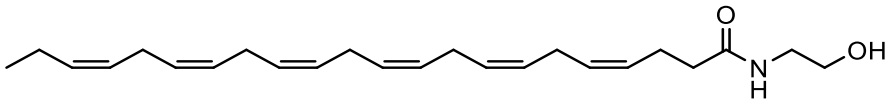
(4Z,7Z,10Z,13Z,16Z,19Z)-N-(2-hydroxyethyl) docosa-4,7,10,13,16,19-hexaenamide (D1)



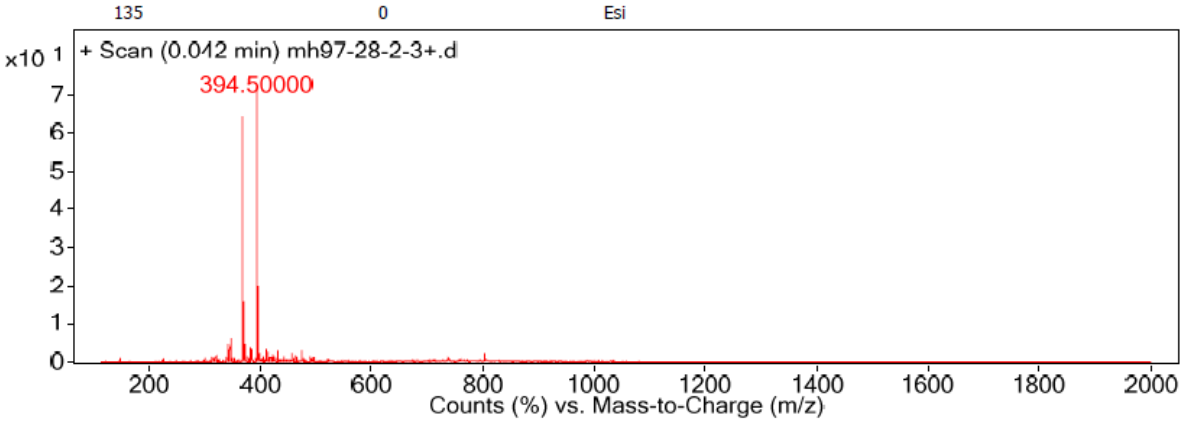


Figure 1. ESI-MS spectrum of compound D1

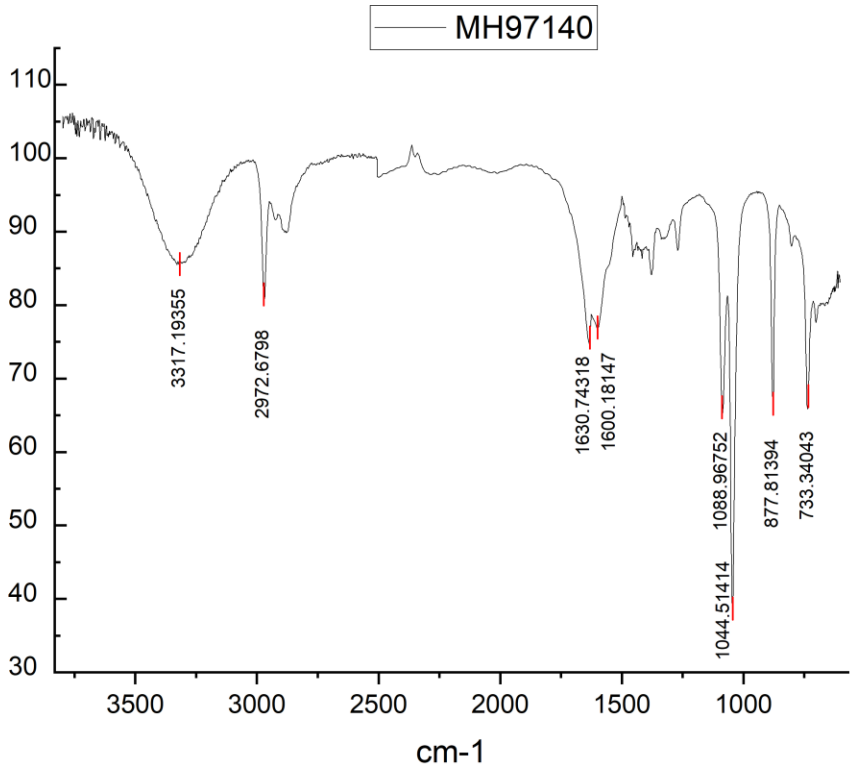


Figure 2. FT-IR spectrum of compound D1

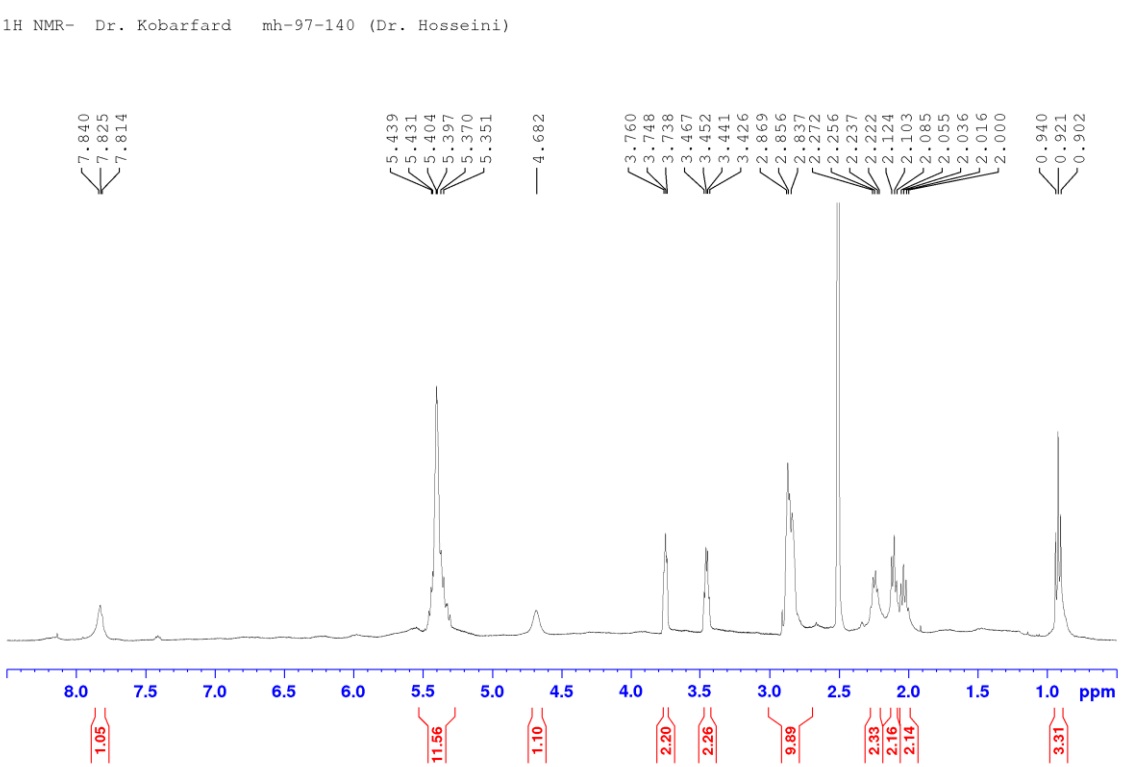


Figure 3. ^{1}H-NMR spectrum of compound D1

(4Z,7Z,10Z,13Z,16Z,19Z)-N,N-bis(2-hydroxyethyl)docosa-4,7,10,13,16,19-hexaenamide (D2)

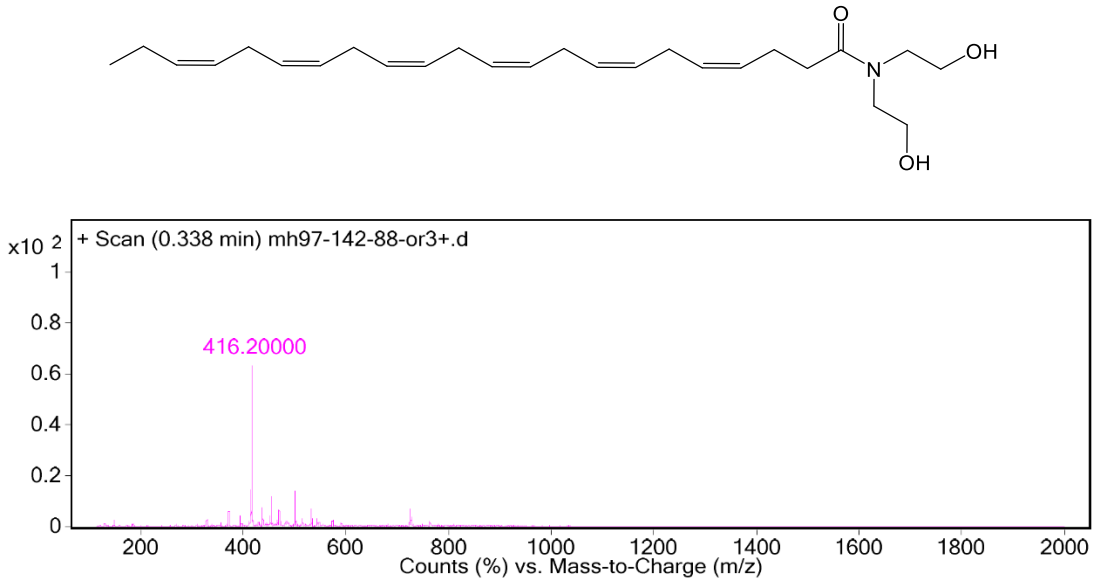


Figure 4. ESI-MS spectrum of compound D2

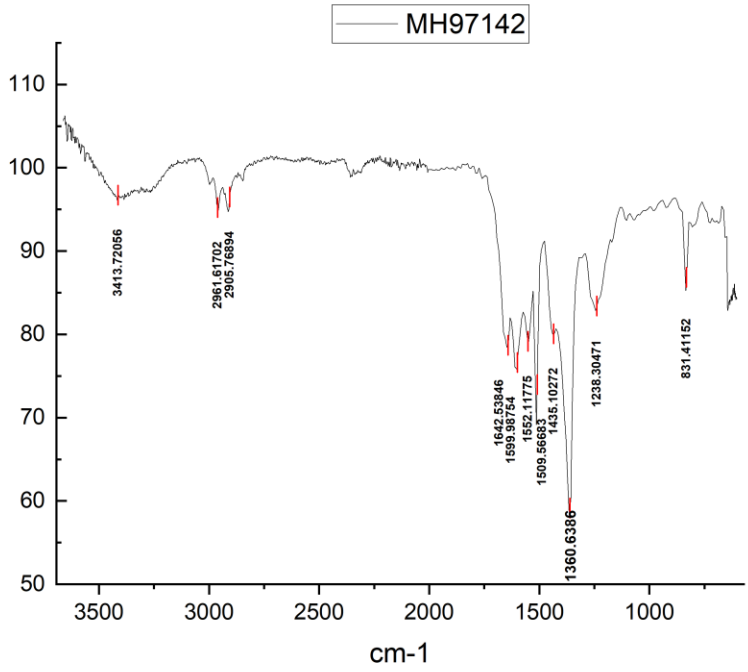


Figure 5. FT-IR spectrum of compound D2

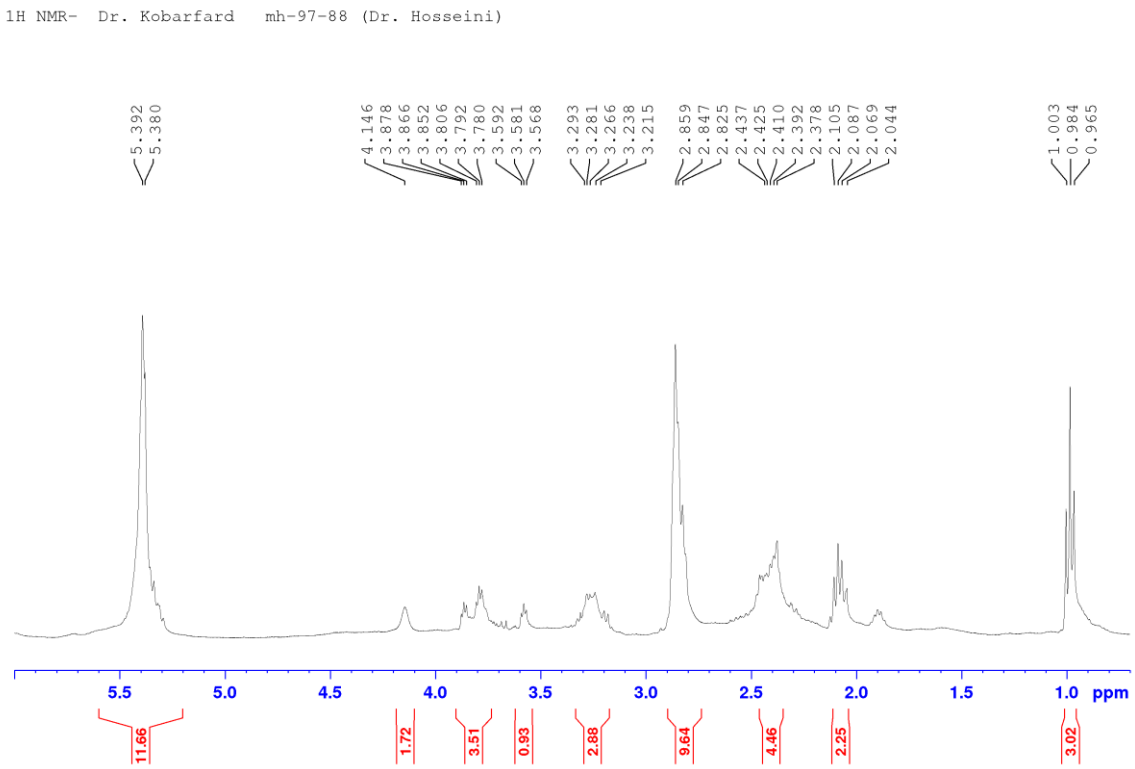


Figure 6. ^{1}H-NMR spectrum of compound D2

4-((4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaen-1-yl)morpholine (D3)

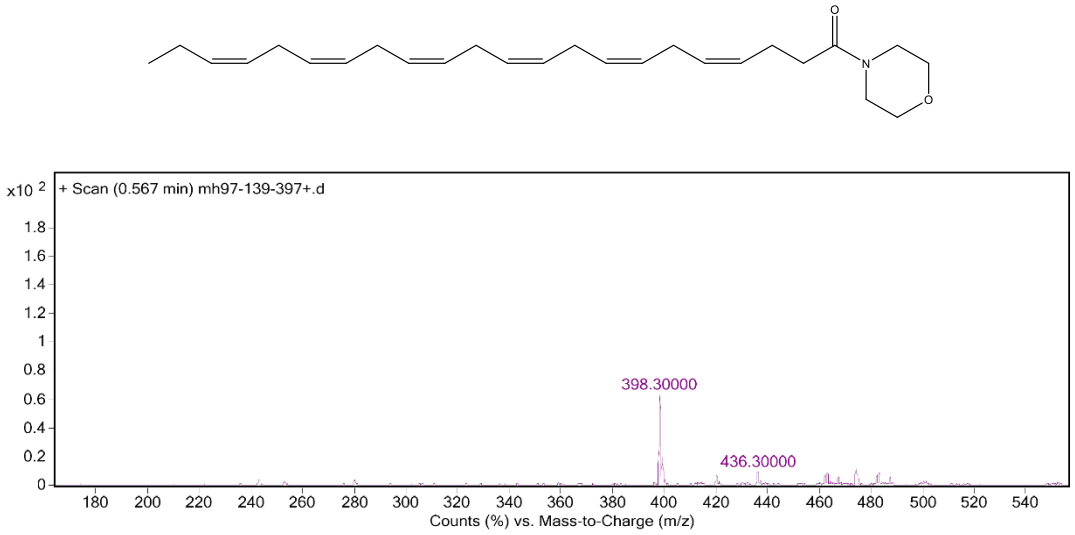


Figure 7. ESI-MS spectrum of compound D3

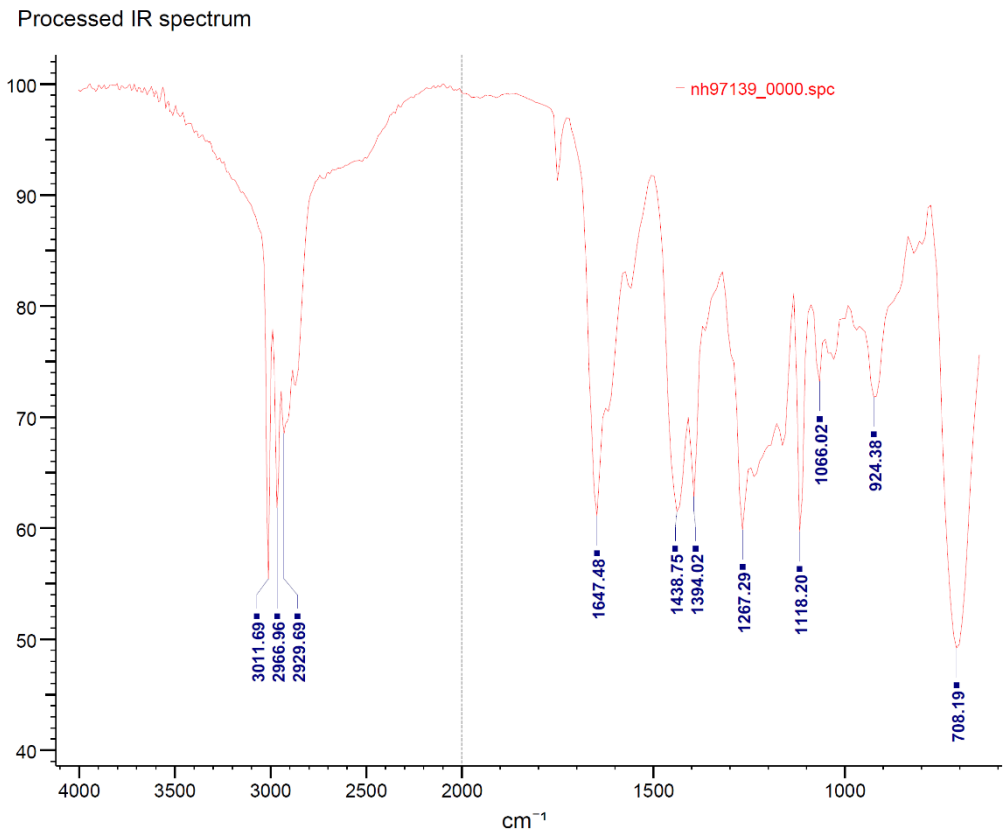


Figure 8. FT-IR spectrum of compound D3

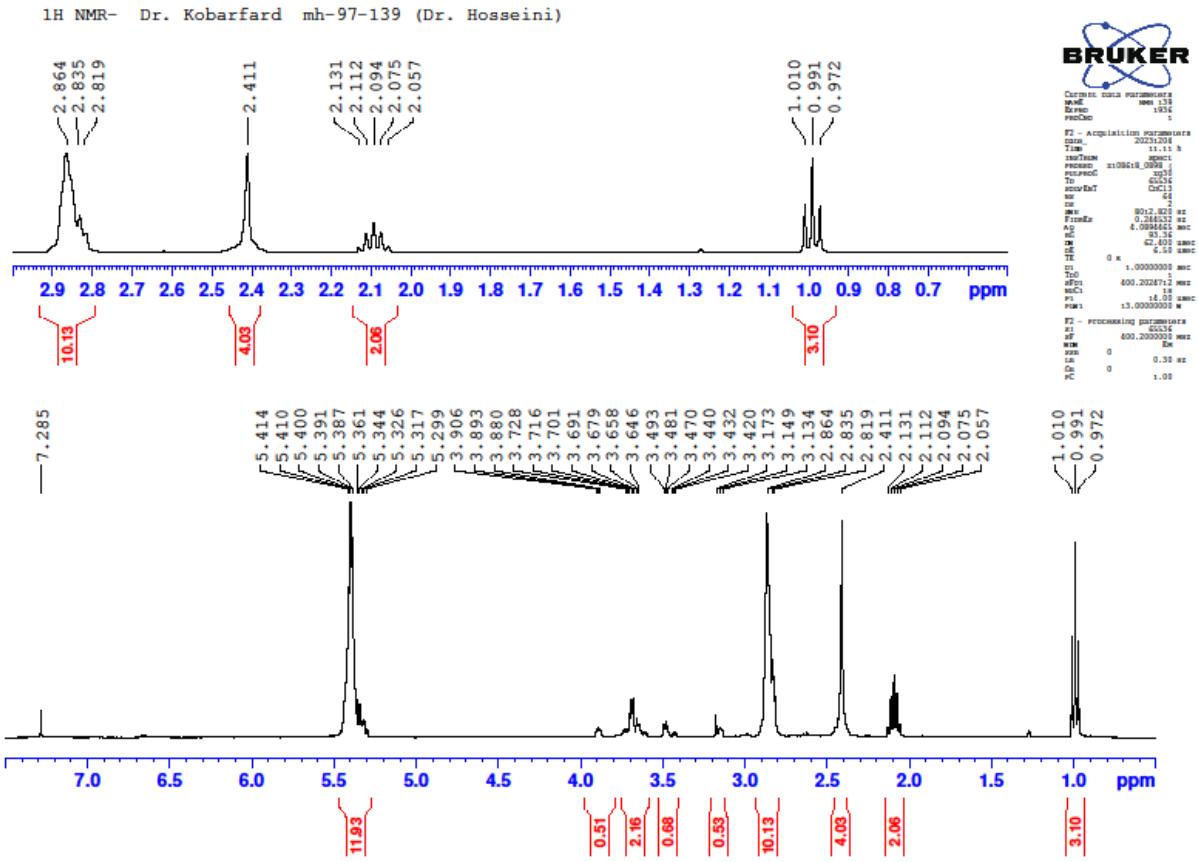


Figure 9. ^{1}H-NMR spectra of compound D3

(4Z,7Z,10Z,13Z,16Z,19Z)-N-(4-hydroxyphenyl)docosa-4,7,10,13,16,19-hexaenamide (D4)

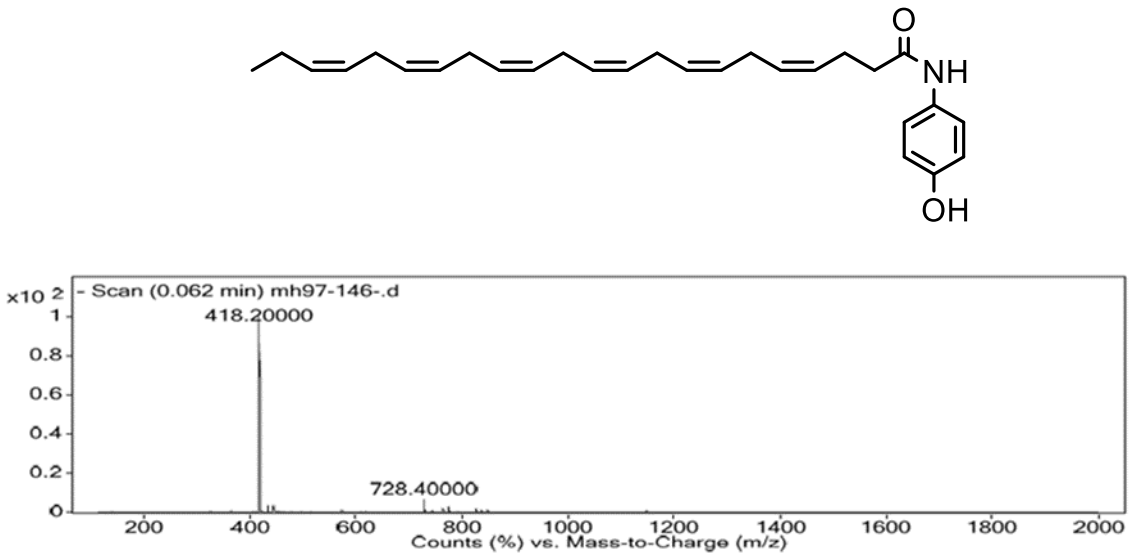


Figure 10. ESI-MS spectrum of compound D4

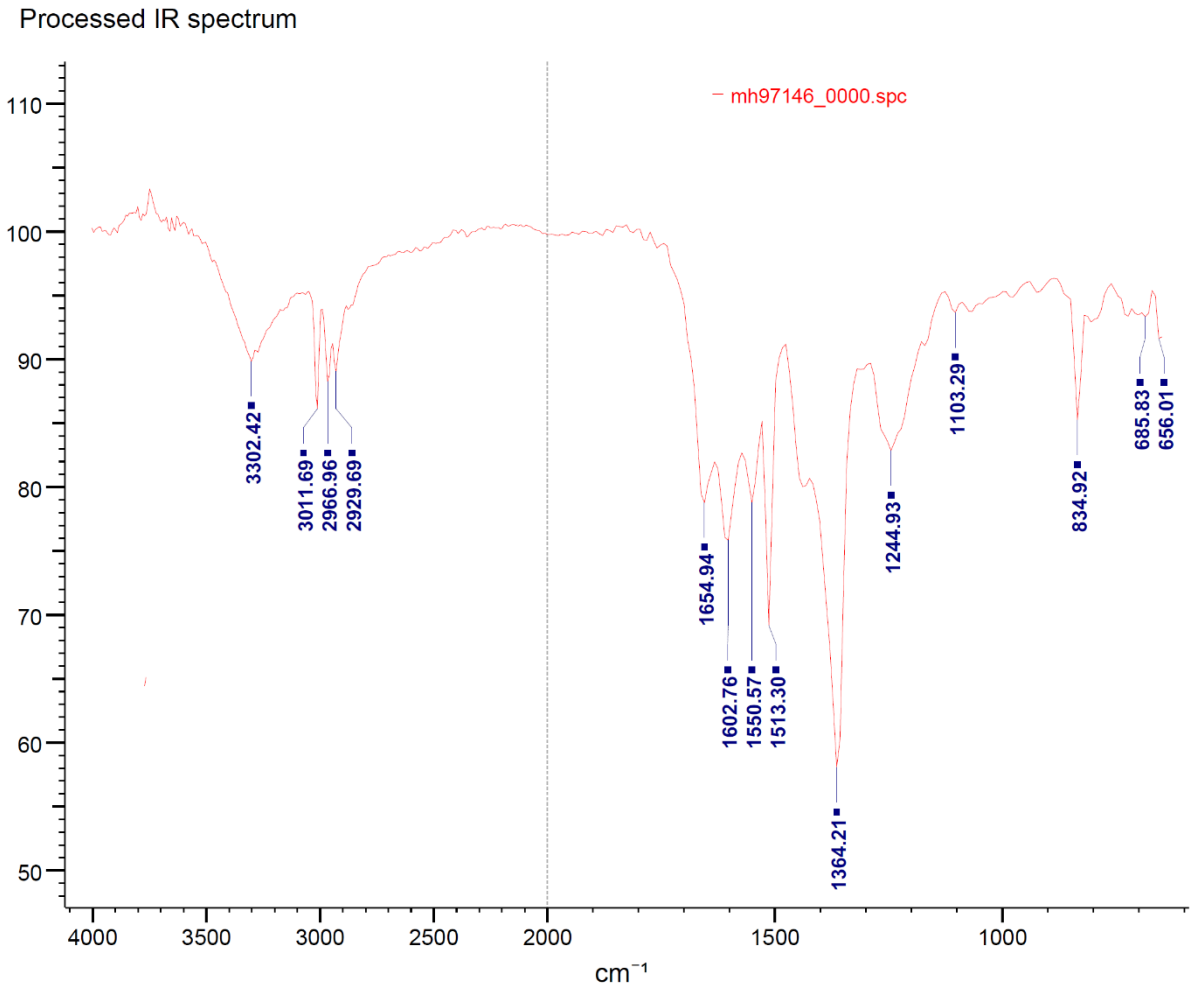


Figure 11. FT-IR spectrum of compound D4

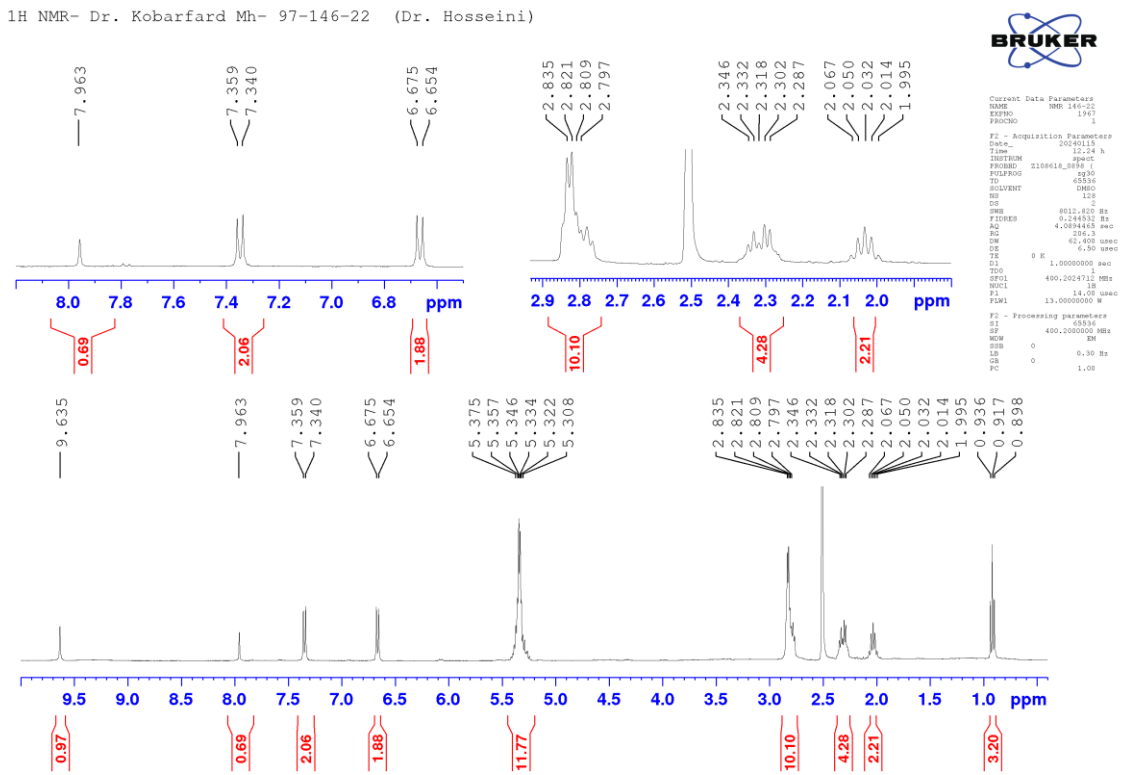
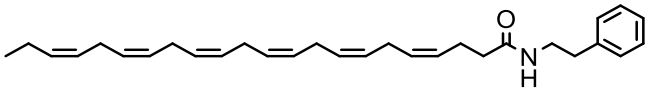


Figure 12.[1]H-NMR spectra of compound D4

(4Z,7Z,10Z,13Z,16Z,19Z)-N-phenethyldocosa-4,7,10,13,16,19-hexaenamide (D5)



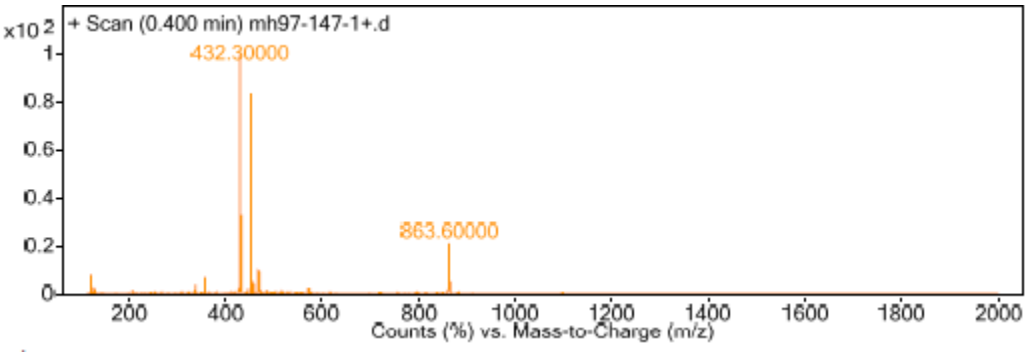


Figure 13. ESI-MS spectrum of compound D5

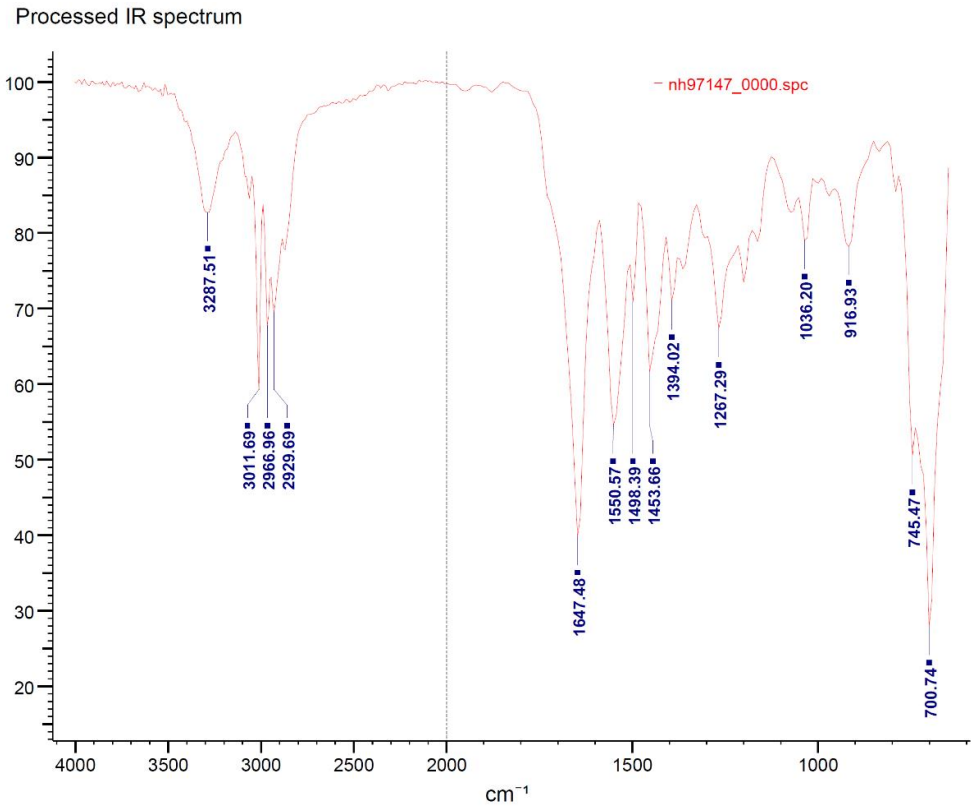


Figure 14. FT-IR spectrum of compound D5

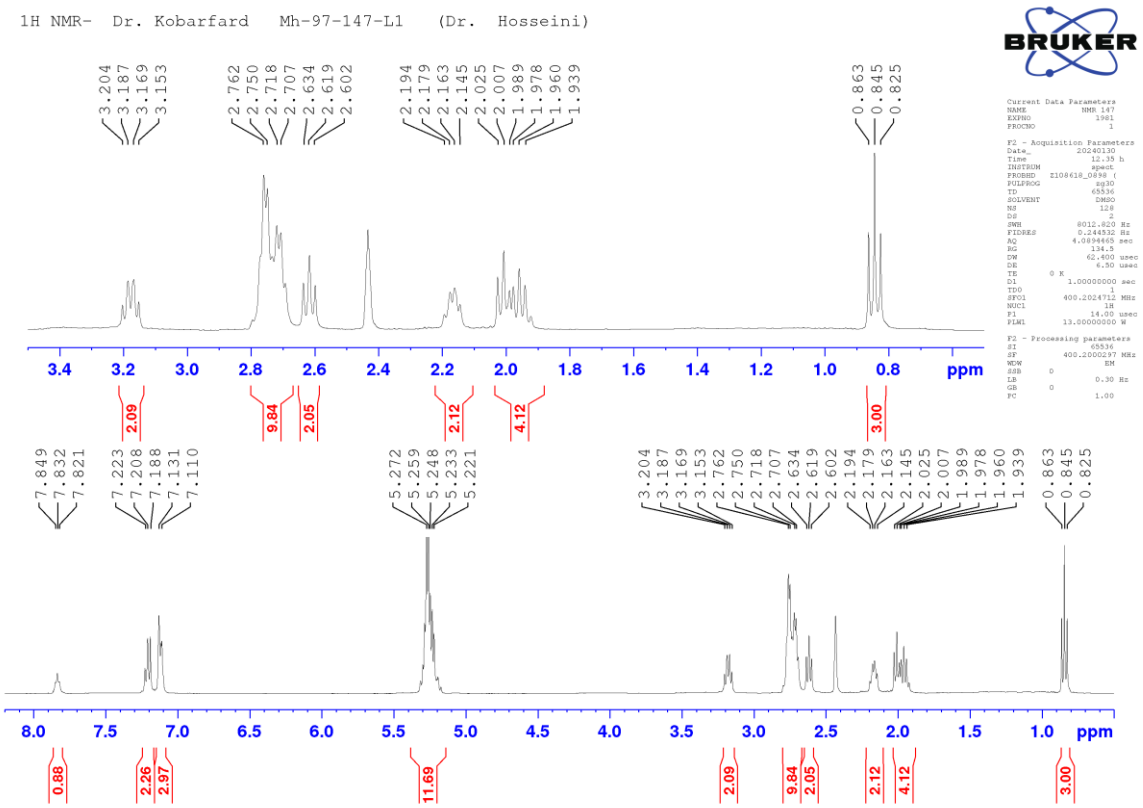


Figure 15. [1]H-NMR spectra of compound D5

(4Z,7Z,10Z,13Z,16Z,19Z)-1-(4-methylpiperazin-1-yl)docosa-4,7,10,13,16,19-hexaen-1-one (D6)

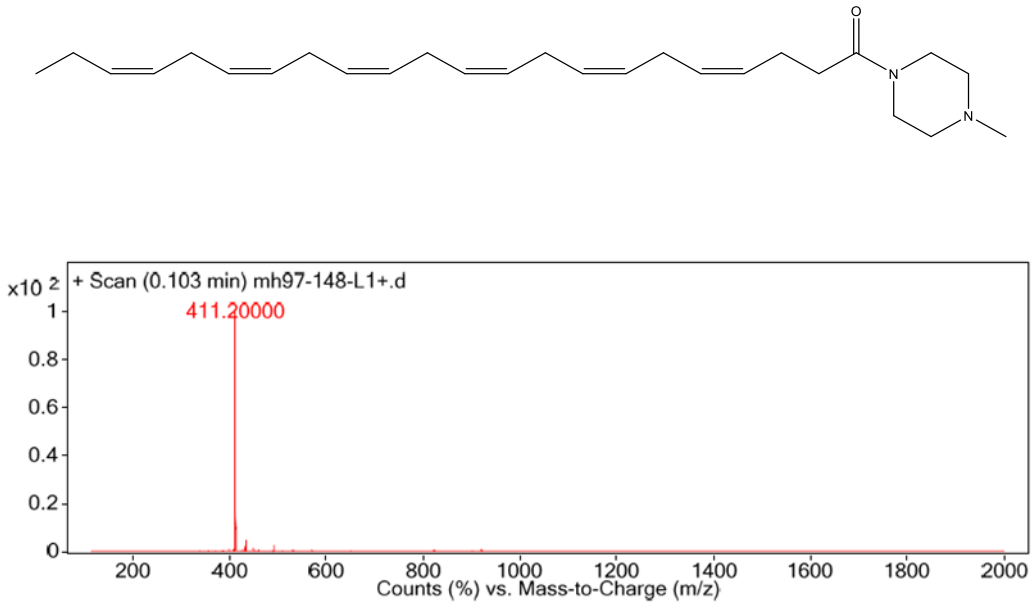


Figure 16. ESI-MS spectrum of compound D6

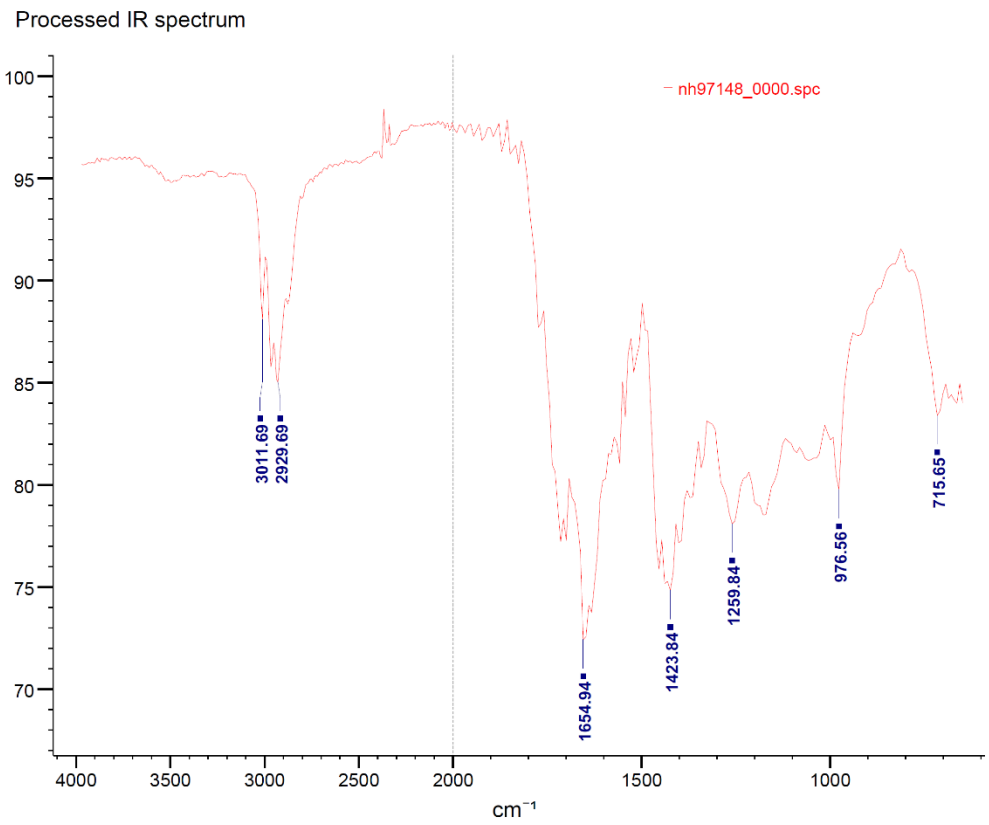


Figure 17. FT-IR spectrum of compound D6

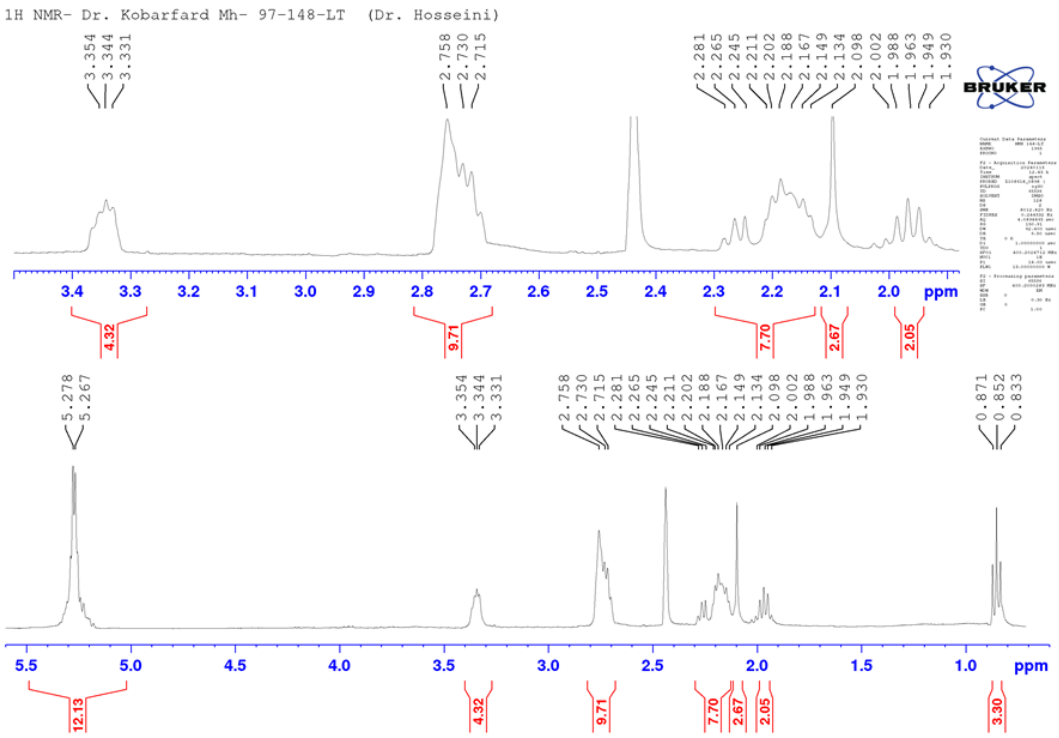
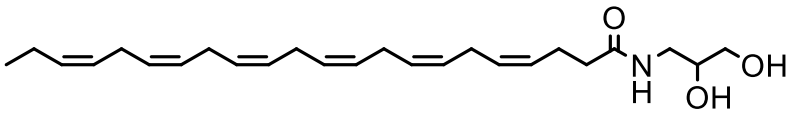


Figure 18. [1]H-NMR spectra of compound D6

(4Z,7Z,10Z,13Z,16Z,19Z)-N-(2,3-dihydroxypropyl)docosa-4,7,10,13,16,19-hexaenamide (D7)



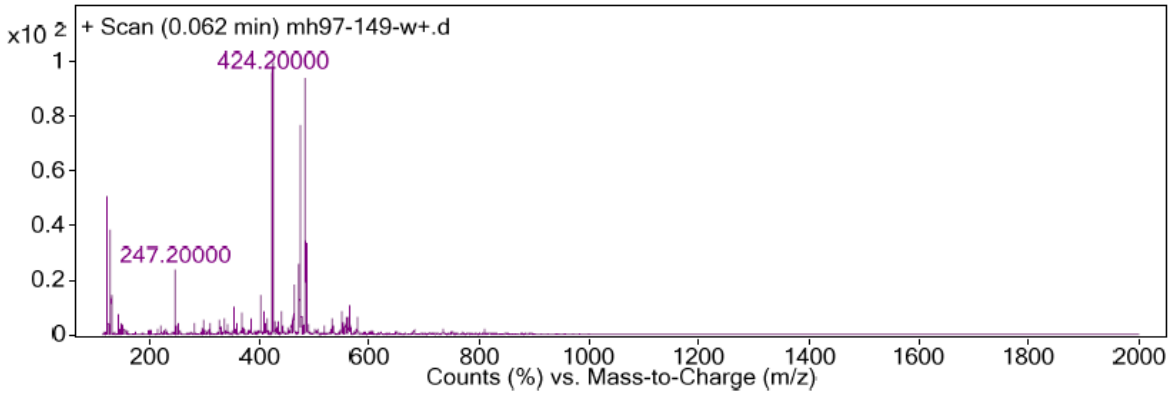


Figure 19. ESI-MS spectrum of compound D7

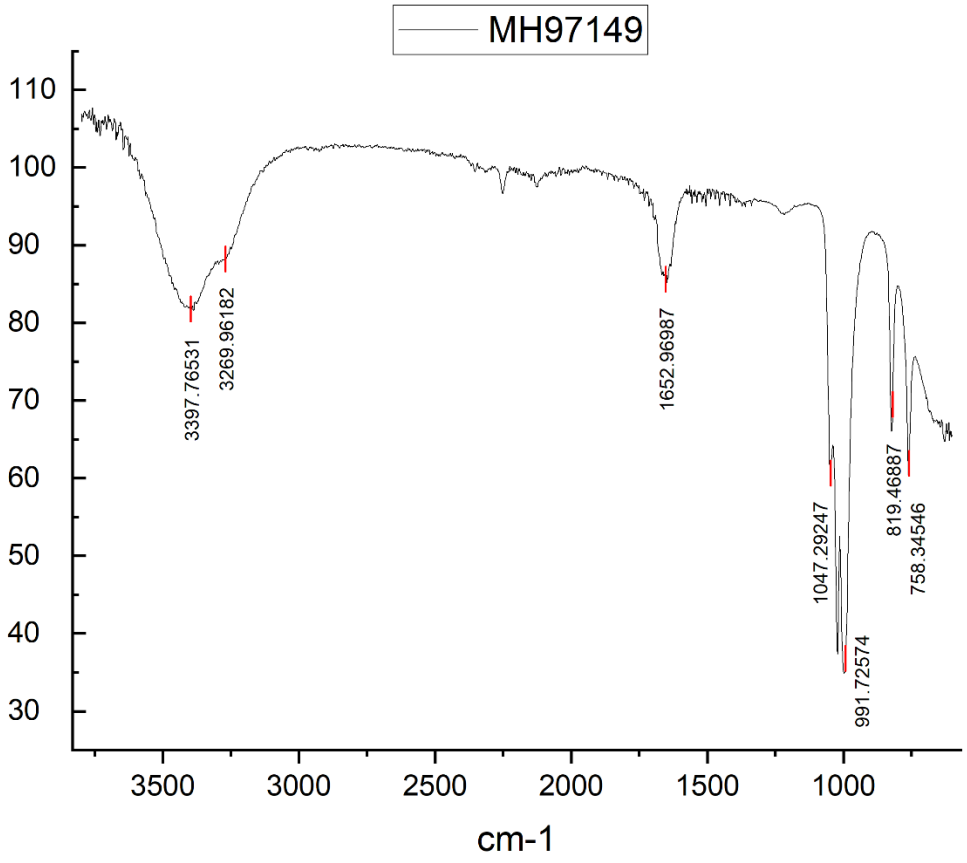


Figure 20. FT-IR spectrum of compound D7

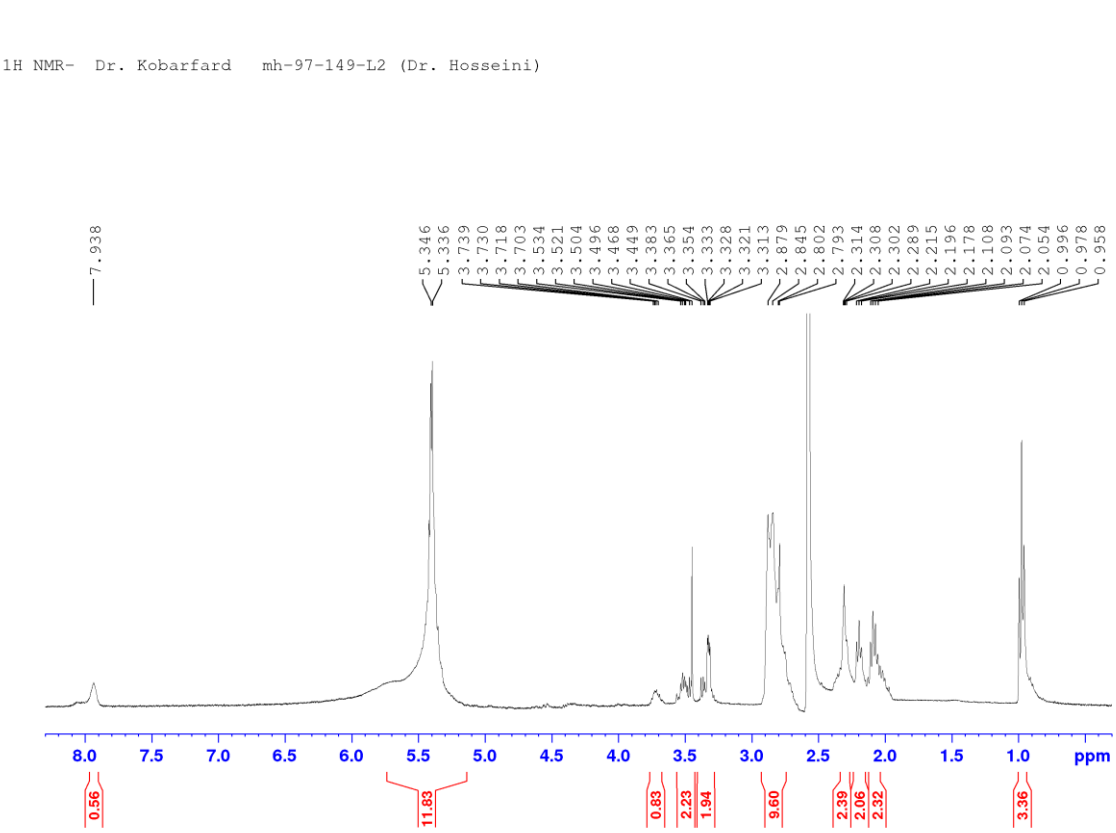
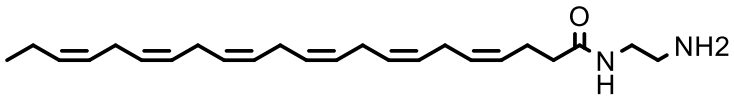


Figure 21.[1]H-NMR spectrum of compound D7

(4Z,7Z,10Z,13Z,16Z,19Z)-N-(2-aminoethyl)docosa-4,7,10,13,16,19-hexaenamide (D8)



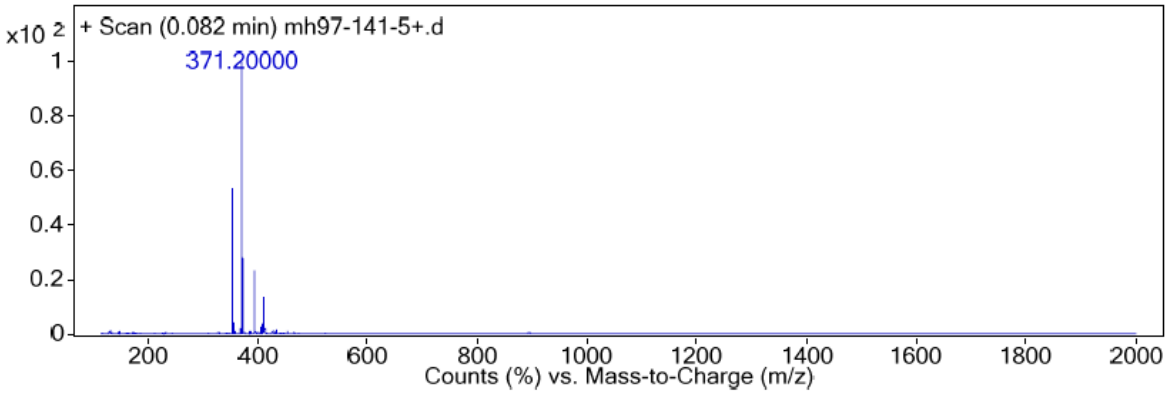


Figure 22. ESI-MS spectrum of compound D8

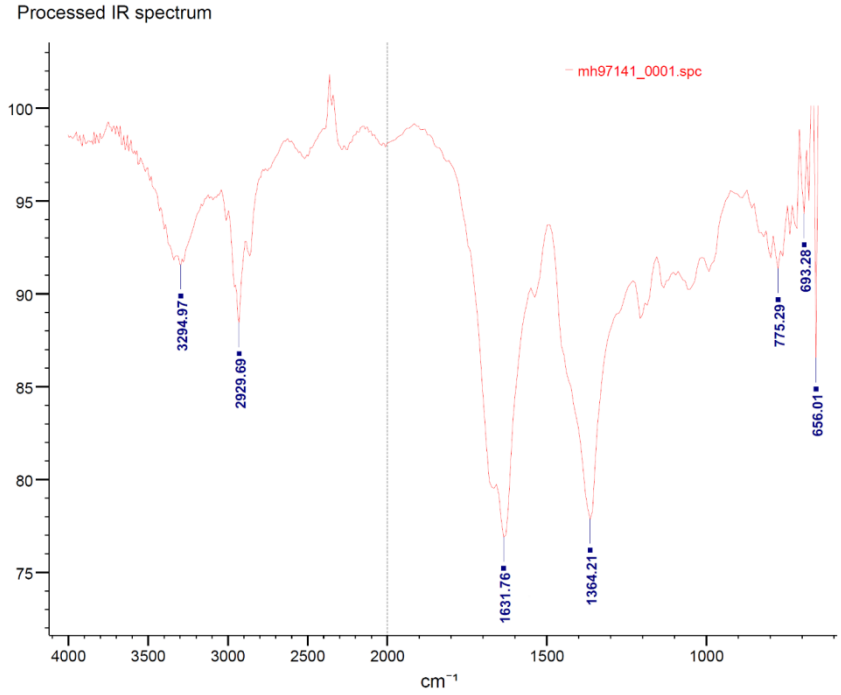


Figure 23. FT-IR spectrum of compound D8

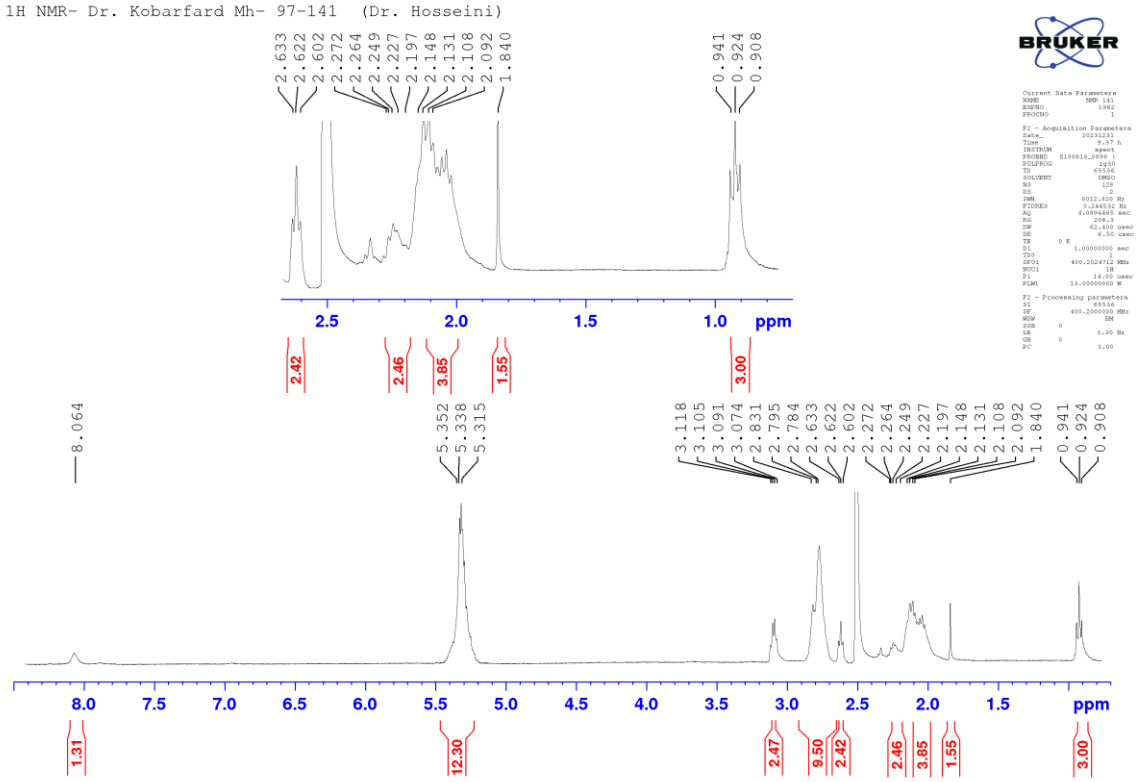
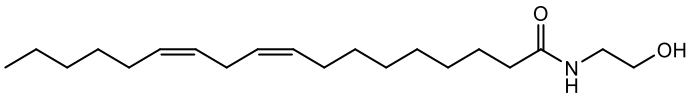


Figure 24. [1]H-NMR spectra of compound D8

(9Z,12Z)-N-(2-hydroxyethyl)octadeca-9,12-dienamide (L1)



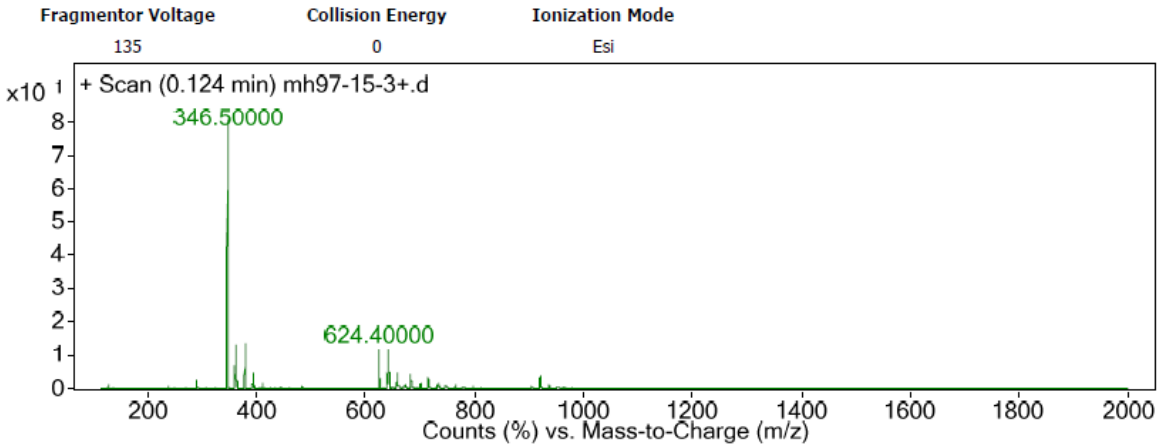


Figure 25. ESI-MS spectrum of compound L1

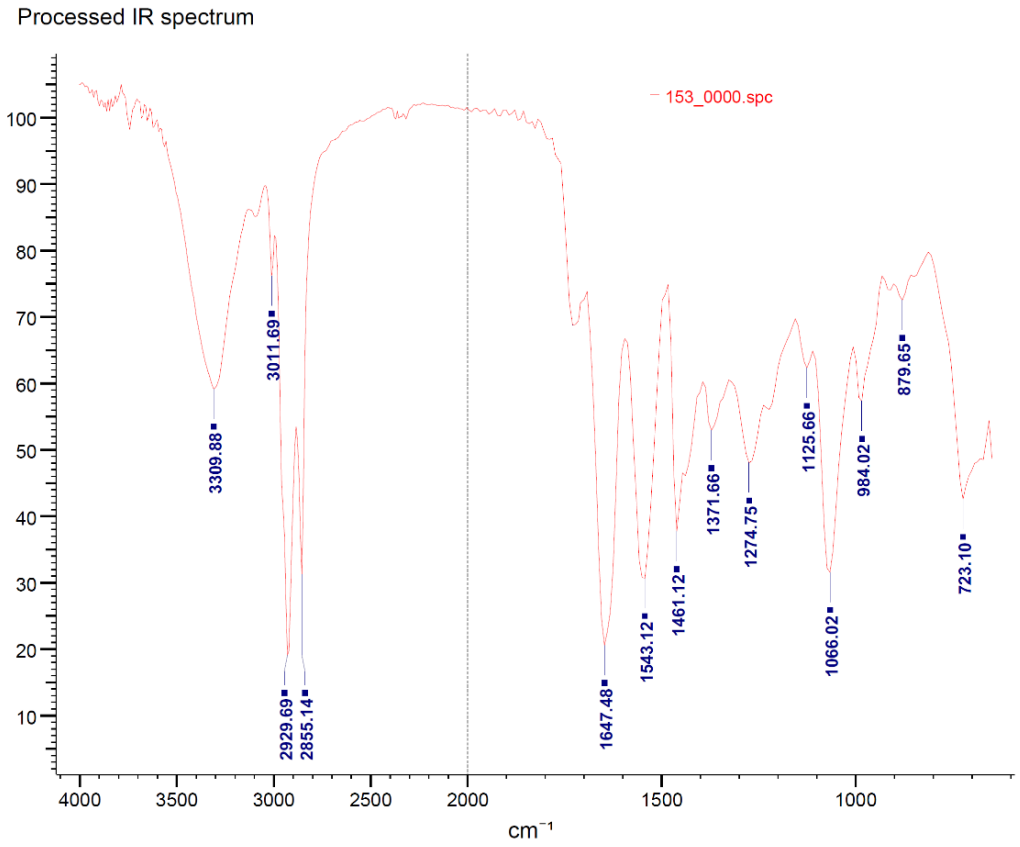


Figure 26. FT-IR spectrum of compound L1

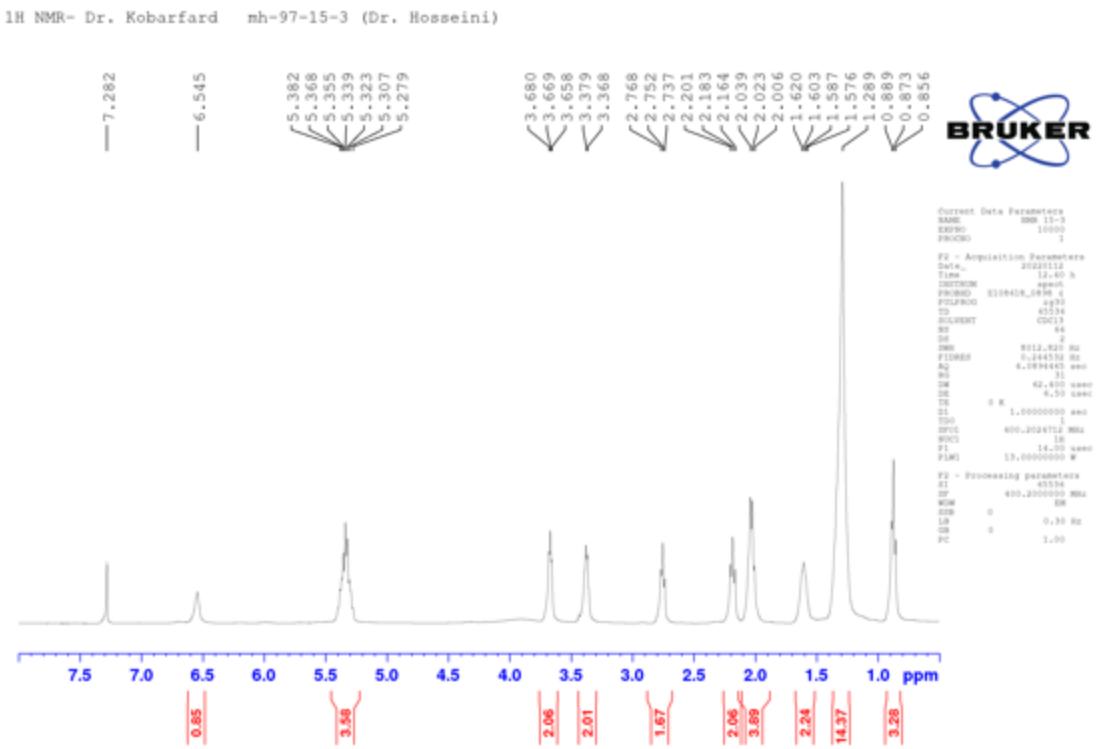
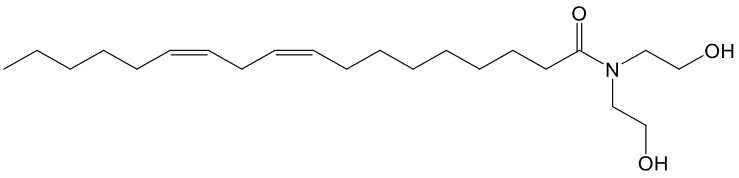


Figure 27. ^{1}H-NMR spectra of compound L1

(14-2,L2): (9Z,12Z)-N,N-bis(2-hydroxyethyl)octadeca-9,12-dienamide (L2)



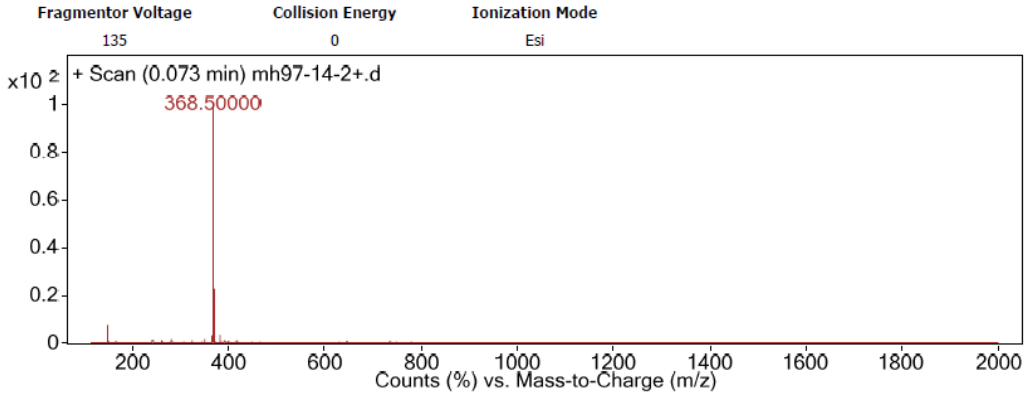


Figure 28. ESI-MS spectrum of compound L2

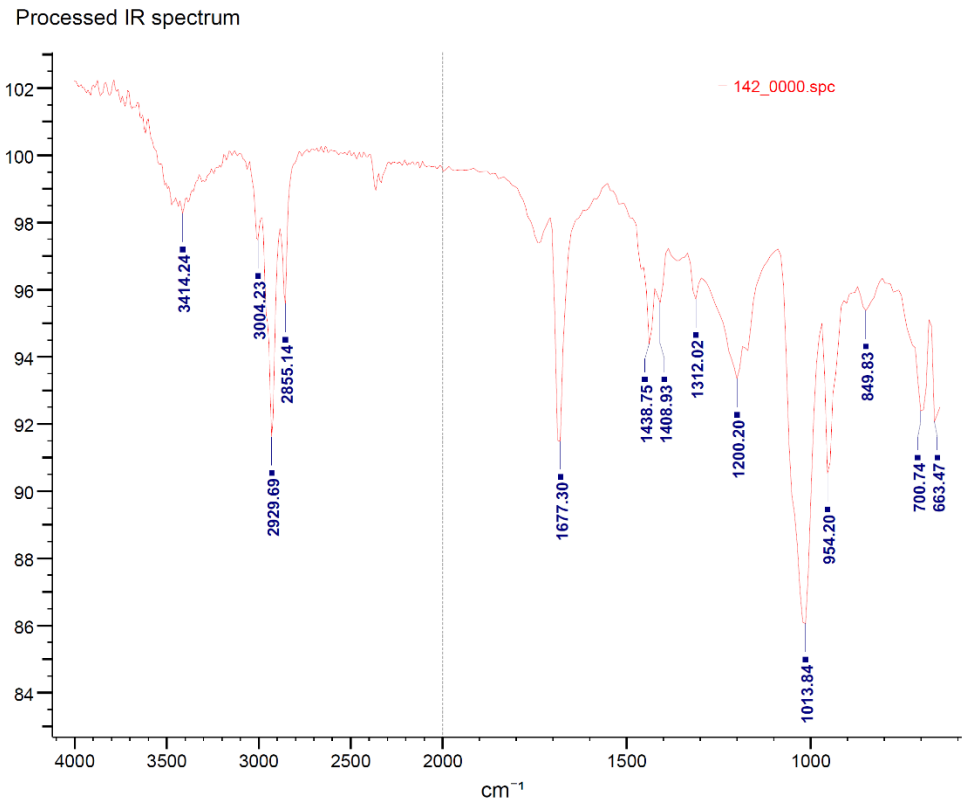


Figure 29. FT-IR spectrum of compound L2

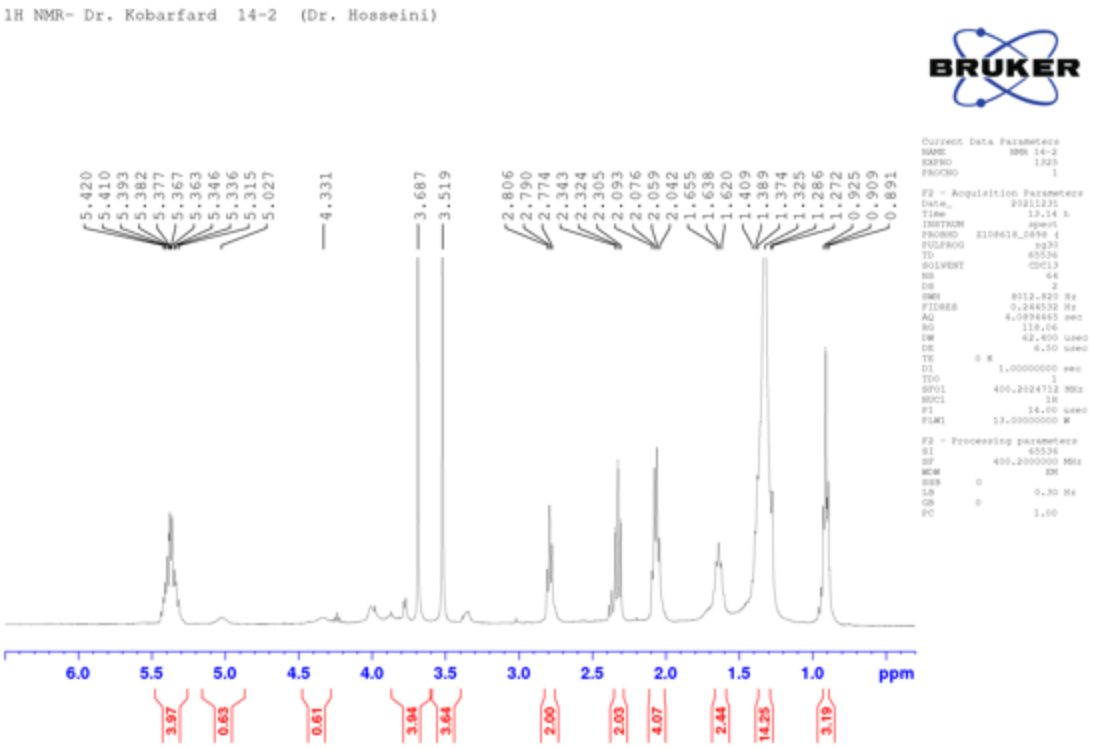


Figure 30. ^{1}H-NMR spectrum of compound L2

(9Z,12Z)-1-morpholinooctadeca-9,12-dien-1-one (L3)

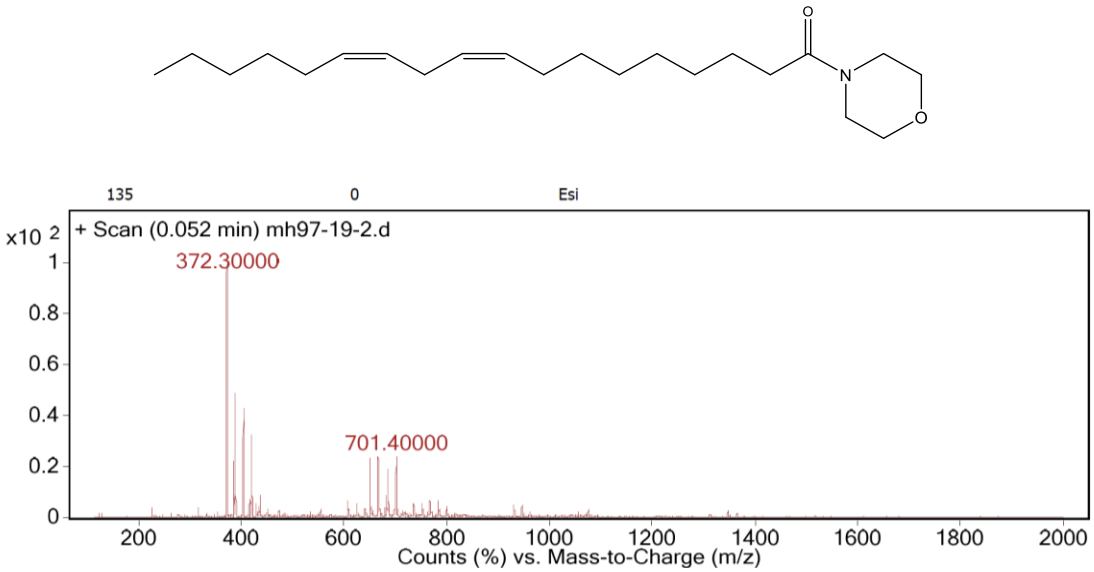


Figure 31. ESI-MS spectrum of compound L3

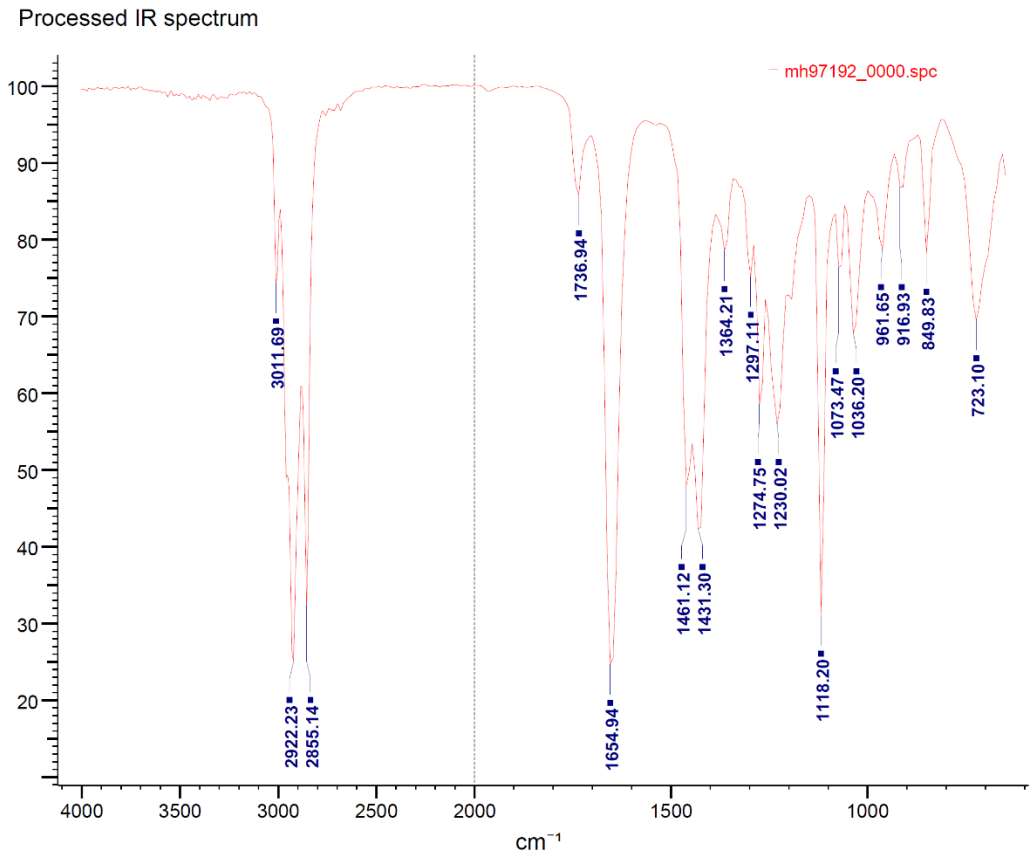


Figure 32. FT-IR spectrum of compound L3

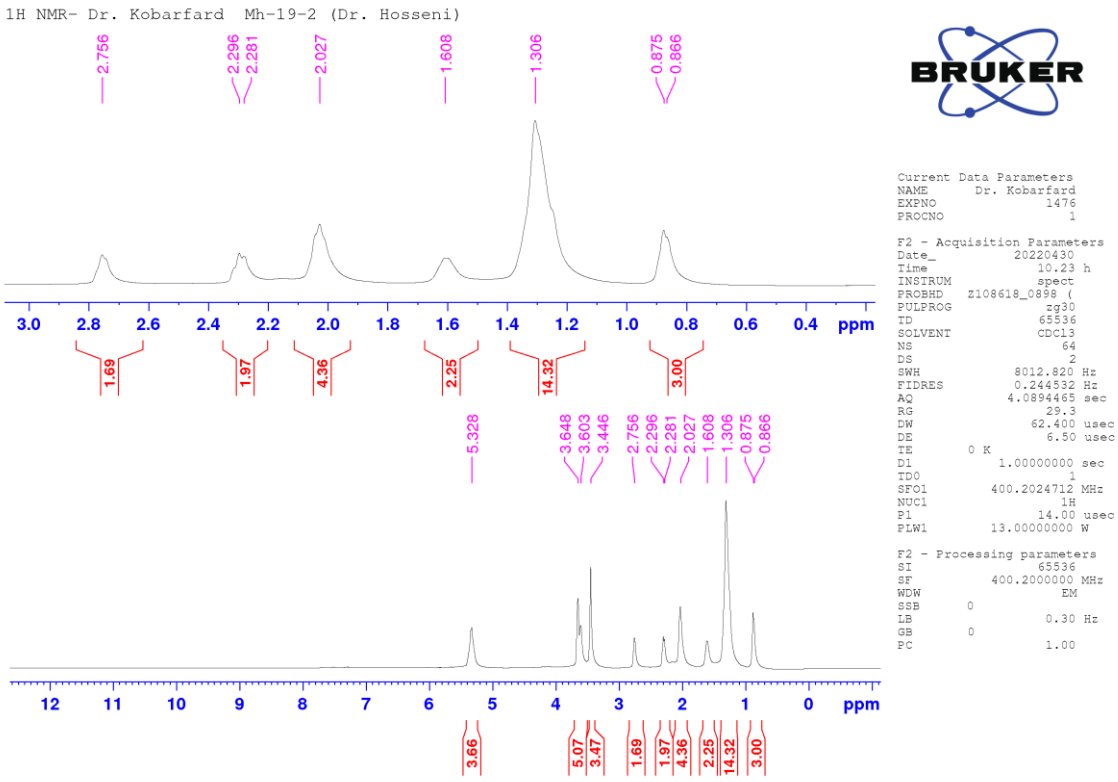
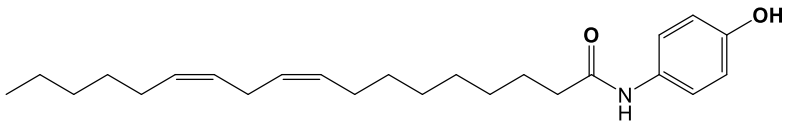


Figure 33. ^{1}H-NMR spectra of compound L3

(9Z, 12Z)-N-(4-hydroxyphenyl) octadeca-9,12-dienamide (L4)



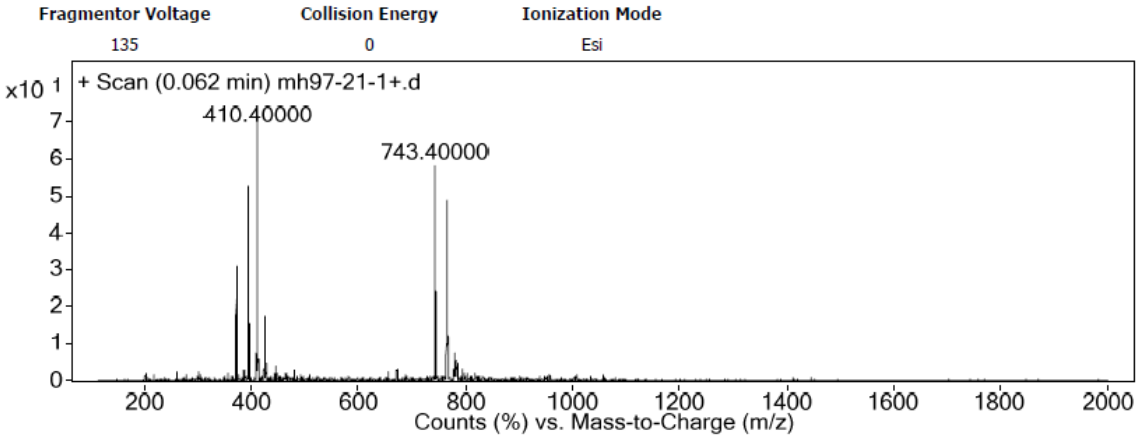


Figure 34. ESI-MS spectrum of compound L4

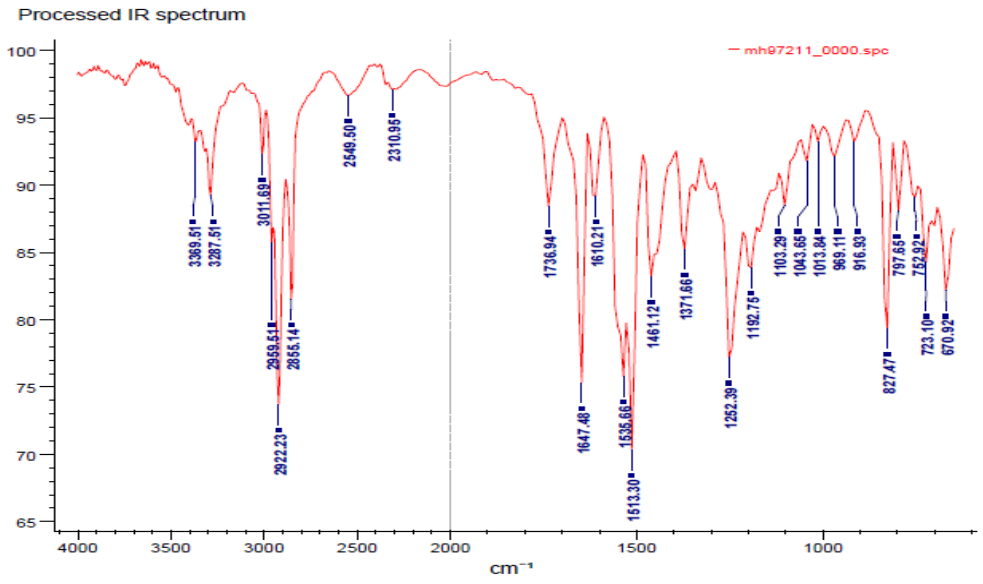


Figure 35. FT-IR spectrum of compound L4

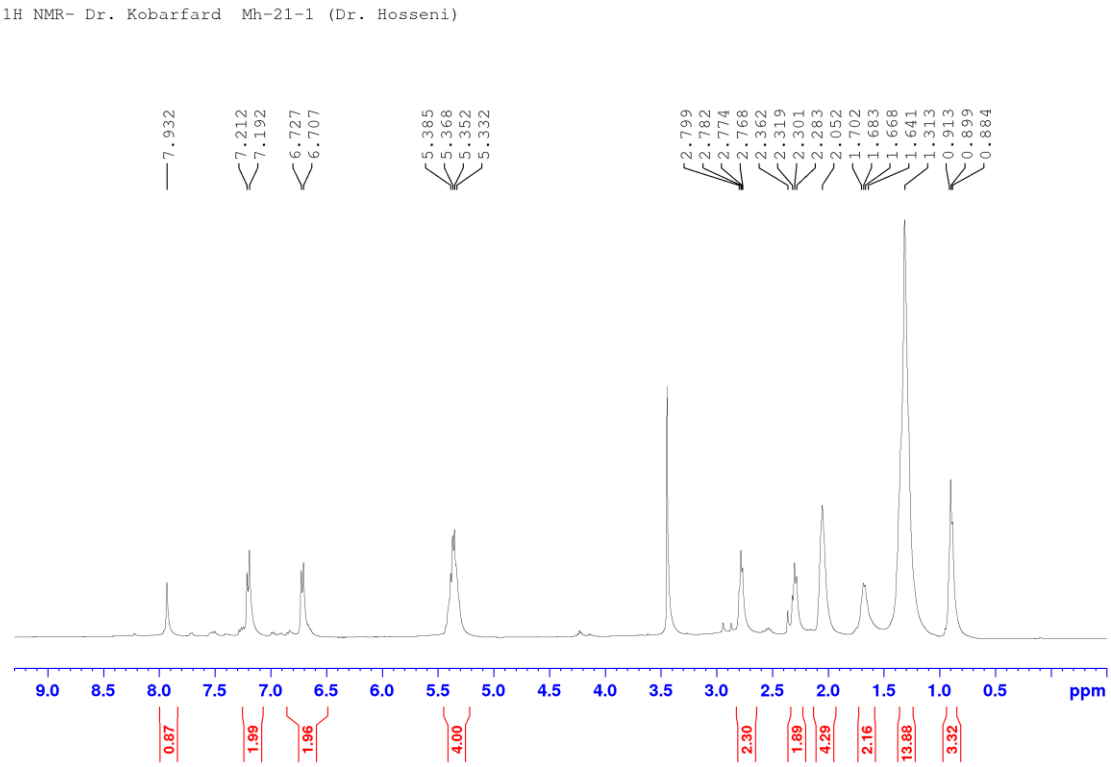


Figure 36. ^{1}H-NMR spectrum of compound L4

(9Z,12Z)-N-phenethyloctadeca-9,12-dienamide (L5)

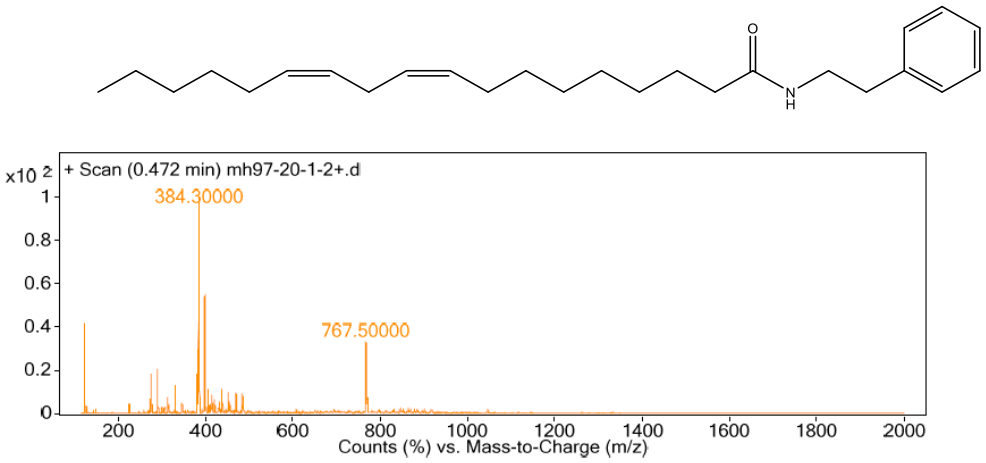


Figure 37. ESI-MS spectrum of compound L5

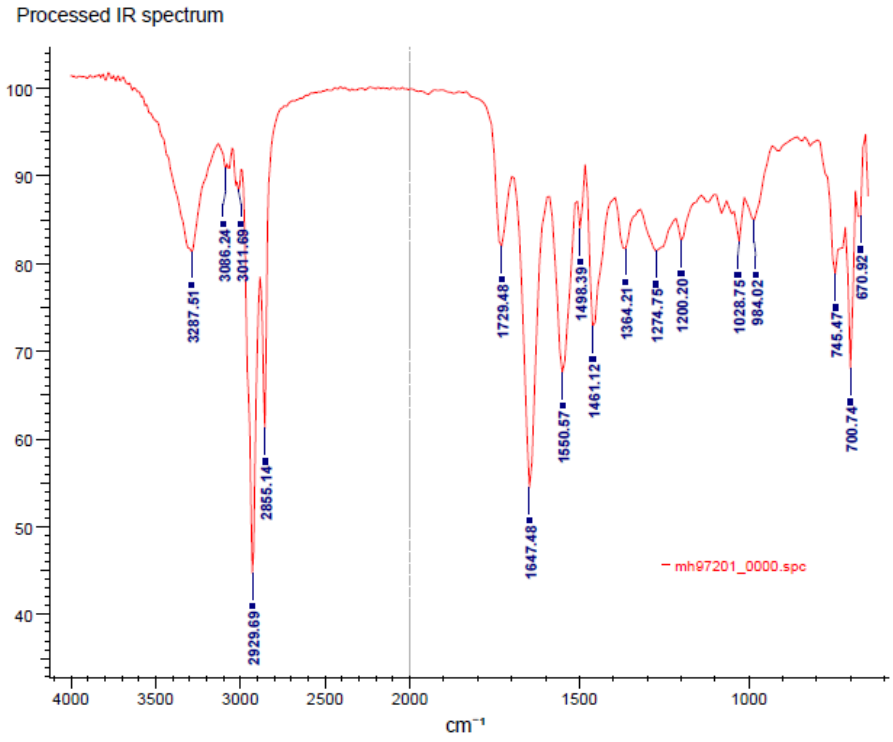


Figure 38. FT-IR spectrum of compound L5

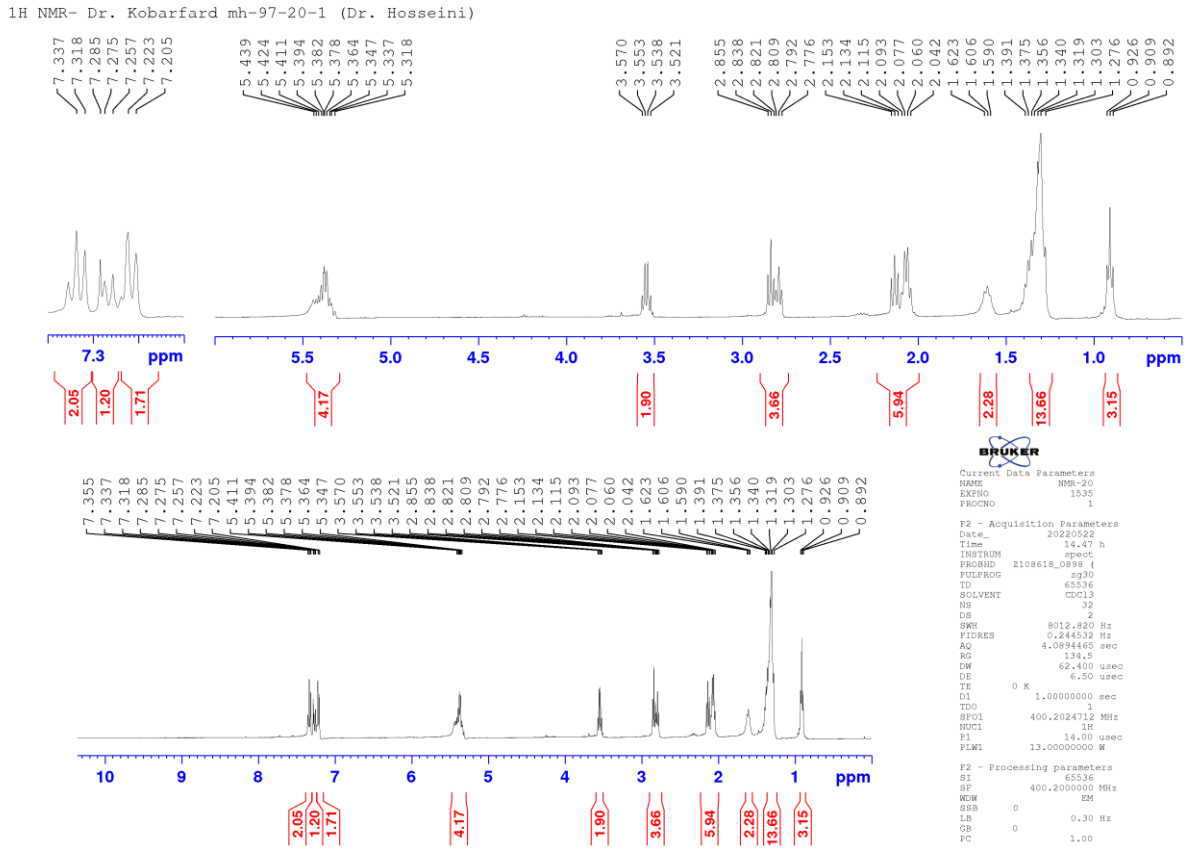


Figure 39. ^{1}H-NMR spectra of compound L5

(9Z,12Z)-1-(4-methylpiperazin-1-yl)octadeca-9,12-dien-1-one (L6)

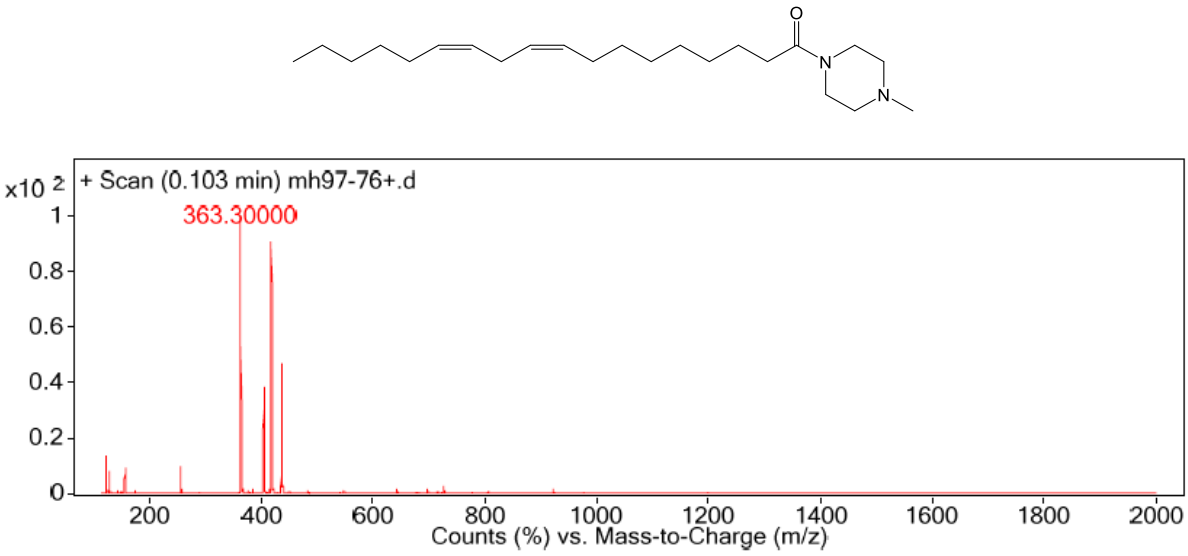


Figure 40. ESI-MS spectrum of compound L6

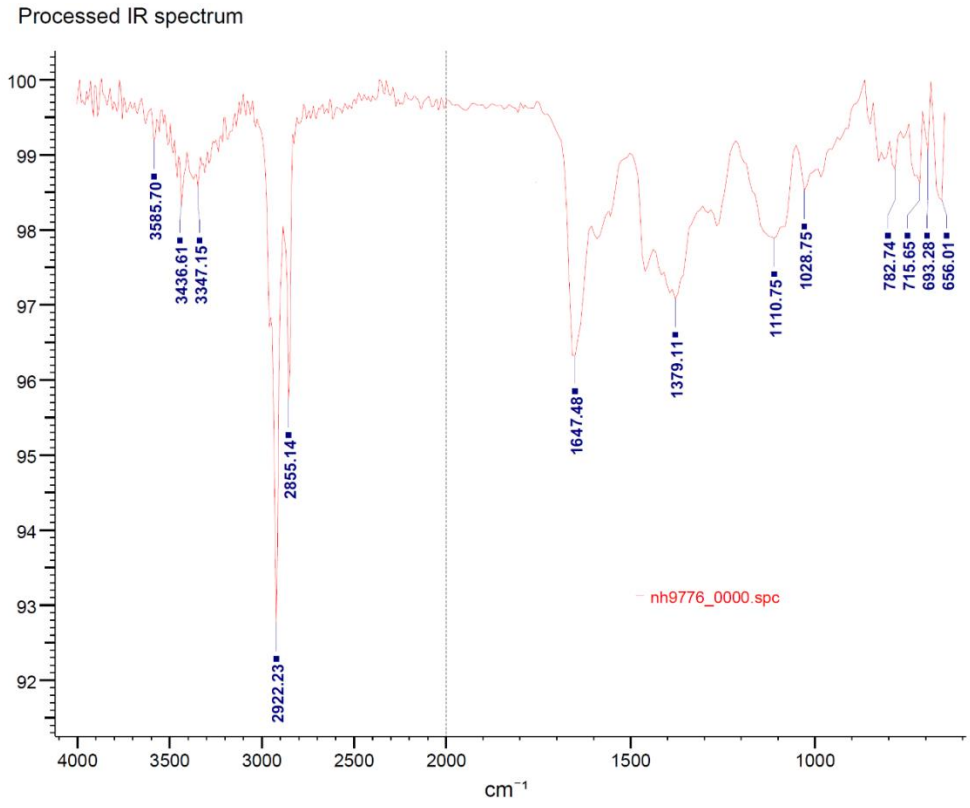


Figure 41. FT-IR spectrum of compound L6

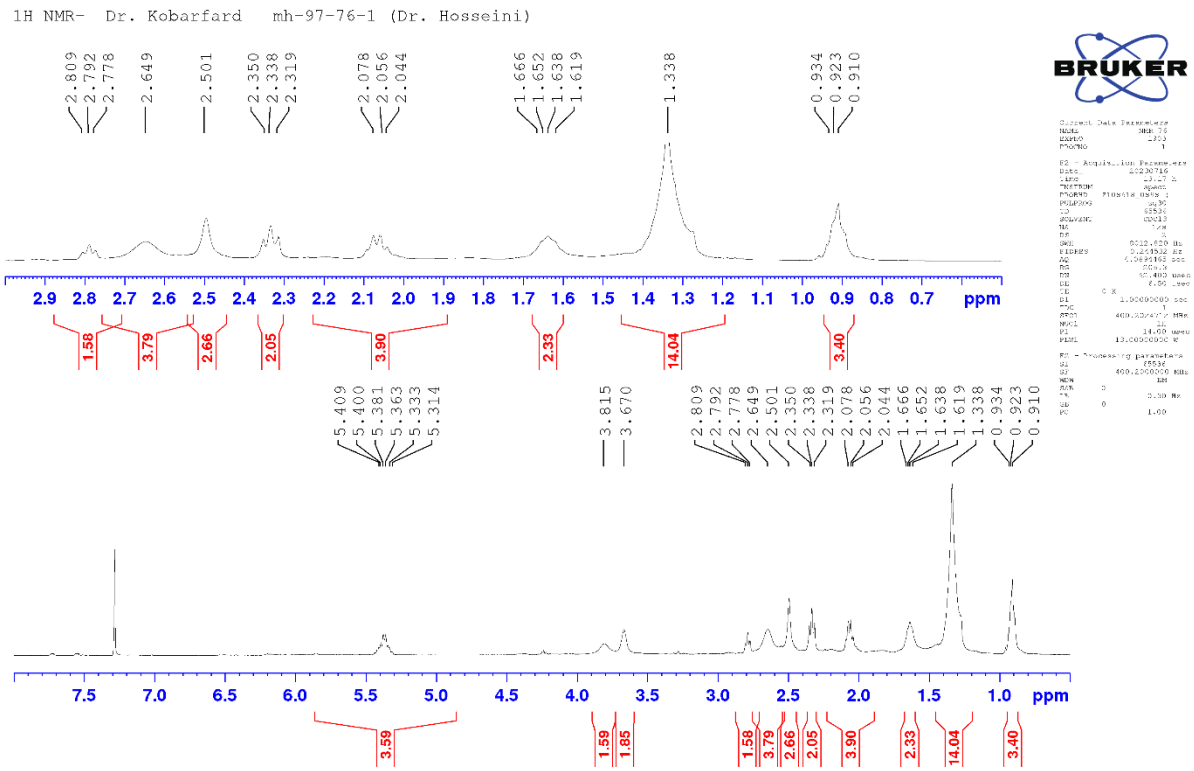
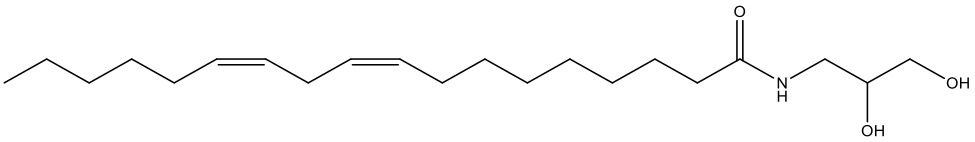


Figure 42. ^{1}H-NMR spectra of compound L6

(9Z,12Z)-N-(2,3-dihydroxypropyl)octadeca-9,12-dienamide (L7)



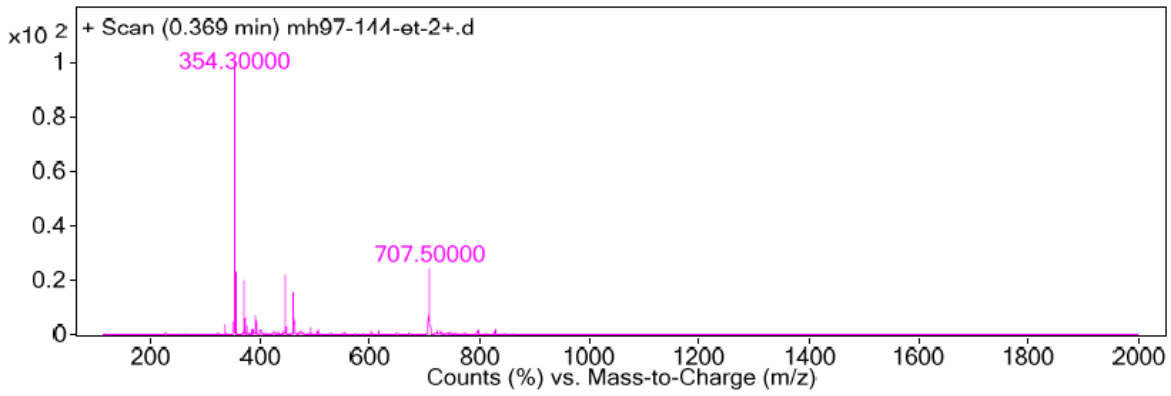


Figure 43. ESI-MS spectrum of compound L7 (m/z: 354 $(M+H)^+$)

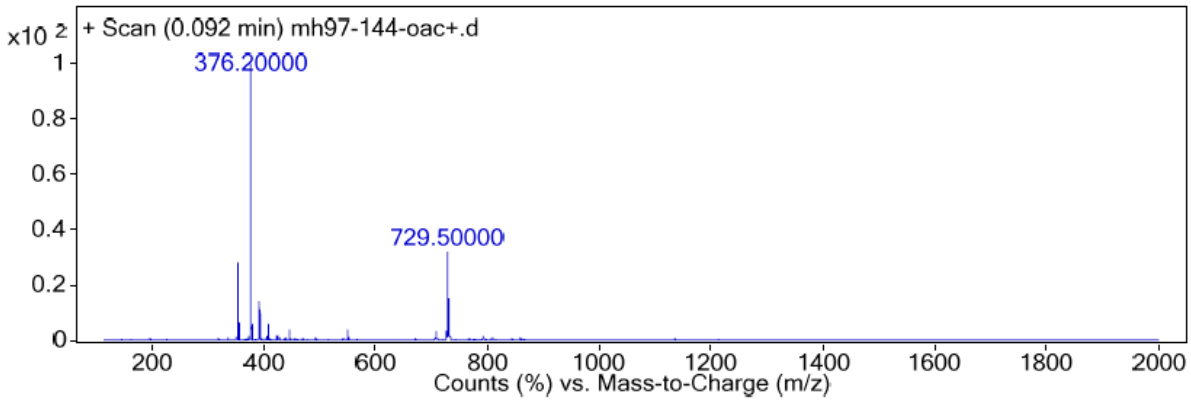


Figure 44. ESI-MS spectrum of compound L7 (m/z: 376 $(M+Na)^+$)

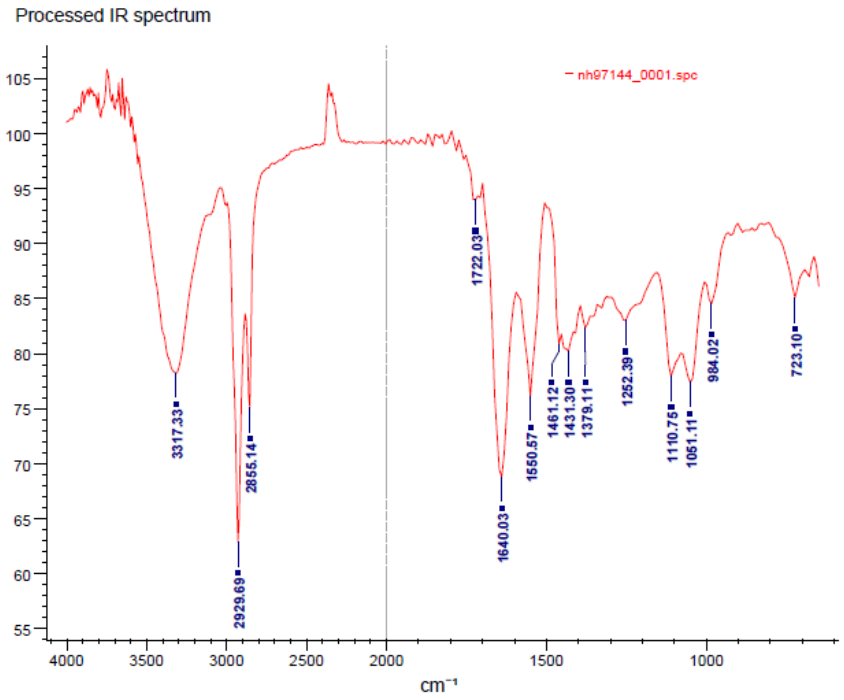


Figure 45. FT-IR spectrum of compound L7

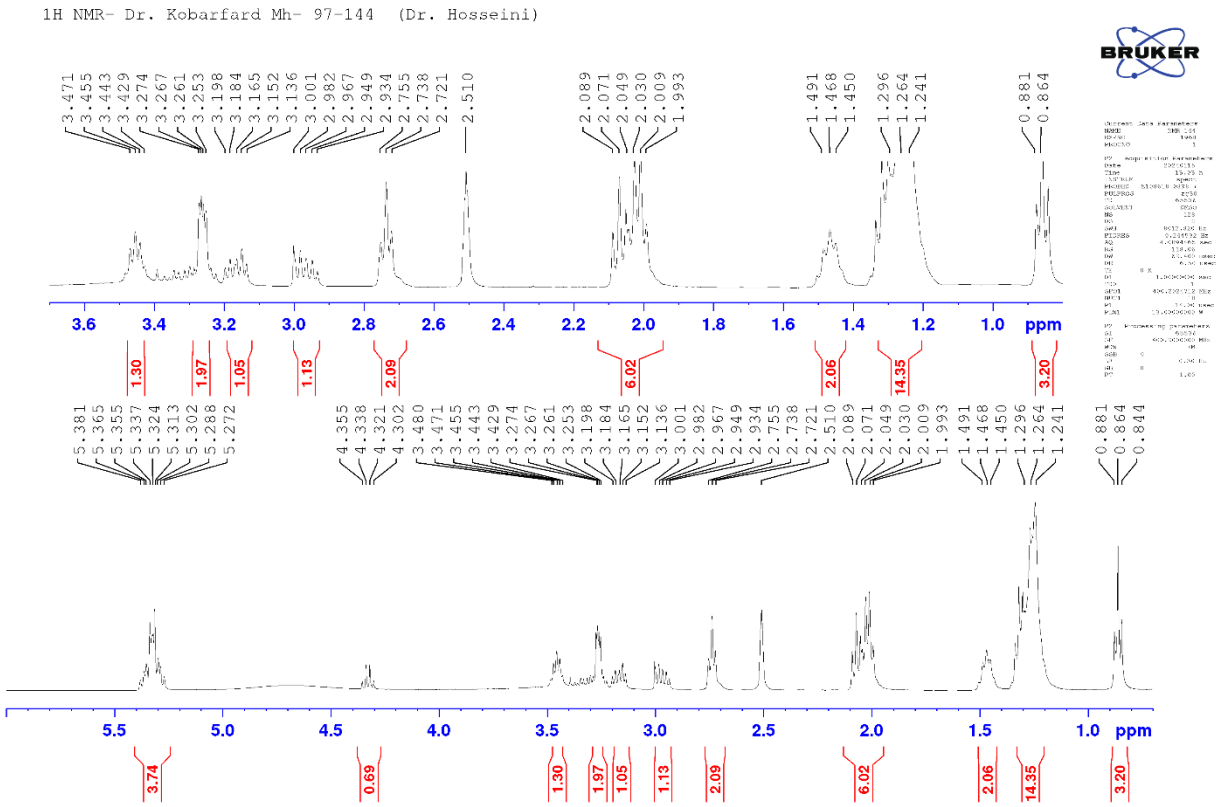
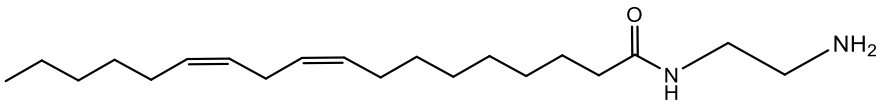


Figure 46. ^{1}H-NMR spectra of compound L7

(9Z,12Z)-N-(2-aminoethyl)octadeca-9,12-dienamide (L8)



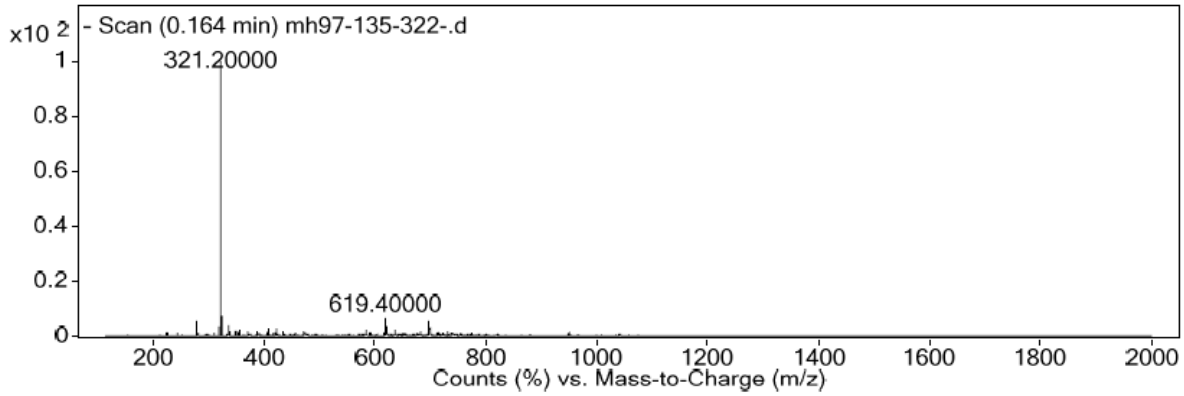


Figure 47. ESI-MS spectrum (negative mode) of compound L8

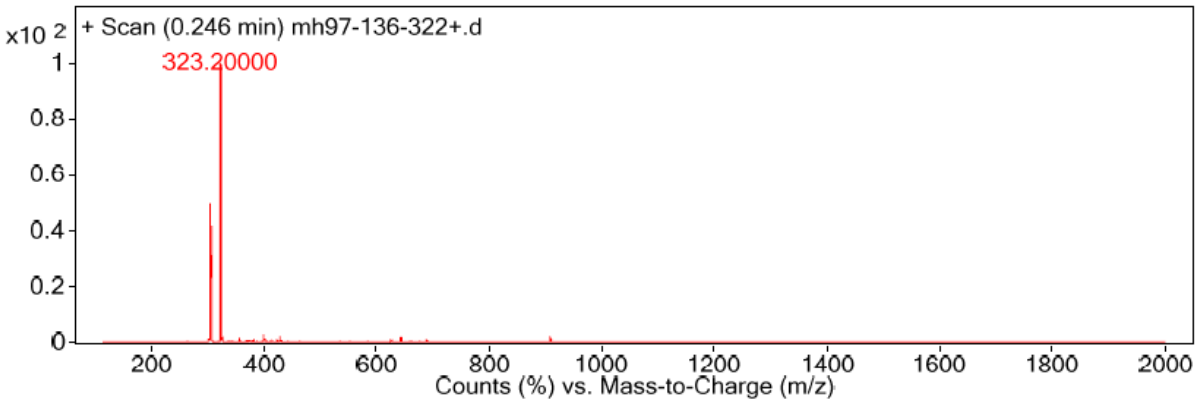


Figure 48. ESI-MS spectrum (positive mode) of compound L8

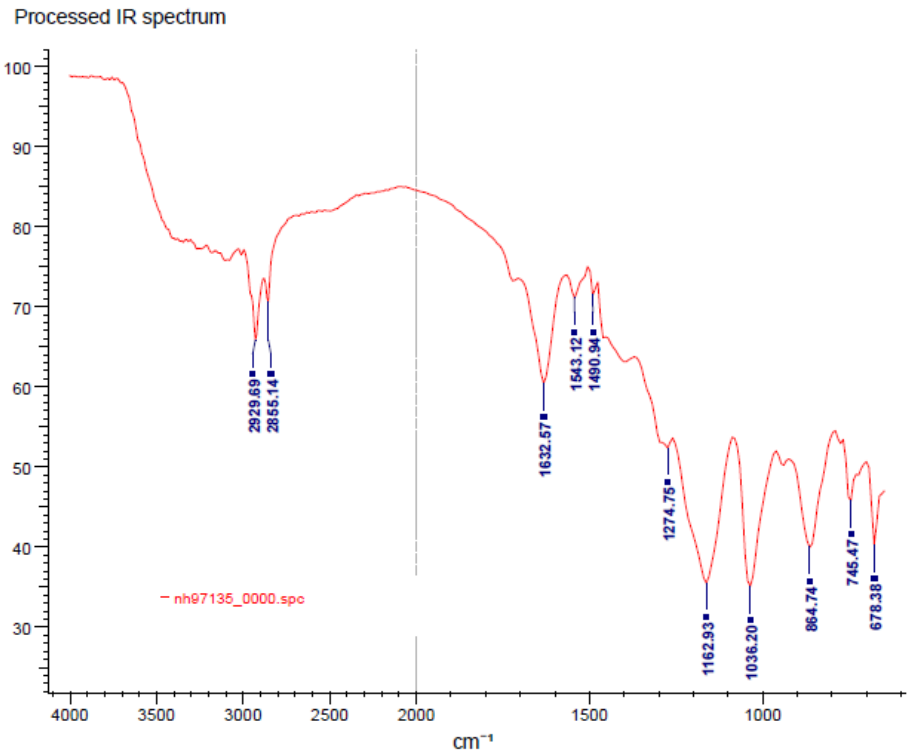


Figure 49. FT-IR spectrum of compound L8

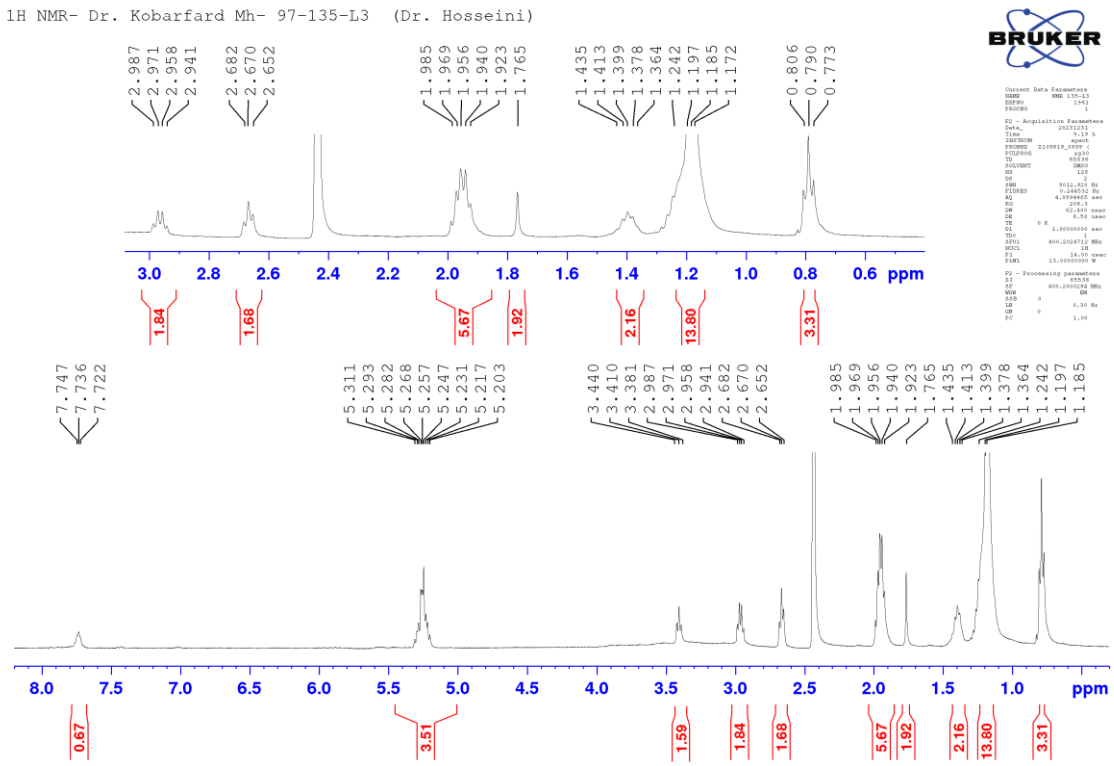
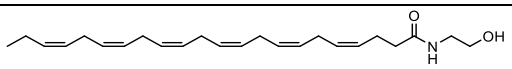
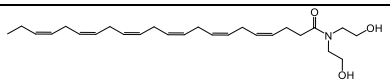
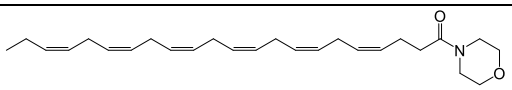
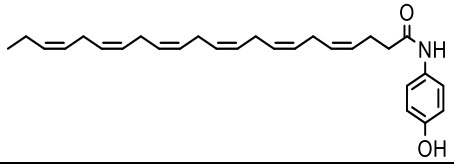
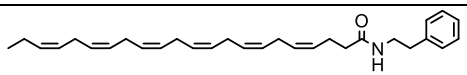
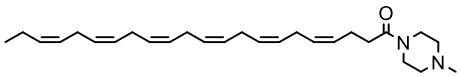
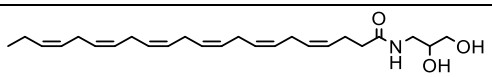
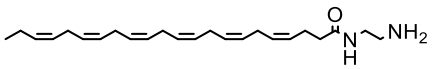
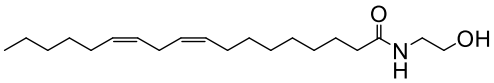
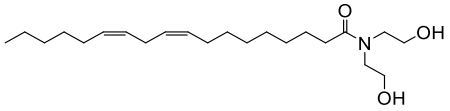
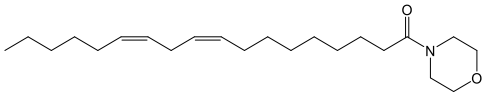
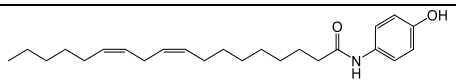
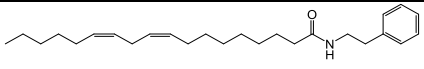
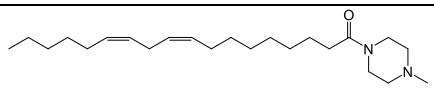
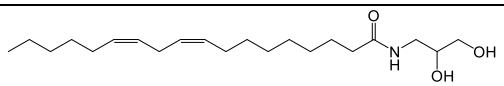
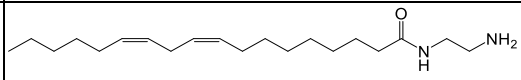
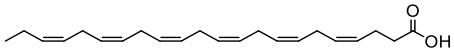


Figure 50. ^{1}H-NMR spectra of compound L8

Table 1: Binding affinity of the synthesized compounds.

Compound	Structure	Binding affinity (Kcal/mol)	
		1Q1M	1T4J
D1		-6.3	-6.2
D2		-6.2	-6.5
D3		-6.0	-6.8
D4		-6.5	-6.9
D5		-6.1	-8.0
D6		-5.7	-6.9
D7		-5.7	-6.5
D8		-5.5	-6.3
L1		-5.4	-5.9
L2		-5.8	-5.6
L3		-5.3	-5.9
L4		-6.0	-6.4
L5		-6.0	-6.7

L6		-6.3	-6.1
L7		-5.7	-5.9
L8		-5.1	-5.8
DHA		-6.3	-5.8