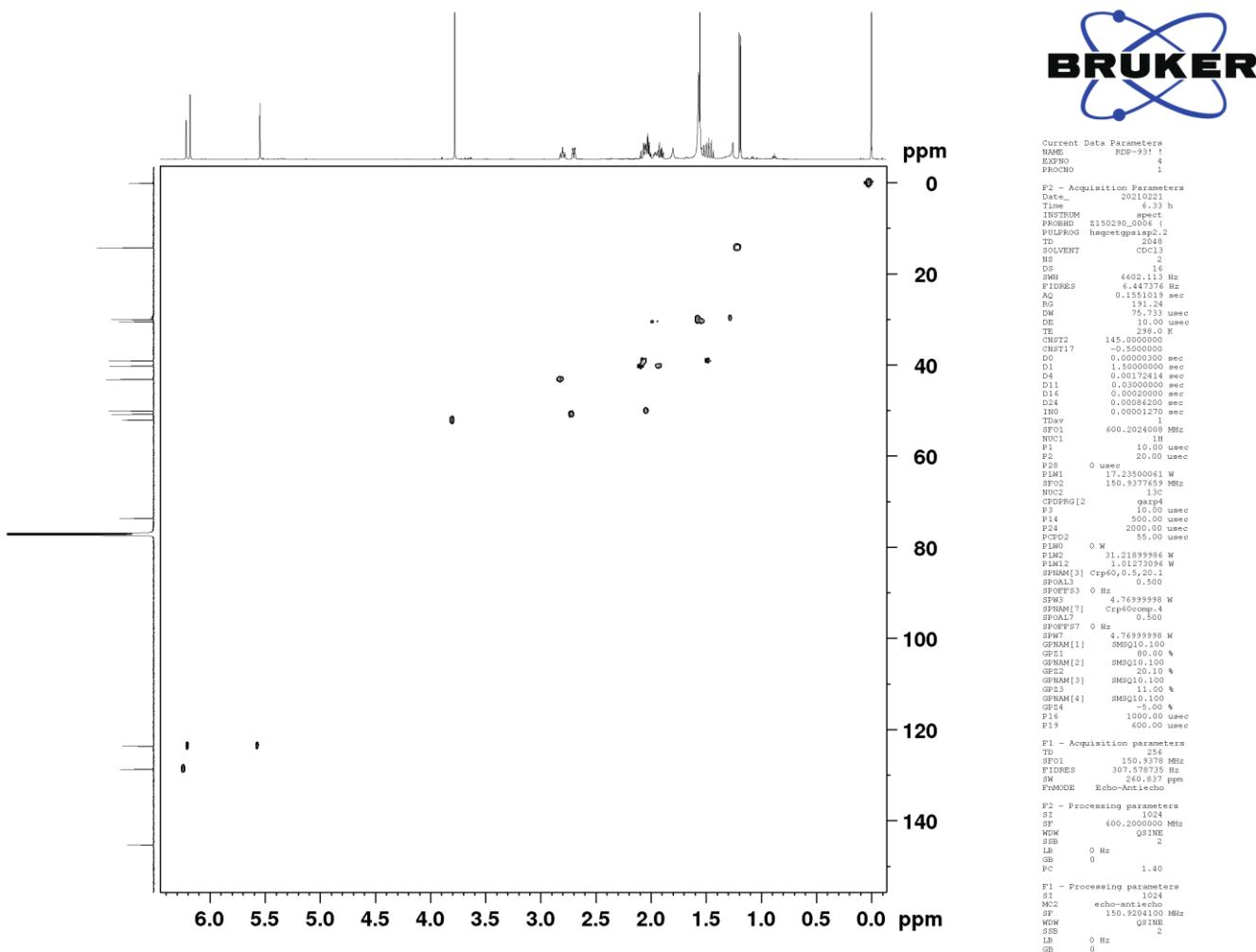
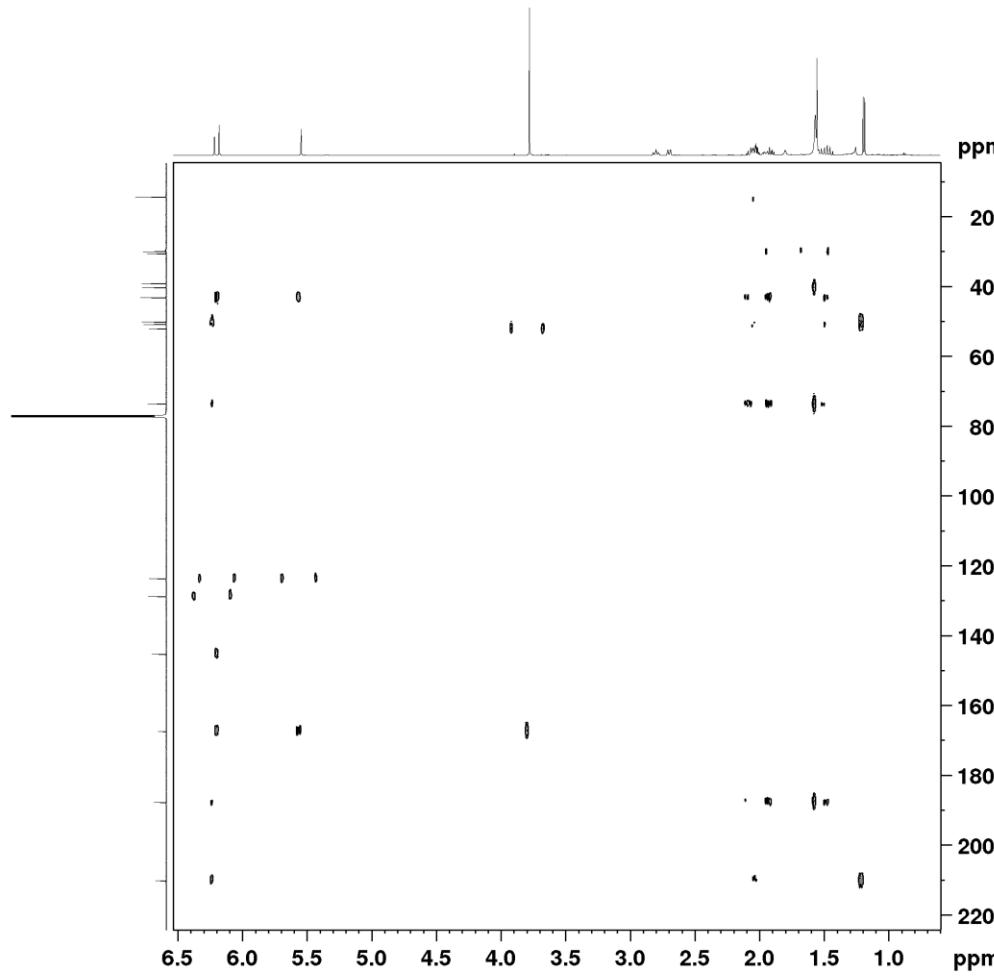


Figure S217 HSQC spectrum (600 MHz, CDCl_3) of compound **39**



Current Data Parameters
NAME RDP-93!
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210221
Time 6.48 h
INSTRUM spect
PROBID Z150290_0001
PULPROG hmbcogn4ir
TD 4096
SOLVENT CDCl3
NS 8
DS 16
SWH 6602.113 Hz
FIDRES 3.223688 Hz
AQ 0.3102037 sec
RG 141.0
DW 75.733 usec
DE 10.00 usec
TE 298.0 K
CNUST13 8.0000000
D0 0.00000300 sec
D1 1.5000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
DNO 0.00001270 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 17.23500061 W
SF02 150.9377651 MHz
NUC2 13C
P3 10.00 usec
PLW2 31.21899986 W
GPNAME[1] SMSQ10.100
GP21 50.00 °
GPNAME[2] SMSQ10.100
GP22 30.00 °
GPNAME[3] SMSQ10.100
GP23 40.10 °
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 150.9378 MHz
FIDRES 615.157471 Hz
SW 260.837 ppm
FhMODE QF

F2 - Processing parameters
SI 4096
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9204100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S218 HMBC spectrum (600 MHz, CDCl_3) of compound **39**

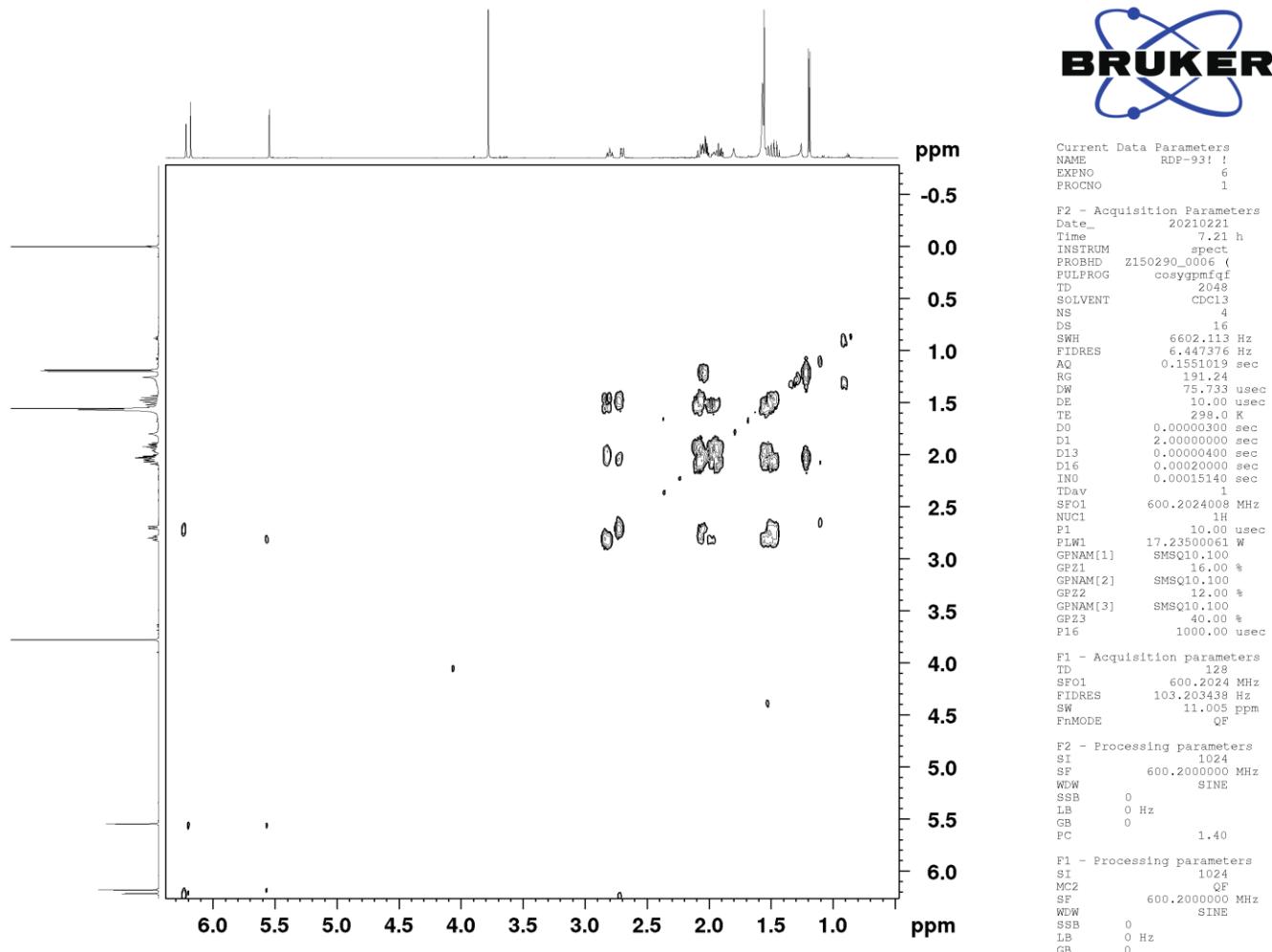
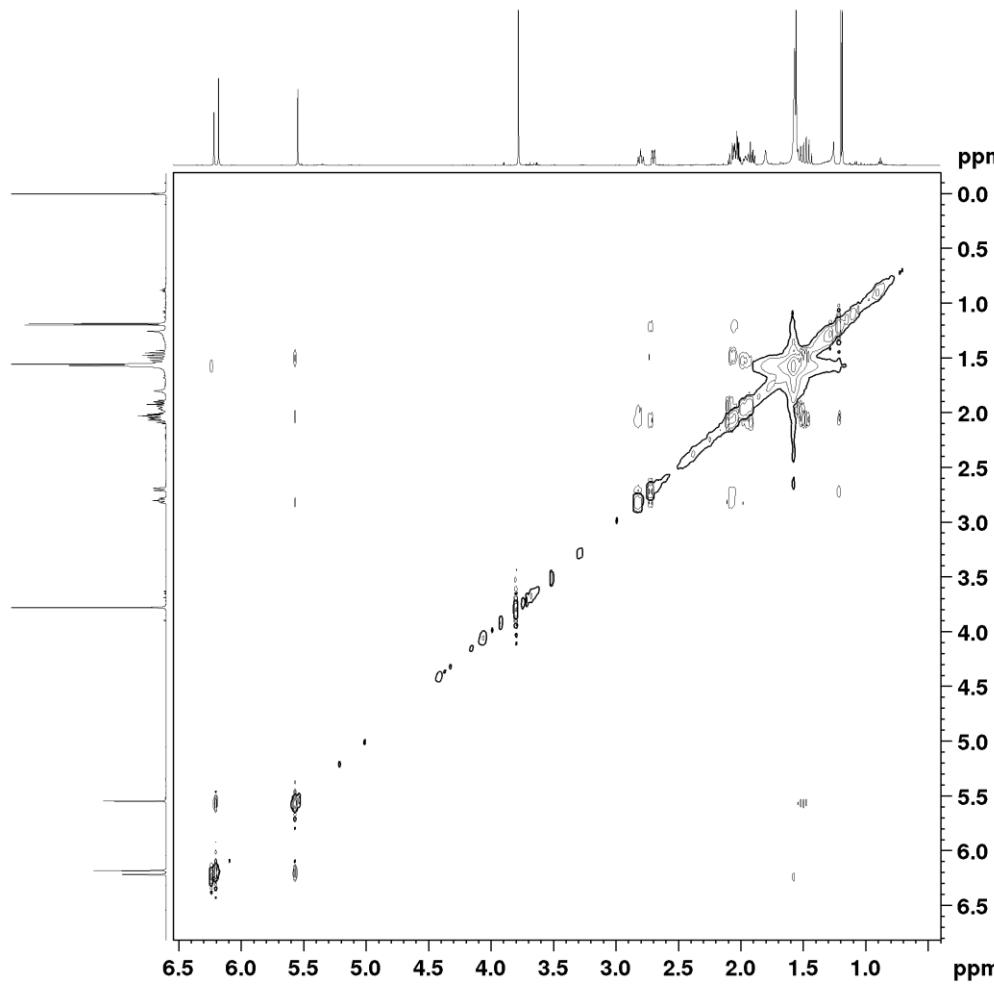


Figure S219 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **39**



Current Data Parameters
NAME RDP-931 !
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210221
Time 7.40 h
INSTRUM spect
PROBHD Z150290_0004 (
PULPROG noeesygrhfp
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 6602.113 Hz
FIDRES 6.447376 Hz
AQ 0.1551019 sec
RG 60.93
DW 75.733 usec
DE 10.00 usec
TE 298.0 K
D0 0.00006297 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00015140 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 51.601719 Hz
SW 11.005 ppm
PwMODE States-TPP1

F2 - Processing parameters
SI 1024
SF 600.200000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-Tpp1
SF 600.2000000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S220 NOESY spectrum (600 MHz, CDCl₃) of compound **39**

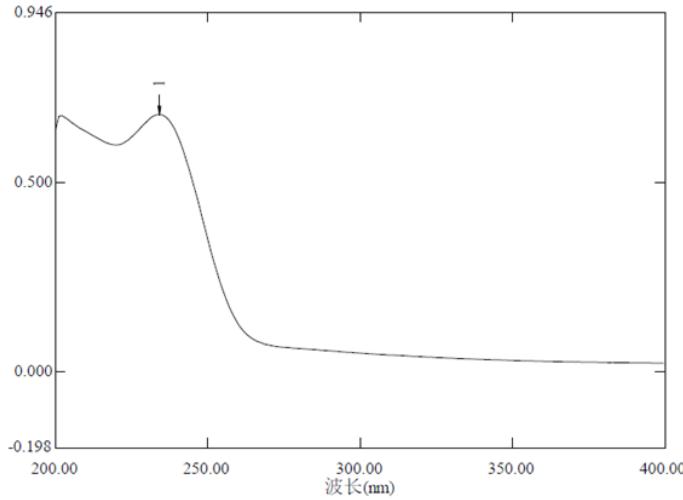
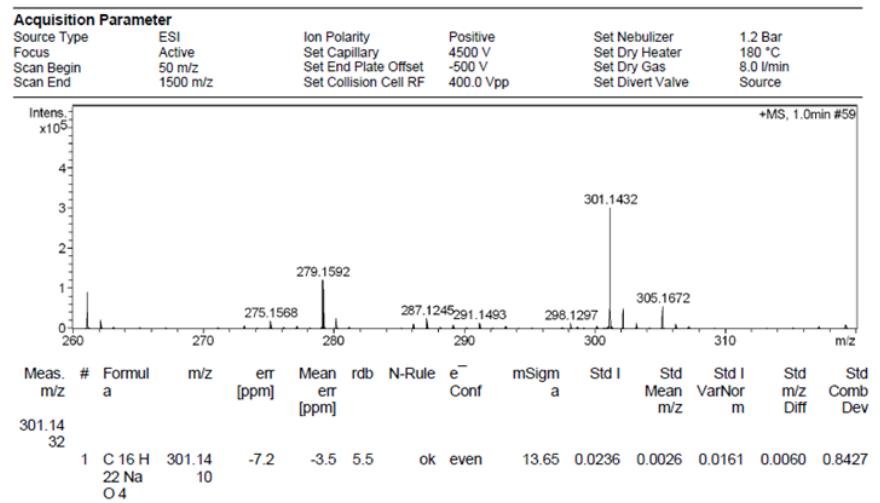


Figure S221 HRESIMS and UV spectra of compound **40**

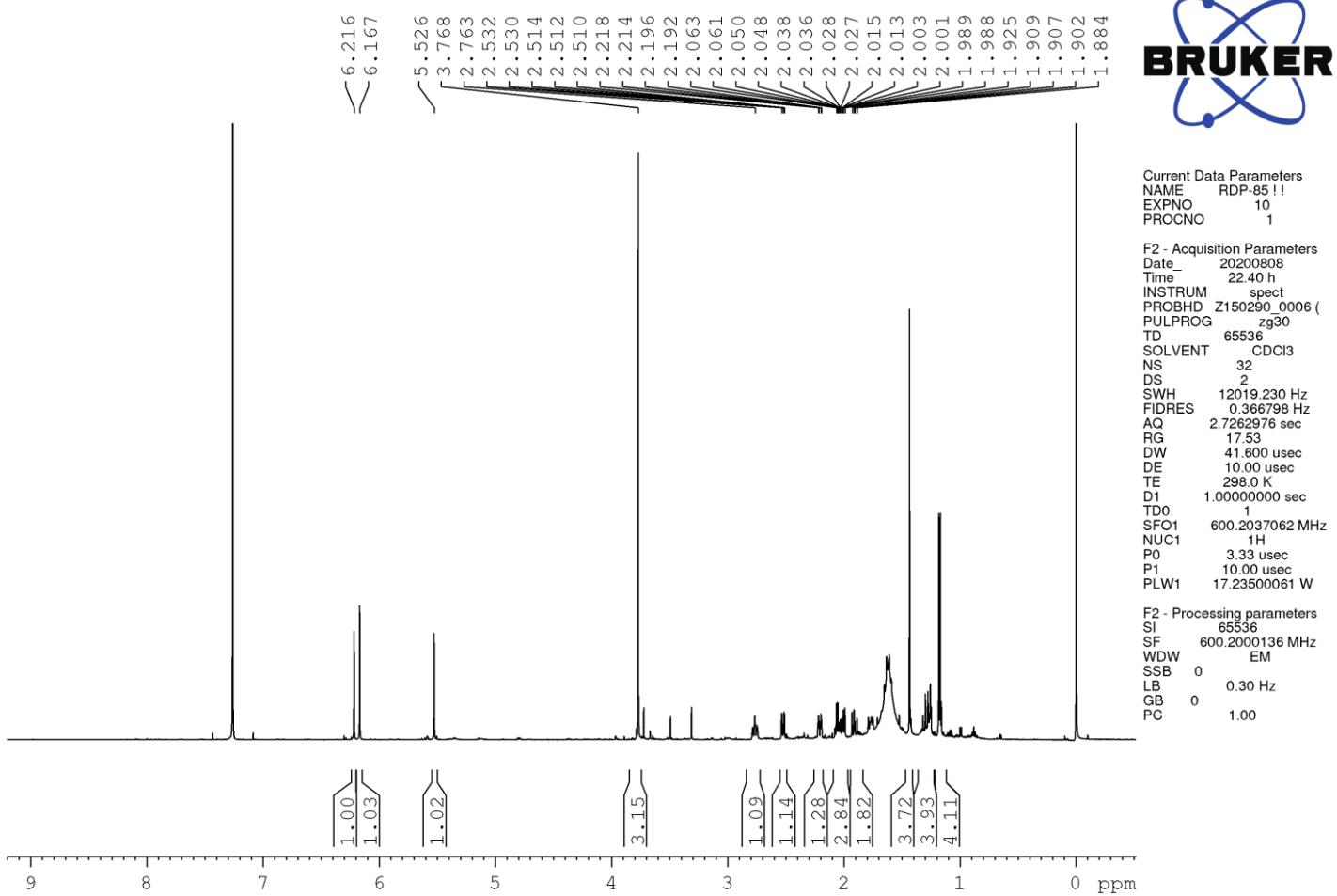
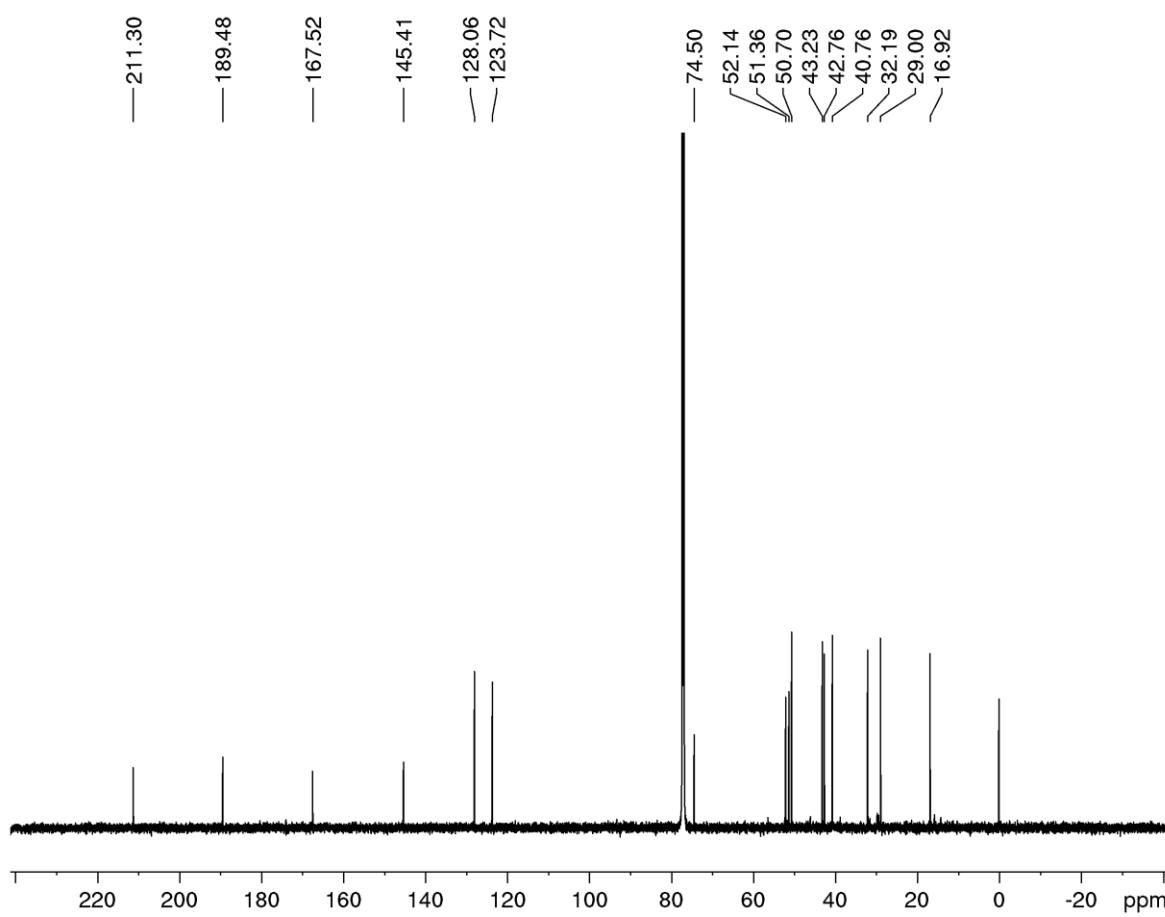


Figure S222 ^1H NMR spectrum (600 MHz, CDCl_3) of compound **40**



Current Data Parameters
NAME RDP-85 !!
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200809
Time 13.57 h
INSTRUM spect
PROBHD Z150290_0006 (
PULPROG zgpg30
TD 65356
SOLVENT CDCl3
NS 1024
DS 4
SWH 42613.637 Hz
FIDRES 1.304047 Hz
AQ 0.7668437 sec
RG 56.02
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 31.21899986 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 17.23500061 W
PLW12 0.25963911 W
PLW13 0.13013110 W

F2 - Processing parameters
SI 32768
SF 150.9203896 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S223 ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **40**

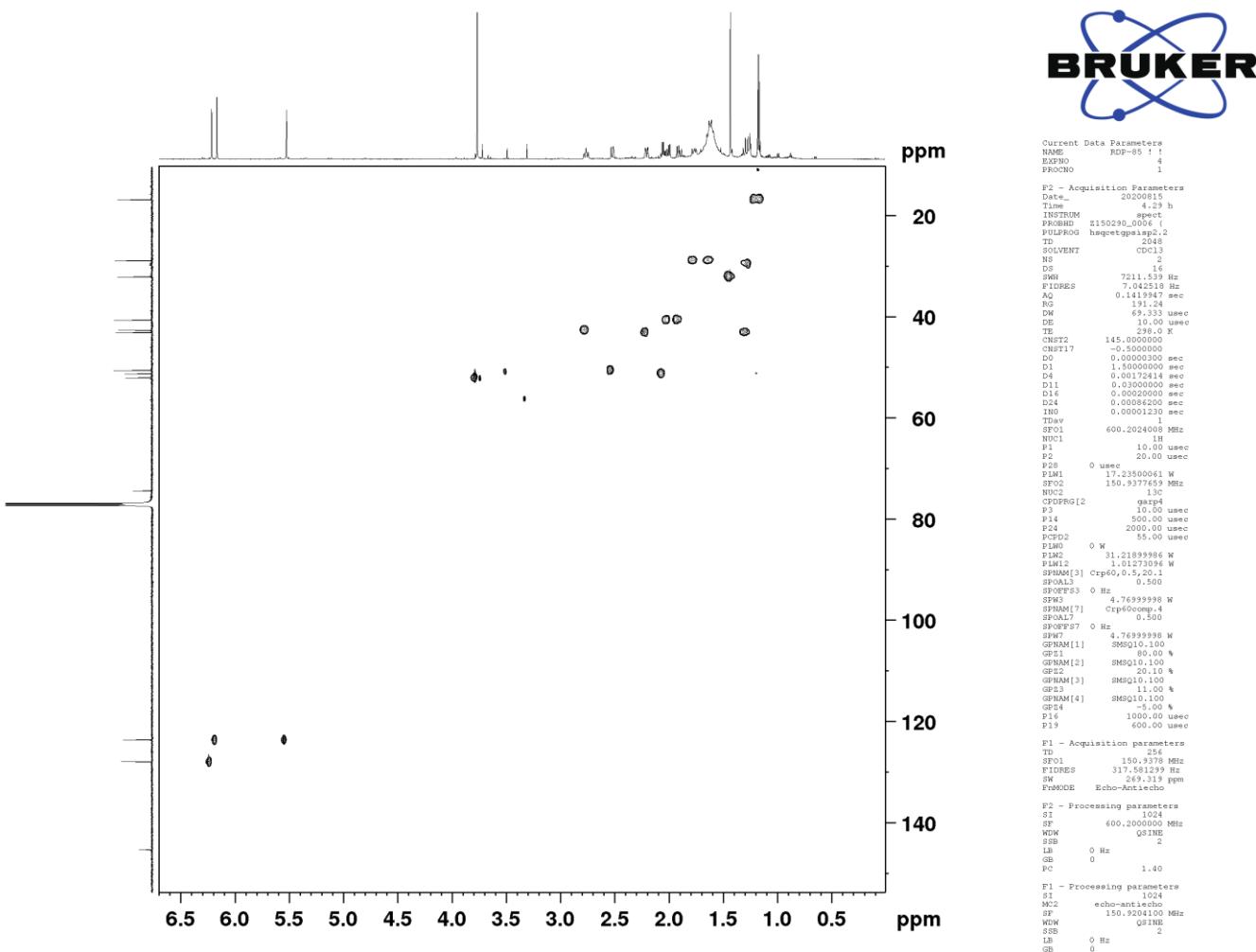


Figure S224 HSQC spectrum (600 MHz, CDCl_3) of compound **40**

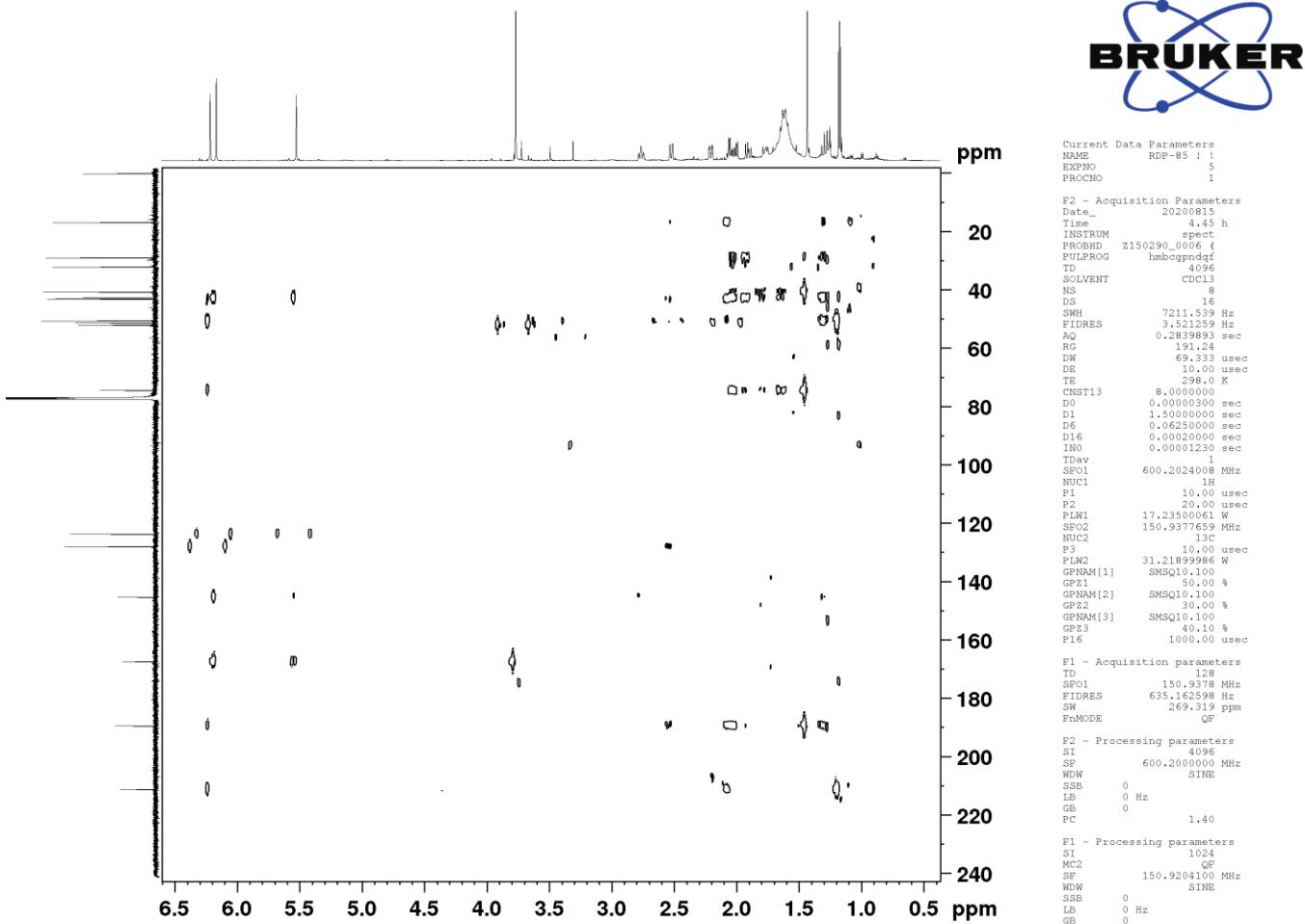
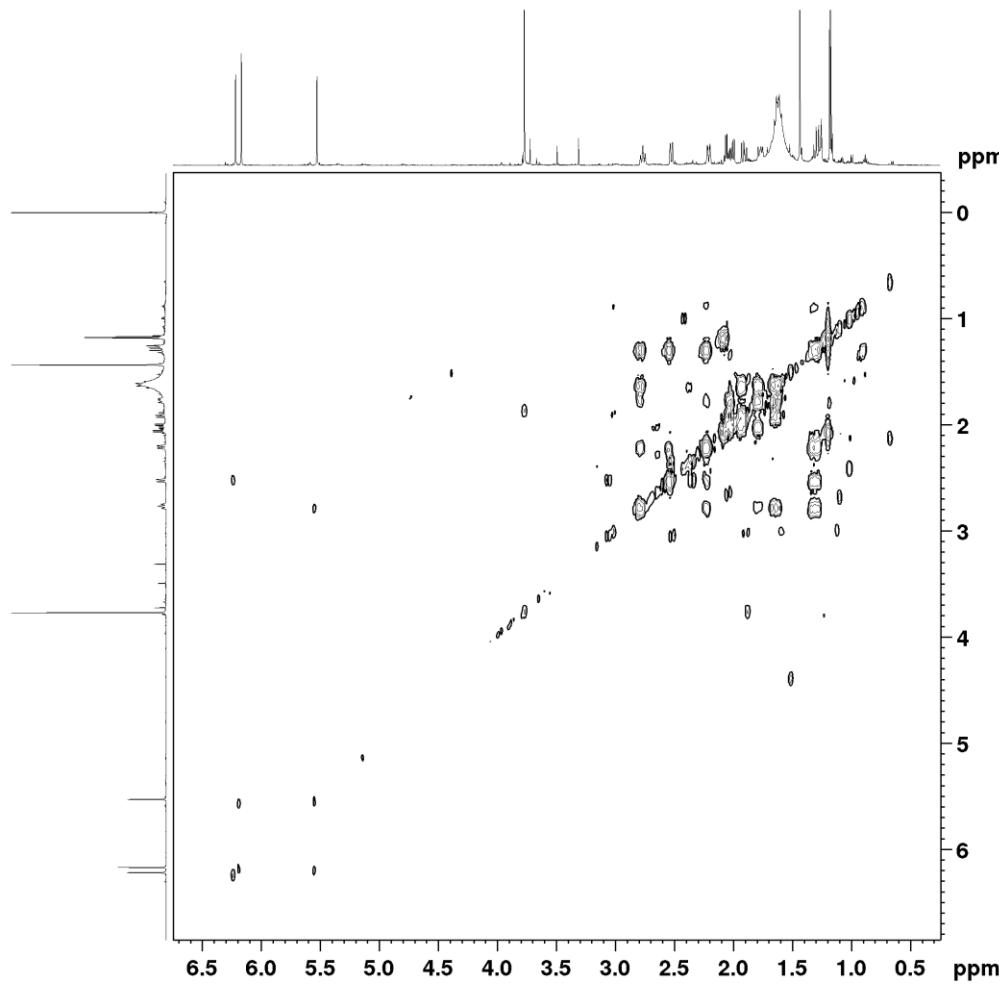


Figure S225 HMBC spectrum (600 MHz, CDCl₃) of compound **40**



Current Data Parameters
NAME RDP-85 !
EXPNO 6
PROCNO 1

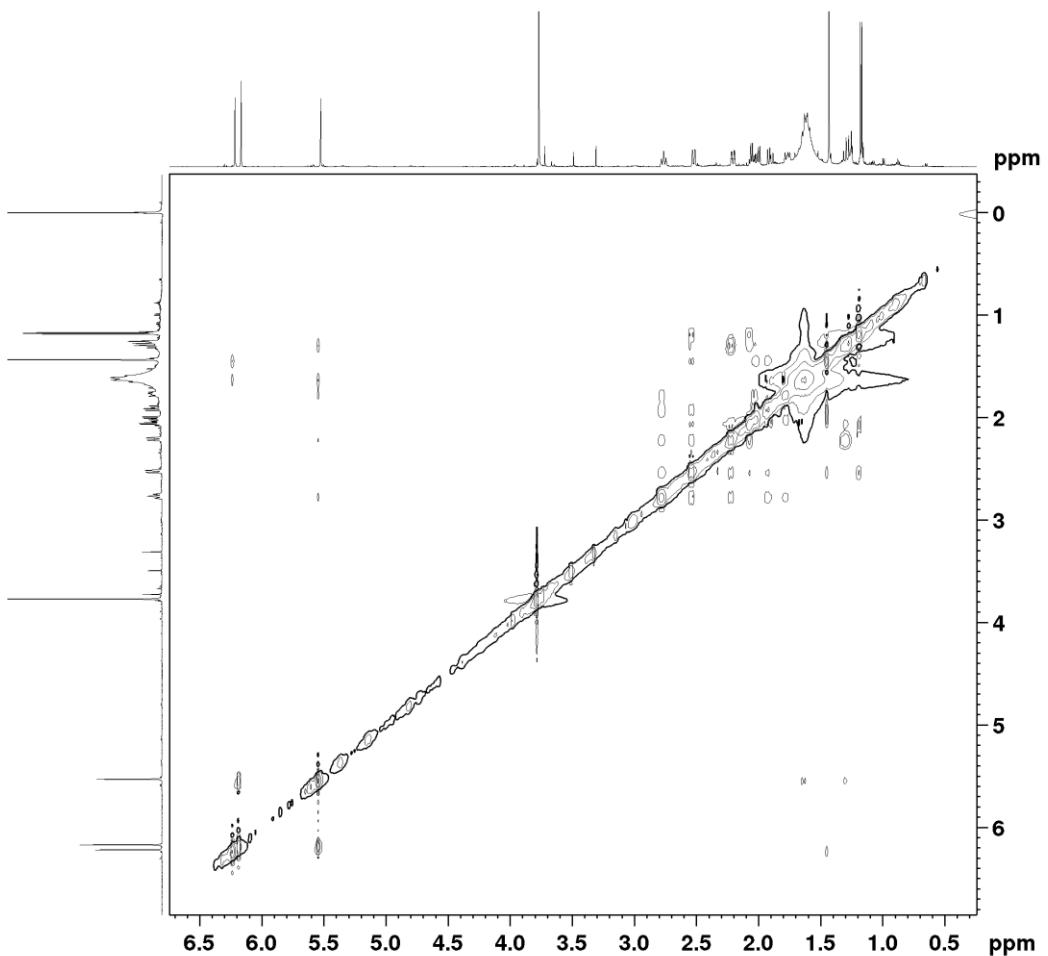
F2 - Acquisition Parameters
Date 20200815
Time 5.18 h
INSTRUM spect
PROBHD Z150290_0006 (cosygppmfr
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 191.24
DW 69.333 usec
DE 10.00 usec
TE 299.0 K
D0 0.00000300 sec
D1 2.0000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013880 sec
TDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.2350061 W
GPNAME[1] SMSQ10.100
GPNAME[2] SMSQ10.100
GPNAME[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.2024 MHz
FIDRES 112.572044 Hz
SW 12.004 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S226 ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **40**



Current Data Parameters
NAME RDP-85 ! !
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200815
Time 5.38 h
INSTRUM spect
PROBHD Z150290_006 ('
PULPROG noeipypphp
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7211.539 Hz
FIDRES 7.042518 Hz
AQ 0.1419947 sec
RG 60
DW 69.333 usec
DB 10.00 usec
TE 298.0 K
D0 0.00005667 sec
D1 2.0000000 sec
D8 0.8000001 sec
D11 0.0300000 sec
D12 0.00002000 sec
D16 0.0002000 sec
D18 0.0001386 sec
DDav 1
SF01 600.2024008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
P17 2500.00 usec
PLW1 17.23500061 W
PLW10 2.75760007 W
GPNAME[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.2024 MHz
FIDRES 56.286022 Hz
SW 12,004 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
SF 600.2000000 MHz
NDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S227 NOESY spectrum (600 MHz, CDCl₃) of compound **40**

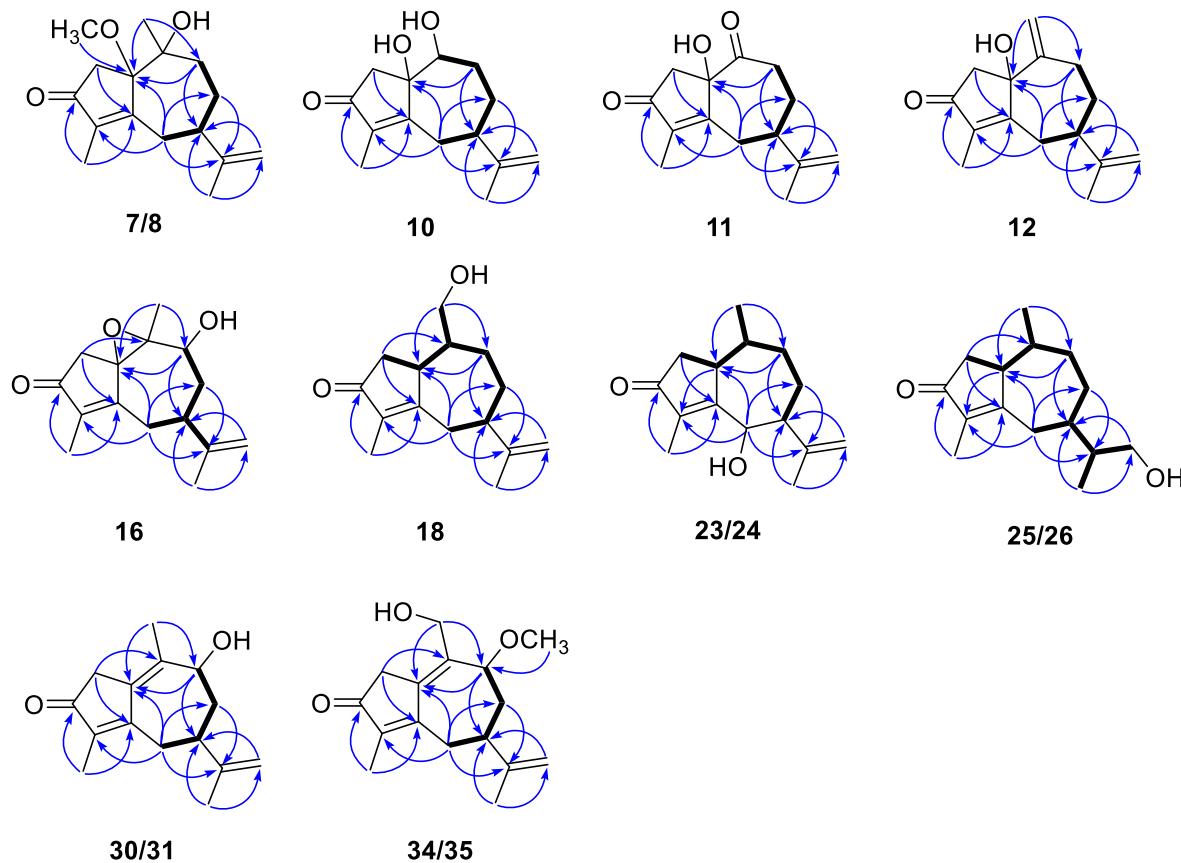


Figure S228 Key correlations from COSY and HMBC of compounds 7–8, 10–12, 16, 18, 23–26, 30–31 and 34–35.

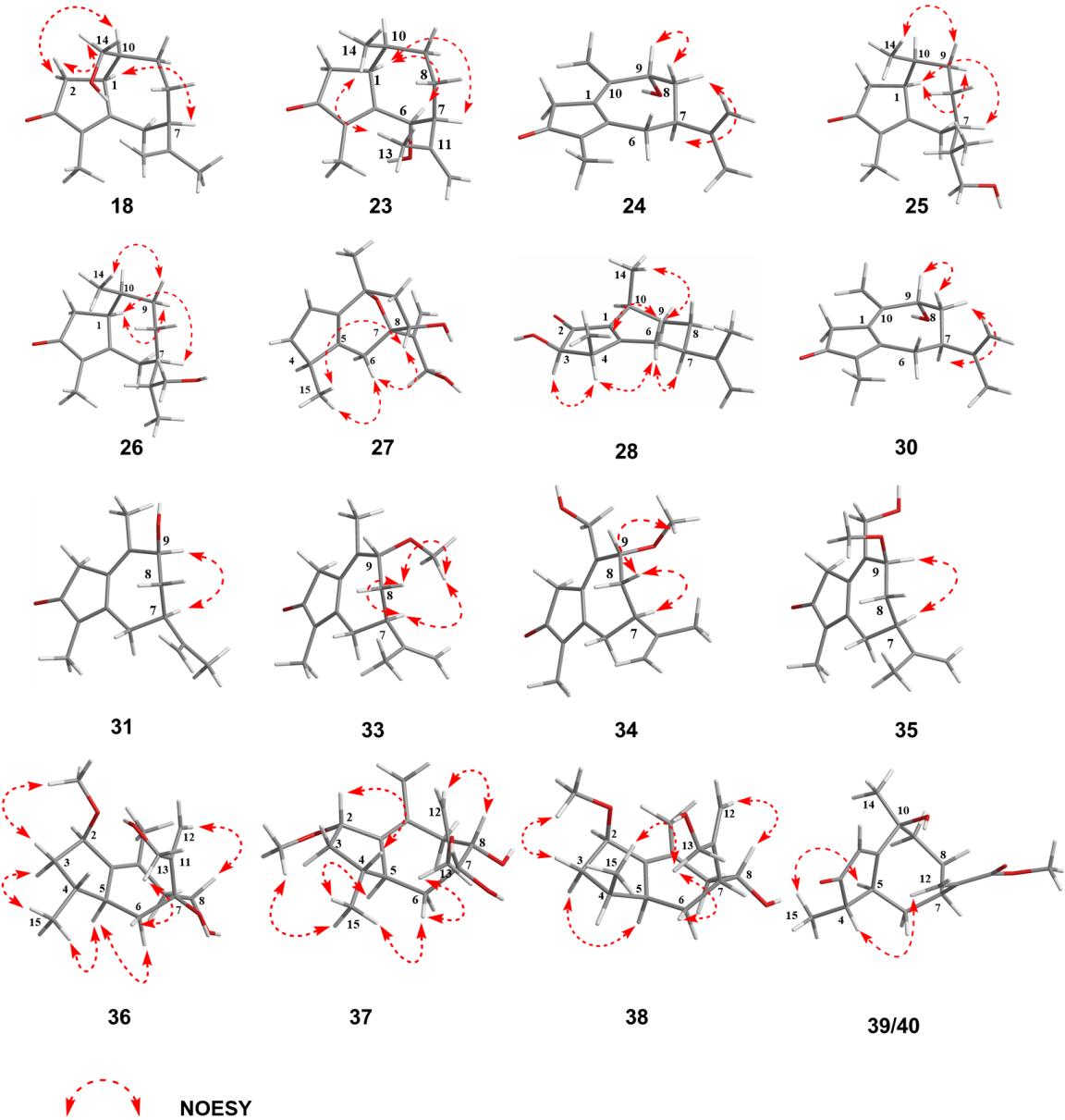


Figure S229 Key NOESY correlations for 18, 23-31 and 33-40.

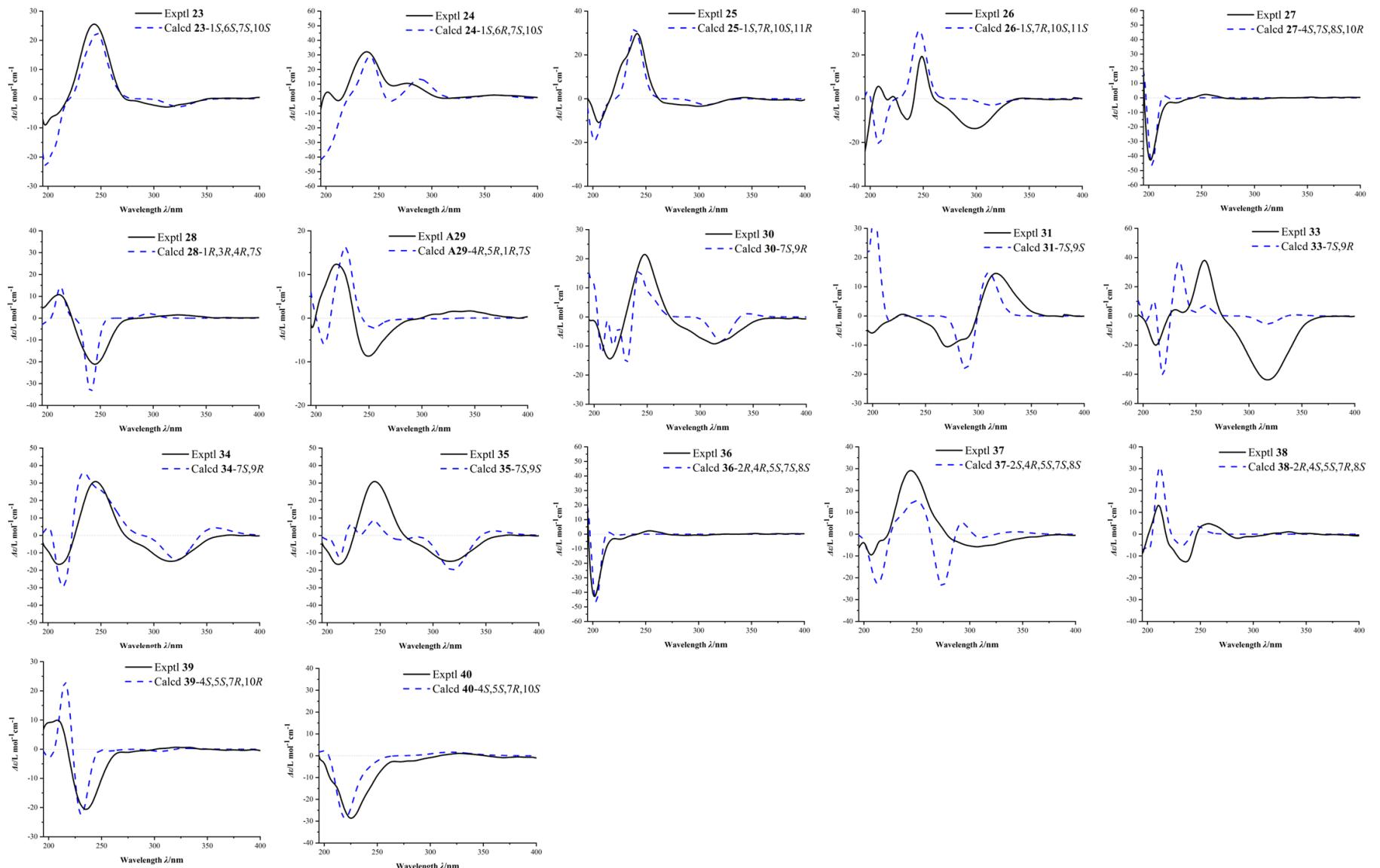


Figure S230 Experimental and calculated ECD spectra for **23-31** and **33-40**.

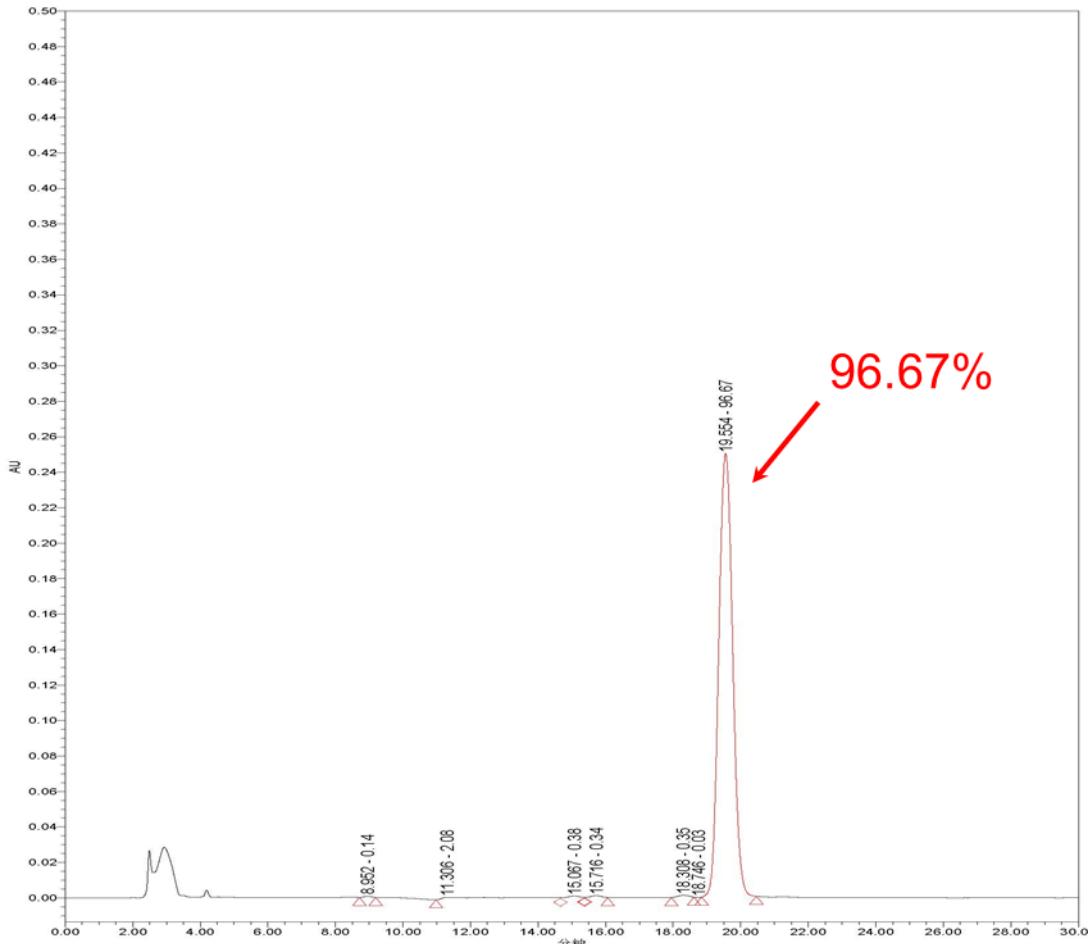


Figure S231 HPLC analysis of compound 7.

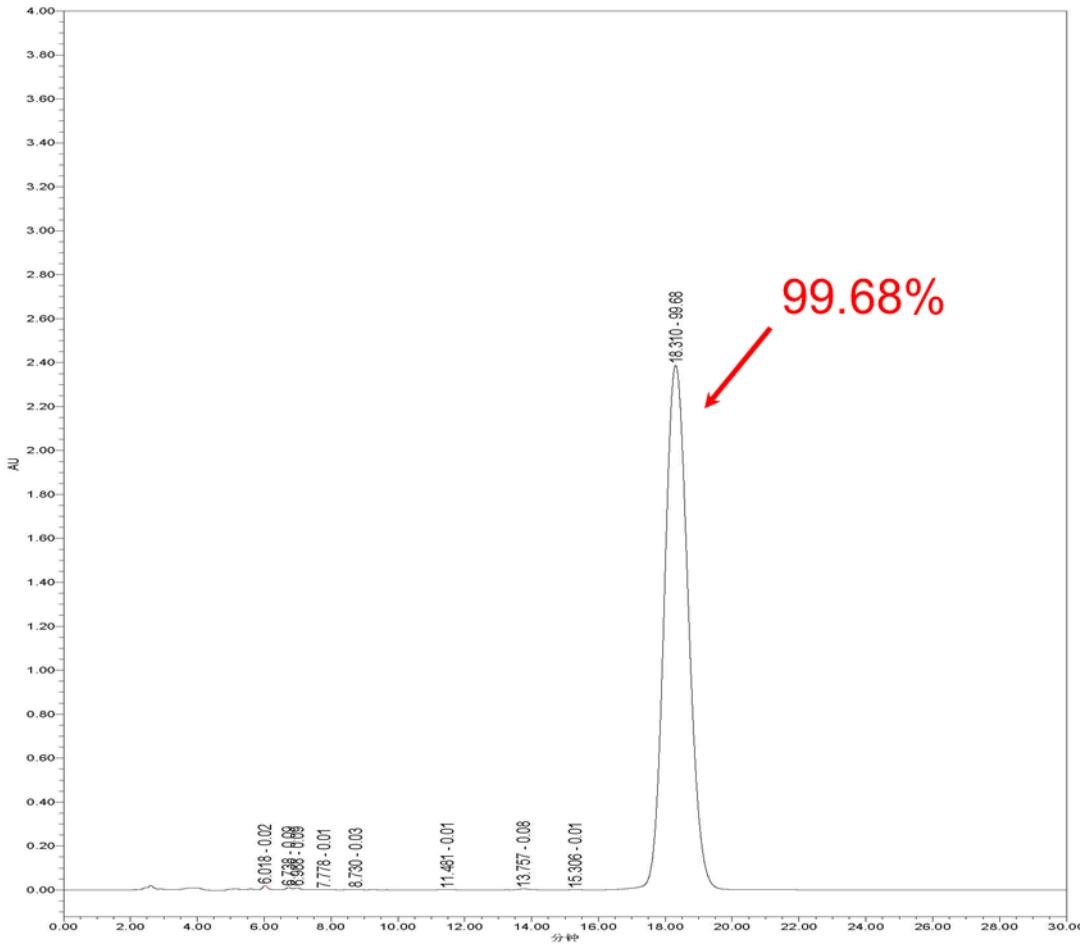


Figure S231 HPLC analysis of compound 15.

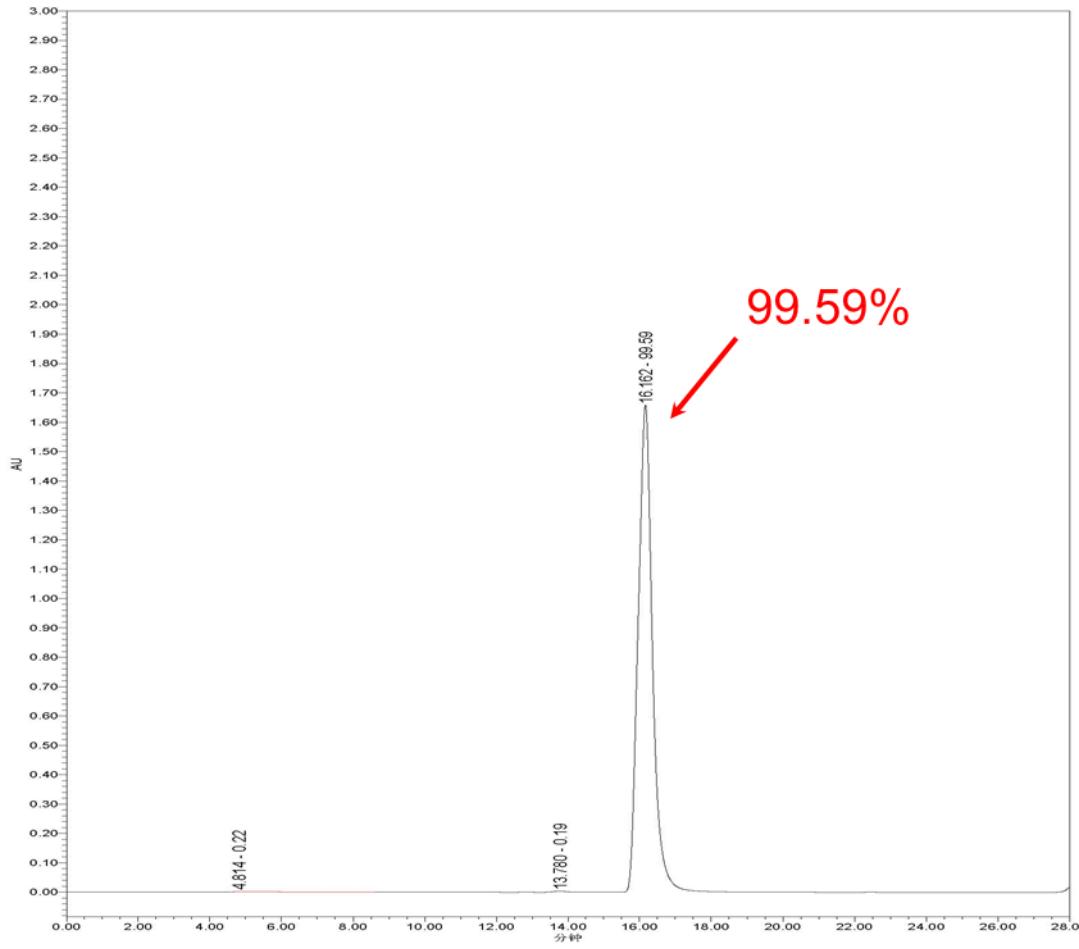


Figure S231 HPLC analysis of compound 16.

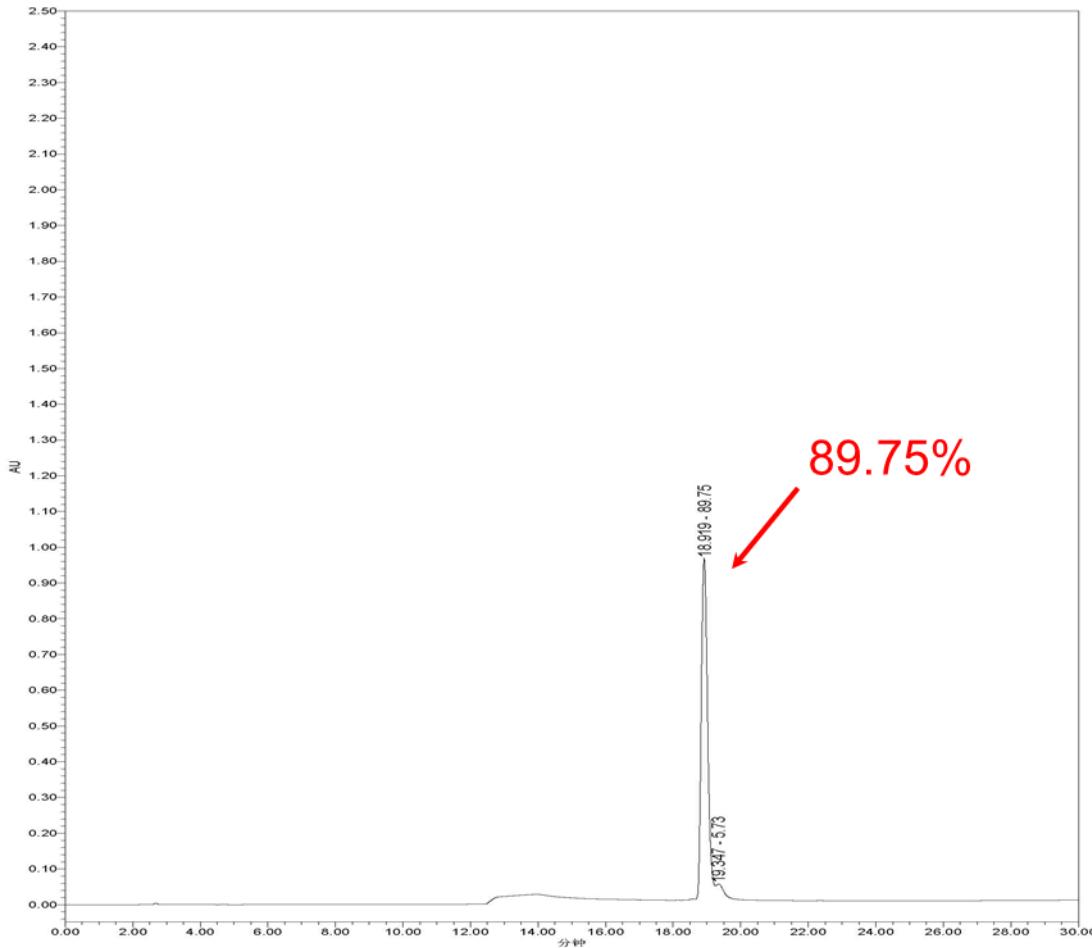


Figure S231 HPLC analysis of compound 38.