

Title: Positive Modulators of *N*-Methyl-*D*-Aspartate Receptor: Structure-Activity Relationship Study on Steroidal C-17 and C-20 Oxime Ethers

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Supporting information

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Table of Contents

¹H and ¹³C NMR spectra of compounds 11-24	2
HR-MS and LC-MS spectra of compounds 11-28.....	11

^1H and ^{13}C NMR spectra of compounds 11-24

Figure S1. ^1H NMR and ^{13}C NMR spectra of compound 11

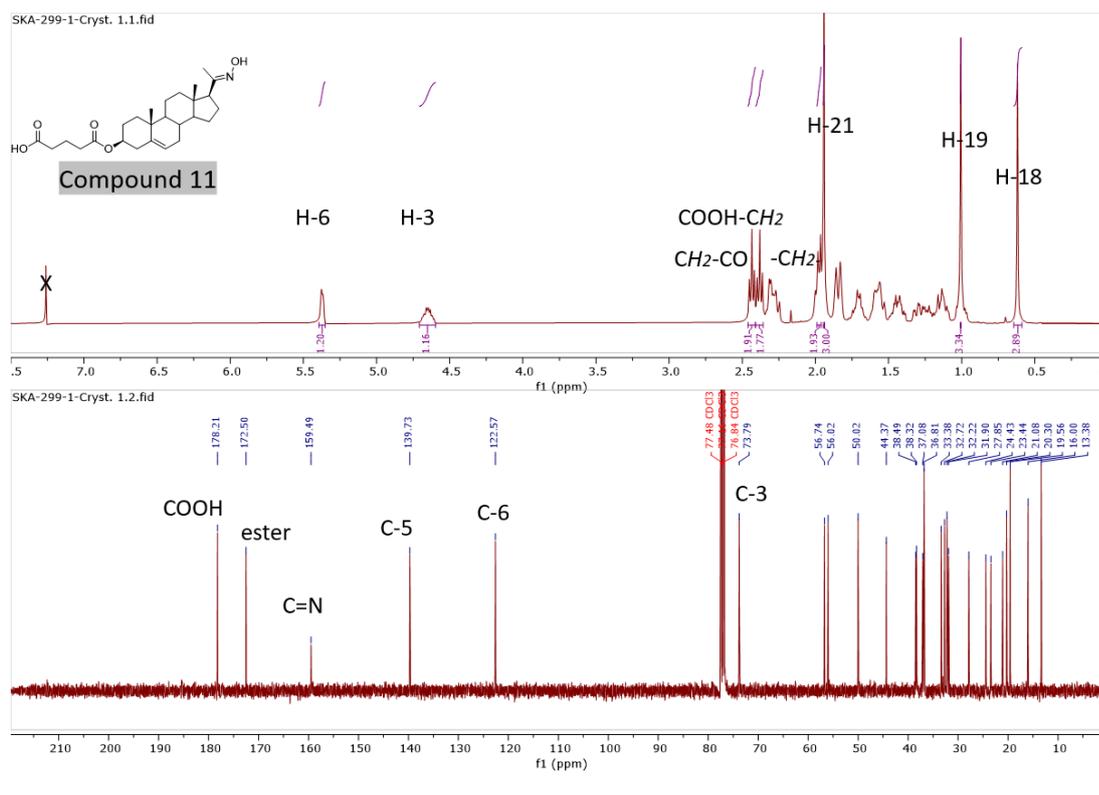


Figure S2. ^1H NMR and ^{13}C NMR spectra of compound 12

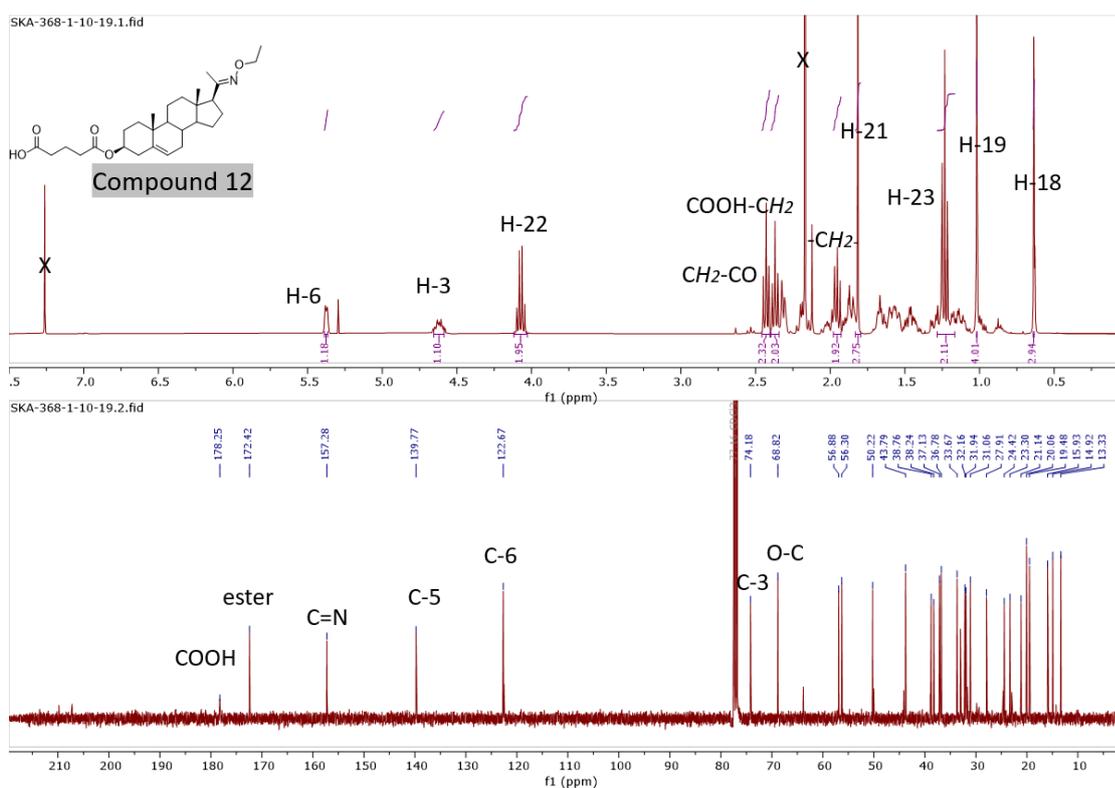


Figure S3. ^1H NMR and ^{13}C NMR and spectra of compound **13**

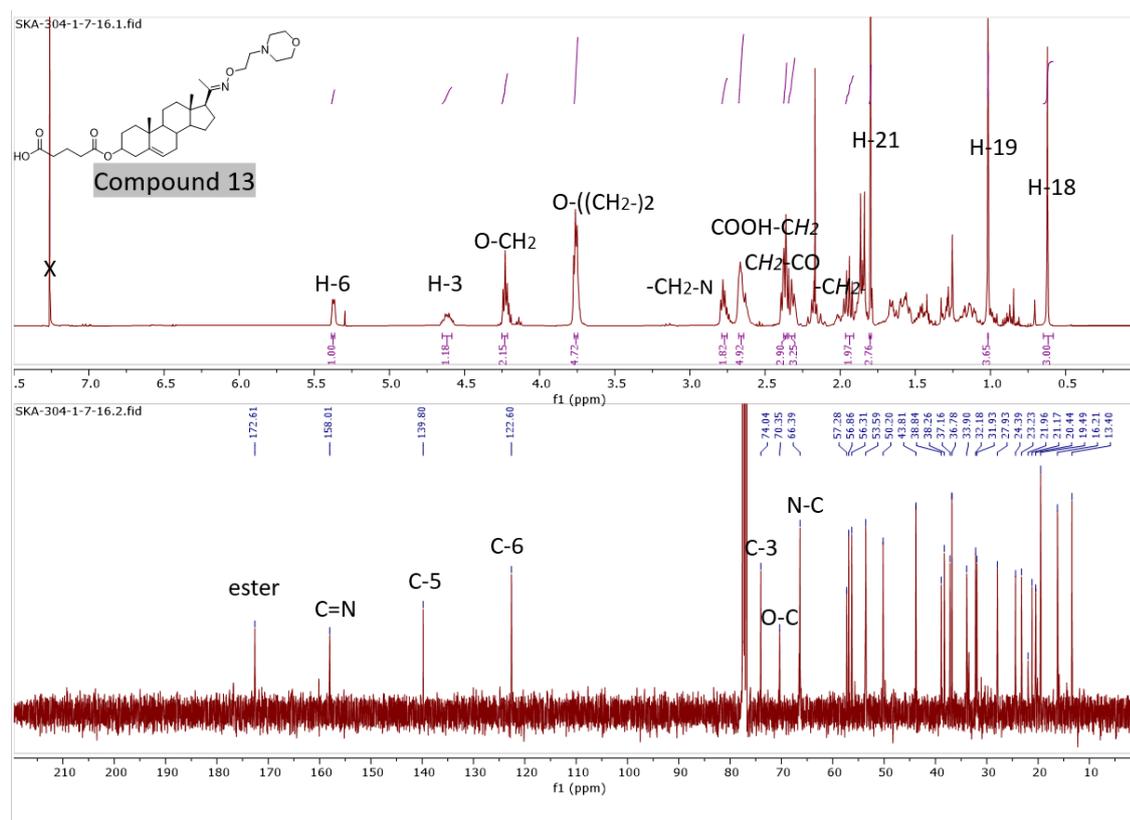


Figure S4. ^1H NMR and ^{13}C NMR and spectra of compound **14**

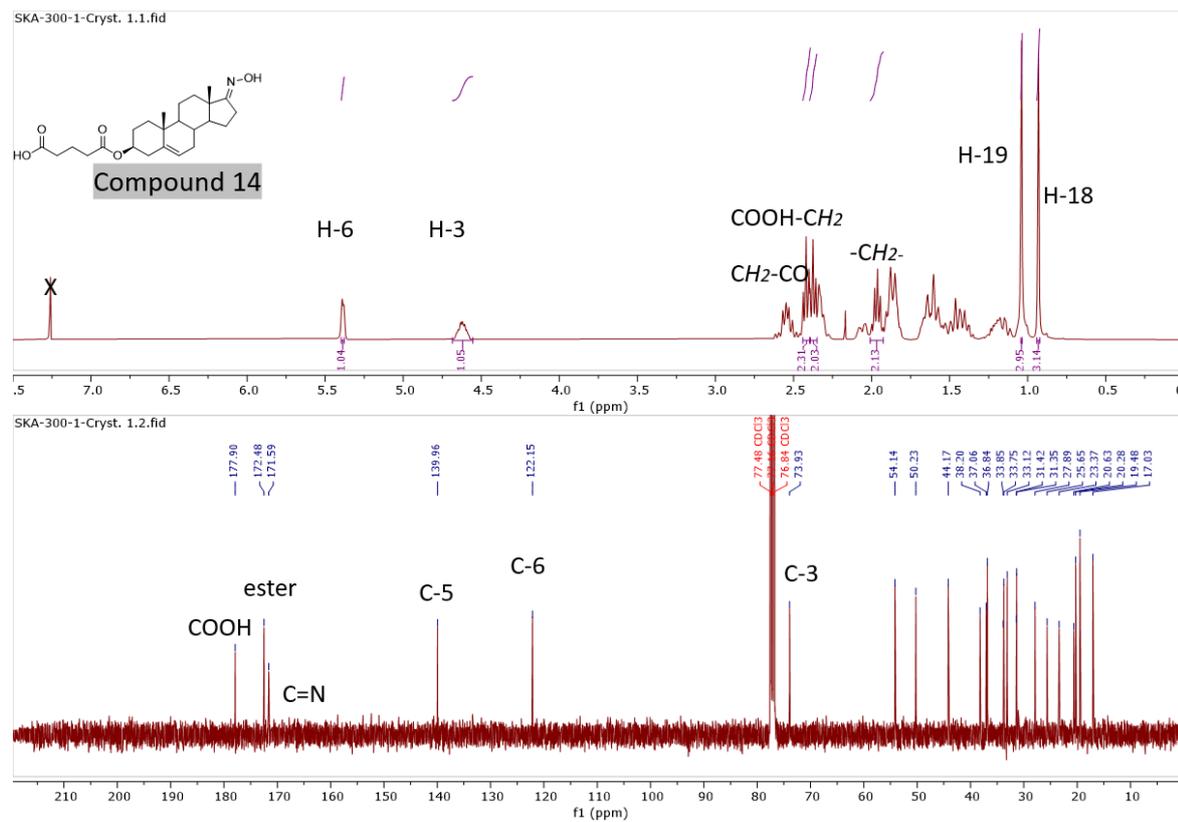


Figure S5. ^1H NMR and ^{13}C NMR and spectra of compound **15**

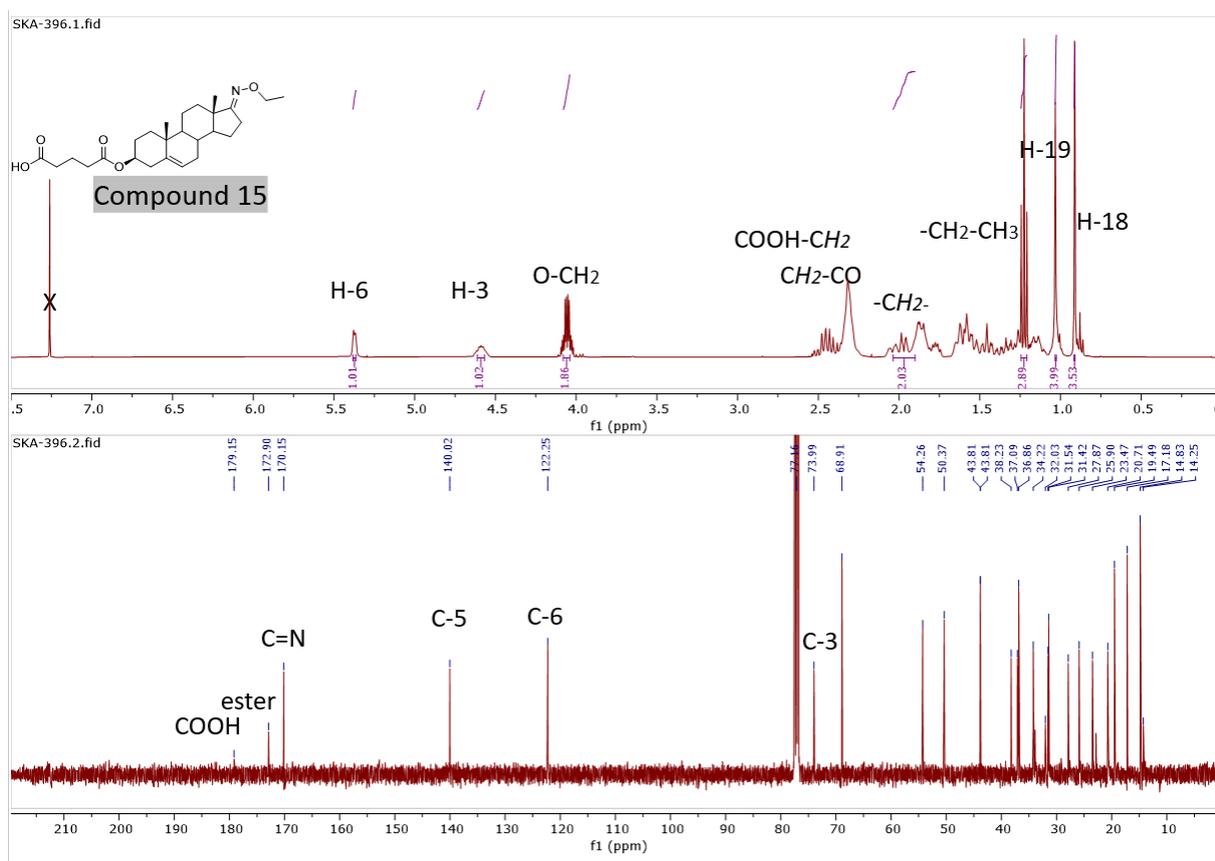


Figure S6. ^1H NMR and ^{13}C NMR and spectra of compound **16**

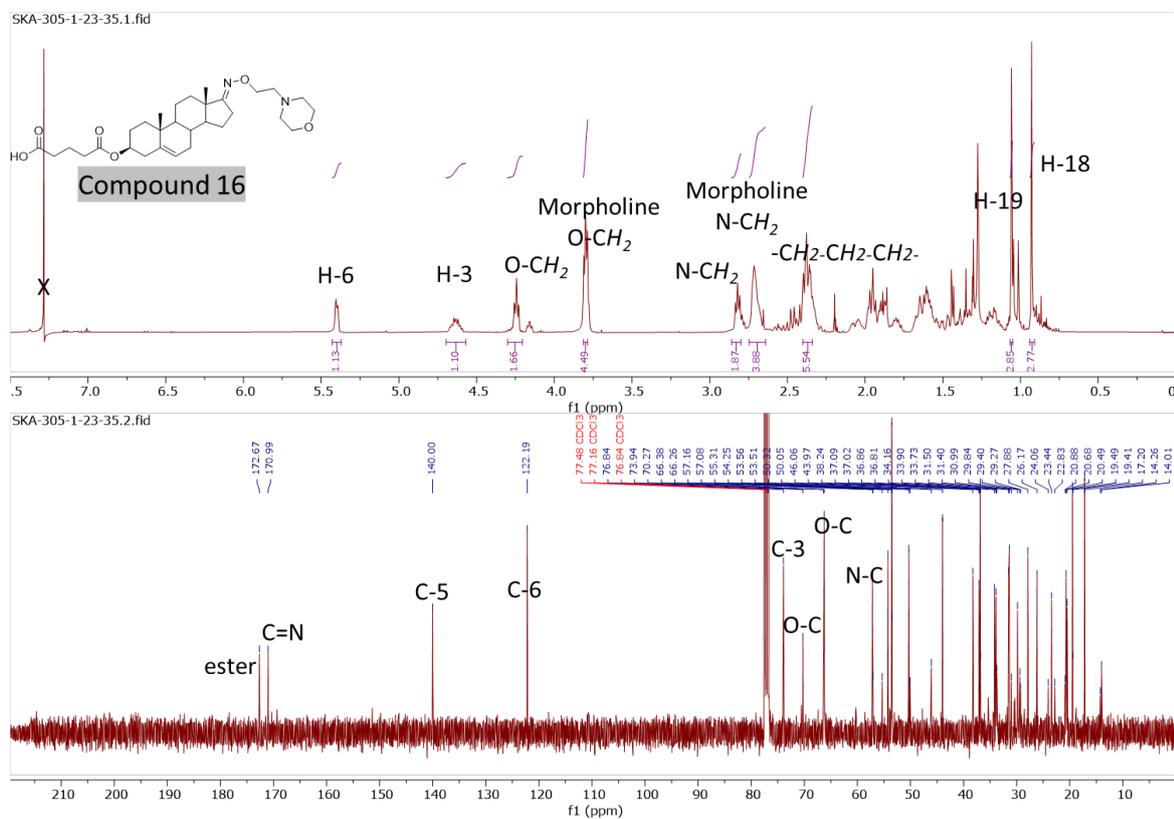


Figure S7. ^1H NMR and ^{13}C NMR and spectra of compound **17**

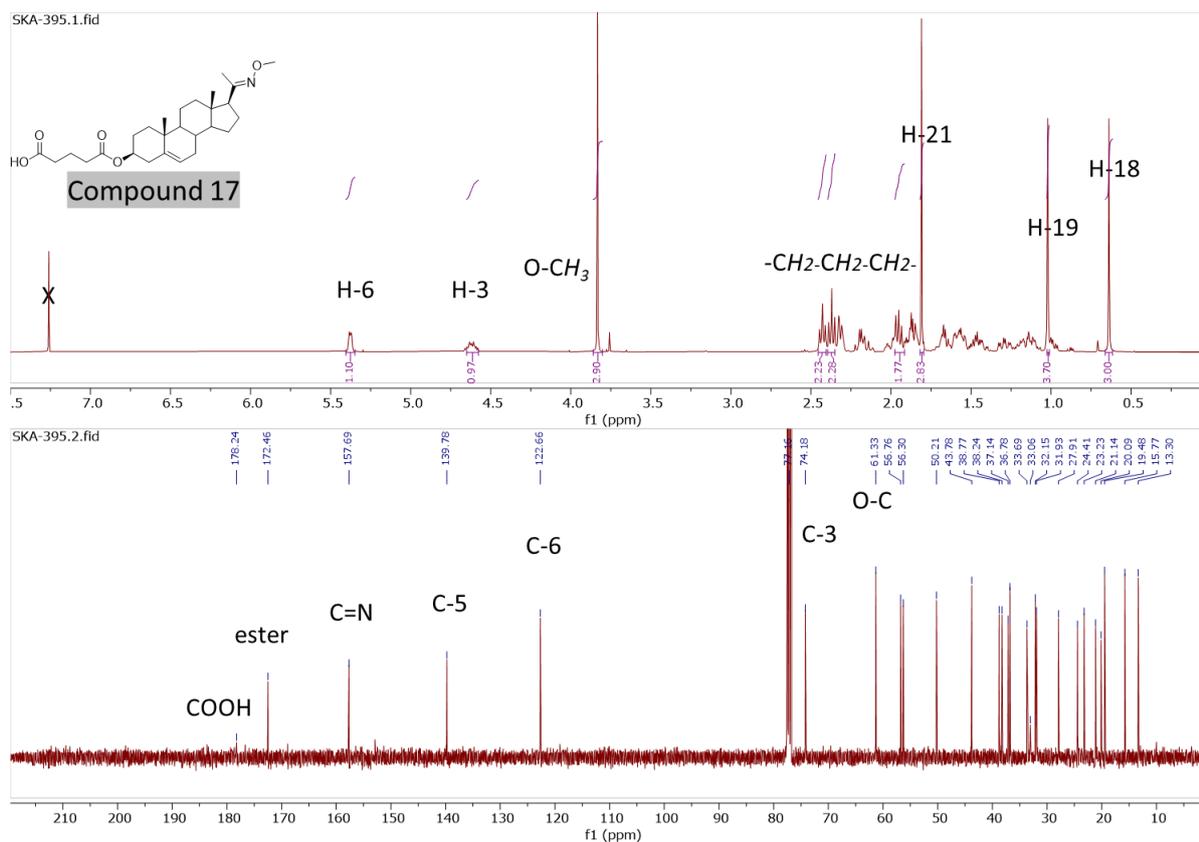


Figure S8. ^1H NMR and ^{13}C NMR and spectra of compound **18**

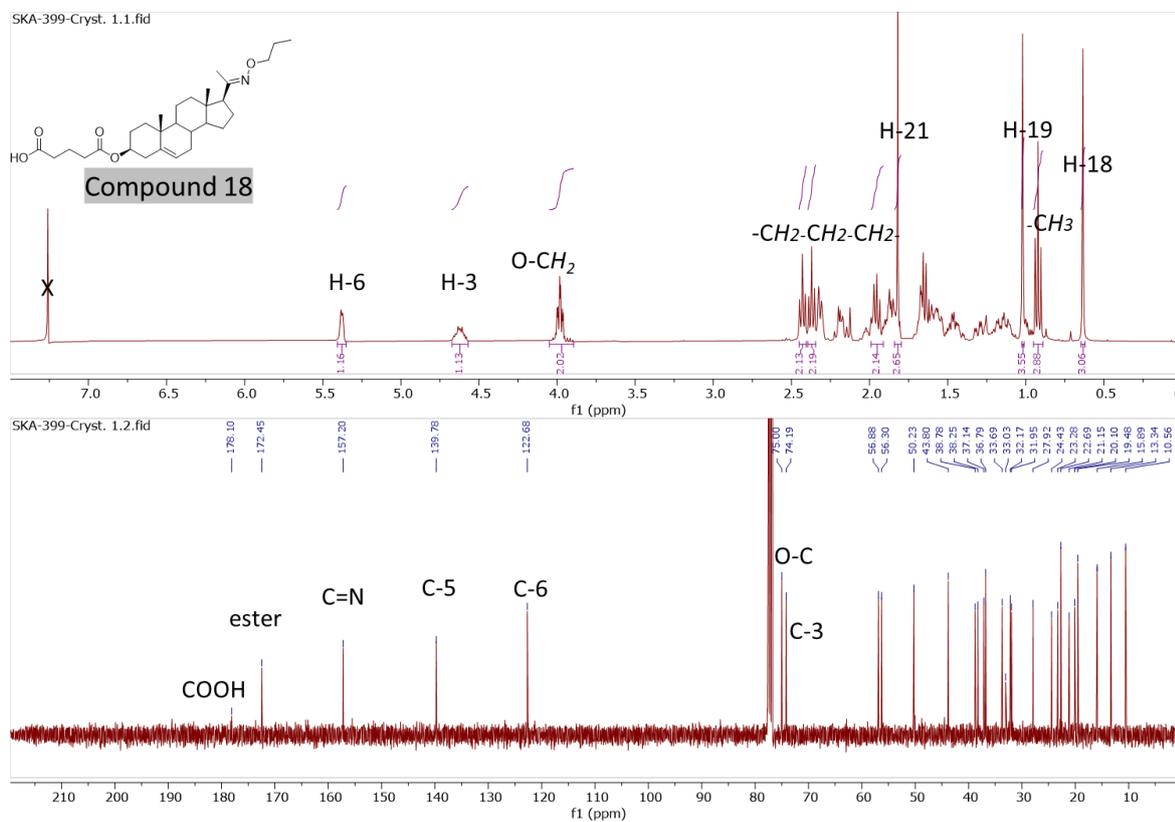


Figure S9. ^1H NMR and ^{13}C NMR and spectra of compound **19**

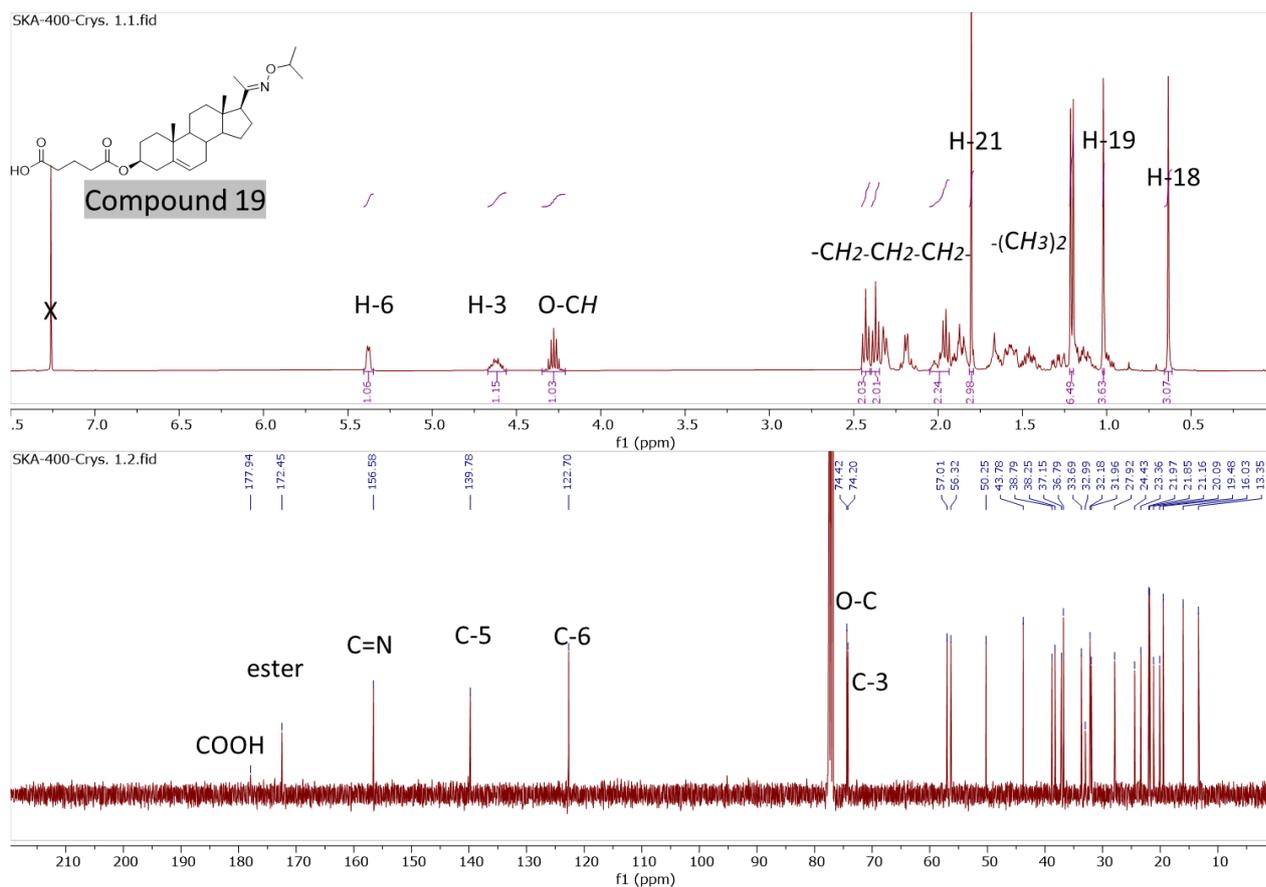


Figure S10. ^1H NMR and ^{13}C NMR and spectra of compound **20**

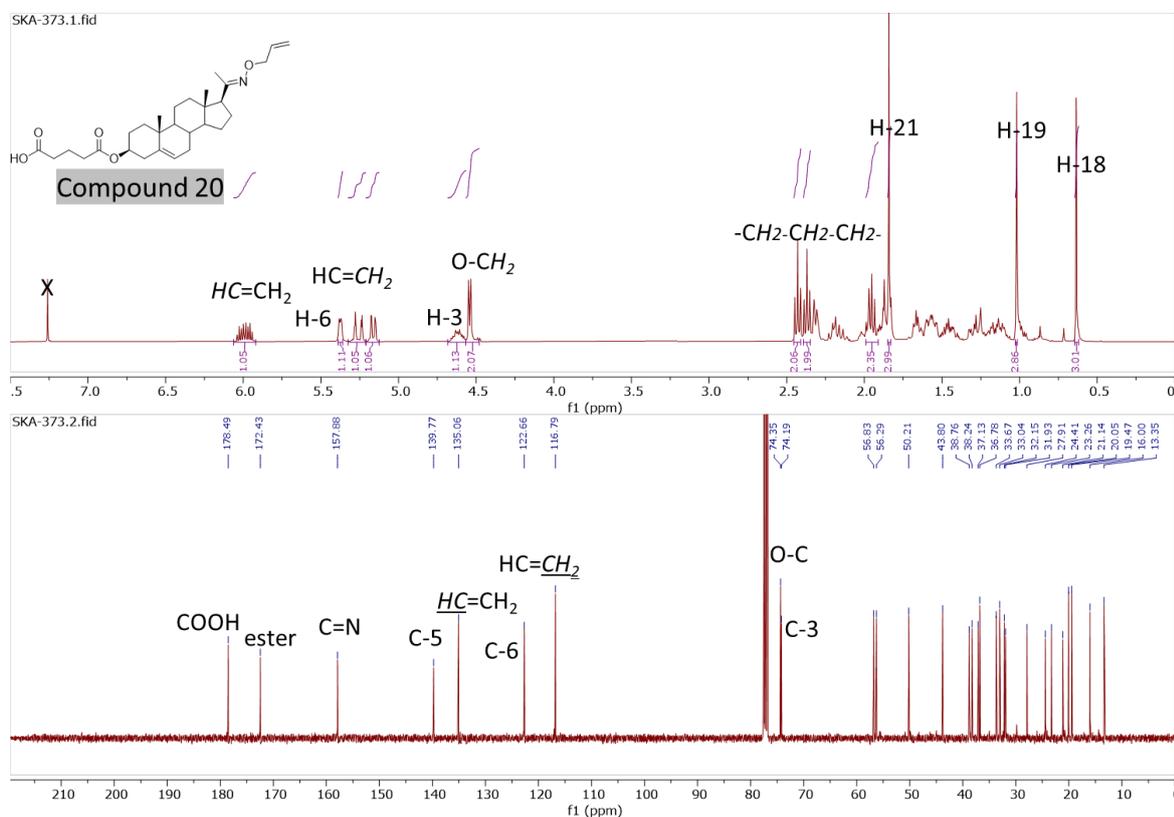


Figure S11. ^1H NMR and ^{13}C NMR and spectra of compound **21**

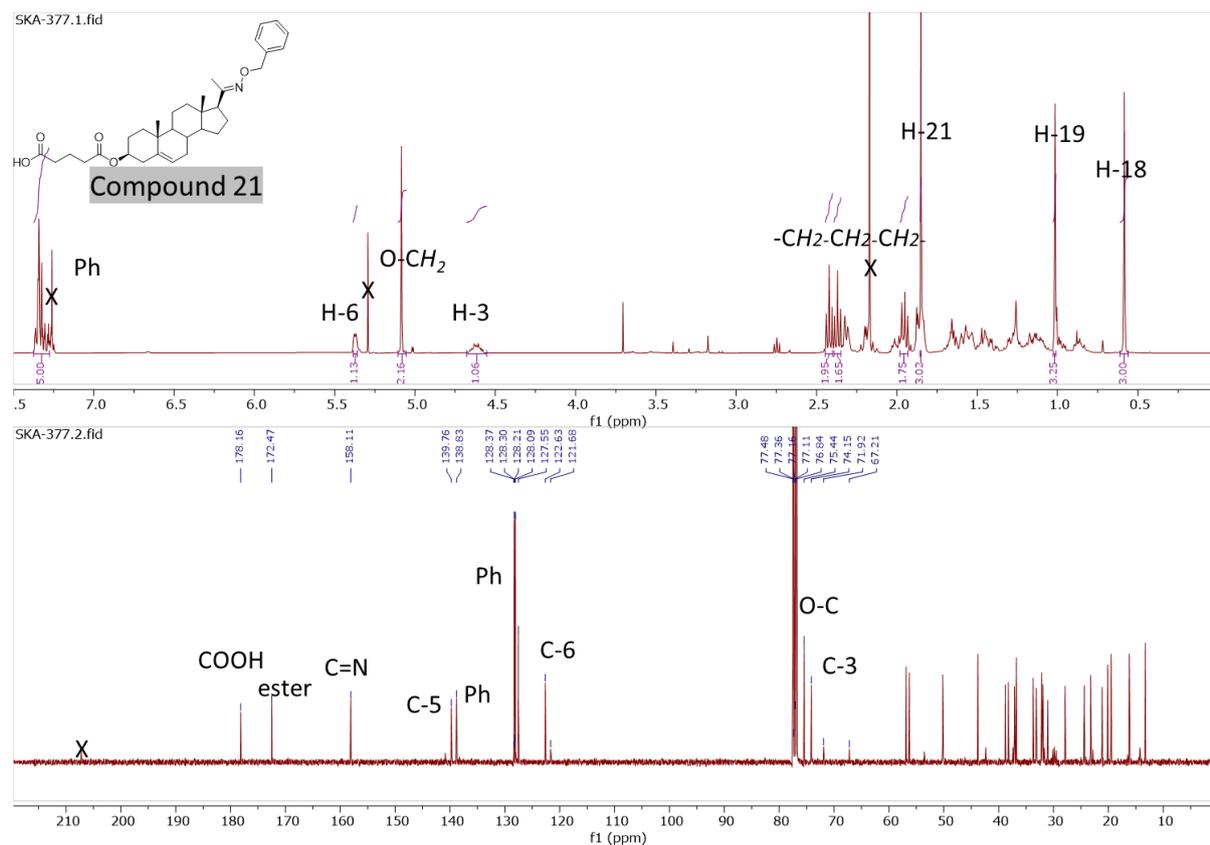


Figure S12. ^1H NMR and ^{13}C NMR and spectra of compound **22**

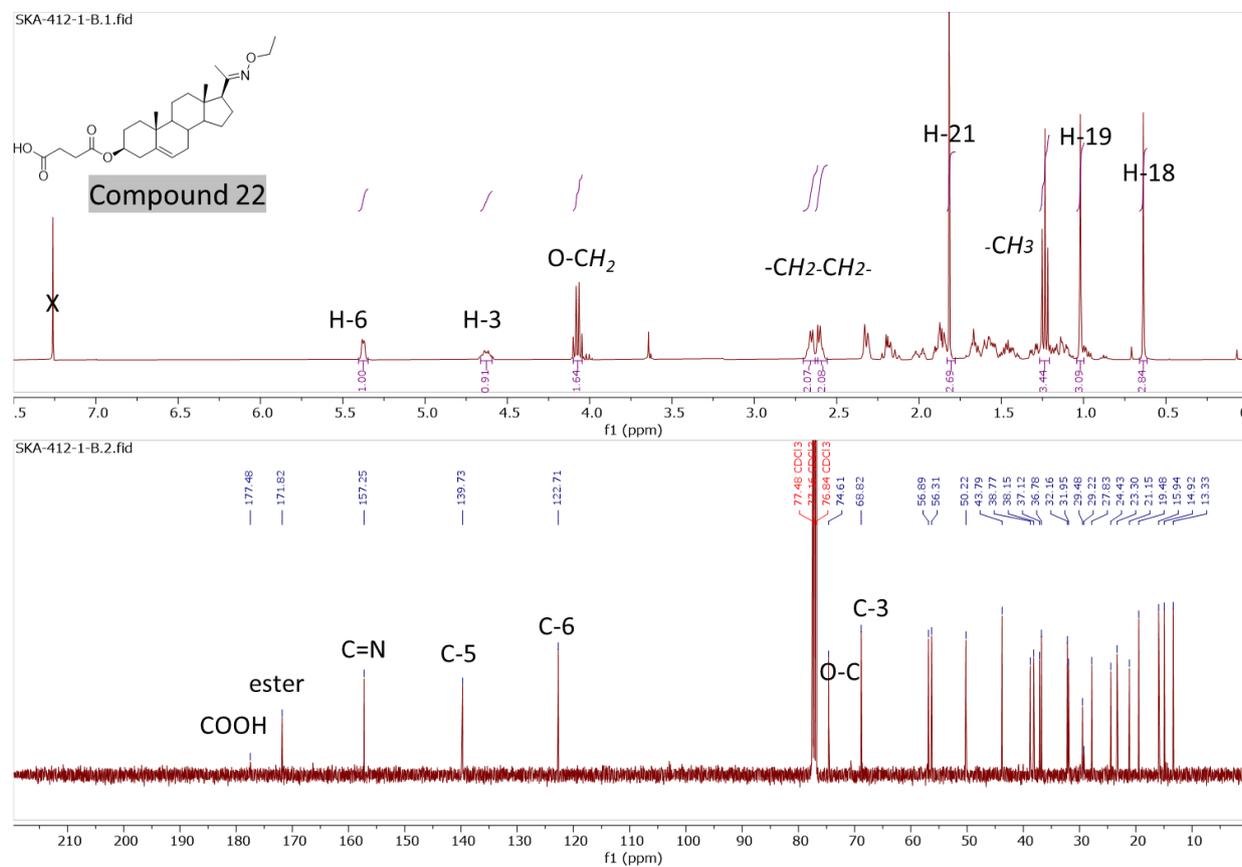


Figure S13. ^1H NMR and ^{13}C NMR and spectra of compound 23

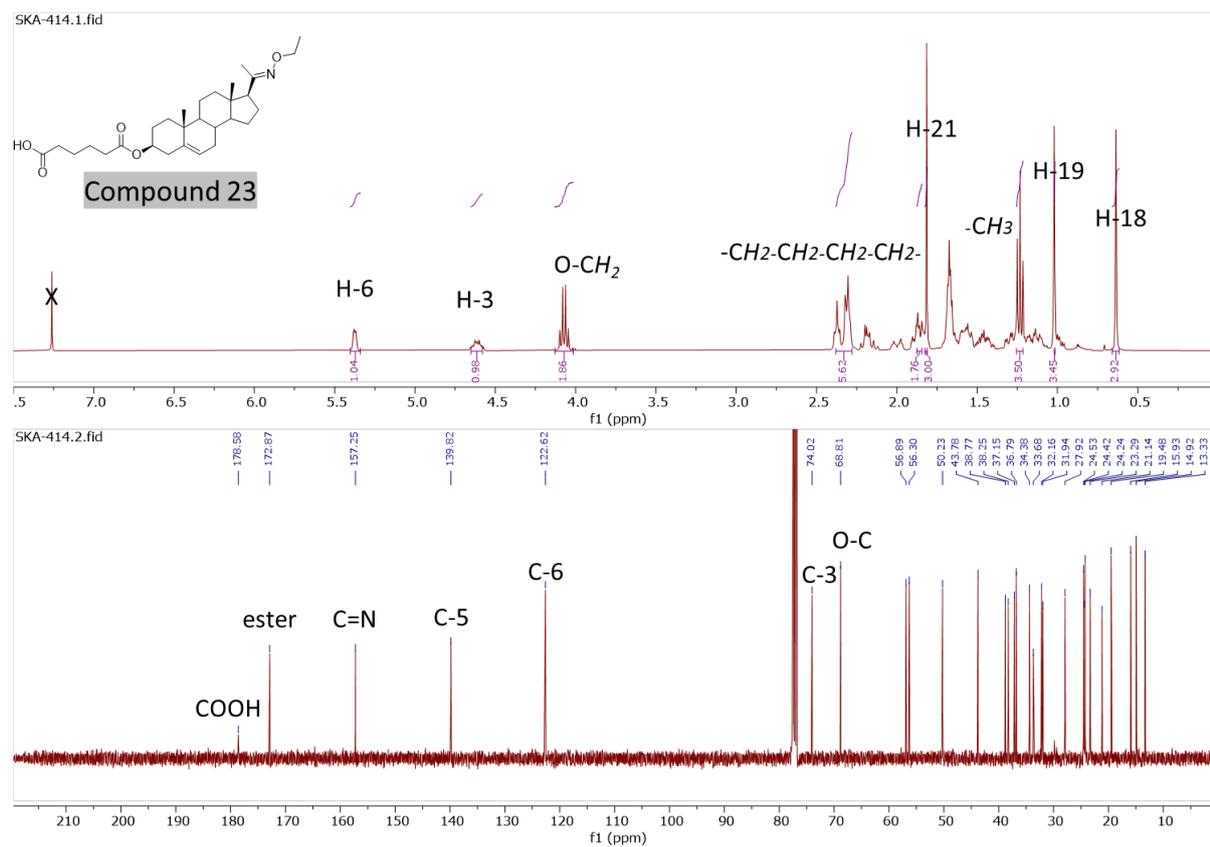


Figure S14. ^1H NMR and ^{13}C NMR and spectra of compound 24

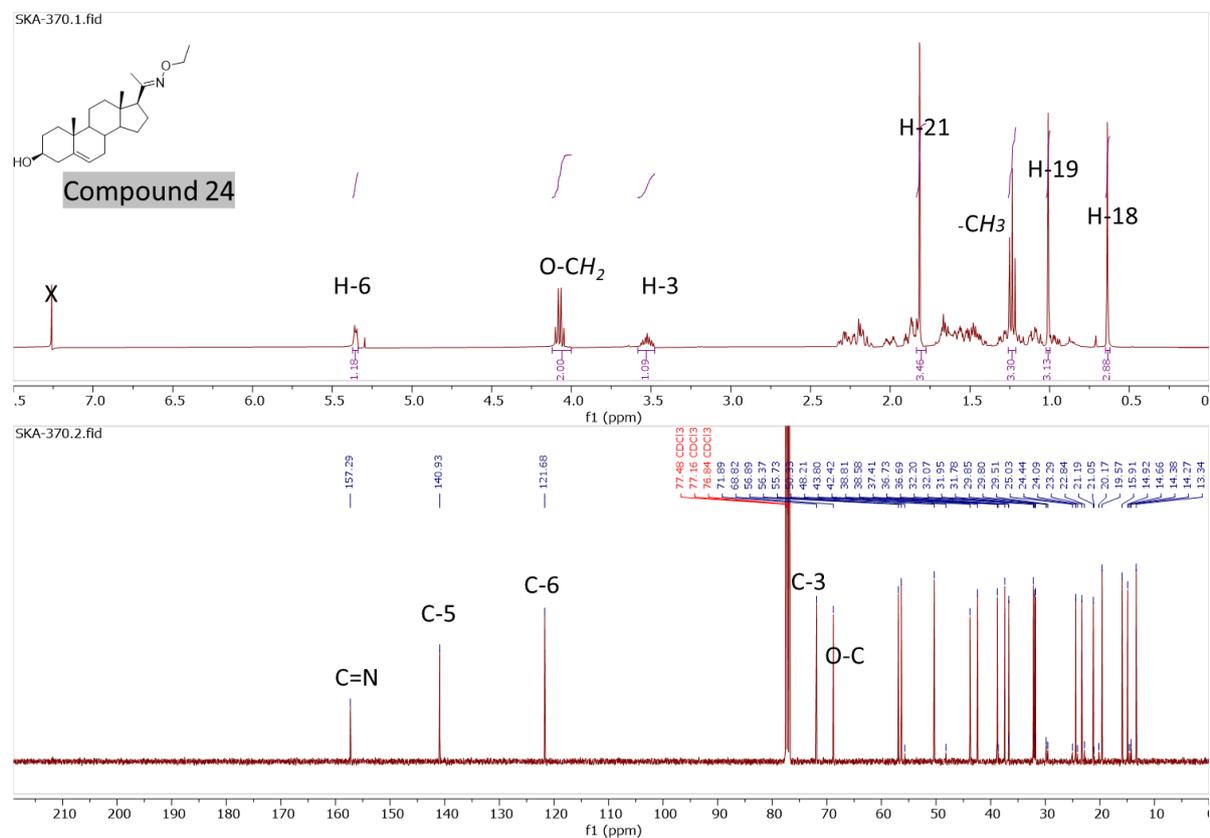


Figure S15. ^1H NMR and ^{13}C NMR and spectra of compound **25**

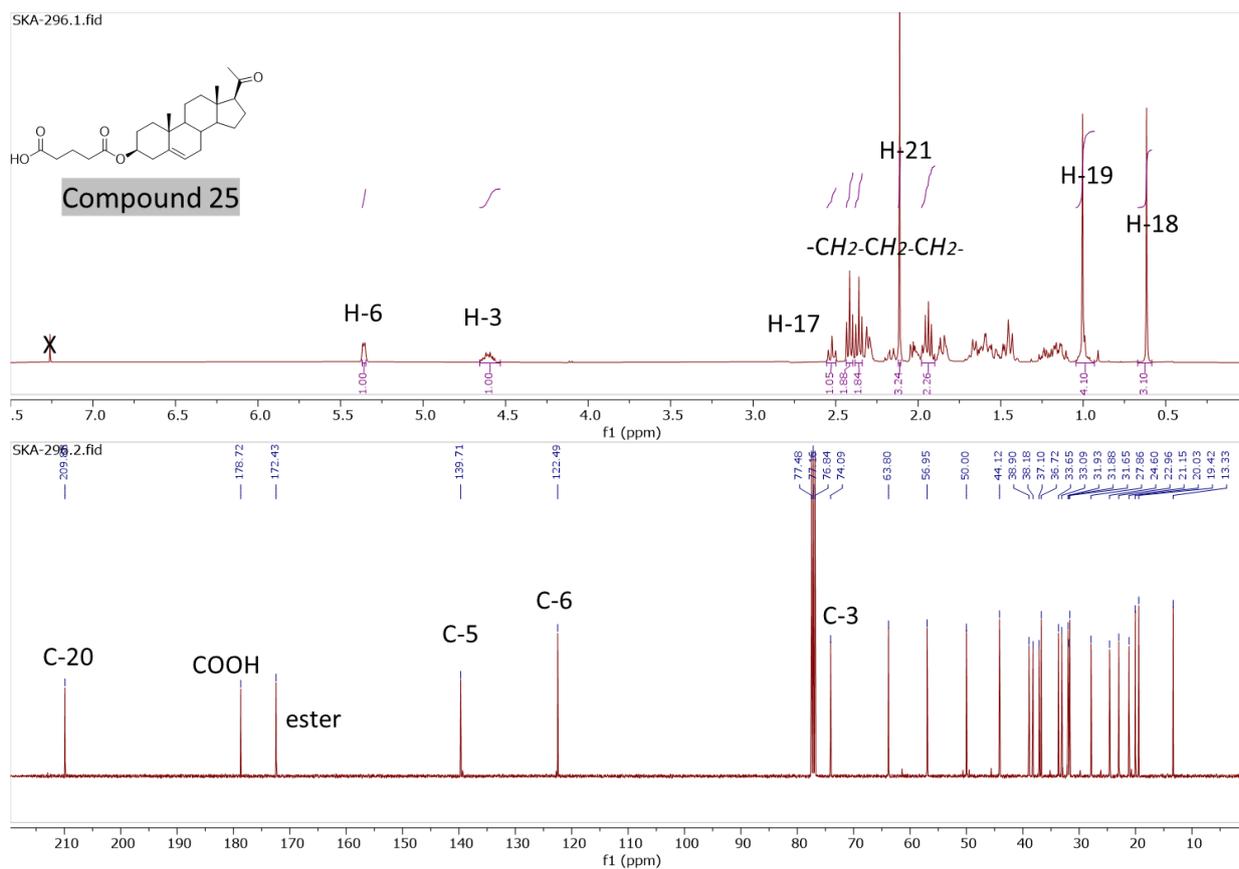


Figure S16. ^1H NMR and ^{13}C NMR and spectra of compound **26**

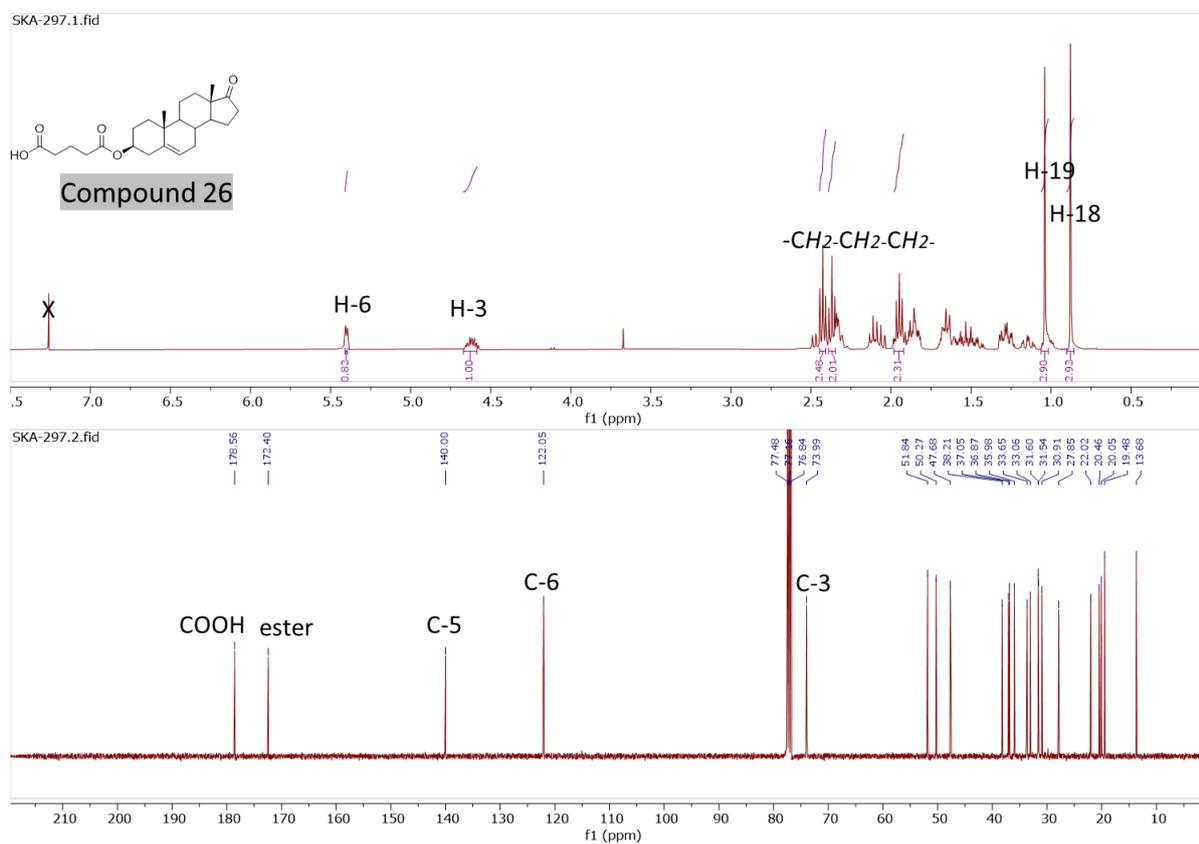


Figure S17. ^1H NMR and ^{13}C NMR and spectra of compound 27

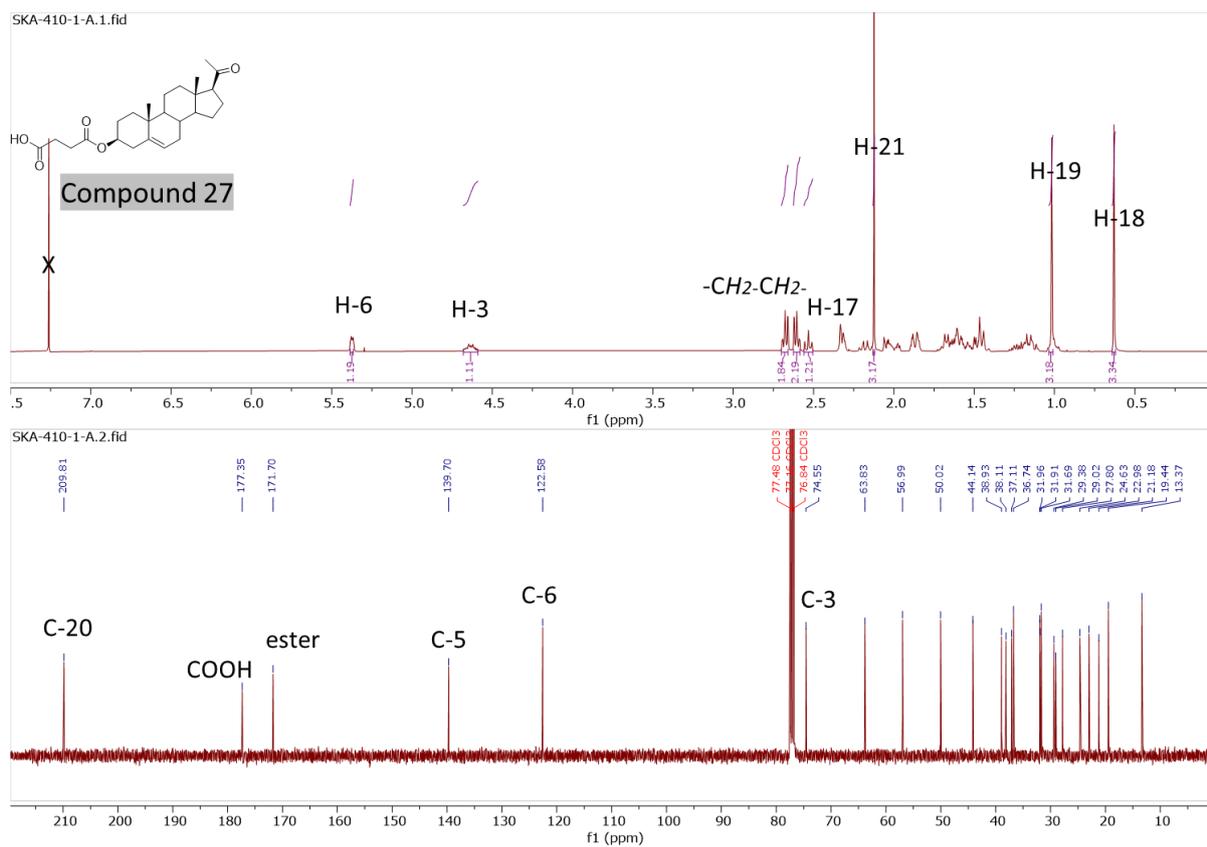
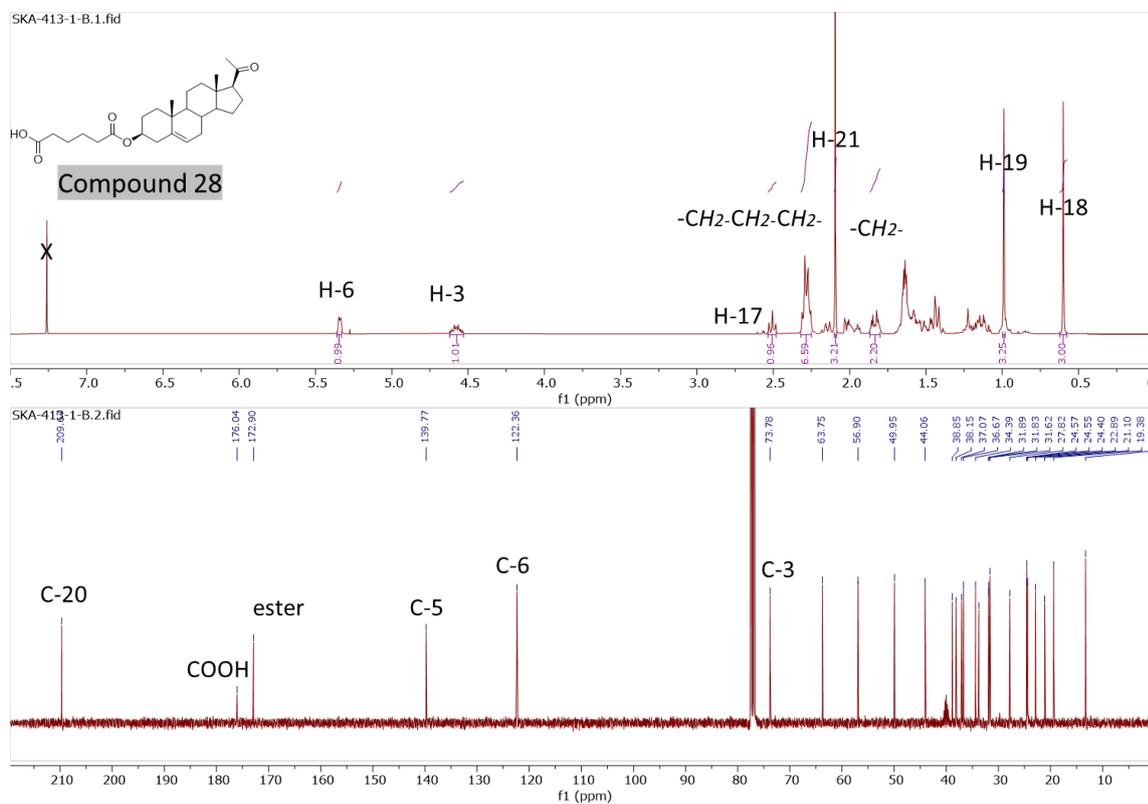


Figure S18. ^1H NMR and ^{13}C NMR and spectra of compound 28



HR-MS and LC-MS spectra of compounds 11-28

Figure S19. HR-MS and LC-MS spectra of compound 11

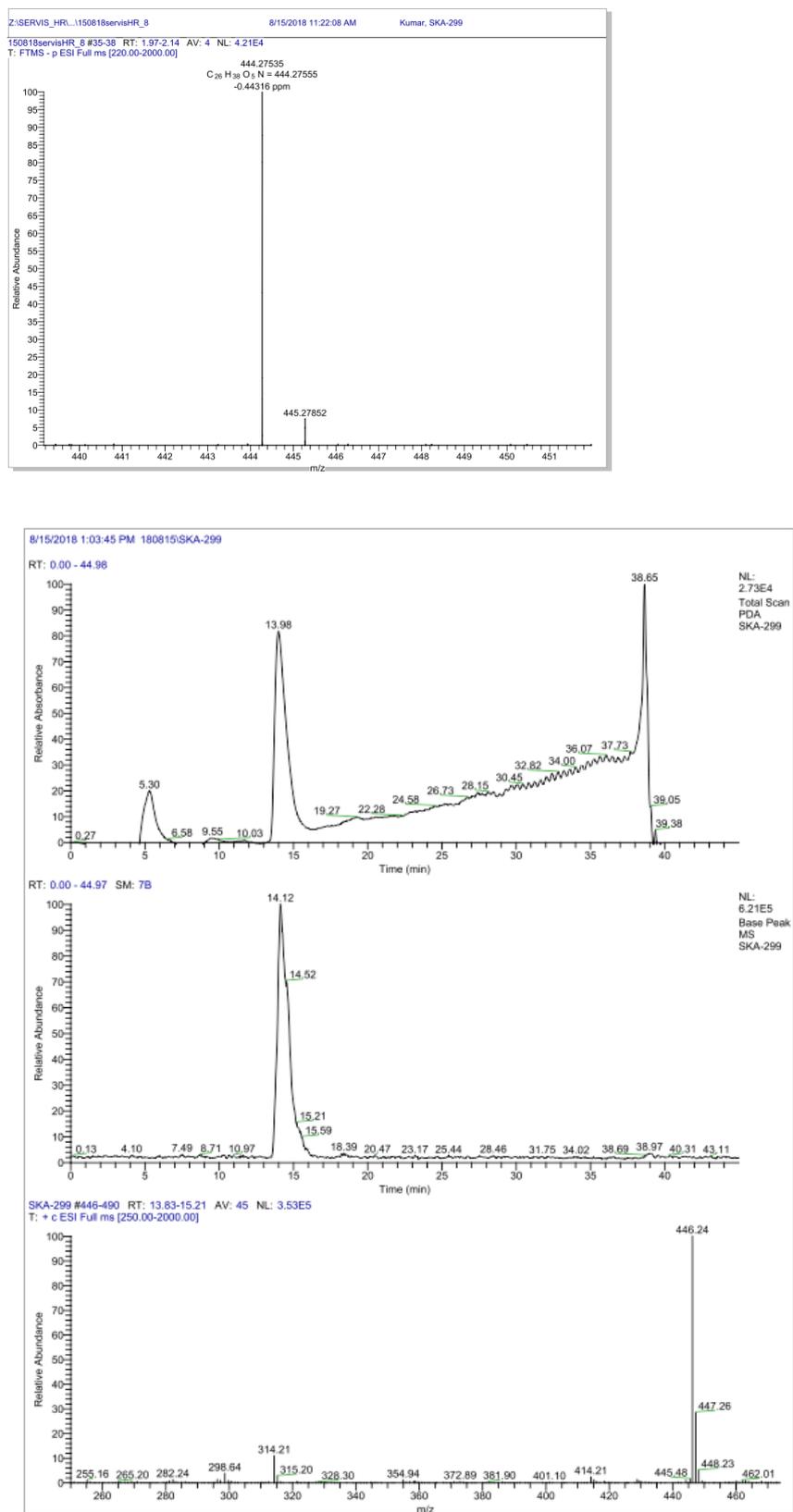


Figure S20. HR-MS and LC-MS spectra of compound 12

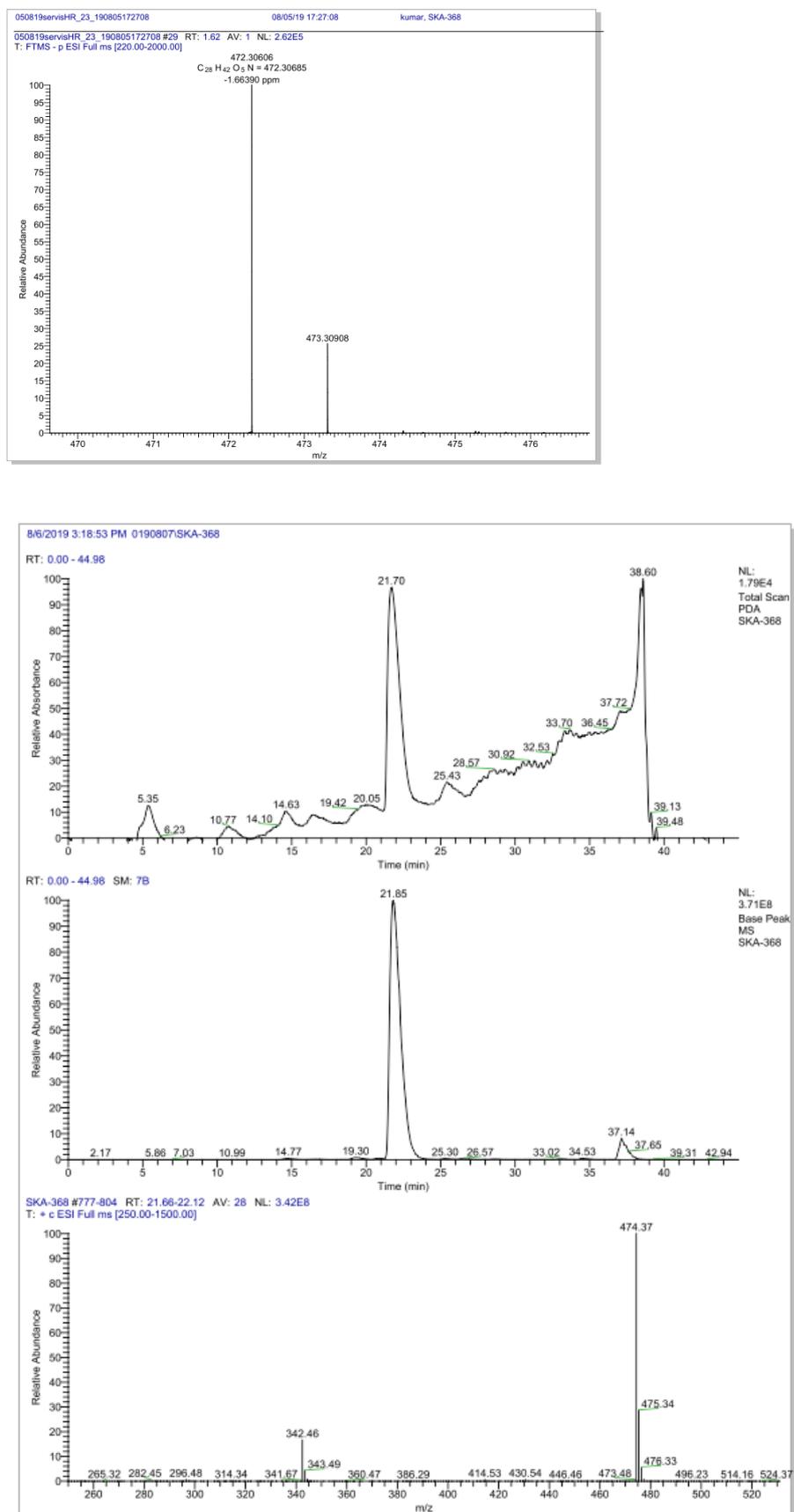


Figure S21. HR-MS and LC-MS spectra of compound **13**

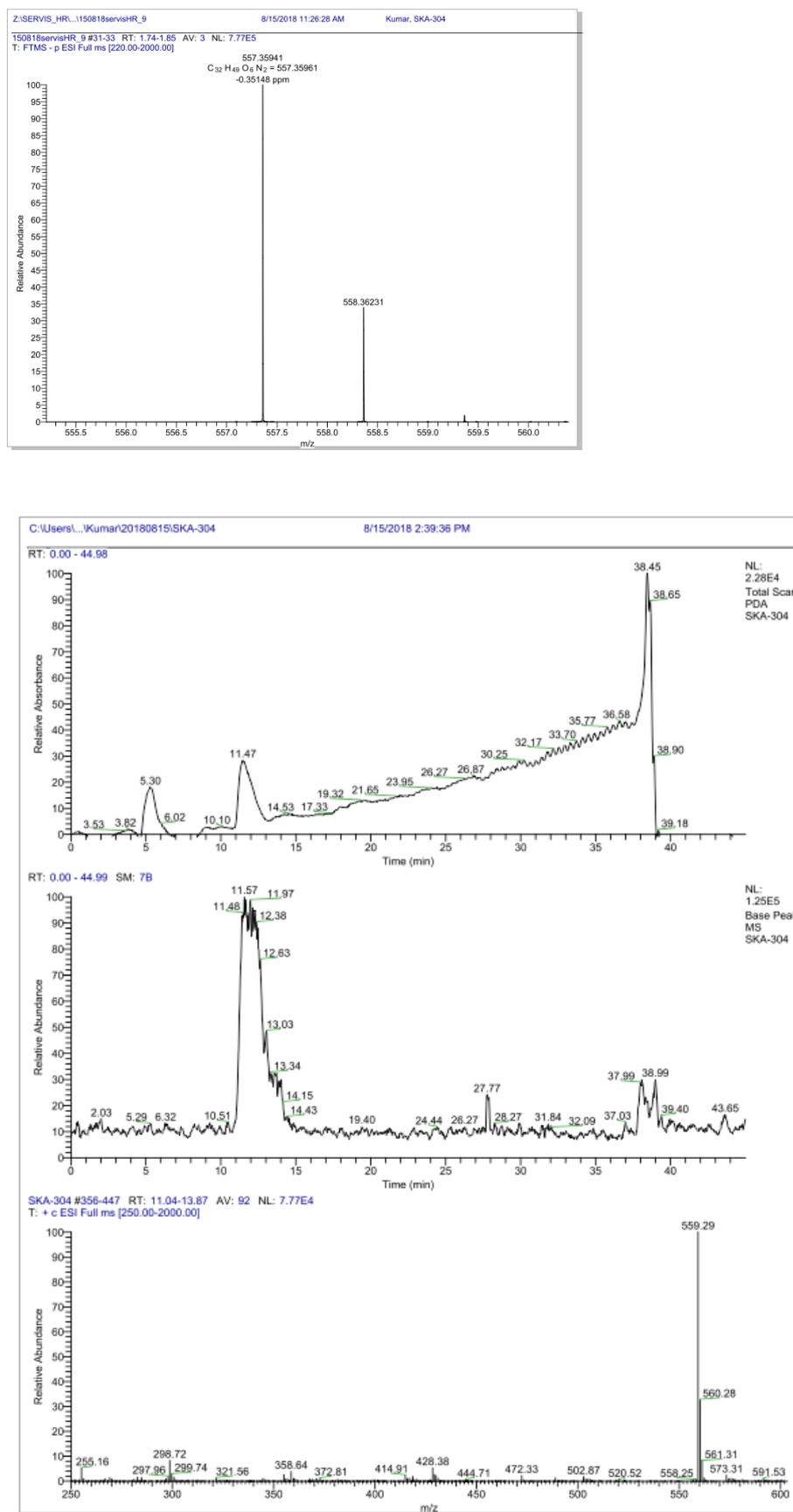


Figure S22. HR-MS and LC-MS spectra of compound 14

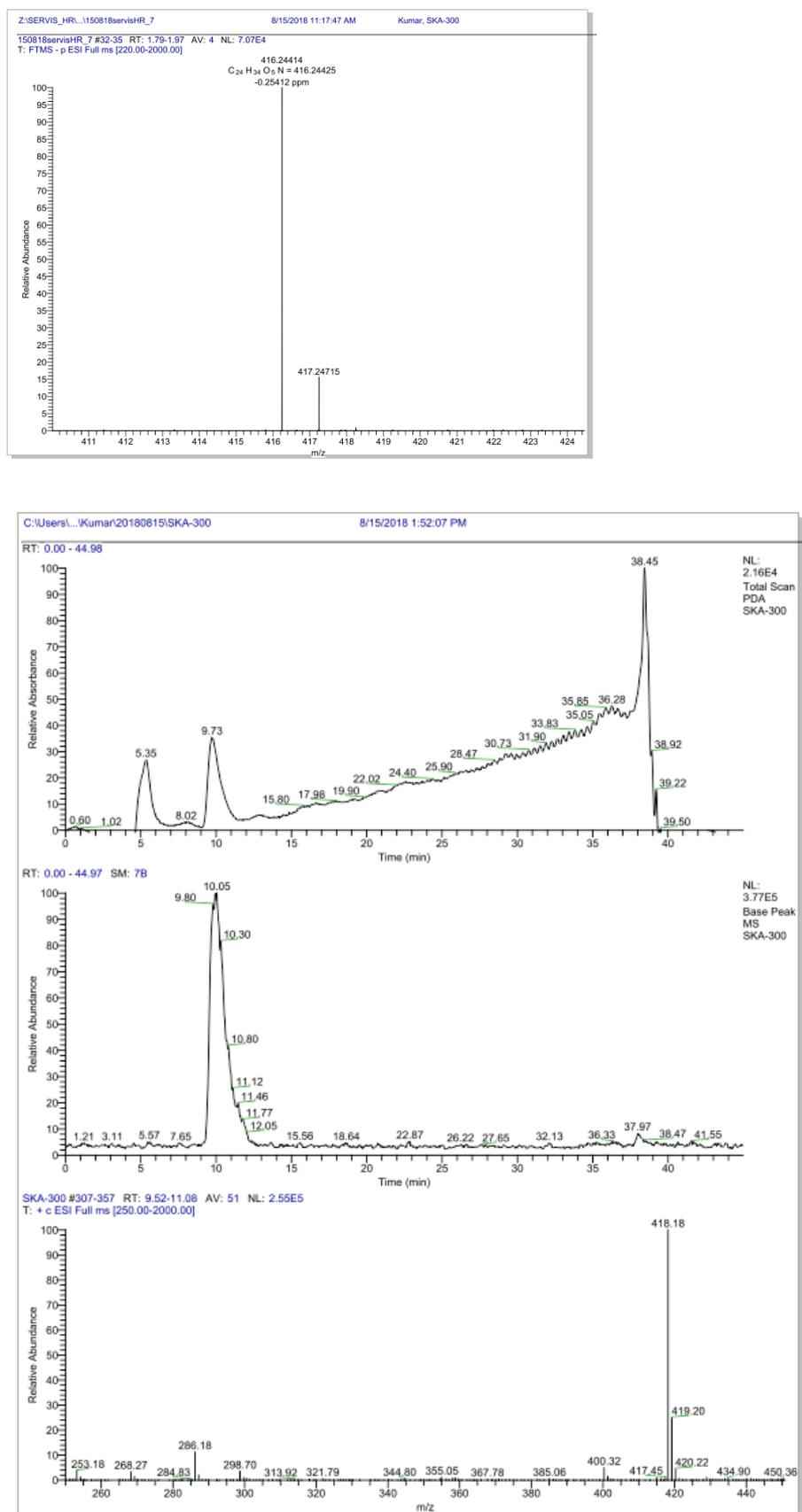


Figure S23. HR-MS and LC-MS spectra of compound **15**

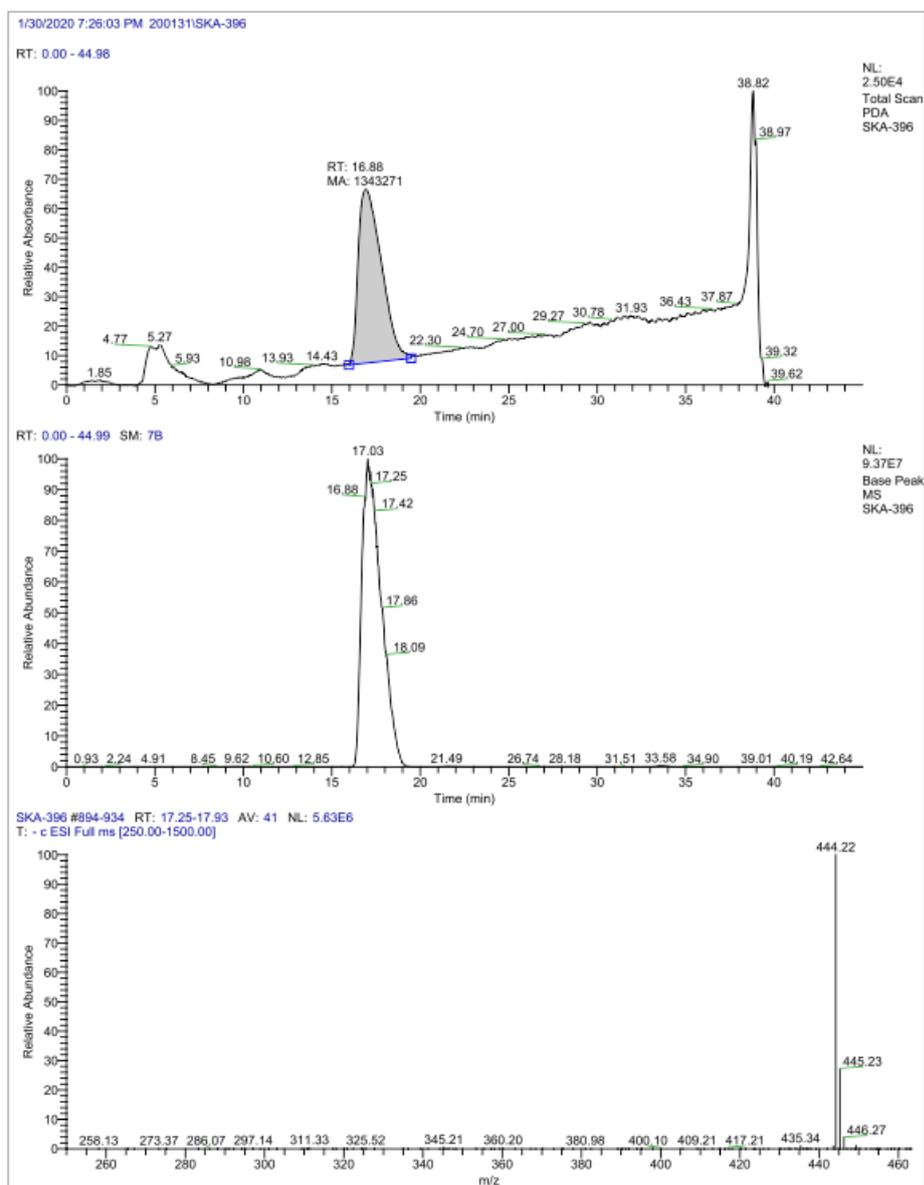
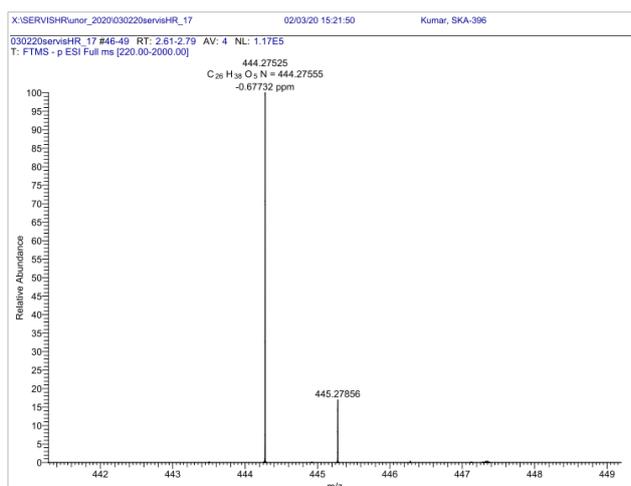


Figure S24. HR-MS and LC-MS spectra of compound **16**

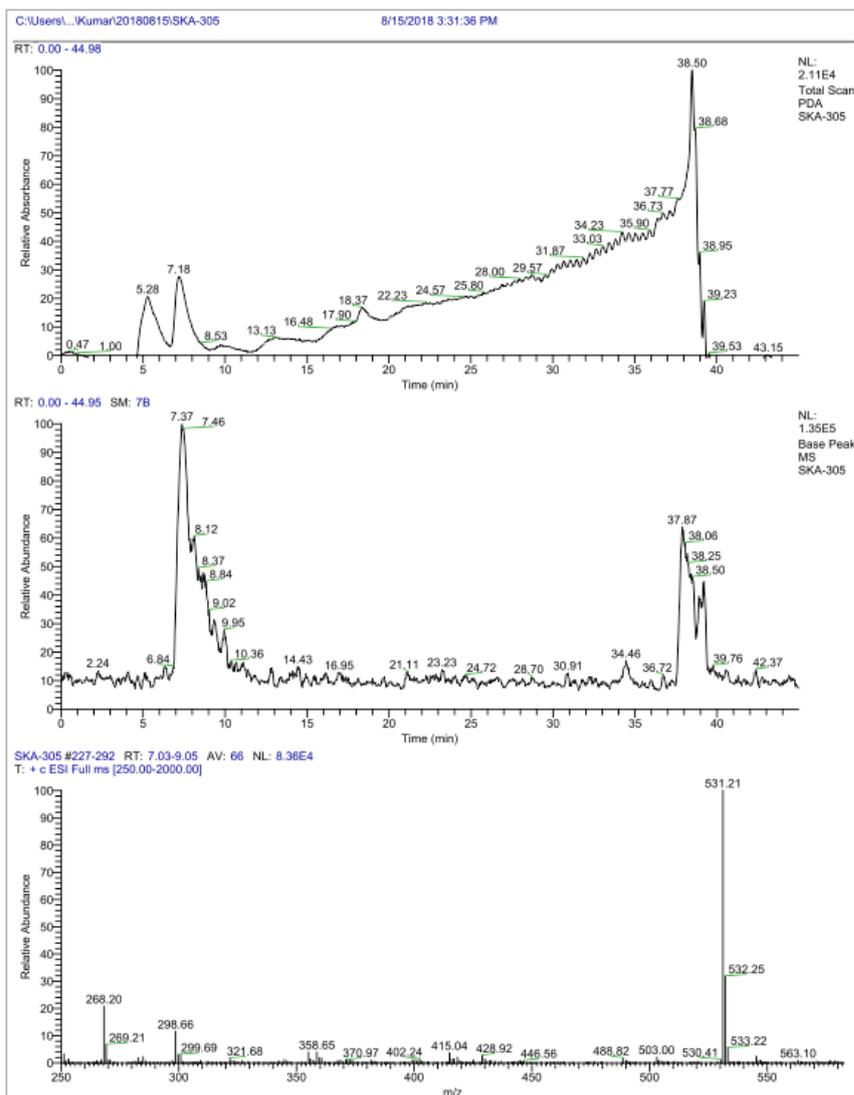
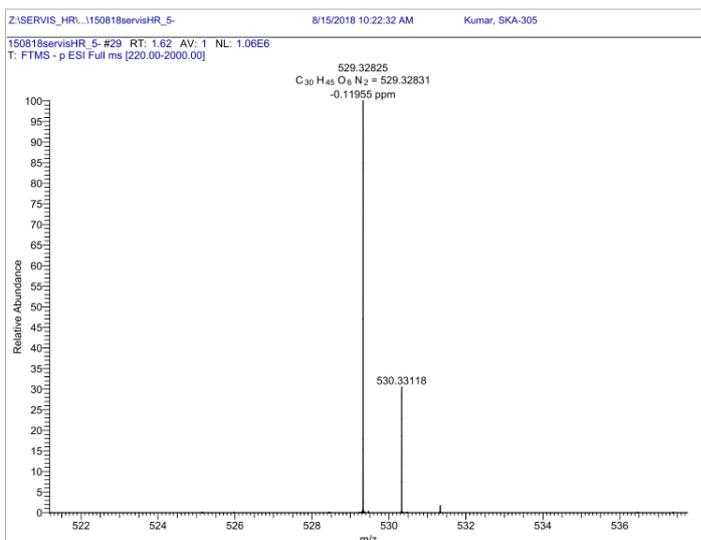
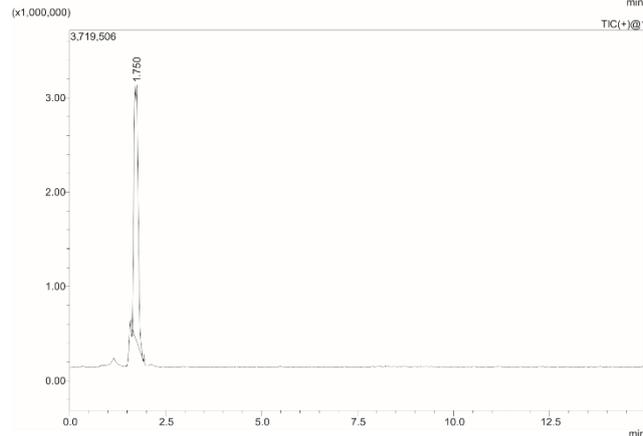
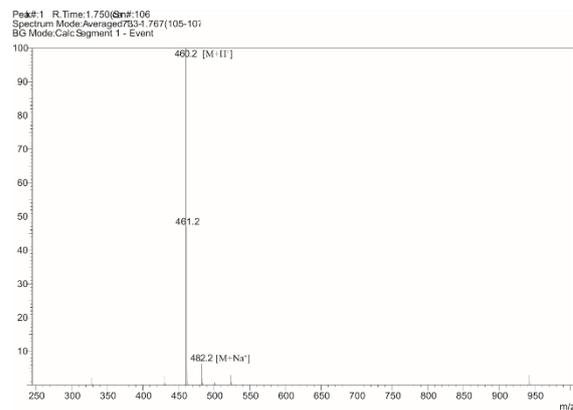
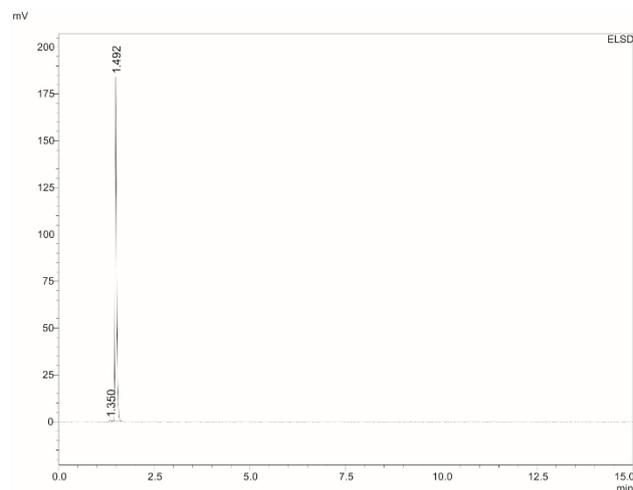
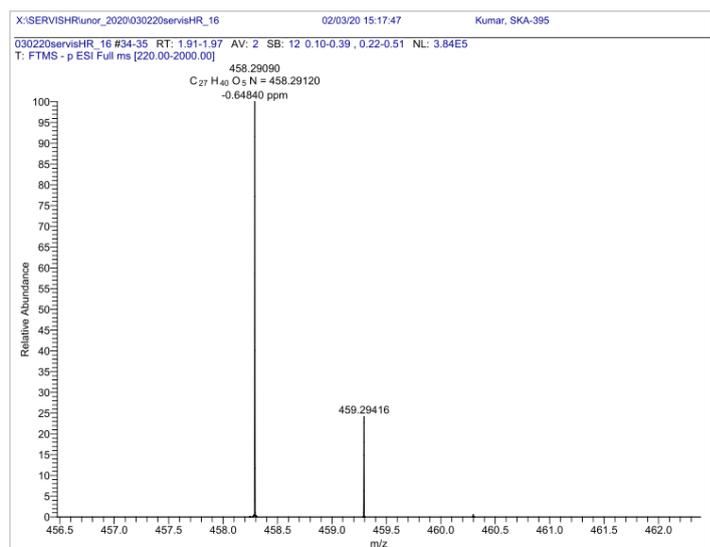


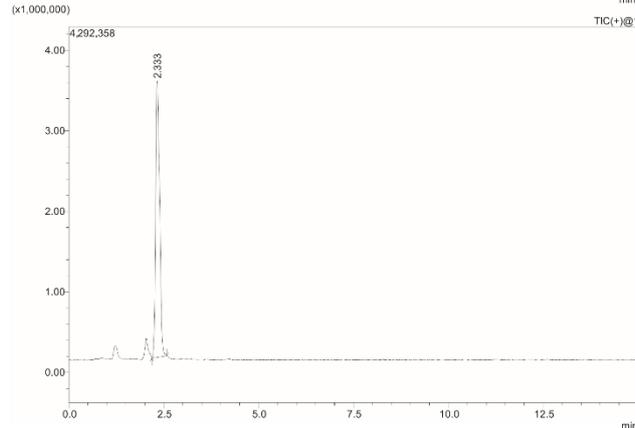
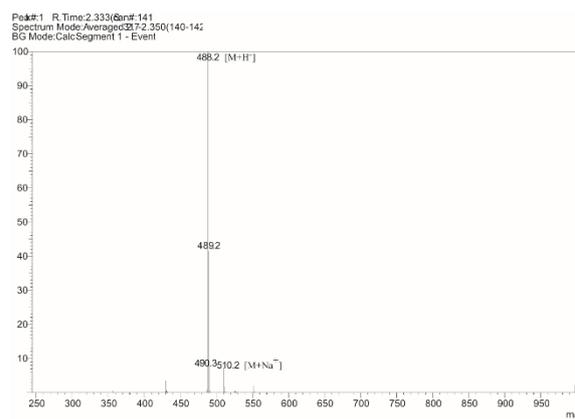
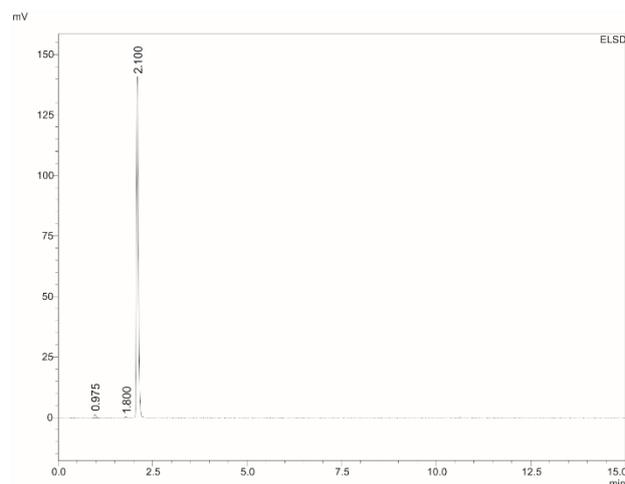
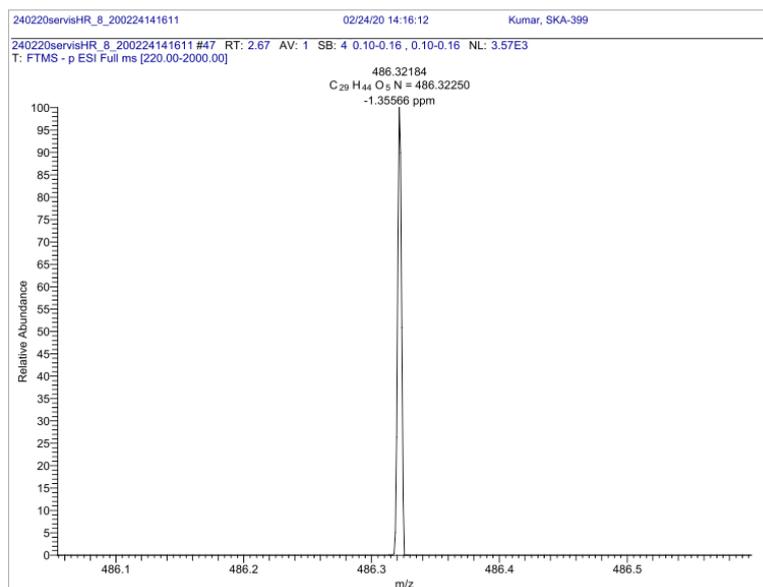
Figure S25. HR-MS and LC-MS spectra of compound **17**



Box :
 Position :
 Method Filename : C8-80,20.lcm
 Vial # : 1-2
 Injection Volume : 0.3 μ L
 Date Acquired : 25-Aug-22 12:30:51
 Comment : Isocratic, A: H₂O, MeOH, FA (950:50:1); B: ACN; A:B (80:20), 0.5 mL/min
 Column, Shim-pack Scepter, C8-120, 1.9 μ m, 2.1x100 mm, (Shimadzu)

ELSD Ret. Time	Area	Area%
1.350	2255	0.410
1.492	548194	99.590
	550450	100.000

Figure S26. HR-MS and LC-MS spectra of compound **18**



Box :
 Position :
 Method Filename : C8-80.20.lcm
 Vial # : 1-3
 Injection Volume : 0.1 uL
 Date Acquired : 25-Aug-22 13:16:04
 Comment : Isocratic, A: H₂O, MeOH, FA (950:50:1); B: ACN; A:B (80:20) 0.5 mL/min
 Column, Shim-pack Scepter, C8-120, 1.9 um, 2.1x100 mm, (Shimadzu)

Ret. Time	Area	Area%
0.975	4439	0.918
1.800	868	0.179
2.100	478375	98.903
	483681	100.000

Figure S27. HR-MS and LC-MS spectra of compound 19

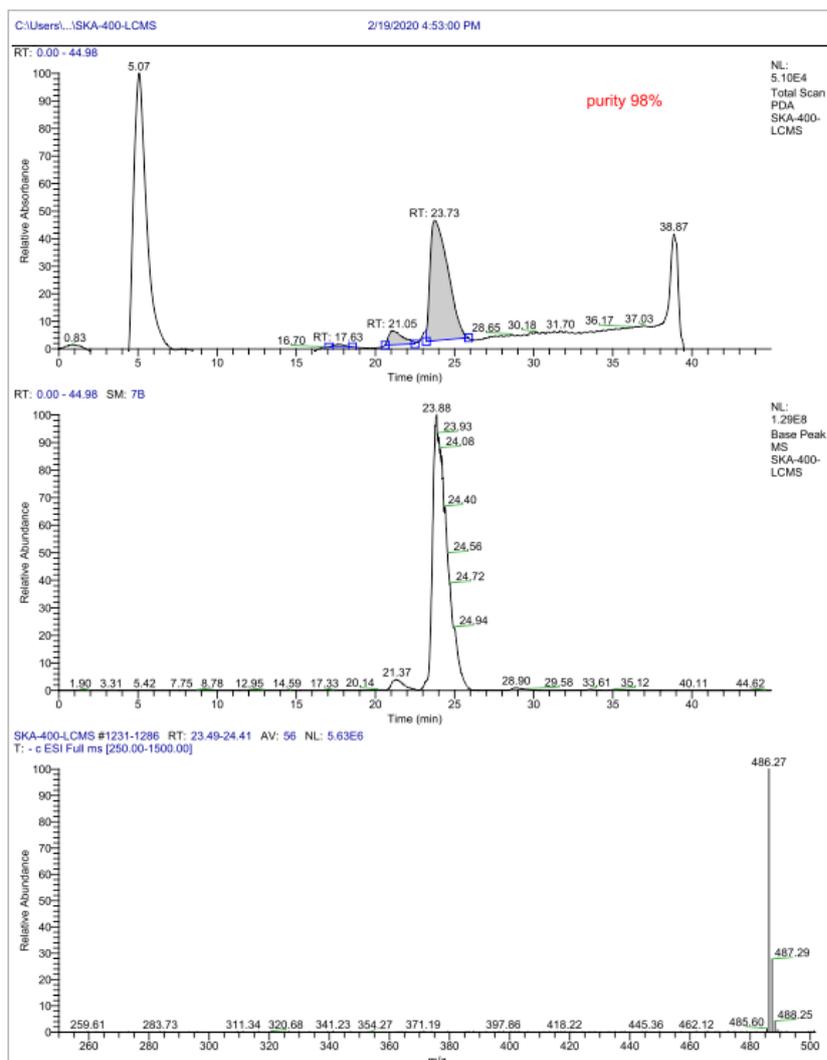
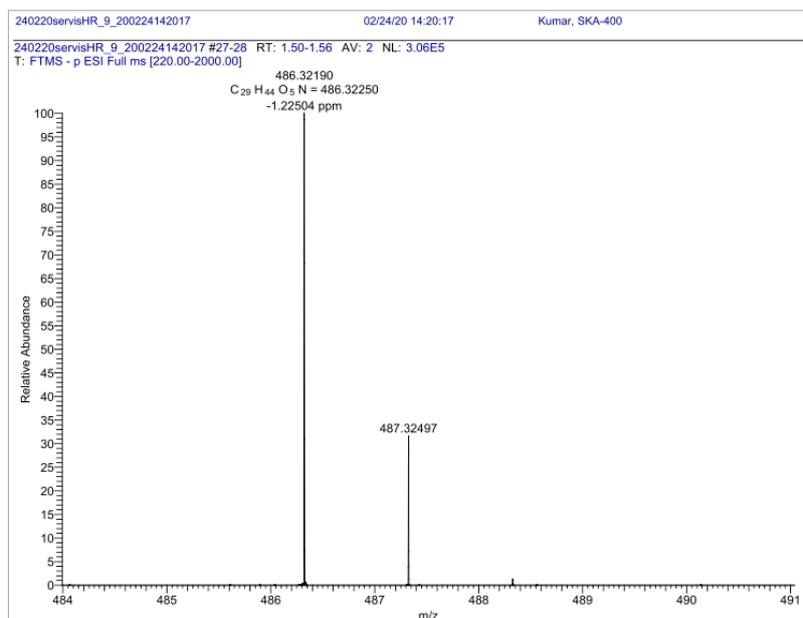


Figure S28. HR-MS and LC-MS spectra of compound **20**

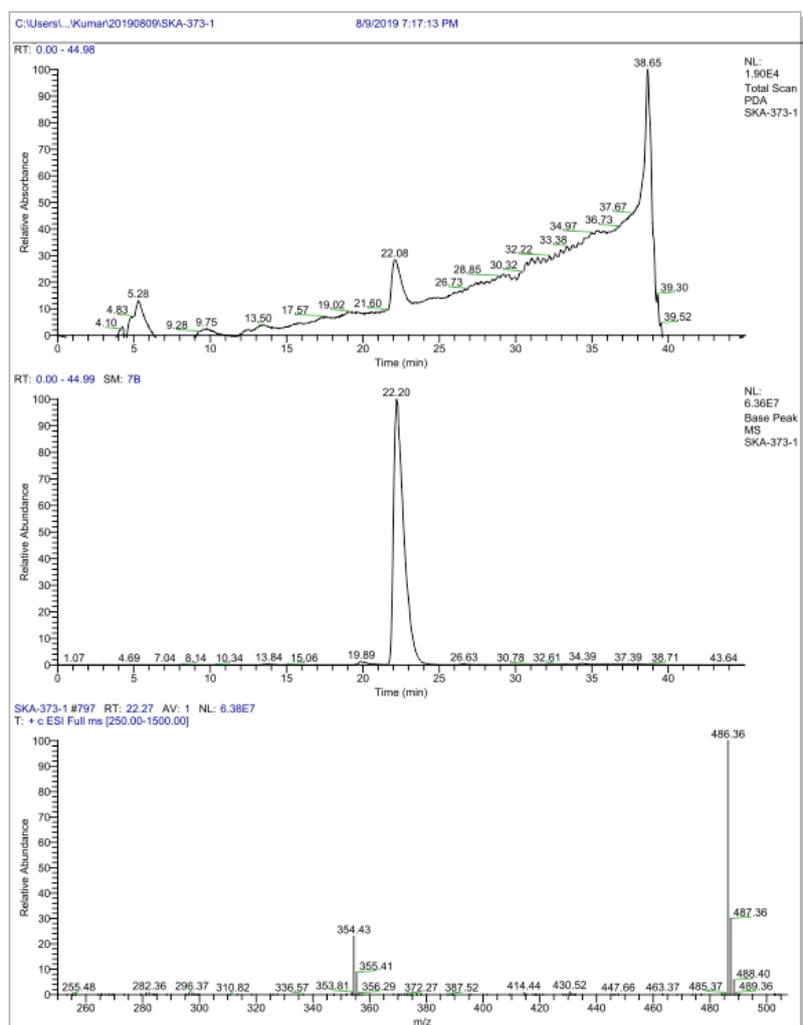
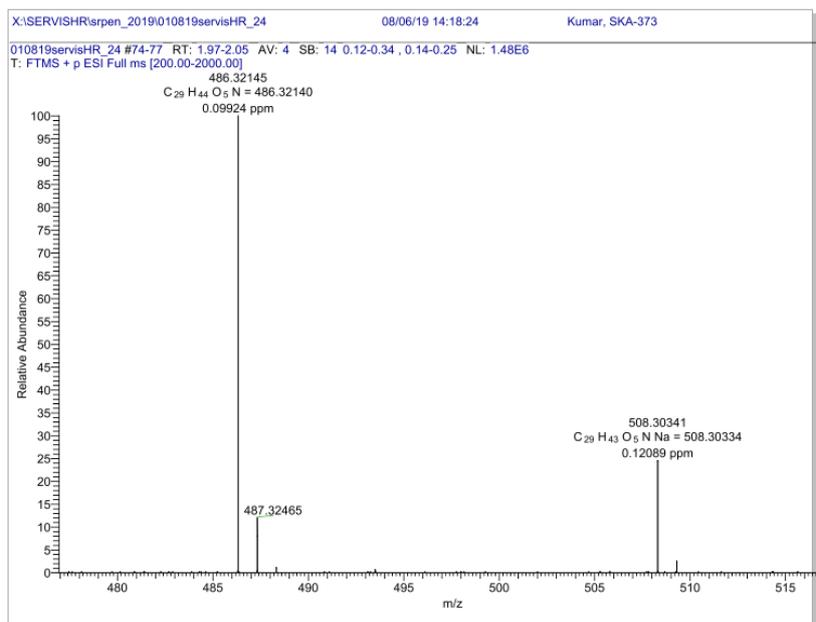


Figure S29. HR-MS and LC-MS spectra of compound **21**

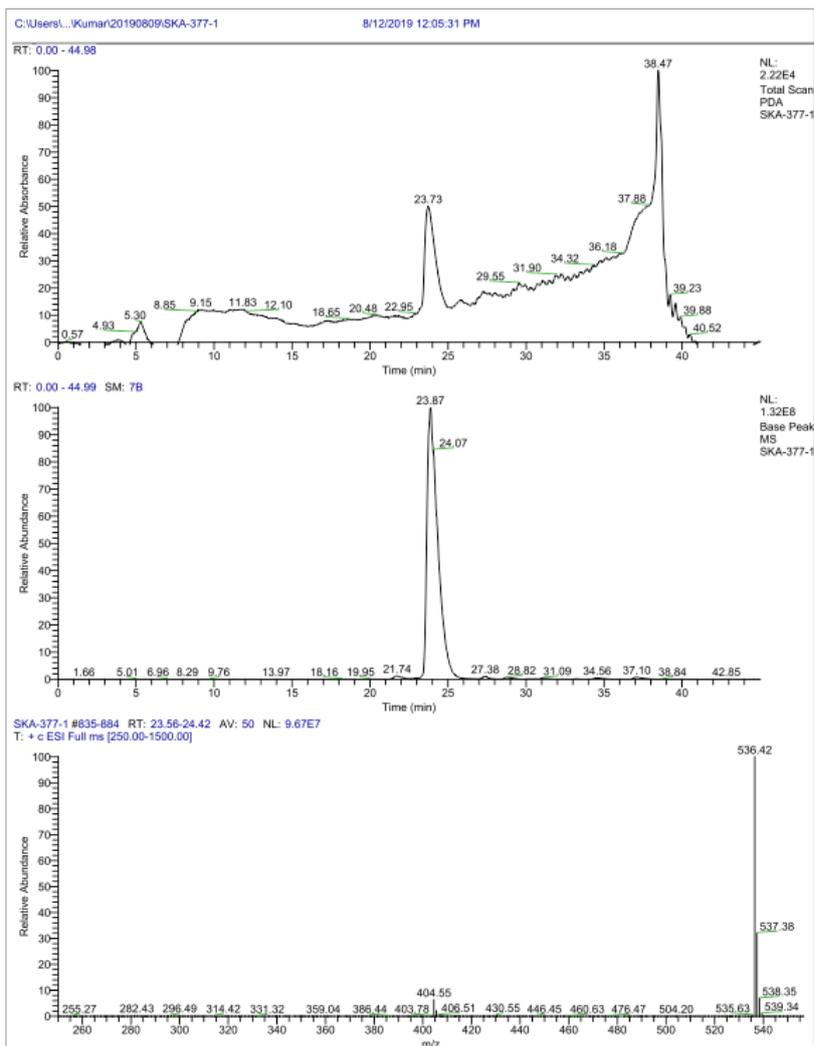
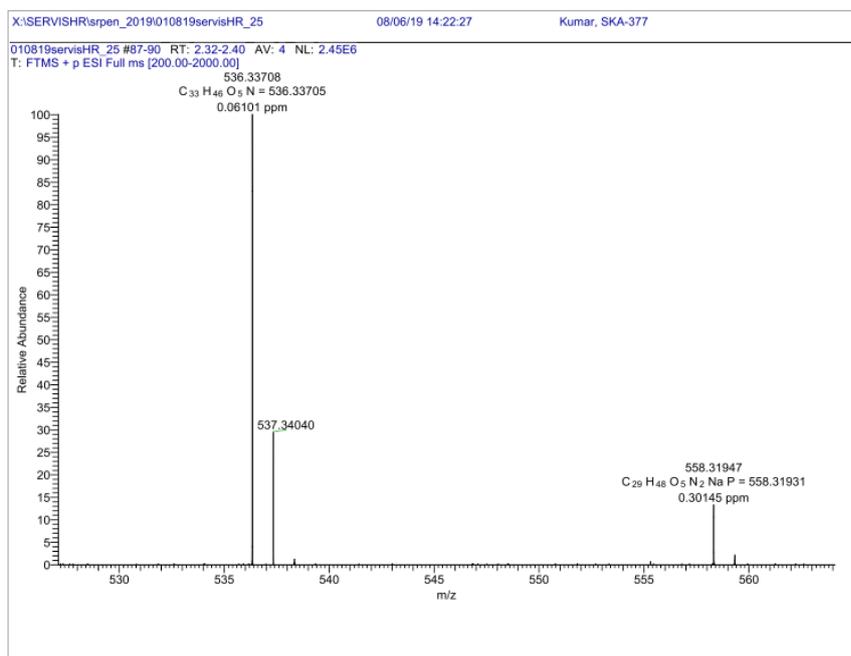


Figure S30. HR-MS and LC-MS spectra of compound **22**

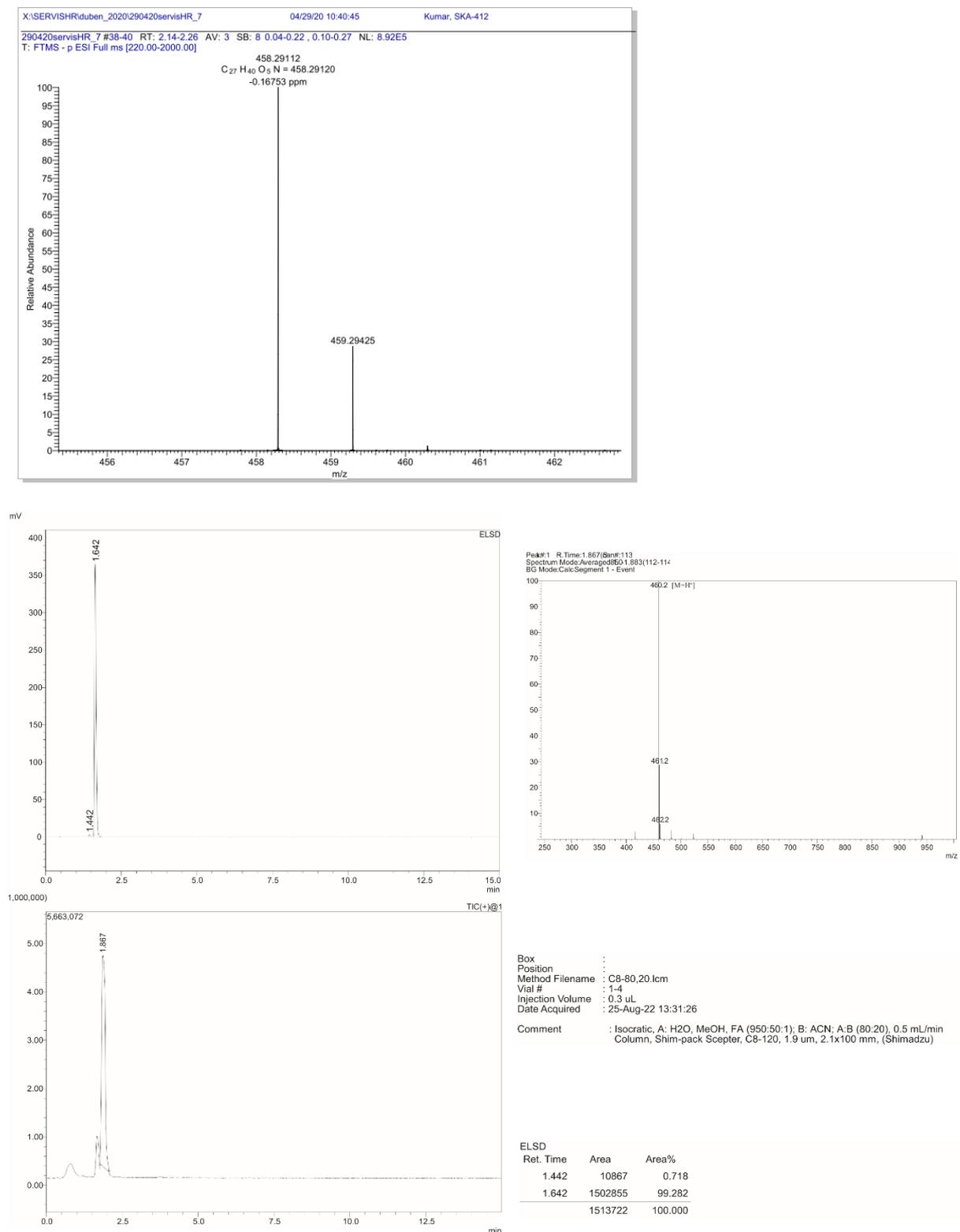


Figure S31. HR-MS and LC-MS spectra of compound **23**

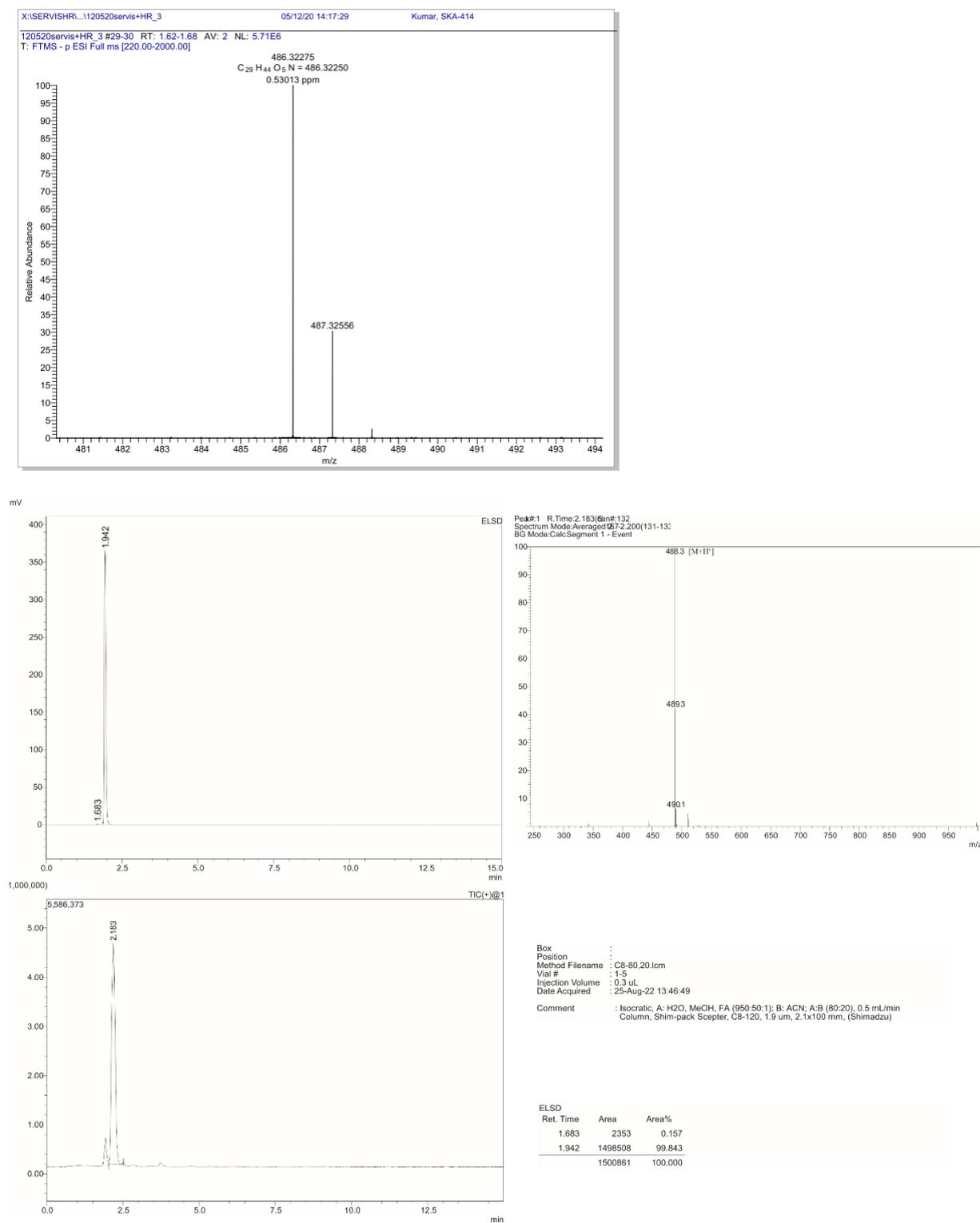


Figure S32. HR-MS and LC-MS spectra of compound **24**

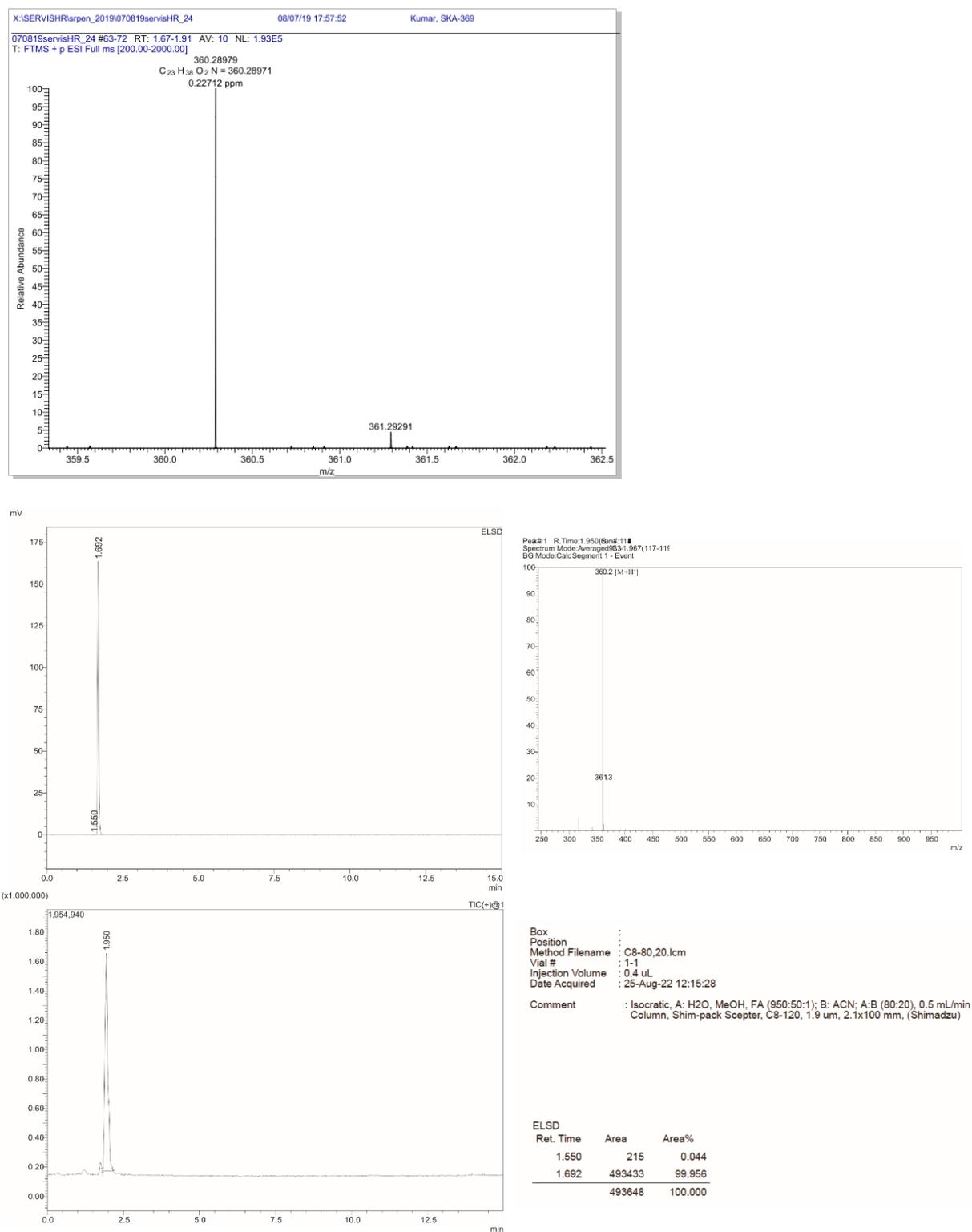


Figure S33. HR-MS and LC-MS spectra of compound **25**

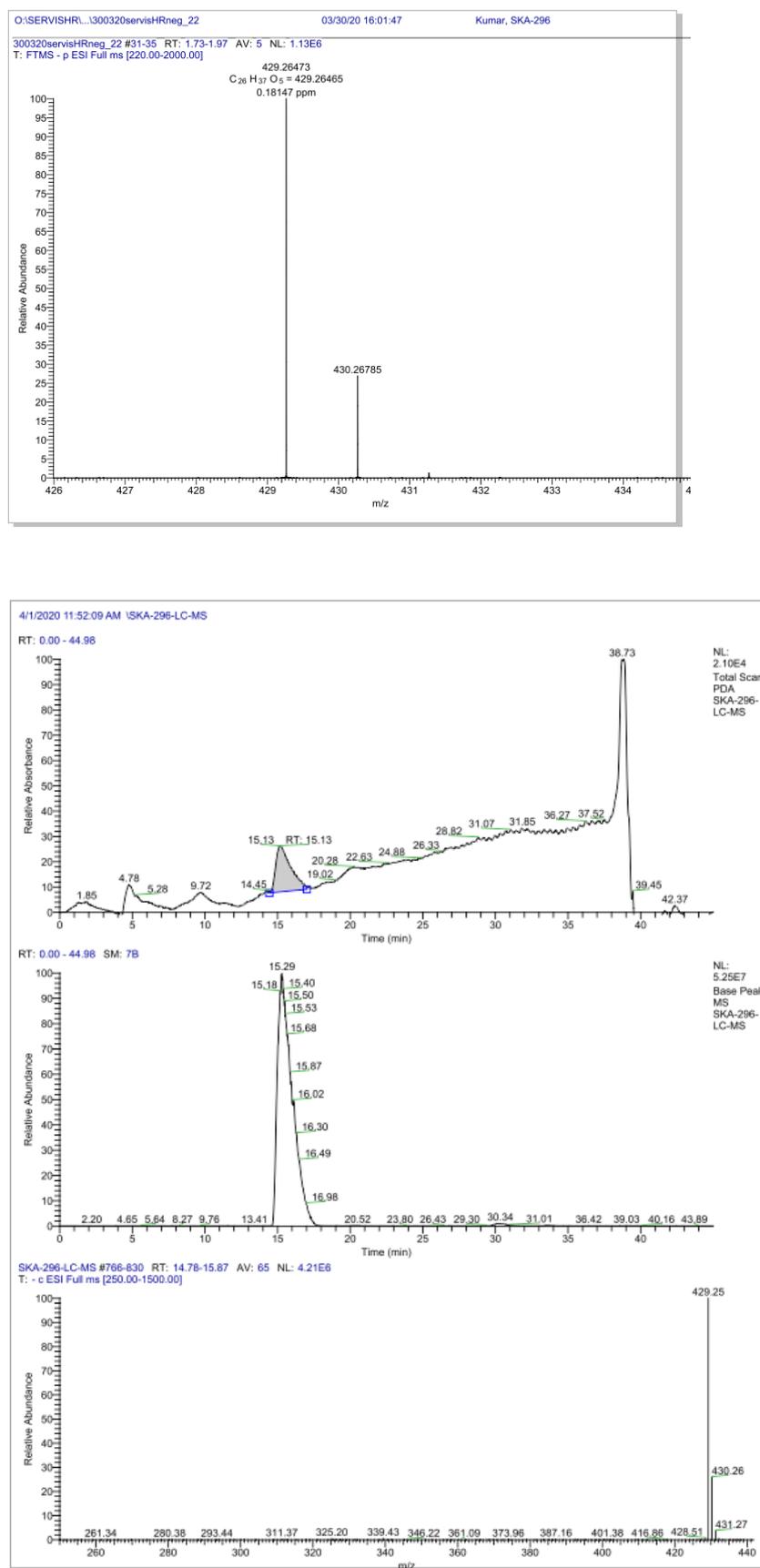


Figure S34. HR-MS and LC-MS spectra of compound 26

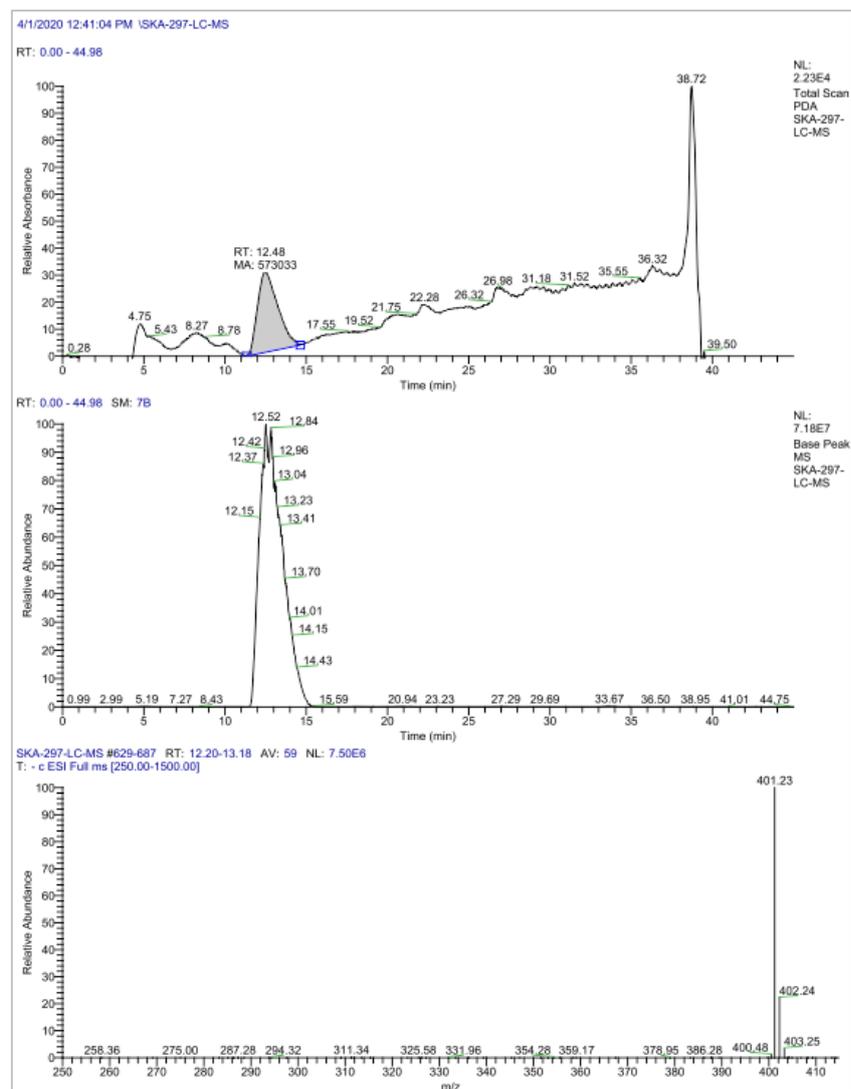
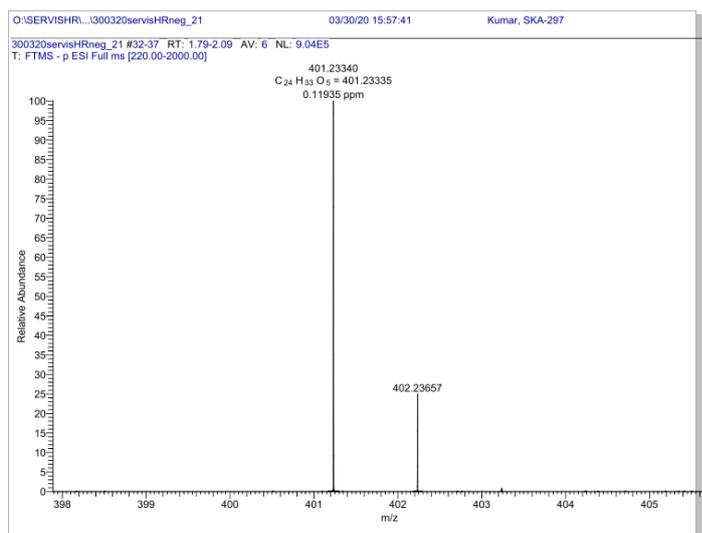


Figure S35. HR-MS and LC-MS spectra of compound **27**

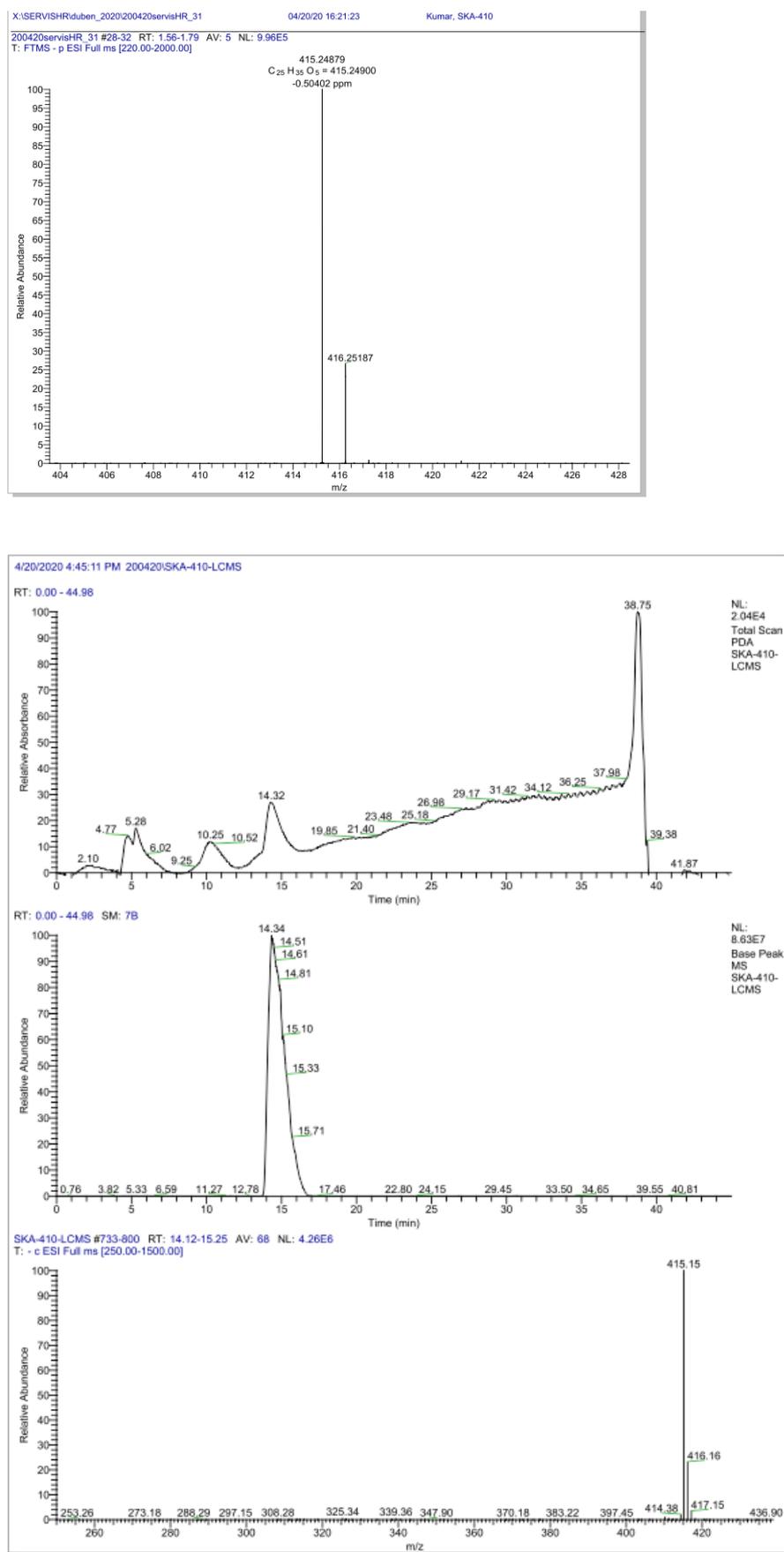


Figure S36. HR-MS and LC-MS spectra of compound **28**

