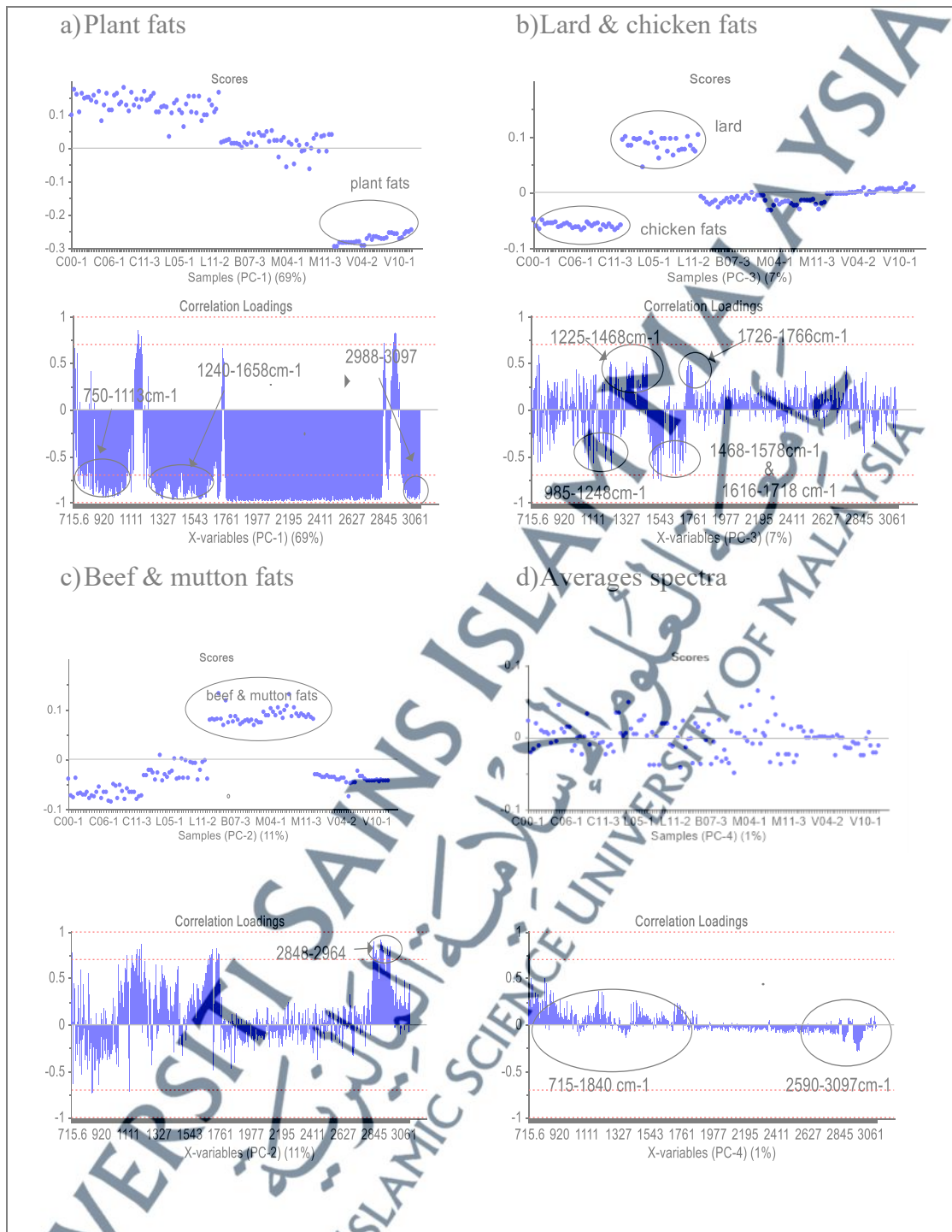
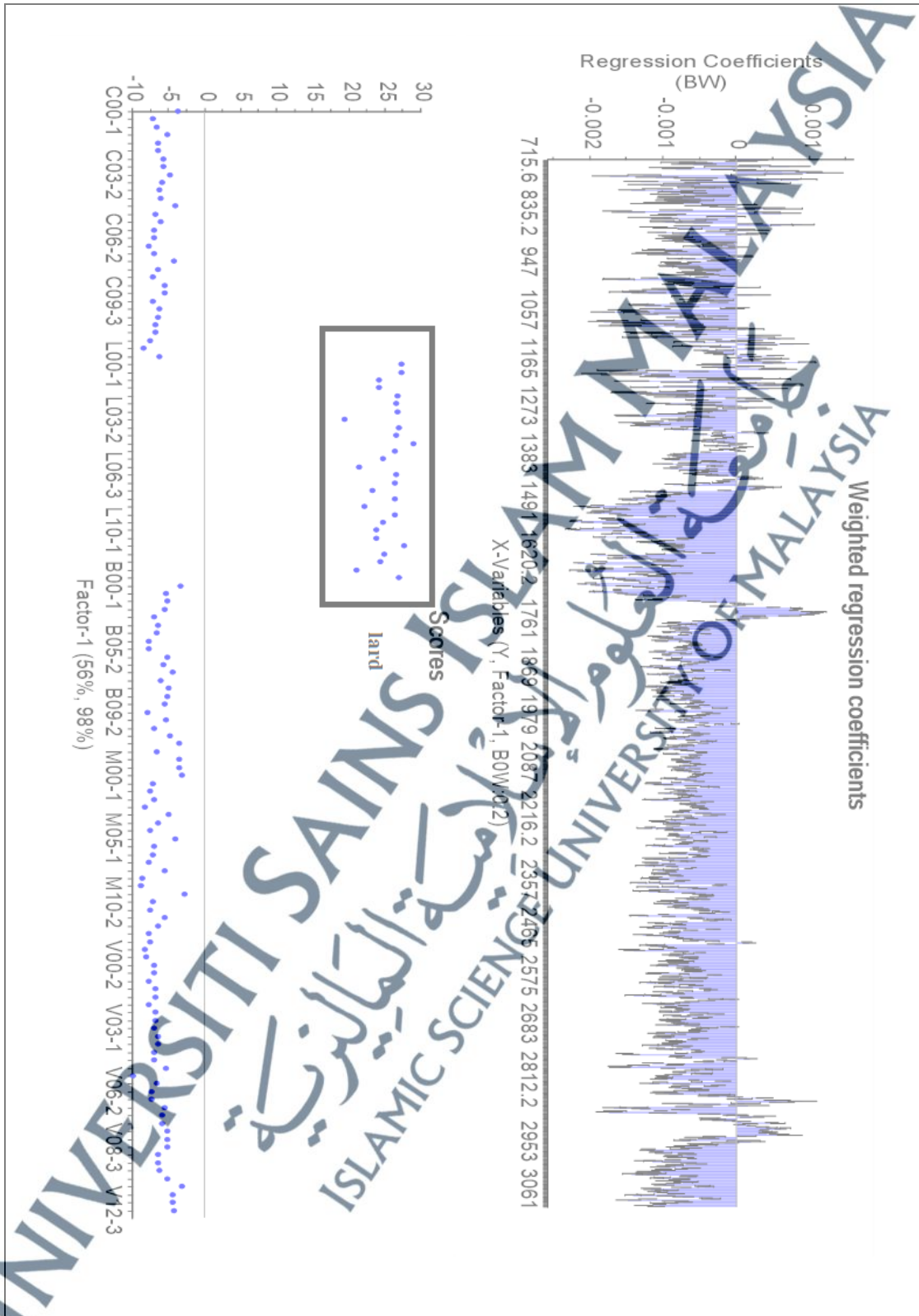


Appendix 2: Loading Plots of FTIR-PCA on Fats.



Appendix 3: Important Variables Selection of FTIR-OSC-PLSR.

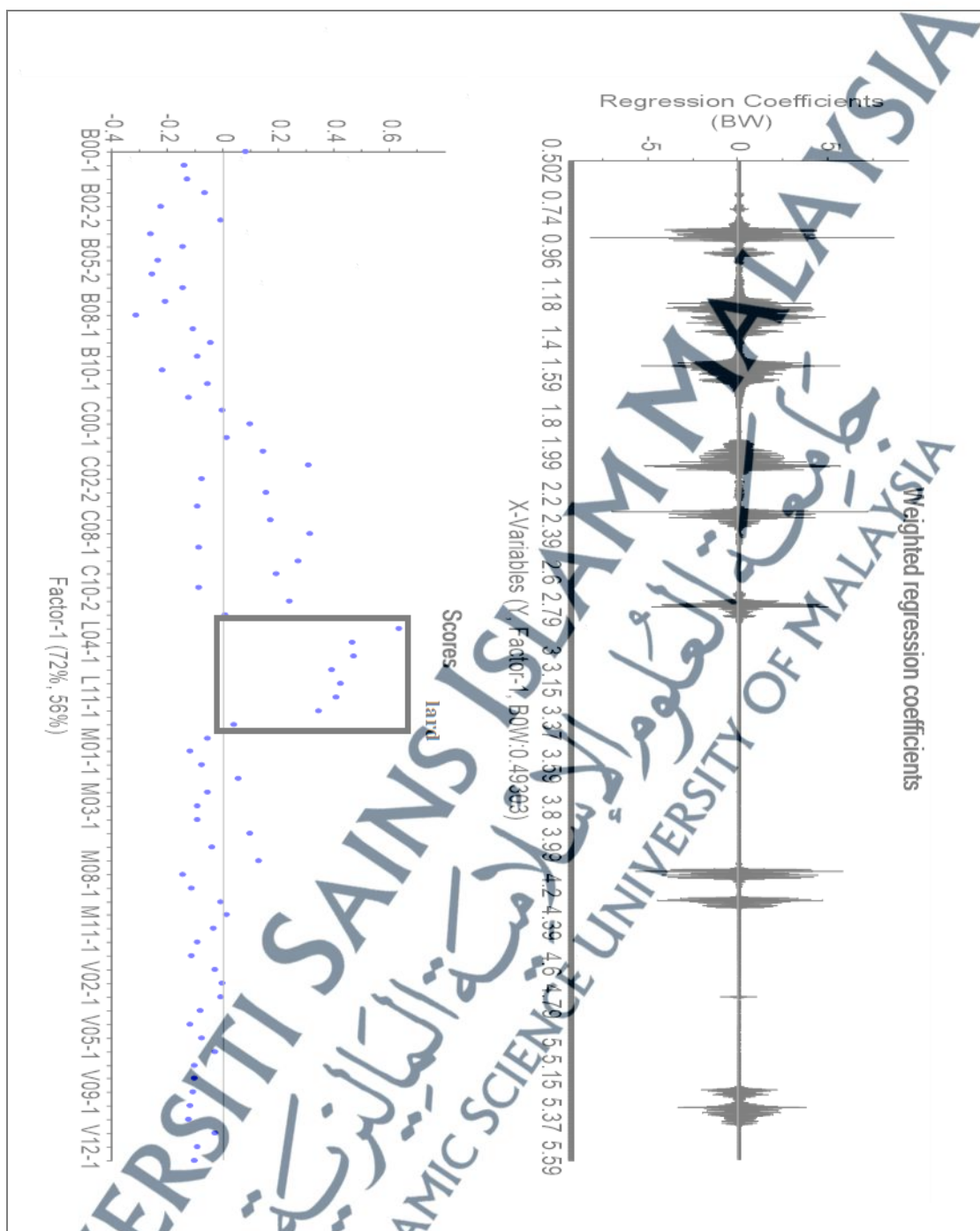


Appendix 4: Assignment of the Main Resonances in the ^1H -NMR.

Chemical shift δ (ppm)	^1H Compound
5.42–5.29	-CHCH- (all unsaturated <i>FA</i>)
5.29–5.22	-CHOCOR (TAG)
4.36–4.24	-CH ₂ OCOR (TAG)
4.20–4.10	-CH ₂ OCOR (TAG)
4.10–4.05	<i>sn</i> -1,3- diacylglycerols (DAG)
4.04–3.98	<i>sn</i> -1,3- DAG
3.76–3.68	<i>sn</i> -1,2- DAG
2.84–2.79	CH-CH ₂ -CH (linolenyl group)
2.79–2.70	CH-CH ₂ -CH (linoleyl group)
2.40–2.20	-OCO-CH ₂ - (all acyl groups)
2.08–1.94	-CH ₂ -CHCH- (oleyl, linoleyl and linolenyl groups)
1.70–1.67	Squalene
1.67–1.50	-OCO-CH ₂ -CH ₂ - (all acyl groups)
1.40–1.14	-(CH ₂) _n - (all acyl groups)
1.02–0.92	-CHCH-CH ₂ -CH ₃ (linolenyl group)
0.92–0.80	-CH ₂ -CH ₂ -CH ₂ -CH ₃ (all acyl groups except linolenyl)

UNIVERSITI SAINS ISLAM MALAYSIA
 جامعة العلوم الإسلامية
 ISLAMIC SCIENCE UNIVERSITY OF MALAYSIA

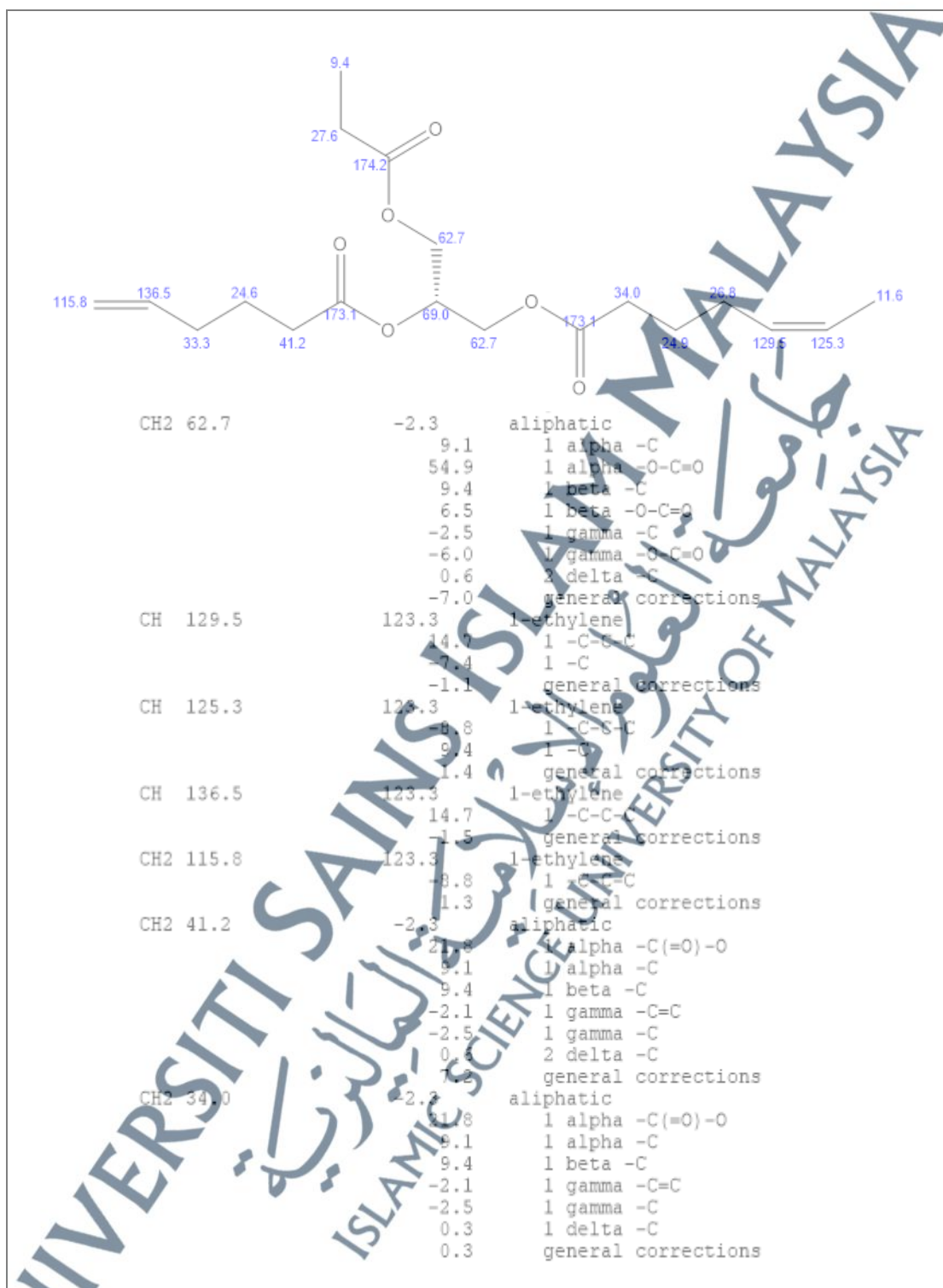
Appendix 5: Important Variables Selection of ¹H-NMR OSC-PLSR.



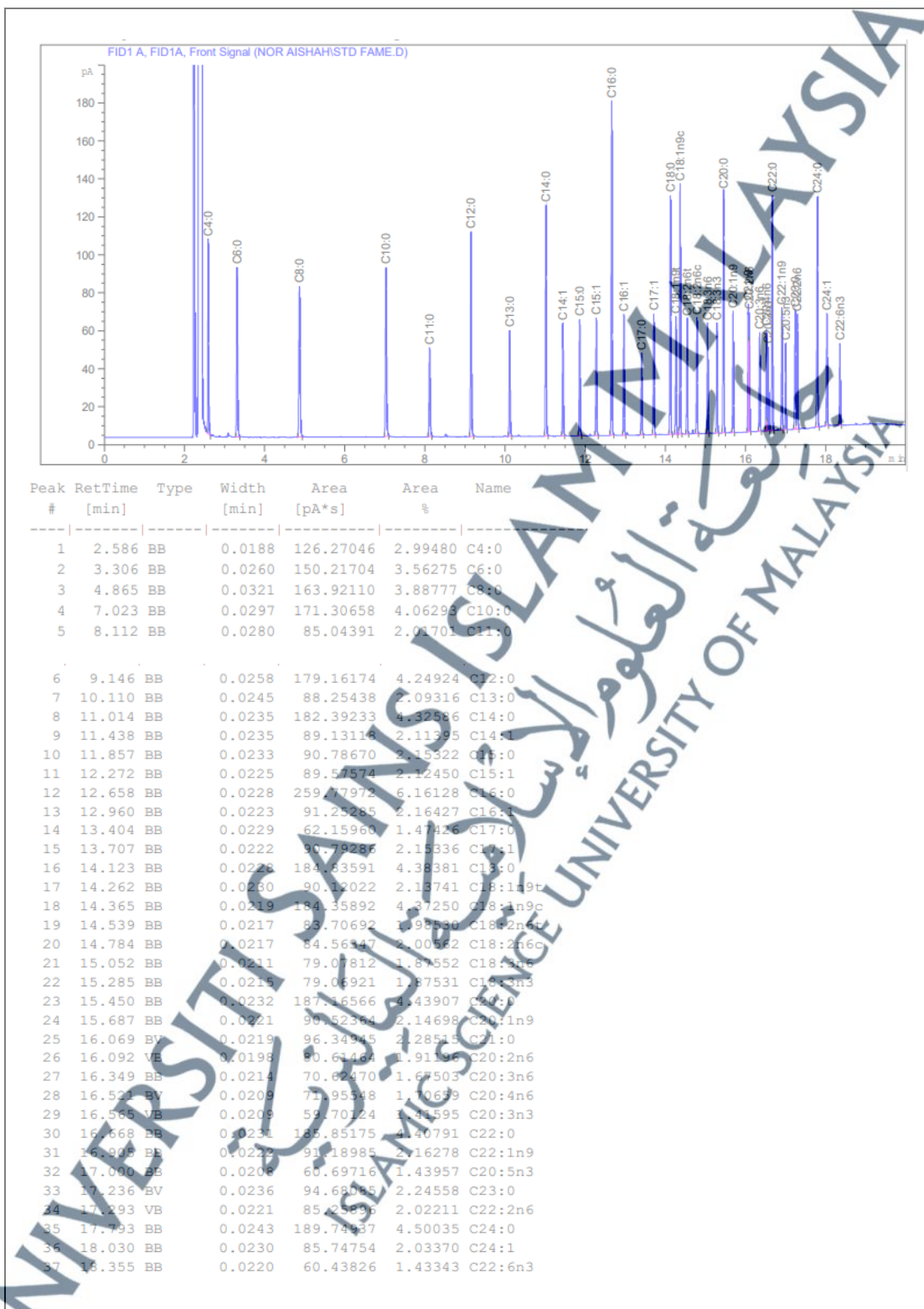
Appendix 6: Assignment of the Main Resonances in the ^{13}C -NMR.

Chemical shift δ (ppm)	^{13}C Compounds	
14.07 - 14.28	C 18(ω 1)	All acyl chains
20.56 - 22.70	C 17(ω 2)	All acyl chains
24.49 - 24.89	C 3	All acyl chains
25.56 - 25.72	C 11	linolenyl
	C 14	Linoleyl & linolenyl
27.22 - 27.38	C 8	Oleyl & linoleyl
	C 11	Oleyl
29.42	C 4 – C 7	All acyl chains
	C 12 – C 15	Oleyl
	C 8 – C 15	Stearoil
	C 8 – C 13	Palmitoil
31.55 - 31.94	C 16 (ω 3)	Linoleyl
34.06 - 34.20	C 2, <i>sn</i> -2	All acyl chains
62.12	CH ₂ O-, <i>sn</i> -1,3	Glycerol (TAG)
	CH ² O-, <i>sn</i> -1	Glycerol (1,2-DAG)
65.07	CH ₂ O-, <i>sn</i> -1	Glycerol (MAG)
68.93	CHO-, <i>sn</i> -2	Glycerol (TAG)
77.01	CDCl ₃	Solvent
127.13 - 127.92	C 12	Linoleyl
	C 10, C 15	Linolenyl
128.10 - 128.47	C 10	Linoleyl
	C 12, C 13	Linolenyl
129.49 - 129.70	C 9,	Oleyl
	C 10,	Linoleyl
130.02 - 130.45 C9	C 13	Linoleyl and linolenyl
172.81	C 1, <i>sn</i> -2	TAG
173.23	C 1, <i>sn</i> -1,3	TAG
130.02 - 130.45	C 9	Linoleyl & linolenyl
	C 13	Linoleyl
172.81	C 1, <i>sn</i> -2	TAG
173.23	C 1, <i>sn</i> -1,3	TAG

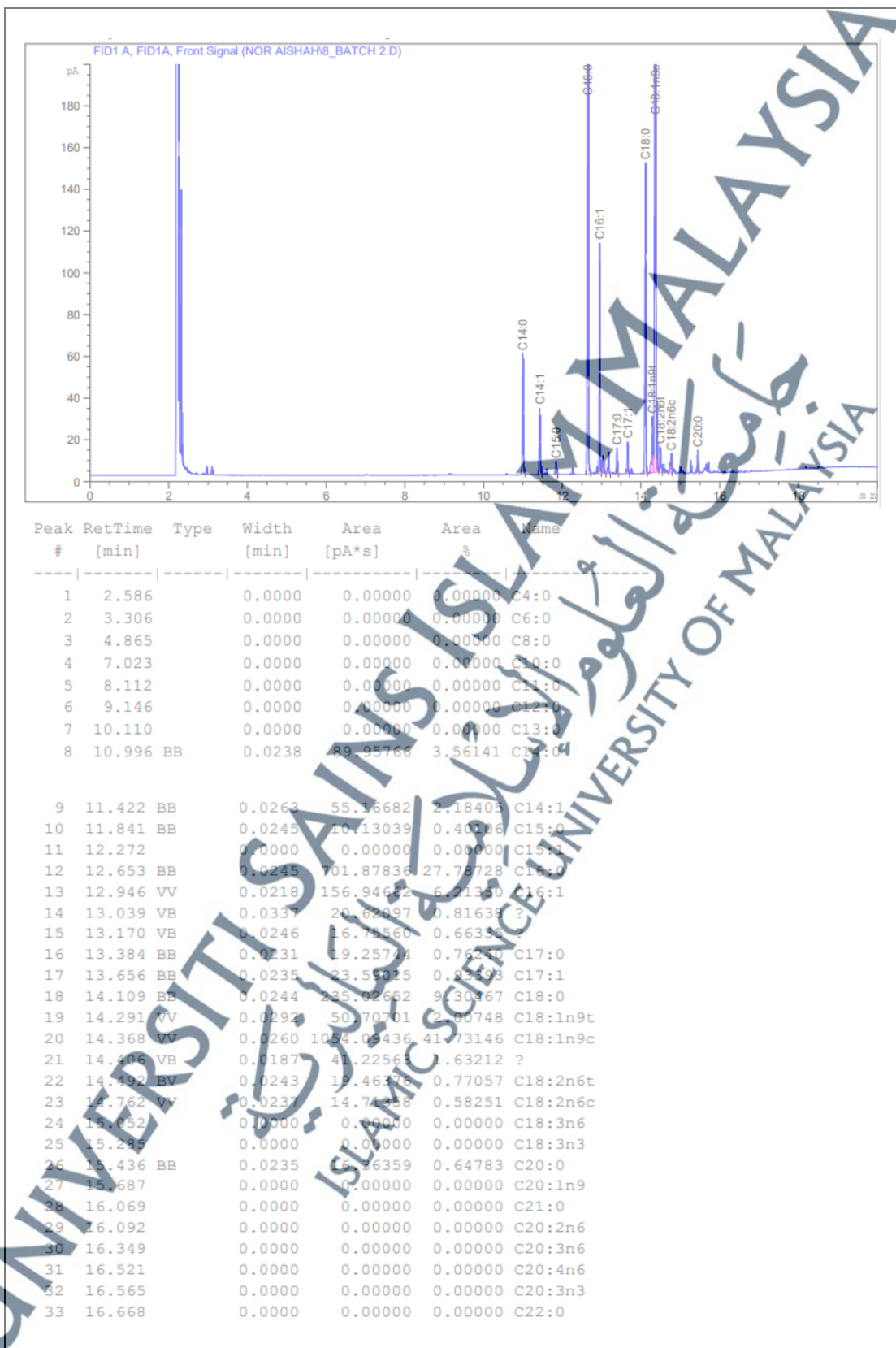
Appendix 7: Estimation of the ^{13}C -NMR



Appendix 8: Standard of FAME Integration.



Appendix 9: Typical Chromatogram of Lard



Appendix 10: Most Prominent FAs GC-FID.

FAs						FAs					
id	C16:0	C18:0	C18:1n9t	C18:1n9c	C18:2n6c	id	C16:0	C18:0	C18:1n9t	C18:1n9c	C18:2n6c
B-01	21.71	8.00	0.00	36.74	23.80	L-01	19.43	9.44	0.00	39.86	25.88
B-02	21.31	9.02	0.00	36.77	23.02	L-02	21.10	8.78	0.38	38.26	22.10
B-03	20.97	8.99	1.49	33.39	18.58	L-03	20.01	9.44	0.00	37.86	24.87
B-04	26.87	8.86	1.59	40.39	0.53	L-04	27.79	9.30	2.01	41.73	0.58
B-05	21.41	8.29	0.47	38.15	20.72	L-05	21.45	8.76	0.00	37.20	22.50
B-06	22.18	8.69	0.23	37.85	20.87	L-06	24.64	4.61	3.77	35.45	10.41
B-07	23.01	28.50	1.08	25.11	1.36	L-07	27.98	9.30	2.00	40.70	0.34
B-08	23.53	30.59	26.87	1.57	1.30	L-08	21.43	9.17	40.82	2.81	23.85
B-09	22.31	8.78	0.00	37.43	21.28	L-09	21.02	8.95	0.12	30.46	22.42
B-10	24.65	4.86	0.16	36.67	22.50	L-10	22.46	4.29	0.00	37.86	22.20
B-11	21.26	29.94	26.48	8.25	0.61	L-11	23.50	32.12	26.44	9.14	1.49
B-12	29.92	9.72	43.33	2.38	0.00	L-12	29.73	9.42	40.91	1.98	0.000
C-01	20.31	9.29	0.00	41.34	22.81	M-01	21.10	9.23	0.00	36.09	22.76
C-02	21.20	8.94	0.00	36.78	22.91	M-02	20.51	8.76	0.00	37.55	23.32
C-03	25.18	5.04	0.00	37.98	22.88	M-03	23.99	4.97	0.00	38.99	22.98
C-04	26.19	16.04	1.76	45.91	0.88	M-04	27.52	16.51	1.87	44.20	0.87
C-05	20.99	8.56	0.00	37.14	22.58	M-05	21.90	8.59	0.38	37.92	21.39
C-06	21.41	9.07	0.00	37.09	22.70	M-06	21.75	8.52	0.00	37.87	22.26
C-07	25.51	4.91	3.92	35.98	10.72	M-07	28.32	36.30	9.27	26.11	0.00
C-08	22.57	8.78	38.01	0.46	20.17	M-08	24.84	34.24	32.86	8.06	0.00
C-09	20.98	8.94	0.11	36.90	22.68	M-09	21.66	3.82	0.00	37.45	21.87
C-10	24.42	4.70	0.00	38.45	22.38	M-10	24.35	4.92	0.00	38.06	22.55
C-11	21.30	29.09	25.82	8.58	0.58	M-11	20.34	29.55	28.58	0.81	0.55
C-12	24.97	13.25	41.86	1.32	0.78	M-12	20.33	28.01	29.01	0.00	0.22
V-07	57.71	5.08	29.90	0.00	4.37	V-01	54.22	3.44	32.33	0.00	7.26
V-08	57.62	4.60	30.30	0.00	5.42	V-02	56.78	3.66	32.12	0.00	6.23
V-09	52.00	3.99	34.67	0.00	4.56	V-03	55.26	4.81	32.30	0.00	5.72
V-10	55.00	3.98	33.11	0.00	5.11	V-04	54.88	3.10	33.23	0.00	2.77
V-11	55.74	4.92	32.29	0.00	5.72	V-05	53.90	4.61	32.40	0.00	7.26
V-12	64.98	5.51	24.18	0.00	1.69	V-06	53.67	4.83	32.28	0.00	7.10

Abbreviation - Fats : C = chicken fat, L = lard, B = Beef fat, M = mutton fat, & V = plant fat
 Temperatures: 120 °C = 01, 02, 03 & 04; 180 °C = 05, 06, 07 & 08; 240° C = 09, 10, 11 & 12
 Duration of heating: 0.5 hr = 01, 05 & 09; 1 hr = 02, 06 & 10; 2 hrs = 03, 07 & 11; 3 hrs = 04, 08 & 12

Appendix 11: Scores Plot of GC-FID-PCA and Clusters.

No.	Clusters	Samples	PC1	No.	Clusters	Samples	PC1
1	1	B-01	-0.23	31	1	M-04	-0.19
2	1	B-02	-0.24	32	1	M-05	-0.23
3	1	B-03	-0.19	33	1	M-06	-0.24
4	1	B-04	-0.18	34	1	M-07	0.00
5	1	B-05	-0.24	35	1	M-09	-0.23
6	1	B-06	-0.23	36	1	M-10	-0.23
7	1	B-07	-0.09	37	2	B-08	0.26
8	1	B-09	-0.23	38	2	B-11	0.19
9	1	B-10	-0.22	39	2	B-12	0.37
10	1	C-01	-0.26	40	2	C-08	0.25
11	1	C-02	-0.23	41	2	C-12	0.34
12	1	C-03	-0.23	42	2	C-11	0.19
13	1	C-04	-0.20	43	2	L-08	0.23
14	1	C-05	-0.24	44	2	L-11	0.19
15	1	C-06	-0.23	45	2	L-12	0.34
16	1	C-07	-0.17	46	2	M-08	0.24
17	1	C-09	-0.23	47	2	M-11	0.27
18	1	C-10	-0.23	48	2	M-12	0.30
19	1	L-01	-0.27	49	3	V-01	0.37
20	1	L-02	-0.24	50	3	V-02	0.38
21	1	L-03	-0.24	51	3	V-03	0.38
22	1	L-04	-0.18	52	3	V-04	0.41
23	1	L-05	-0.23	53	3	V-05	0.37
24	1	L-06	-0.18	54	3	V-06	0.36
25	1	L-07	-0.17	55	3	V-07	0.37
26	1	L-09	-0.24	56	3	V-08	0.37
27	1	L-10	-0.24	57	3	V-09	0.39
28	1	M-01	-0.23	58	3	V-10	0.38
29	1	M-02	-0.24	59	3	V-11	0.38
30	2	M-03	-0.23	60	3	V-12	0.38

Abbreviation - Fats : C = chicken fat, L = lard, B = Beef fat, M = mutton fat, & V = plant fat
 Temperatures: 120 °C = 01, 02, 03 & 04; 180 °C = 05, 06, 07 & 08; 240° C = 09, 10, 11 & 12
 Duration of heating: 0.5 hr = 01, 05 & 09; 1 hr = 02, 06 & 10; 2 hrs = 03, 07 & 11; 3 hrs = 04, 08 & 12.

Appendix 12: Lipid Classes of the LC-MS/MS.

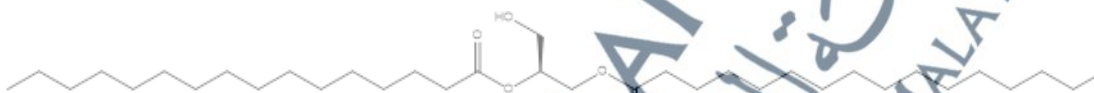
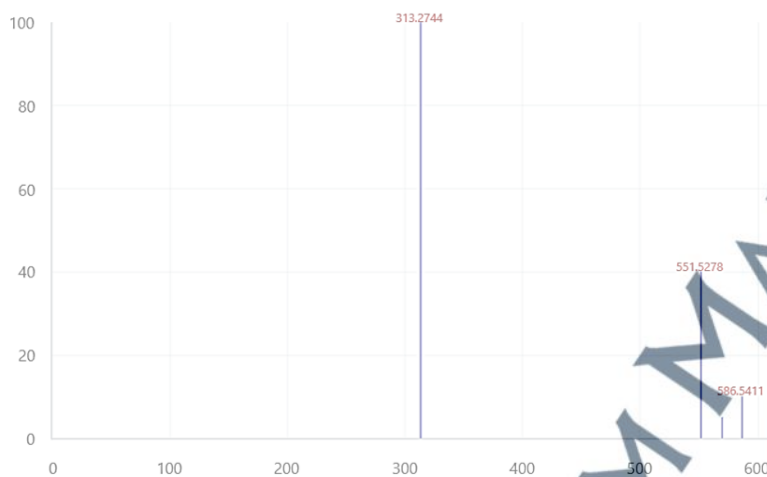
bil	m/z	lipid species compound +ion adduct	bil	m/z	lipid species compound +ion adduct	bil	m/z	lipid species compound +ion adduct
1	264.5	MAG 10:0+NH4	41	572.5	DAG 31:0+NH4	81	656.5	DAG 37:0+NH4
2	278.5	MAG 11:0+NH4	42	574.5	DAG 32:6+NH4	82	658.5	DAG 38:6+NH4
3	318.5	MAG 14:1+NH4	43	576	DAG 32:5+NH4	83	660.5	DAG 38:5+NH4
4	332.5	MAG 15:1+NH4	44	576.5	DAG 32:5+NH4	84	662.5	DAG 38:4+NH4 MGDG
5	334.5	MAG 15:0+NH4	45	578.5	DAG 32:4+NH4	85	664	DAG 38:0+NH4
6	346.5	MAG 16:1+NH4	46	586.5	DAG 32:0+NH4	86	664.5	DAG 38:3+NH4
7	348.5	MAG 16:0+NH4	47	588.5	DAG 33:6+NH4	87	666.5	DAG 38:2+NH4
8	360.5	MAG 17:1+NH4	48	591	DAG 33:5+NH4	88	668.5	DAG 39:8+NH4
9	362.5	MAG 17:0+NH4	49	592.5	DAG 33:4+NH4	89	669.5	SQDG 23:0
10	374.5	MAG 18:1+NH4	50	600.5	DAG 33:0+NH4	90	670.5	DAG 39:7+NH4
11	376.5	MAG 18:0+NH4	51	602.5	DAG 34:6+NH4	91	672.5	DAG 39:6+NH4 MGDG
12	390.5	MAG 19:0+NH4	52	604.5	DAG 34:5+NH4	92	674.5	DAG 39:2+NH4
13	402.5	MAG 20:1+NH4	53	606.5	DAG 34:4+NH4	93	676.5	DAG 39:4+NH4
14	404.5	MAG 20:0+NH4	54	608.5	DAG 34:3+NH4	94	679	DAG 39:3+NH4
15	418.5	DAG 20:0+NH4	55	614.5	DAG 34:0+NH4	95	680.5	DAG 40:9+NH4
16	420.5	MAG 22:6+NH4	56	616.5	DAG 35:6+NH4	96	681	SQDG 24:1
17	430	MAG 22:1+NH4	57	618.5	DAG 35:5+NH4	97	683.5	DAG 40:8+NH4
18	430.5	MAG 22:1+NH4	58	620.5	DAG 35:4+NH4	98	683.5	SQDG 24:0
19	432.5	DAG 21:0+NH4	59	622.5	DAG 35:3+NH4	99	684.5	DAG 39:0+NH4 MGDG
20	446.5	MAG 23:0+NH4	60	624.5	DAG 35:2+NH4	100	686	DAG 38:3+NH4
21	458.5	MAG 24:1+NH4	61	626.5	DAG 36:1+NH4	101	686.5	DAG 40:6+NH4
22	460.5	MAG 24:0+NH4	62	627.5	SQDG 20:0	102	688.5	DAG 40:5+NH4
23	472.5	DAG 24:1+NH4	63	628.5	DAG 35:0+NH4	103	690.5	DAG 40:4+NH4
24	474.5	DAG 24:0+NH4	64	630.5	DAG 36:6+NH4	104	692.5	DAG 40:3+NH4
25	486.5	DAG 25:1+NH4	65	632	DAG 36:5+NH4	105	694.5	DAG 40:2+NH4
26	488.5	DAG 25:0+NH4	66	632.5	DAG 36:5+NH4	106	696	SQDG 25:1
27	500.5	DAG 26:1+NH4	67	634	DAG 36:4+NH4 MGDG	107	697.5	SQDG 25:0 MGDG
28	502.5	DAG 26:0+NH4	68	635	DAG 36:4+NH4 24:1+NH4	108	700	DAG 29:3+NH4 MGDG
29	514.5	DAG 27:1+NH4	69	636.5	DAG 36:3+NH4	109	700.5	DAG 29:3+NH4 MGDG
30	516.5	DAG 27:0+NH4	70	638.5	DAG 36:2+NH4	110	702	DAG 29:2+NH4 MGDG
31	528.5	DAG 28:1+NH4	71	640.5	DAG 36:1+NH4	111	702.5	DAG 41:5+NH4
32	530.5	DAG 28:0+NH4	72	641.5	SQDG 21:0	112	704.5	DAG 42:11+NH4 DAG
33	542.5	DAG 29:1+NH4	73	642.5	DAG 36:0+NH4	113	706.5	DAG 42:10+NH4
34	544.5	DAG 29:0+NH4	74	644.5	DAG 37:6+NH4	114	708.5	DAG 41:2+NH4
35	548.5	DAG 30:5+NH4	75	646.5	DAG 37:5+NH4	115	709	SQDG 26:1
36	560.5	DAG 30:4+NH4	76	648.5	DAG 37:4+NH4	116	709.5	SQDG 26:1
37	566.5	DAG 30:1+NH4	77	650.5	DAG 37:3+NH4	117	716.5	DAG 42:5+NH4
38	558.5	DAG 30:0+NH4	78	652.5	DAG 37:2+NH4	118	718.5	DAG 42:4+NH4
39	562.5	DAG 31:5+NH4	79	654.5	DAG 37:1+NH4	119	720.5	DAG 42:3+NH4
40	564.5	DAG 31:4+NH4	80	655.5	SQDG 22:0	120	721.5	SQDG 27:2

bil	m/z	lipid species compound +ion adduct	bil	m/z	lipid species compound +ion adduct	bil	m/z	lipid species compound +ion adduct
121	722	TAG 41:2+NH4	141	797	TAG 47:7+NH4	161	859.5	SQDG 37:3
122	723	DAG 42:2+NH4	142	799.5	SQDG 33:5	162	866	SQDG 37:0
123	723.5	SQDG 27:1	143	802	MGDG 36:1+NH4	163	868	SQDG 38:6
124	728	MGDG 31:3+NH4	144	805.5	SQDG 33:2	164	870	SQDG 38:5
125	732.5	DAG 43:4+NH4	145	811.5	SQDG 34:6	165	873	TAG 52:4+NH4
126	734.5	DAG 44:10+NH4	146	814	SQDG 34:5	166	873.5	SQDG 38:3
127	757.5	SQDG 30:5	147	816	SQDG 34:4	167	874.5	TAG 52:3+NH4
128	761	SQDG 30:3	148	820	MGDG 38:6+NH4	168	875.5	SQDG 38:2
129	762	SQDG 30:3	149	822	SQDG 34:1	169	876.5	TAG 52:2+NH4
130	764	SQDG 30:2	150	825.5	SQDG 35:6	170	877.5	SQDG 39:8
131	766	SQDG 30:1	151	828	SQDG 35:5	171	879.5	SQDG 38:0
132	772	SQDG 31:5	152	830	SQDG 35:4	172	880.5	TAG 53:7+NH4
133	773.5	SQDG 31:4	153	832	SQDG 35:3	173	881	TAG 52:0+NH4
134	779.5	SQDG 31:1	154	844	SQDG 36:4	174	883	MGDG 43:3+NH4
135	783	DAG 46:0+NH4	155	849.5	SQDG 36:1	175	886	SQDG 39:4
136	783.5	SQDG 32:6	156	851.5	SQDG 37:7	176	888	SQDG 39:3
137	785.5	SQDG 32:5	157	852	MGDG 40:4+NH4	177	890	SQDG 40:9
138	788	MGDG 35:1+NH4	158	855	MGDG 40:3+NH4	178	891.5	SQDG 40:8
139	789.5	SQDG 32:3	159	856.5	TAG 51:5+NH4	179	893.5	SQDG 40:7
140	794	SQDG 32:1	160	857	TAG 51:5+NH4	180	895	TAG 54:7+NH4

bil	m/z	lipid species compound +ion adduct	bil	m/z	lipid species compound +ion adduct	bil	m/z	lipid species compound +ion adduct
181	896	SQDG 40:6	201	922	SQDG 41:0	221	951.5	SQDG 44:6
182	897	MGDG 43:3+NH4	202	924	SQDG 42:6	222	953.5	SQDG 44:5
183	897.5	SQDG 40:5	205	925.5	SQDG 42:5	223	956.5	MGDG 47:1+NH4
184	898.5	TAG 54:5+NH4	204	927.5	TAG 46:5+NH4	224	963.5	MADAG 59:1+NH4
185	899.5	SQDG 40:4	205	929.5	SQDG 42:3	225	965.5	MADAG 59:0+NH4
186	900.5	TAG 55:11+NH4	206	930.5	TAG 46:3+NH4			
187	901.5	SQDG 40:3	207	931.5	SQDG 42:2			
188	902.5	TAG 54:3+NH4	208	932.5	TAG 56:2+NH4			
189	903.5	SQDG 40:2	209	933.5	SQDG 42:1			
190	904.5	TAG 54:2+NH4	210	934.5	MGDG 46:5+NH4			
191	905.5	SQDG 40:1	211	935.5	SQDG 42:0			
192	906.5	TAG 54:1+NH4	212	936.5	TAG 56:0+NH4			
193	907.5	SQDG 40:0	213	937.5	SQDG 43:6			
194	908	TAG 54:0+NH4	214	938.5	TAG 57:6+NH4			
195	910	SQDG 41:6	215	940.5	TAG 57:5+NH4			
196	912	SQDG 41:5	216	943.5	SQDG 43:3			
197	913.5	SQDG 41:4	217	946.5	TAG 57:2+NH4			
198	916	SQDG 42:10	218	948.5	TAG 57:1+NH4			
199	917.5	SQDG 42:9	219	949.5	SQDG 43:0			
200	920	SQDG 41:1	220	950.5	TAG 57:0+NH4			

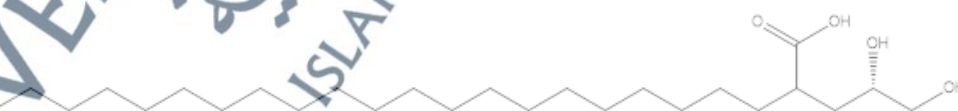
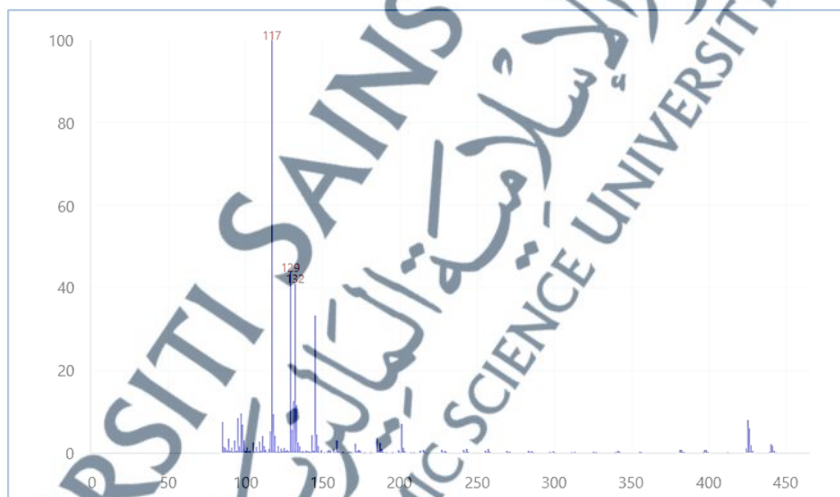
Appendix 13: Typical Spectra of Glycerolipids (GL).

A) DAG 32:0



1,2 dihexadecanonyl-sn-glycerol

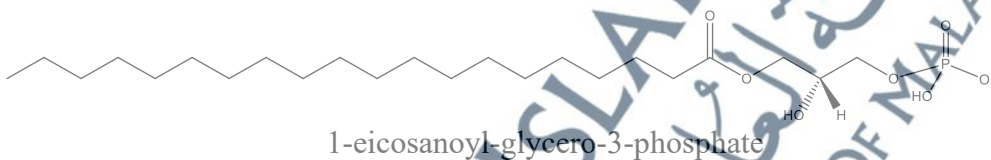
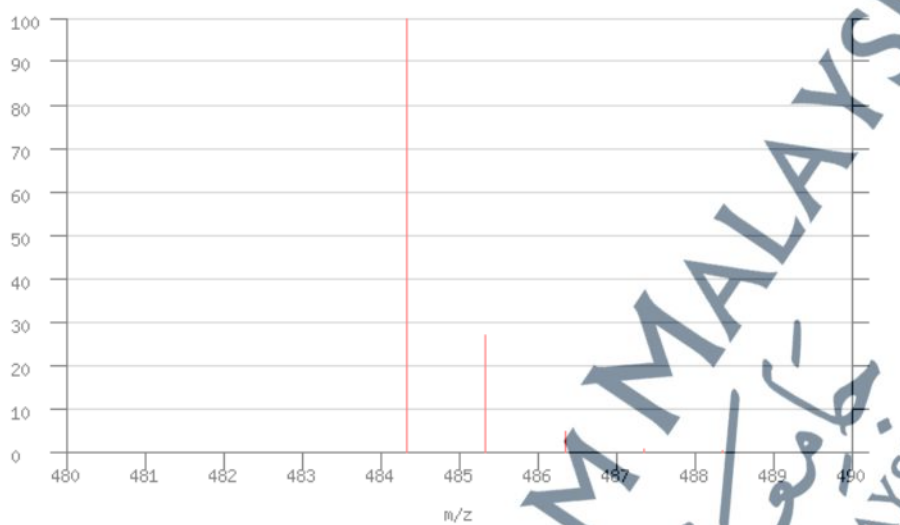
B) MAG 24:0



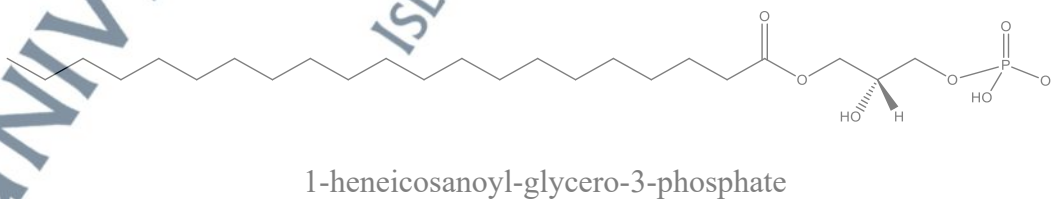
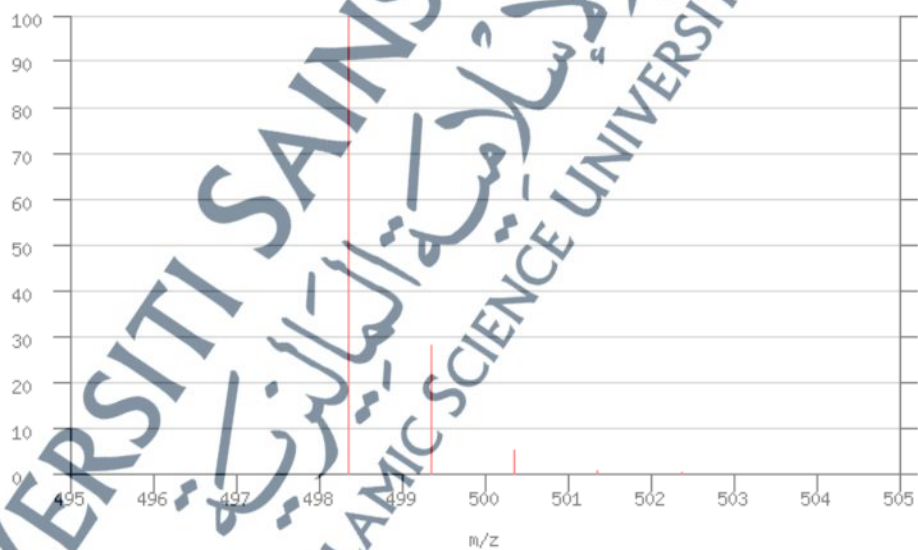
tetracosanoic acid

Appendix 14: Typical Spectra of Glycerophospholipids (GPPL)

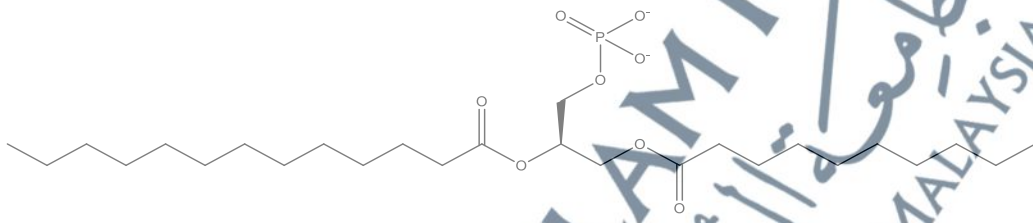
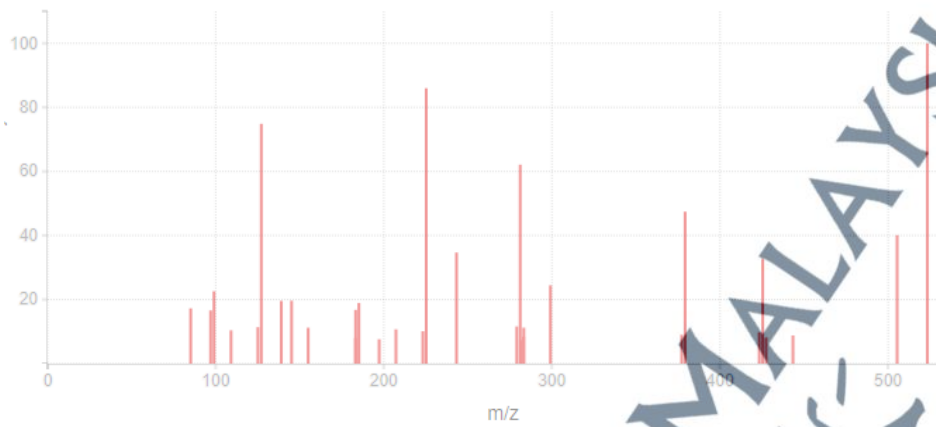
A) PA(20:0)



B) PA(21:0)

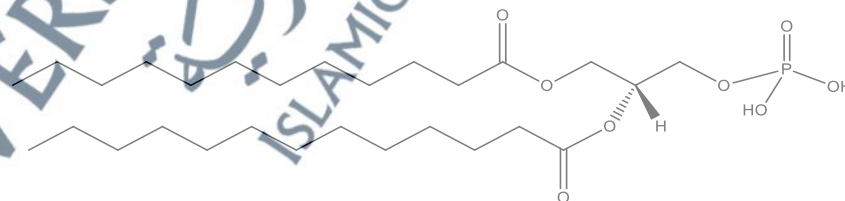


C) PA(23:0)



1-decanoyl-2-tridecyloyl-sn-glycero-3-phosphate

D) PA(25:0)



1-dodecanoyl-2-tridecanoyl-sn-glycero-3-phosphate

Appendix 15: List of Publications.

1. Salleh, N. A. M., Hassan, M. S., Jumal, J., Harun, F. W., & Jaafar, M. Z. 2018. Differentiation of Edible Fats from Selected Sources after Heating Treatments using Fourier Transform Infrared Spectroscopy (FTIR) and Multivariate Analysis. *In AIP Conference Proceedings* 2017, June, AIP Publishing LLC. Vol. 1972. (1): p. 030015.
2. Salleh, N. A. M., & Hassan, M. S. 2019. Discrimination of Lard and other Edible Fats after Heating Treatments using Partial Least Square Regression (PLSR), Principal Component Regression (PCR), and Linear Support Vector Machine Regression (SVMR). *In Journal of Physics: Conference Series*. November 2019. IOP Publishing. Vol. 1366. (1): p. 012114.
3. Salleh, N. A. M., Yahaya, N., Rosli, D., Azizan, M. F., Yamin, B. M., & Hassan, M. S. 2022. Characterization of Lard Profile from Different Geographical Regions of Husbandries and Body Parts of Pig using FTIR Technique Combined with Chemometrics. *International Journal on Advanced Science Engineering Information Technology*. Vol.12 (2022): p. 1565-1573.