

Supplementary Materials

for the paper

“Synthesis and evaluation of antimicrobial and cytotoxic activity of oxathiine fused quinone-thioglycoside conjugates of substituted 1,4-naphthoquinones”

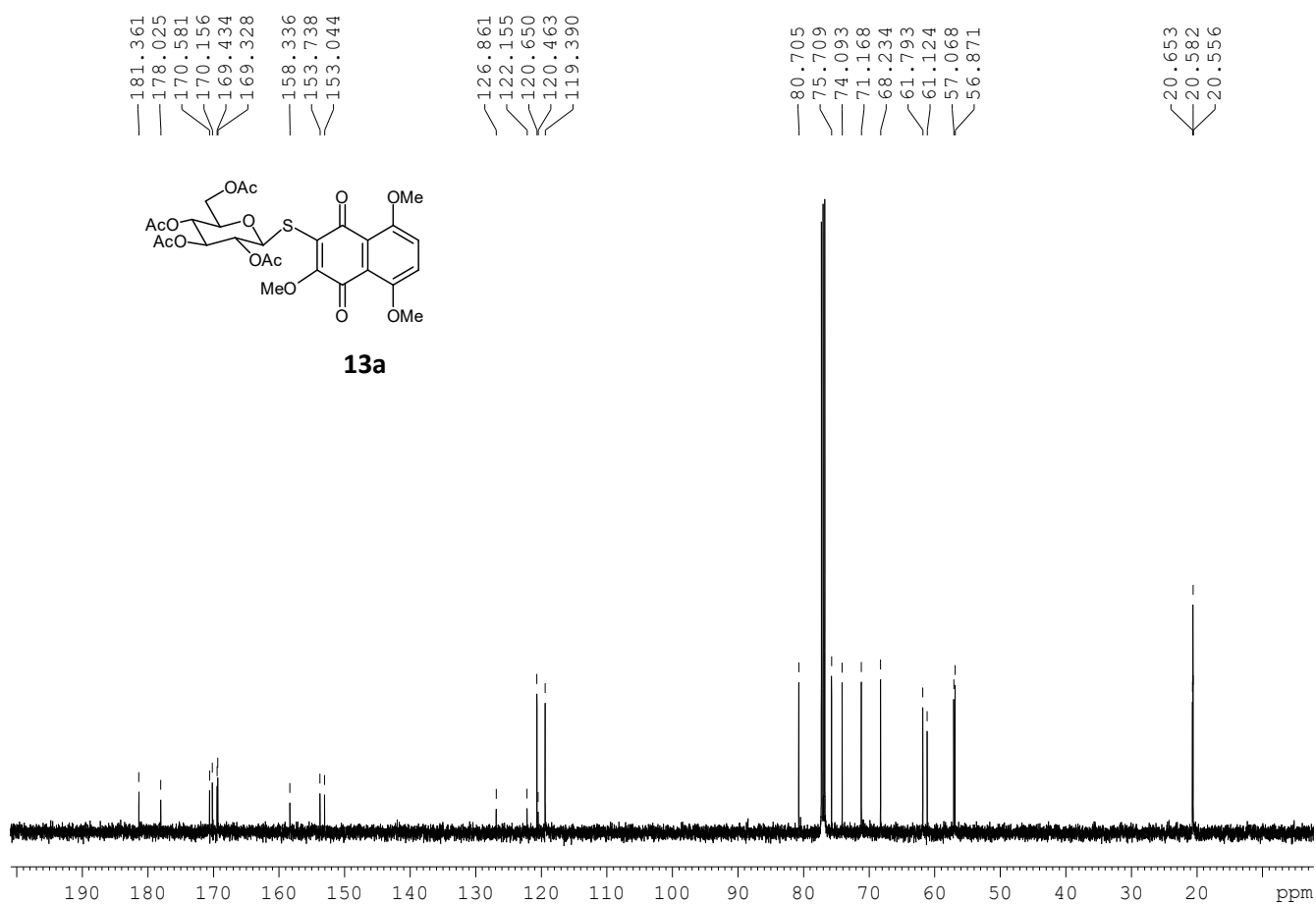
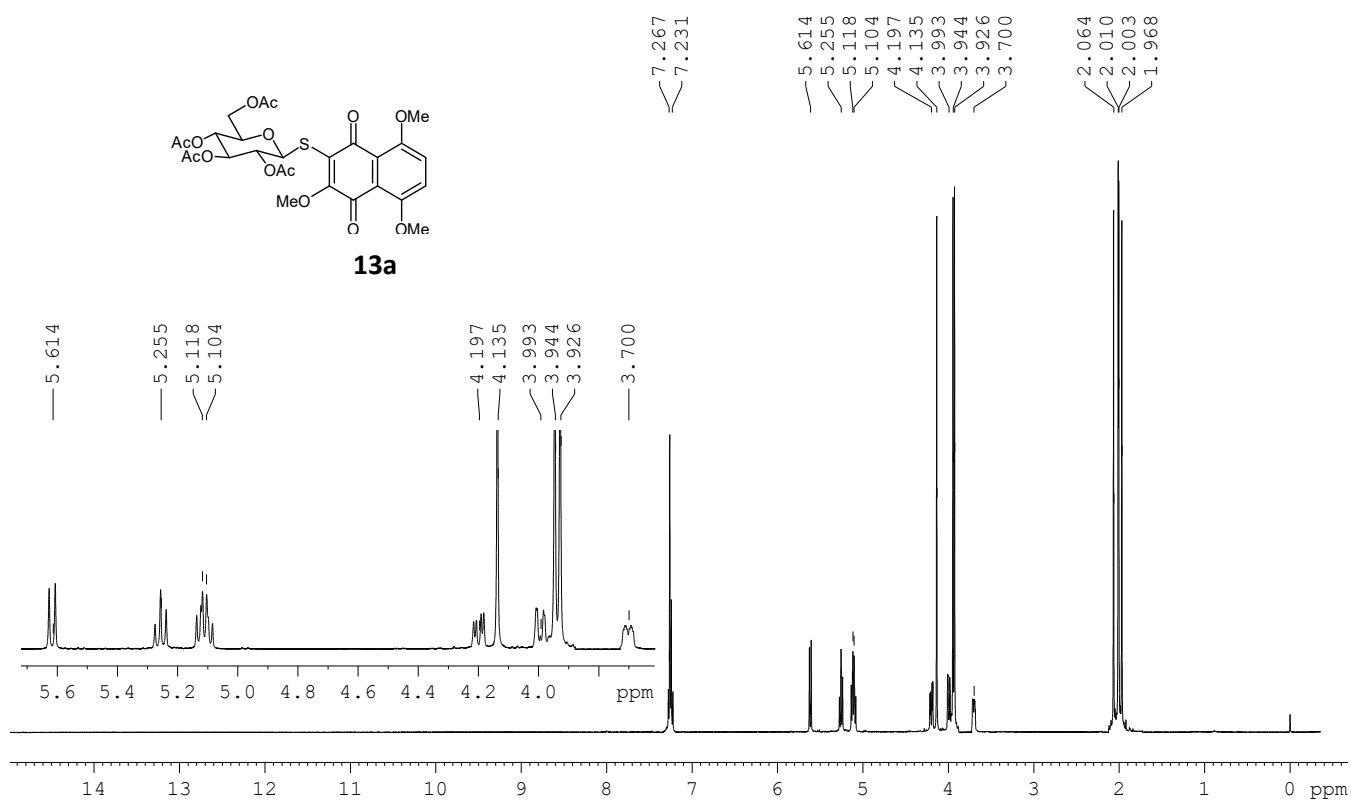
Yuri E. Sabutski, Ekaterina S. Menchinskaya, Ludmila S. Shevchenko, Ekaterina A. Chingizova, Artur R. Chingizov, Roman S. Popov, Vladimir A. Denisenko, Valery V. Michailov, Dmitry L. Aminin, Sergey G. Polonik

Content

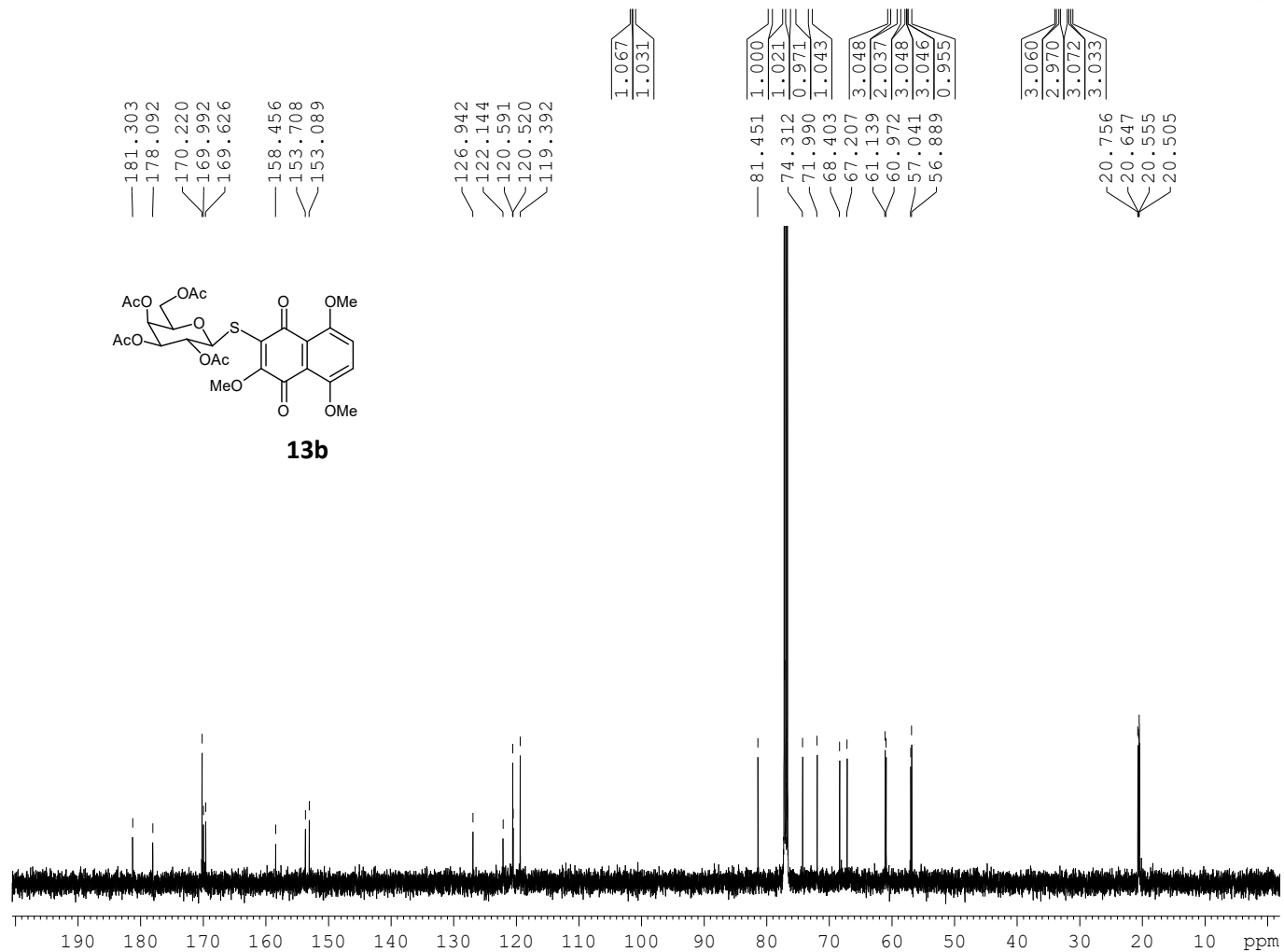
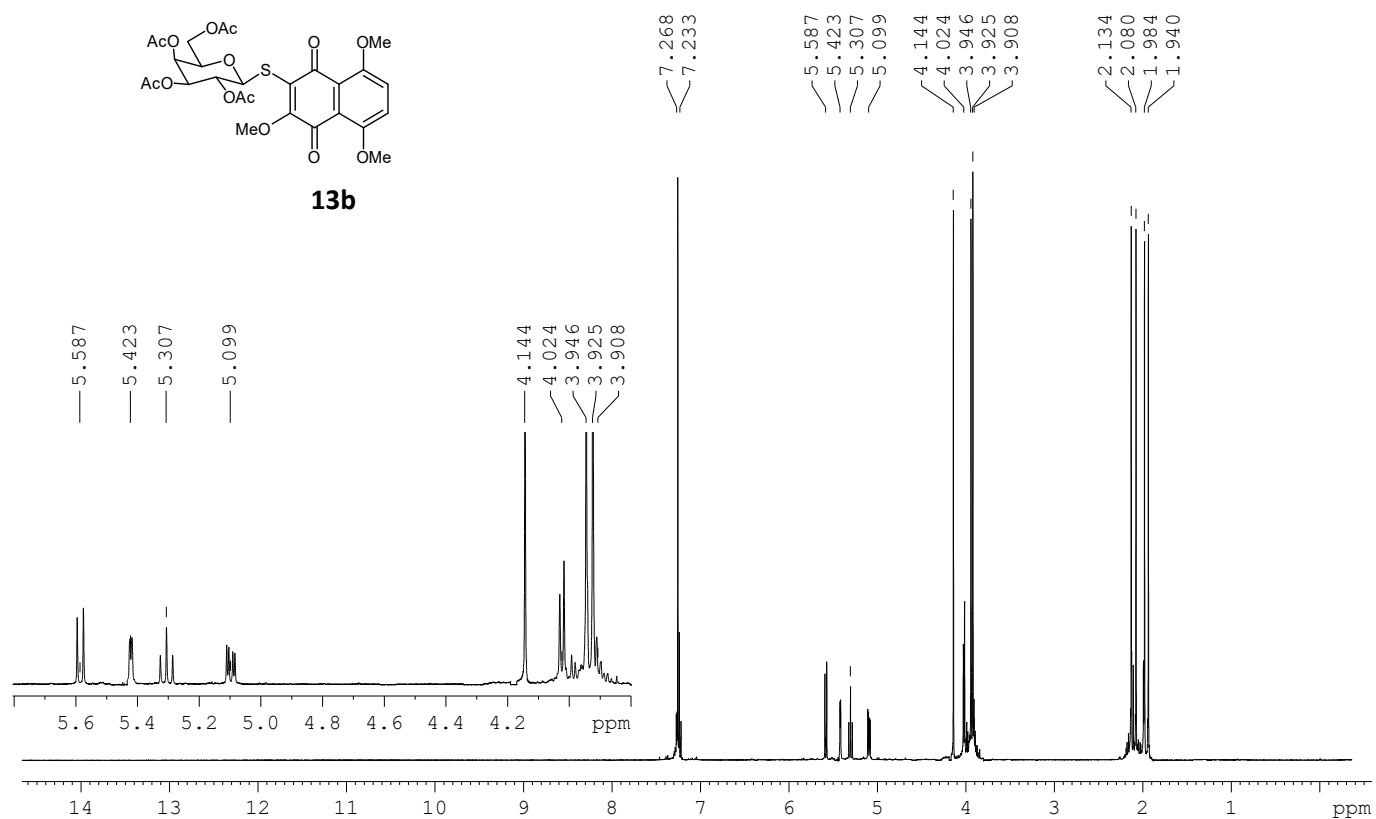
¹H and ¹³C NMR spectra for synthesized compounds

S2-S33

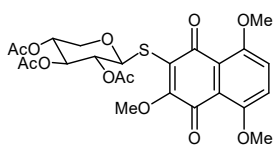
2-(2,3,4,6-Tetra-O-acetyl- β -D-glucopyranosyl-1-thio)-3,5,8-trimethoxy-1,4-naphthoquinone (**13a**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



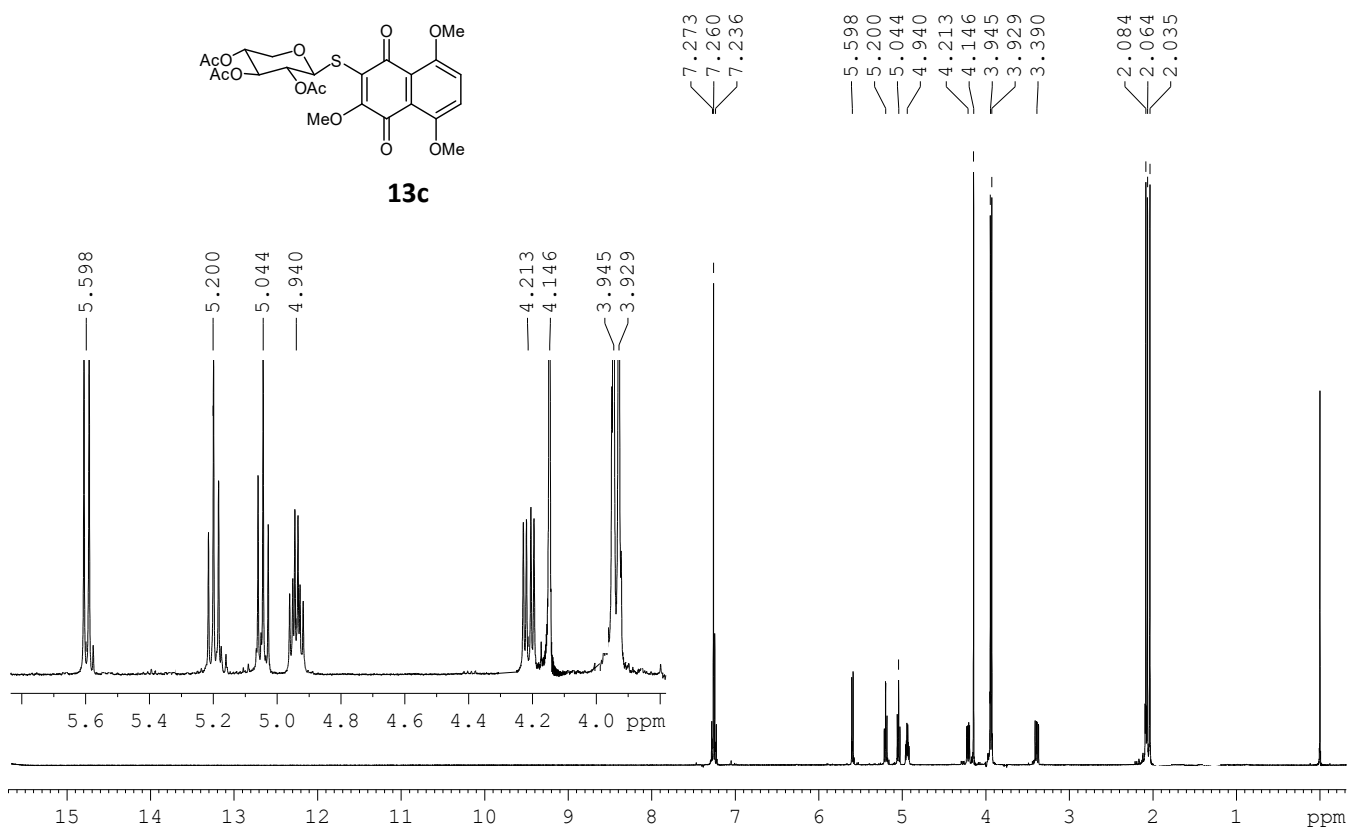
2-(2,3,4,6-Tetra-O-acetyl- β -D-galactopyranosyl-1-thio)-3,5,8-trimethoxy-1,4-naphthoquinone (**13b**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



2-(2,3,4-Tri-O-acetyl- β -D-xylopyranosyl-1-thio)-3,5,8-trimethoxy-1,4-naphthoquinone (**13c**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



13c

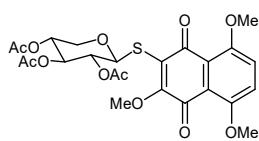


181.318
178.342
169.816
169.747
169.424
159.429
153.765
153.316

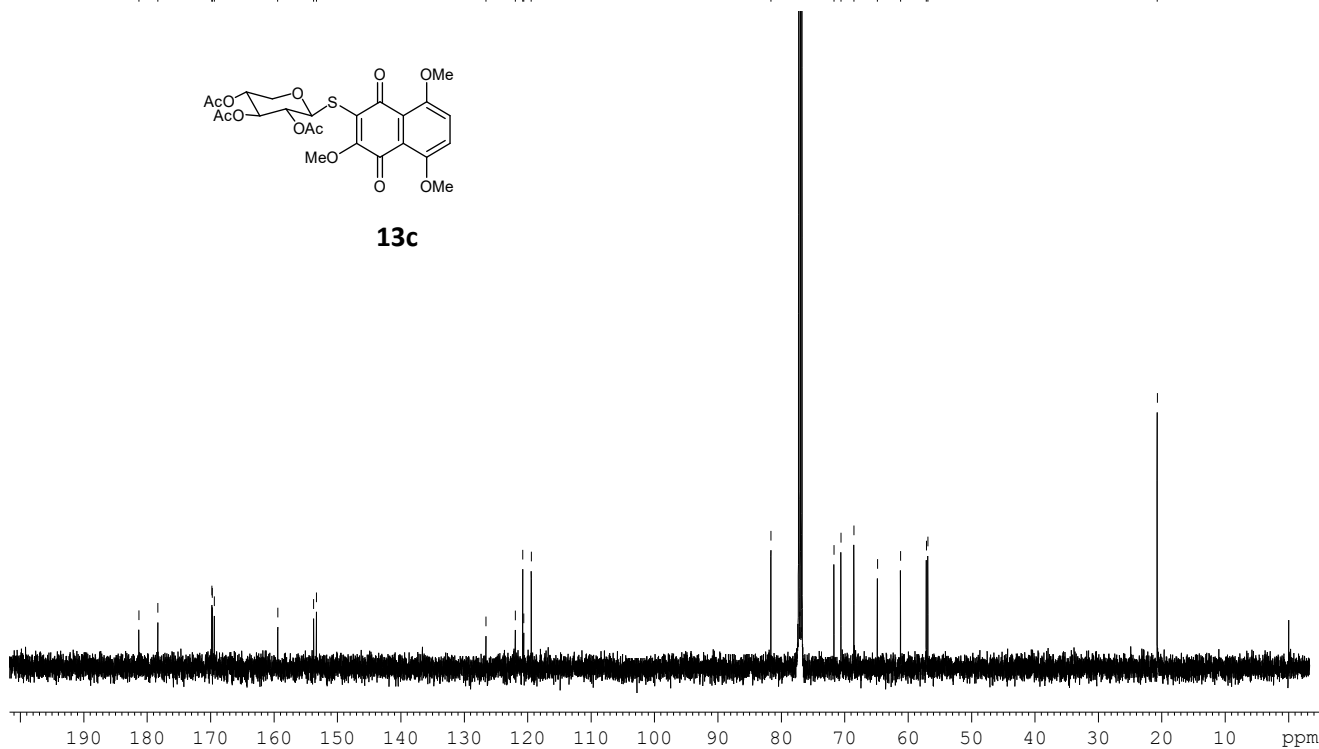
126.590
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56.894

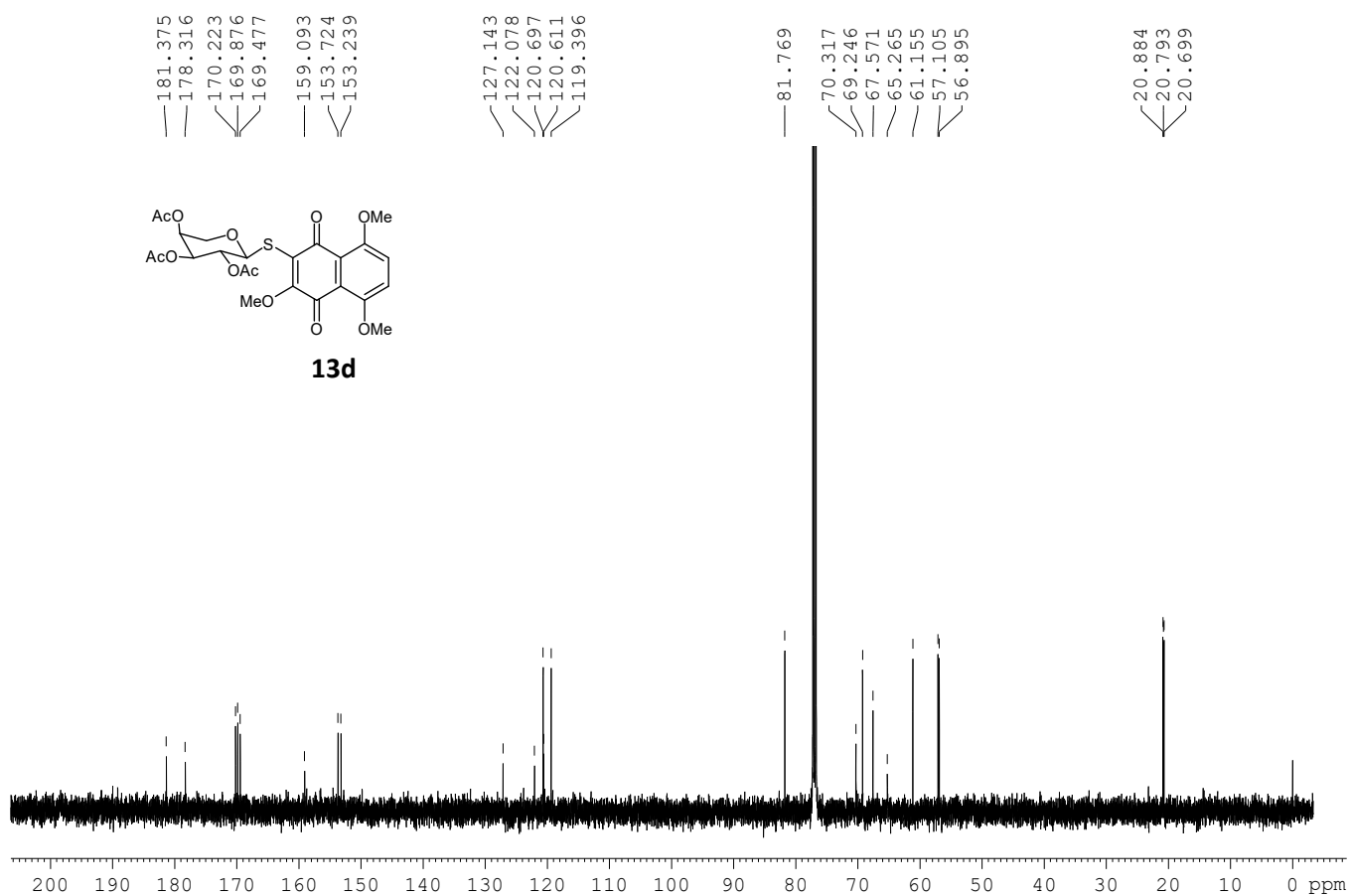
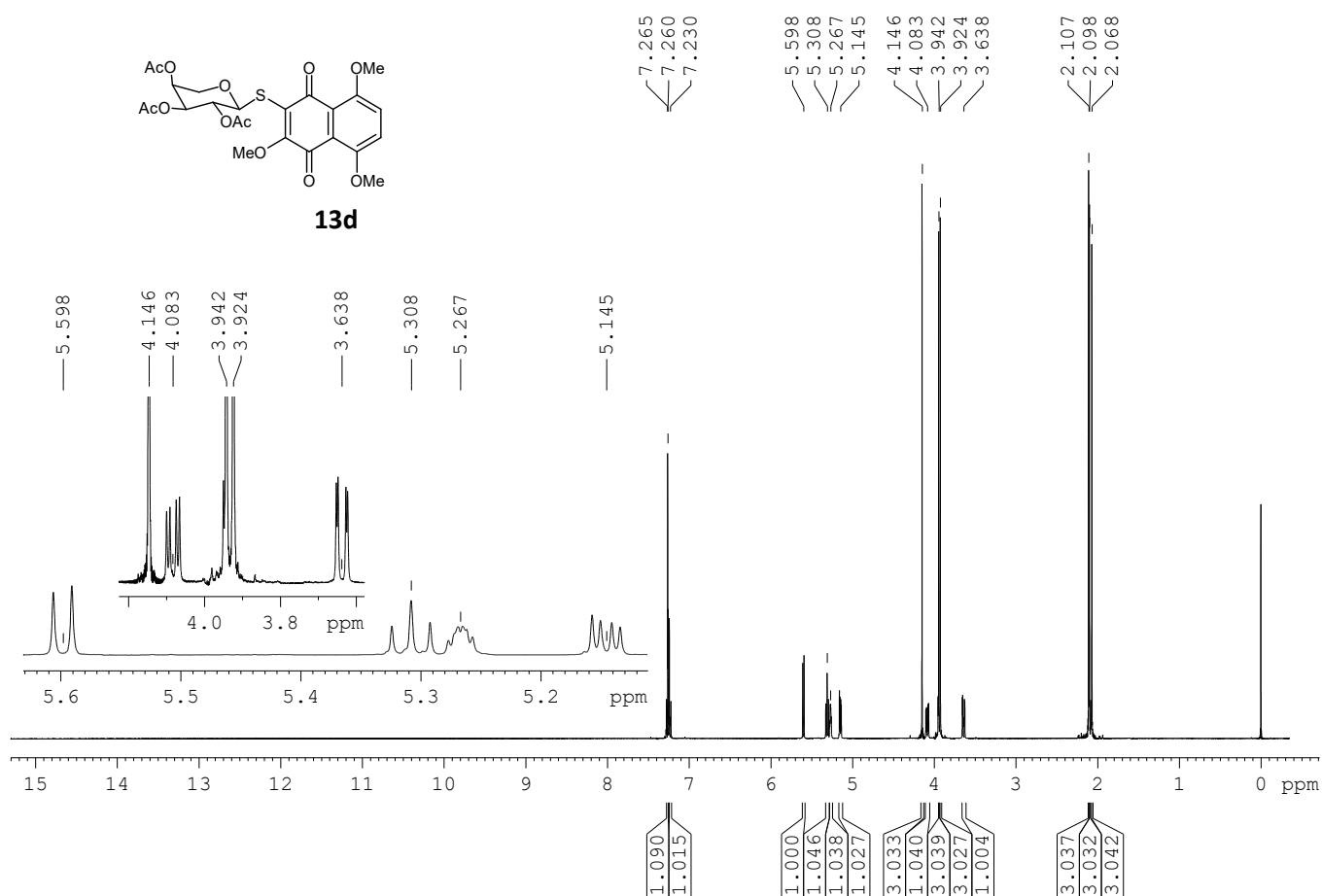
20.716



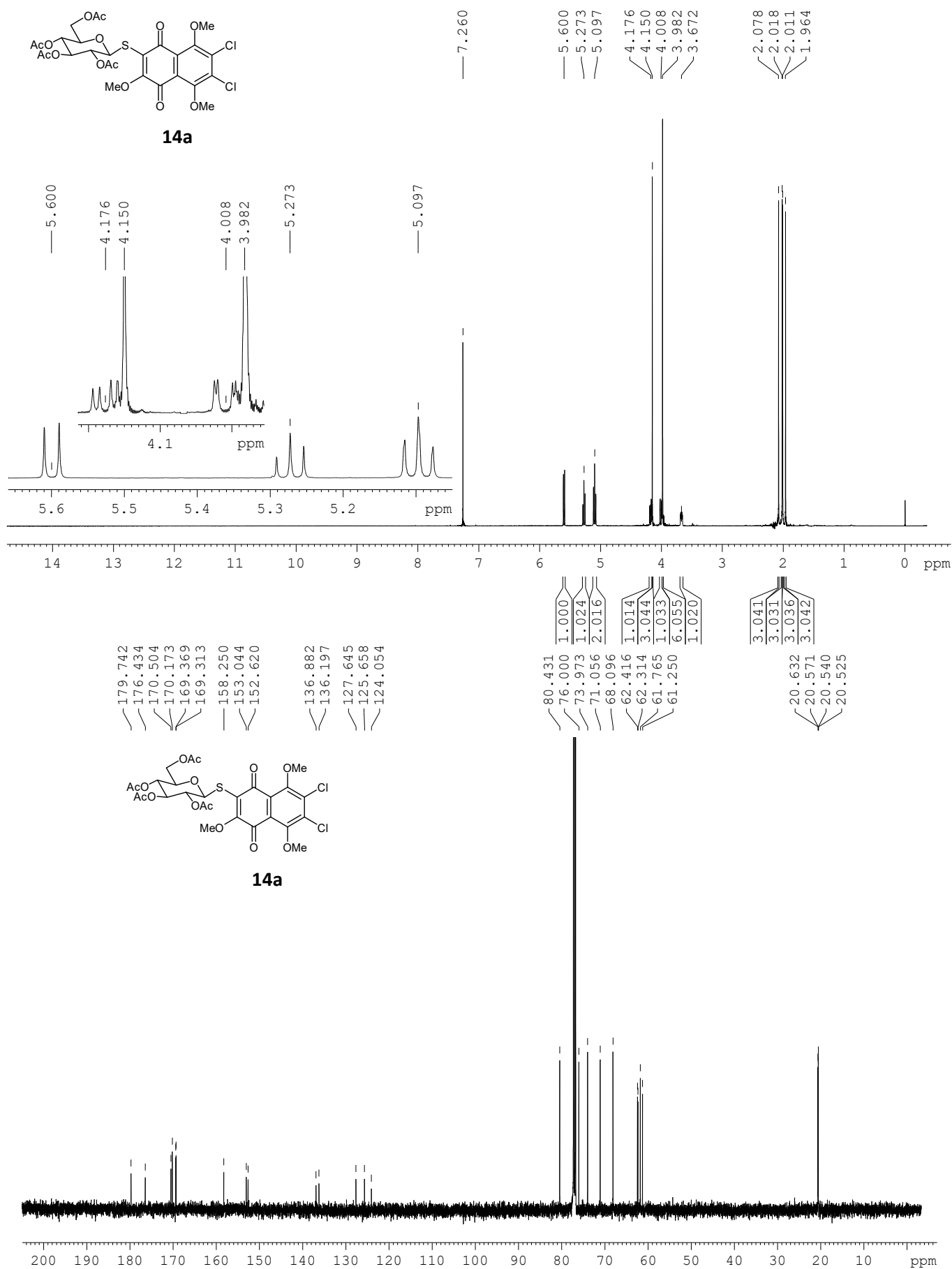
13c



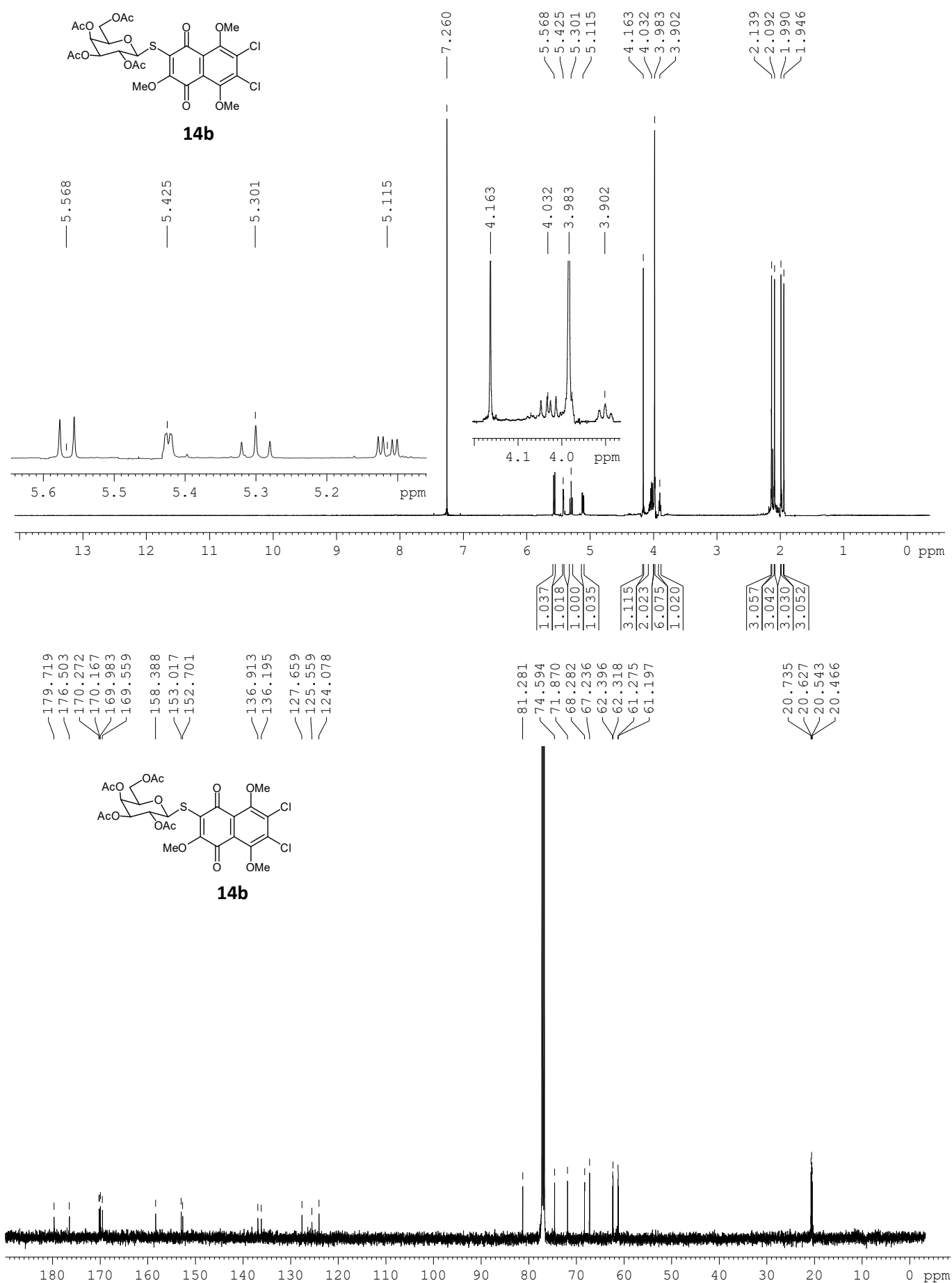
2-(2,3,4-Tri-O-acetyl- α -L-arabinopyranosyl-1-thio)-3,5,8-trimethoxy-1,4-naphthoquinone (**13d**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



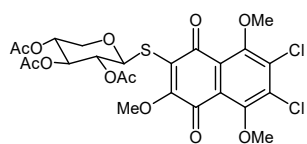
2-(2,3,4,6-Tetra-O-acetyl- β -D-glucopyranosyl-1-thio)-6,7-dichloro-3,5,8-trimethoxy-1,4-naphthoquinone (**14a**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



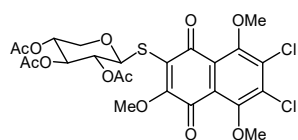
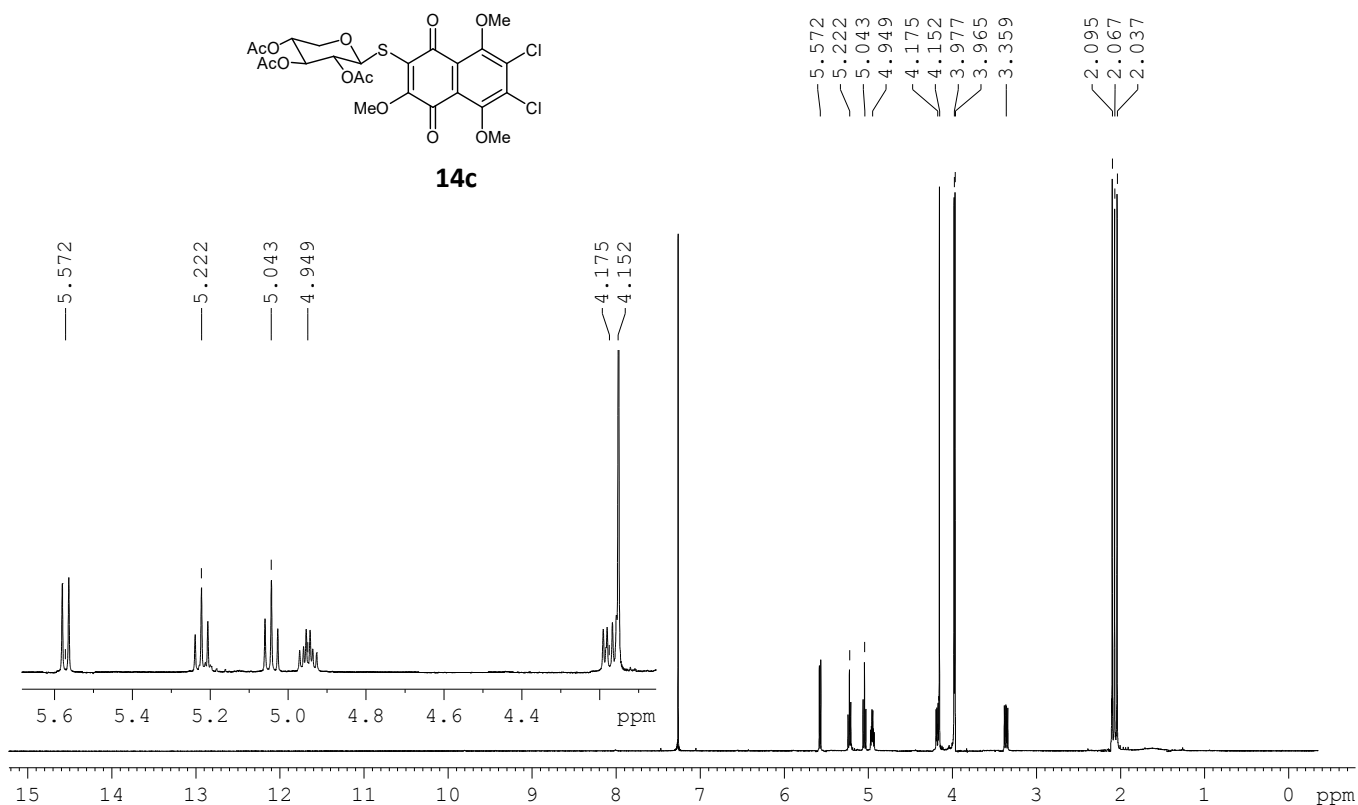
2-(2,3,4,6-Tetra-O-acetyl- β -D-galactopyranosyl-1-thio)-6,7-dichloro-3,5,8-trimethoxy-1,4-naphthoquinone (**14b**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



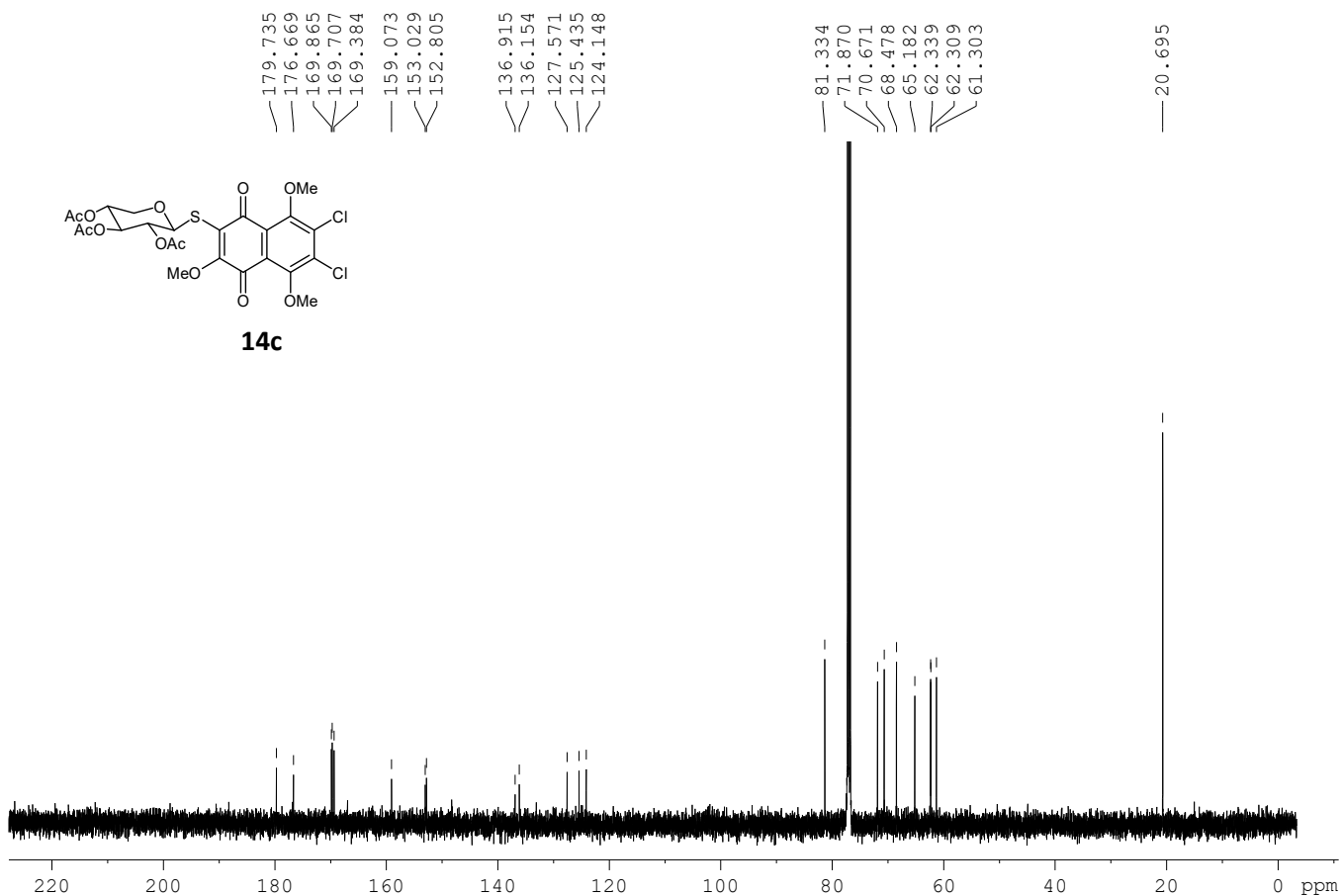
2-(2,3,4-Tri-O-acetyl- β -D-xylopyranosyl-1-thio)-6,7-dichloro-3,5,8-trimethoxy-1,4-naphthoquinone (**14c**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



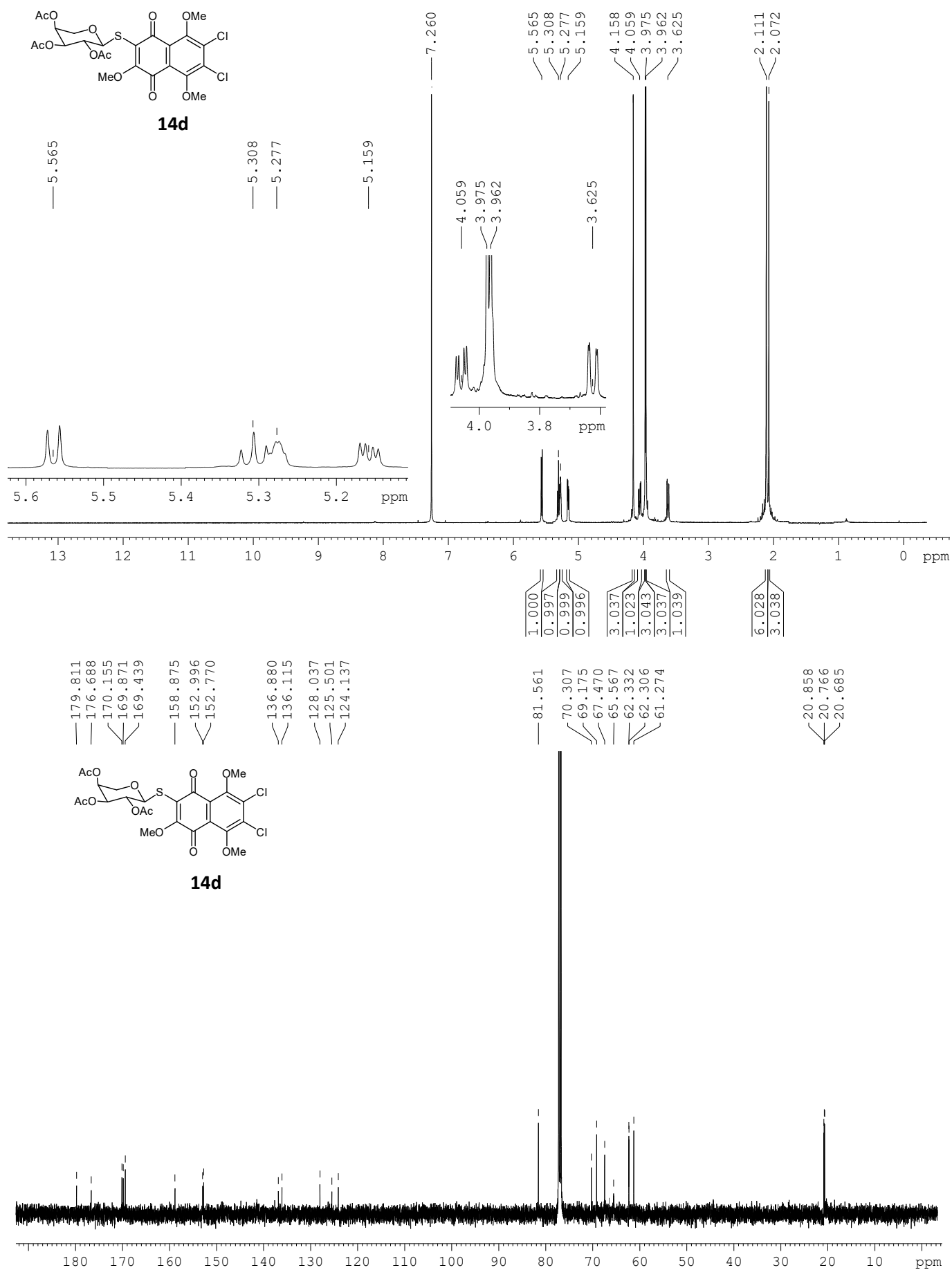
14c



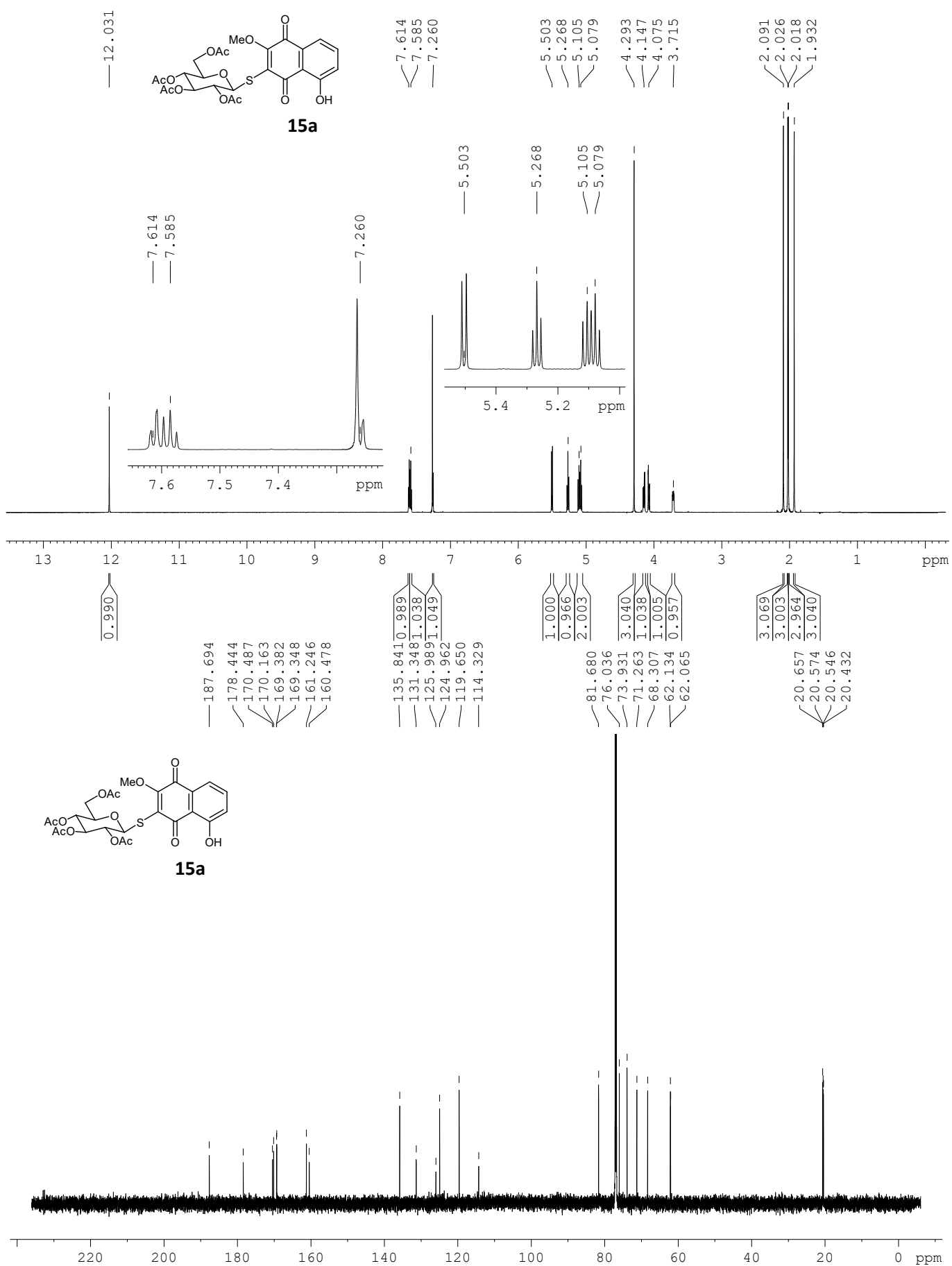
14c



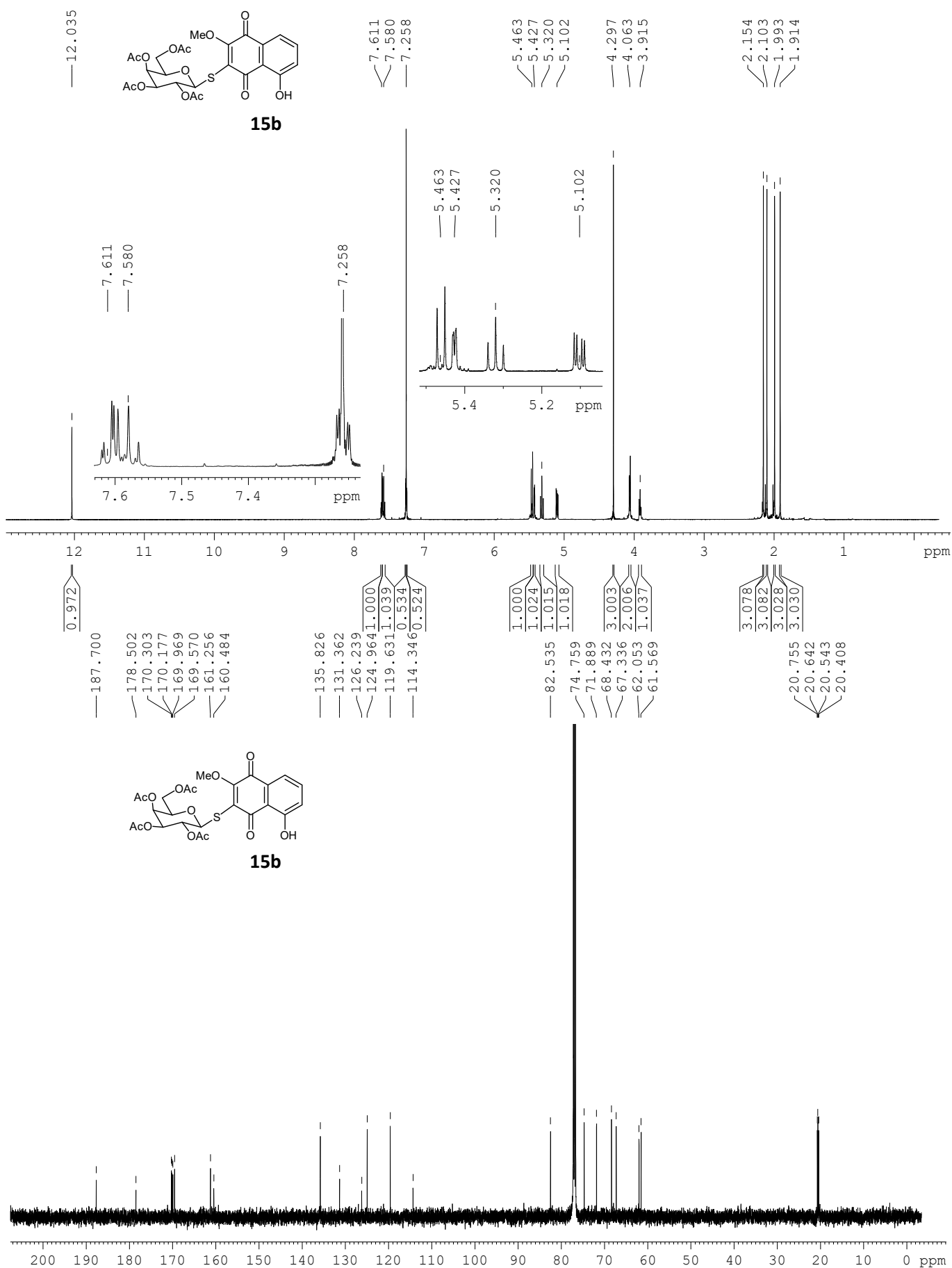
2-(2,3,4-Tri-O-acetyl- α -L-arabinopyranosyl-1-thio)-6,7-dichloro-3,5,8-trimethoxy-1,4-naphthoquinone (**14d**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



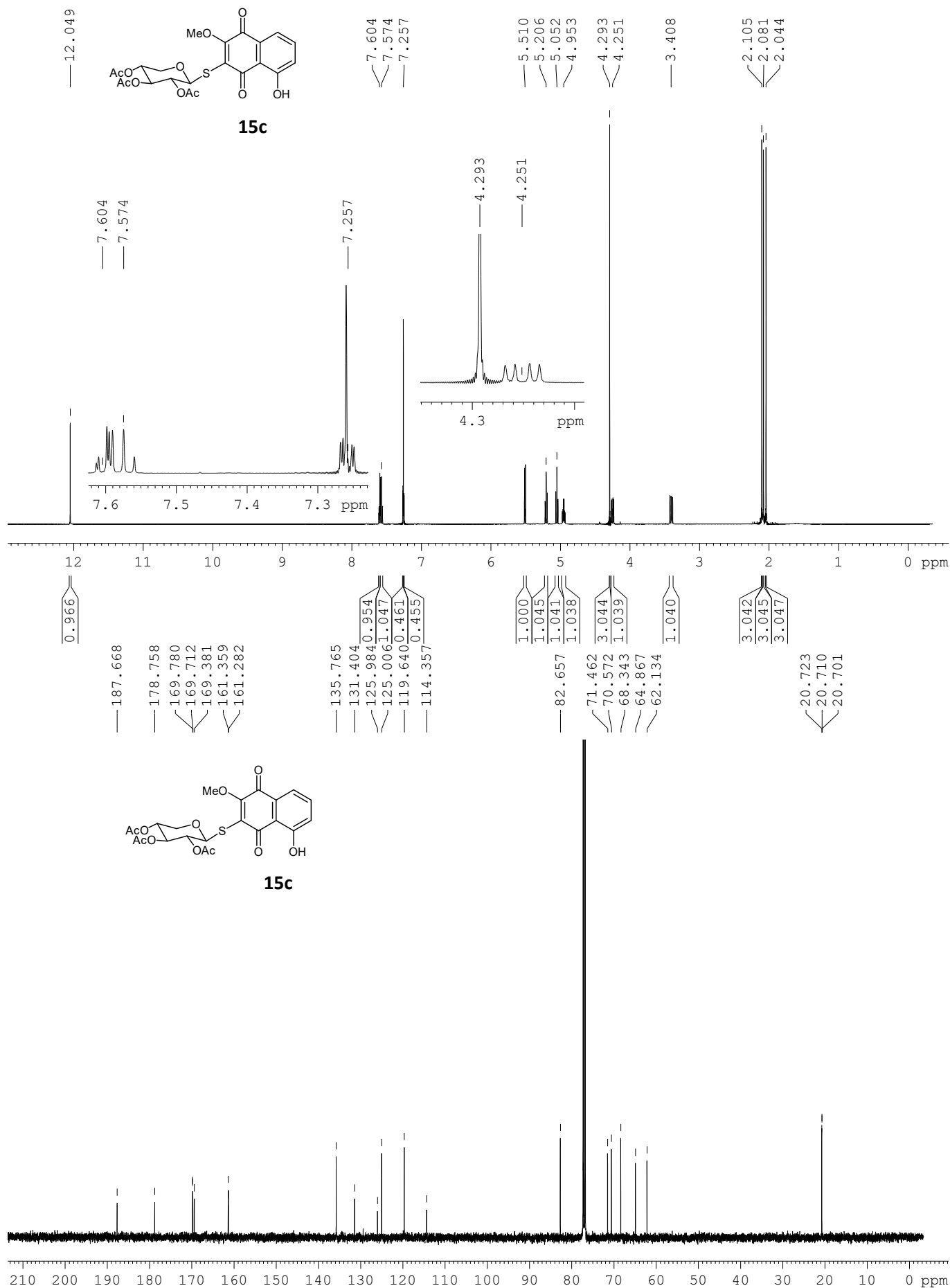
2-(2,3,4,6-Tetra-O-acetyl- β -D-glucopyranosyl-1-thio)-8-hydroxy-3-methoxy-1,4-naphthoquinone (**15a**), (^1H NMR - 700 MHz, ^{13}C NMR - 176 MHz, solvent - CDCl_3)



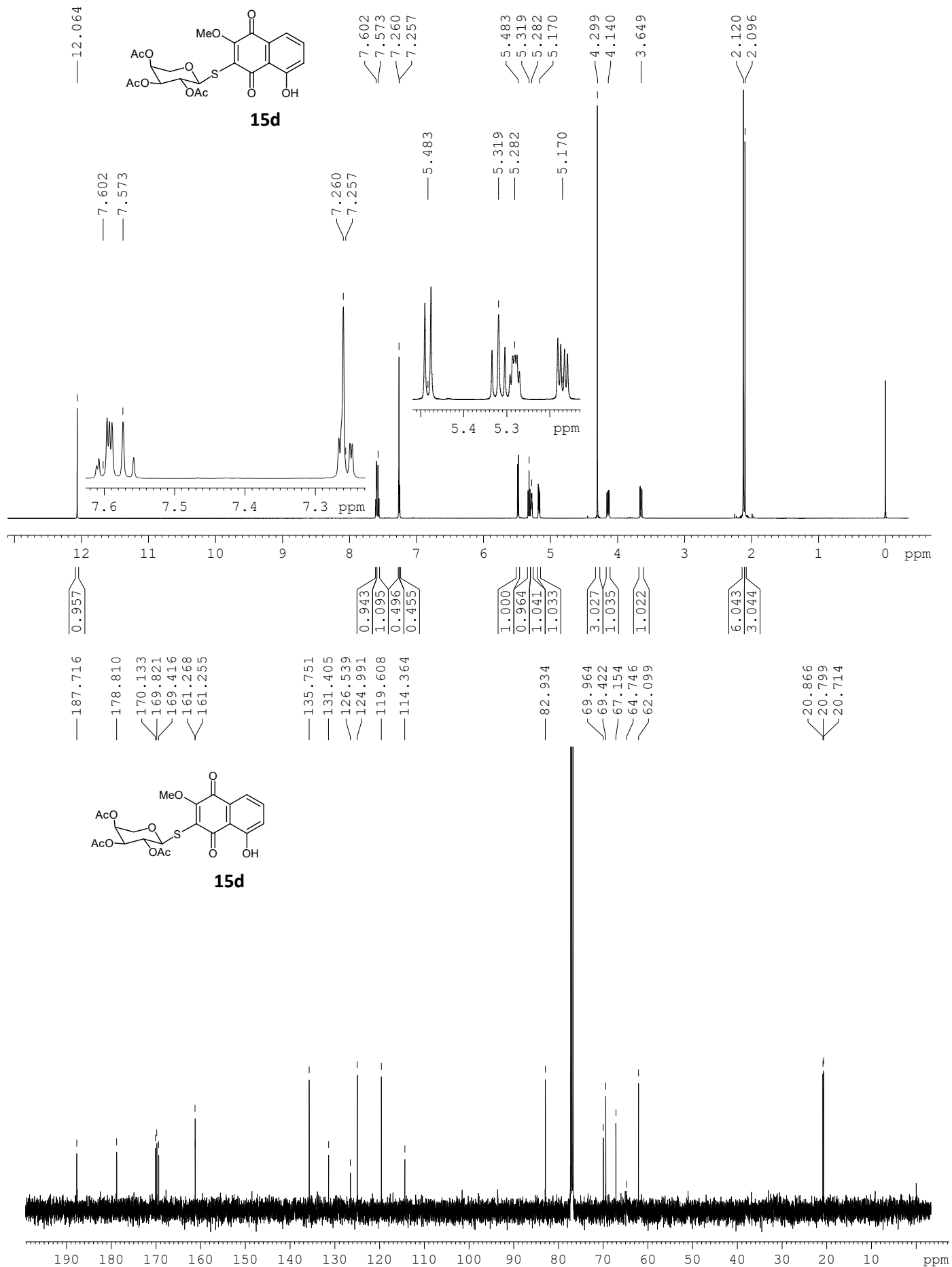
2-(2,3,4,6-Tetra-O-acetyl- β -D-galactopyranosyl-1-thio)-8-hydroxy-3-methoxy-1,4-naphthoquinone (**15b**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



2-(2,3,4-Tri-O-acetyl- β -D-xylopyranosyl-1-thio)-8-hydroxy-3-methoxy-1,4-naphthoquinone (**15c**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



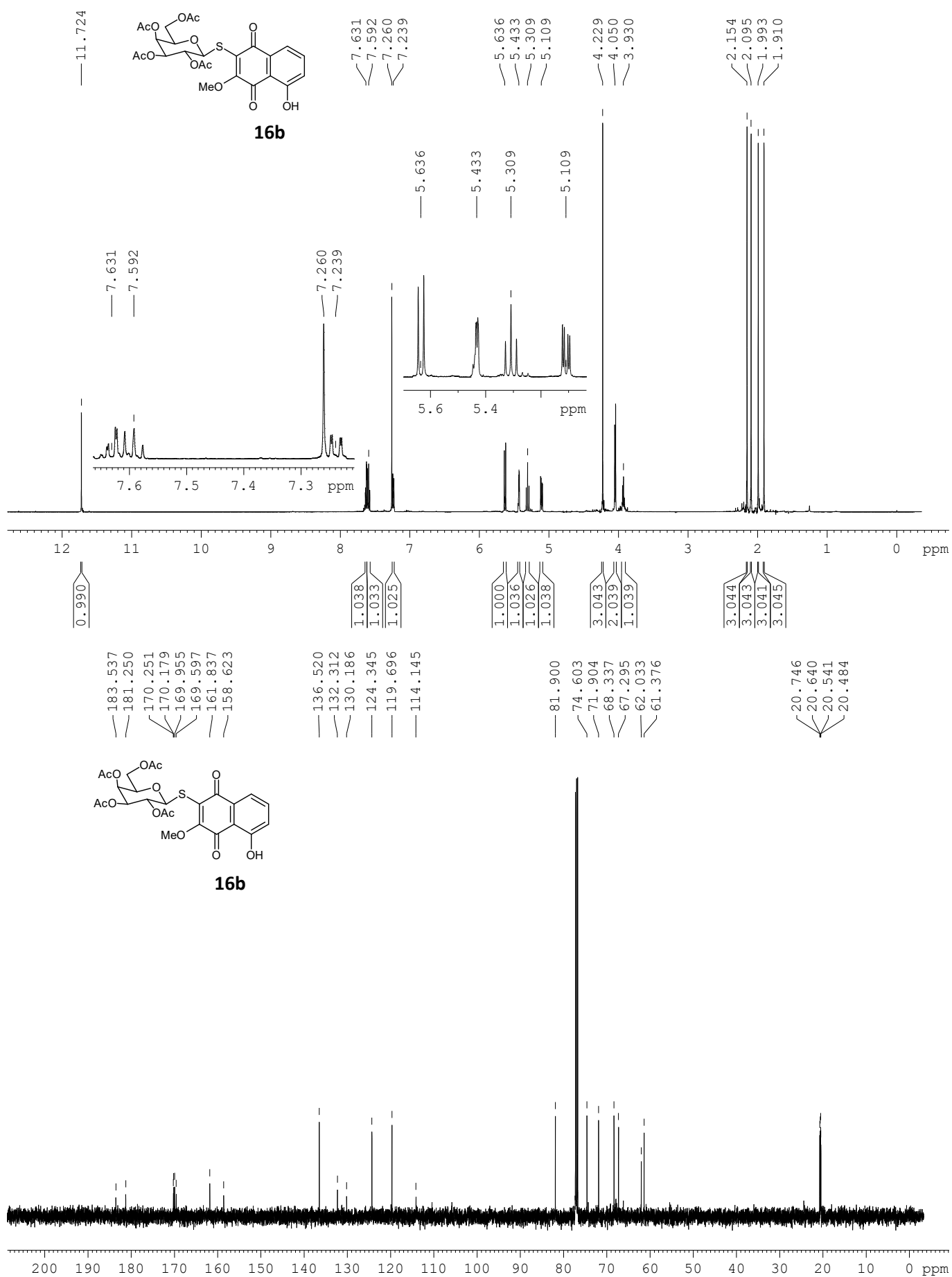
2-(2,3,4-Tri-O-acetyl- α -L-arabinopyranosyl-1-thio)-8-hydroxy-3-methoxy-1,4-naphthoquinone (**15d**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



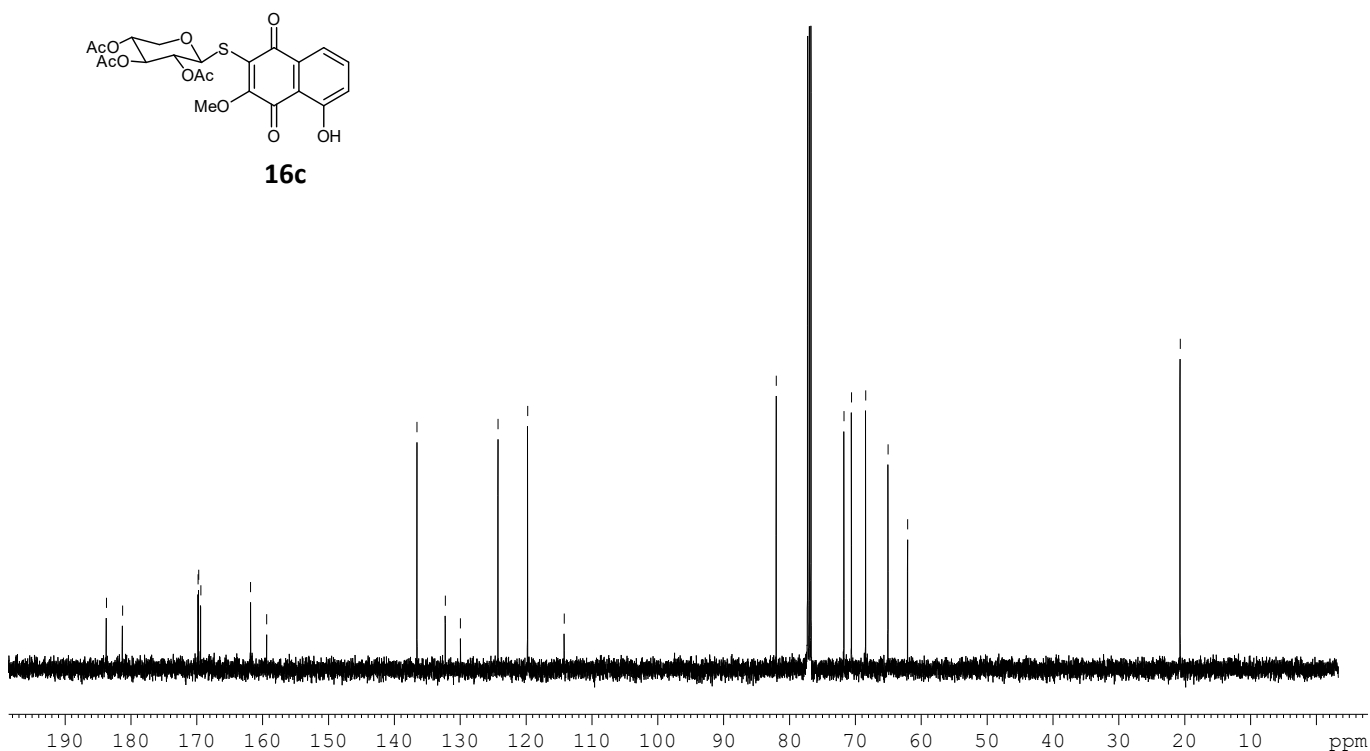
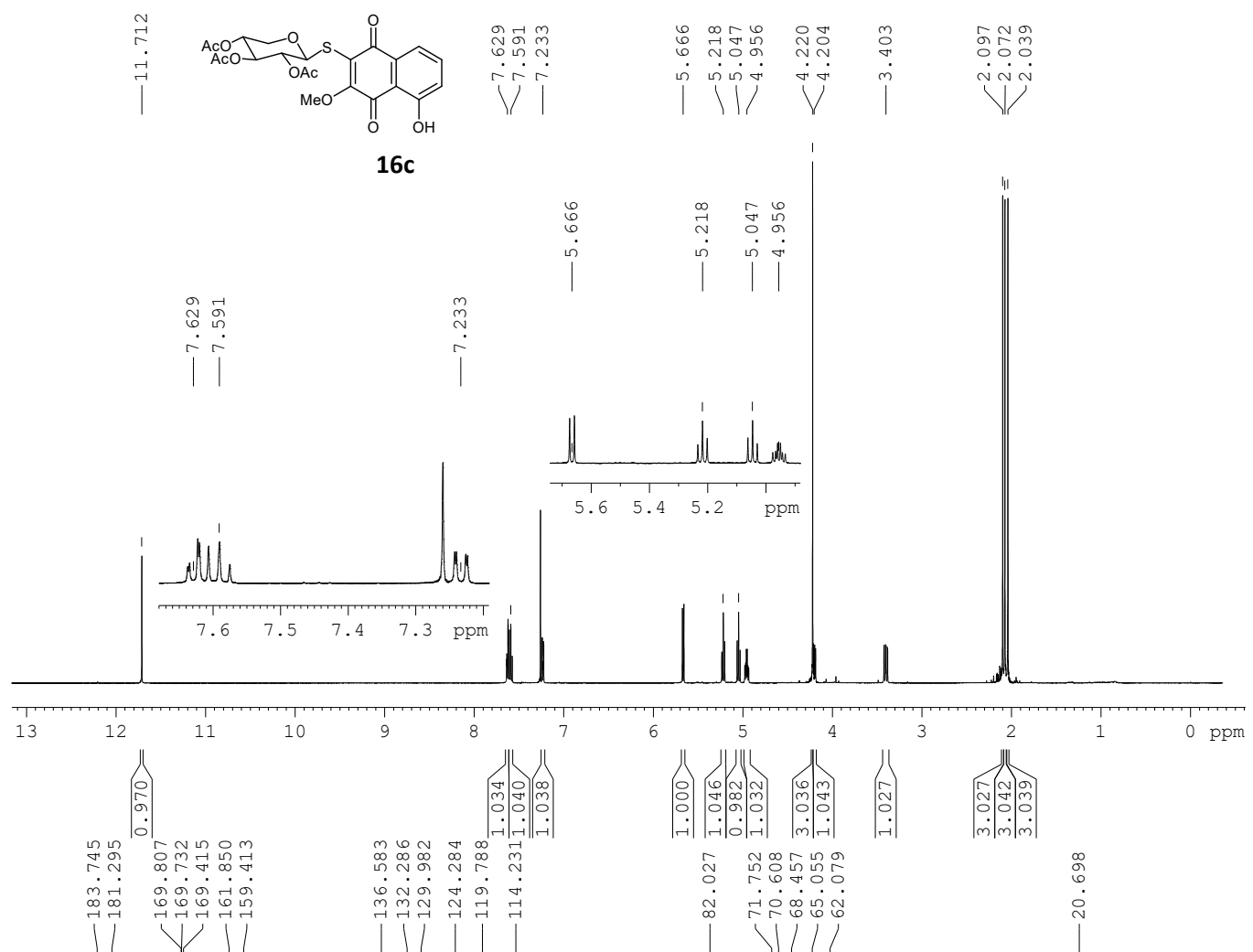
2-(2,3,4,6-Tetra-O-acetyl- β -D-glucopyranosyl-1-thio)-5-hydroxy-3-methoxy-1,4-naphthoquinone (**16a**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



2-(2,3,4,6-Tetra-O-acetyl- β -D-galactopyranosyl-1-thio)-5-hydroxy-3-methoxy-1,4-naphthoquinone (**16b**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



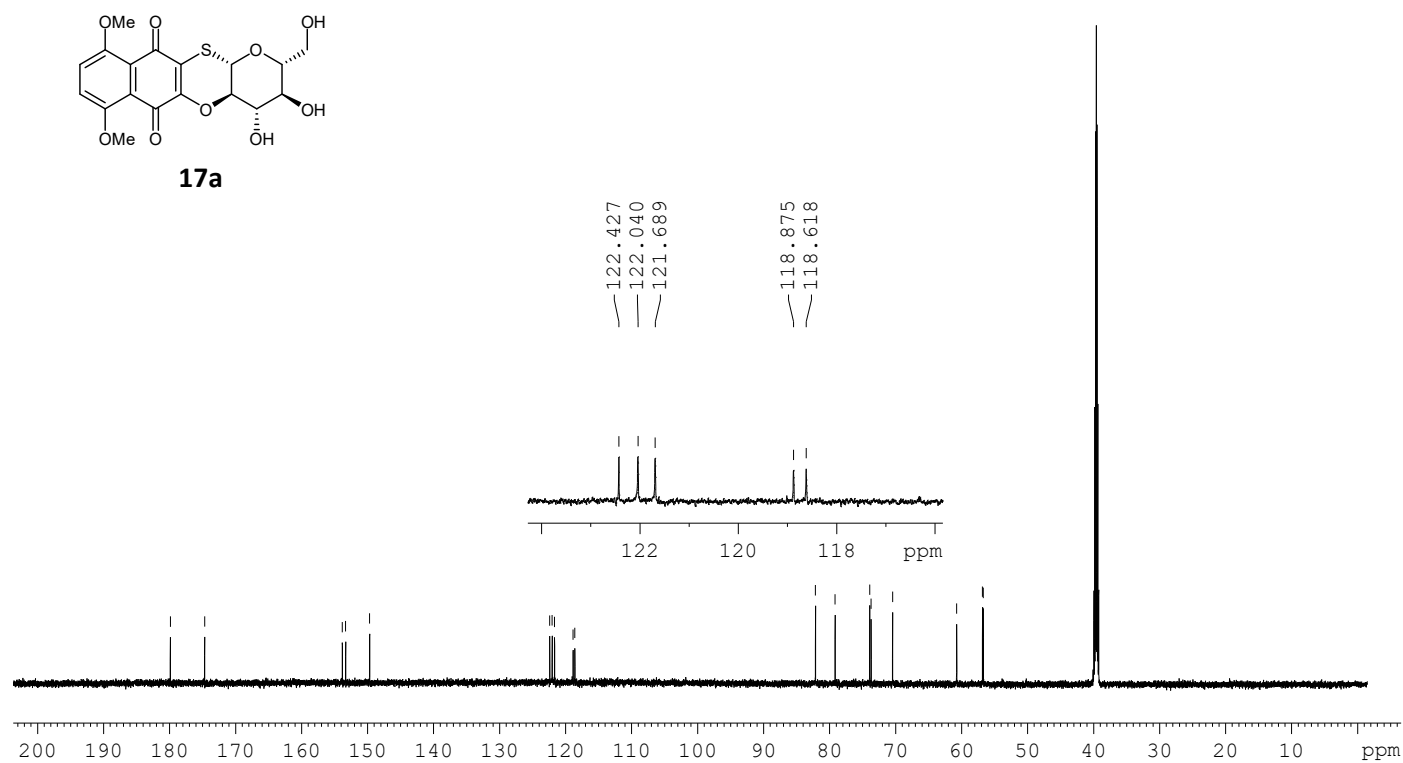
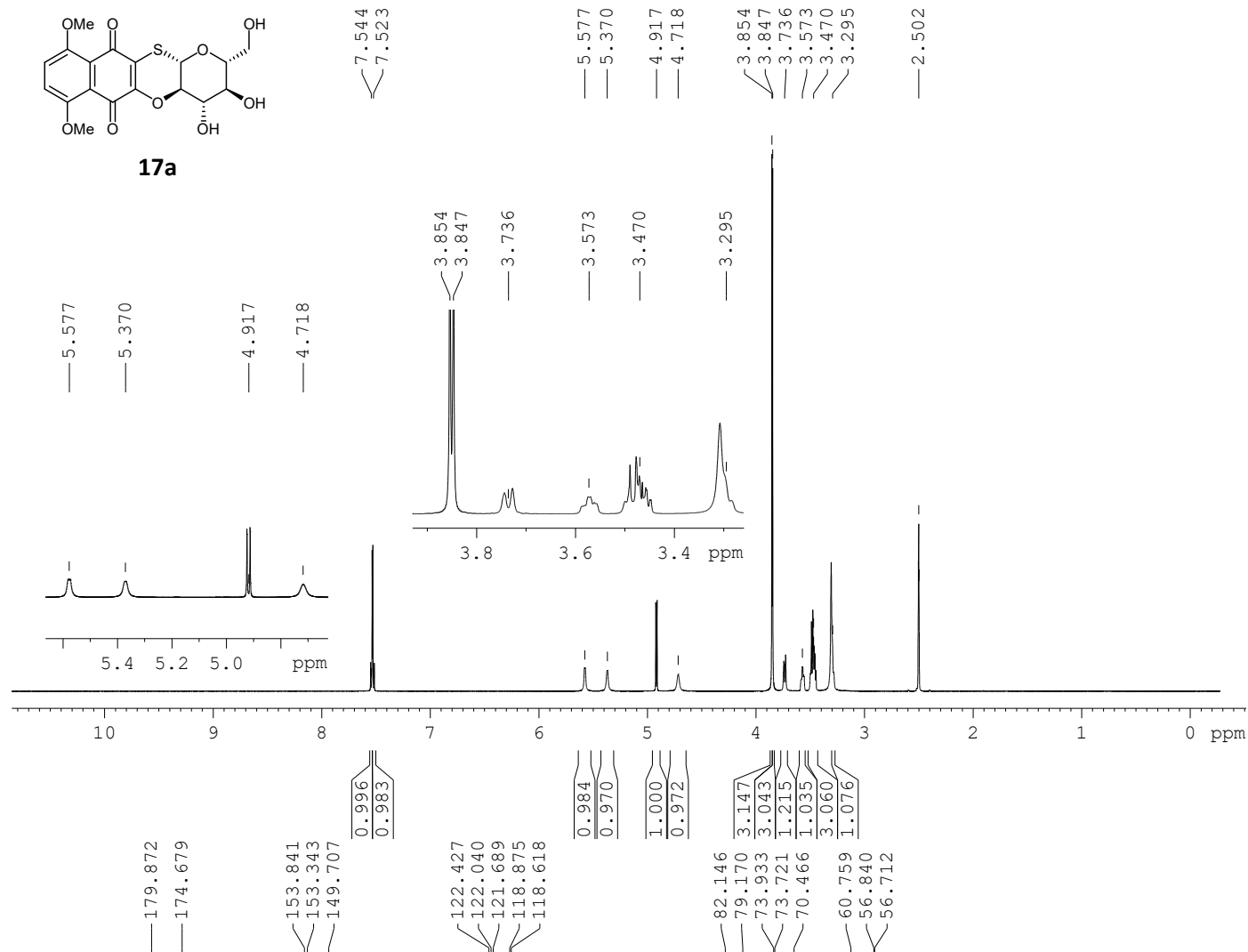
2-(2,3,4-Tri-O-acetyl- β -D-xylopyranosyl-1-thio)-5-hydroxy-3-methoxy-1,4-naphthoquinone (**16c**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



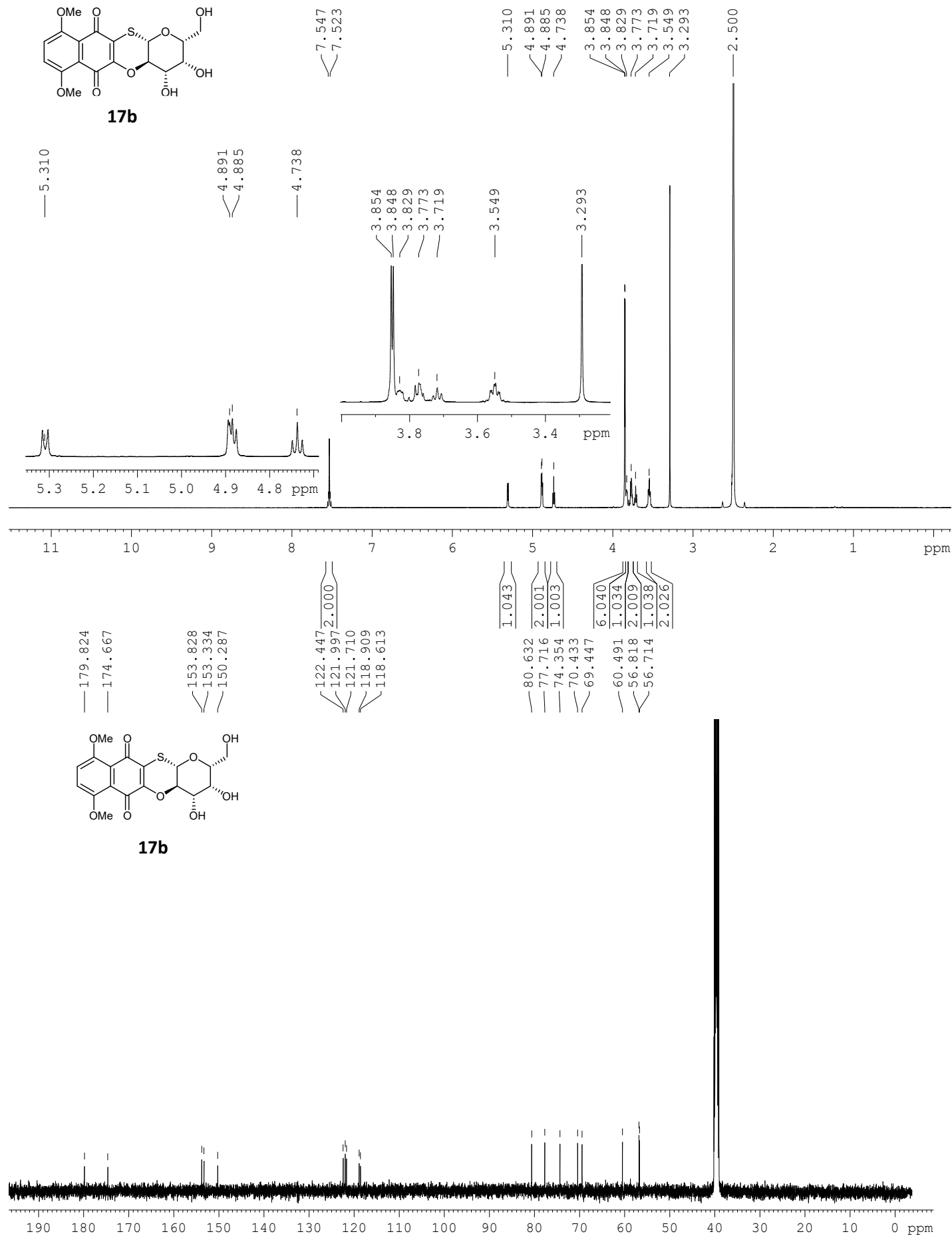
2-(2,3,4-Tri-O-acetyl- α -L-arabinopyranosyl-1-thio)-5-hydroxy-3-methoxy-1,4-naphthoquinone (**16d**), (^1H NMR - 700 MHz, ^{13}C NMR - 176 MHz, solvent - CDCl_3)



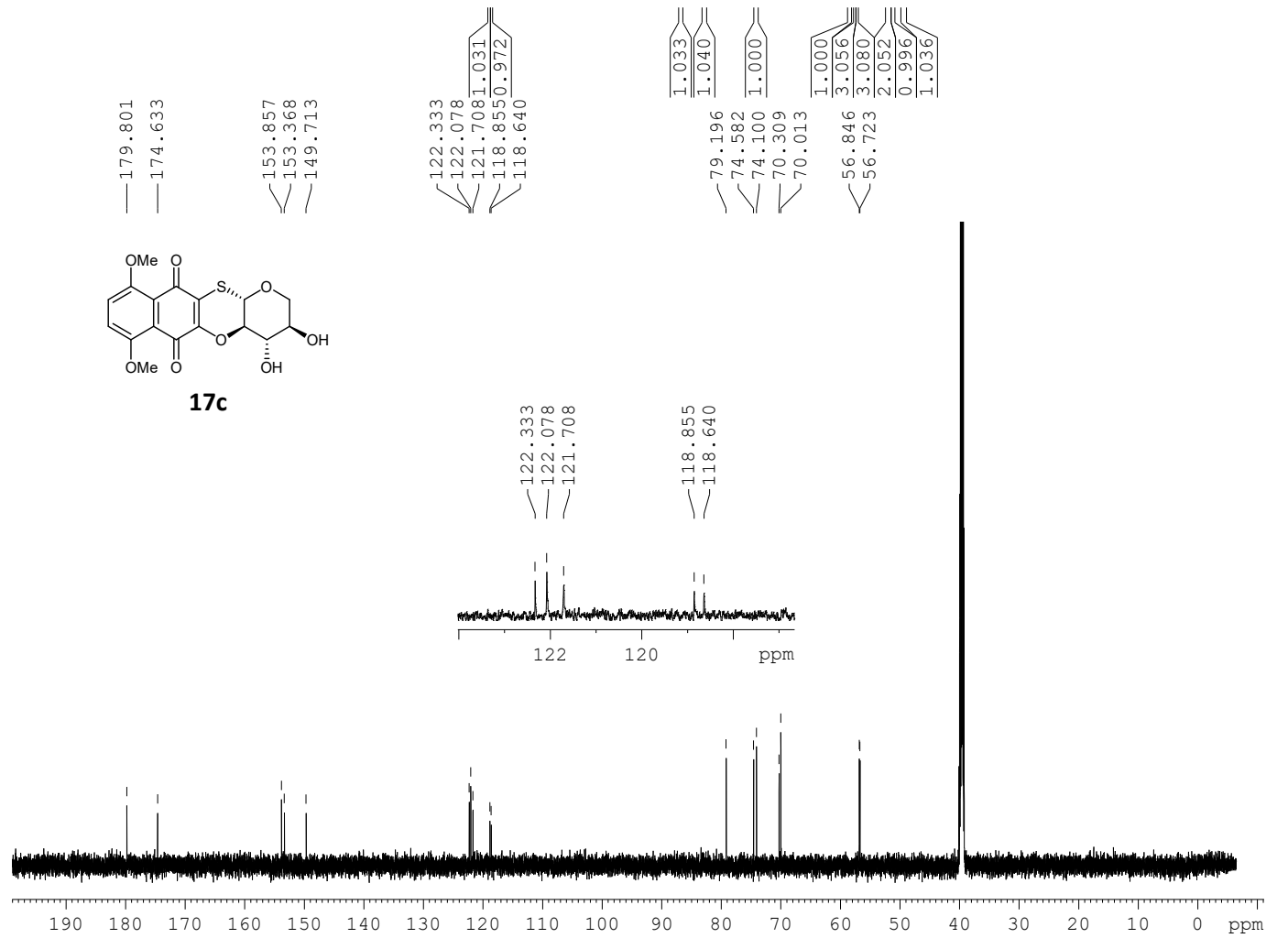
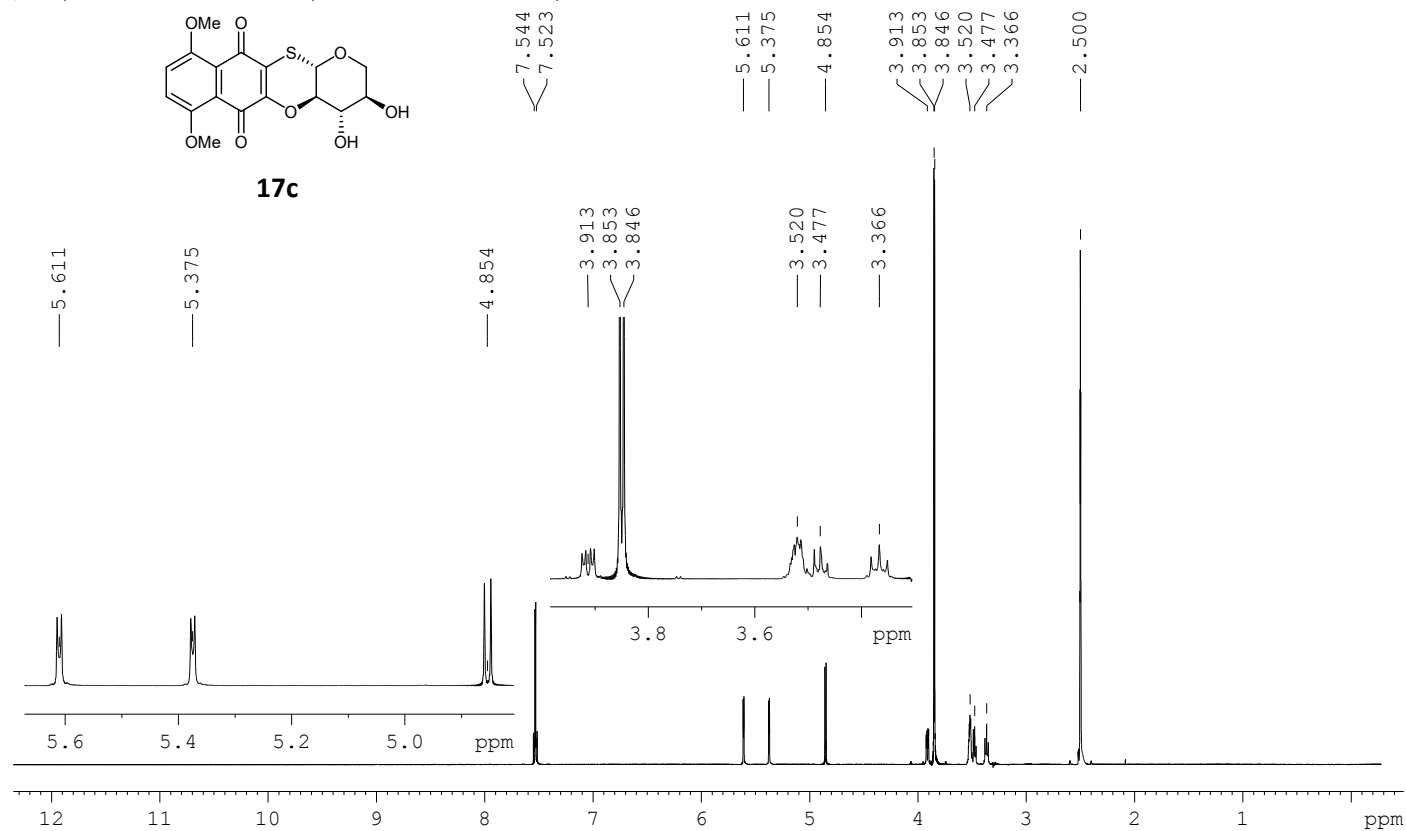
(2*R*,3*S*,4*S*,4*aR*,12*aS*)-3,4-Dihydroxy-2-hydroxymethyl-7,10-dimethoxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**17a**), (¹H NMR - 700 MHz, ¹³C NMR - 176 MHz, solvent - DMSO-*d*₆)



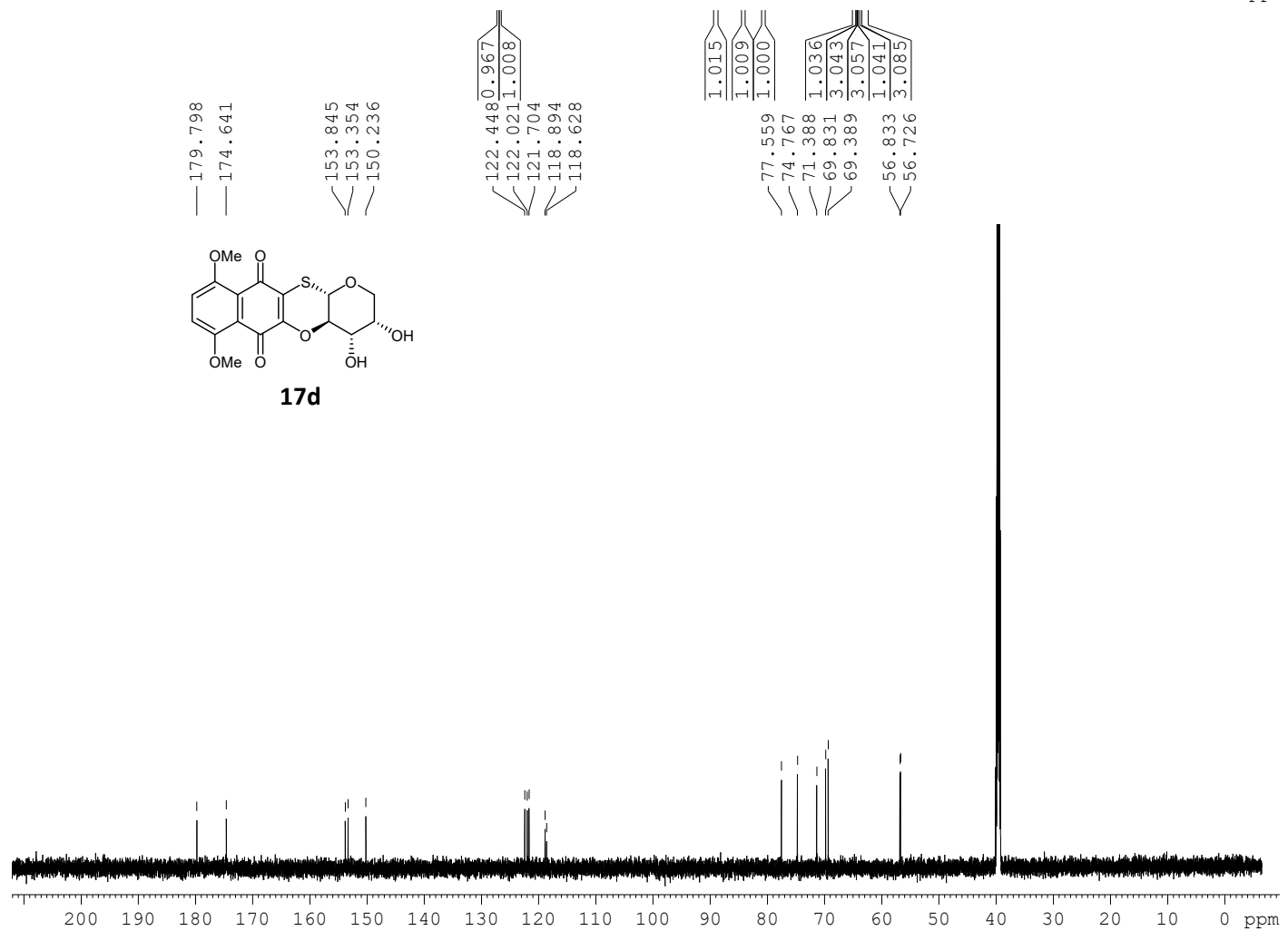
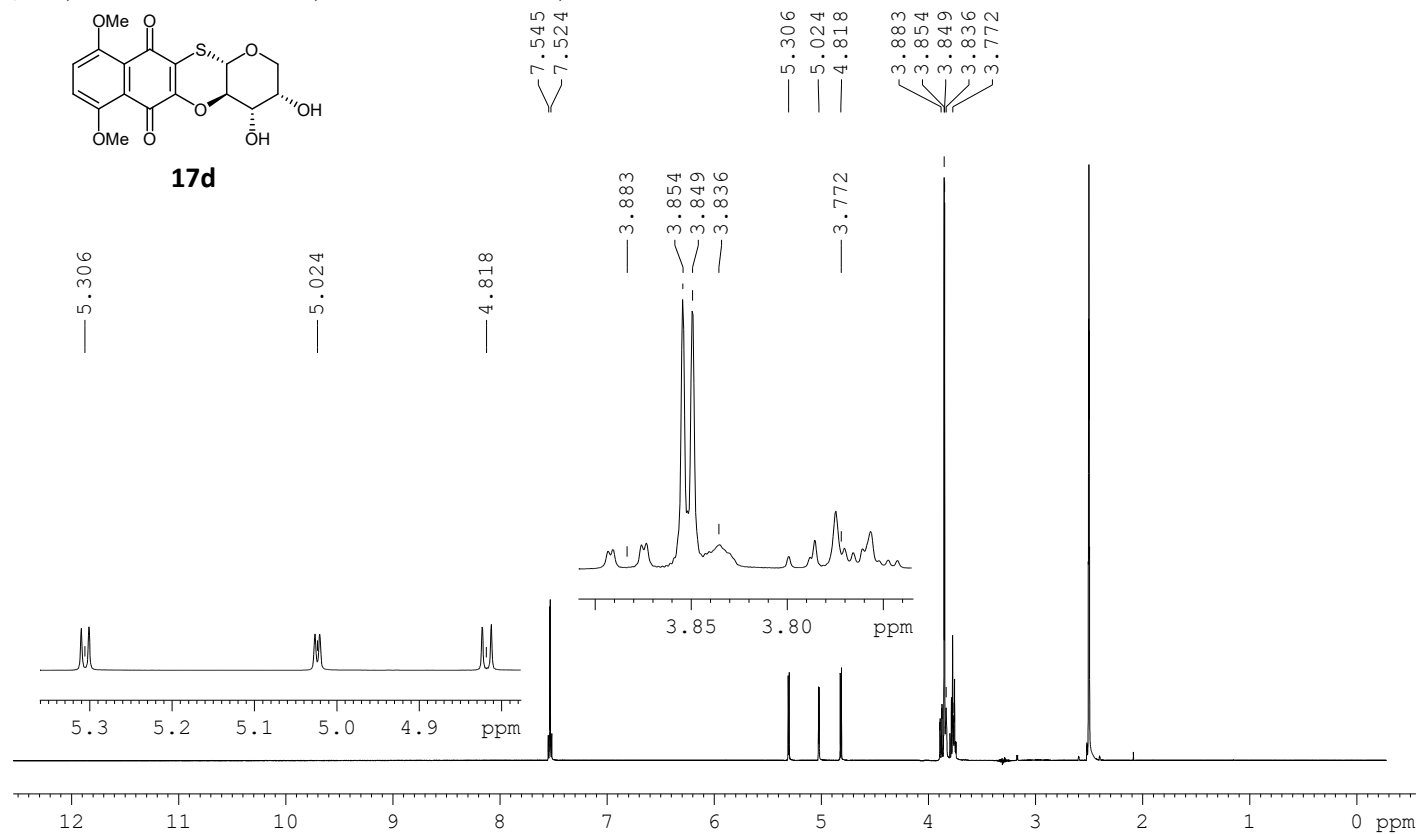
(2*R*,3*R*,4*S*,4*aR*,12*aS*)-3,4-Dihydroxy-2-hydroxymethyl-7,10-dimethoxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**17b**), (¹H NMR - 500 MHz, ¹³C NMR - 125 MHz, solvent - DMSO-*d*₆)



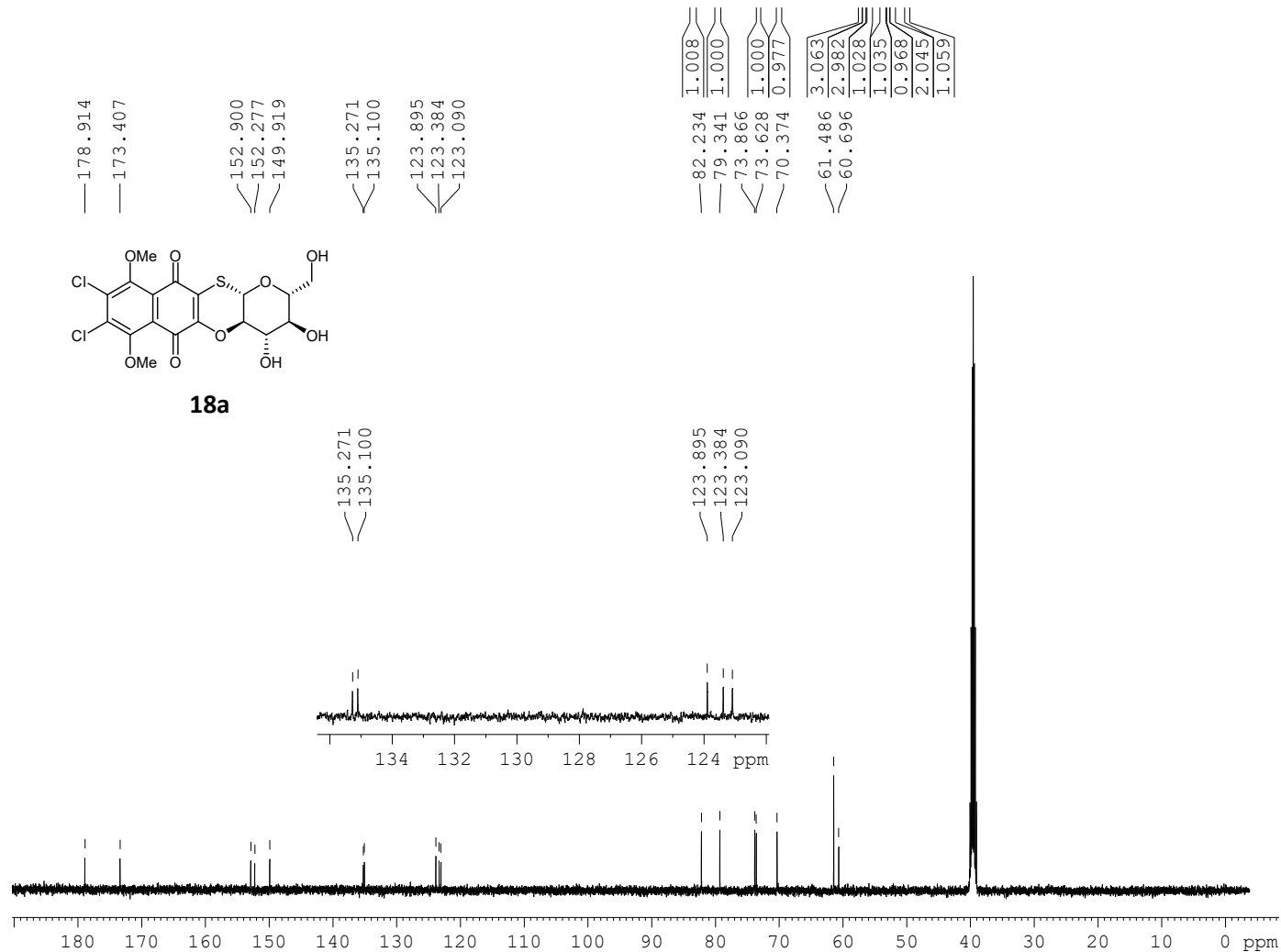
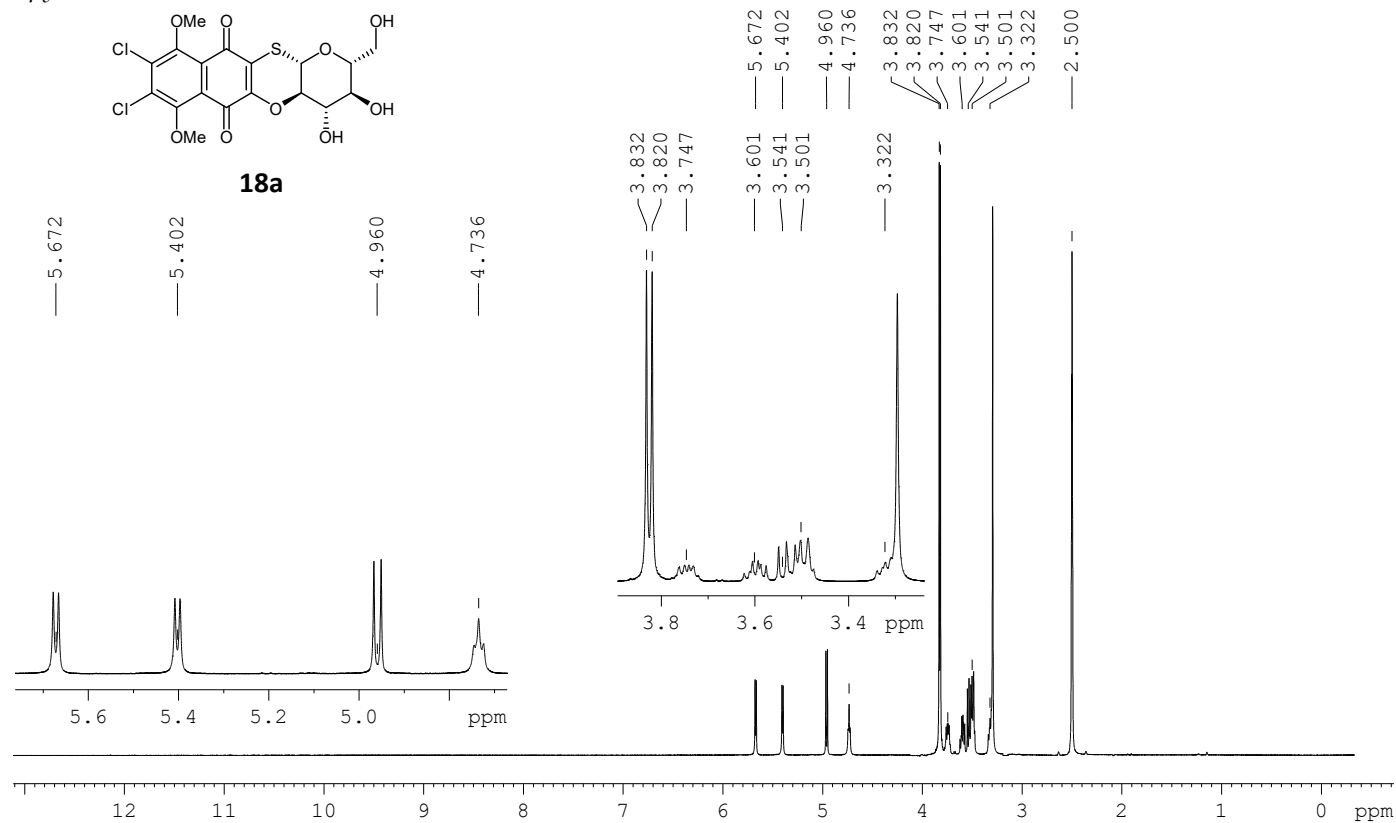
(3*R*,4*S*,4*aR*,12*aS*)-3,4-Dihydroxy-7,10-dimethoxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**17c**), (¹H NMR - 700 MHz, ¹³C NMR - 176 MHz, solvent - DMSO-*d*₆)



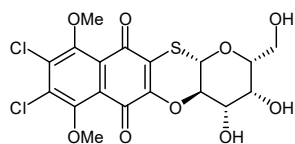
(3*S*,4*S*,4*aR*,12*aS*)-3,4-Dihydroxy-7,10-dimethoxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione
(17d), (¹H NMR - 700 MHz, ¹³C NMR - 176 MHz, solvent - DMSO-*d*₆)



(2*R*,3*S*,4*S*,4*aR*,12*aS*)-8,9-Dichloro-3,4-dihydroxy-2-hydroxymethyl-7,10-dimethoxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**18a**), (¹H NMR - 500 MHz, ¹³C NMR - 125 MHz, solvent - DMSO-*d*₆)

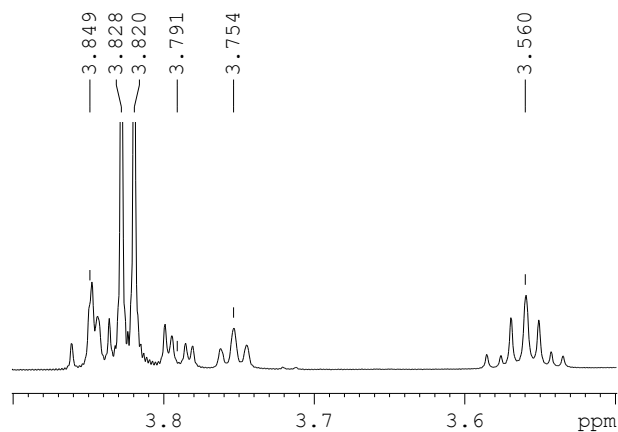


(2R,3R,4S,4aR,12aS)-8,9-Dichloro-3,4-dihydroxy-2-(hydroxymethyl)-7,10-dimethoxy-3,4,4a,12a-tetrahydro-2H-naphtho[2,3-b]pyrano[2,3-e][1,4]oxathiine-6,11-dione (**18b**), (¹H NMR - 700 MHz, ¹³C NMR - 176 MHz, solvent - DMSO-d₆)



18b

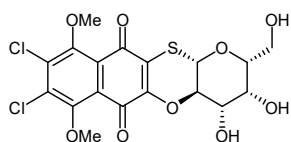
— 5.401
 — 4.925
 — 4.803
 — 3.849
 — 3.828
 — 3.820
 — 3.791
 — 3.754
 — 3.560
 — 2.500



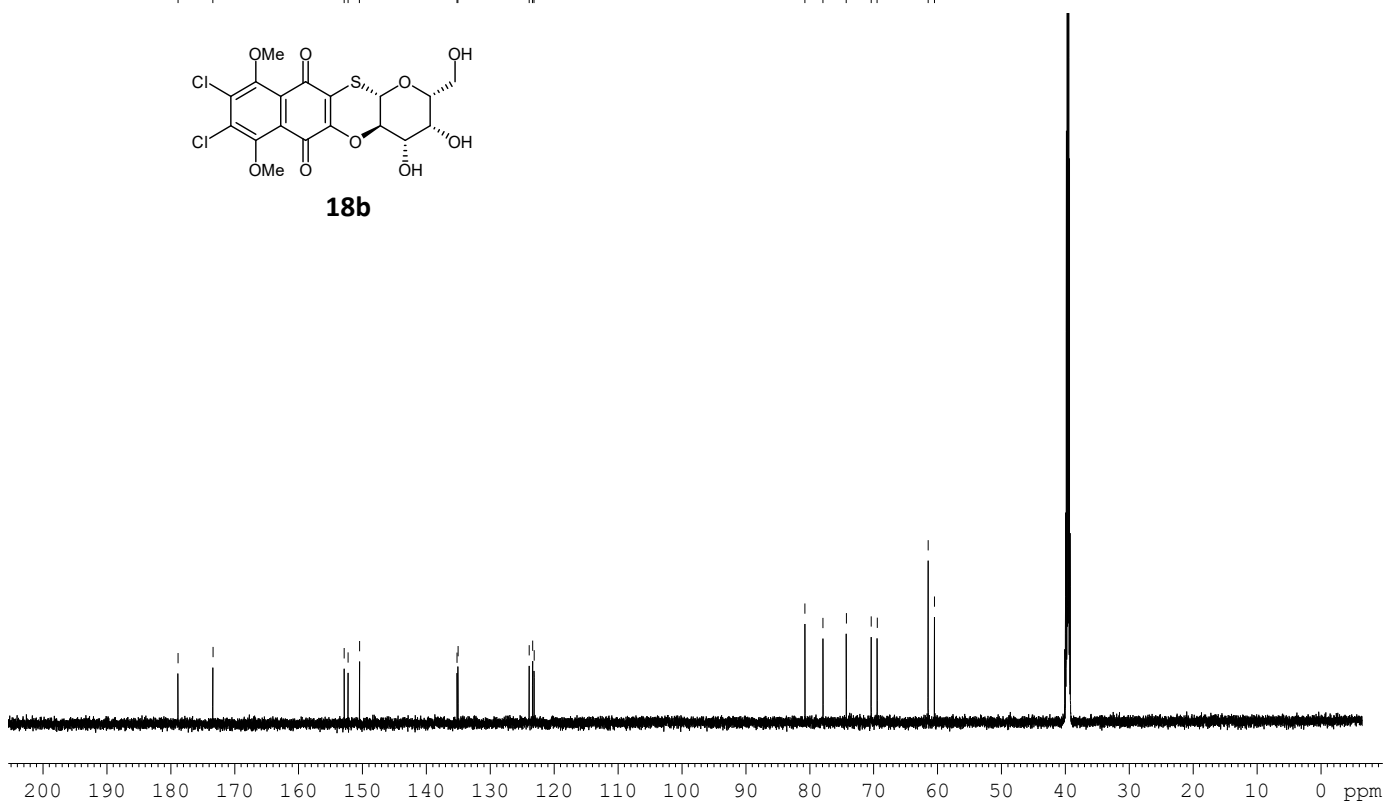
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

— 178.872
 — 173.414
 — 152.877
 — 152.272
 — 150.473
 — 135.215
 — 135.071
 — 123.920
 — 123.391
 — 123.157

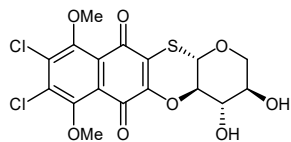
— 1.027
 — 1.000
 — 1.950
 — 2.029
 — 3.035
 — 3.033
 — 1.032
 — 0.999
 — 2.043



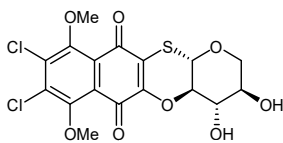
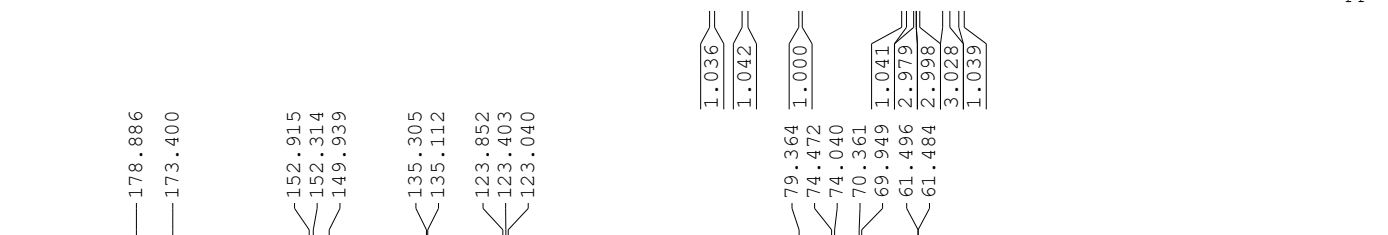
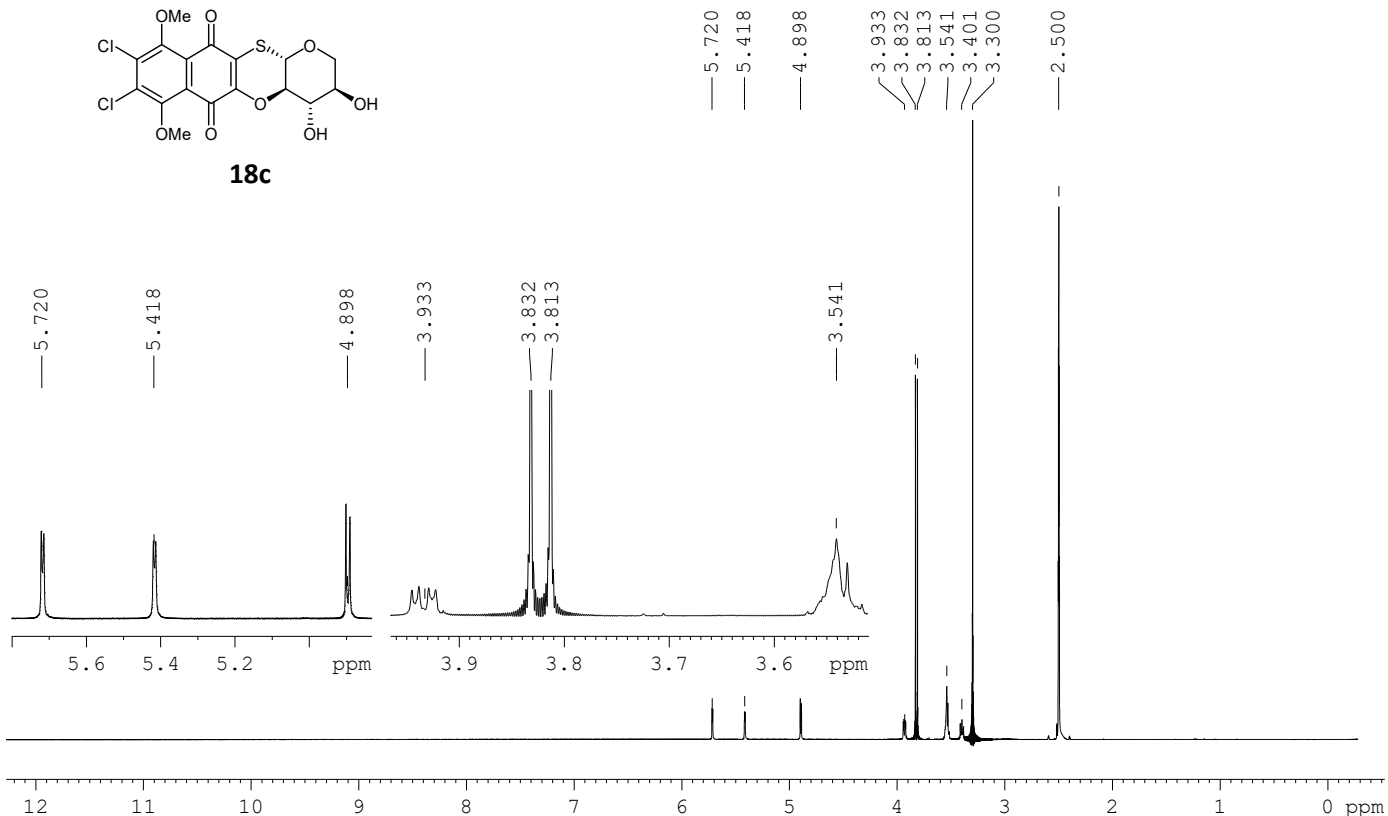
18b



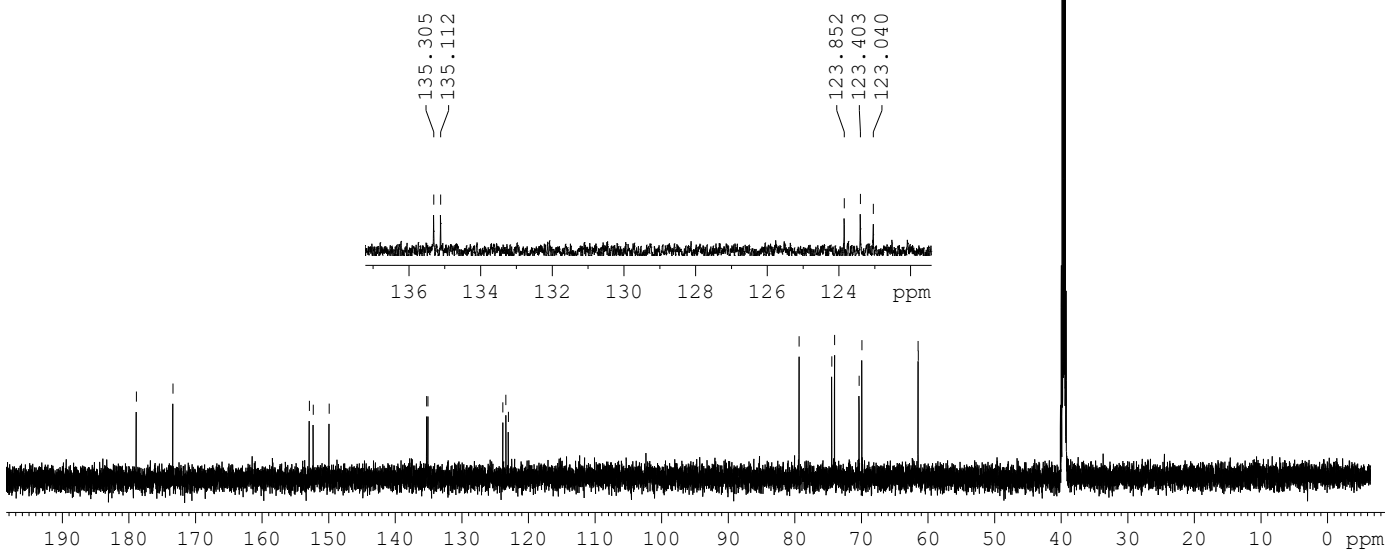
(3*R*,4*S*,4*aR*,12*aS*)-8,9-Dichloro-3,4-dihydroxy-7,10-dimethoxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**18c**), (¹H NMR - 700 MHz, ¹³C NMR - 176 MHz, solvent - DMSO-*d*₆)



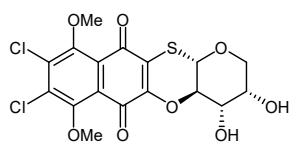
18c



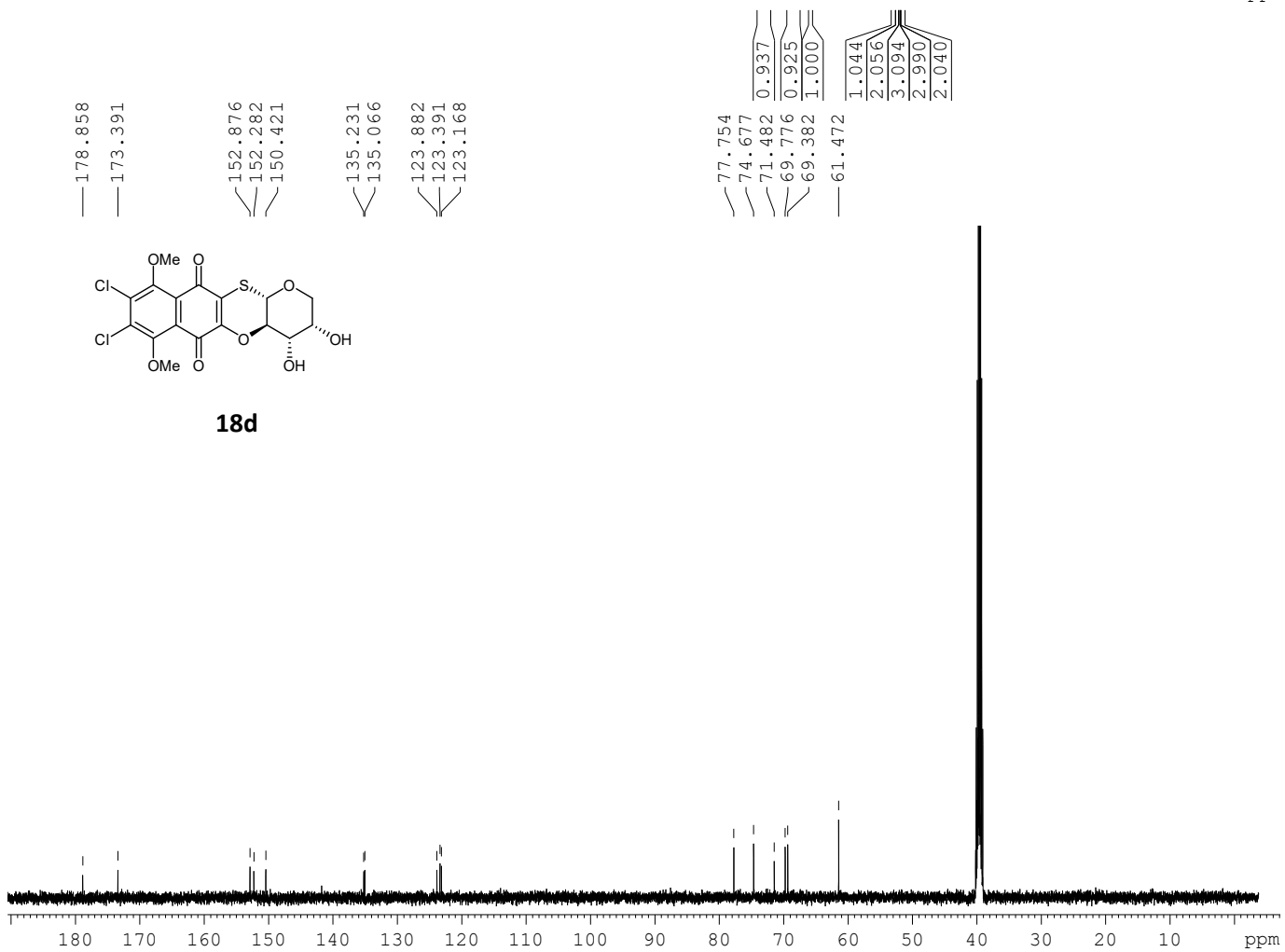
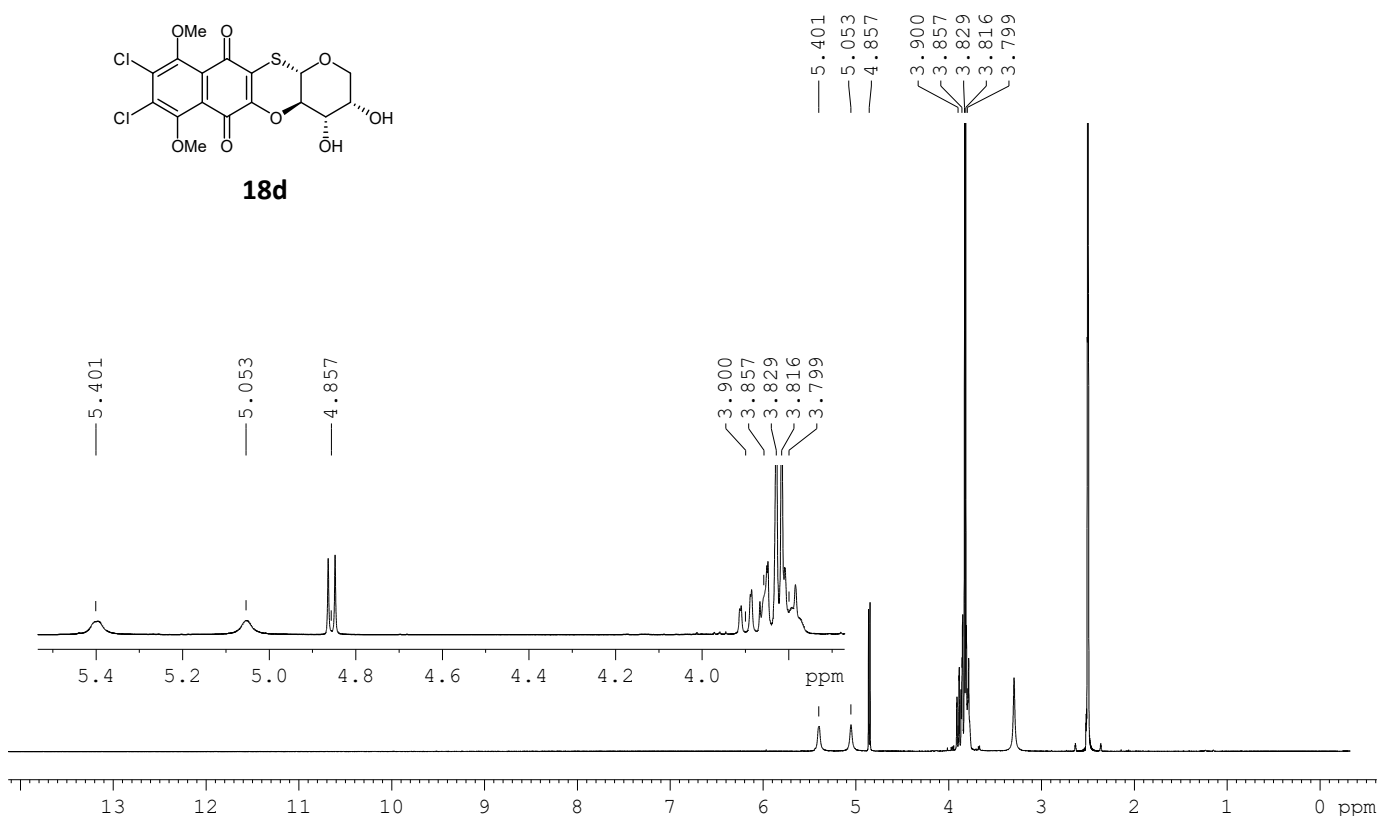
18c



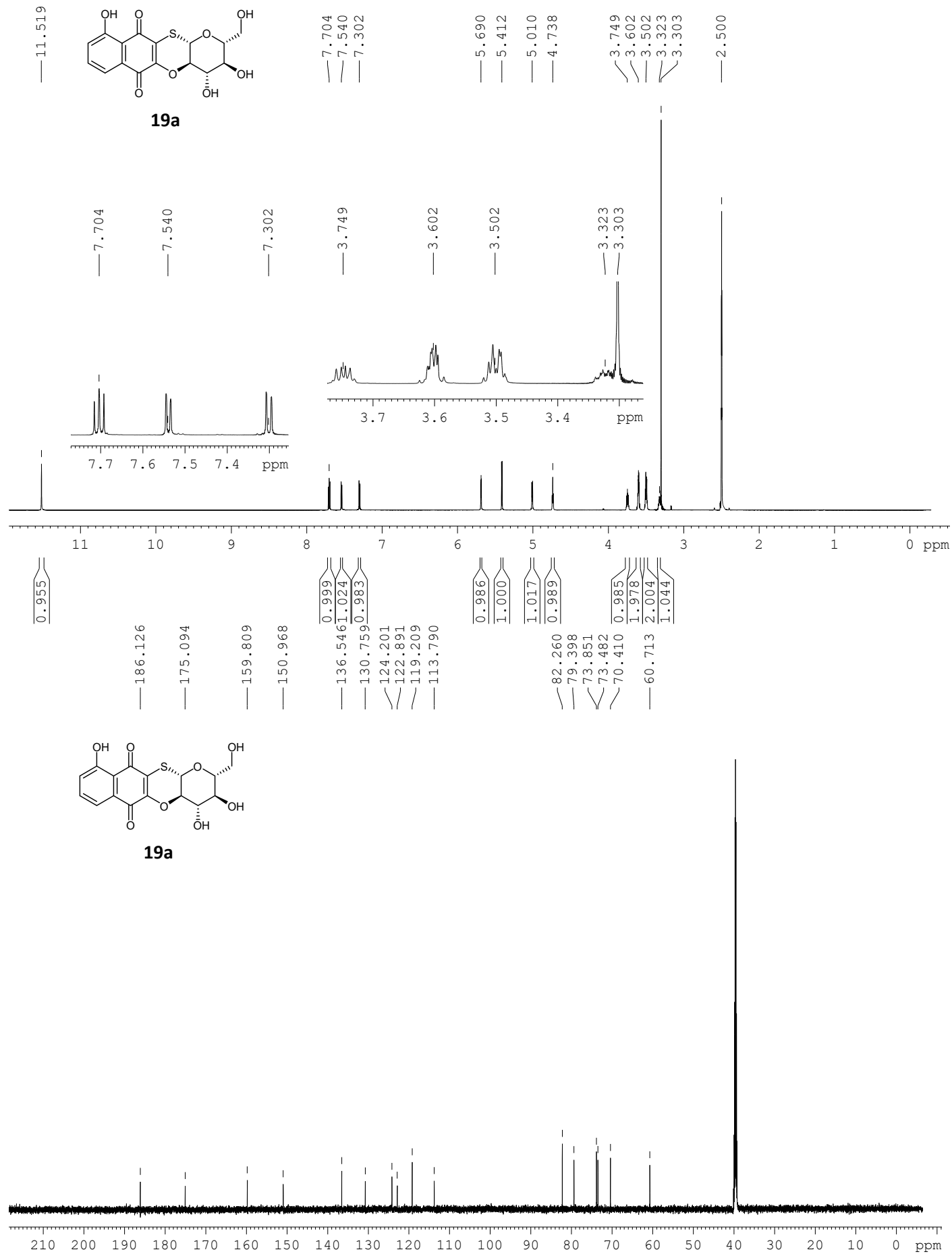
(3*S*,4*S*,4*aR*,12*aS*)-8,9-Dichloro-3,4-dihydroxy-7,10-dimethoxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**18d**), (¹H NMR - 500 MHz, ¹³C NMR - 125 MHz, solvent - DMSO-*d*₆)



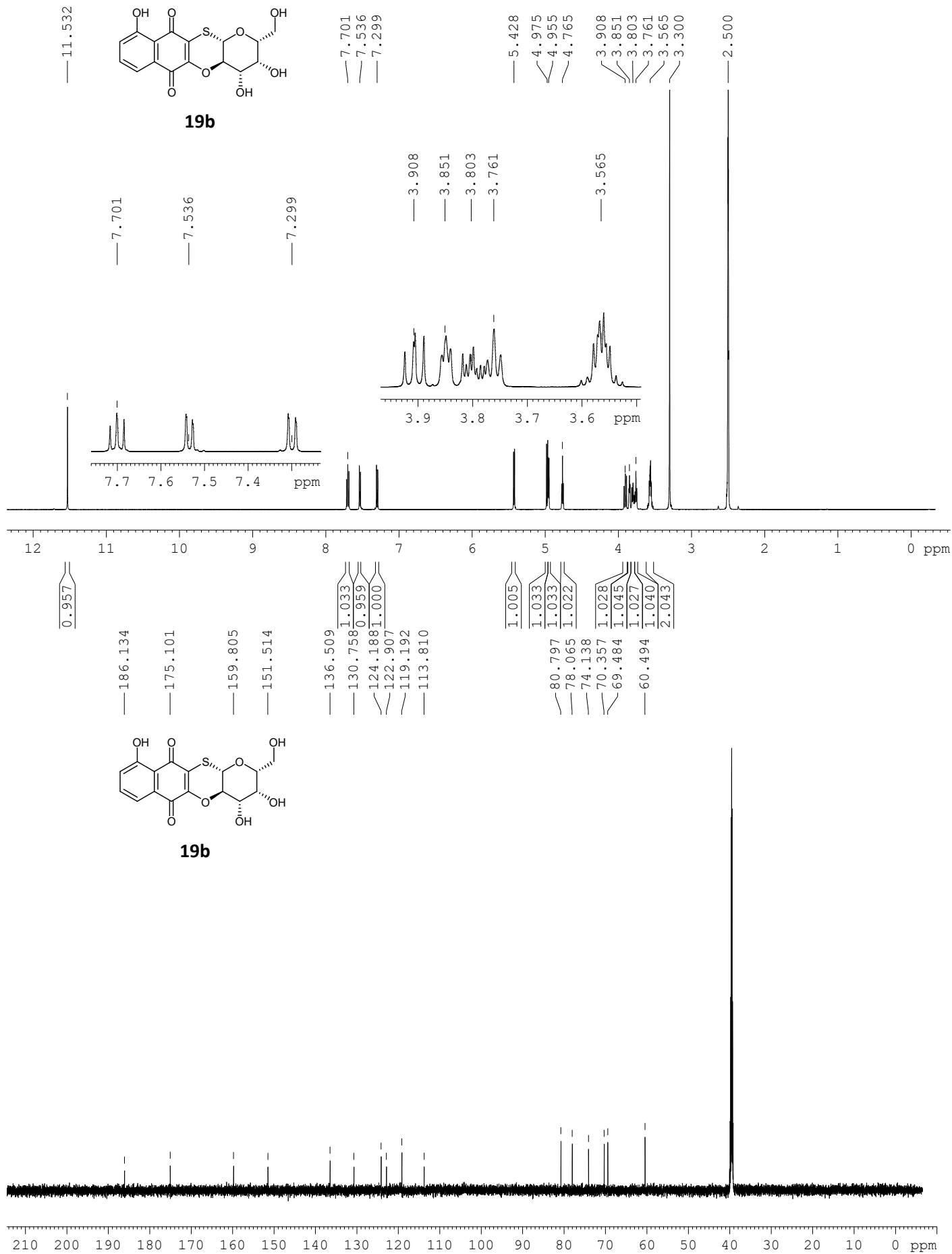
18d



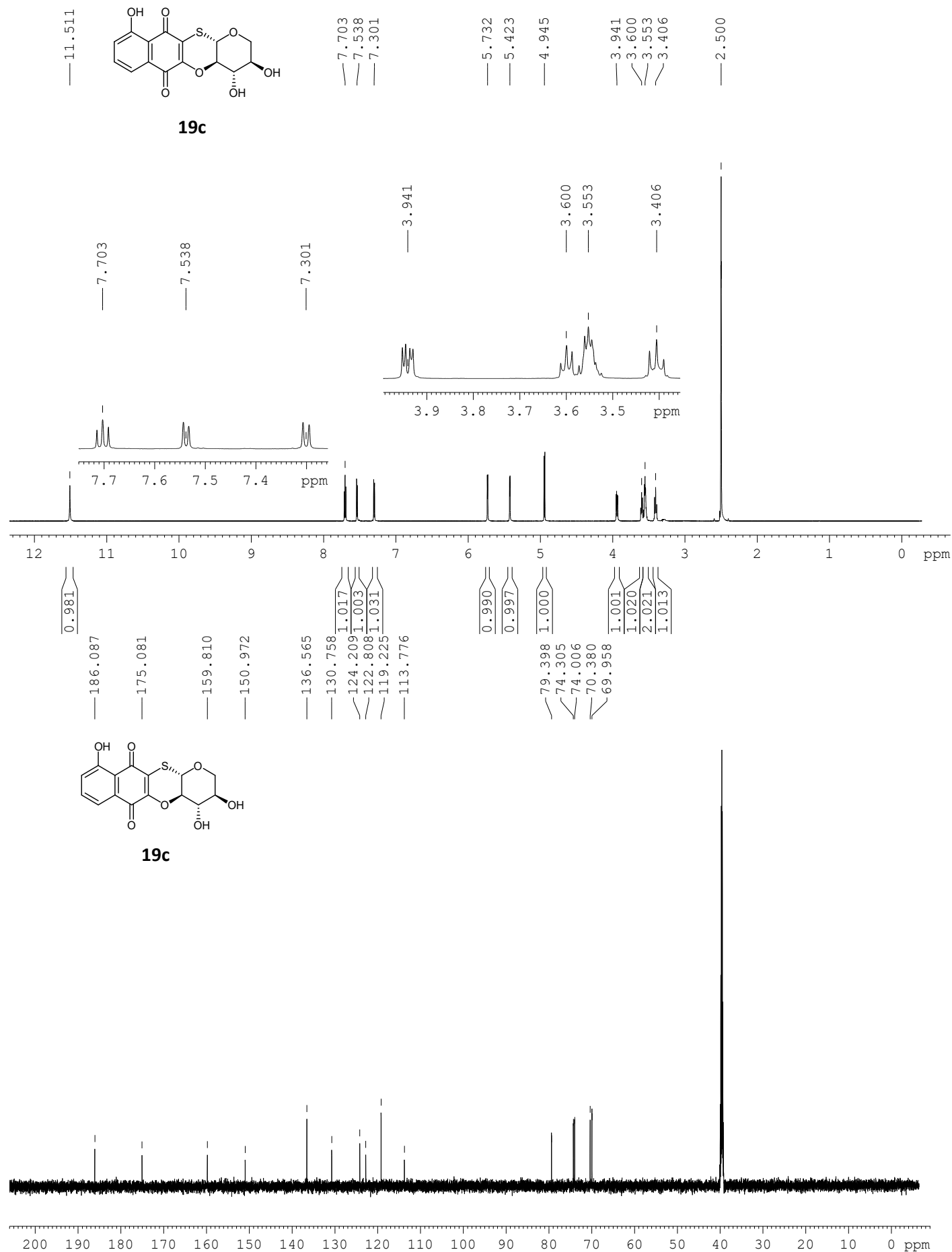
(2*R*,3*S*,4*S*,4*aR*,12*aS*)-3,4,10-Trihydroxy-2-hydroxymethyl-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**19a**), (¹H NMR - 700 MHz, ¹³C NMR - 176 MHz, solvent - DMSO-*d*₆)



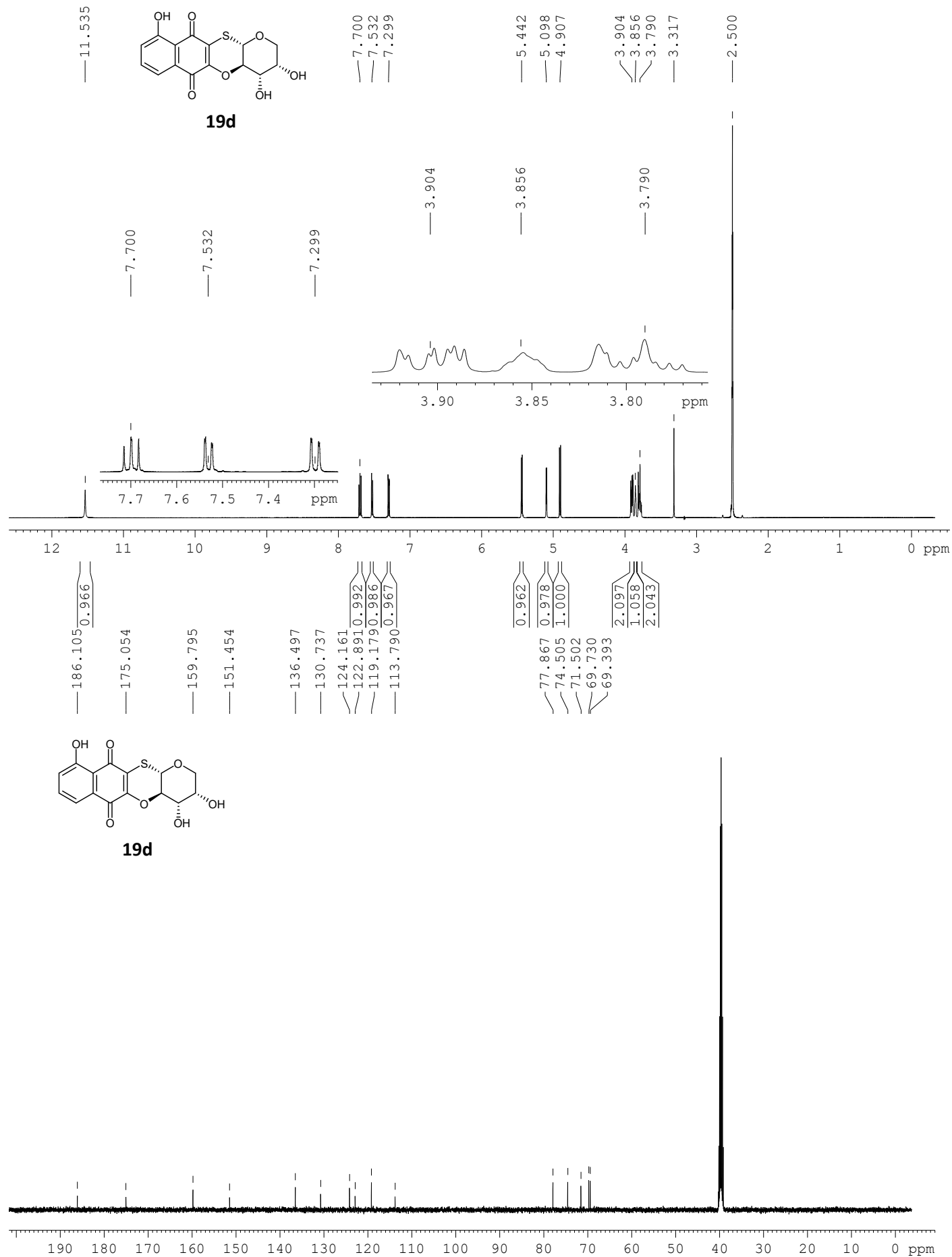
(2R,3R,4S,4aR,12aS)-3,4,10-Trihydroxy-2-hydroxymethyl-3,4,4a,12a-tetrahydro-2H-naphtho[2,3-b]pyrano-[2,3-e][1,4]oxathiine-6,11-dione (**19b**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



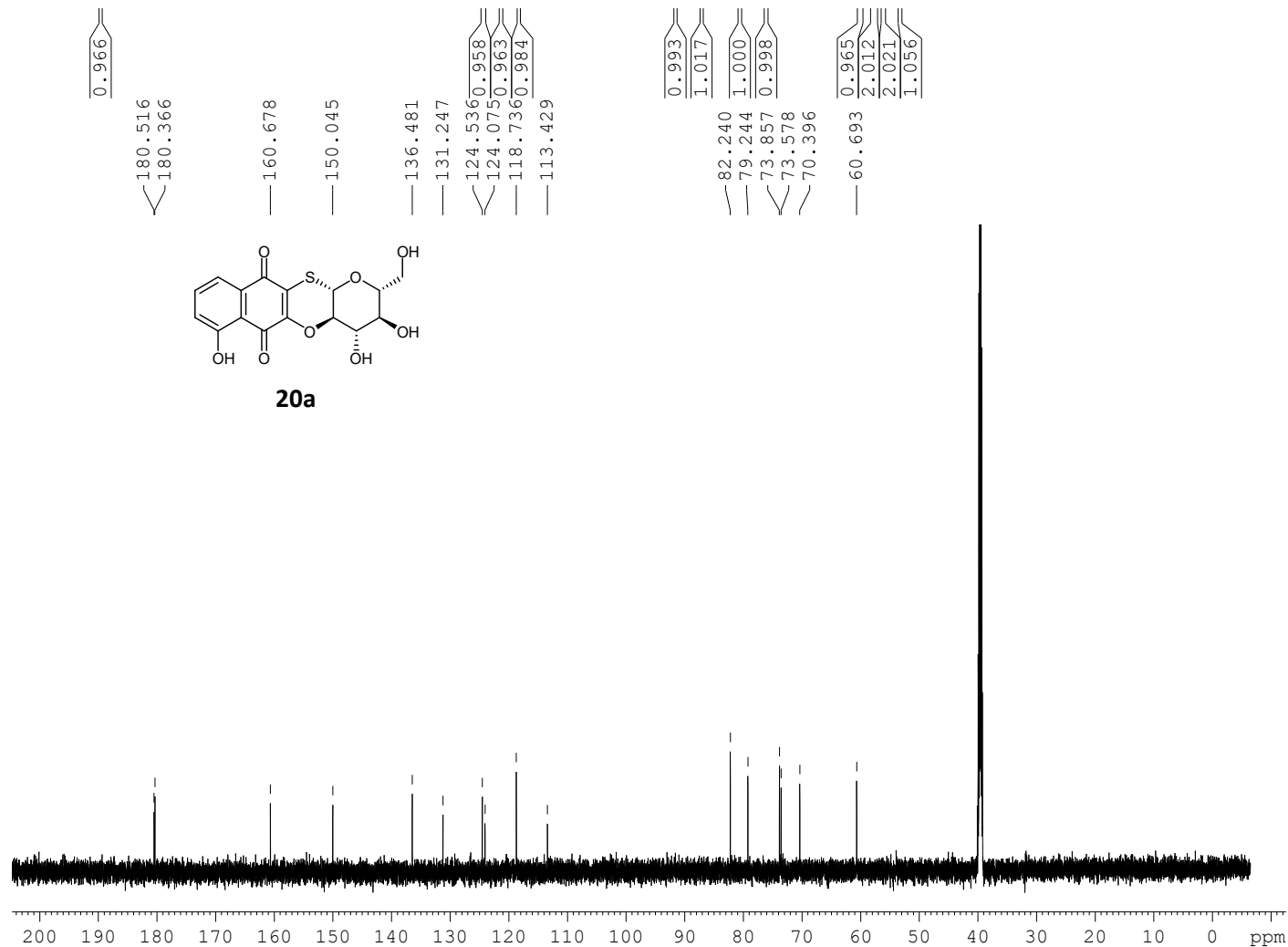
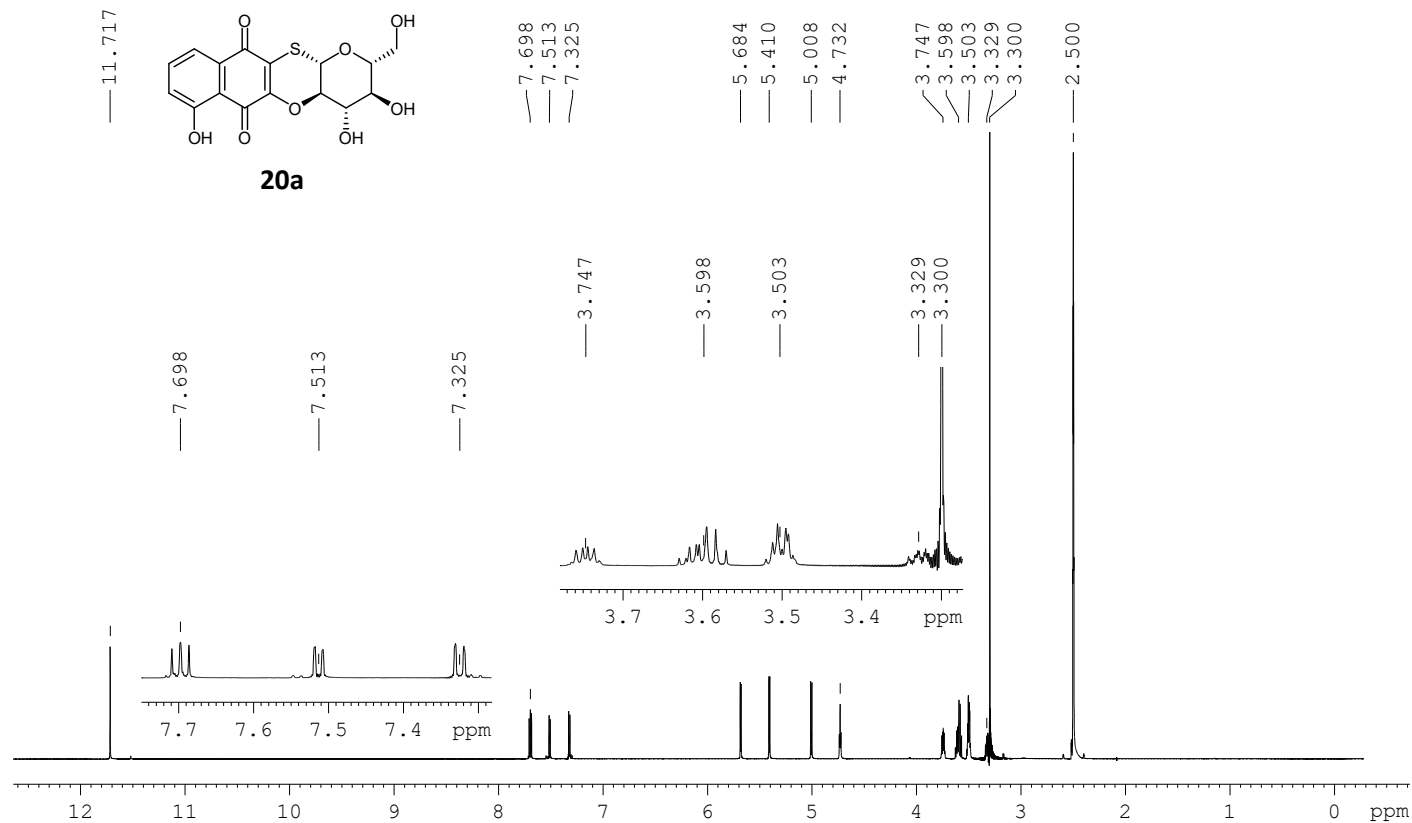
(3*R*,4*S*,4*aR*,12*aS*)-3,4,10-Trihydroxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**19c**), (¹H NMR - 700 MHz, ¹³C NMR - 176 MHz, solvent - DMSO-*d*₆)



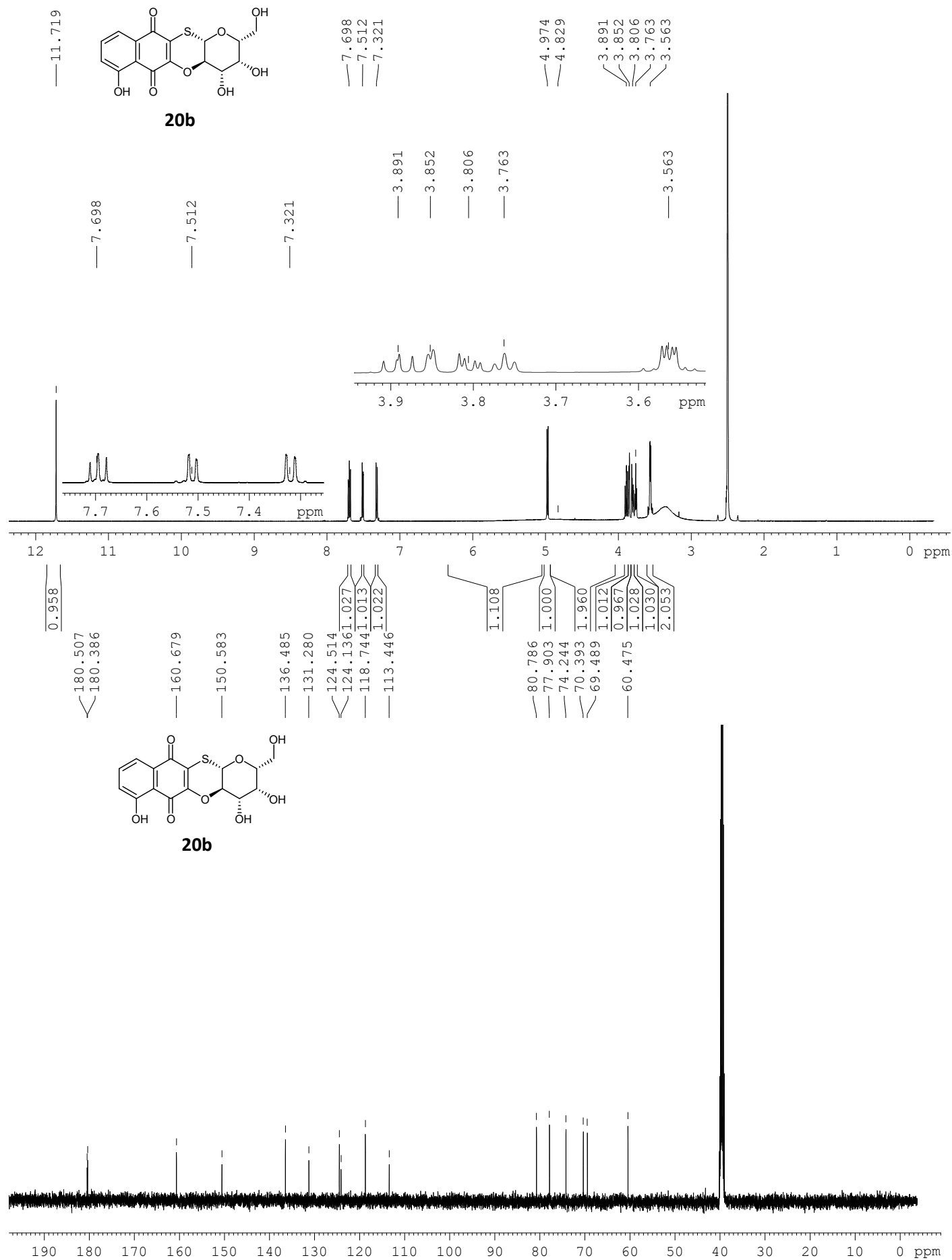
(3*S*,4*S*,4*aR*,12*aS*)-3,4,10-Trihydroxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**19d**), (¹H NMR - 500 MHz, ¹³C NMR - 125 MHz, solvent - DMSO-*d*₆)



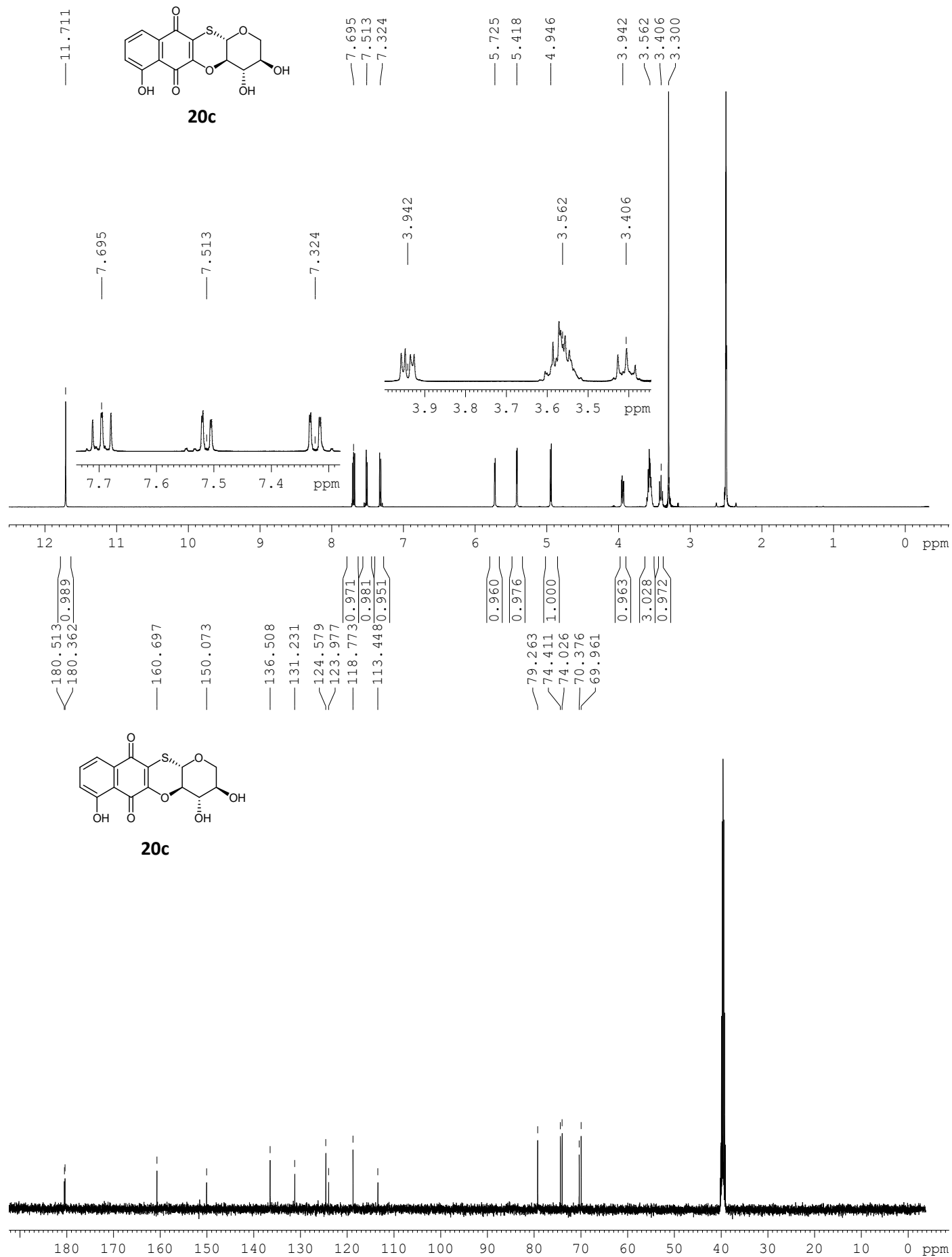
(2*R*,3*S*,4*S*,4*aR*,12*aS*)-3,4,7-Trihydroxy-2-(hydroxymethyl)-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano-[2,3-*e*][1,4]oxathiine-6,11-dione (**20a**), (¹H NMR - 700 MHz, ¹³C NMR - 176 MHz, solvent - DMSO-*d*₆)



(2R,3R,4S,4aR,12aS)-3,4,7-Trihydroxy-2-hydroxymethyl-3,4,4a,12a-tetrahydro-2H-naphtho[2,3-b]pyrano[2,3-e][1,4]oxathine-6,11-dione (**20b**), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



(3*R*,4*S*,4*aR*,12*aS*)-3,4,7-Trihydroxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**20c**), (¹H NMR - 500 MHz, ¹³C NMR - 125 MHz, solvent - DMSO-*d*₆)



(3*S*,4*S*,4*a**R*,12*a**S*)-3,4,7-Trihydroxy-3,4,4*a*,12*a*-tetrahydro-2*H*-naphtho[2,3-*b*]pyrano[2,3-*e*][1,4]oxathiine-6,11-dione (**20d**), (¹H NMR - 500 MHz, ¹³C NMR - 125 MHz, solvent - DMSO-*d*₆)

