

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

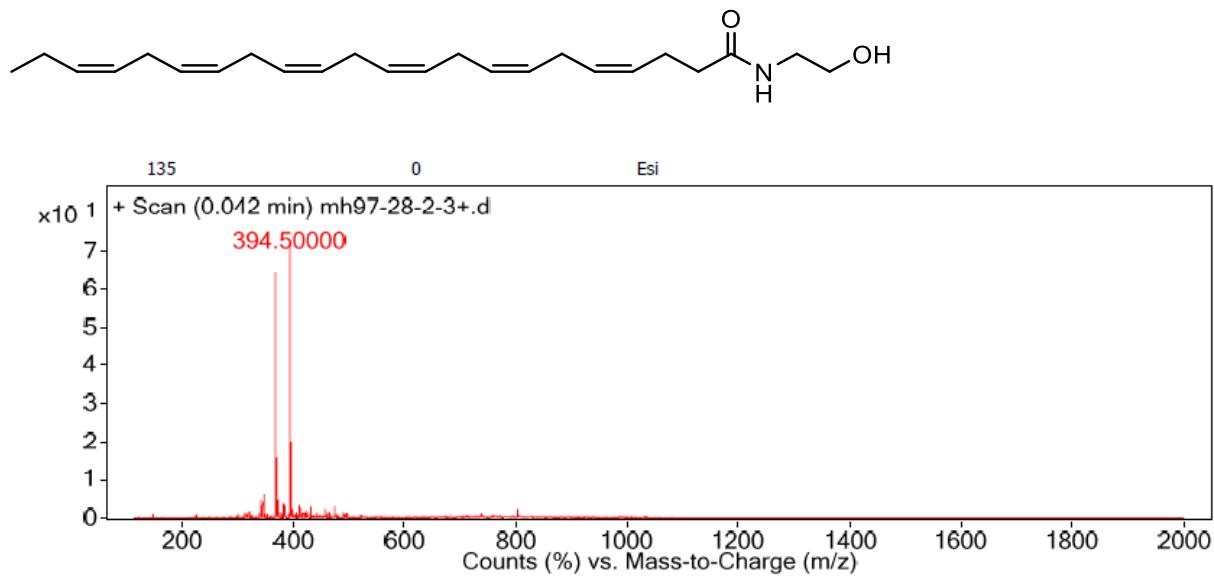


Figure 1. ESI-MS spectrum of compound D1

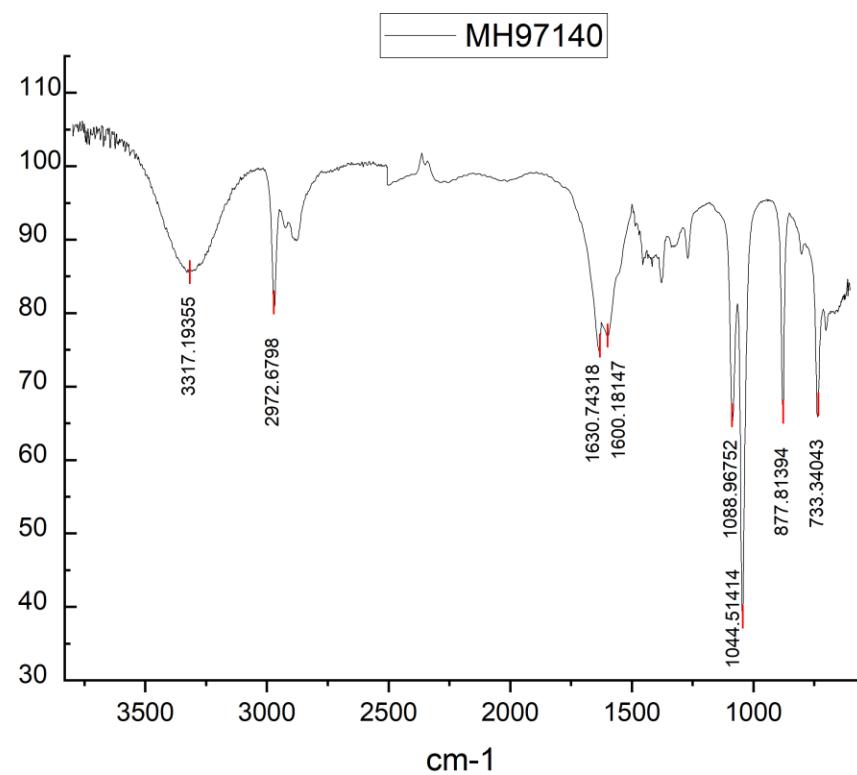


Figure 2. FT-IR spectrum of compound D1

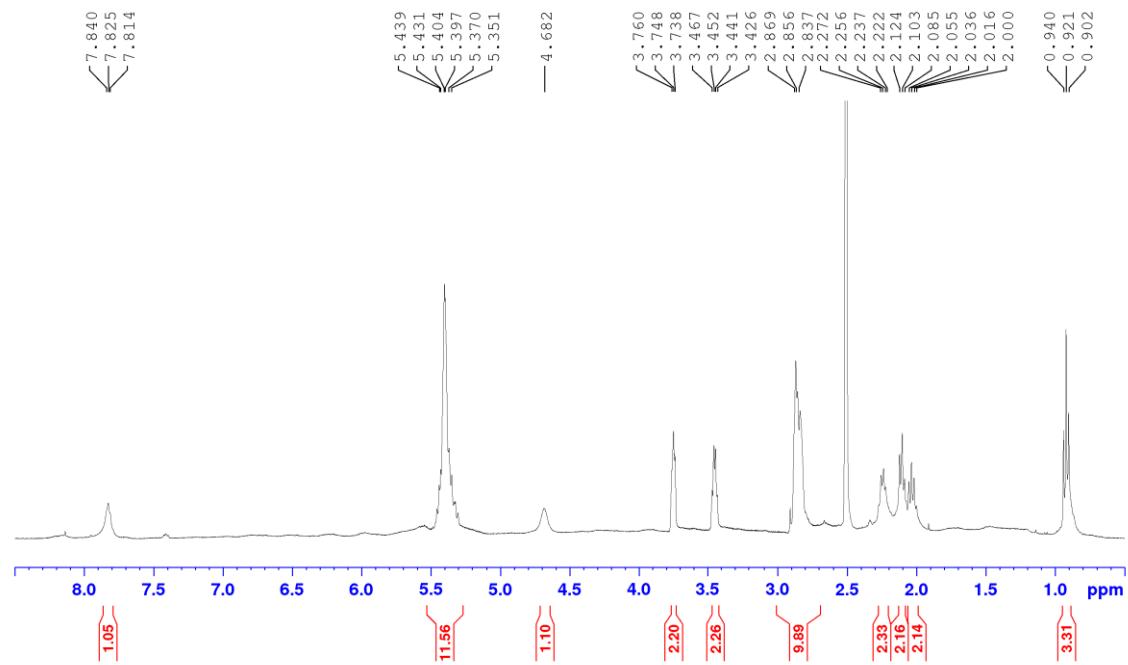


Figure 3. ¹H-NMR spectrum of compound D1

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

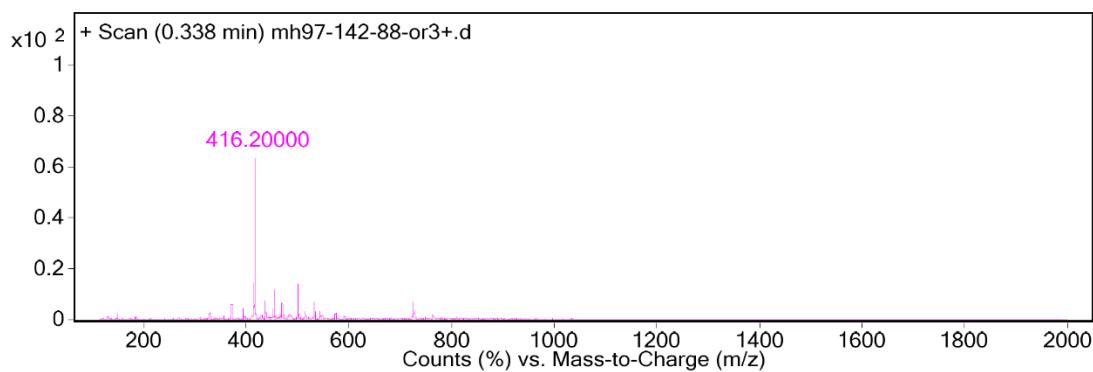
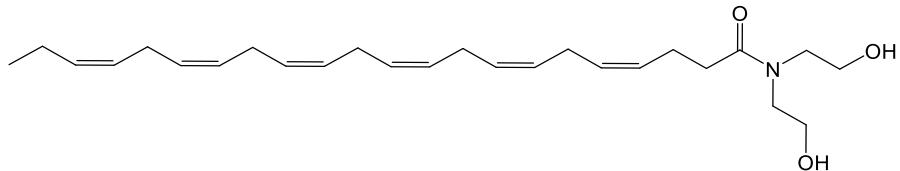


Figure 4. ESI-MS spectrum of compound D2

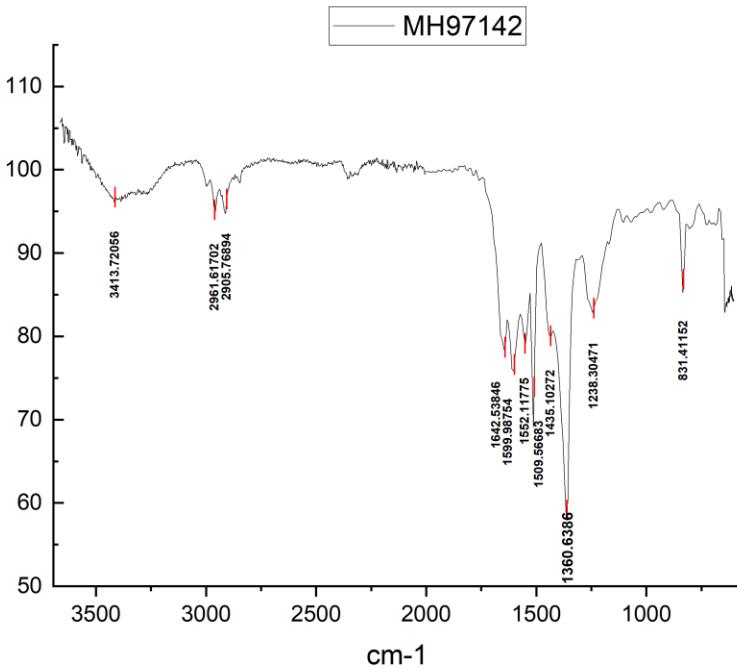


Figure 5. FT-IR spectrum of compound D2

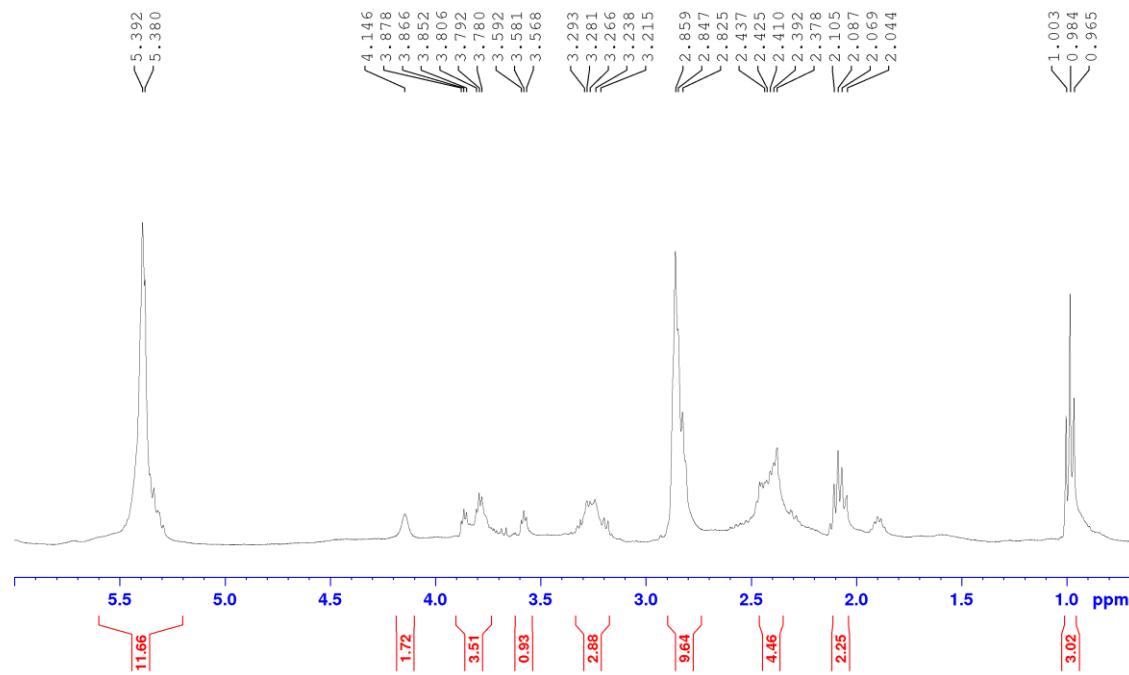


Figure 6. ¹H-NMR spectrum of compound D2

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

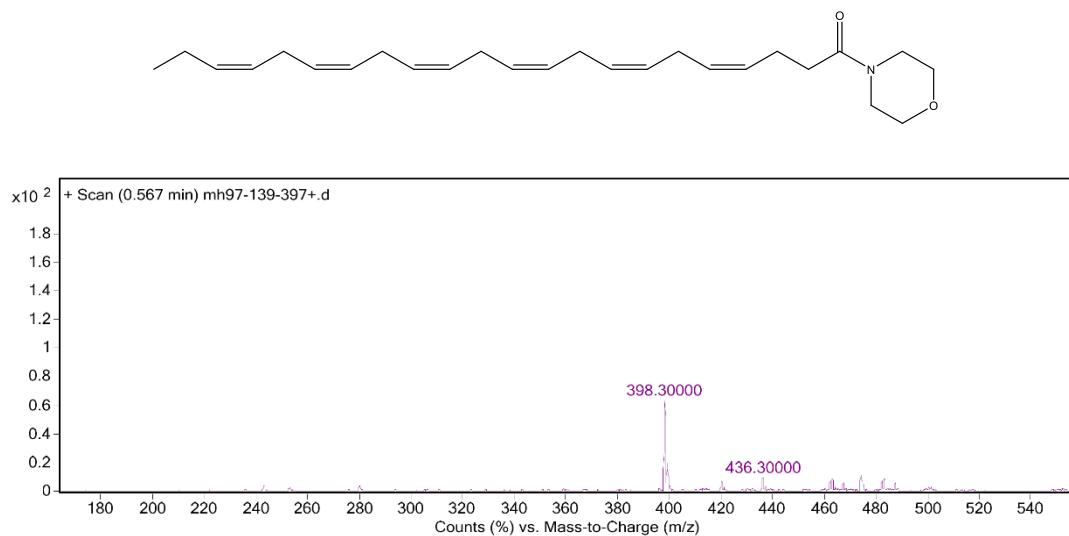


Figure 7. ESI-MS spectrum of compound D3

Processed IR spectrum

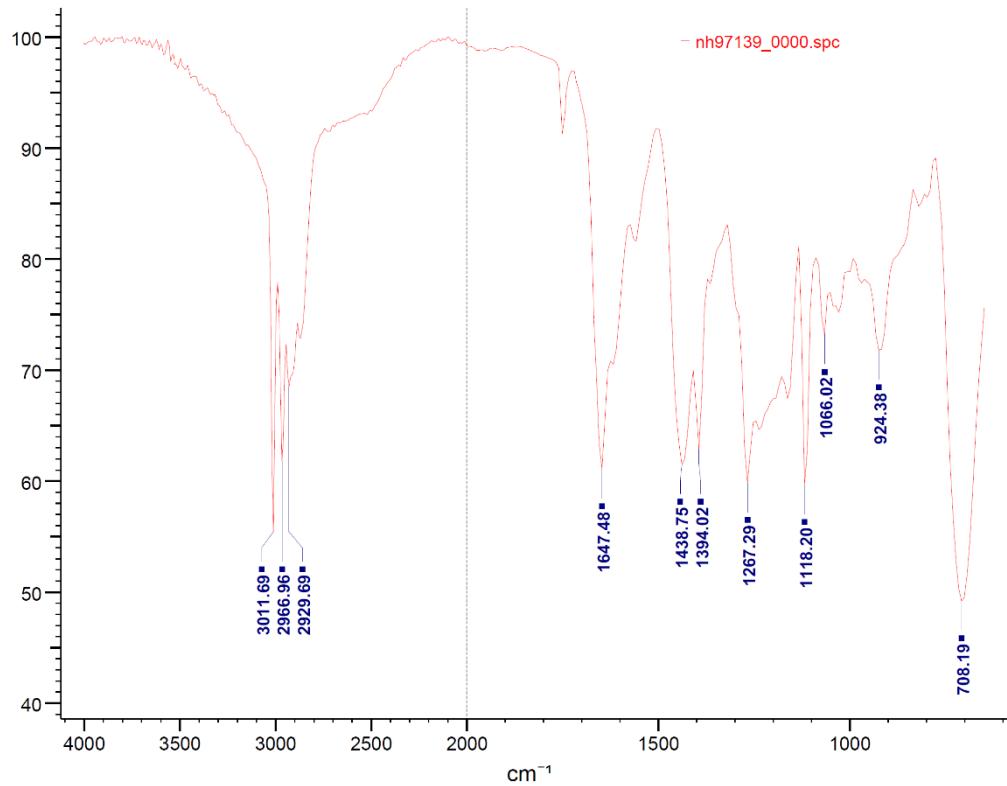


Figure 8. FT-IR spectrum of compound D3

¹H NMR- Dr. Kobarfard mh-97-139 (Dr. Hosseini)

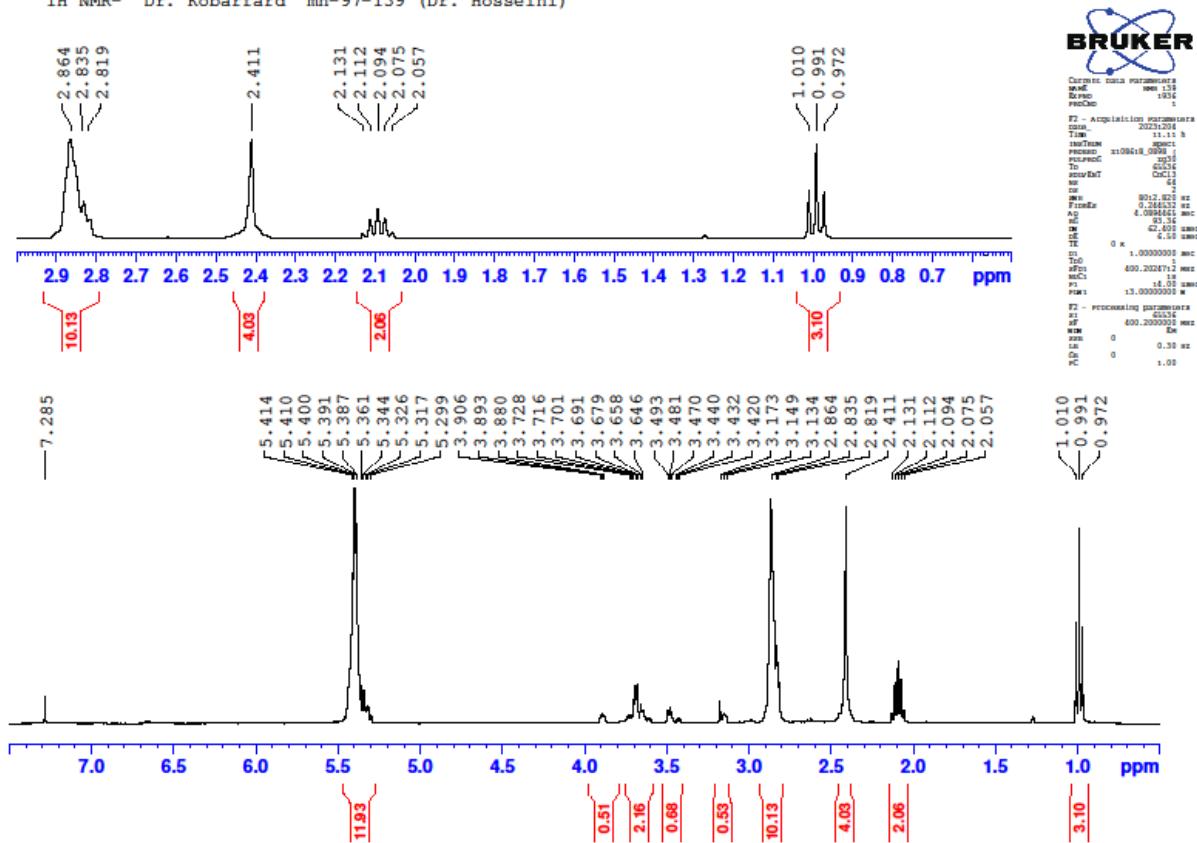


Figure 9. ¹H-NMR spectra of compound D3

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

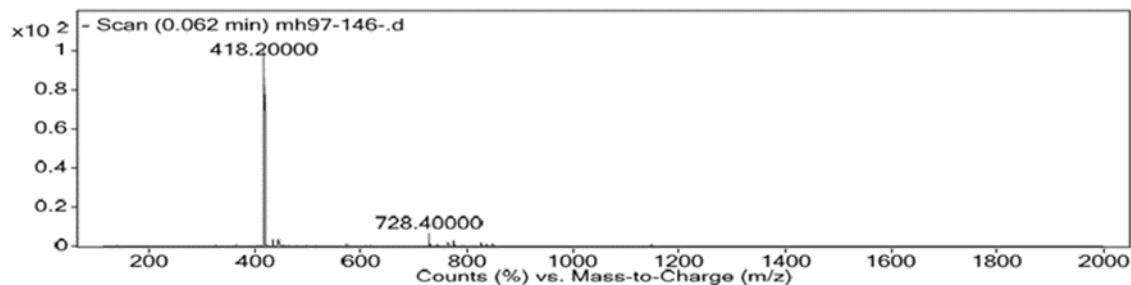
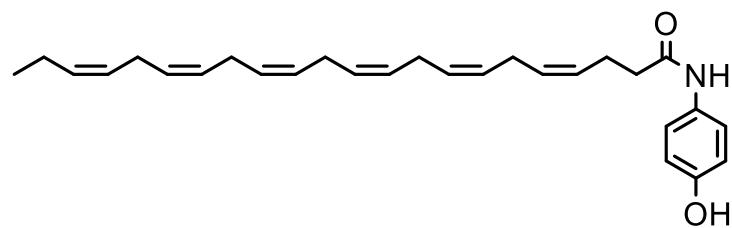


Figure 10. ESI-MS spectrum of compound D4

Processed IR spectrum

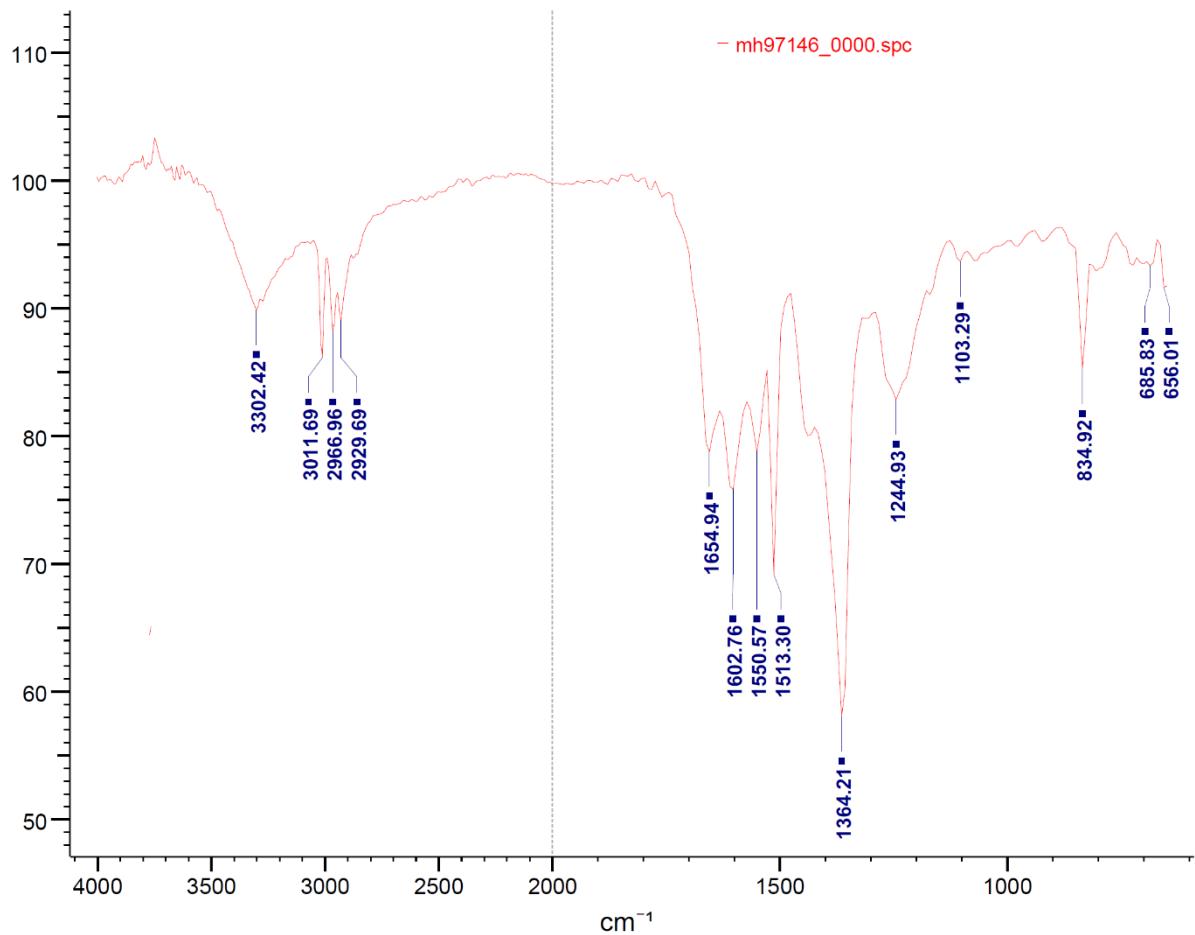
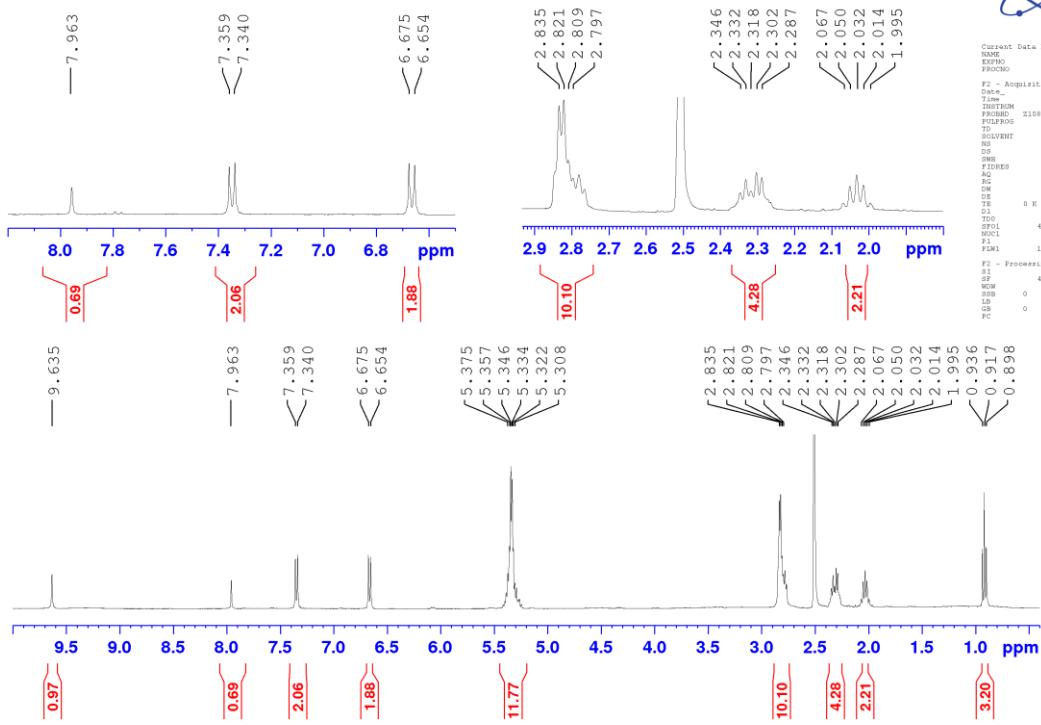


Figure 11. FT-IR spectrum of compound D4



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

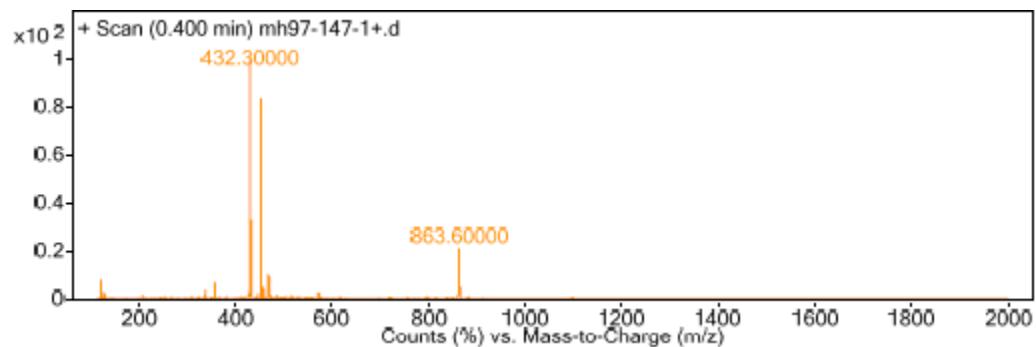
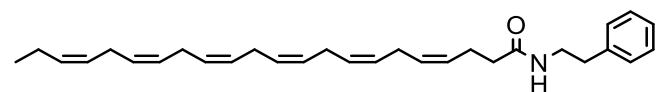


Figure 13. ESI-MS spectrum of compound D5

Processed IR spectrum

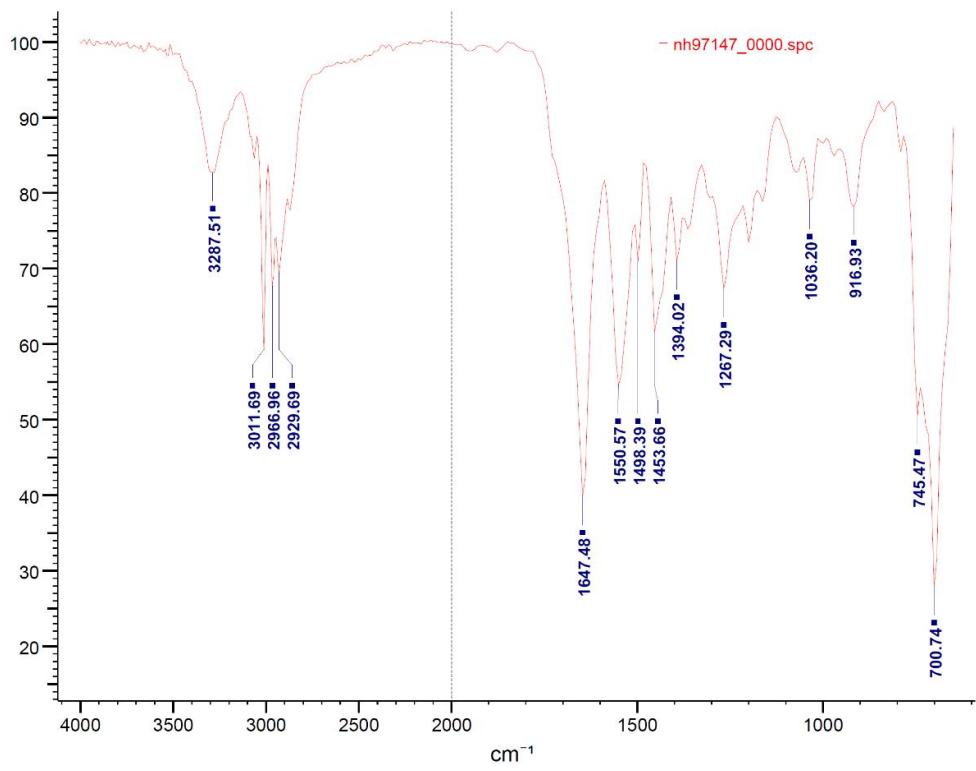


Figure 14. FT-IR spectrum of compound D5

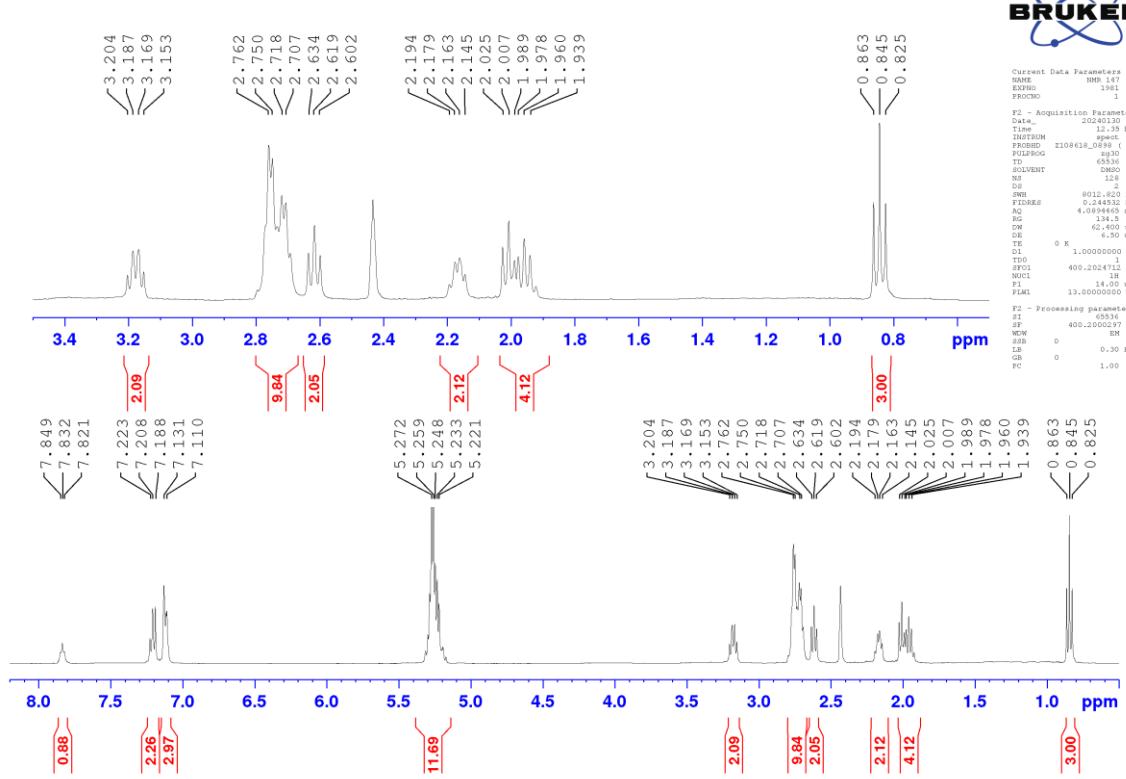


Figure 15. ^1H -NMR spectra of compound D5

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

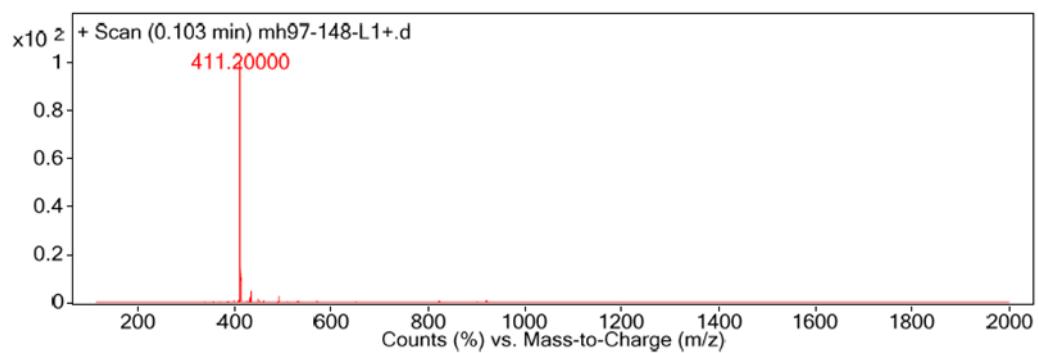
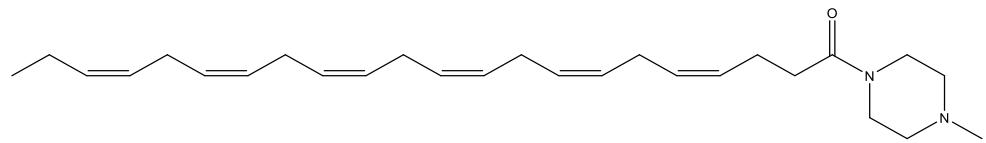


Figure 16. ESI-MS spectrum of compound D6

Processed IR spectrum

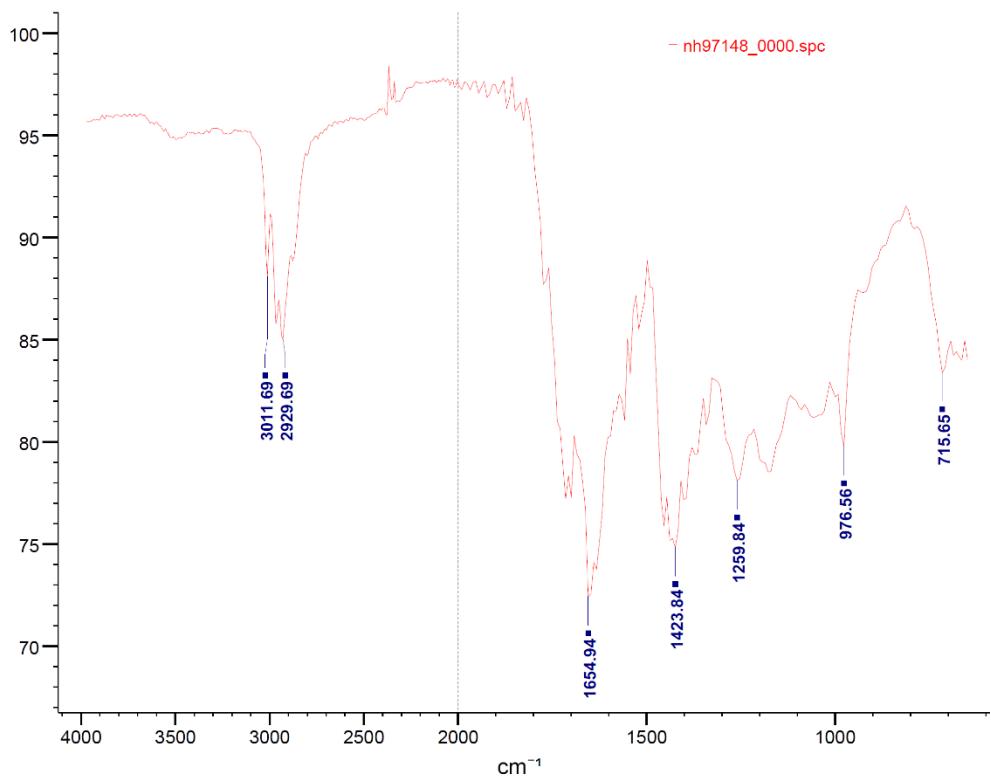


Figure 17. FT-IR spectrum of compound D6

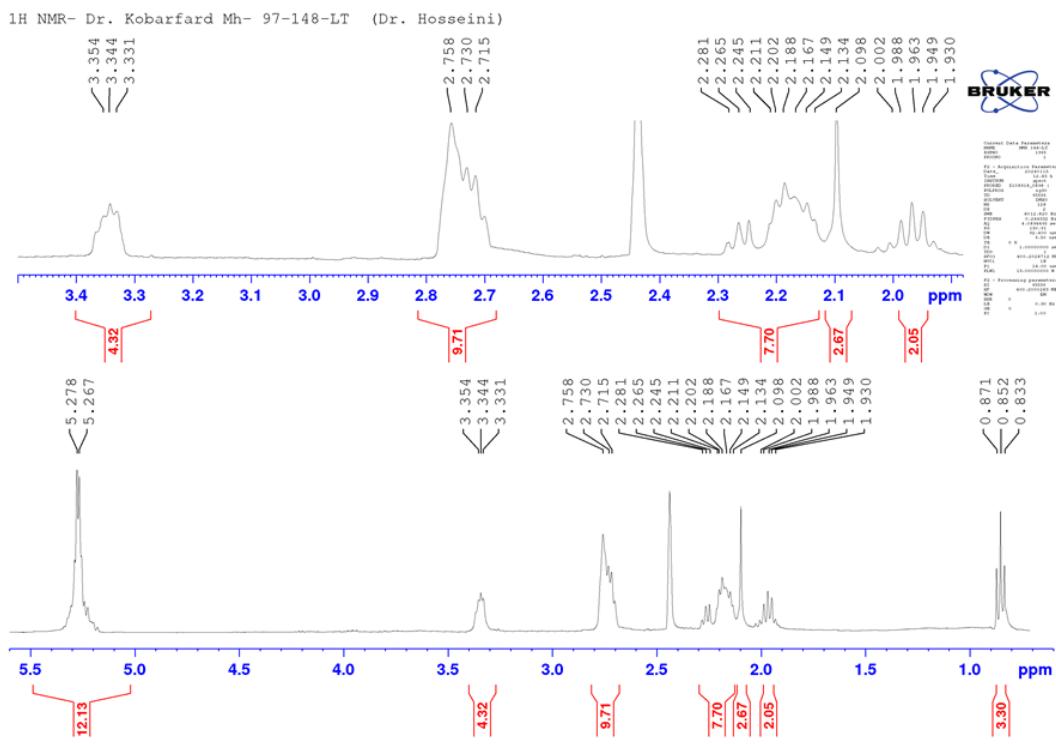


Figure 18. ^1H -NMR spectra of compound D6

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

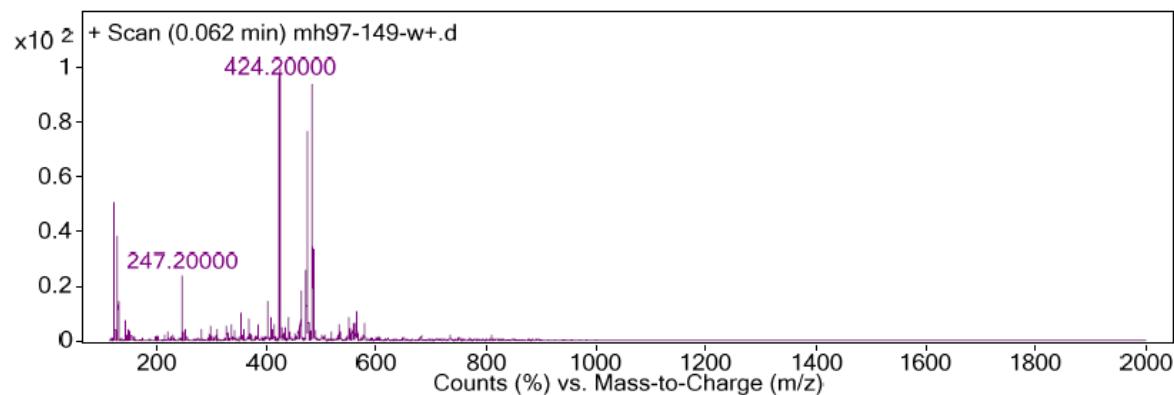
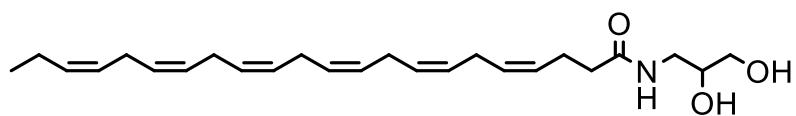


Figure 19. ESI-MS spectrum of compound D7

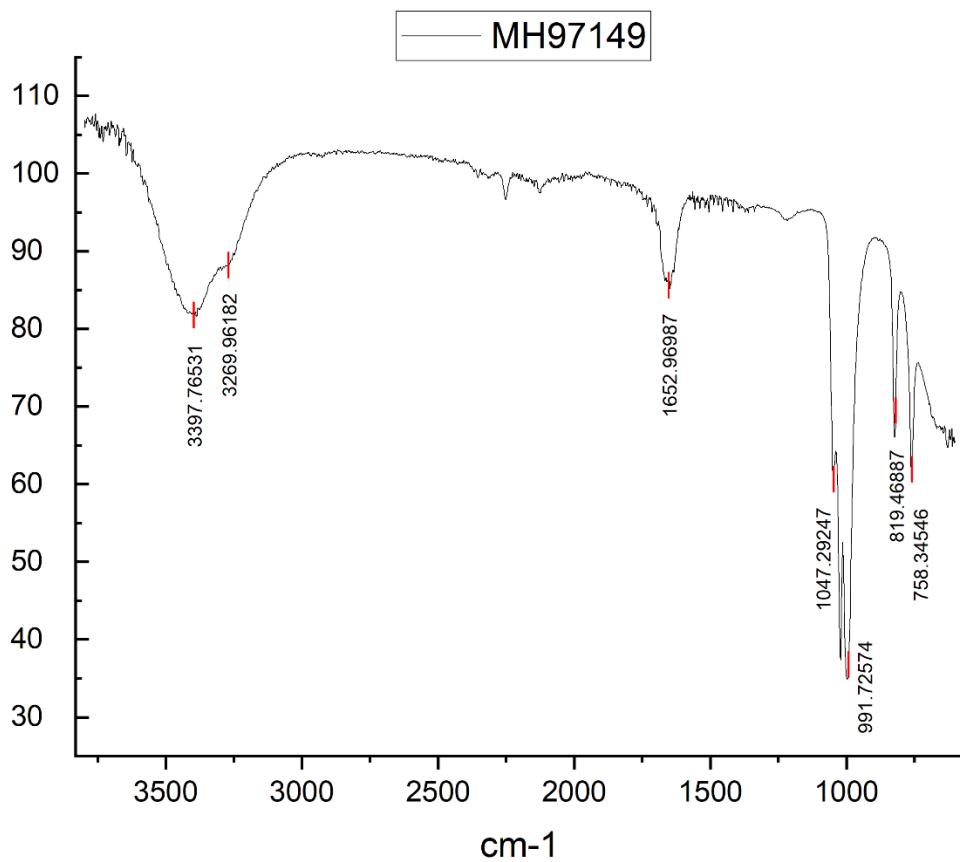


Figure 20. FT-IR spectrum of compound D7

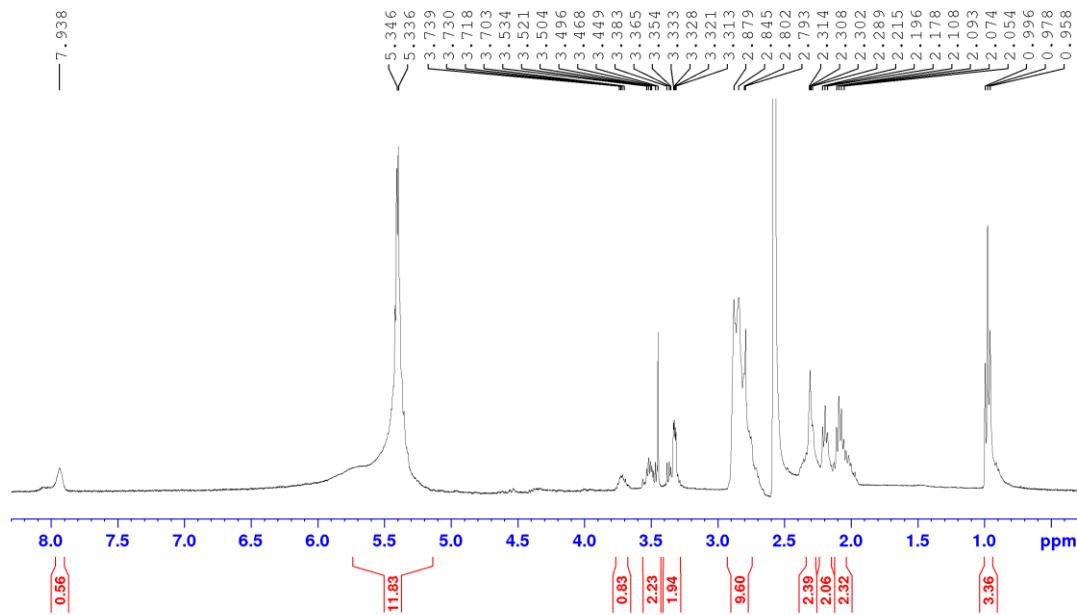


Figure 21.¹H-NMR spectrum of compound D7

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

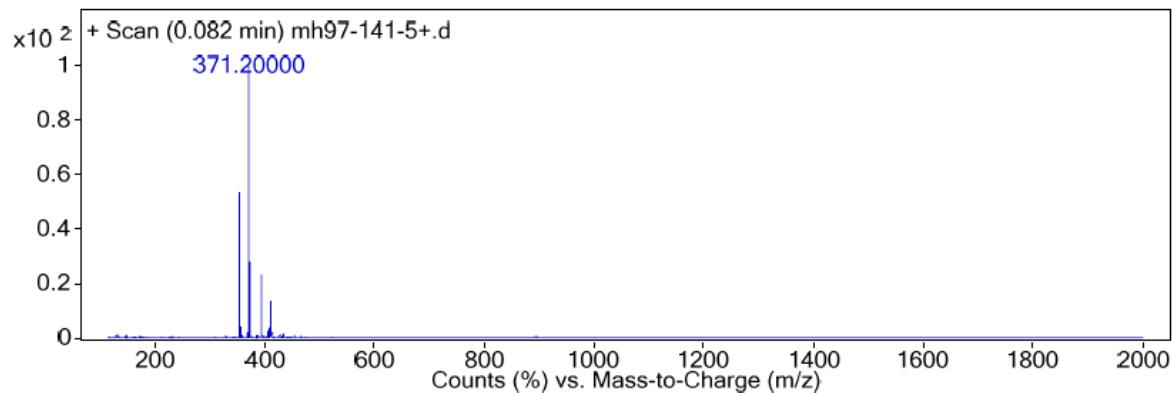
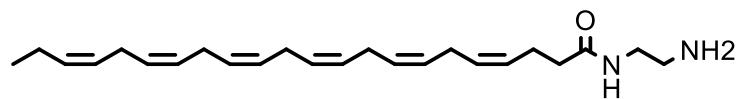


Figure 22. ESI-MS spectrum of compound D8

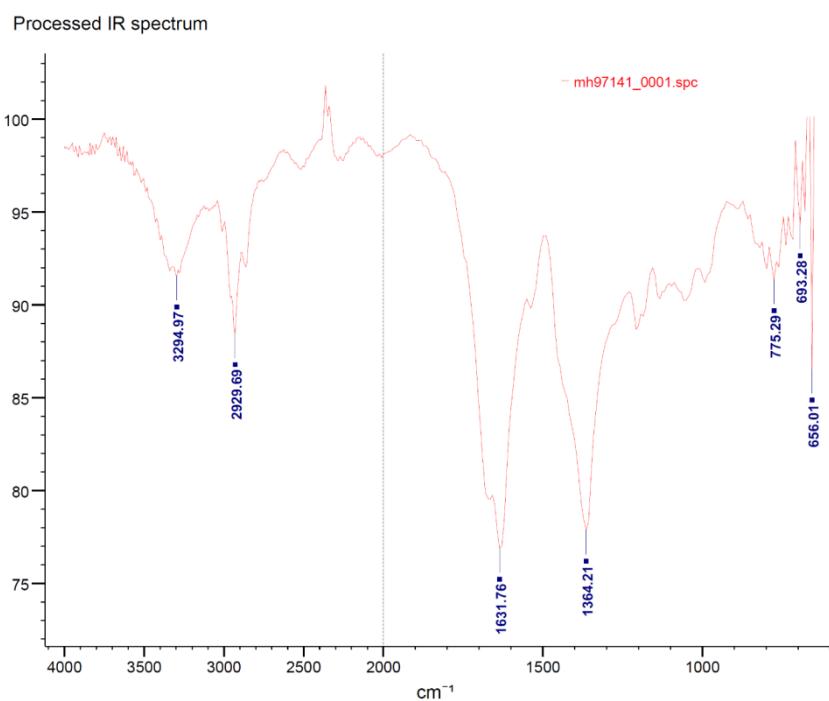


Figure 23. FT-IR spectrum of compound D8

¹H NMR- Dr. Kobarfard Mh- 97-141 (Dr. Hosseini)

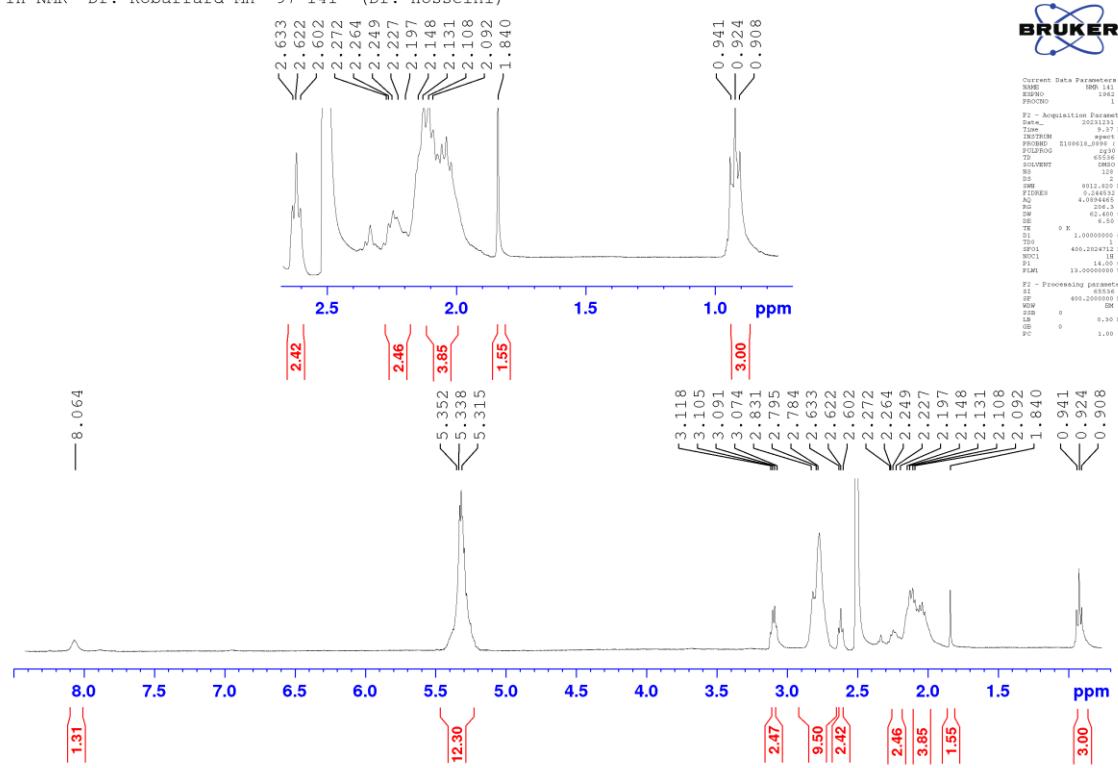


Figure 24. ¹H-NMR spectra of compound D8

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

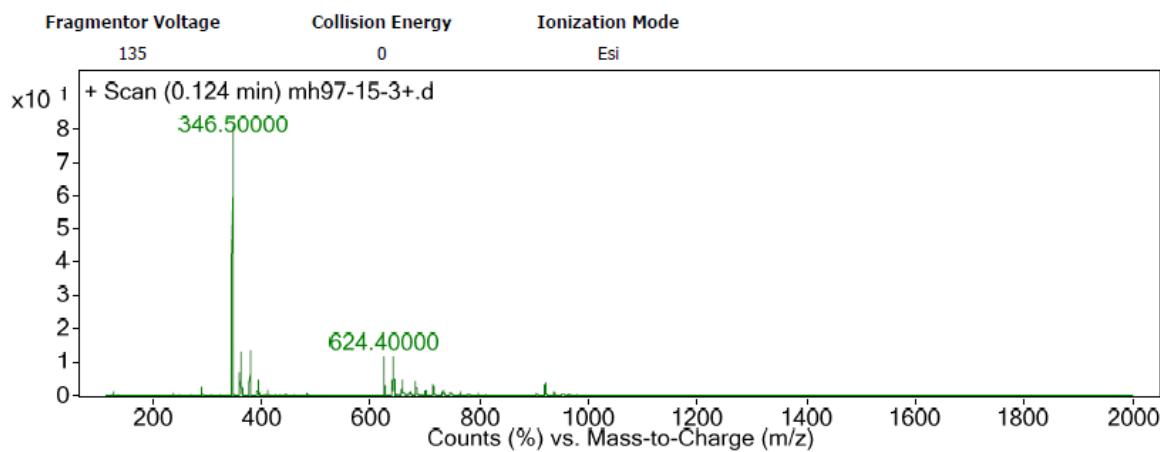
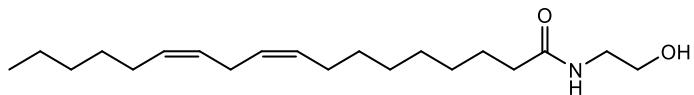


Figure 25. ESI-MS spectrum of compound L1

Processed IR spectrum

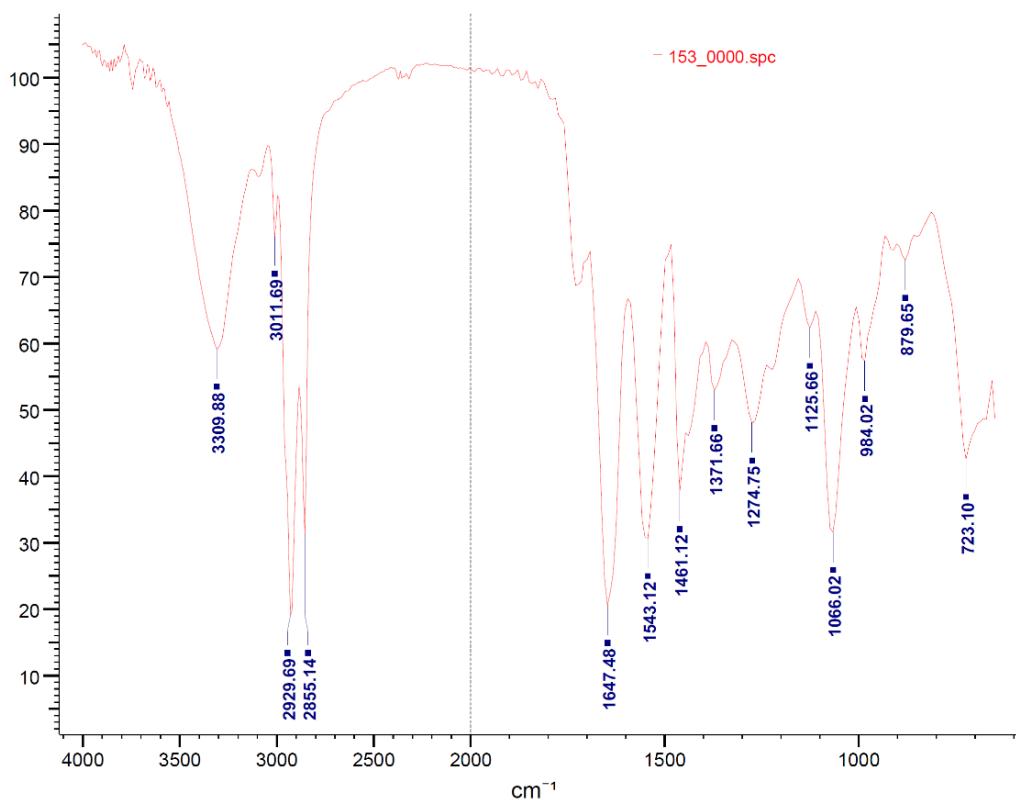


Figure 26. FT-IR spectrum of compound L1

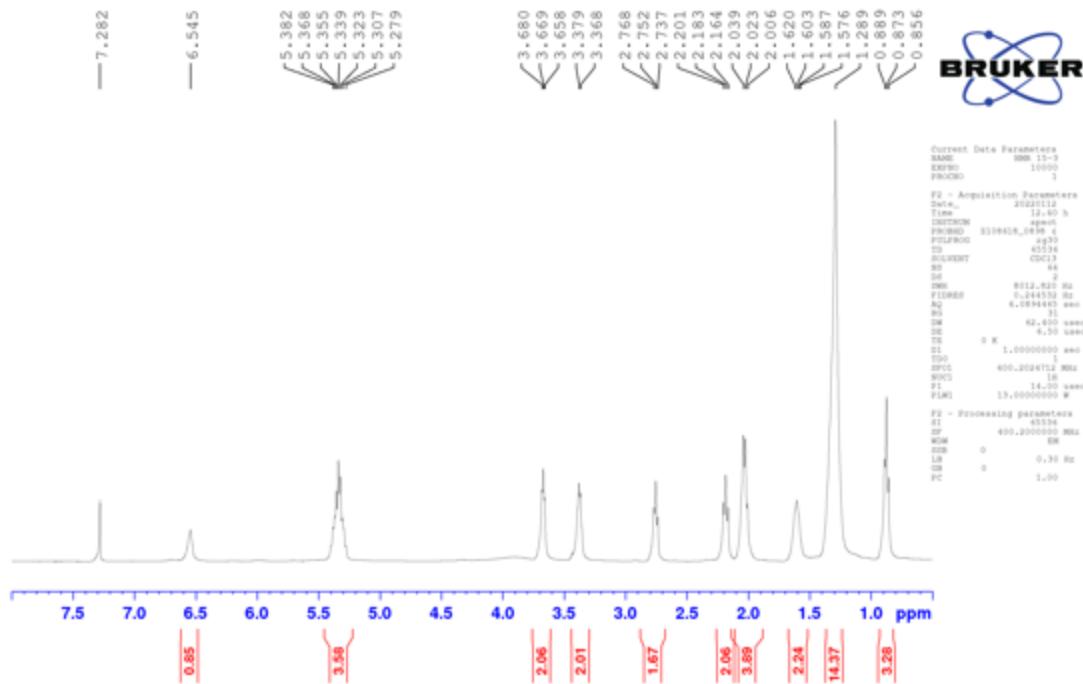


Figure 27. ¹H-NMR spectra of compound L1

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

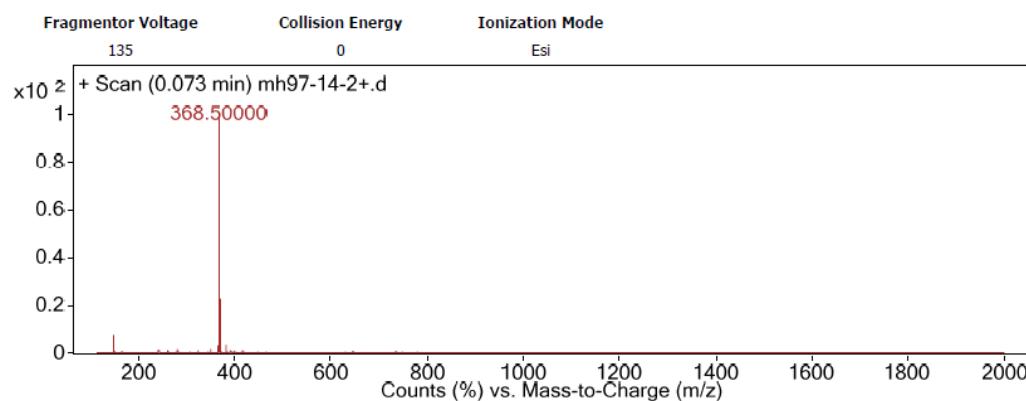
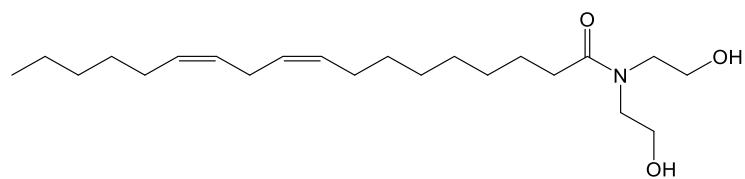


Figure 28. ESI-MS spectrum of compound L2

Processed IR spectrum

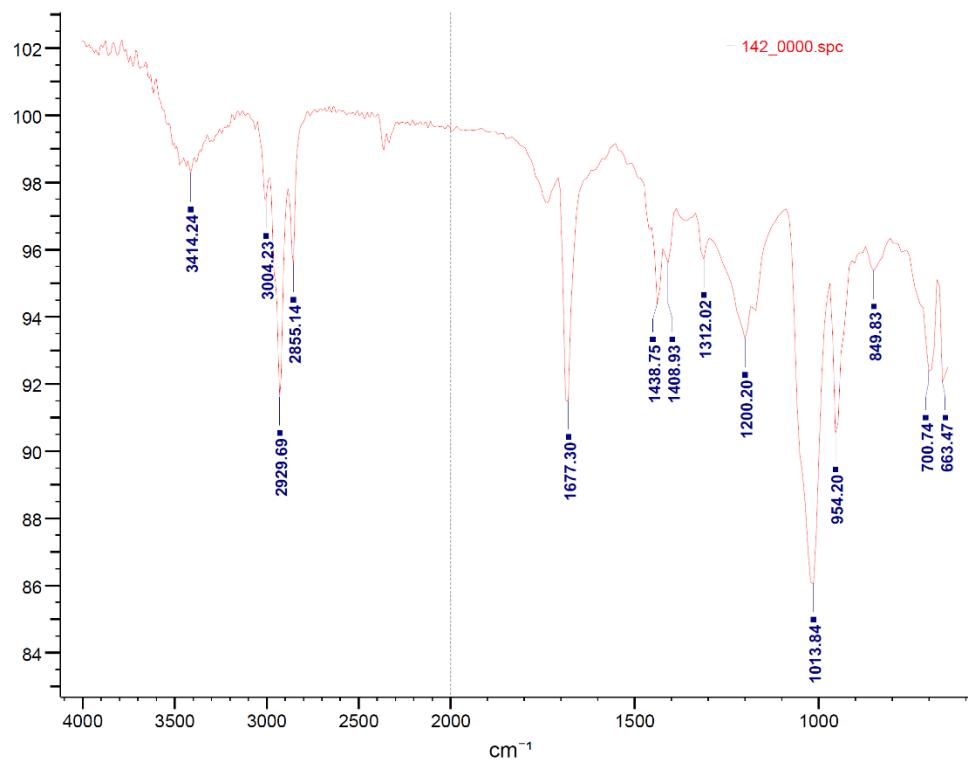
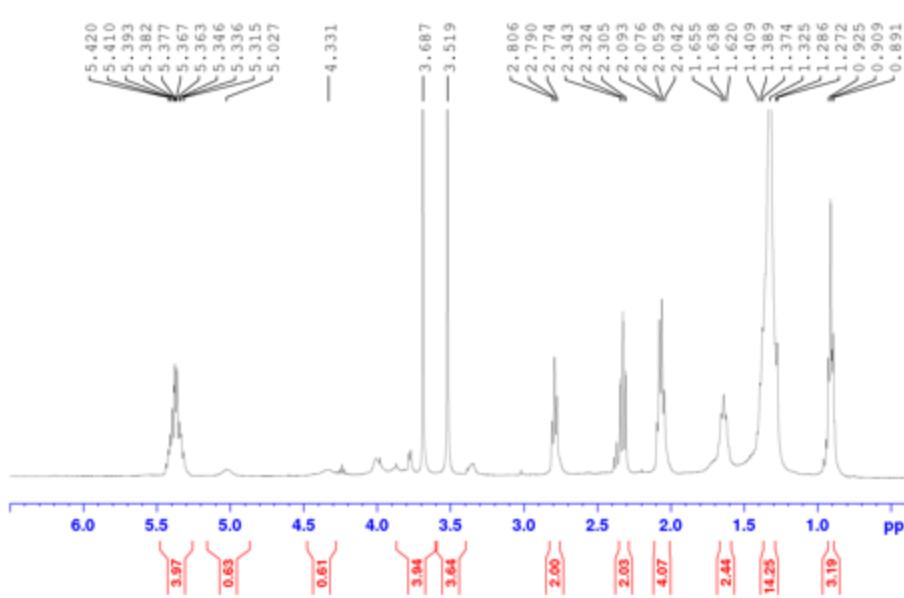


Figure 29. FT-IR spectrum of compound L2



Current Data Parameters
NAME: HNN 14-2
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date: 20111231
Time: 13:14:26
INSTRUM: spect
PROBPC: Z10861E_3991
PULPROG: zg3d90f
TD: 65536
SOLVENT: CDCl3
NS: 64
DS: 2
SW0: 8012.420 Hz
FIDRES: 0.244032 Hz
AQ: 4.000000 sec
RG: 118.04
DM: 62.400 used
DE: 6.00 used
TE: 0.0 K
D1: 1.00000000 sec
TDO: 1
RHO1: 400.2024712 MHz
NUC1: 1H
P1: 14.00 usec
PSWI: 13.00000000 W

F2 - Processing parameters
SI: 65536
SF: 400.2000000 MHz
RM: 8K
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

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

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

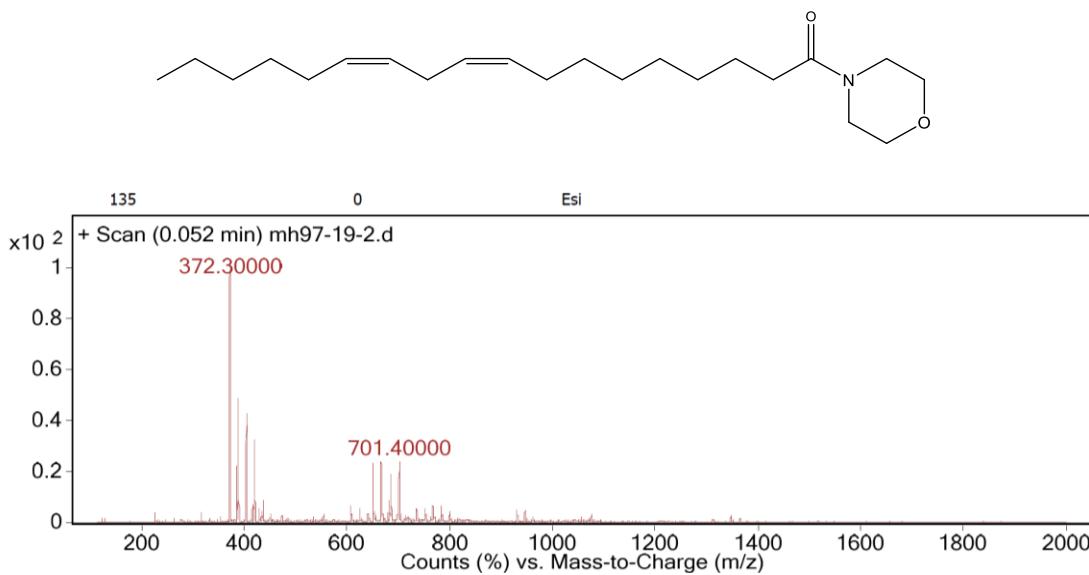


Figure 31. ESI-MS spectrum of compound L3

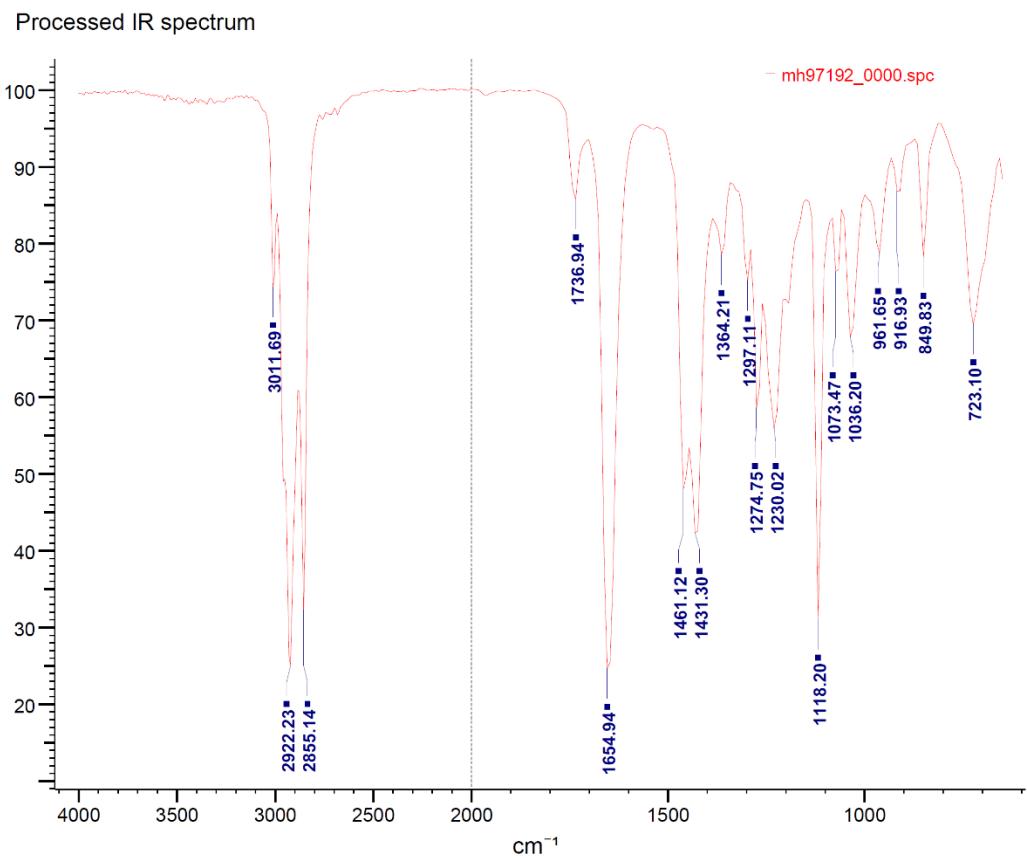


Figure 32. FT-IR spectrum of compound L3

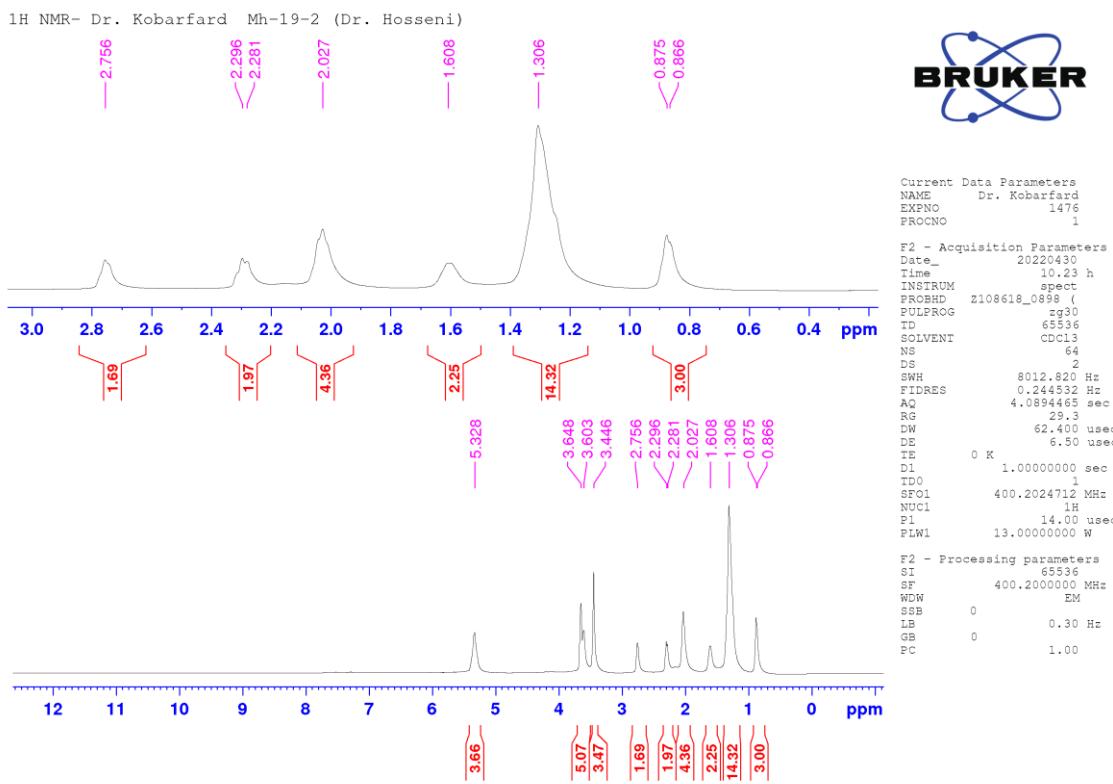


Figure 33. ^1H -NMR spectra of compound L3

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

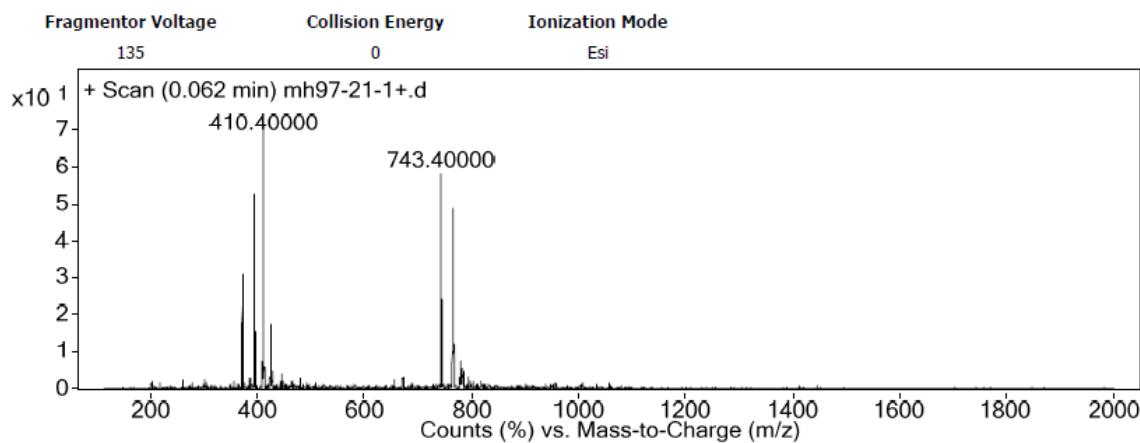
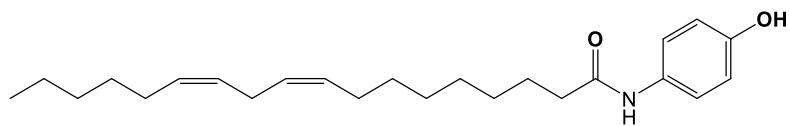


Figure 34. ESI-MS spectrum of compound L4

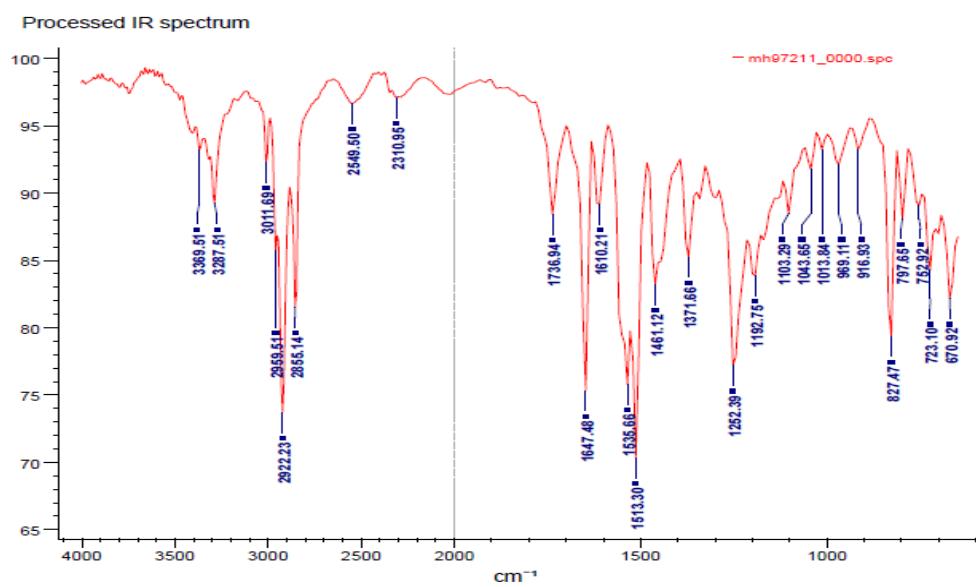


Figure 35. FT-IR spectrum of compound L4

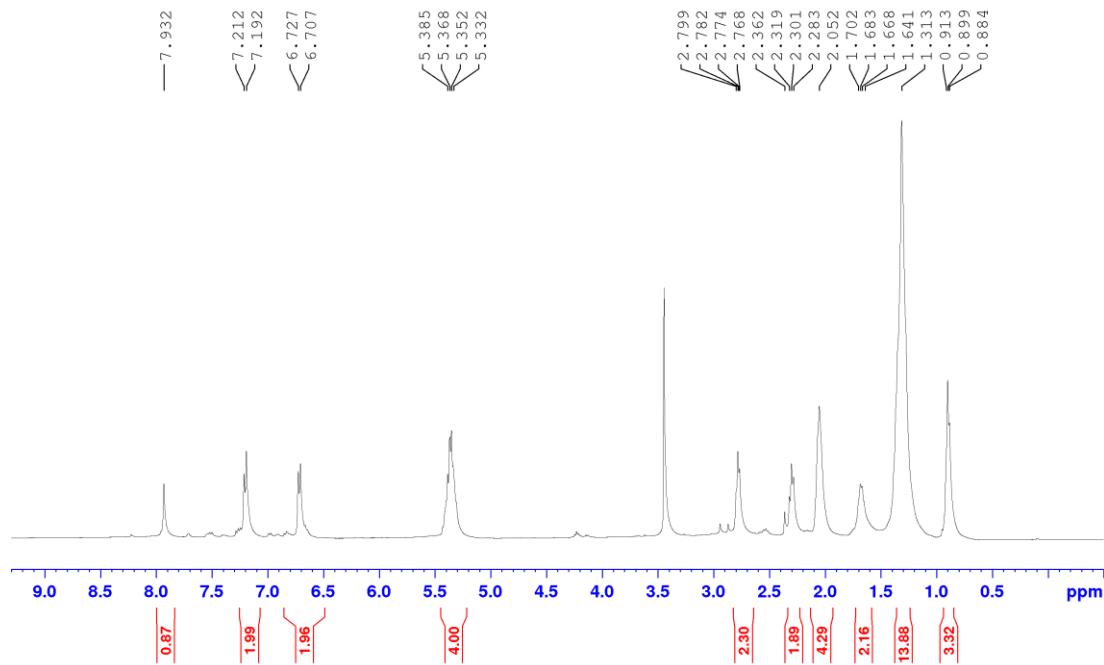


Figure 36. ¹H-NMR spectrum of compound L4

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

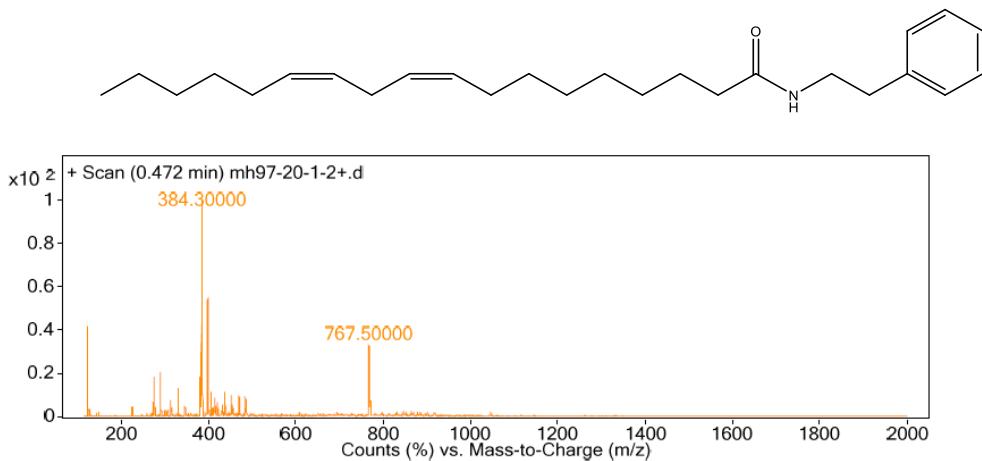


Figure 37. ESI-MS spectrum of compound L5

Processed IR spectrum

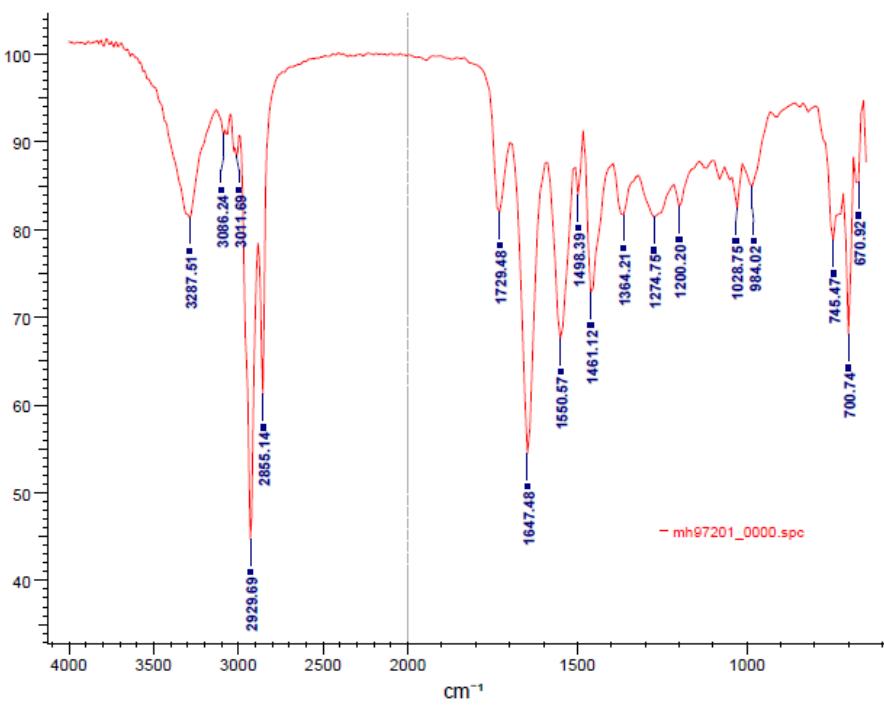
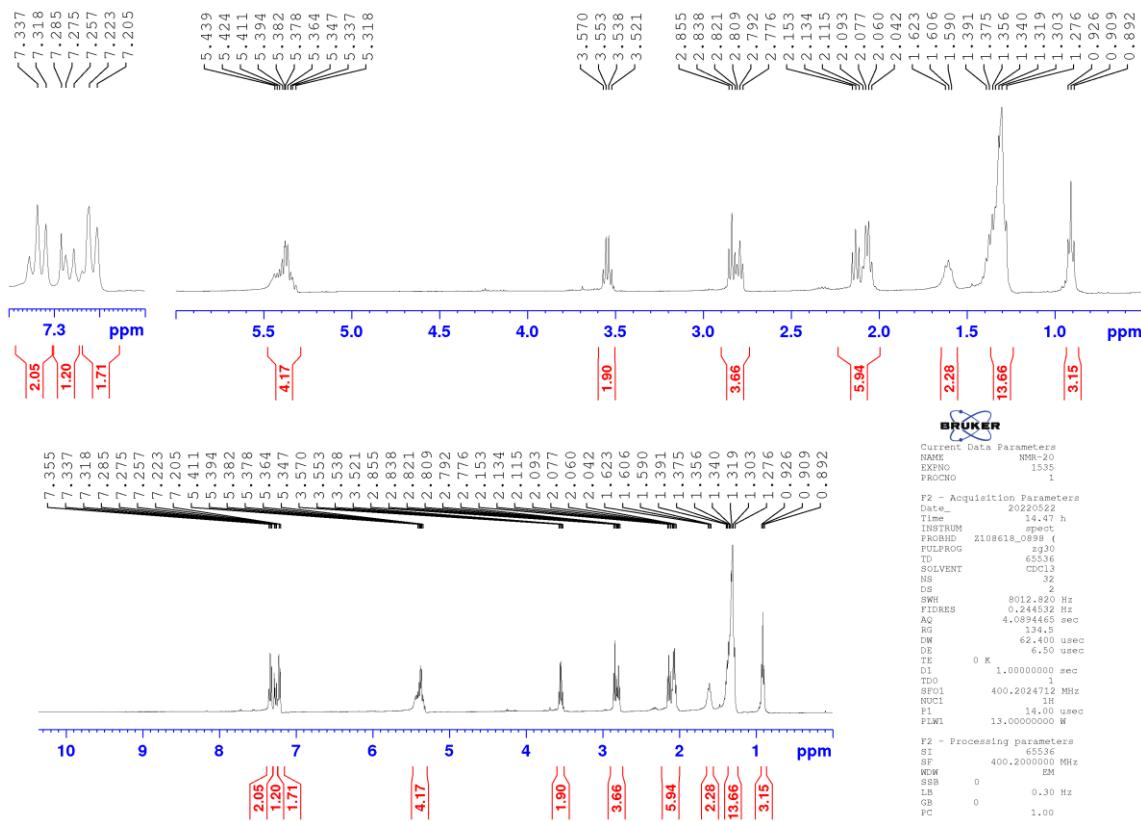


Figure 38. FT-IR spectrum of compound L5



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

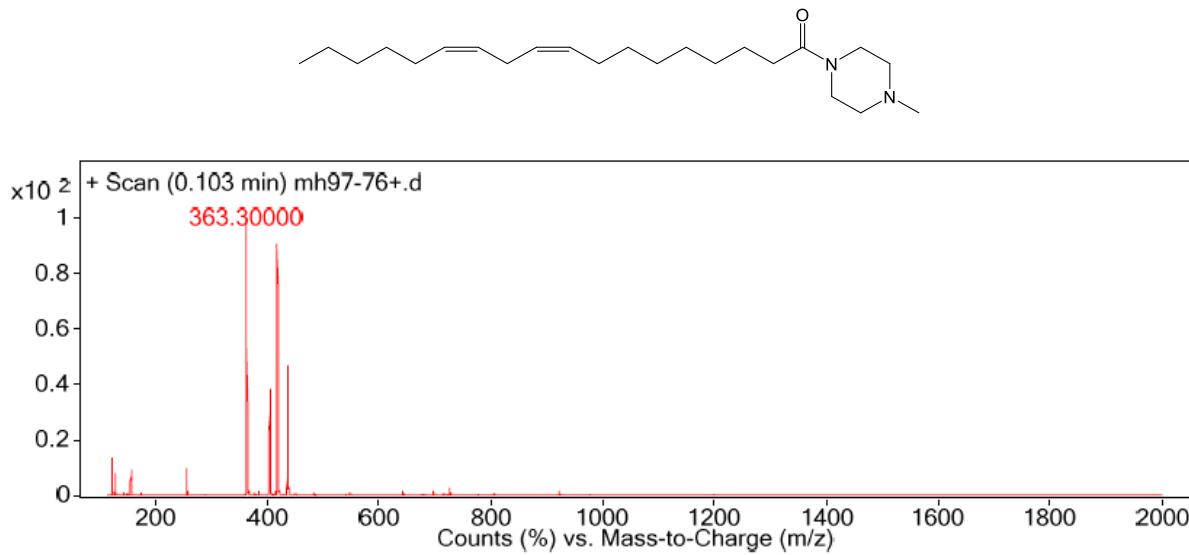


Figure 40. ESI-MS spectrum of compound L6

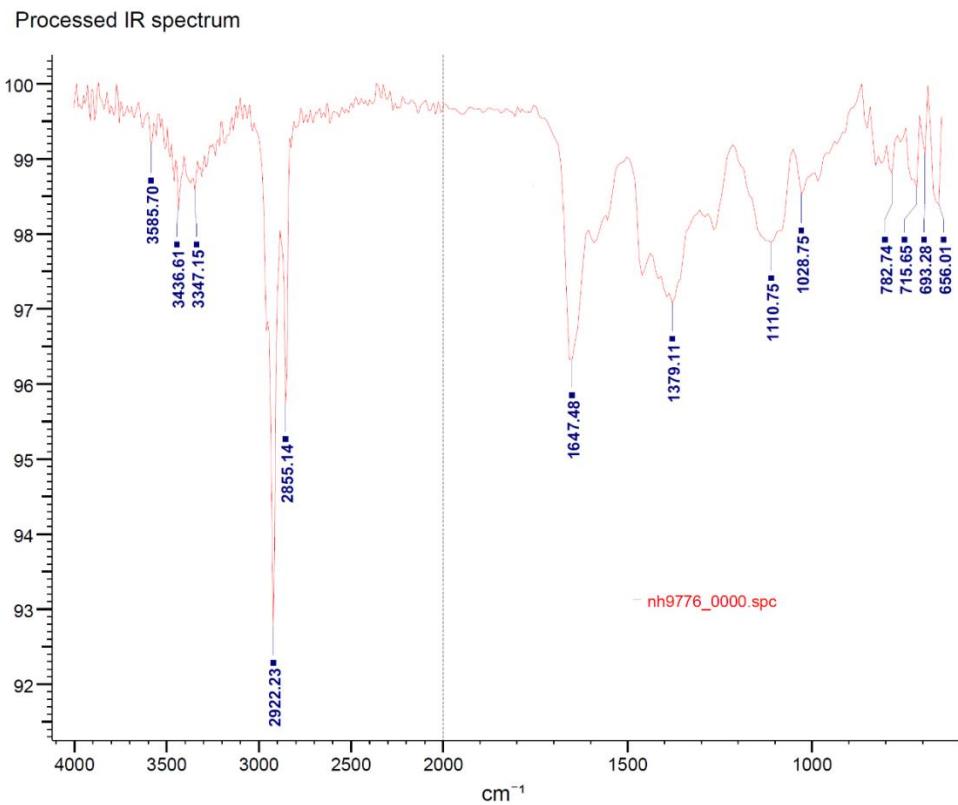
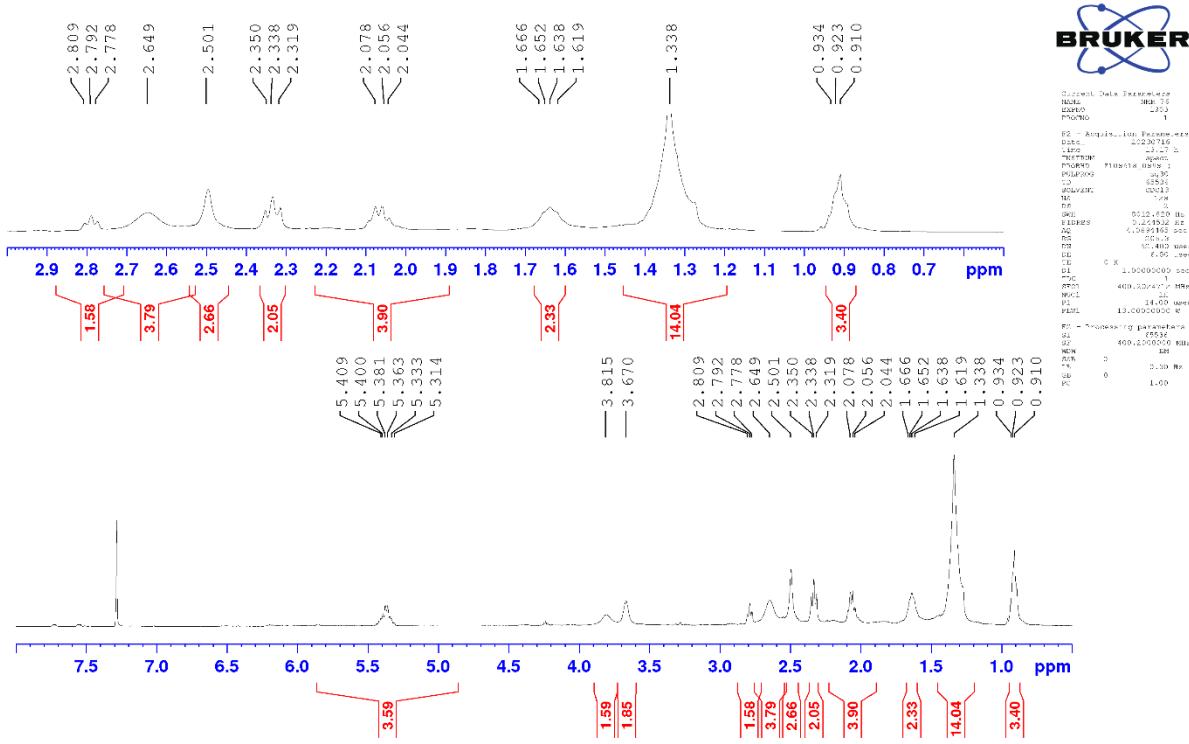


Figure 41. FT-IR spectrum of compound L6

¹H NMR - Dr. Kobarfard mh-97-76-1 (Dr. Hosseini)



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

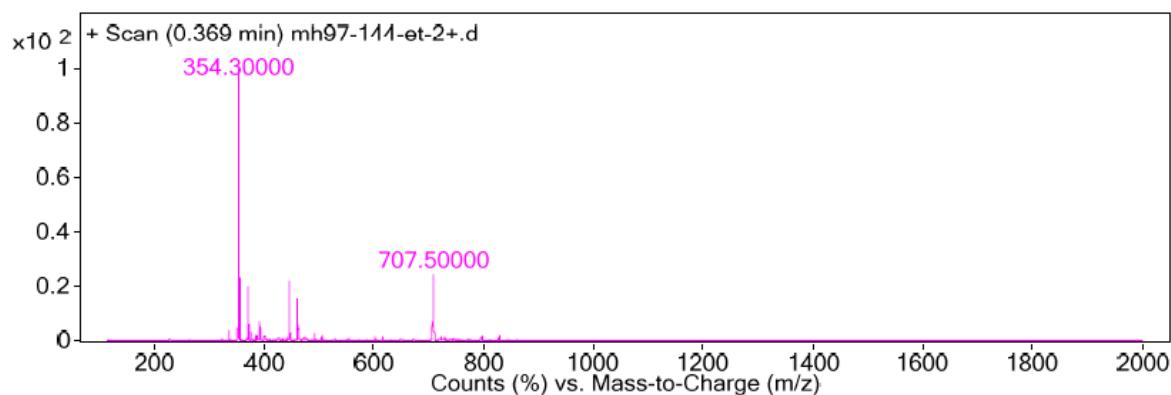
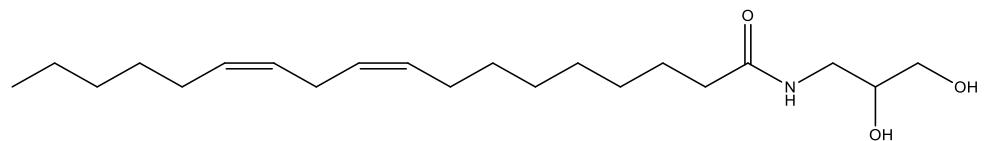


Figure 43. ESI-MS spectrum of compound L7 (m/z : 354 ($M+H$) $^+$)

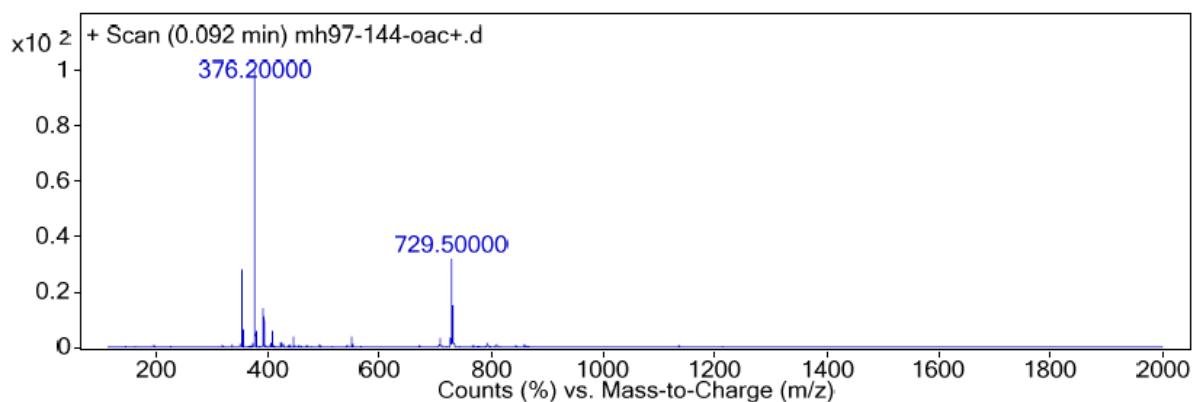


Figure 44. ESI-MS spectrum of compound L7 (m/z : 376 ($M+Na$) $^+$)

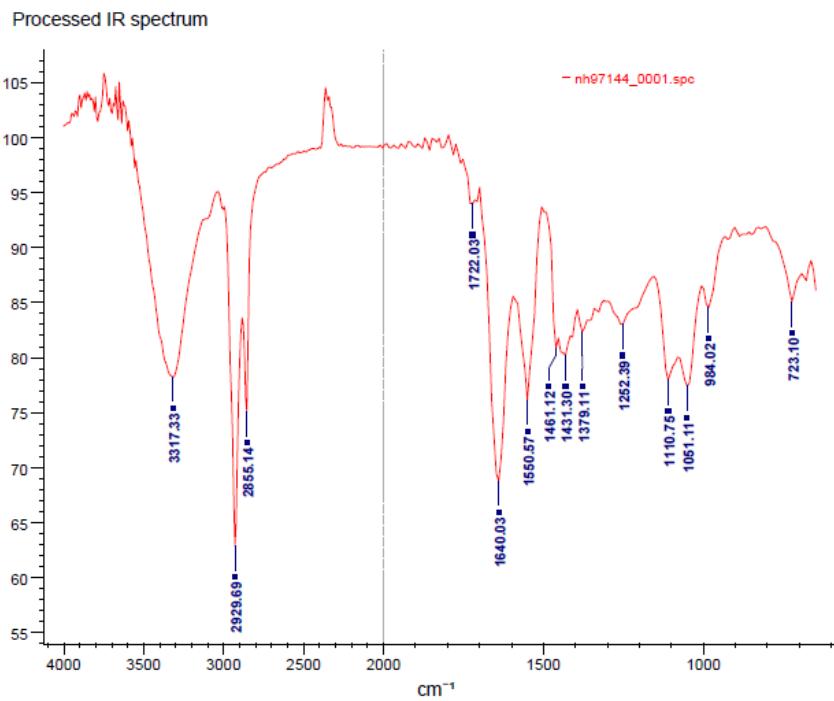


Figure 45. FT-IR spectrum of compound L7

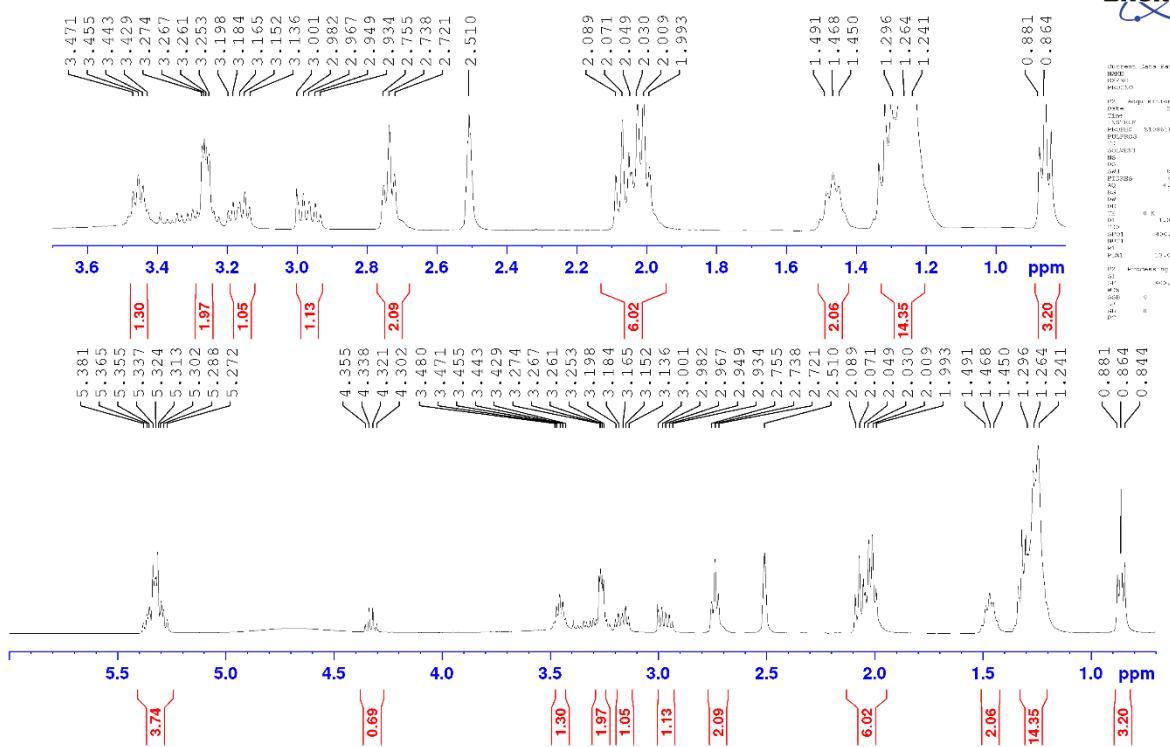


Figure 46. ¹H-NMR spectra of compound L7

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

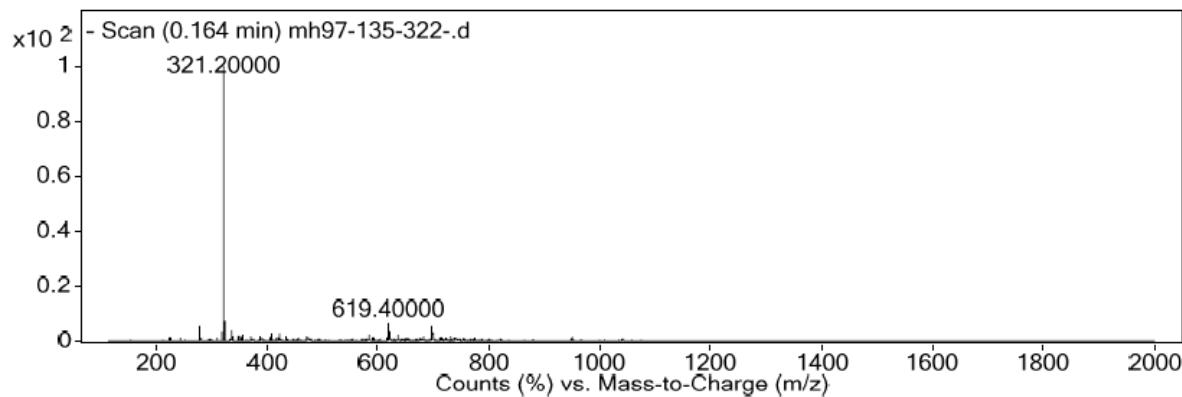
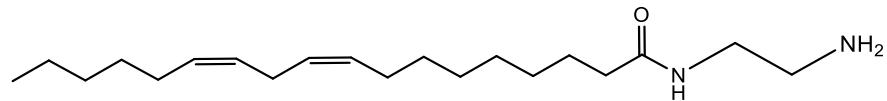


Figure 47. ESI-MS spectrum (negative mode) of compound L8

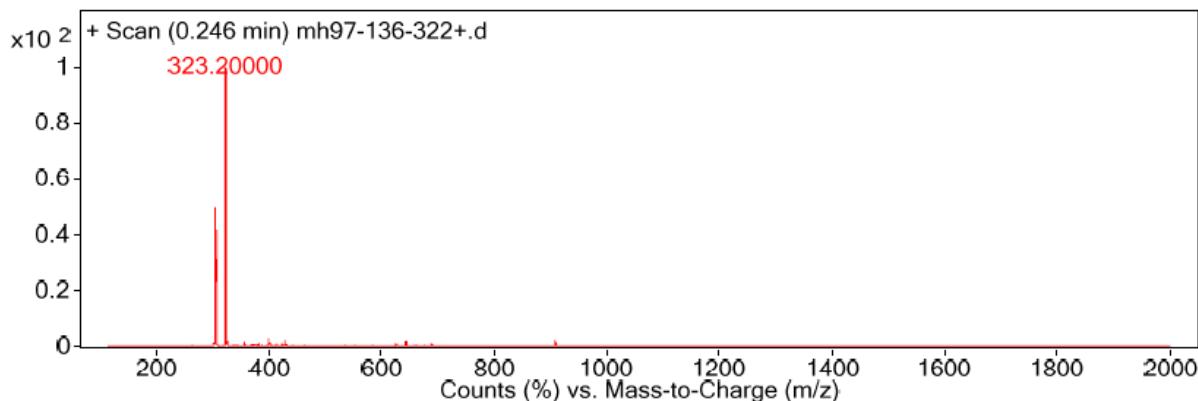


Figure 48. ESI-MS spectrum (positive mode) of compound L8

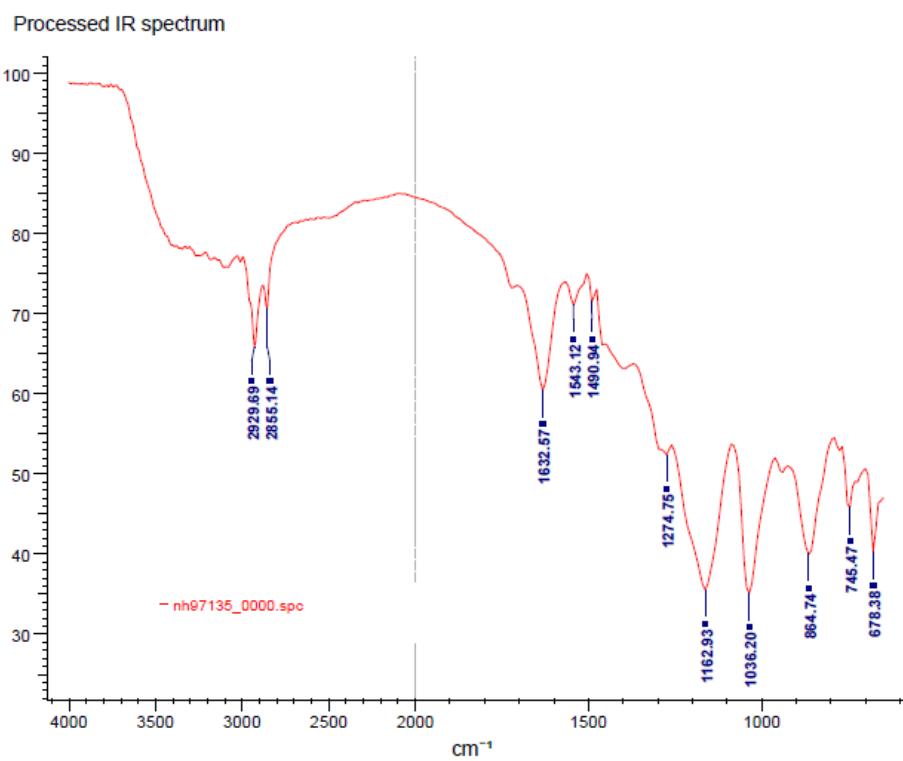


Figure 49. FT-IR spectrum of compound L8

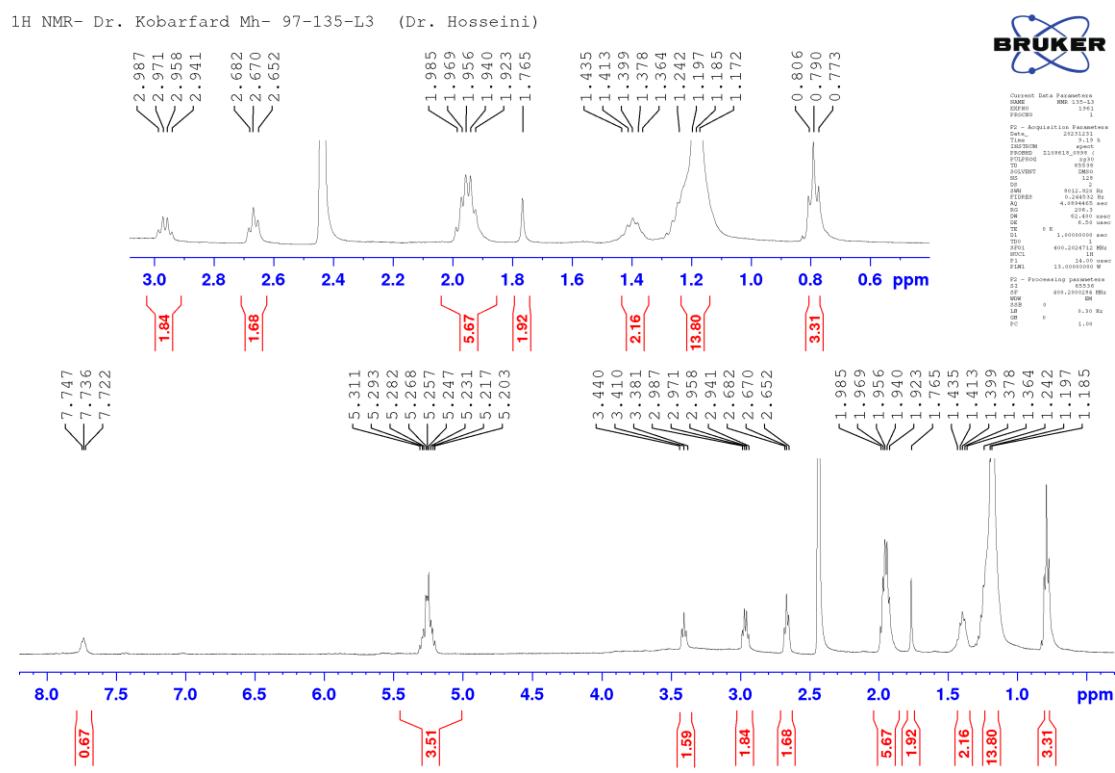
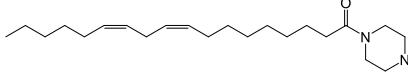
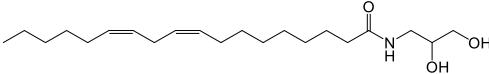
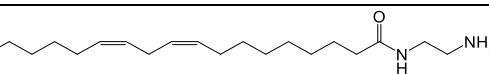
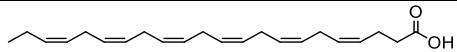


Figure 50. ^1H -NMR spectra of compound L8

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