Supplementary Material

Synthesis and anticancer activity evaluation of some new 1,2,3,5-tetrazine derivatives attached to benzothiazole moiety

Joseph Tsemeugne[a]*, Yetiny A. Bah[a], Jean P. Dzoyem[b,c], Jérôme N. Ndefongang[a], Ibukun M. Famuyide[c], Lyndy J. McGaw[c], Pamela K. Nangmo[a], Blandine M. W. Ouahouo[a], Pierre Mkounga[a], Giles Edwards[d], Peter F. W. Simon[e], Apollinaire Tsopmo[f], Emmanuel F. Sopbué[b]*, and Augustin E. Nkengfack[a]

[a]Univ. of Yaounde I, P.O. Box 812 Yaounde, Cameroon; [b]Univ. of Dschang, PO Box 67 Dschang, Cameroon; [c]Univ. of Pretoria, Private Bag X04, Onderstepoort 0110, Pretoria, South Africa; [d]The Univ. of Manchester; Oxford Road; Manchester; M13 9PL; United Kingdom; [e]Rhein-Waal Univ. of Applied Sciences, Marie-Curie Straße 1, 47533 Kleve, Germany; [f]Carleton Univ. 1125 Colonel By DriveK1S 5B6, Ottawa, Canada
Email: tsemeugne@yahoo.fr; sopbue@yahoo.fr

Table of Contents

Figure 1. UV spectrum of compound **4a** in methanol as solvent S3
Figure 2. IR spectrum of compound **4a**.....S3
Figure 3. ^{1}H-NMR (DMSO-d$_6$, 400 MHz) spectrum of compound **4a**.....S4
Figure 4. ^{13}C(H)-NMR ^{1}H (DMSO-d_6, 100 MHz) of compound **4a**.....S4
Figure 5. HRMS ESI-Positive mode of compound **4a**.....S5
Figure 6. UV spectrum of compound **4a'** in methanol as solvent.....S5
Figure 7. IR spectrum of compound **4a'**.....S6
Figure 8. ^{1}H-NMR (DMSO-d_6, 400 MHz) spectrum of compound **4a'** and expanded ^{1}H-NMR spectrum S7
Figure 9. ^{13}C(H)-NMR ^{1}H (DMSO-d_6, 100 MHz) of compound **4a**' and expanded ^{13}C spectrum S9
Figure 10. HRMS ESI-Positive mode of compound **4a'**.....S9
Figure 11. UV spectrum of compound **4b** in methanol as solvent.....S10
Figure 12. IR spectrum of compound **4b**.....S10
Figure 13. ^{1}H-NMR (DMSO-d_6, 400 MHz) spectrum of compound **4b**.....S11
Figure 14. ^{13}C(H)-NMR ^{1}H (DMSO-d_6, 100 MHz) of compound **4b**.....S11
Figure 15. HRMS ESI-Positive mode of compound **4b**.....S12
Figure 16. UV spectrum of compound **4c** in methanol as solvent.....S12
Figure 17. IR spectrum of compound **4c**.....S13
Figure 18. ^{1}H-NMR (DMSO-d_6, 400 MHz) spectrum of compound **4c**.....S13
Figure 19. ^{13}C(H)-NMR ^{1}H (DMSO-d_6, 100 MHz) of compound **4c**.....S14
Figure 20. DEPT-135 ^{13}C(H)-NMR ^{1}H (DMSO-d_6, 100 MHz) spectrum of compound **4c** S14
Figure 21. HSQC (DMSO-d_6, 100MHz spectrum of compound **4c** S15
Figure 22. HMBC (DMSO-d_6, 100MHz spectrum of compound **4c** S15
Figure 23. COSY ^{1}H-^{1}H (DMSO-d_6, 100MHz spectrum of compound **4c** S16
Figure 24. NOESY (DMSO-d_6, 100MHz spectrum of compound **4c** S16
Figure 25. HRMS ESI-Positive mode of compound **4c**.....S17
Figure 26. UV spectrum of compound **4c'** in methanol as solvent.....S18
Figure 27. IR spectrum of compound **4c'**.....S18

 ©AUTHOR(S)

Figure 28. ^{1}H-NMR (DMSO-d_6, 400 MHz) spectrum of compound **4c'**…… S19
Figure 29. ^{13}C(H)-NMR ^{1}H (DMSO-d_6, 100 MHz) of compound **4c'**……S19
Figure 30. DEPT-135 ^{13}C(H)-NMR ^{1}H (DMSO-d_6, 100MHz spectrum of compound **4c'**.....S20
Figure 31. HSQC (DMSO-d_6, 100MHz spectrum of compound **4c'** S20
Figure 32. HRMS ESI-Positive mode of compound **4c'**……S21

 ©AUTHOR(S)

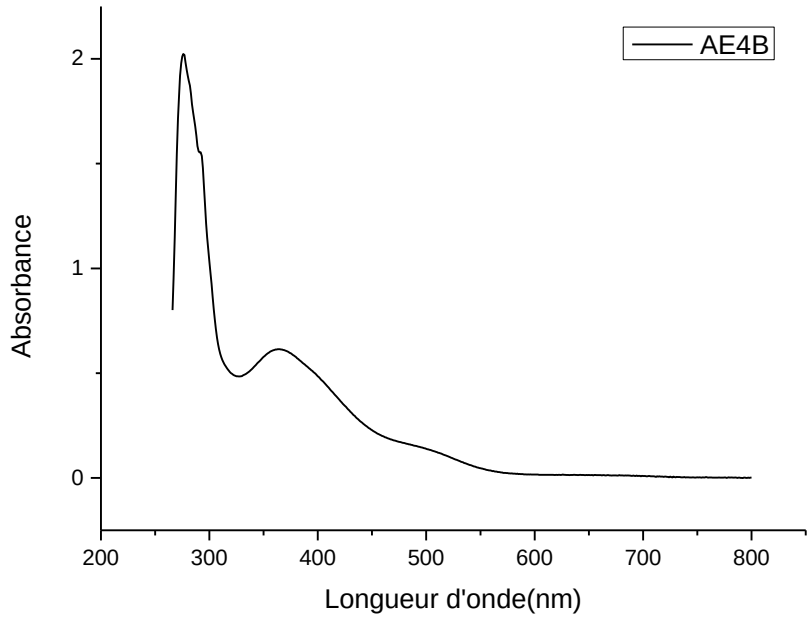


Figure 1. UV spectrum of compound **4a** in methanol as solvent.

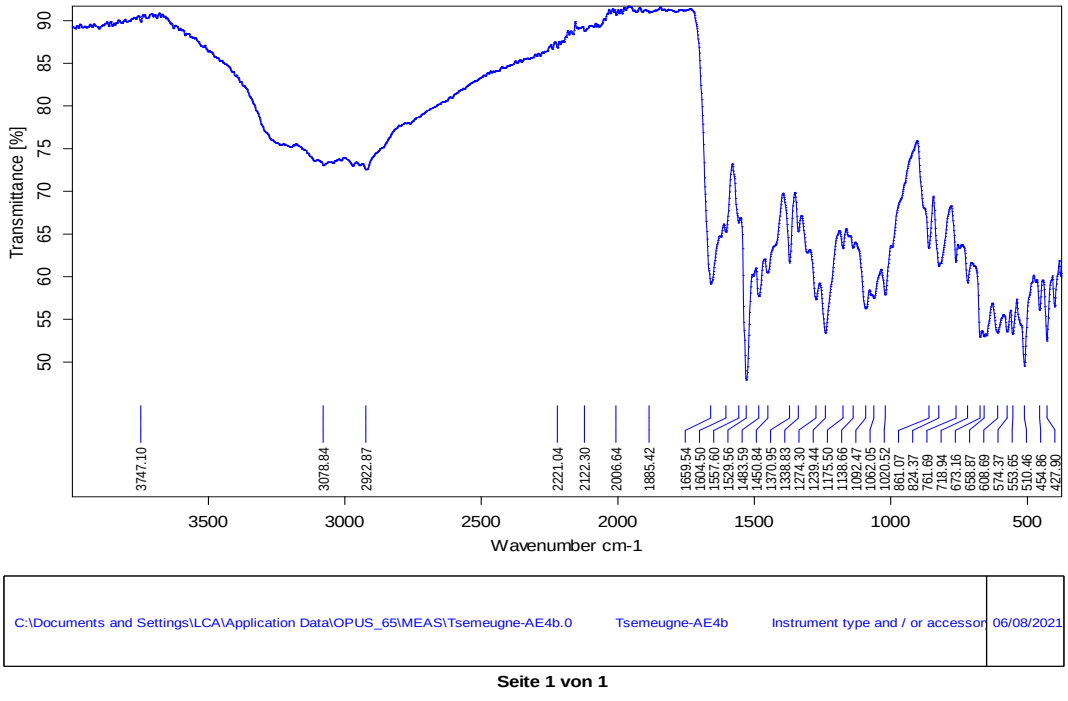


Figure 2. IR spectrum of compound **4a.**

©AUTHOR(S)

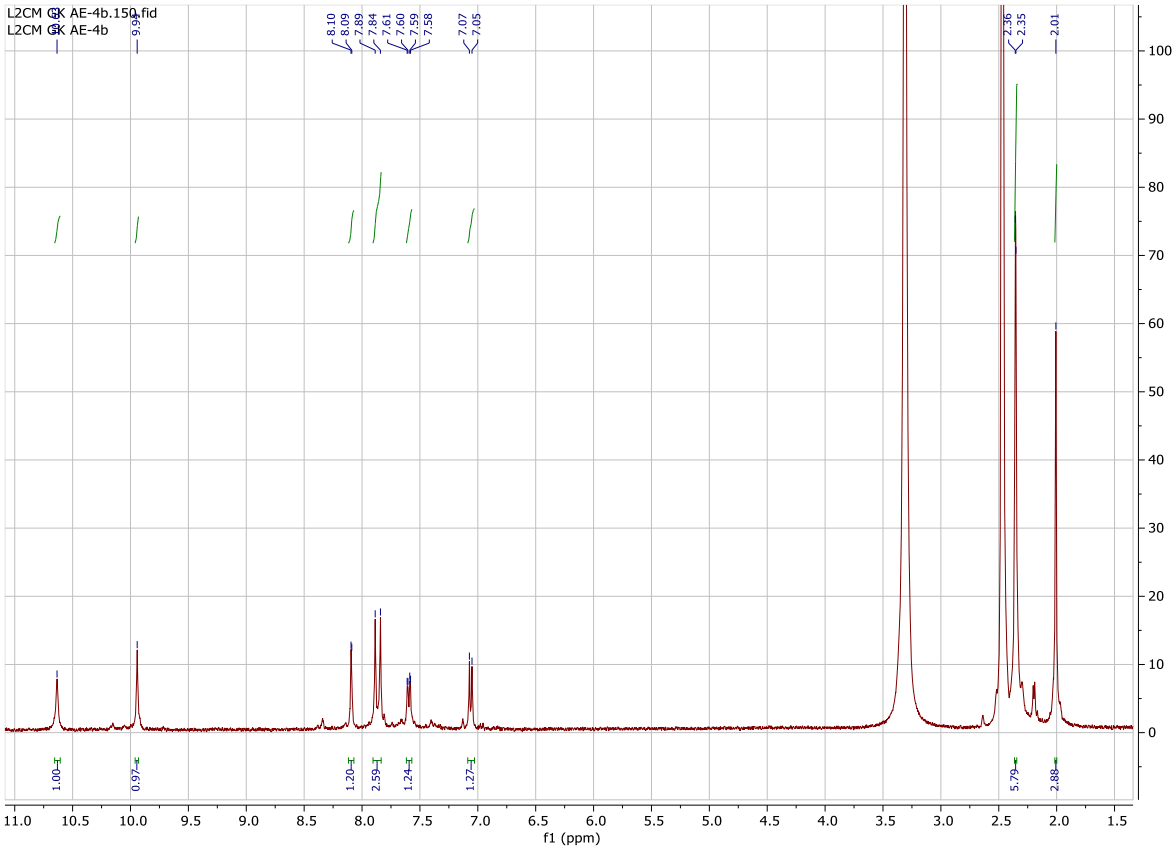


Figure 3 . ^{1}H-NMR (DMSO-d$_6$, 400 MHz) spectrum of compound **4a.**

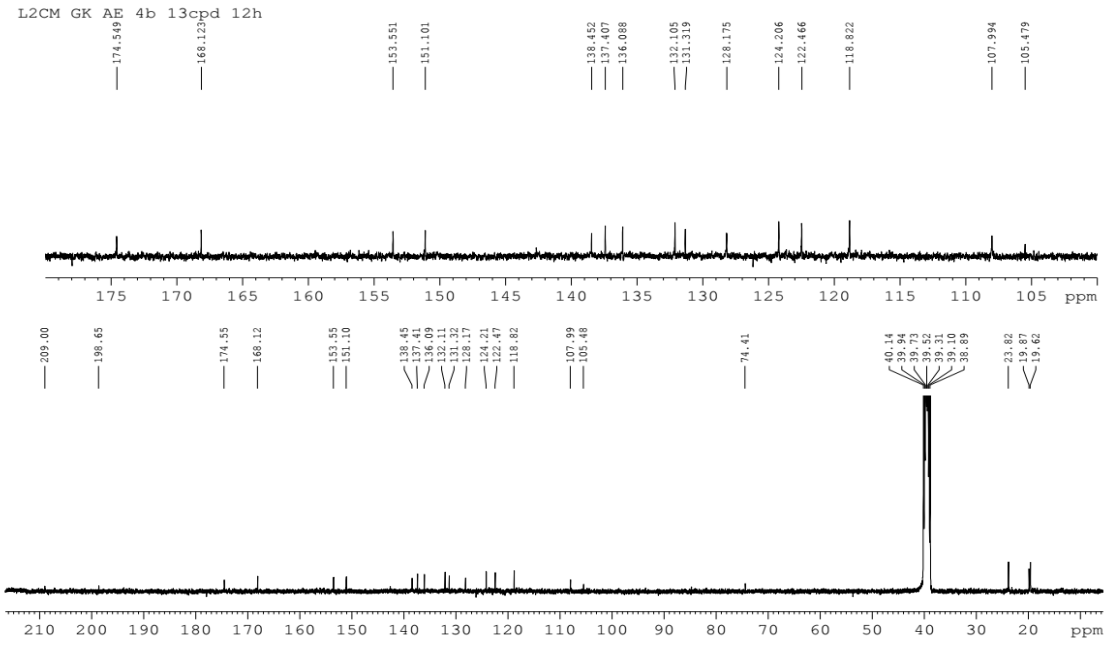


Figure 4. ^{13}C(H)-NMR ^{1}H (DMSO-d$_6$, 100 MHz) of compound **4a.**

©AUTHOR(S)

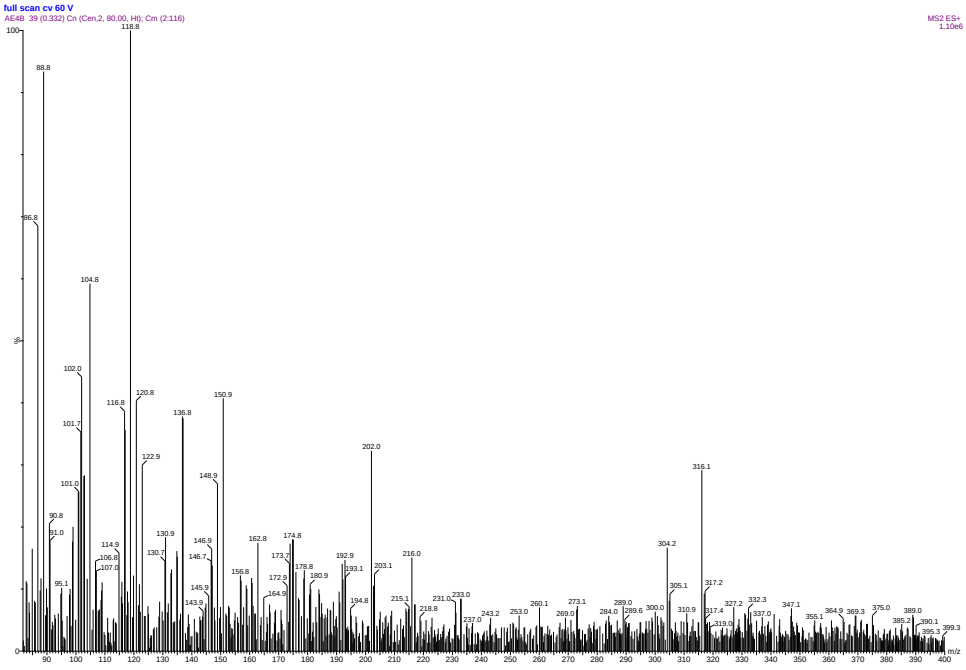


Figure 5. HRMS ESI-Positive mode of compound **4a.**

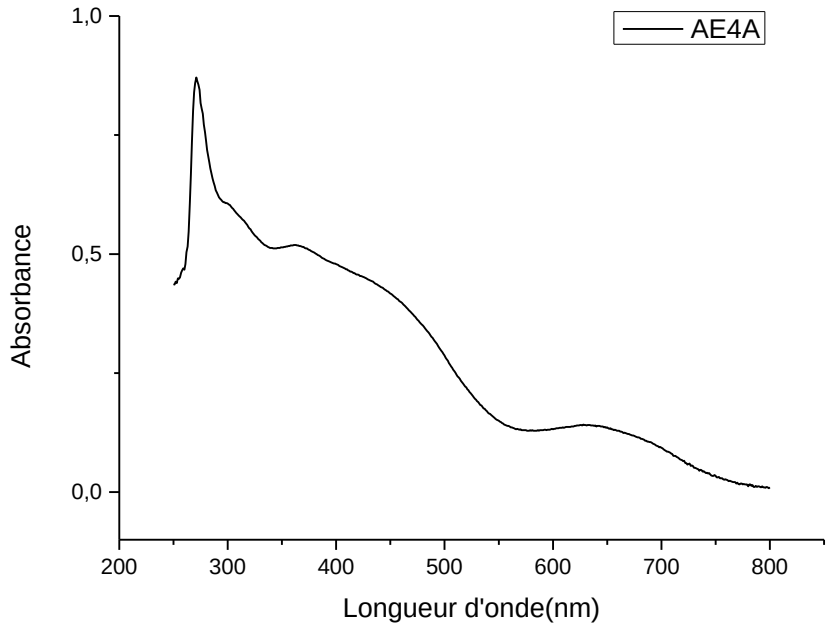


Figure 6. UV spectrum of compound **4a'** in methanol as solvent.

©AUTHOR(S)

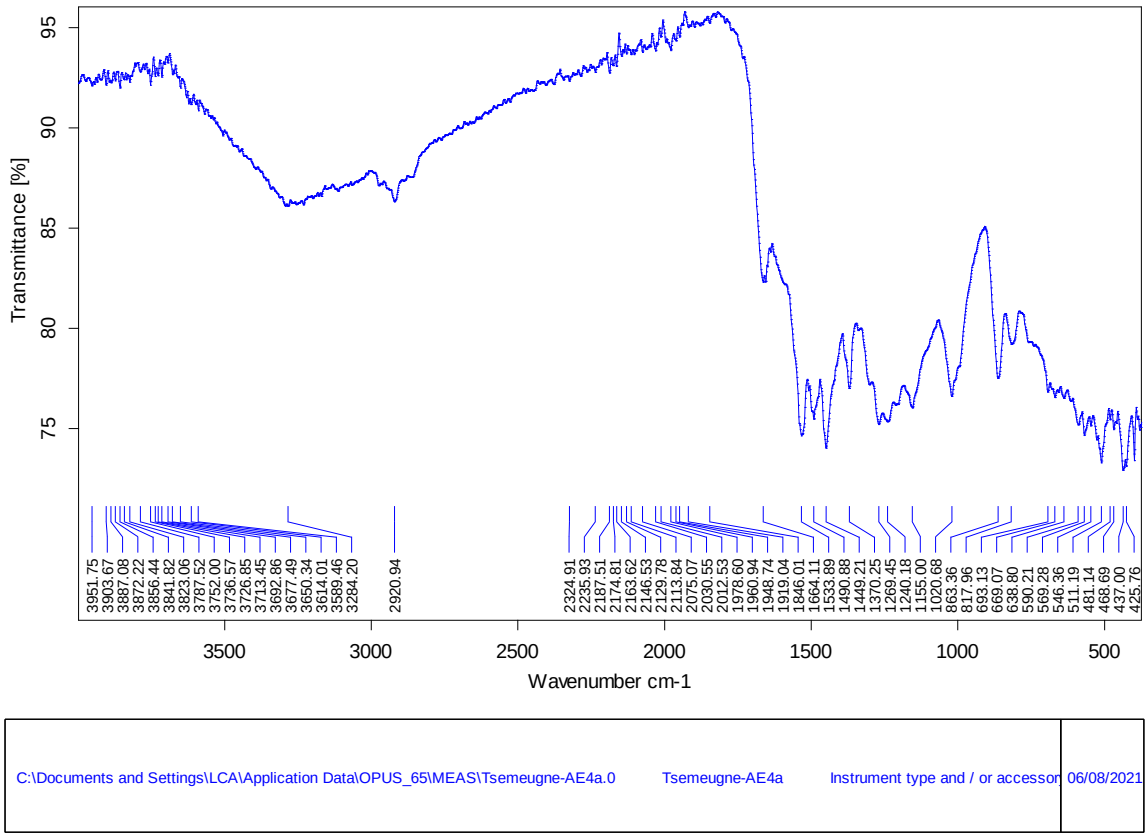
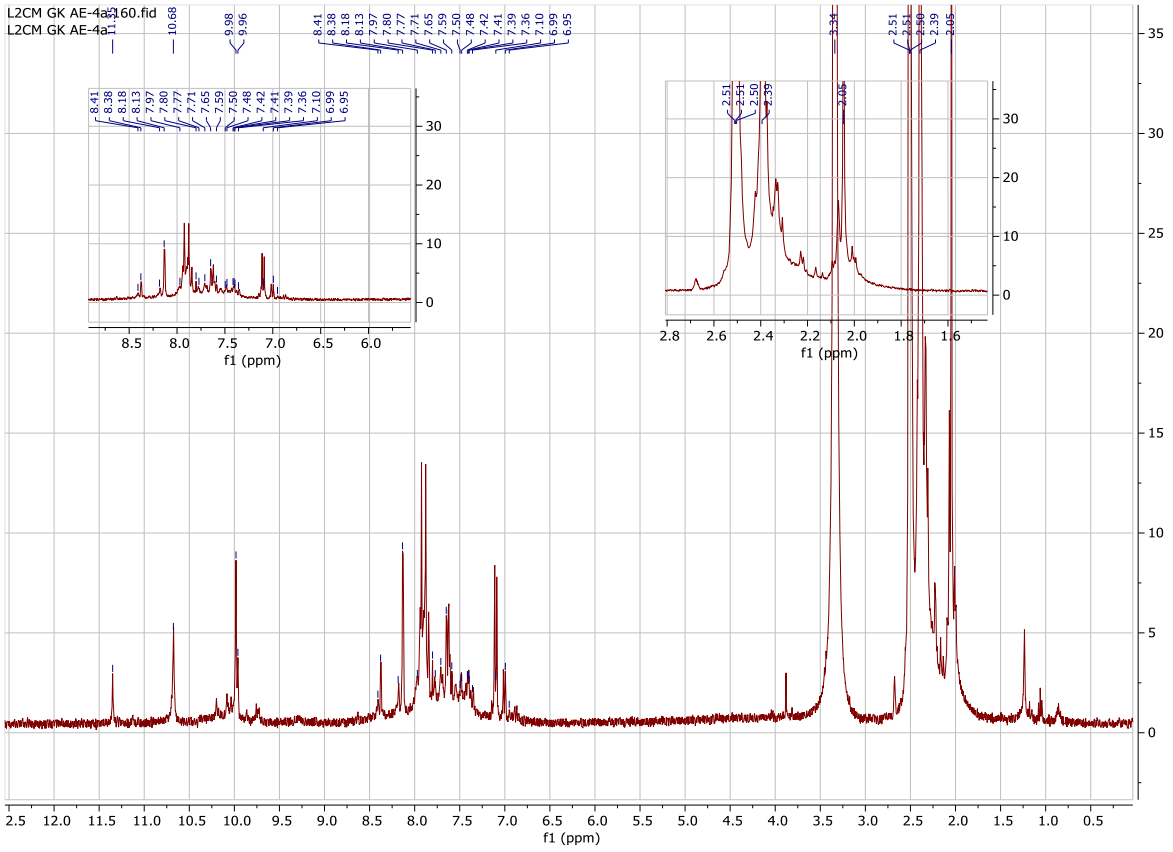


Figure 7. IR spectrum of compound **4a'.**



©AUTHOR(S)

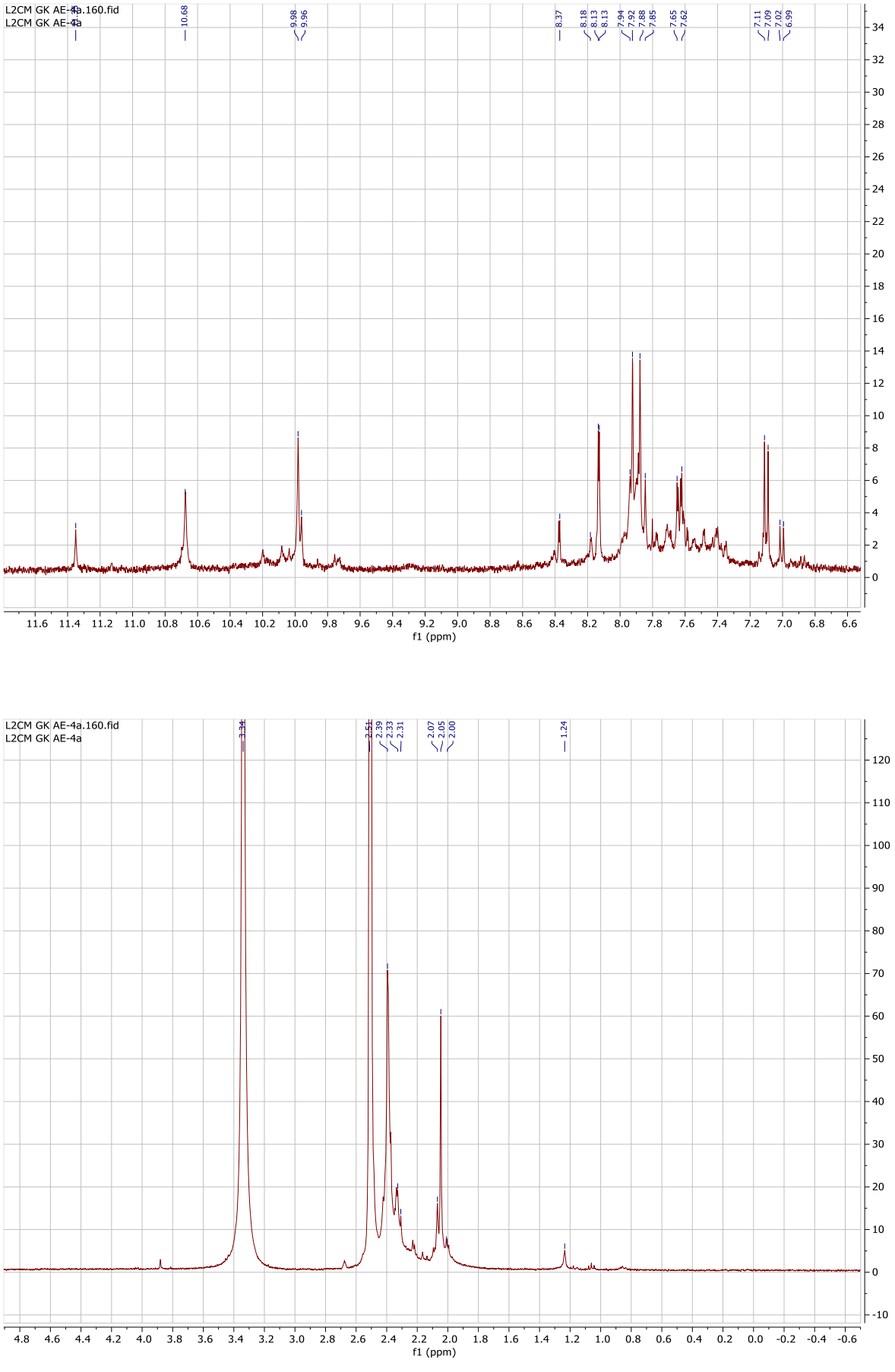
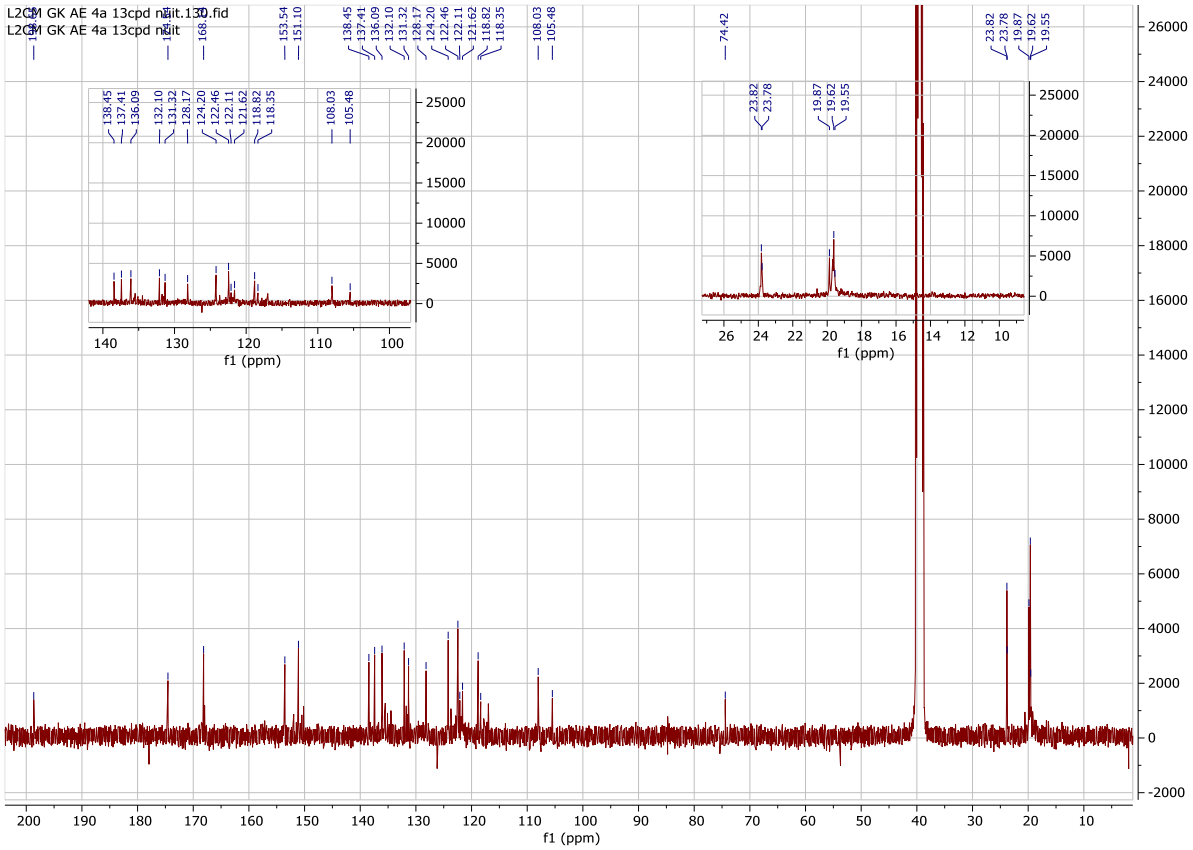
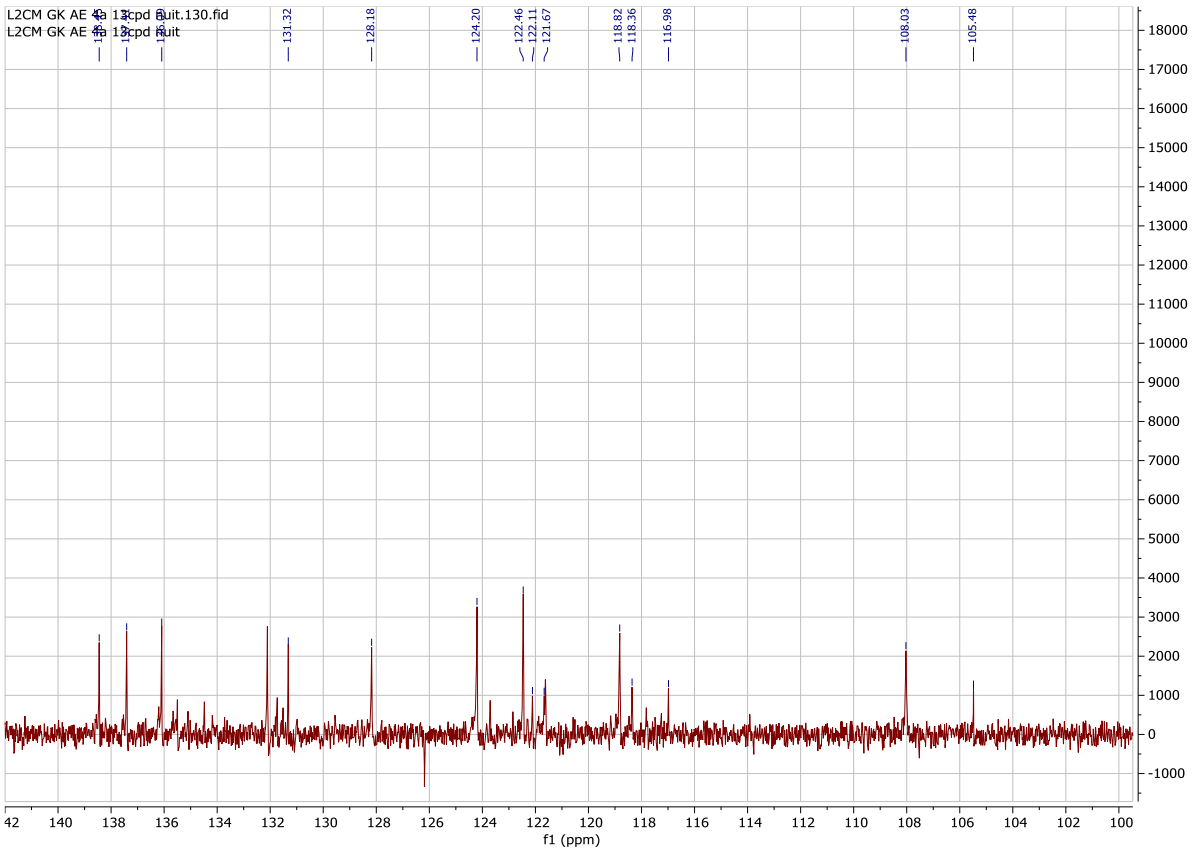


Figure 8. ^{1}H-NMR (DMSO-d_6, 400 MHz) spectrum of compound **4a'.**

©AUTHOR(S)


L2CM GK AE 4a 13cpd nuit.130.fid
L2CM GK AE 4a 13cpd nuit
153.54
151.10
138.45
137.41
136.09
132.10
131.32
128.17
124.20
122.46
122.11
121.62
118.82
118.35
108.03
105.48
74.42
23.82
23.78
19.87
19.62
19.55
f1 (ppm)


L2CM GK AE 4a 13cpd nuit.130.fid
L2CM GK AE 4a 13cpd nuit
131.32
128.18
124.20
122.46
122.11
121.67
118.82
118.36
116.98
108.03
105.48
f1 (ppm)

©AUTHOR(S)

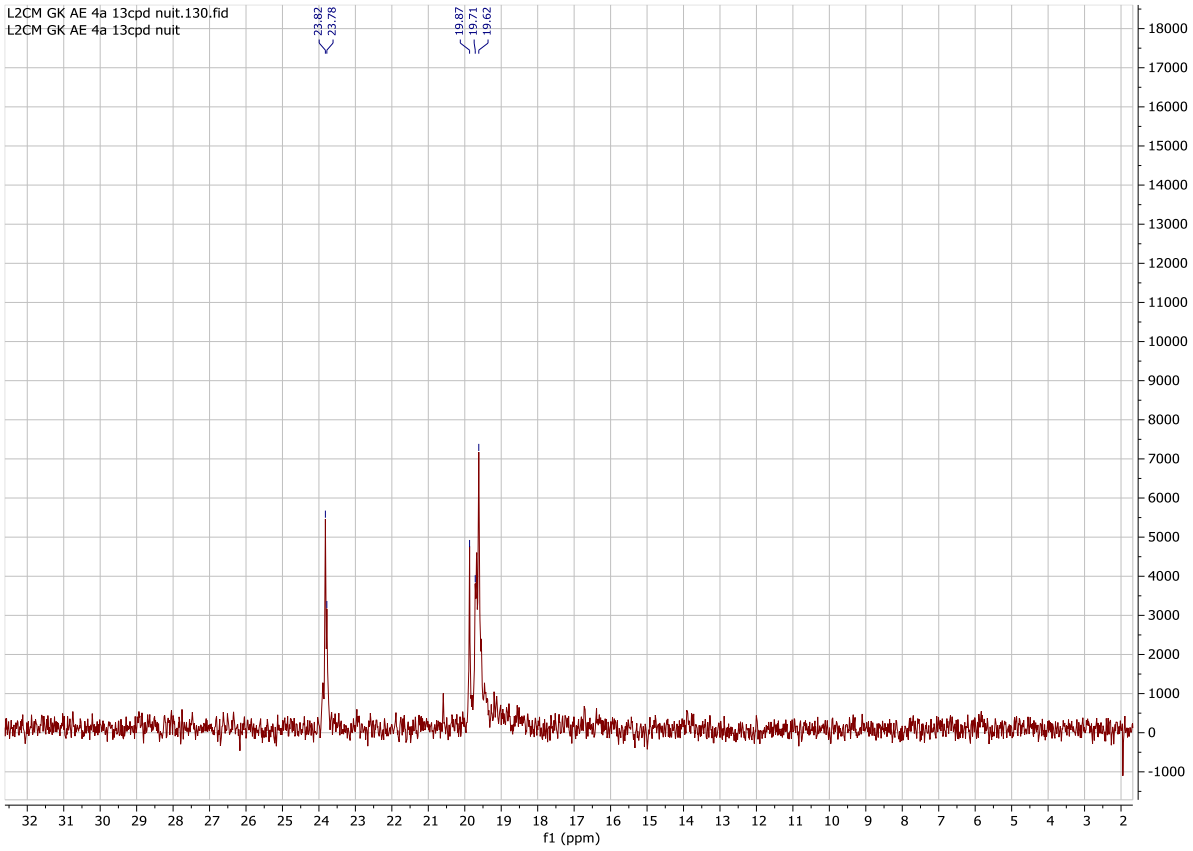


Figure 9. ^{13}C(H)-NMR ^{1}H (DMSO-d$_6$, 100 MHz) of compound **4a'.**

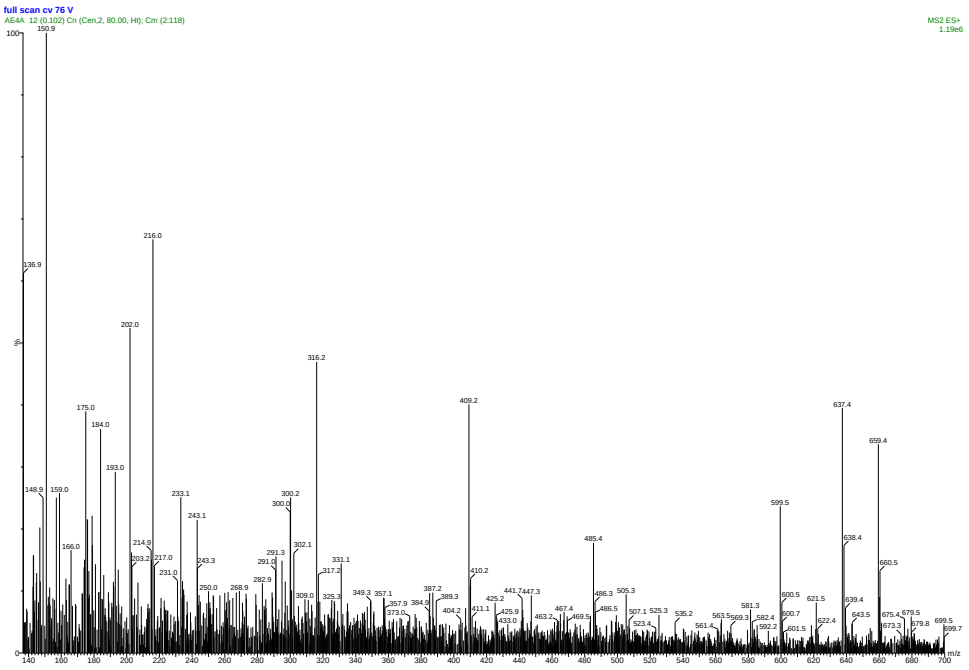


Figure 10. HRMS ESI-Positive mode of compound **4a'.**

©AUTHOR(S)

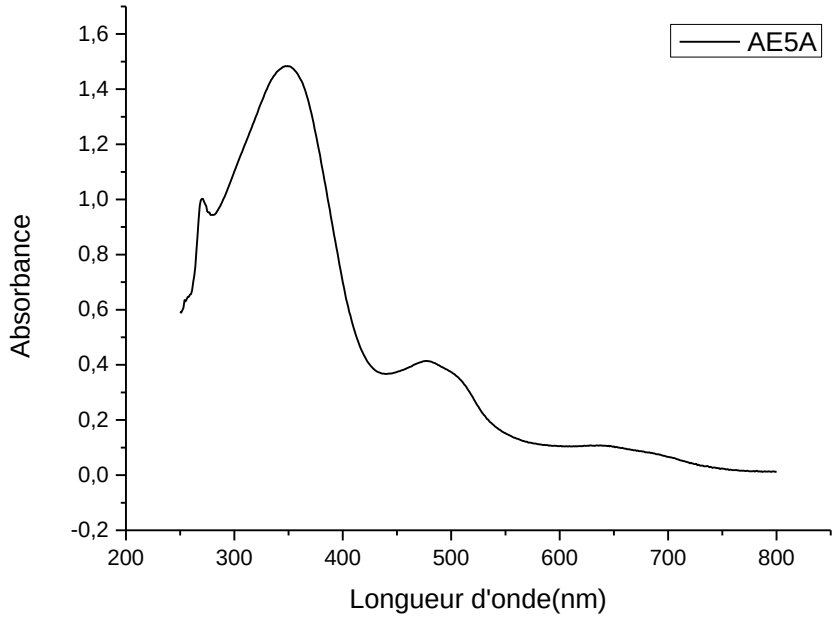


Figure 11. UV spectrum of compound **4b** in Methanol as solvent.

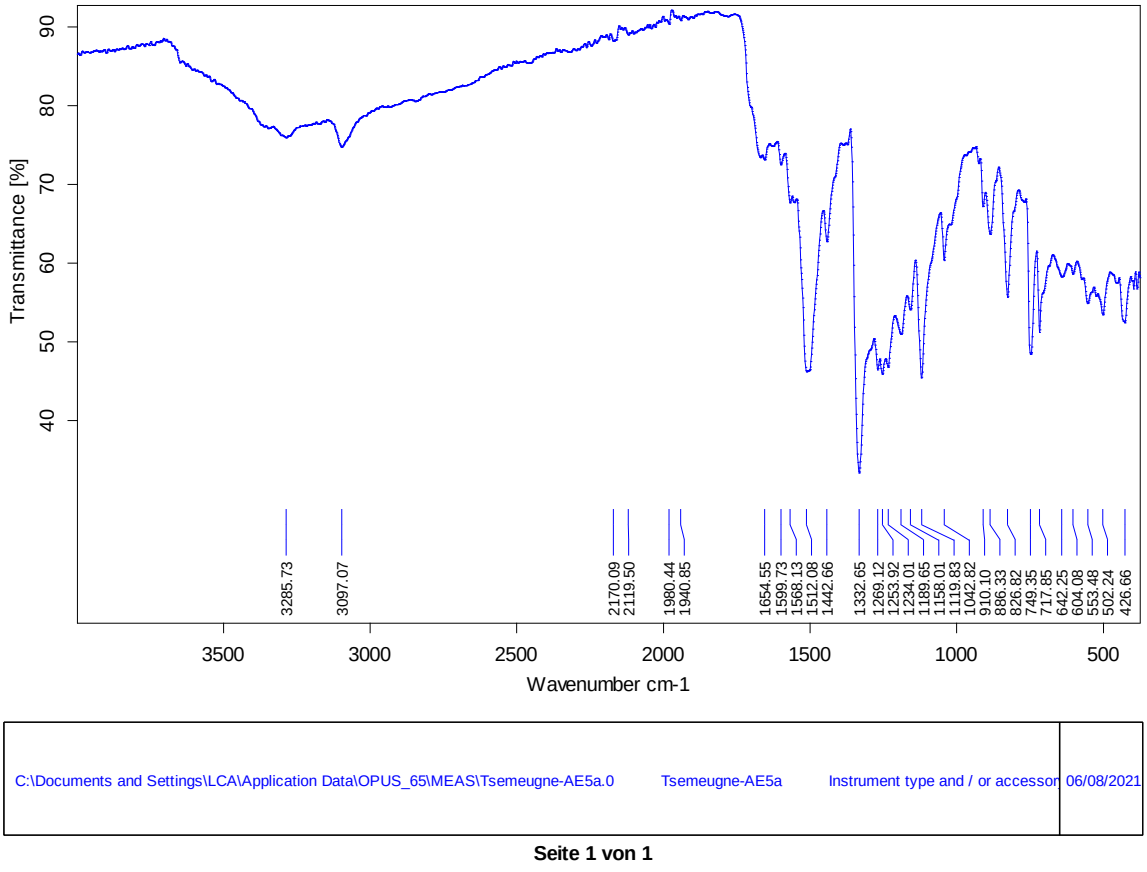


Figure 12. IR spectrum of compound **4b.**

©AUTHOR(S)

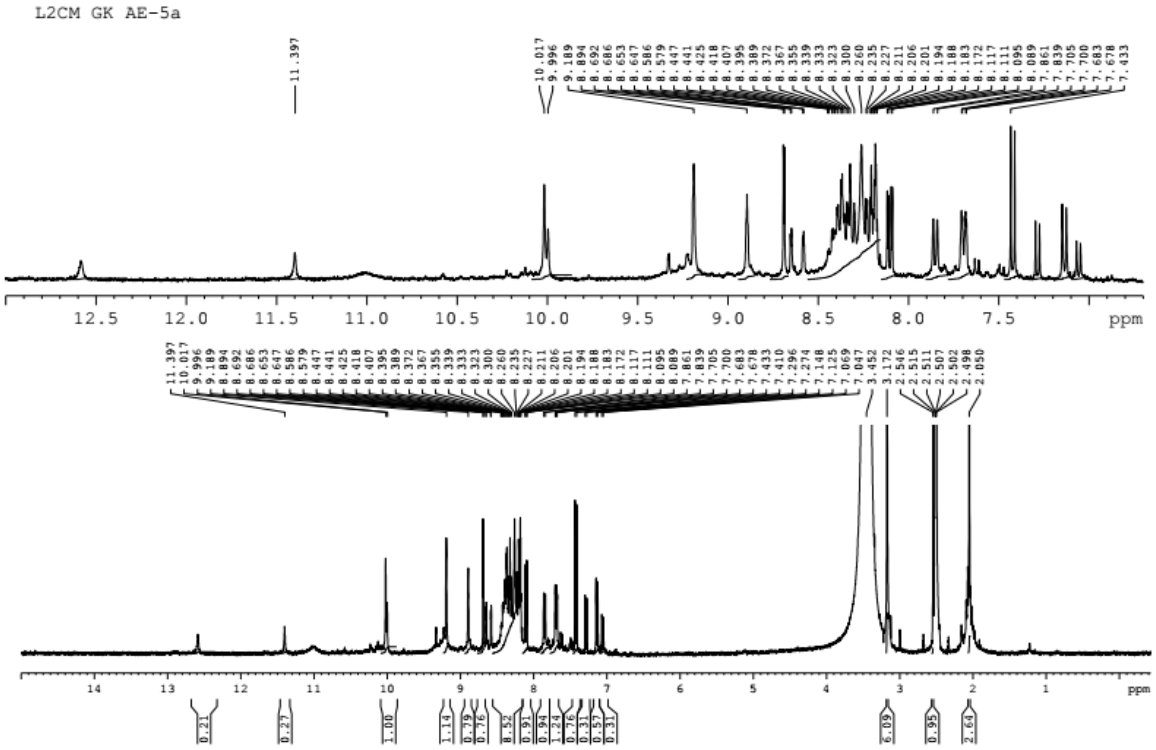


Figure 13. ^{1}H-NMR (DMSO-d_6, 400 MHz) spectrum of compound **4b.**

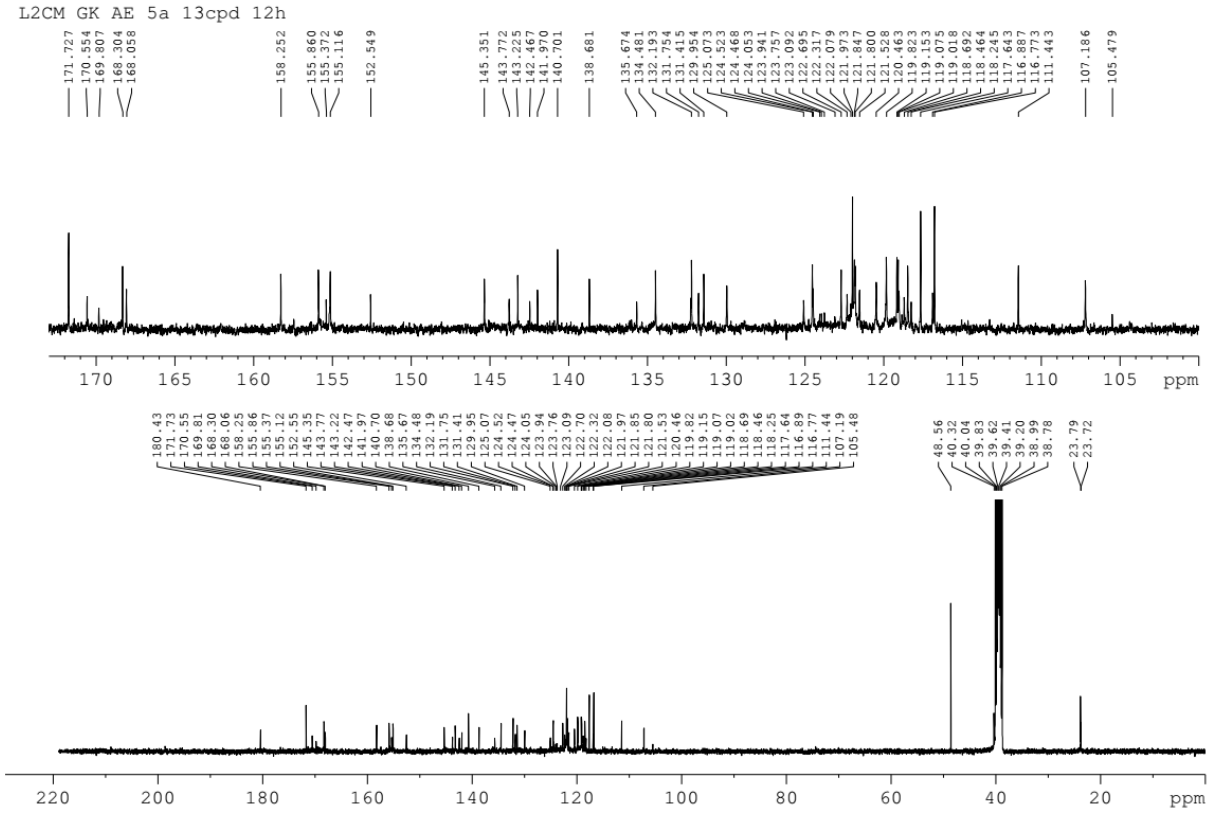


Figure 14. ^{13}C(^{1}H)-NMR (DMSO-d_6, 100 MHz) of compound **4b.**

©AUTHOR(S)

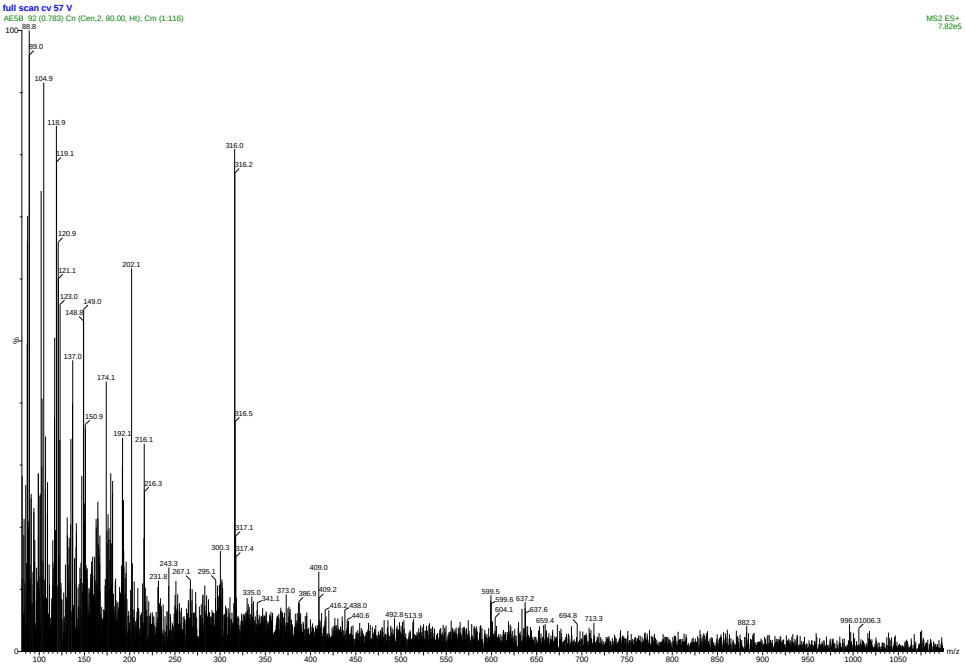


Figure 15. HRMS ESI-Positive mode of compound **4b.**

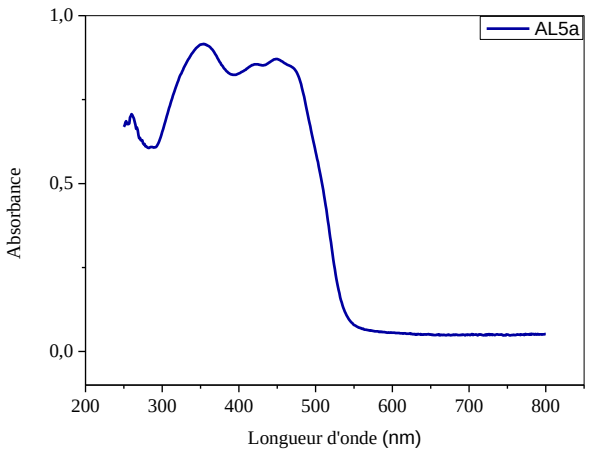


Figure 16. UV spectrum of compound **4c** in methanol as solvent.

©AUTHOR(S)

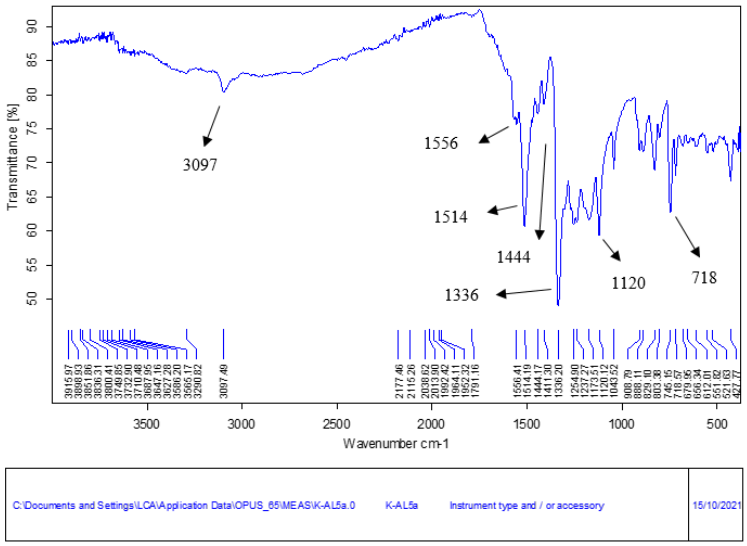


Figure 17. IR spectrum of compound **4c.**

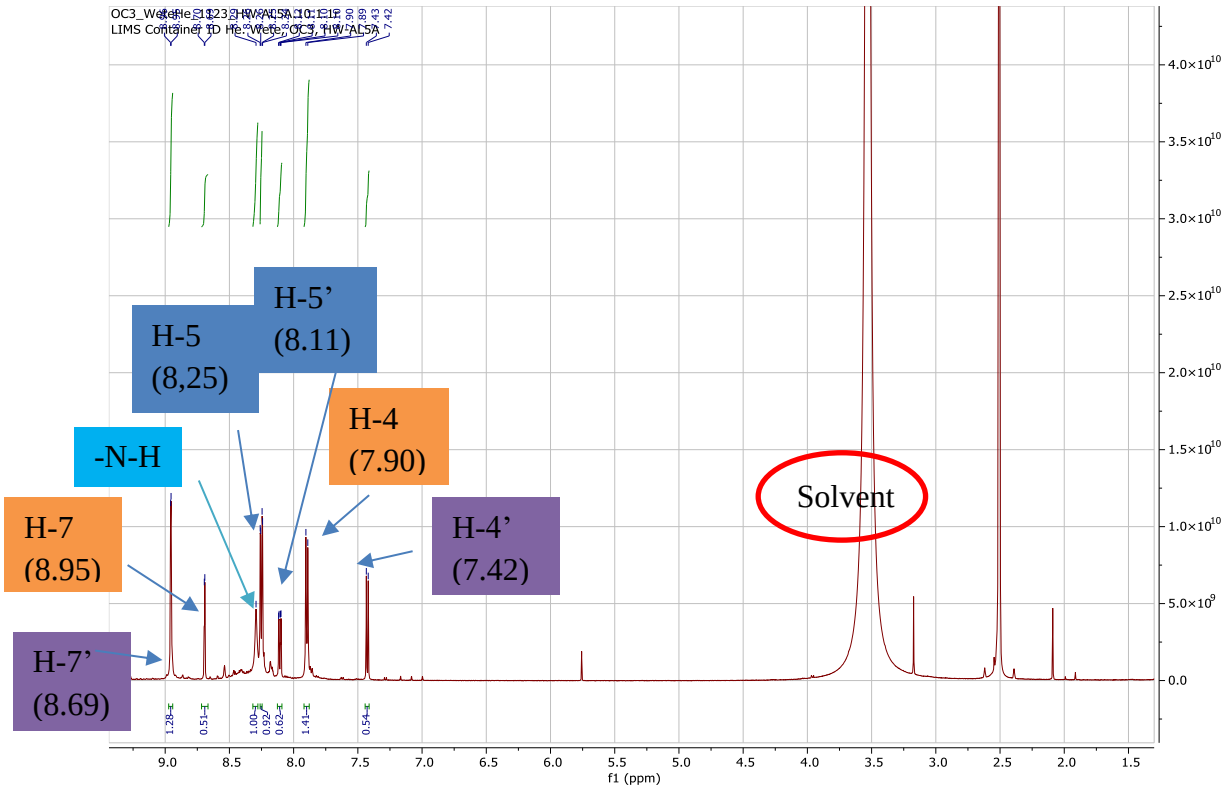


Figure 18. ^{1}H-NMR (DMSO-d_6, 400 MHz) spectrum of compound **4c.**

©AUTHOR(S)

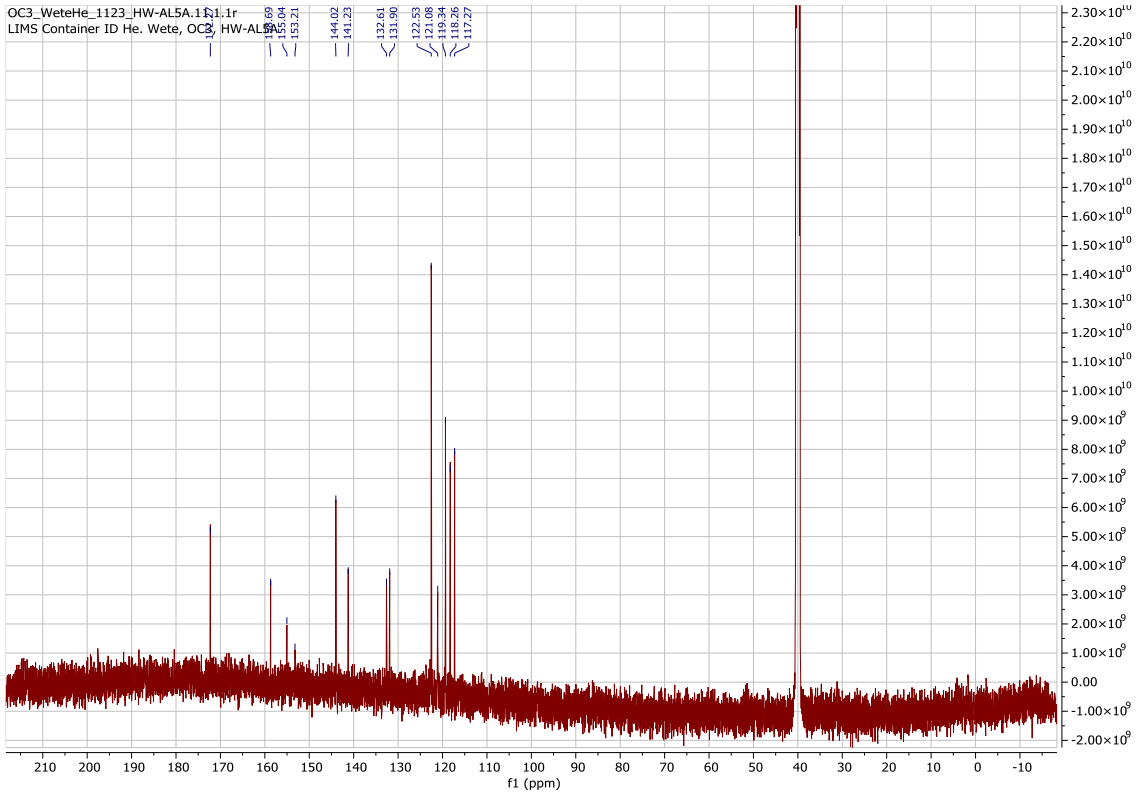


Figure 19. ^{13}C(H)-NMR ^{1}H (DMSO-d$_6$, 100 MHz) of compound **4c.**

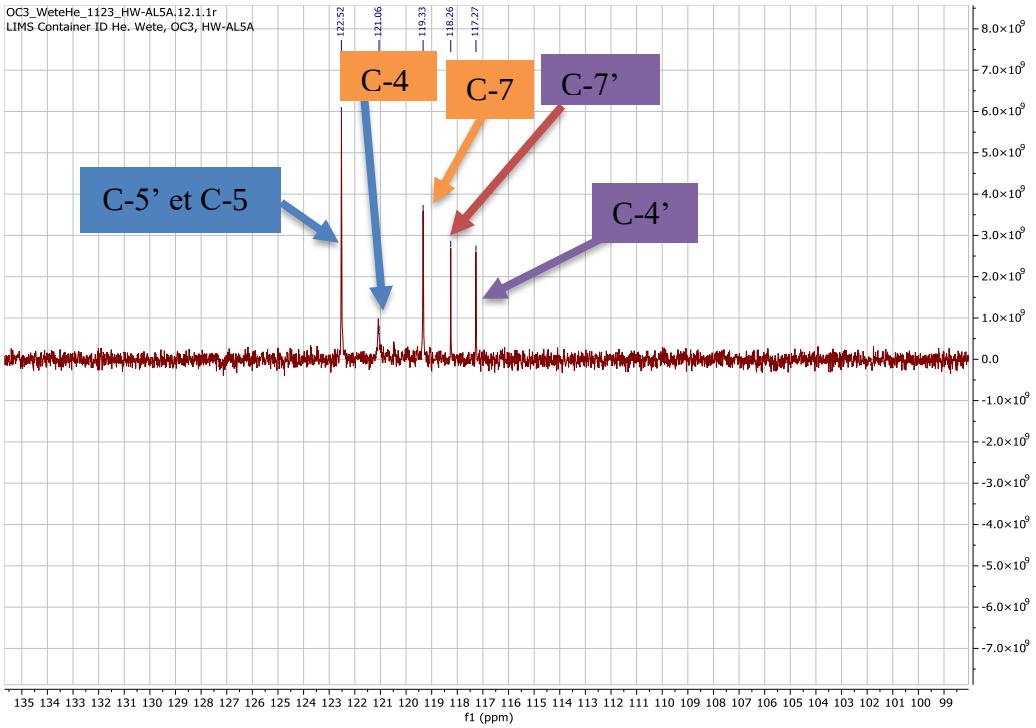


Figure 20. DEPT-135 (DMSO-d$_6$, 100 MHz) of compound **4c.**

©AUTHOR(S)

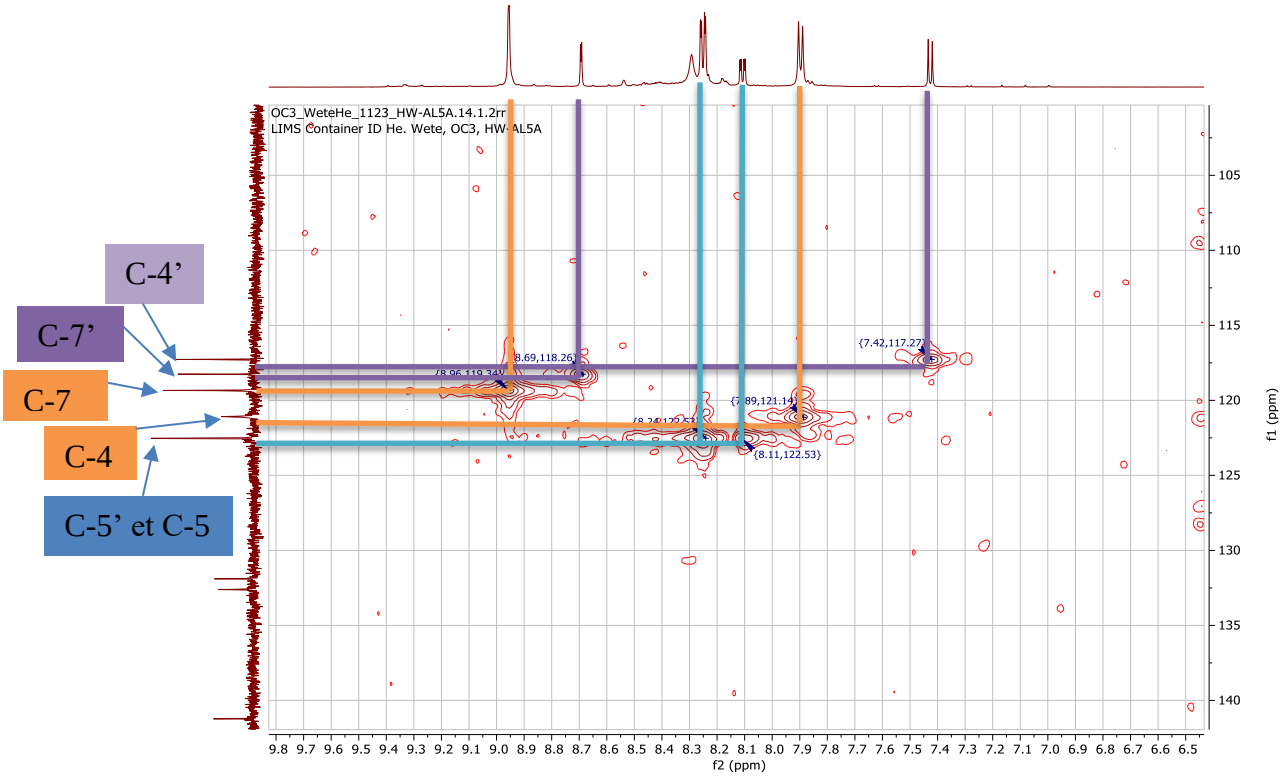


Figure 21. HSQC spectrum of compound **4c.**

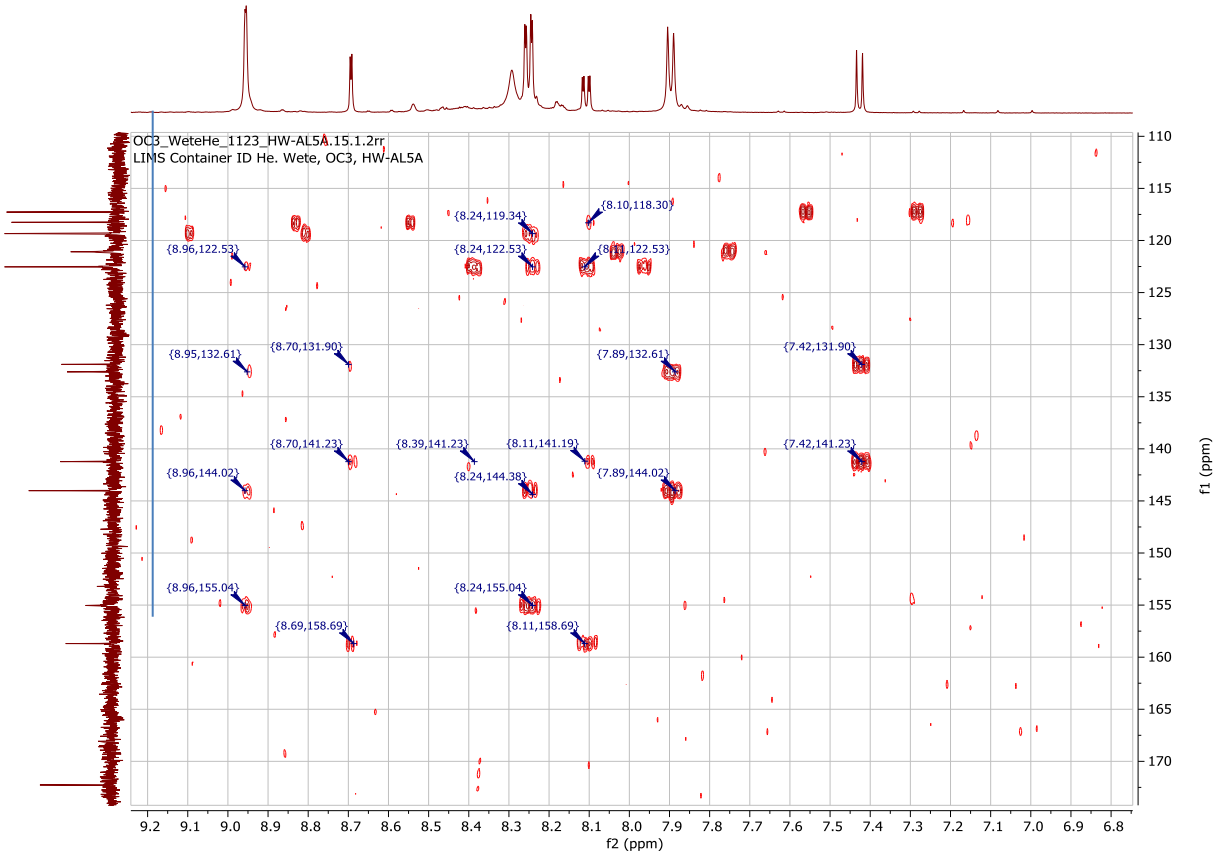


Figure 22. HMBC spectrum of compound **4c.**

©AUTHOR(S)

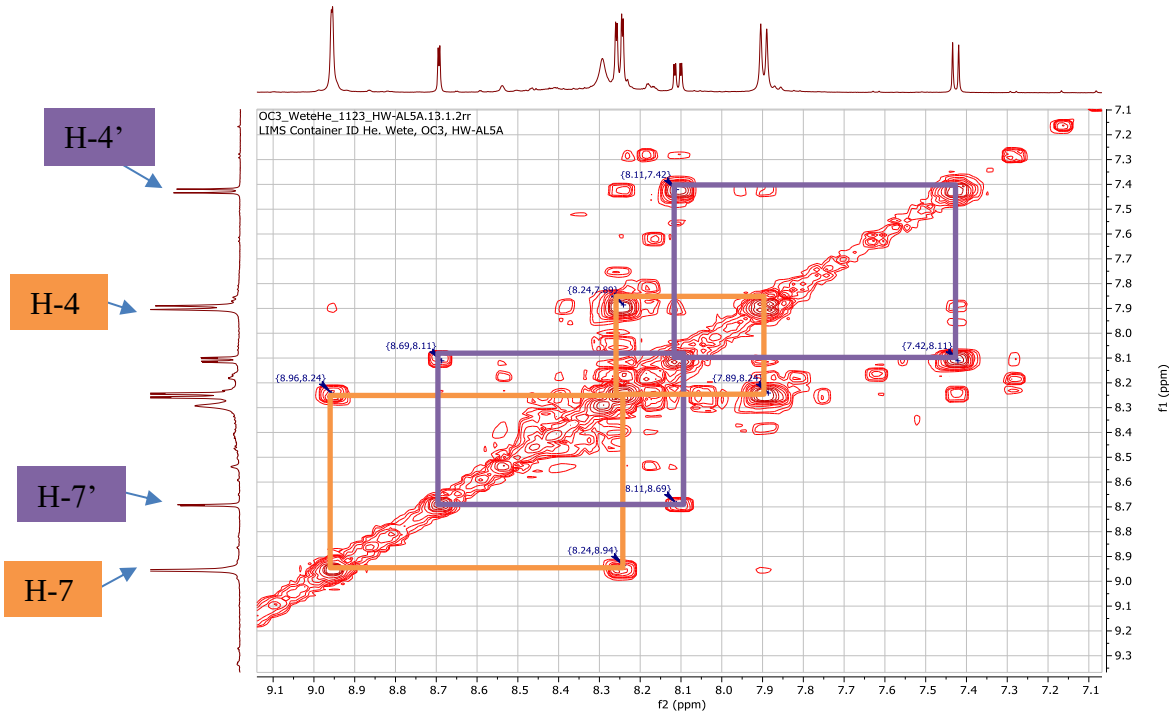


Figure 23. COSY ^{1}H-^{1}H spectrum of compound **4c.**

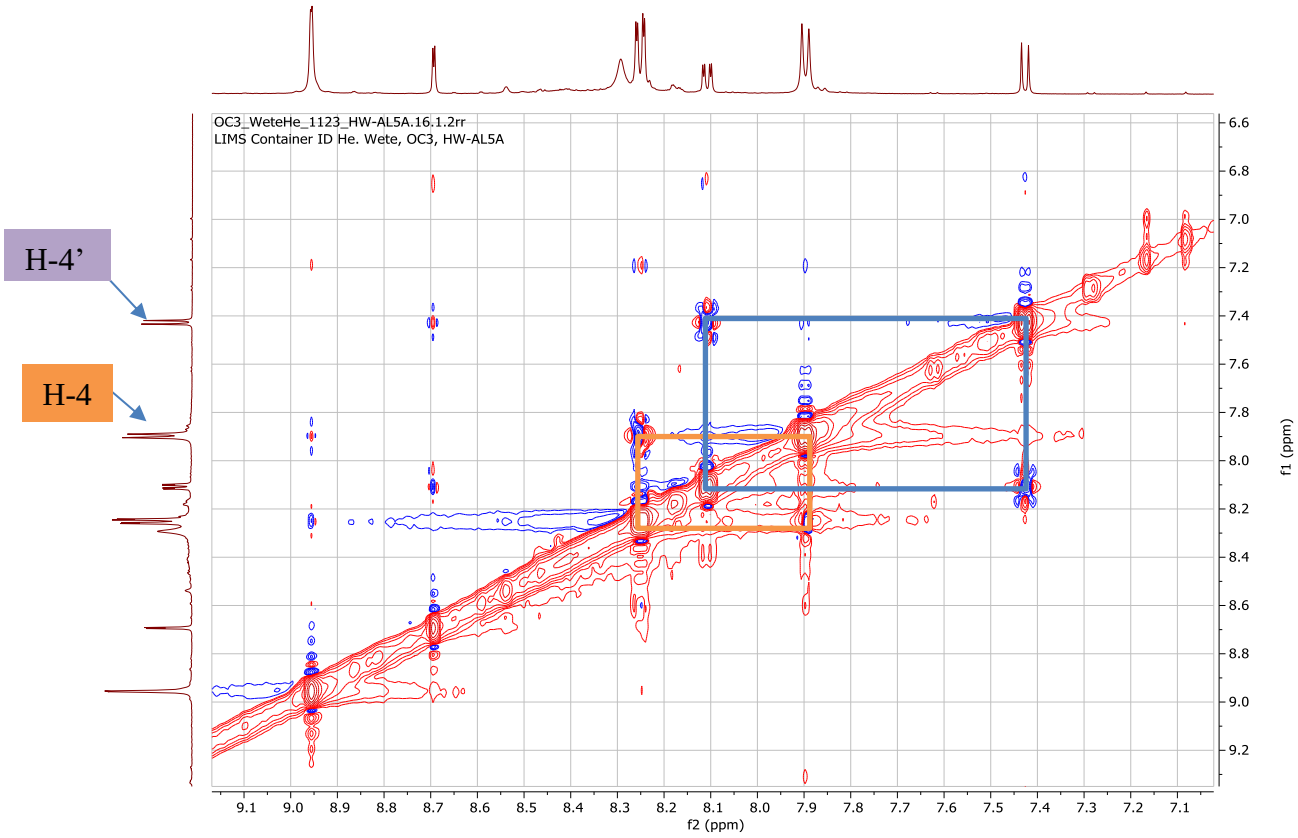


Figure 24. NOESY spectrum of compound **4c.**

©AUTHOR(S)

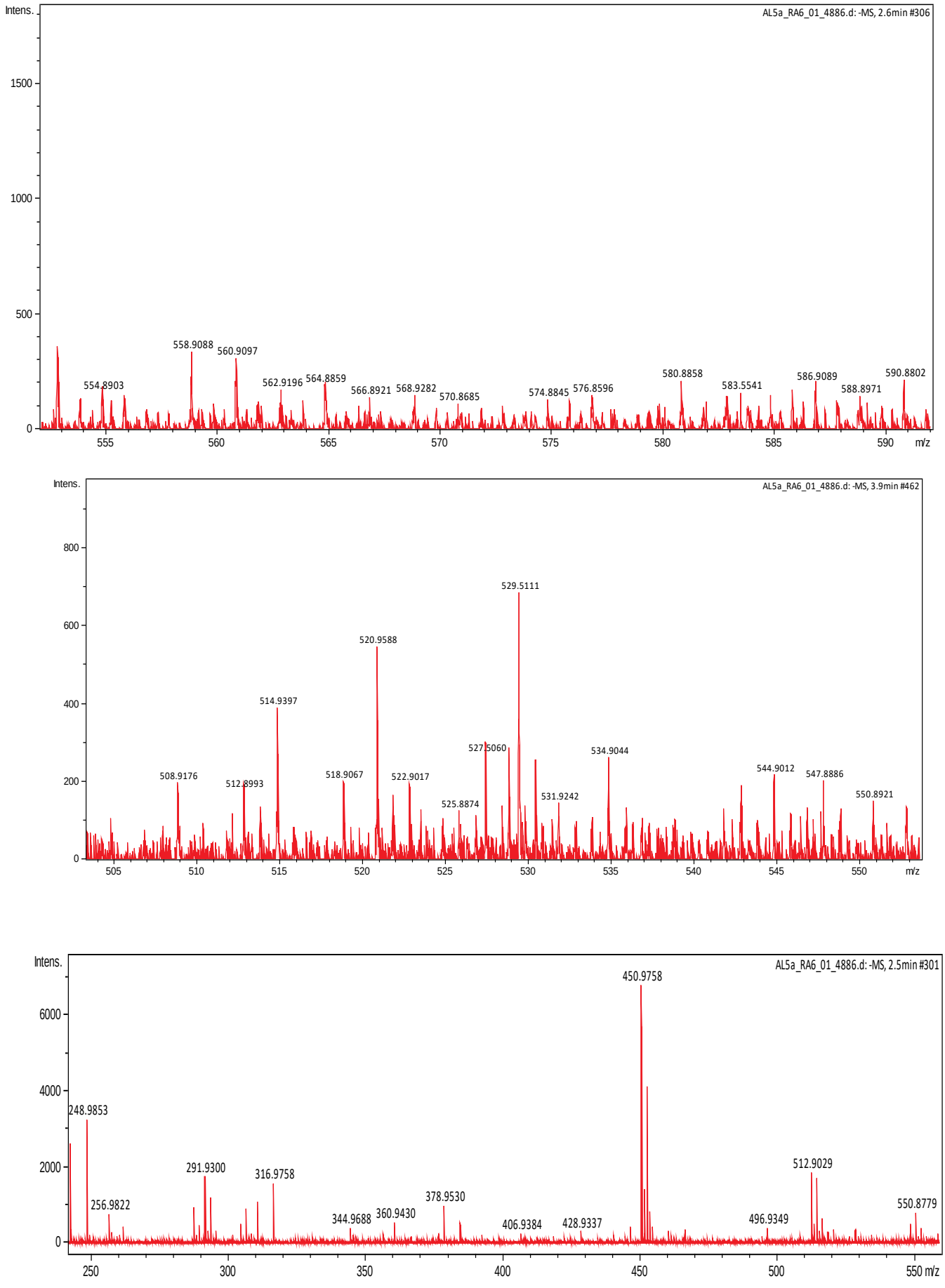


Figure 25. HRMS ESI-Positive mode of compound **4c.**

©AUTHOR(S)

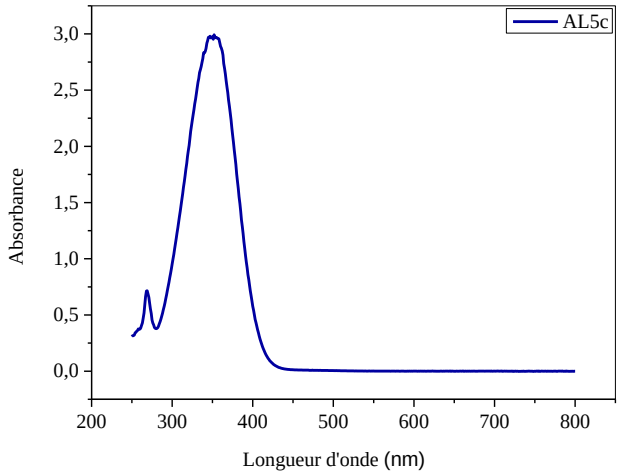


Figure 26. UV spectrum of compound **4c'** in methanol as solvent.

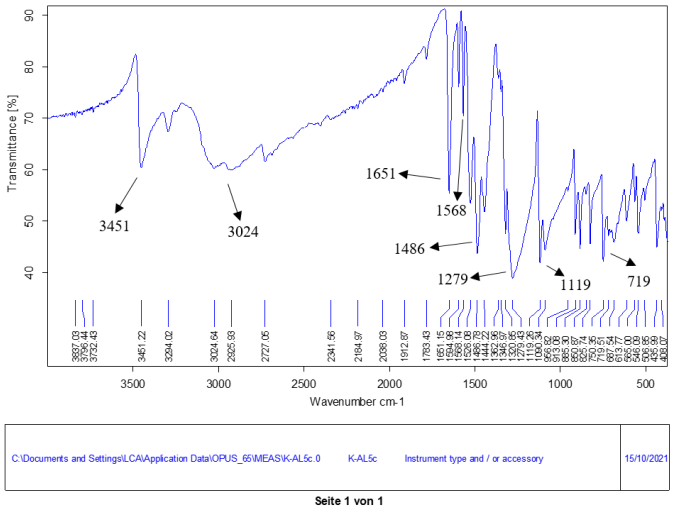


Figure 27. IR spectrum of compound **4c'.**

©AUTHOR(S)

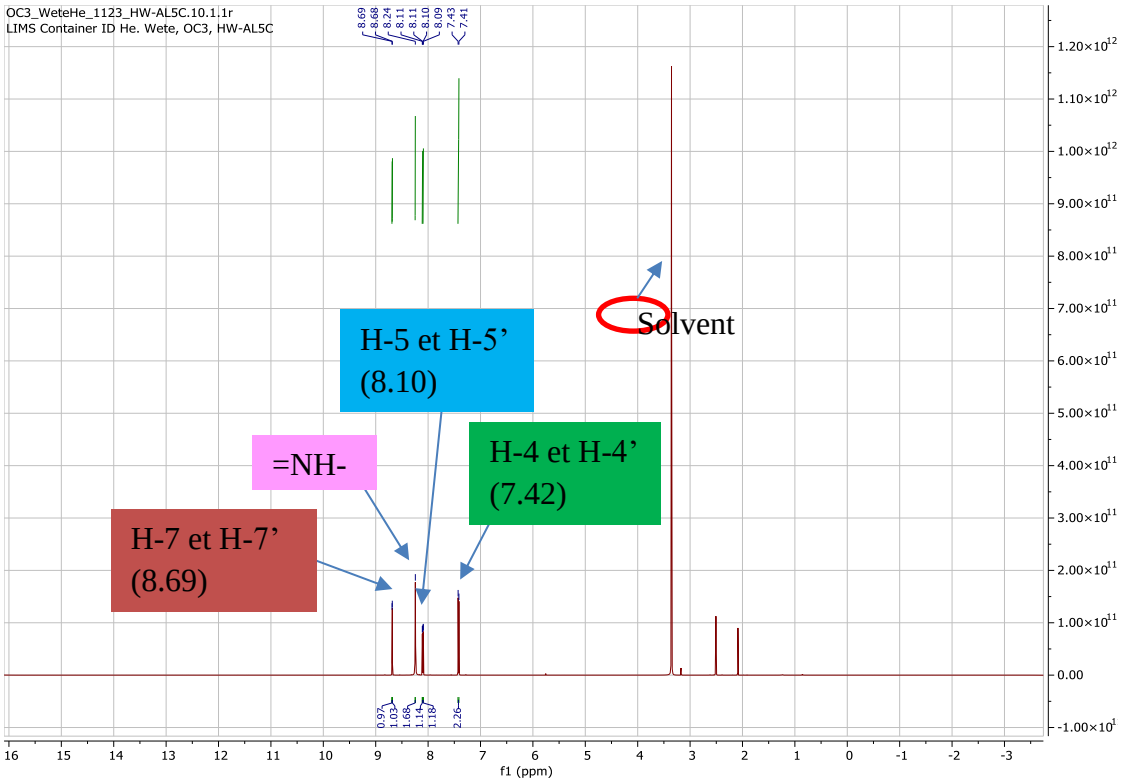


Figure 28. ^{1}H-NMR (DMSO-d_6, 400 MHz) spectrum of compound **4c'.**

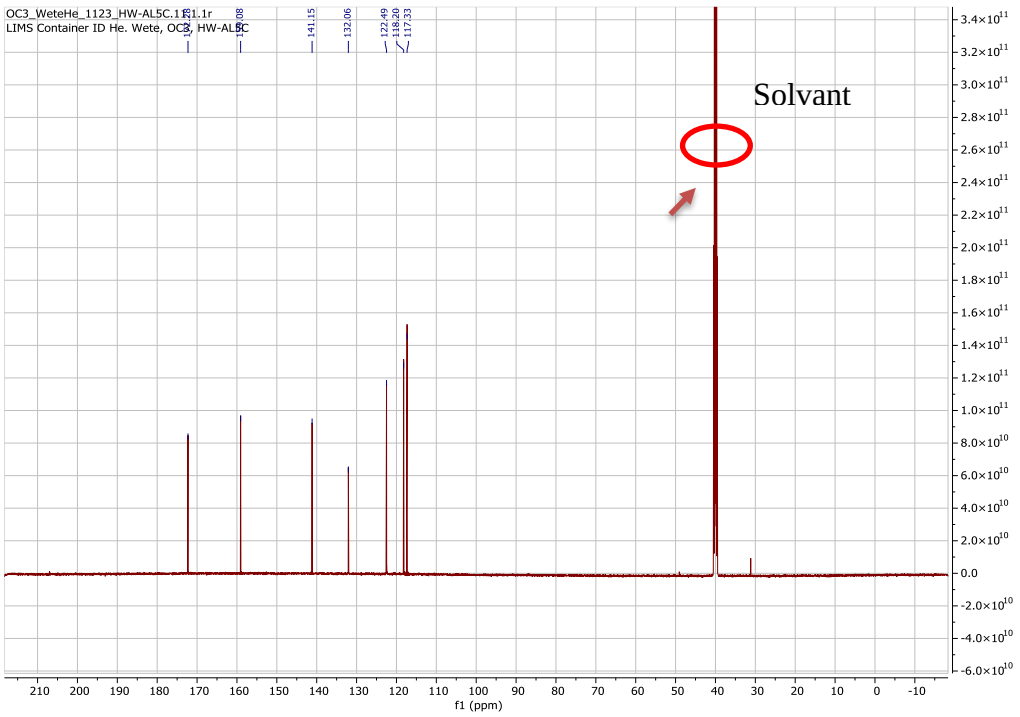


Figure 29. ^{13}C(H)-NMR ^{1}H (DMSO-d_6, 100 MHz) of compound **4c'.**

©AUTHOR(S)

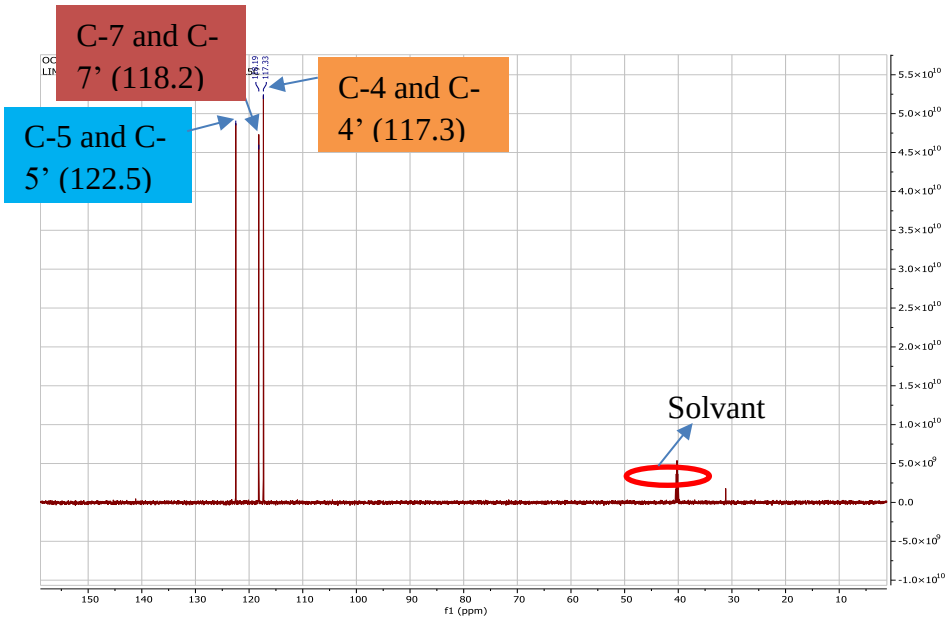


Figure 30. DEPT-135 (DMSO-d_6, 100 MHz) of compound **4c'.**

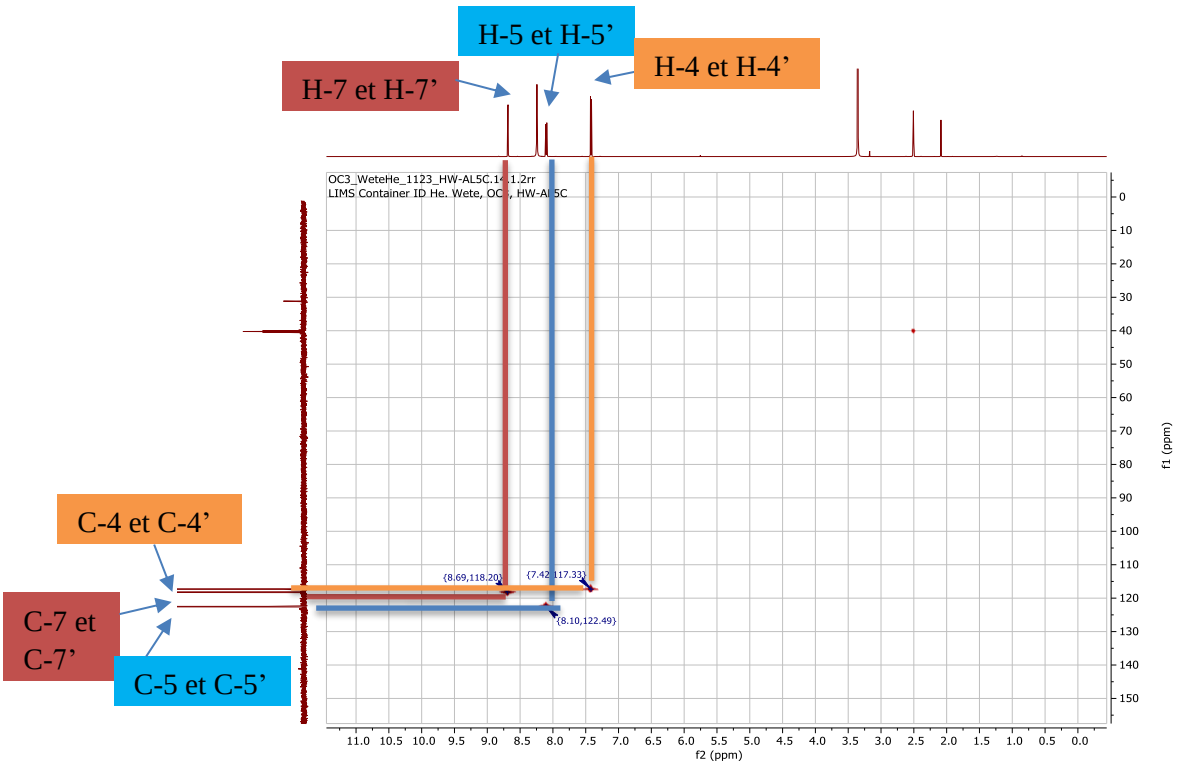


Figure 31. HSQC spectrum of compound **4c'.**

©AUTHOR(S)

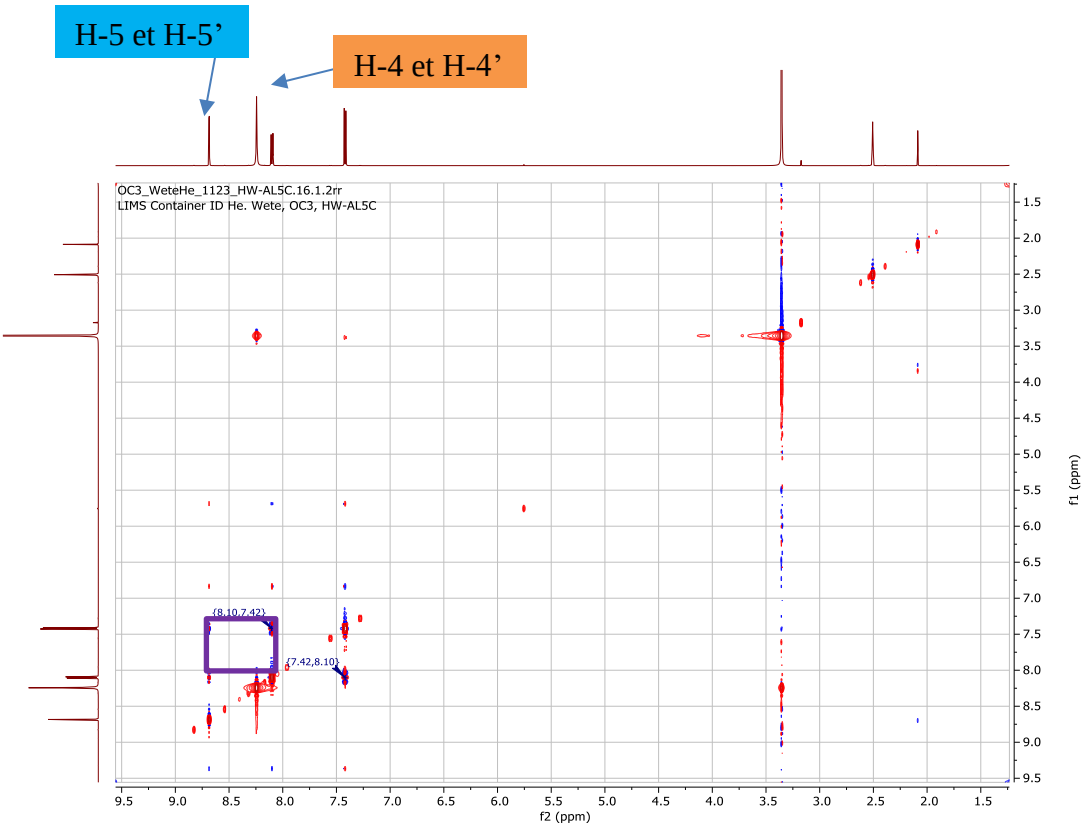
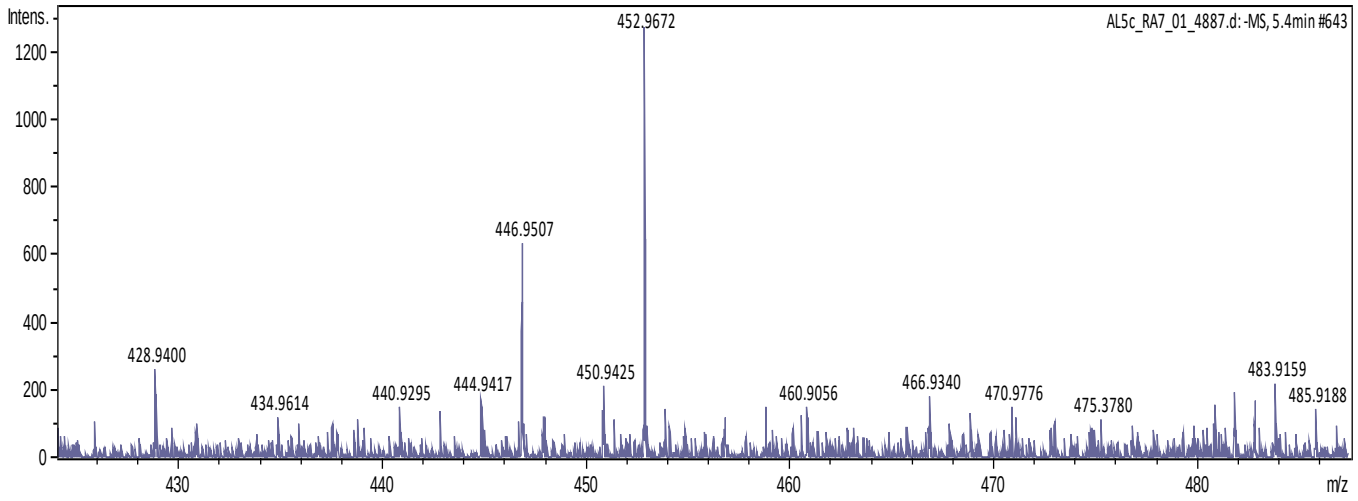


Figure 32. HRMS ESI-Positive mode of compound **4c'.**



©AUTHOR(S)