

S1. In-silico results.

Table 1 Docking score for the top 7 chemical moieties identified through GC-MS.

Sl. No.	Molecules	Docking score (Kcal/mol)	Amino acid residues for hydrogen bond	H-bond distance
1.	9,12-Octadecadienoic acid	102.333	O19-Arg268	2.256
2.	Palmitoleic acid	89.868	H48-Thr73	2.320
3.	trans-13-Octadecenoic acid	99.797	O19-Arg17 O20-Arg17	2.221 2.478
4.	9,12-Octadecadienoic acid (Z, Z)	99.682	O19-Arg268 O19-Arg17	1.796 2.364
5.	9-Hexadecenoic acid	88.909	O17-Arg268	2.067
6.	cis-13-Eicosenoic acid	100.97	O21-Arg268	2.029
7.	cis-13-Octadecenoic acid	99.047	O20-Arg17 O19-Arg268	2.399 2.164

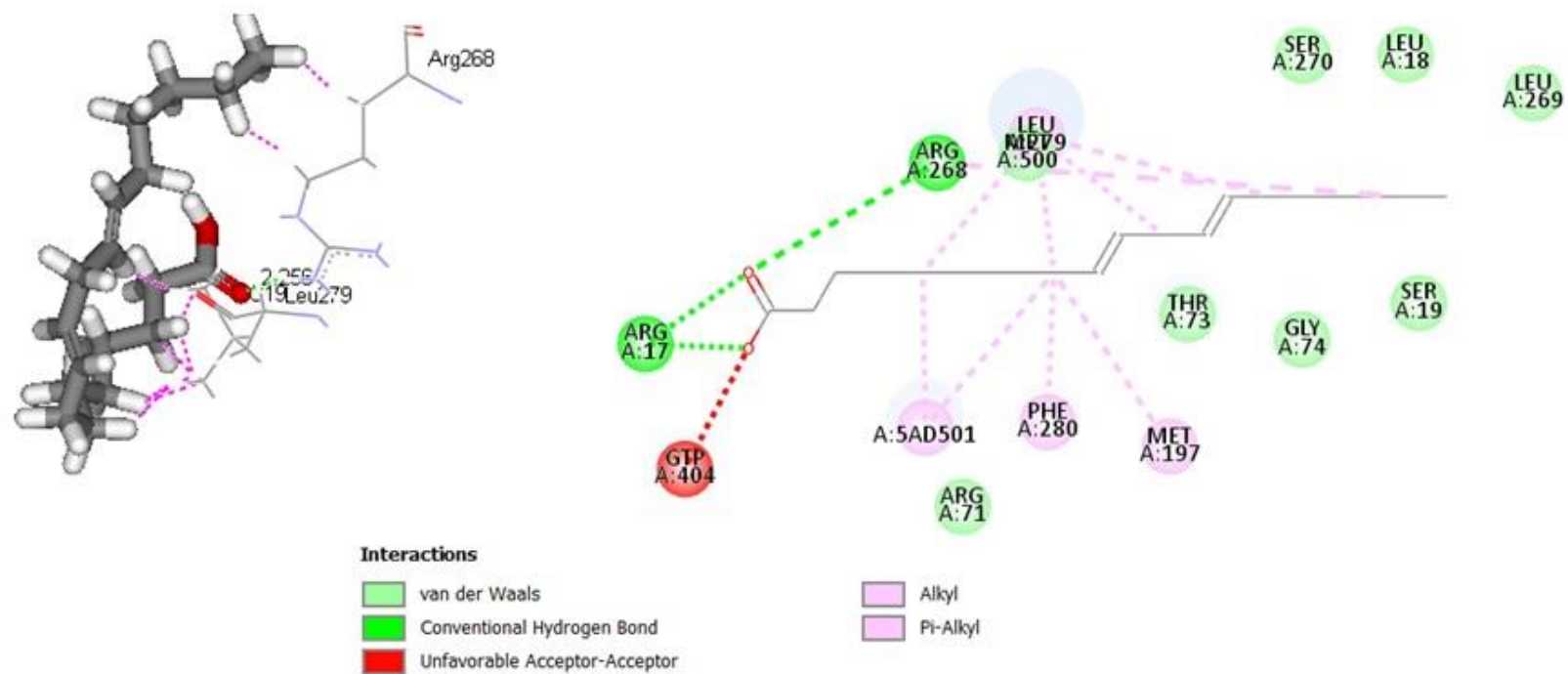


Figure 1 2D and 3D interactions of 9,12-Octadecadienoic acid with MAO-A enzyme active site.

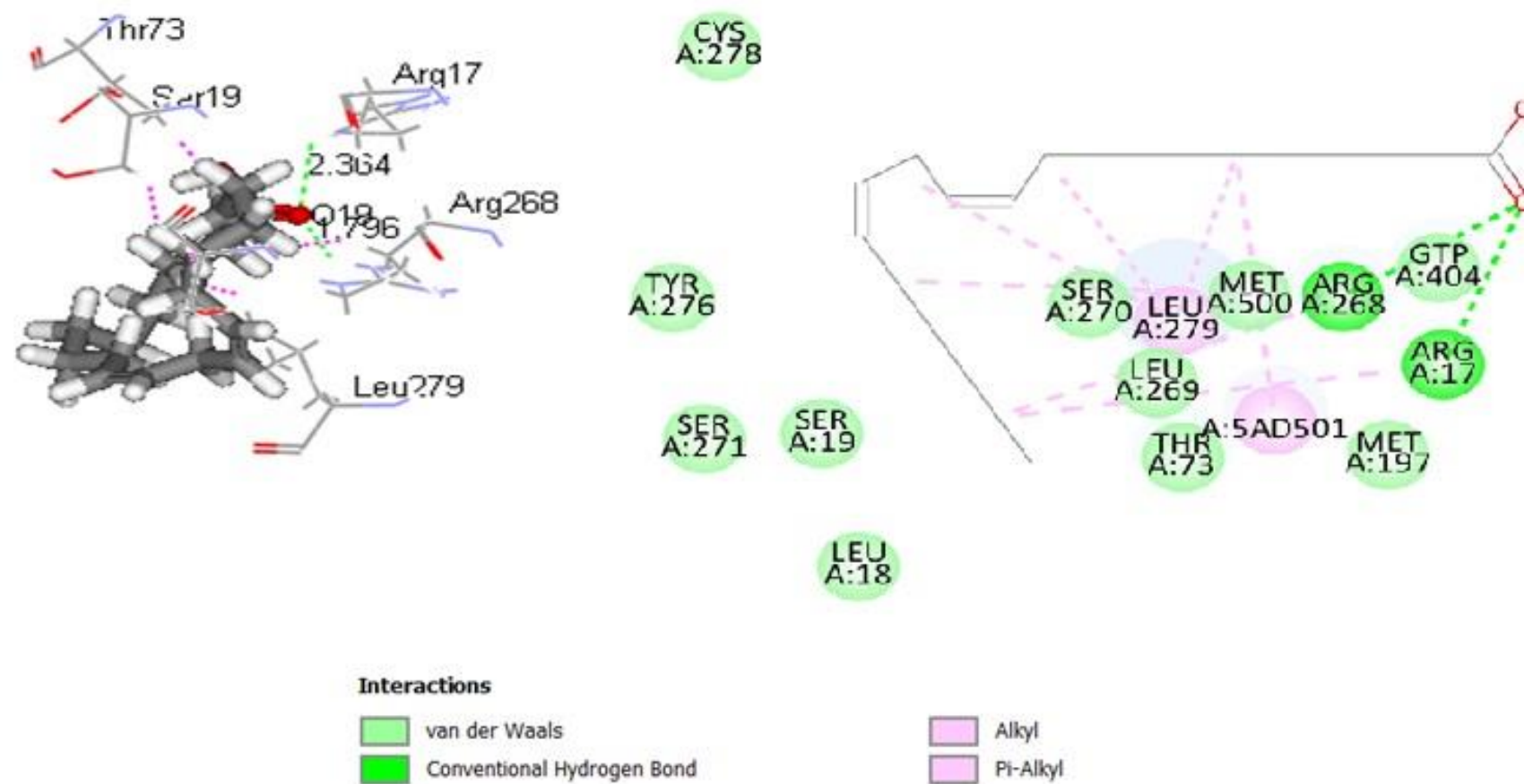


Figure 2 2D and 3D interactions of 9,12-Octadecadienoic acid (Z,Z) with MAO-A enzyme active site.

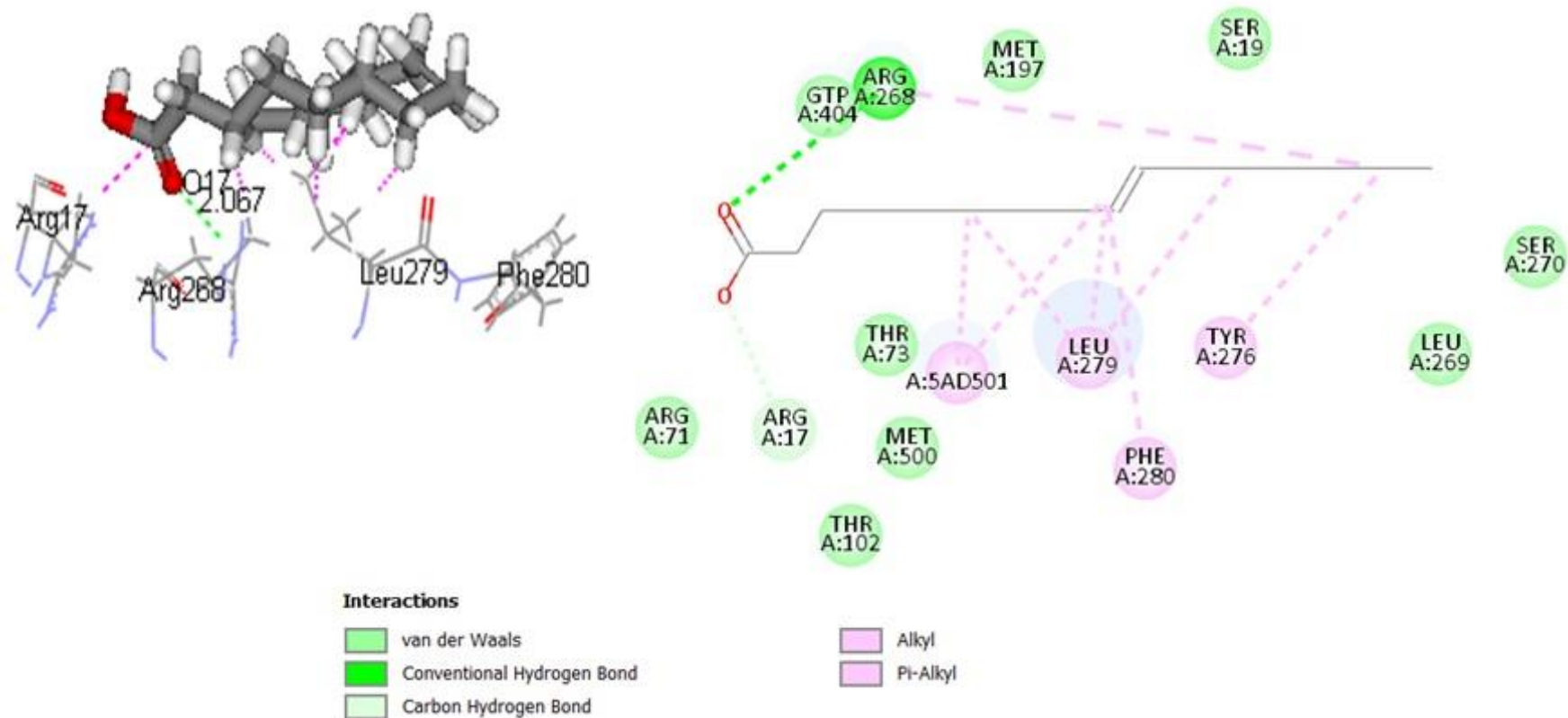


Figure 3 2D and 3D interactions of 9-Hexadecenoic acid with MAO-A enzyme active site.

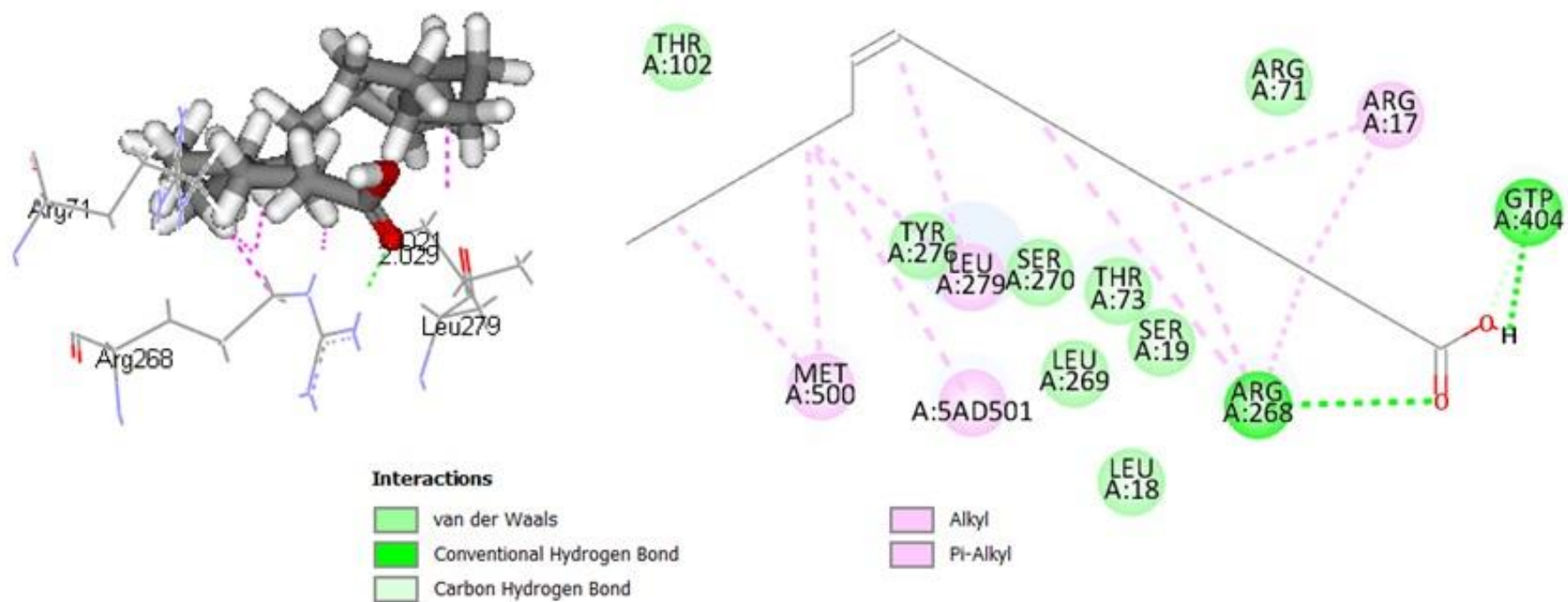


Figure 4 2D and 3D interactions of cis-13-Eicosenoic acid with MAO-A enzyme active site.

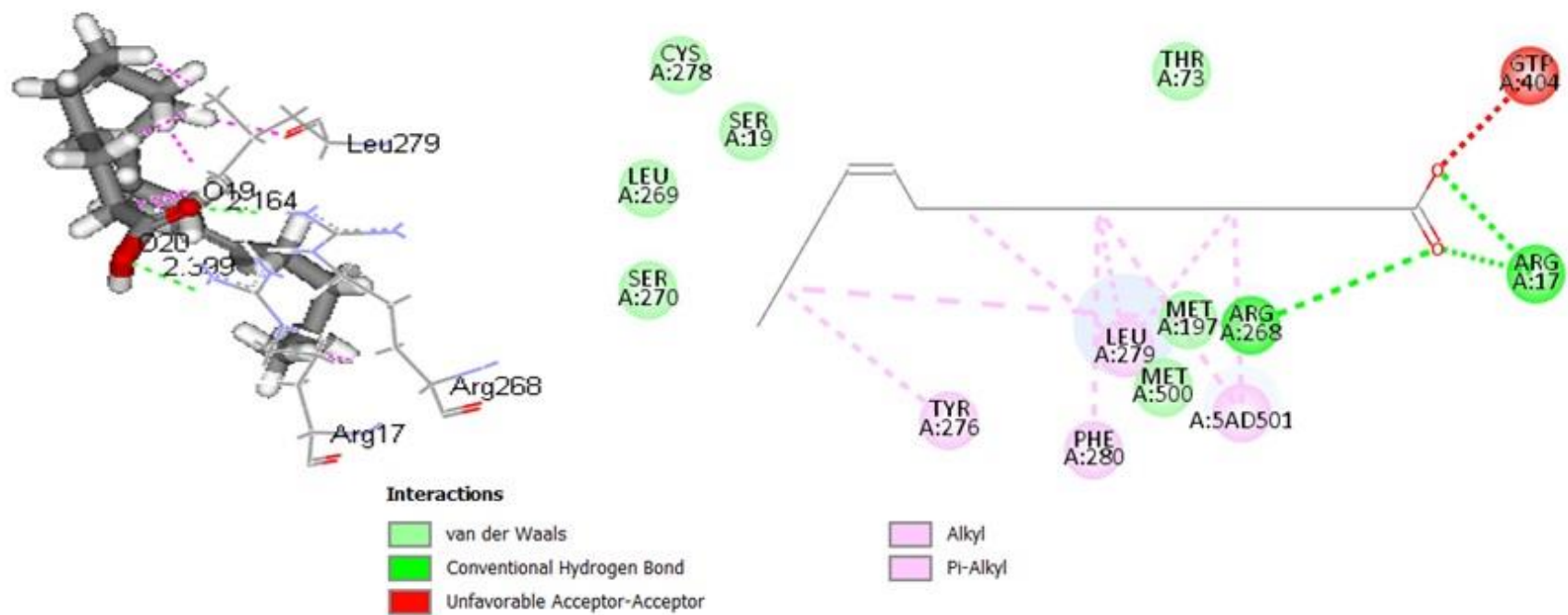


Figure 5 2D and 3D interactions of cis-13-Octadecenoic acid with MAO-A enzyme active site.

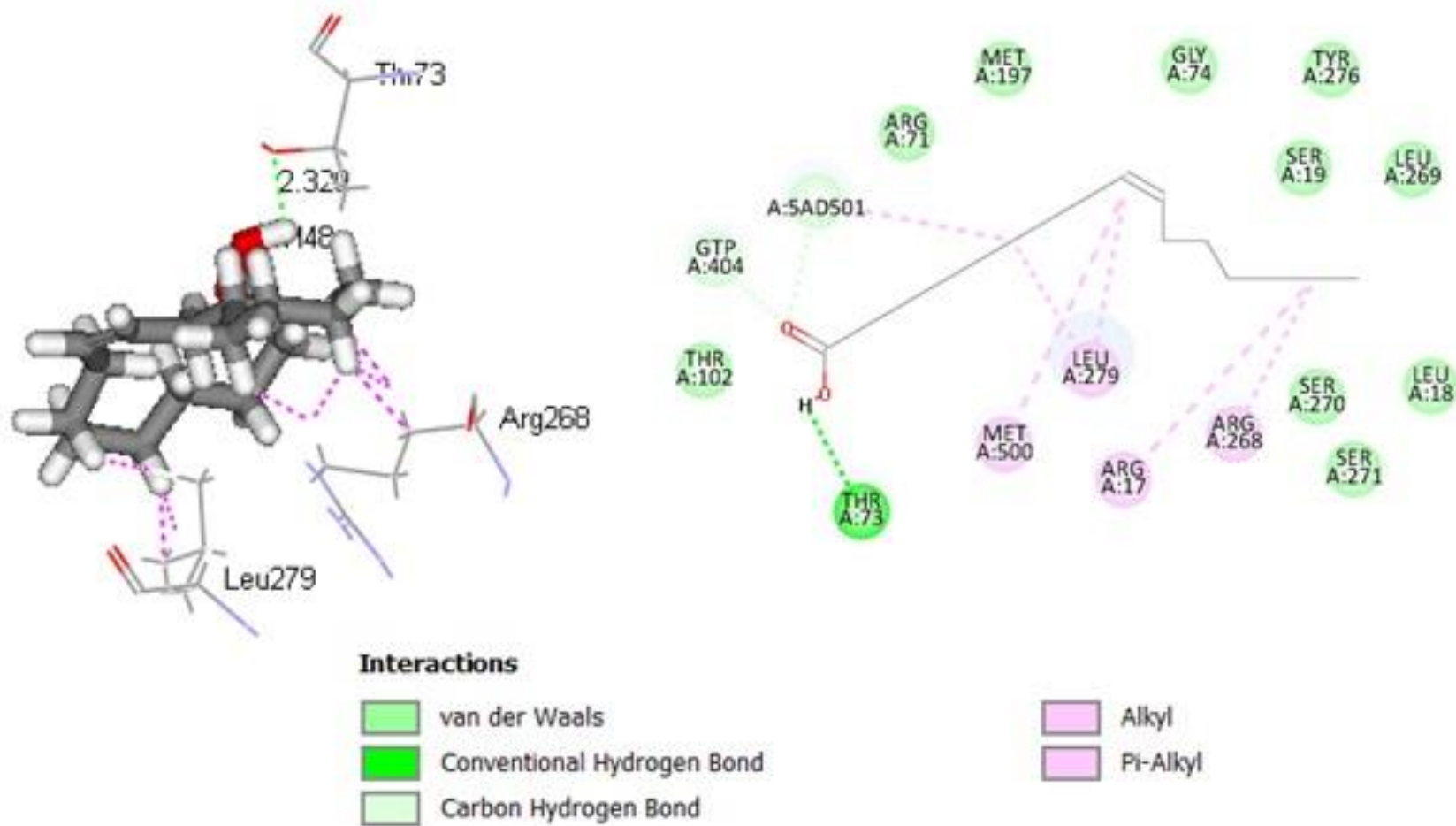
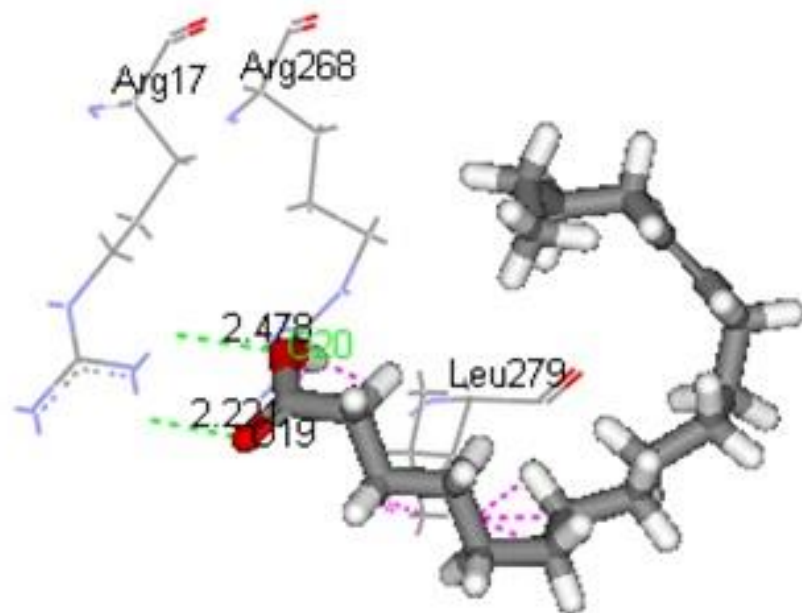
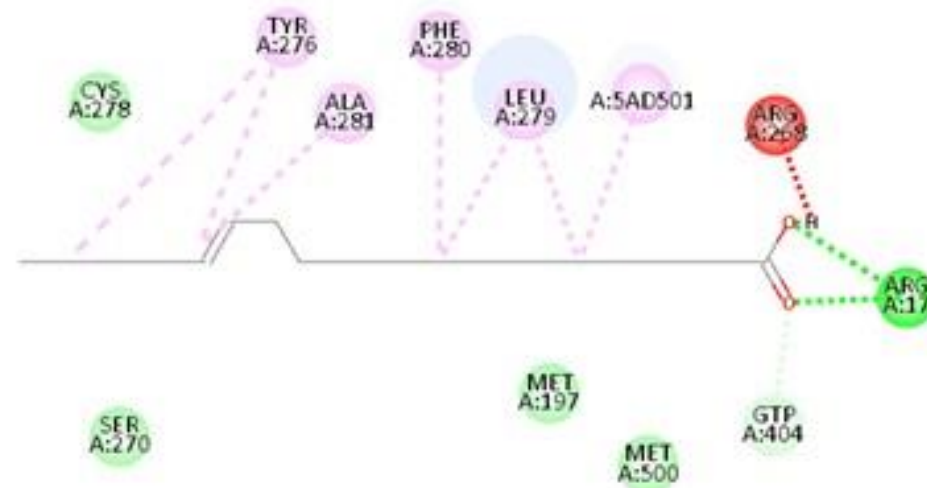


Figure 6 2D and 3D interactions of Palmitoleic acid with MAO-A enzyme active site.



Interactions

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond



- Unfavorable Donor-Donor
- Alkyl
- Pi-Alkyl

Figure 7 2D and 3D interactions of trans-13-Octadecenoic acid with MAO-A enzyme active site.

S1. GC-MS results of 7 compounds (enlisted in Table 1) identified to be effective *in-silico*.

RT: 0.00 - 28.08

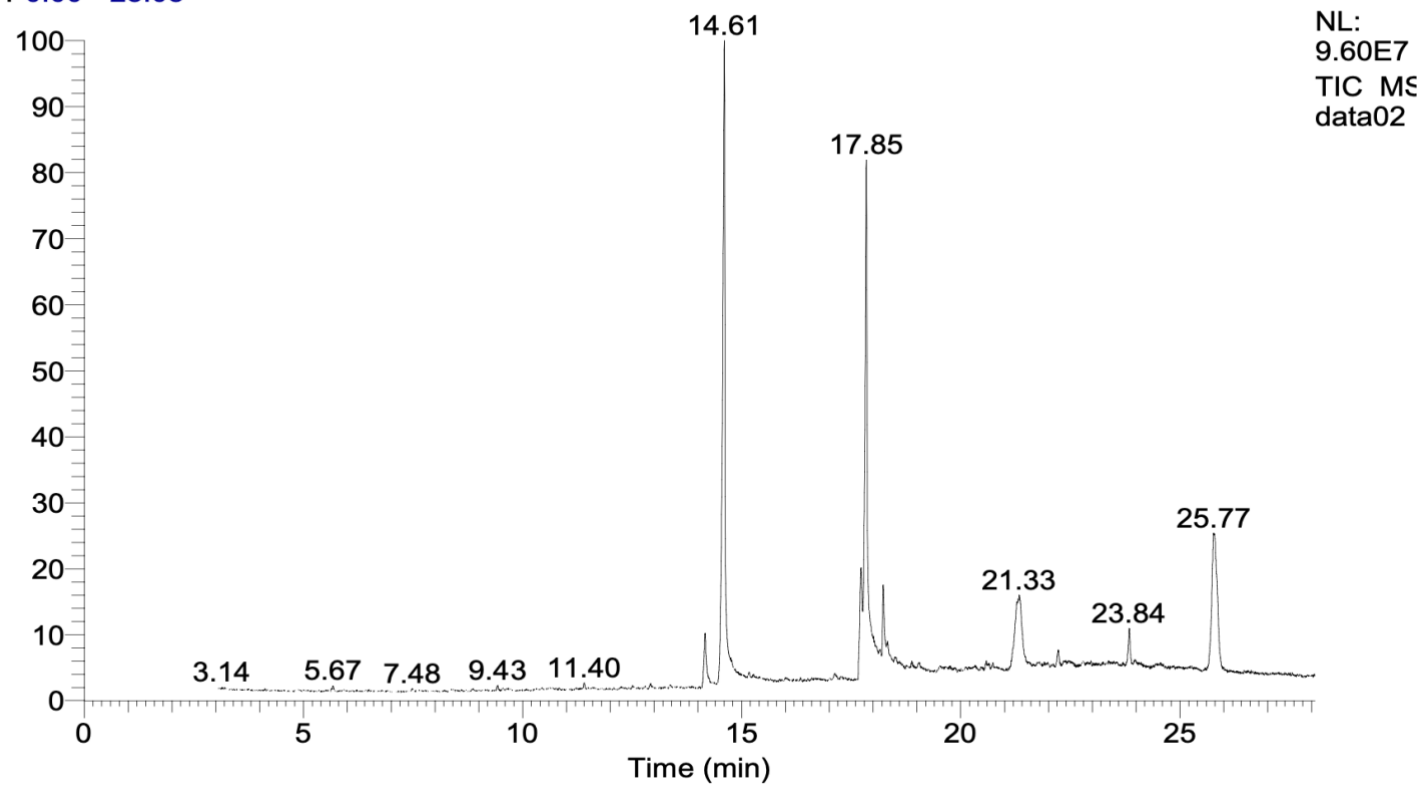


Figure 8 Gas chromatogram of *A. foveolus* oil extract.

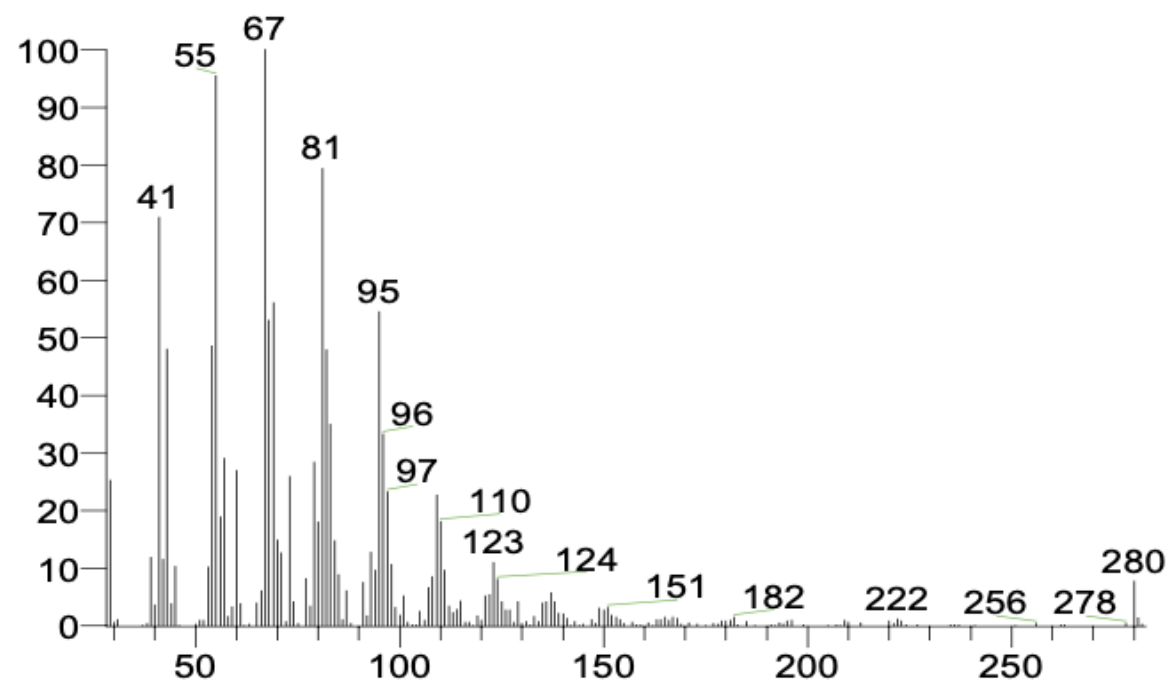


Figure 9 Mass spectrum of 9,12-Octadecadienoic acid (Z, Z) or 9,12-Octadecadienoic acid.

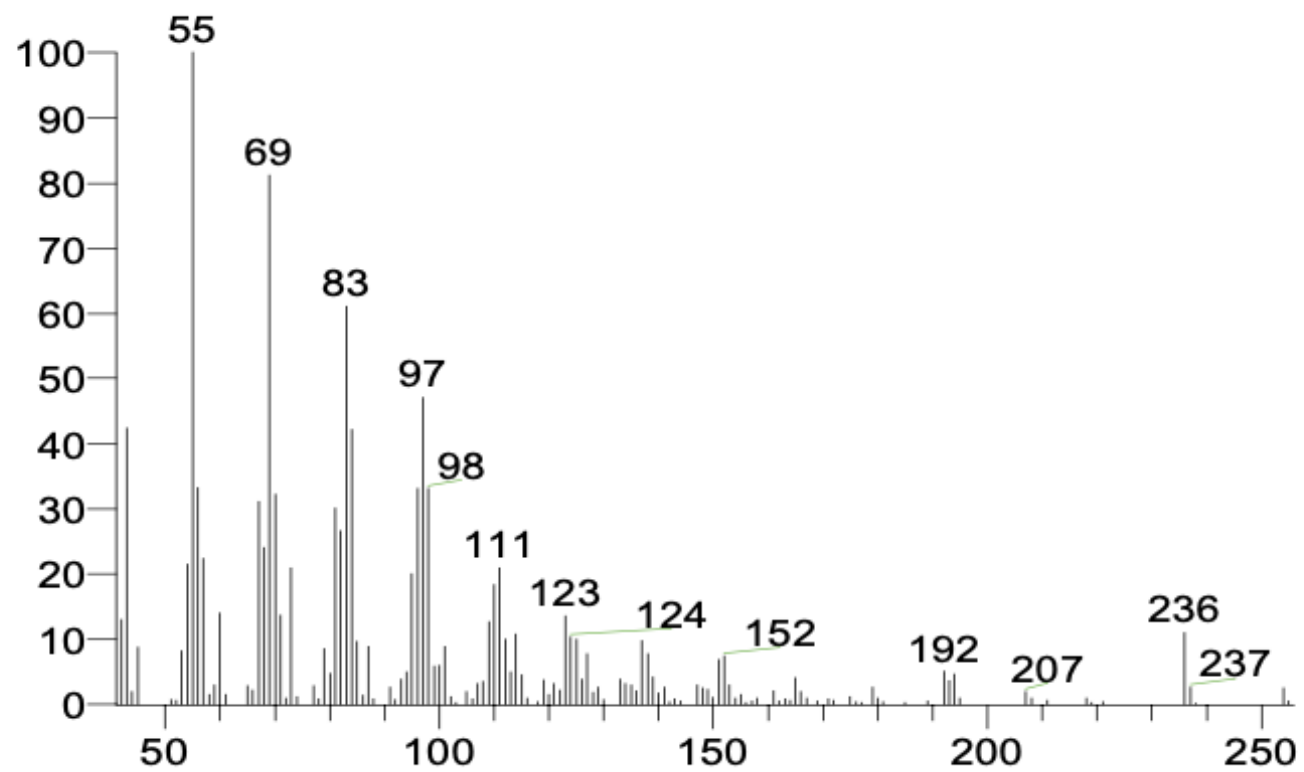


Figure 10 Mass spectrum of Palmitoleic acid.

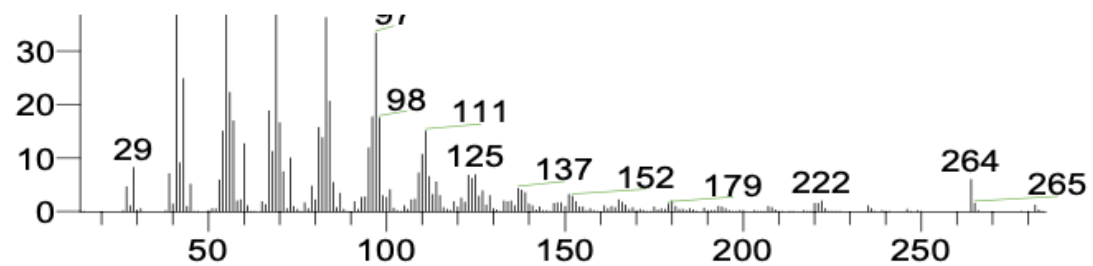
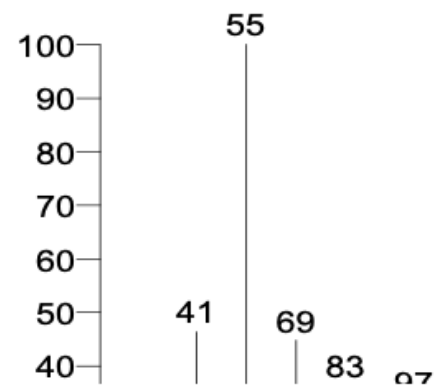


Figure 11 Mass spectrum of *trans*-13-Octadecenoic acid.

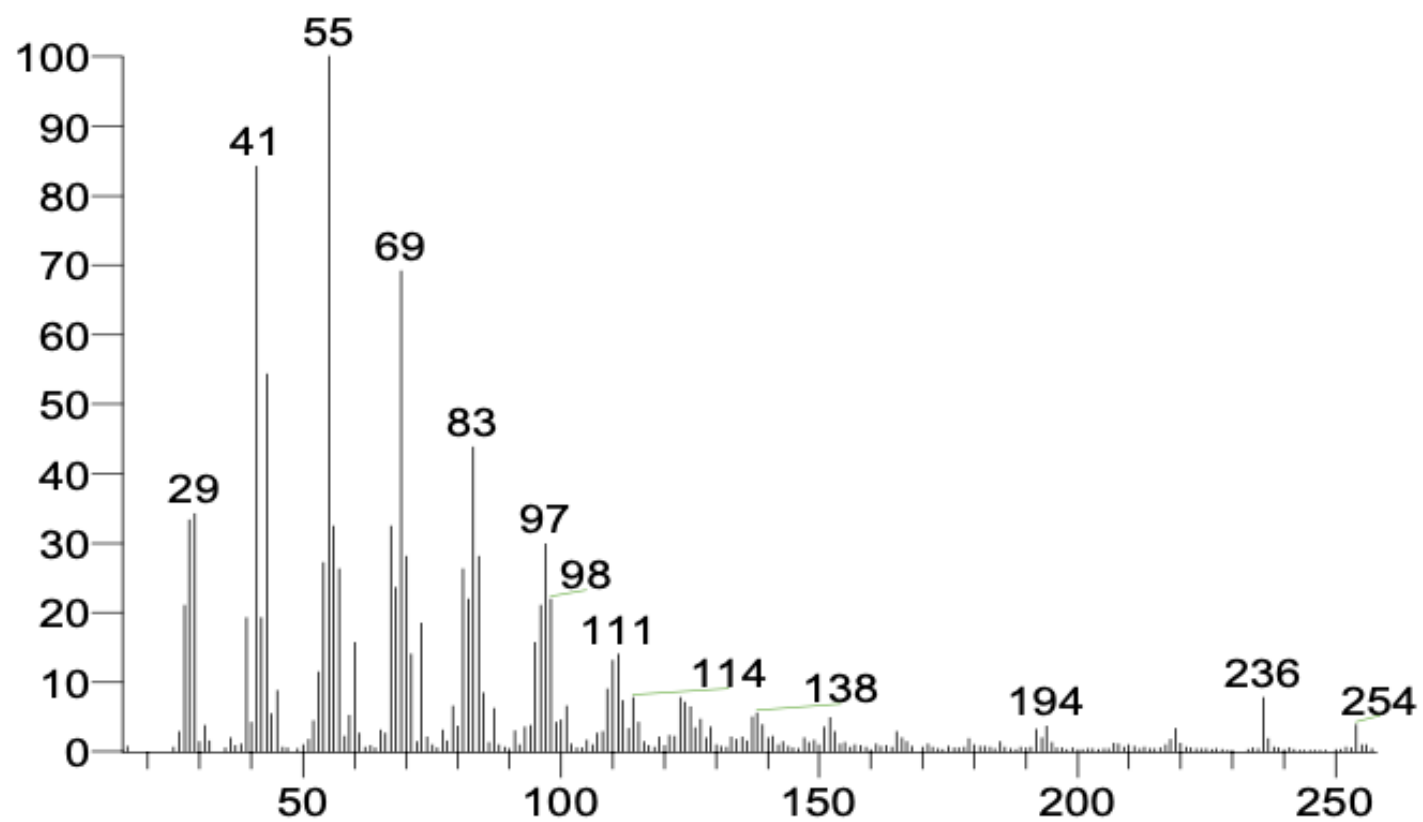


Figure 12 Mass spectrum of 9-Hexadecenoic acid.

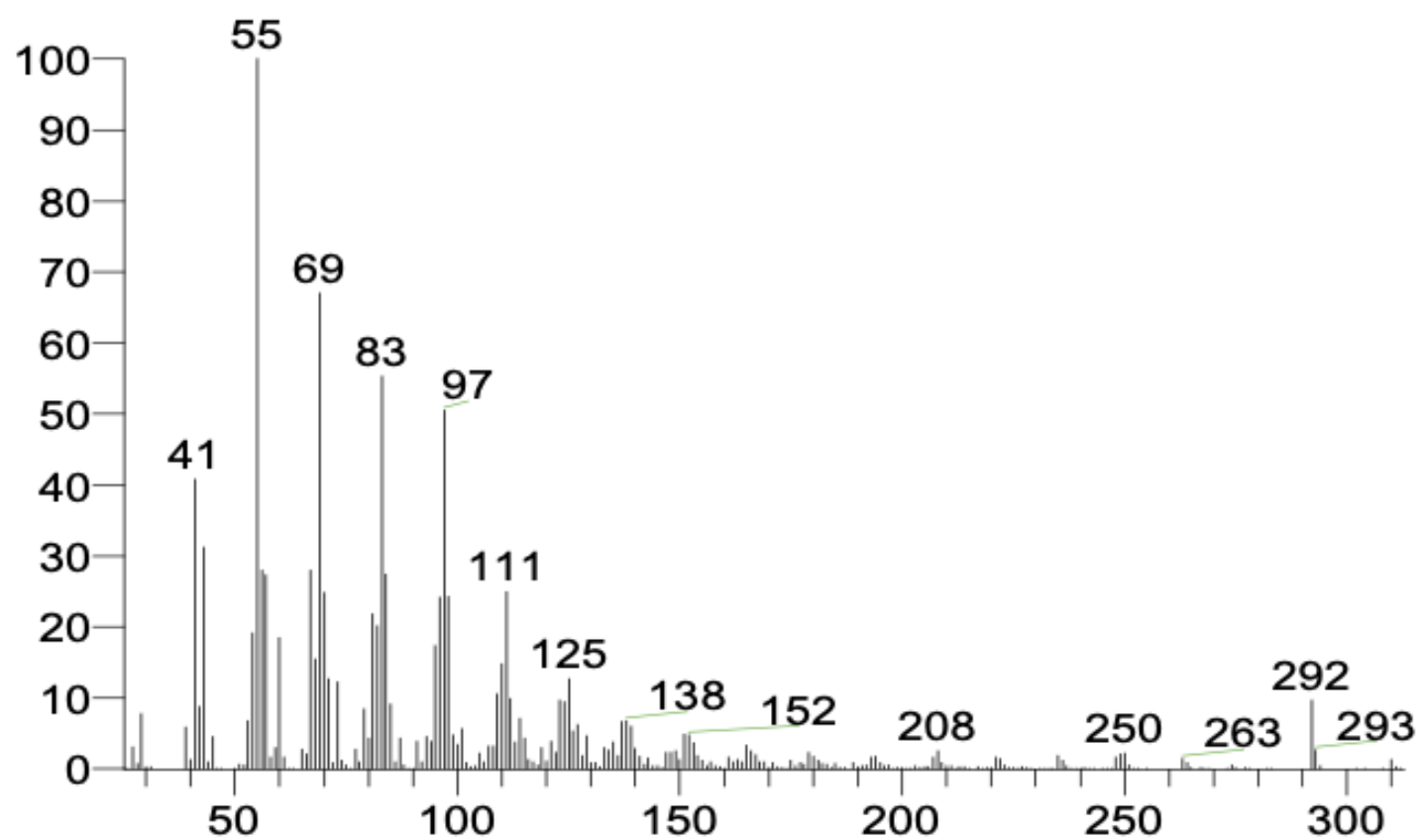


Figure 13 Mass spectrum of cis-13-Eicosenoic acid.

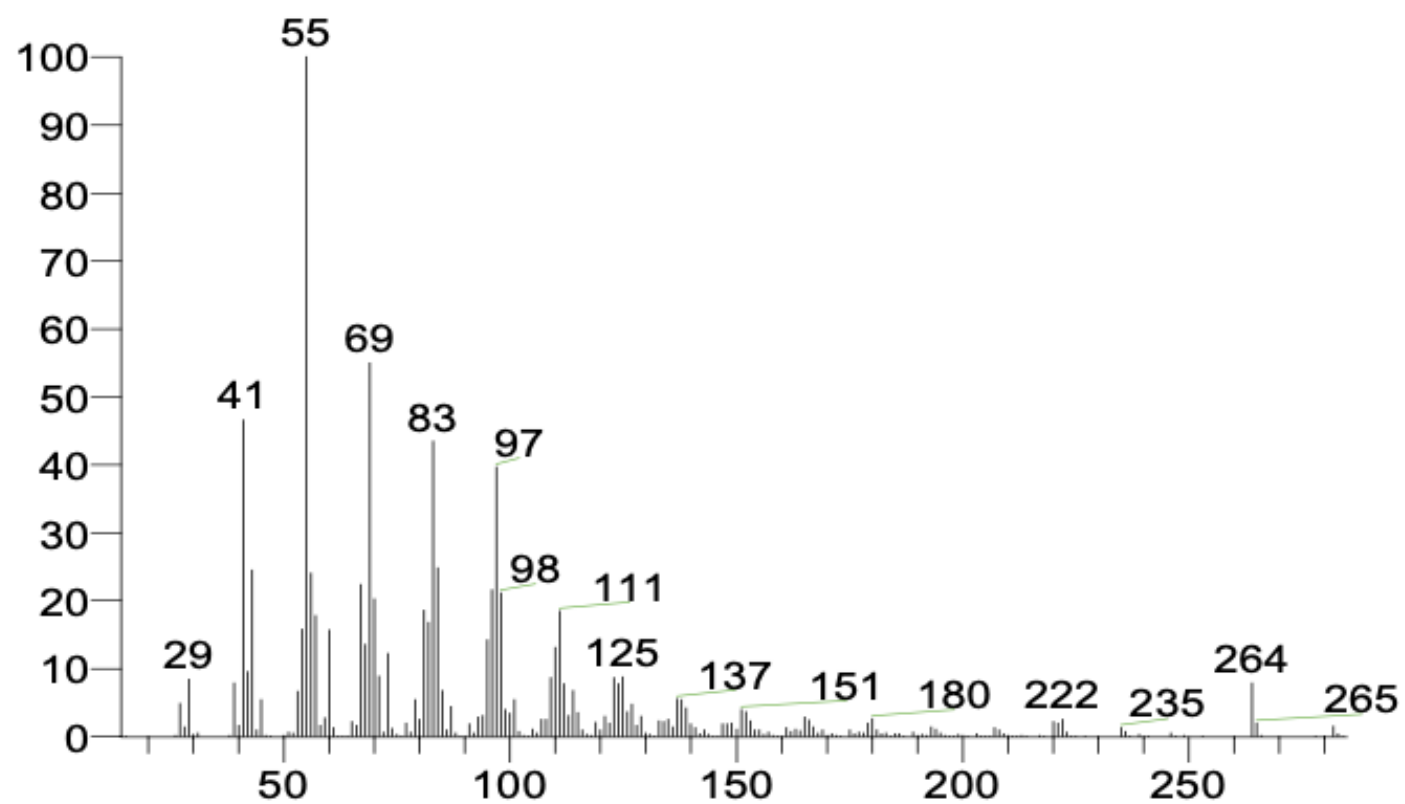


Figure 14 Mass spectrum of *cis*-13-Octadecenoic acid.