APPENDICES

Appendix 1: BUCHI 20/40/60 rule for rotary evaporator

University of Wollongong
School of Chemistry

Buchi 20/40/60 rule for Rotary Evaporators

Optimal Distillation parameters for a rotary evaporator vary according to solvent in use:

1. Set **water bath temperature** to **60°C** – It does not need to be higher!
2. The **cooling water** temperature should be below **20°C**.
3. Adjust the needed **vacuum** for a solvent boiling point of **40°C** according to list below.

Solvent	Formula	Vacuum [mbar] for bp at 40 °C
Acetic acid	$C_2H_4O_2$	44
Acetone	C_3H_6O	556
Acetonitrile	C_2H_3N	226
n-Amylalcohol, n-Pentanol	$C_5H_{12}O$	11
n-Butanol	C_4H_{10}	25
tert-Butanol, 2-Methyl-2-Propanol	$C_4H_{10}O$	130
Butylacetate	$C_6H_{12}O_2$	39
Chlorobenzene	C_6H_5Cl	36
Chloroform	$CHCl_3$	474
Cyclohexane	C_6H_{12}	235
Dichloromethane, Methylene chloride	CH_2Cl_2	atm. press.*
Diethylether	$C_4H_{10}O$	atm. press.*
1,2,-Dichloroethylene (trans)	$C_2H_2Cl_2$	751
Diisopropylether	$C_6H_{14}O$	375
Dioxane	$C_4H_8O_2$	107
Dimethylformamide (DMF)	C_3H_7NO	11
Ethanol	C_2H_6O	175
Ethylacetate	$C_4H_8O_2$	240
Ethylmethylketone	C_4H_8O	243
Heptane	C_7H_{16}	120
Hexane	C_6H_{14}	335
Isopropylalcohol	C_3H_8O	137
Isoamylalcohol, 3-Methyl-1Butanol	$C_5H_{12}O$	14
Methanol	CH_4O	337
Pentane	C_5H_{12}	atm. press.*
n-Propylalcohol	C_3H_8O	67
Pentachloroethane	C_2HCl_5	13
1,1,2,2,-Tetrachloroethane	$C_2H_2Cl_4$	35
1,1,1,-Trichloroethane	$C_2H_3Cl_3$	300
Tetrachloroethylene	C_2Cl_4	53
Tetrachloromethane	CCl_4	271
Tetrahydrofurane (THF)	C_4H_8O	357
Toluene	C_7H_8	77
Trichloroethylene	C_2HCl_3	183
Water	H_2O	72
Xylene	C_8H_{10}	25

*~850 mbar recommended

Reference: Buchi: List of Solvents

Doc: CHEMFS rotovap pressure-temp
Created: Feb 2005
Custodian: Dept. Chem. School Safety Coordinator
Last Review: Dec 2010
Page 1 of 1
Next Review: Dec 2013

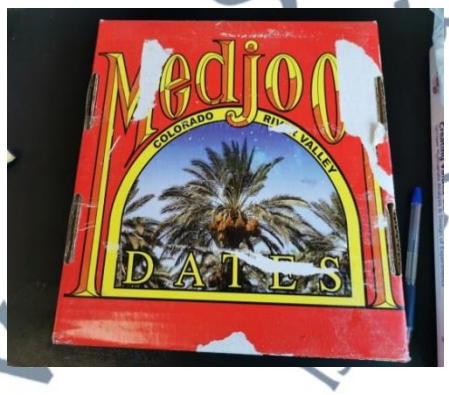
Appendix 2: Different Varieties of Dates Fruits Used in FTIR Analysis.

Ajwa Dates (K1)

Safawi Dates (K2)

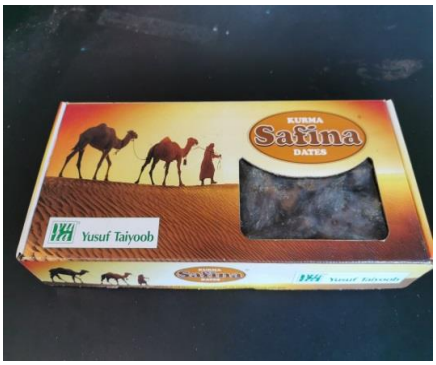
Mariami Dates (K3)

Ajwa Dates used in this Study (K4)



Medjool Dates (K5)

Safia Dates (K6)



Safina Dates (K7)

Ameera Dates (K8)

Raziz Dates (K9)

Sunseed Dates (K10)

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Appendix 3: GC-MS Setting

```
                              INSTRUMENT CONTROL PARAMETERS:    GCMS
                              -------------------------------------

   D:\METHODS\ELMA.M
      Fri Jan 15 16:37:44 2016

Control Information
------- -----------

Sample Inlet      :  GC
Injection Source  :  GC ALS
Mass Spectrometer :  Enabled

Oven
Equilibration Time                          0 min
Oven Program                                On
    80 °C for 3 min
    then 7 °C/min to 250 °C for 15 min
Run Time                                    42.286 min



Front Injector
Syringe Size                                10 µL
Injection Volume                            1 µL
Solvent A Washes (PreInj)                   5
Solvent A Washes (PostInj)                  5
Solvent A Volume                            8 µL
Solvent B Washes (PreInj)                   0
Solvent B Washes (PostInj)                  0
Solvent B Volume                            8 µL
Sample Washes                               1
Sample Wash Volume                          8 µL
Sample Pumps                                2
Dwell Time (PreInj)                         0 min
Dwell Time (PostInj)                        0 min
Solvent Wash Draw Speed                     300 µL/min
Solvent Wash Dispense Speed                 6000 µL/min
Sample Wash Draw Speed                      300 µL/min
Sample Wash Dispense Speed                  6000 µL/min
Injection Dispense Speed                    6000 µL/min
Viscosity Delay                             0 sec
Sample Depth                                Disabled
Injection Type                              Standard
L1 Airgap                                   0 µL


Front SS Inlet He
Mode                                        Splitless
Heater                                      On    250 °C
Pressure                                    On    10.785 psi
Total Flow                                  On    52.3 mL/min
Septum Purge Flow                           On    1 mL/min
Gas Saver                                   On    20 mL/min After 2 min
Purge Flow to Split Vent                    50 mL/min at 2 min


Thermal Aux 2 {MSD Transfer Line}
Heater                                      On
Temperature Program                         On
    280 °C for 0 min
Run Time                                    42.286 min


Column #1
DB-5MS UI (30m X 0.25mm X 0.25DB-5MS UI (30m X 0.25mm X 0.25
325 °C: 30 m x 250 µm x 0.25 µm
In: Front SS Inlet He
Out: Vacuum
```

(Initial)	80 °C
Pressure	12.758 psi
Flow	1.3 mL/min
Average Velocity	42.148 cm/sec
Holdup Time	1.1863 min
Flow Program	On
1.3 mL/min for 0 min	
Run Time	42.286 min

Signals	
Test Plot	Save Off
	50 Hz
Test Plot	Save Off
	50 Hz
Test Plot	Save Off
	50 Hz
Test Plot	Save Off
	50 Hz

MS ACQUISITION PARAMETERS

General Information

Tune File	: atune.u
Acquistion Mode	: Scan

MS Information

Solvent Delay	: 6.00 min
EMV Mode	: Relative
Relative Voltage	: 0
Resulting EM Voltage	: 1682

[Scan Parameters]

Low Mass	: 45.0
High Mass	: 600.0
Threshold	: 150
Sample #	: 2 A/D Samples 4
Plot 2 low mass	: 50.0
Plot 2 high mass	: 550.0

[MSZones]

MS Source	: 230 C maximum 250 C
MS Quad	: 150 C maximum 200 C

END OF MS ACQUISITION PARAMETERS

TUNE PARAMETERS for SN: US92023506

Trace Ion Detection is OFF.

EMISSION : 34.610

ENERGY	:	69.922		
REPELLER	:	25.935		
IONFOCUS	:	90.157		
ENTRANCE_LE	:	35.000		
EMVOLTS	:	1682.353		
			Actual EMV :	1682.35
			GAIN FACTOR :	0.74
AMUGAIN	:	2742.000		
AMUOFFSET	:	120.625		
FILAMENT	:	1.000		
DCPOLARITY	:	0.000		
ENTLENSOFFS	:	18.322		
MASSGAIN	:	-275.000		
MASSOFFSET	:	-35.000		

END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

Appendix 4: LC-QToF-MS Setting

LC conditions

LC system: ACQUITY UPLC I-Class with FTN Sample Manager

Column: ACQUITY UPLC HSS T3 2.1 x 100 mm, 1.8 µm

Column temp.: 40 °C

Sample temp.: 15 °C

Injection volume (µL): 10

Mobile phase: A: water (0.1% formic acid); B: acetonitrile

Gradient:

Time	Flow rate (mL/min)	Solvent A	Solvent B
0	0.6	99	1
0.5	0.6	99	1
16	0.6	65	35
18	0.6	0	100
20	0.6	99	1

MS conditions

MS system: Vion IMS QTof

Acquisition range: 100-1500 Da

Scan time: 0.1 s

Acquisition mode: HDMS*, ESI- and ESI+ in sensitive mode

Lock mass: Leucine Enkephalin (LE) 1 ppm (scan for 0.3 s, interval: 60 s)

Capillary voltage: 1.5 kV (ESI+)/1.5 kV (ESI-)

Cone voltage: 40 V

Collision energy (eV): low CE: 4/High CE: 10-40

Source temp.: 120 °C

Desolvation temp.: 550 °C

Cone gas flow: 50 L/h

Desolvation gas flow: 800 L/h

Acquisition time: 20 min

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Appendix 5: FTIR Setting

Spectrum One Instrument Settings

Monday, December 09, 2019 12:16 PM Malay Peninsula Standard Time
Serial number 79884

Sample Parameters

Name	Oh-a
Description:	Urine
Comments:	

Scan Parameters

Start:	4000.00	cm-1
End:	600.00	cm-1
Number of Scans:	4	
Data Type:	Sample	
Units:	%T	

Beam Parameters

Detector Type:	MIR TGS	
Detector Site:	Int2	
Source Type:	MIR	
Source Site:	Int1	
Beamsplitter:	OptKBr	
Filter Wheel:	none	
J Stop Wavenumber	4000.00	cm-1
J Stop Image Size:	8.94	mm

Accessory Parameters

User Defined Configuration:	
Accessory:	Not Fitted/Unknown

Instrument Parameters

Resolution:	4.00	cm-1
Data Interval:	1.000	cm-1
Apodization:	Strong	
Phase Correction:	Magnitude	
Scan Speed:	0.20	cm/s
CO2/H2O:	Yes	
AVI:	No	
Look Ahead:	No	

Quality Parameters

Water Vapor	No
Carbon Dioxide	No
Baseline Low	No
Baseline High	No
Baseline Slope	No
Strong Bands	No
Weak Bands	No
High Noise	No
Fringes	No
Vignetting	No
Blocked Beam	No
Negative Bands	No
Stray Light	No
Zero Transmission	No
Window Cutoff	No

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Appendix 6: Consent Form

CONSENT FORM FOR PARTICIPATING IN RESEARCH PROJECT

RESEARCH TITLE:

METABOLOMIC STUDY ON HUMAN URINE ON CONSUMPTION OF DATE FRUITS.

AGREEMENT:

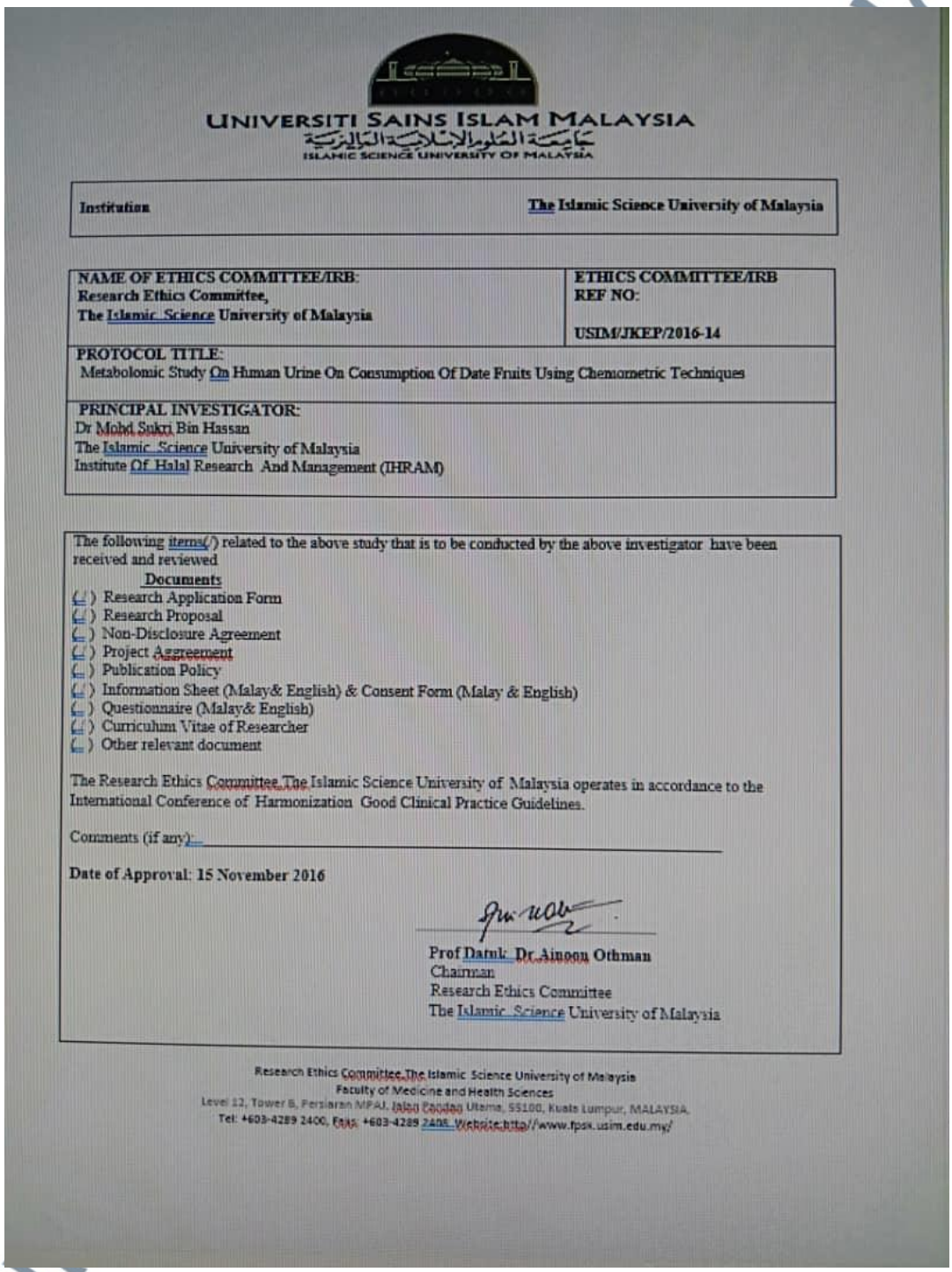
I have read the information of the research study above and have been informed of the nature of this metabolomics study in terms of methodology and possible adverse effects. I understand the possible advantages and disadvantages of participating in this research. I understand that I have the right to know about this research study and the findings. I know I can quit from this research study at any time.

I agree / disagree to participate and using my urine as sample for this research study.

Name of Participant	**Identity Card No**	**Signature**
Ahmad Solehin Ab Sabar	950302-06-5387	
Muhammad Nabil Bazli	950603-08-5373	
Muhamad Syukur Kamarudin	950917-01-6661	
Mohamad Tarmizi Mohd Nasir	951105-06-5569	
Mohd Zulhilmi Mohd Noor	950101-11-5069	
Nurul 'Izzati Mohd Jihadi	950327-02-5170	
Nur Syamira Zainudin	950608-04-5370	
Ana Syahmi Muhamad Sahri	950713-10-6104	
Asmaa' Mardhiah Rohisham	950117-03-5418	
Siti Nazurah Md Jusoh	951124-11-5154	

Witness's Name	**Identity Card No.**	**Signature**
Nurul Elma Sabri	890407-08-5120	

Appendix 7: Letter of Ethics Approval



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Institution	The Islamic Science University of Malaysia

NAME OF ETHICS COMMITTEE/IRB: Research Ethics Committee, The Islamic Science University of Malaysia	ETHICS COMMITTEE/IRB REF NO: USIM/JKEP/2016-14
PROTOCOL TITLE: Metabolomic Study On Human Urine On Consumption Of Date Fruits Using Chemometric Techniques	
PRINCIPAL INVESTIGATOR: Dr Mohd Sukri Bin Hassan The Islamic Science University of Malaysia Institute Of Halal Research And Management (IHRAM)	

The following items(/) related to the above study that is to be conducted by the above investigator have been received and reviewed

Documents

(/) Research Application Form
(/) Research Proposal
(_) Non-Disclosure Agreement
(/) Project Agreement
(_) Publication Policy
(/) Information Sheet (Malay& English) & Consent Form (Malay & English)
(_) Questionnaire (Malay& English)
(/) Curriculum Vitae of Researcher
(_) Other relevant document

The Research Ethics Committee The Islamic Science University of Malaysia operates in accordance to the International Conference of Harmonization Good Clinical Practice Guidelines.

Comments (if any):_____

Date of Approval: 15 November 2016

Prof Datuk Dr Ainoon Othman
Chairman
Research Ethics Committee
The Islamic Science University of Malaysia

Research Ethics Committee The Islamic Science University of Malaysia
Faculty of Medicine and Health Sciences
Level 12, Tower B, Persiaran MPAJ, Jalan Pandan Utama, 55100, Kuala Lumpur, MALAYSIA.
Tel: +603-4289 2400, Faks: +603-4289 2406 Website:http//www.fpsk.usim.edu.my/

Appendix 8: Diet Diary for Volunteers

PATIENT'S DIARY OF METABOLOMIC STUDY

NAME: _____

AGE: _____ GENDER: _____

NATIONALITY: _____

WEIGHT: _____ HEIGHT: _____

BMI: _____

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MAKLUMAT UNTUK IBUBAPA/PENJAGA/PESAKIT

Tajuk penyelidikan
Kajian Metabolomik ke atas air kencing manusia terhadap pemakanan kurma

Pengenalan
Kajian metabolomik adalah salah satu kajian "omics" dimana pemfokusan ke atas metabolit-metabolit dengan mengambil kira perubahan metabolit yang terdapat di dalam tisu badan manusia dan cecair dalam badan manusia seperti darah dan air kencing. Pemakanan harian memberi faktor terhadap perubahan metabolit dalam badan manusia. Dalam kajian ini, perubahan metabolit di dalam air kencing manusia sebelum dan selepas memakan kurma akan dikaji untuk melihat kepentingan buah kurma terhadap badan manusia.

Apa yang akan dilakukan
Tempoh kajian ini adalah selama 7 hari dari hari Isnin hingga Ahad. Sampel air kencing akan
dikumpulkan 2 kali sehari pada pukul 7am dan 7pm, dari hari Isnin hingga Ahad. Kecuali pada hari Selasa, sampel air kencing akan dikumpulkan sebanyak 4 kali pada pukul 7am, 11am, 3pm dan 7pm. Ini kerana selepas pengumpulan sampel air kencing pada pukul 7am, pesakit akan diberi 7 biji buah kurma untuk dimakan. Sampel air kencing perlu dikumpulkan setiap 4jam selepas pemakanan buah kurma (lihat lampiran Maklumat kajian metabolomik untuk pesakit).

Faedah penyelidikan
Penyelidikan ini dapat menyumbang kepada perkembangan sains dan perubatan. Ia akan
meningkatkan pengetahuan tentang kebaikan buah kurma untuk system metabolik badan
manusia.

Risiko
Tiada risiko tambahan kerana penyelidikan hanya mengumpul air kencing dan pengawalan
pemakanan yang mengikut piawai.

Kerahsiaan
Keputusan yang diperolehi akan dimaklumkan secara keseluruhan (kolektif) dan tidak akan
merujuk pada nama individu pesakit. Justeru maklumat dan keputusan dari setiap pesakit
adalah sulit. Sebagai ibubapa/pesakit anda berhak mengetahui keputusan bagi anda sahaja.

Perlukah saya mengambil bahagian
Penglibatan dalam penyelidikan ini adalah secara sukarela. Sekiranya anda tidak setuju, anda
tidak perlu memberikan sebab dan anda juga boleh menarik diri pada bila-bila masa sahaja.

Bayaran dan pampasan
Anda tidak akan dikenakan apa-apa bayaran dan anda juga tidak akan dibayar bagi penglibatan dalam penyelidikan ini. Sekiranya hasil dari penyelidikan ini dapat mengembangkan satu produk yang boleh dipasarkan, anda tidak boleh menuntut hakmilik
kepada harta intelek dan juga keuntungan dari produk yang terhasil dan dikomersilkan, jika
ada.

Jika ada sebarang pertanyaan, sila hubungi:
Nama: Alamat & No Telefon:

INFORMATION FOR PARENT/GUARDIAN/PATIENT

Research title
Metabolomic study on human urine on consumption of dates fruits

Introduction
Metabolomic is one of "omics" study which focus on metabolites by evaluating the changes of metabolites in tissues and body fluids such as blood and urine. Daily diet may change the metabolites in body. In this study, metabolites changes in human urine before and after consumption of dates will be studied to investigate the benefit of dates to human.

What will be done?
The study duration is 7 days from Monday to Sunday. The urine samples will be collected for twice per day at 7am and 7pm, from Monday to Sunday. Except for Tuesday, the urine will be collected 4 times at 7am, 11am, 3pm and 7pm. This is because, after urine collection at 7am on Tuesday, the patient will be given 7 dates fruits to consume. The urine need to be collected every 4 hours after consuming the dates fruits (see Information of metabolomic study for Patient sheet).

Research significant
This research can give advantages in science and medical field. This research can increase the people awareness about the benefit of consuming dates fruits on human metabolic system.

Risk
No additional risks because this research is only collect the urine sample and control diet according to standard daily diet.

Privacy
The findings/results for this research will be published in collective data and will not mention patient's name, individually. Thus, all the informations are private & confidential (P&C).

Do I need to participate?

Participation in this research is voluntarily. You don't have to give an excuse if disagree to participate and you can quit from this research at any time.

Payment and compensation
No payment fee and you will not be paid as volunteer. If this research can produce a new market product, you cannot claim for any benefit, if any.

Any inquiries, don't hesitate to contact:
Name:
Address:
Phone Number:

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Information of metabolomic study for volunteers

Table 1: Summary of urine collection

	DAY 1	DAY 2	DAY 3	DAY 4	DAY 5	DAY 6	DAY 7
6-7 AM	/	/	/	/	/	/	/
11 AM		/					
3 PM		/					
6-7 PM	/	/	/	/	/	/	/

Inclusion/ Exclusion criteria:

- Healthy (5 males 5 females)
- Non-smokers
- Not in any medication/ supplement
- Aged between 20-25 years old
- Body mass index (BMI) not more than 30

Design of study

- The study duration is 7 days from Monday to Sunday. The urine samples will be collected for every early morning around 6-7 am starting from Monday, and the second round of sample collection is at 6-7 pm on the same day.
- On Tuesday, urine sample will be collected at 6-7 am, and after collection, the volunteers will be given 7 dates fruits to consume. Urine will be collected 4 hours after consuming the date fruit which is around at 11 am (second round), and 4 hours after that which is at 3 pm (third round), urine will be taken. The fourth round is at 6-7 pm, urine will be taken on the same day.
- From Wednesday to Sunday, urine will be collected in the early morning at 6-7 am and after 12 hours which is at 6-7 pm. The summary of urine collection had been shown in Table 1.

Menu

- Given to volunteers after considering their food allergy and so on.
- Volunteers are required to follow the control diet (food will be provided during experiment).
- The menu is consist of rice, a protein dish (chicken or fish)
- Only mineral water is allowed during experiment.
- No nescafe, coca cola, pepsi or any bicarbonate drinks
- No fruits and vegetables

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BORANG KEIZINAN UNTUK PESERTA

Saya
……(Nama Penuh)……..

No Kad Pengenalan …… beralamat ……..
(Alamat)
……
…….

Dengan ini bersetuju untuk mengambil bahagian dalam kajian metabolomik seperti berikut:-

Tajuk Kajian:

KAJIAN METABOLOMIK PEMAKANAN KURMA TERHADAP URIN MANUSIA

Tujuan kajian ini telah dijelaskan kepada saya oleh **Dr Mohd Sukri Hassan** (Penyelidik) dan **Nurul Elma Sabri** (Pelajar PhD) sebaik mungkin dalam **Bahasa Melayu**.

Saya juga telah dimaklumkan berkenaan asas kajian metabolomik dari sudut metodologi dan kemungkinan kesan sampingan. Saya memahami kemungkinan kelebihan dan kekurangan daripada penyertaan dalam kajian ini. Saya dengan ini sukarela untuk menyertai kajian seperti dijelaskan diatas yang merangkumi pengawalan diet, butiran aktiviti dan makanan yang diambil melalui diari eksperimen dan persampelan urin

Saya memahami seluruh data adalah sulit dan persendirian (P&C) dan hanya akan digunakan untuk kajian metabolomik (diterbitkan tanpa mendedahkan identity peserta).

Tarikh: …… Tandatangan:
……

DI HADAPAN

Nama: Dr Mohd Sukri Hassan

No Kad Pengenalan: 620203086631 Tandatangan:

……

Jawatan: Researcher

Nama: Nurul Elma Sabri

No Kad Pengenalan: 890407085120 Tandatangan:

……

Jawatan: PhD Student

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CONSENT FORM FOR VOLUNTEER

I

……(Full Name)……

……

Identity Card No ……

of……

……

(Address)

……

hereby agree to participate in the metabolomics study specified below:-

Title of Study:

METABOLOMICS STUDY ON HUMAN URINE ON CONSUMPTION OF DATES FRUITS

the nature and purpose of which has been explained to me by **Dr Mohd Sukri Hassan** (Researcher) and interpreted by **Nurul Elma Sabri** (PhD Student) to the best of his/her ability in **Malay** language/dialect.

I have been informed of the nature of this metabolomics study in terms of methodology and possible adverse effects. I understand the possible advantages and disadvantages of participating in this research. I voluntarily to participate in this research specified above which

involves control diet, details of activities and food taken throughout the experiment (diary) and urine sampling.

I understand that all data would be private and confidential (P&C) and only used for metabolomics study (publication without reveal the identity of volunteer).

Date: …… Signature:
……

IN THE PRESENCE OF

Name: Dr Mohd Sukri Hassan
Identity Card No: 620203086631 Signature:
…….
Designation: Researcher

Name: Nurul Elma Sabri
Identity Card No: 890407085120 Signature:
…….
Designation: PhD Student

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DAY: _____ DATE _____

YOU HAVE TO REPORT EVERY SINGLE THINGS THAT YOU DID AND WHAT YOU EAT FOR THE WHOLE DAY

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DAY: _____ DATE _____

YOU HAVE TO REPORT EVERY SINGLE THINGS THAT YOU DID AND WHAT YOU EAT FOR THE WHOLE DAY

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DAY: _____ DATE _____

YOU HAVE TO REPORT EVERY SINGLE THINGS THAT YOU DID AND WHAT YOU EAT FOR THE WHOLE DAY

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DAY: _____ DATE _____

YOU HAVE TO REPORT EVERY SINGLE THINGS THAT YOU DID AND WHAT YOU EAT FOR THE WHOLE DAY

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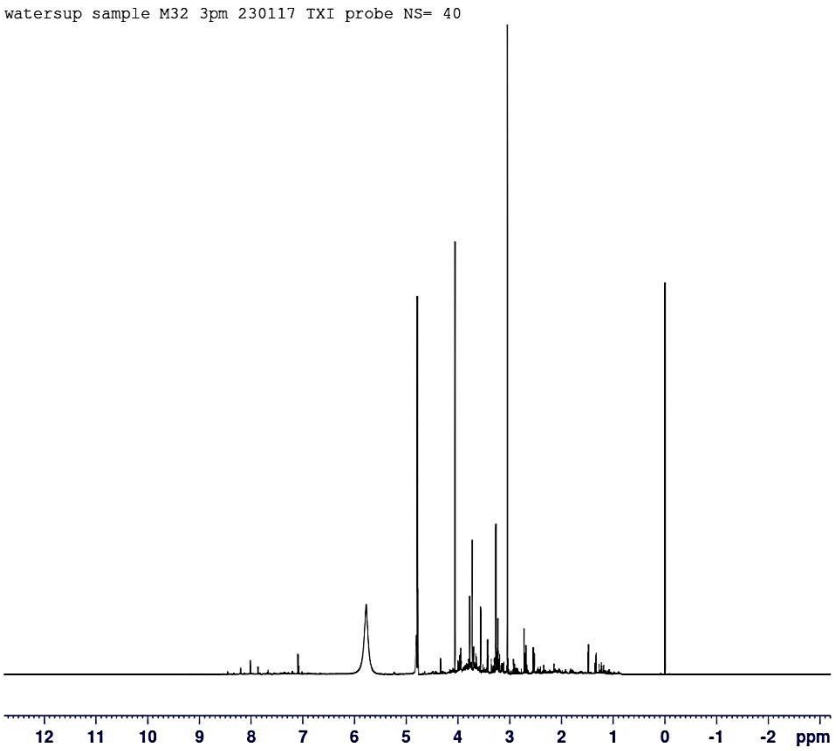
Appendix 9: ^{1}H-NMR Setting



GENOMMALAYSIA
Malaysia Genome Institute

```
Current Data Parameters
NAME            Elma_USIM
EXPNO                  21
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170123
Time                17.52
INSTRUM             spect
PROBHD   5 mm PATXI 1H-
PULPROG      noesygppr1d
TD                  32768
SOLVENT       Urine_USIM
NS                     40
DS                      4
SWH             11194.030 Hz
FIDRES           0.341615 Hz
AQ               1.4636374 sec
RG                   16.16
DW                 44.667 usec
DE                  7.92 usec
TE                 298.0 K
D1              2.00000000 sec
D8              0.01000000 sec
D12             0.00002000 sec
D16             0.00020000 sec
TD0                     1
ZGOPTNS       -DFLAG_BLK

======== CHANNEL f1 ========
SFO1          700.3032919 MHz
NUC1                   1H
P0                   9.82 usec
P1                   9.82 usec
PLW1         13.99600029 W
PLW9          0.00005399 W

====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPNAM[2]       SMSQ10.100
GPZ1                50.00 %
GPZ2               -10.00 %
P16               1000.00 usec

F2 - Processing parameters
SI                  16384
SF            700.2999402 MHz
WDW                    EM
SSB         0
LB          0 Hz
GB          0
PC                   4.00
```

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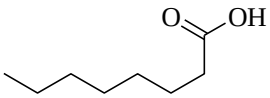
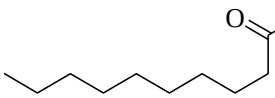
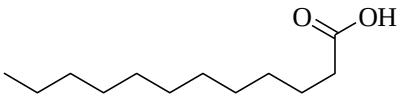
Appendix 10: Chemical Structures of Compounds Identified in Ajwa Dates using GC-MS



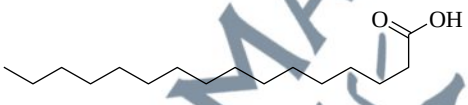
octanoic acid



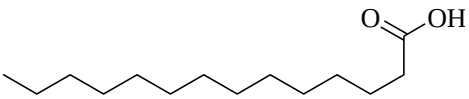
n-decanoic acid



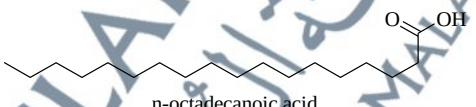
n-dodecanoic acid



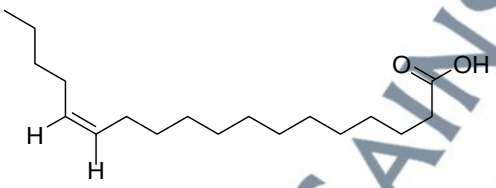
n-hexadecanoic acid



n-tetradecanoic acid

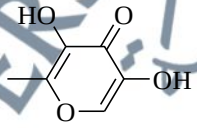


n-octadecanoic acid

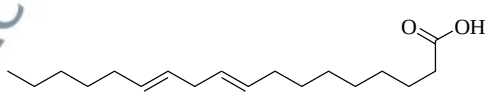


cis-13-octadecenoic acid

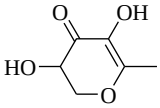
9-octadecenoic acid



3,5-dihydroxy-2-methyl-4H-pyran-4-one



9, 12-octadecadienoic acid



2,3-dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one

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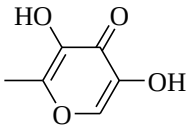
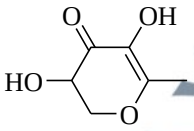
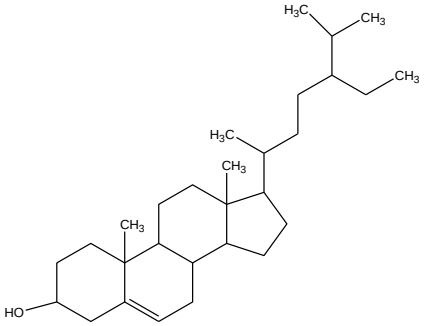


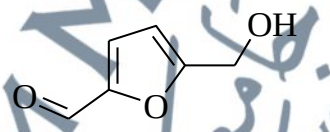
3, 5-dihydroxy-2-methyl-4H-pyran-4-one



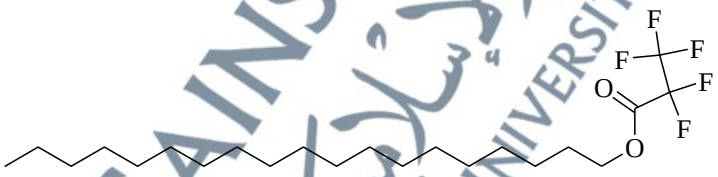
2,3-dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one



β-sitosterol



5-Hydroxymethylfulfural



nonadecyl pentafluoropropionate

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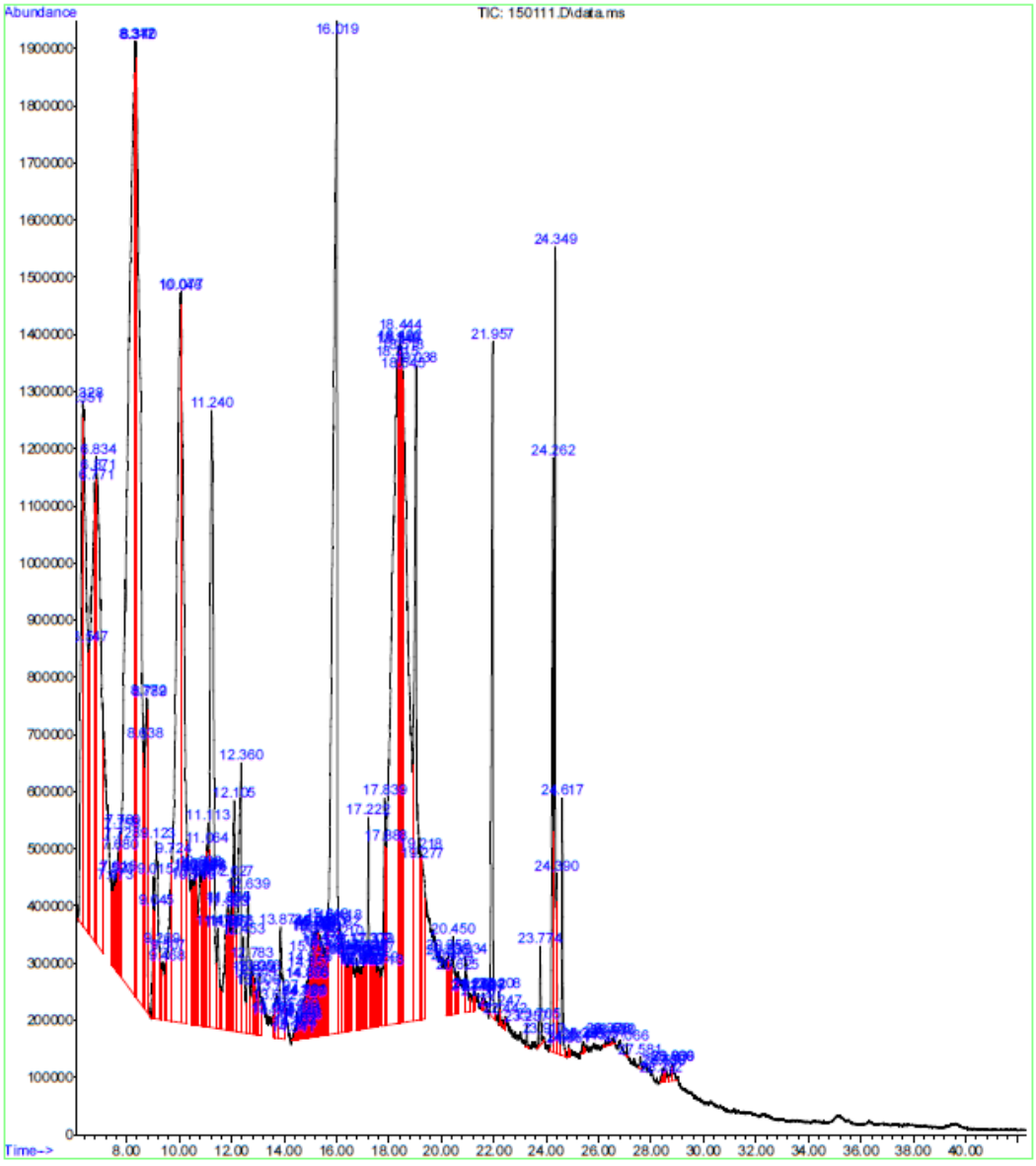
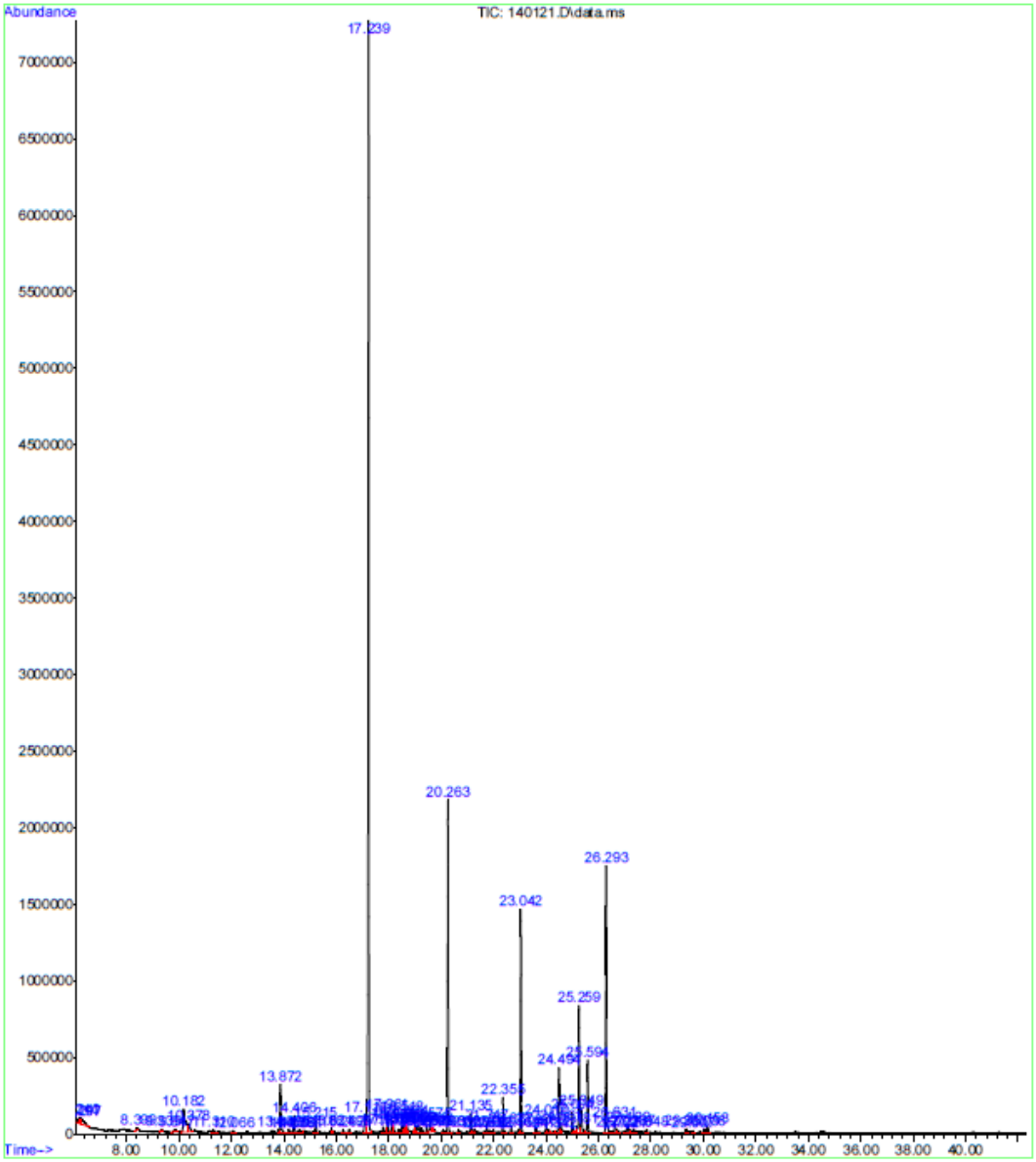
Appendix 11: GC-MS Chromatogram of Methanol Extract (D1)

```
Data Path : D:\DATA\sample 2016\
Data File : 150111.D
Acq On    : 15 Jan 2016  16:01
Operator  :
Sample    : AD1
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   C:\Database\NIST11.L              Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```



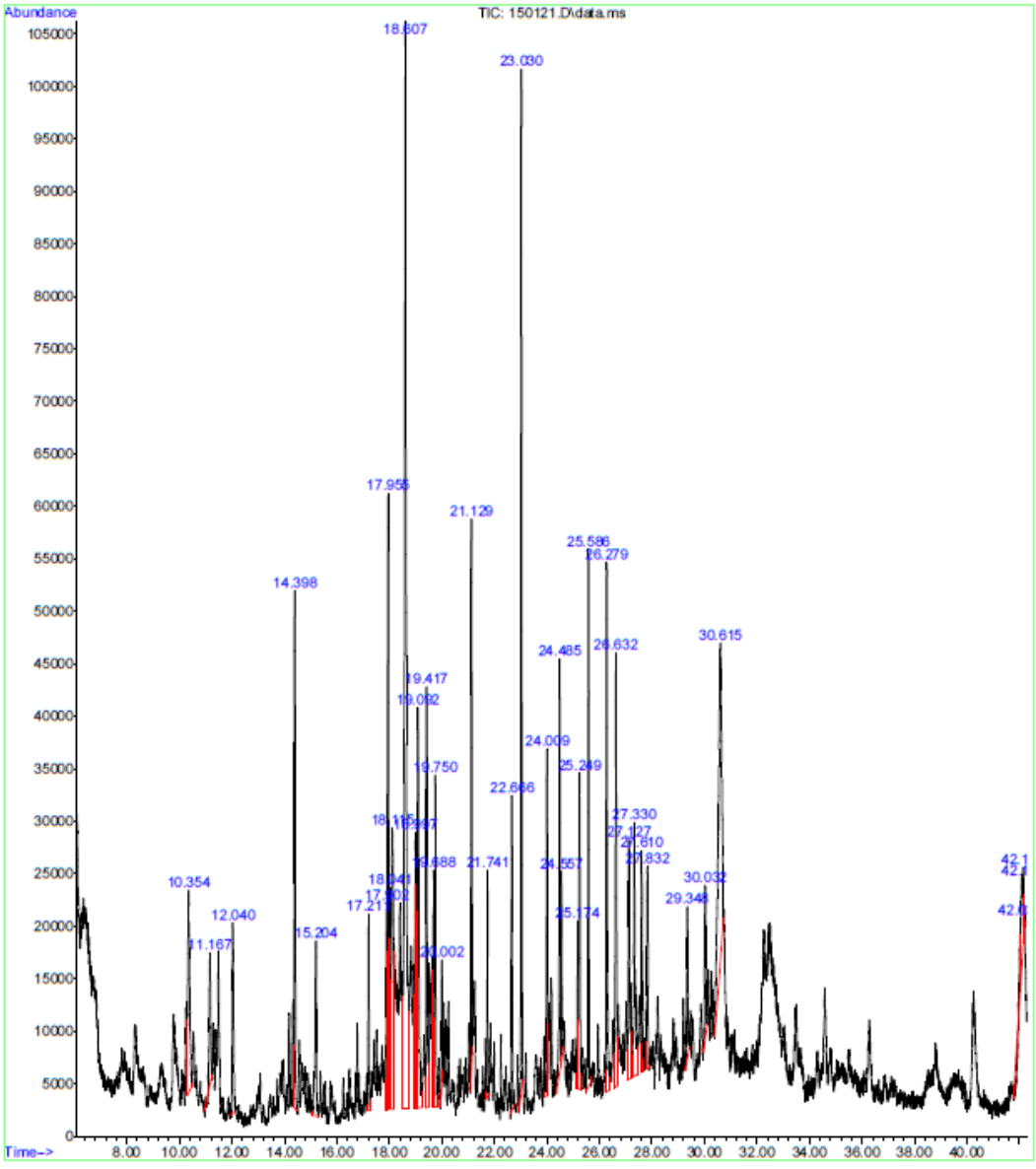
Appendix 12: GC-MS Chromatogram of Chloroform Extract (D2)

```
Data Path : D:\DATA\sample 2016\
Data File : 140121.D
Acq On    : 14 Jan 2016  14:45
Operator  :
Sample    : AD2
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   C:\Database\NIST11.L              Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```



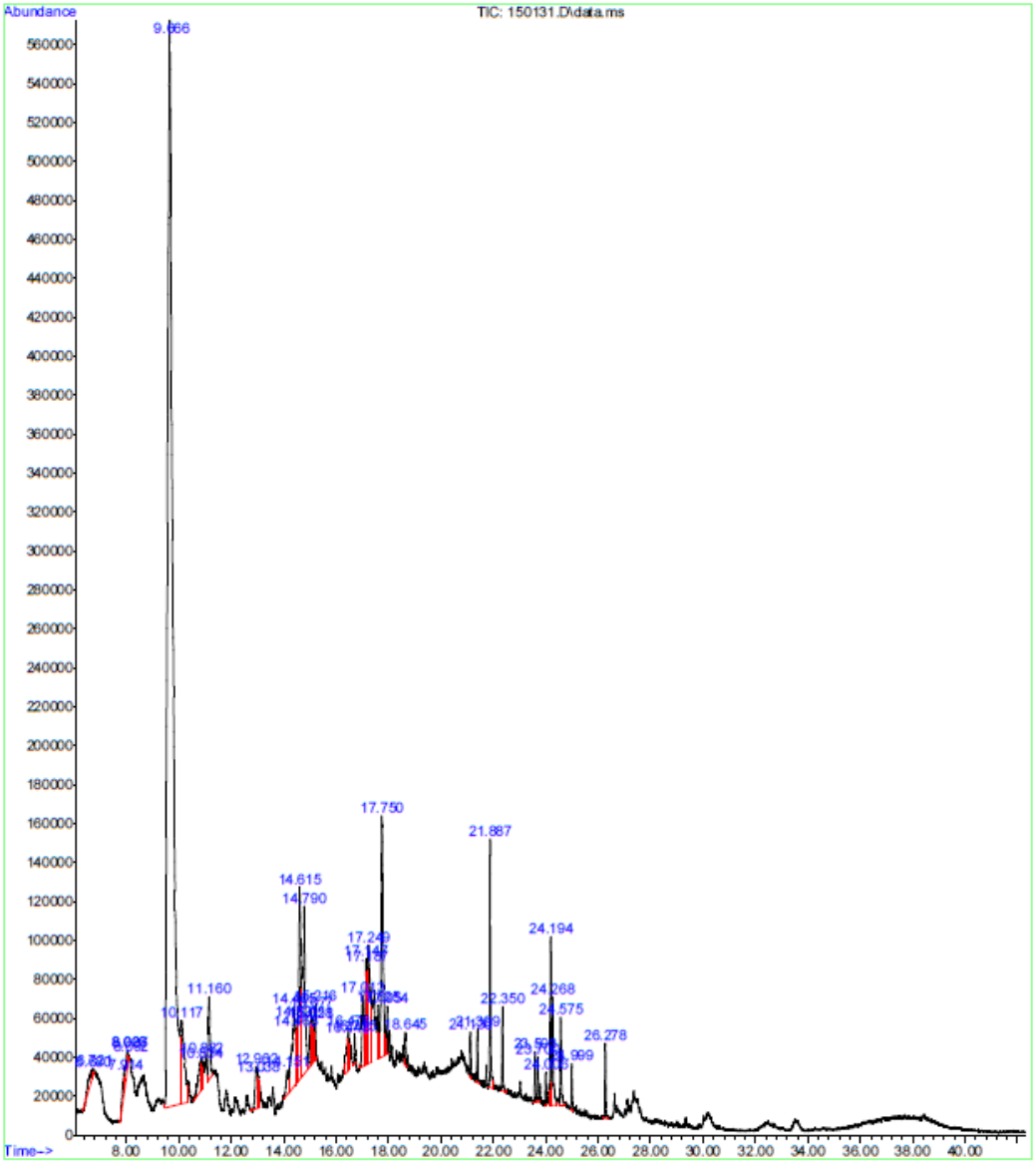
Appendix 13: GC-MS Chromatogram of Hexane Extract (D3)

```
Data Path : D:\DATA\sample 2016\
Data File : 150121.D
Acq On    : 15 Jan 2016  16:45
Operator  :
Sample    : AD3
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   C:\Database\NIST11.L              Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```



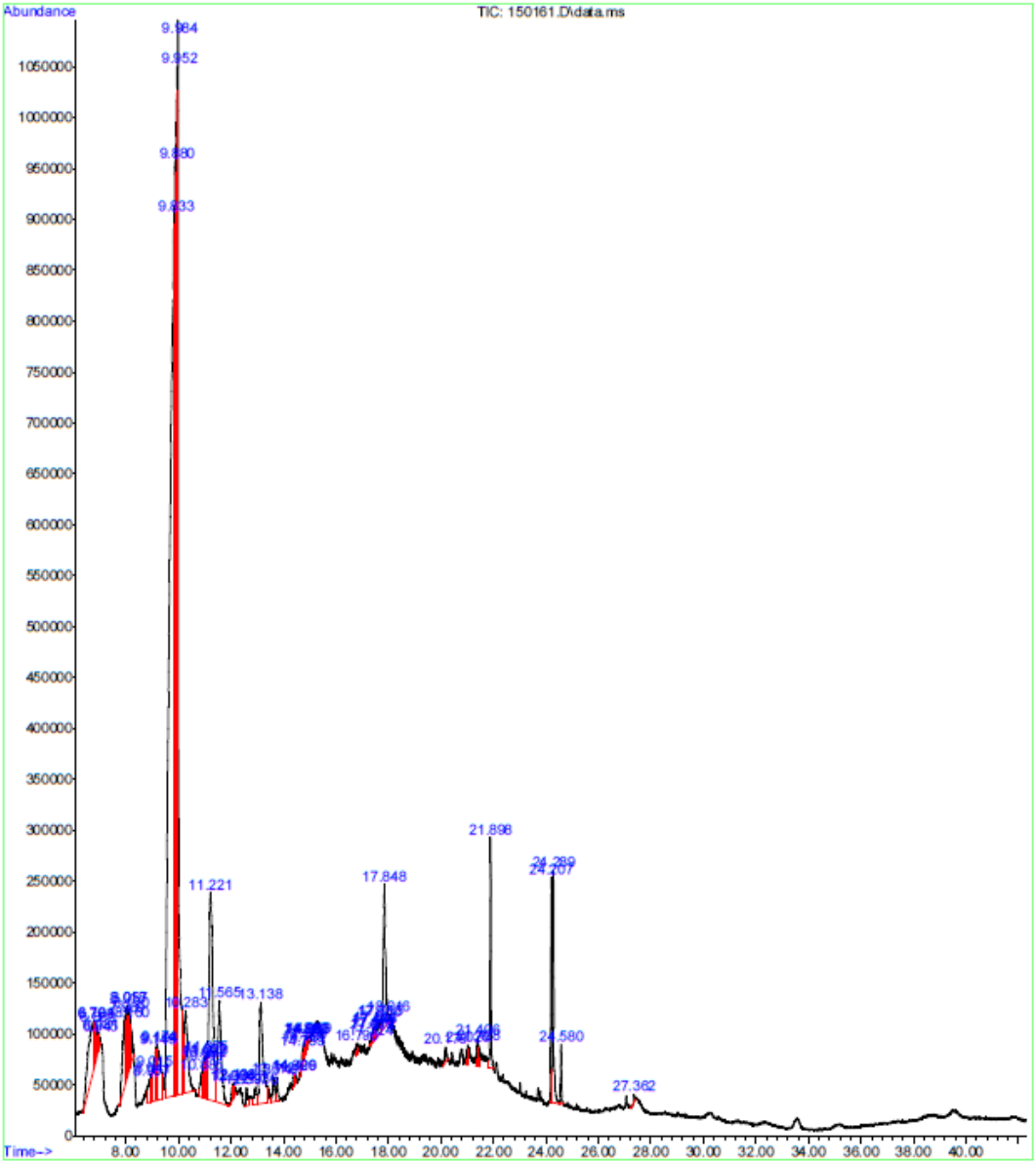
Appendix 14: GC-MS Chromatogram of Methanol: Chloroform Extract (D4)

```
Data Path : D:\DATA\sample 2016\
Data File : 150131.D
Acq On    : 19 Jan 2016    8:58
Operator  :
Sample    : AD4
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   C:\Database\NIST11.L              Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```



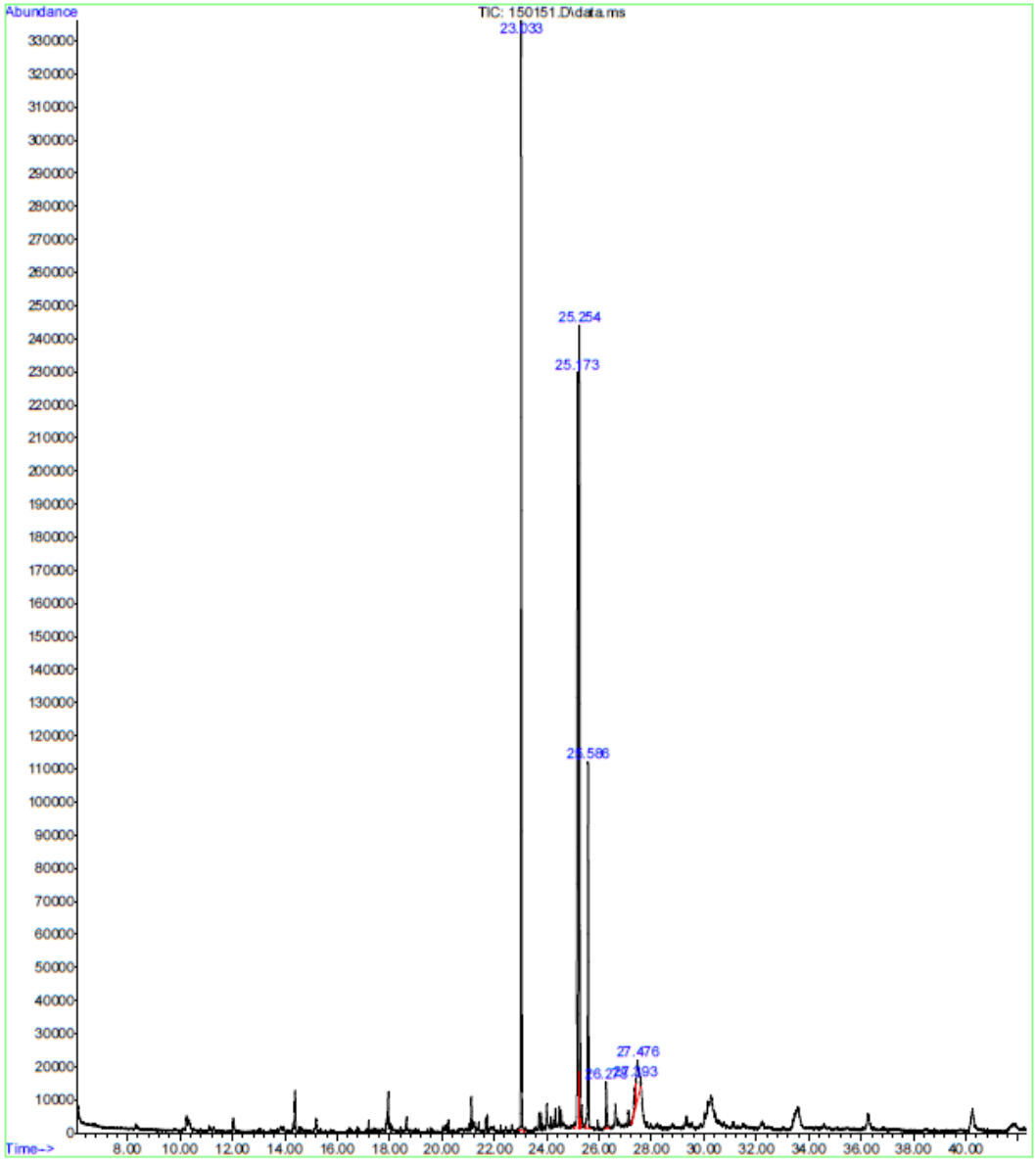
Appendix 15: GC-MS Chromatogram of Methanol: Hexane Extract (D5M)

```
Data Path : D:\DATA\sample 2016\
Data File : 150161.D
Acq On    : 19 Jan 2016  11:11
Operator  :
Sample    : AD5M
Misc      :
ALS Vial  : 6   Sample Multiplier: 1

Search Libraries:   C:\Database\NIST11.L              Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```



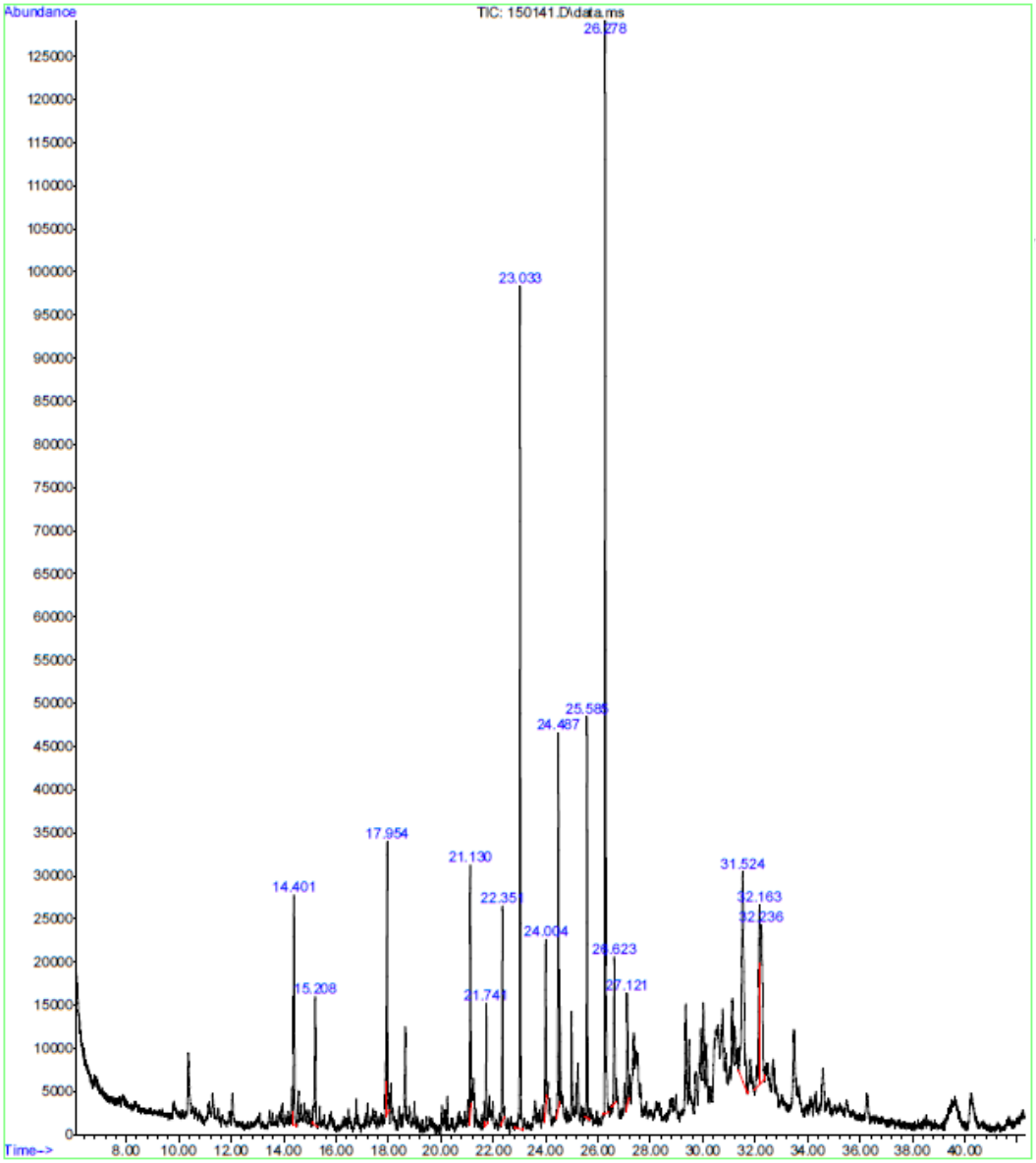
Appendix 16: GC-MS Chromatogram of Methanol: Hexane Extract (D5H)

```
Data Path : D:\DATA\sample 2016\
Data File : 150151.D
Acq On    : 19 Jan 2016  10:27
Operator  :
Sample    : SD5H
Misc      :
ALS Vial  : 5   Sample Multiplier: 1

Search Libraries:   C:\Database\NIST11.L              Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```



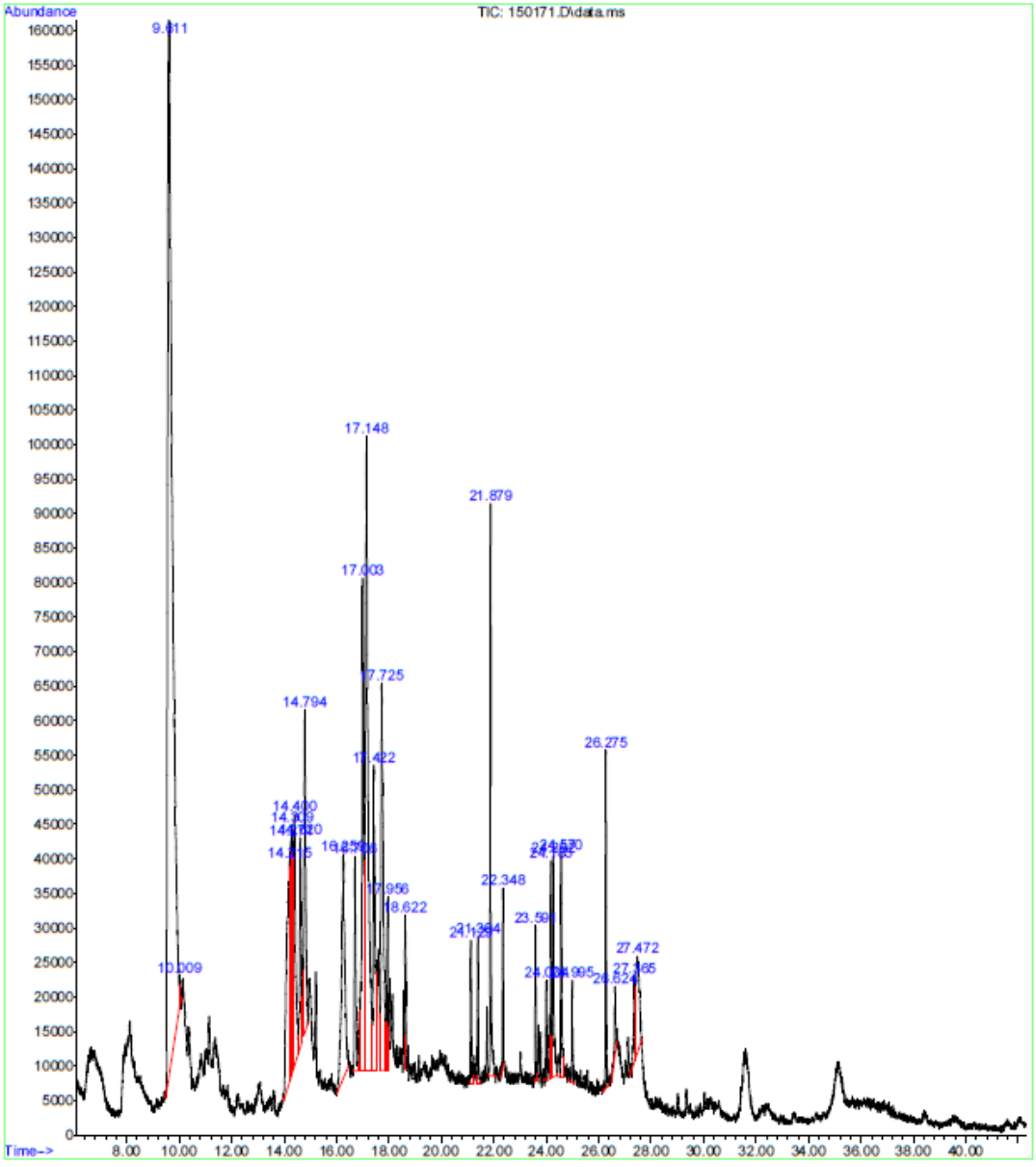
Appendix 17: GC-MS Chromatogram of Chloroform: Hexane Extract (D6)

```
Data Path : D:\DATA\sample 2016\
Data File : 150141.D
Acq On    : 19 Jan 2016    9:42
Operator  :
Sample    : AD6
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   C:\Database\NIST11.L              Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```

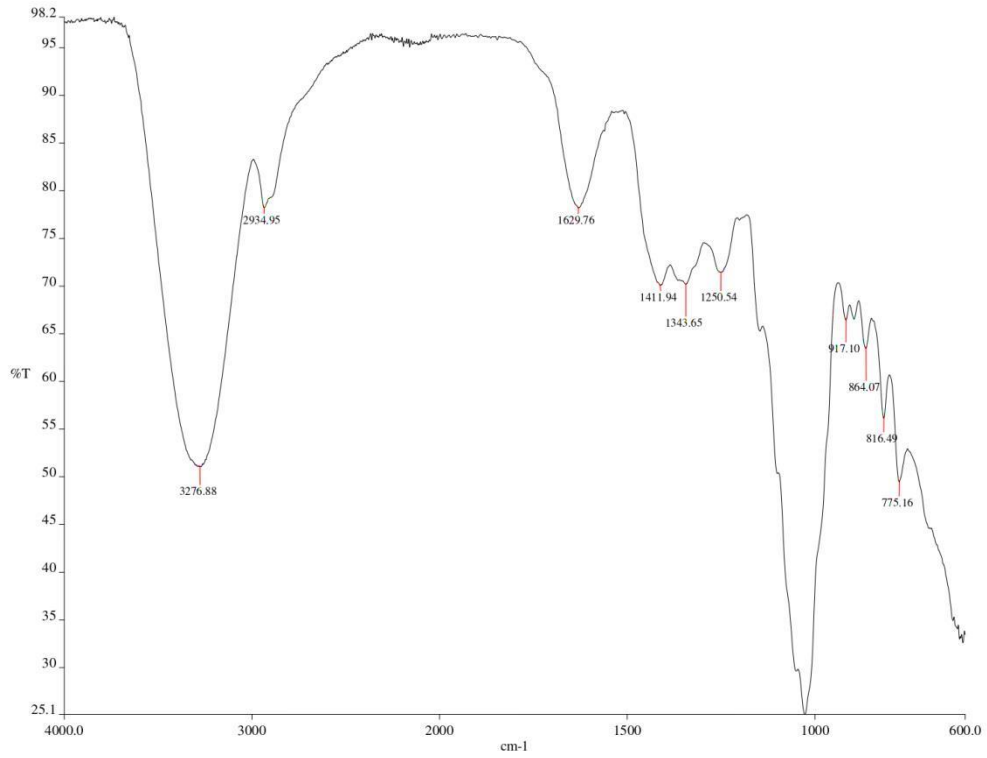


Appendix 18: GC-MS Chromatogram of Methanol: Chloroform: Hexane Extract (D7)

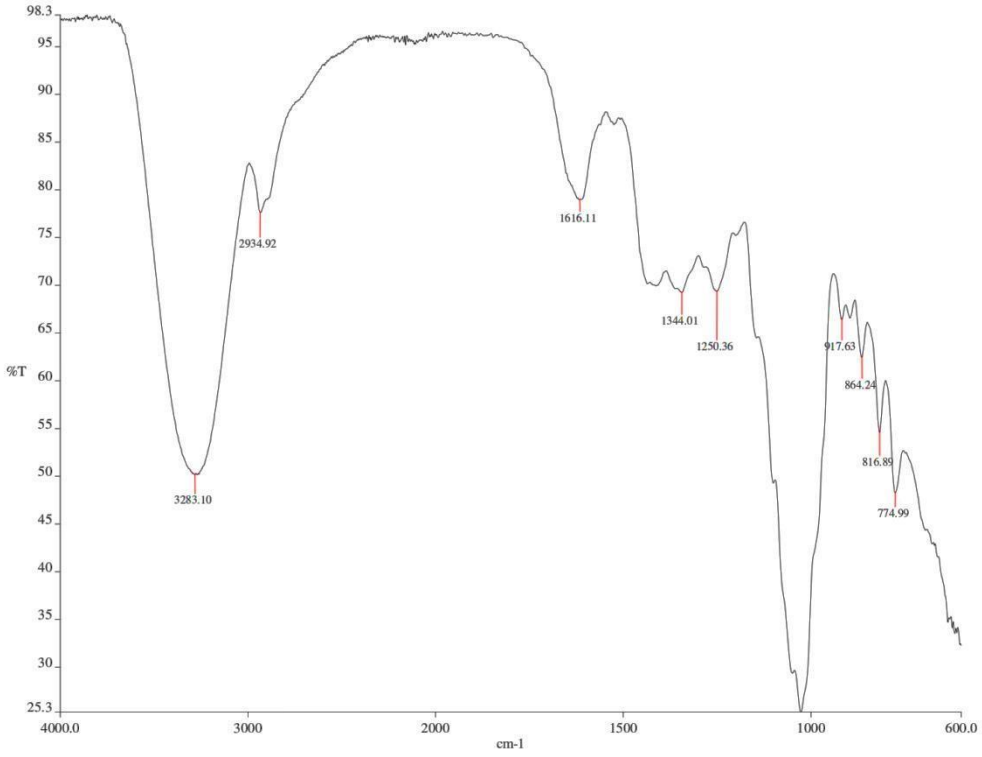
```
Data Path : D:\DATA\sample 2016\
Data File : 150171.D
Acq On    : 19 Jan 2016  11:56
Operator  :
Sample    : AD7
Misc      :
ALS Vial  : 7   Sample Multiplier: 1

Search Libraries:   C:\Database\NIST11.L            Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```



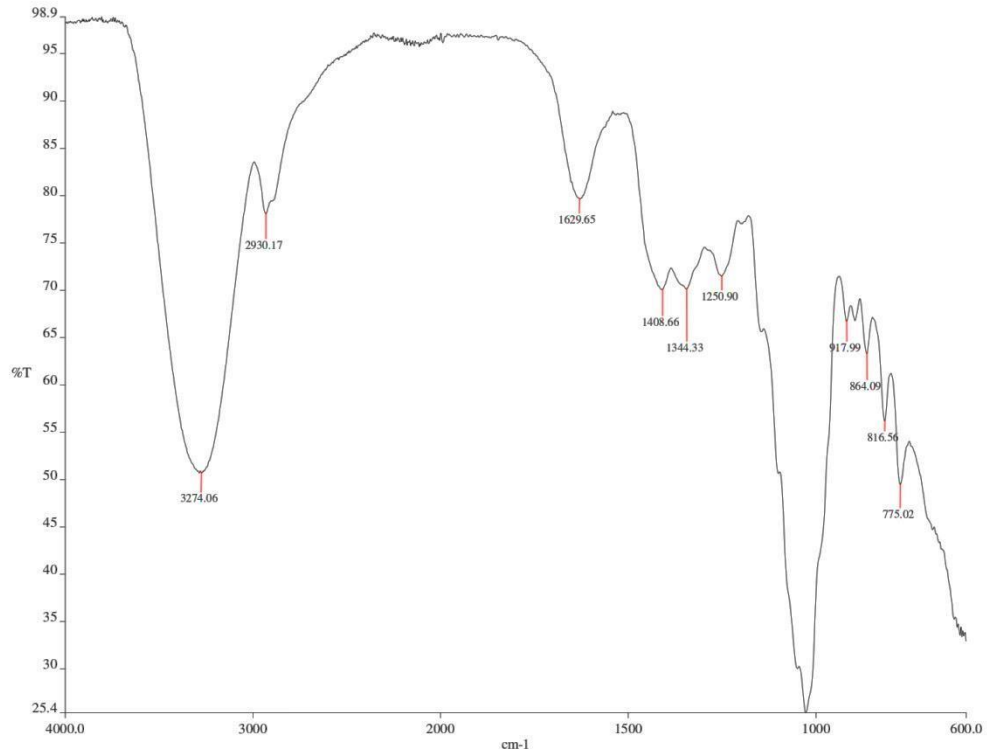
Appendix 19: FTIR Spectra for Ajwa Dates from K1 to K10 (a to j)



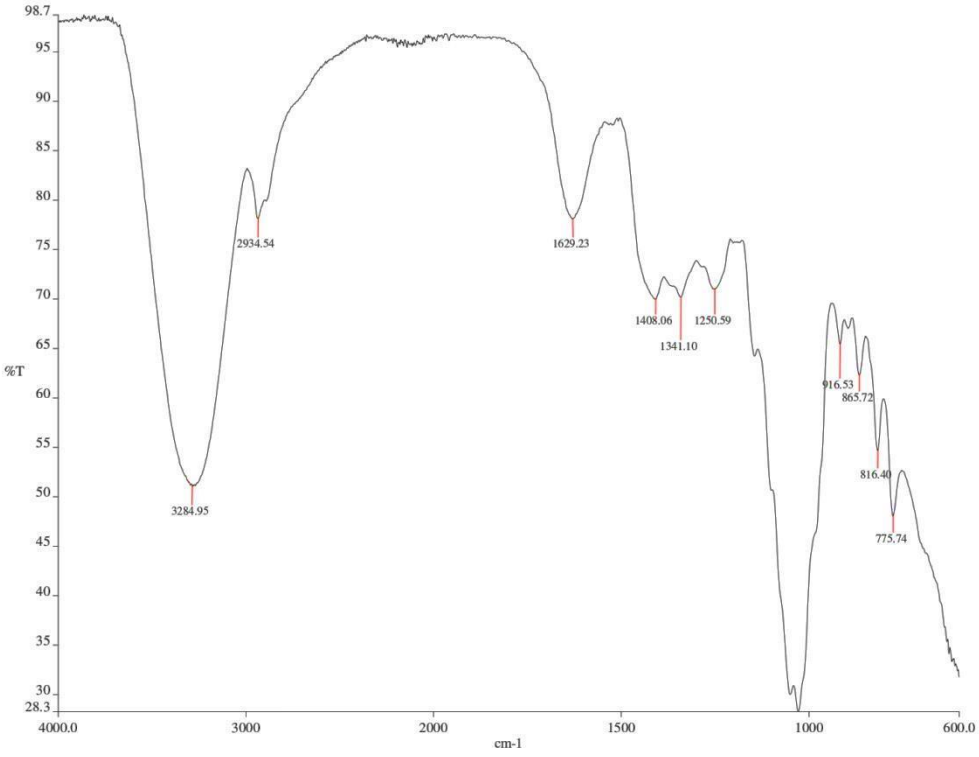
Appendix 19 a): FTIR Spectrum of K1



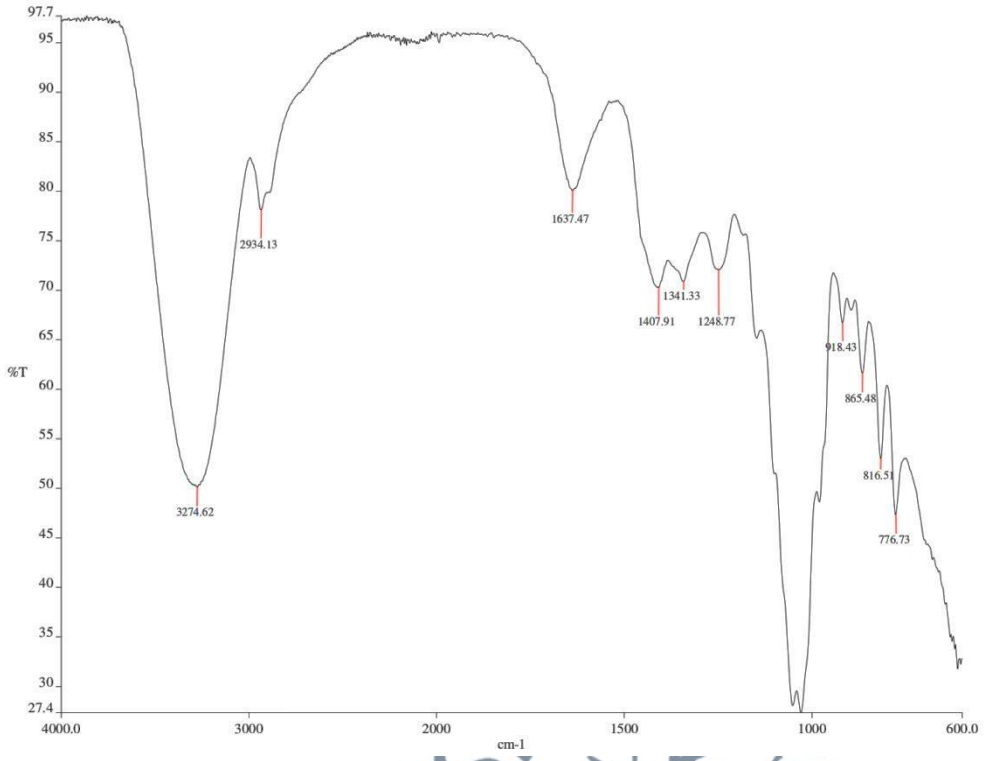
Appendix 19 b): FTIR Spectrum of K2



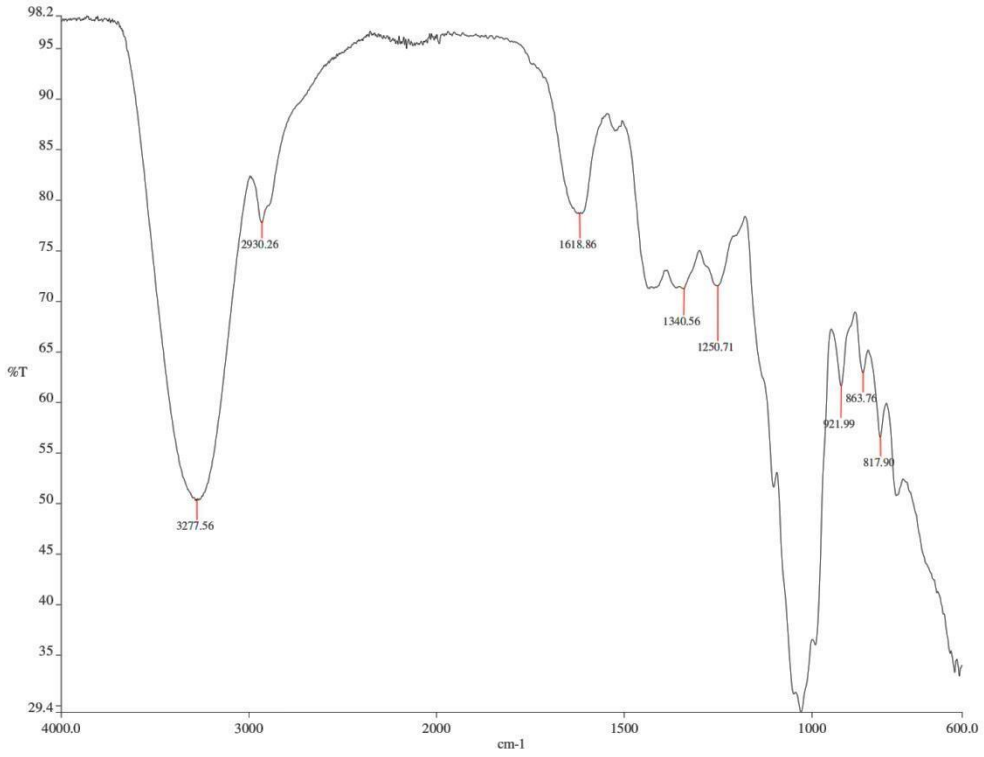
Appendix 19 c): FTIR Spectrum of K3



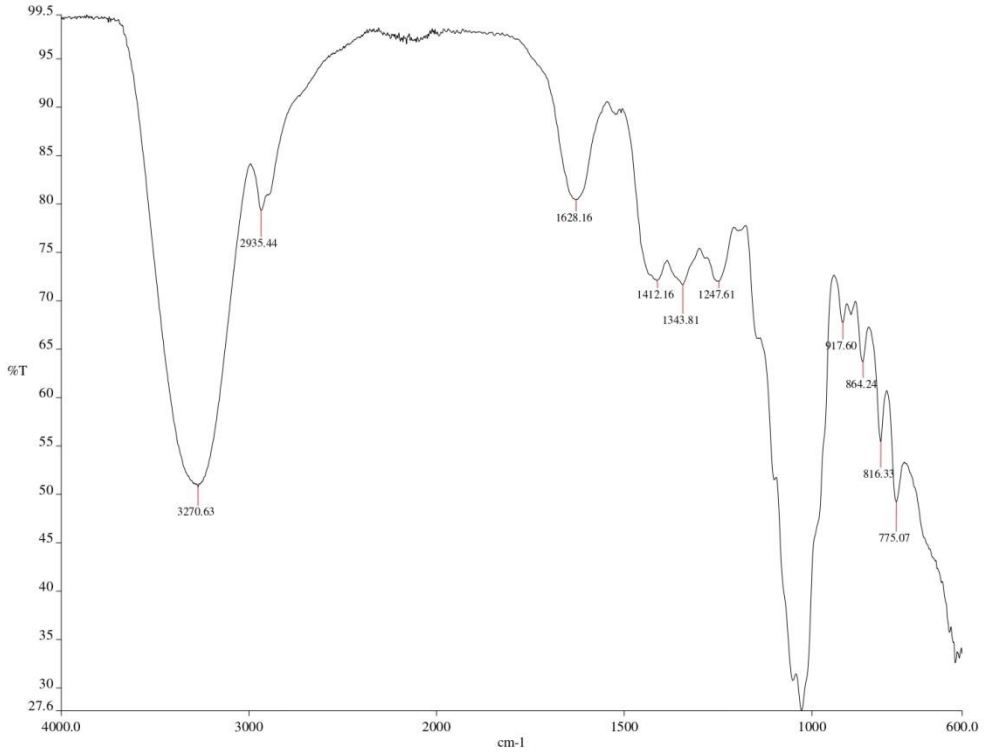
Appendix 19 d): FTIR Spectrum of K4



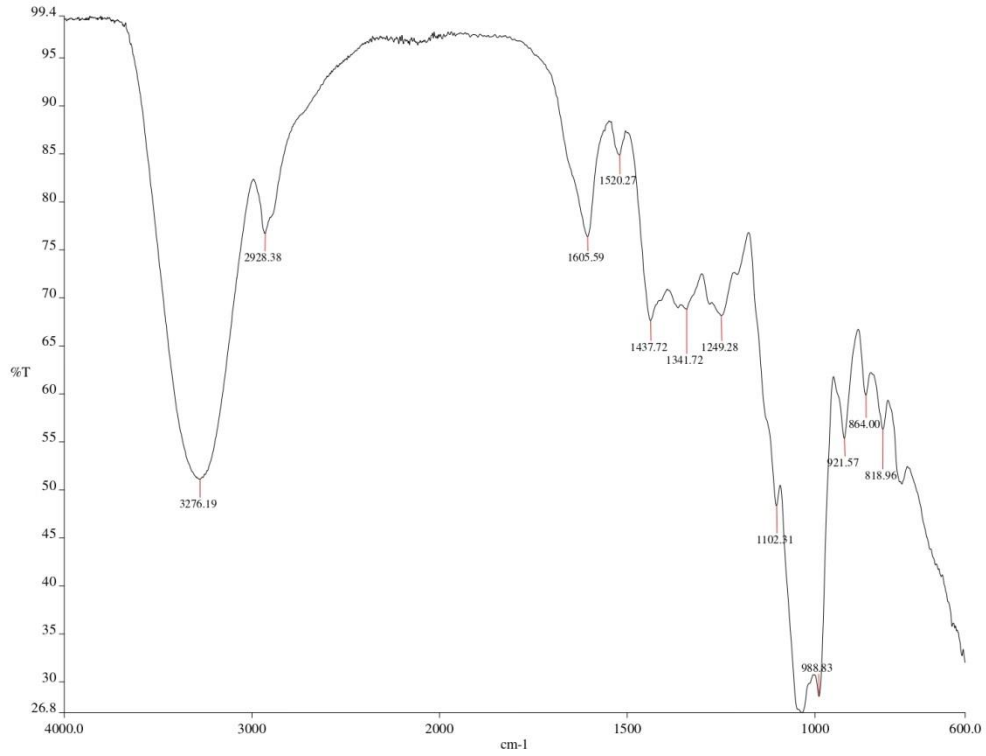
Appendix 19 e): FTIR Spectrum of K5



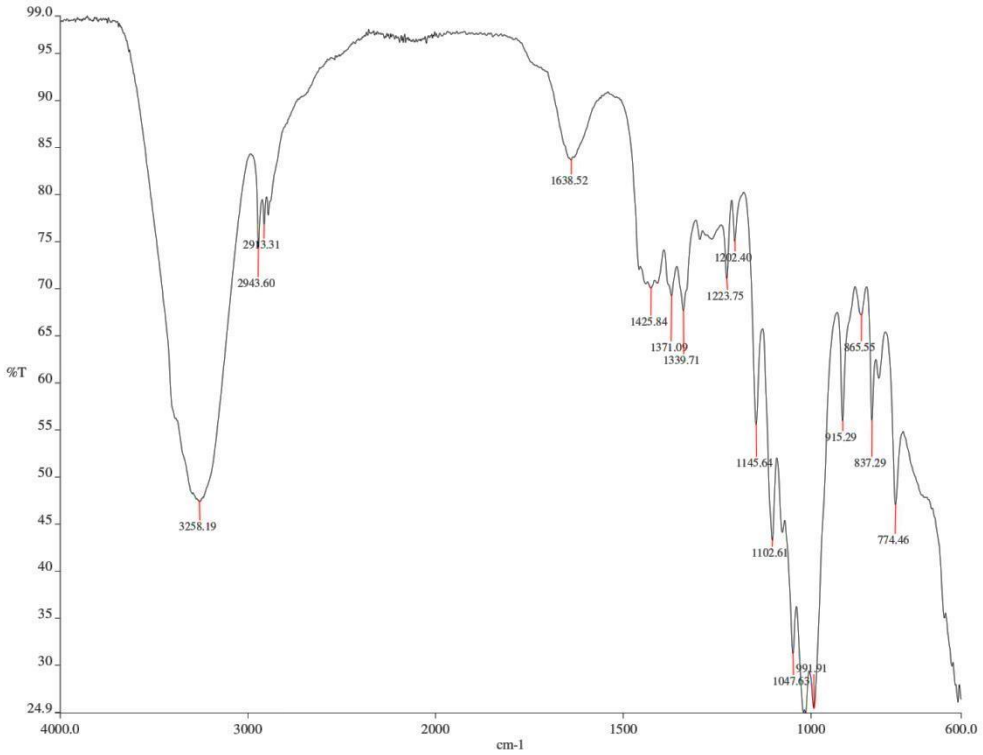
Appendix 19 f): FTIR Spectrum of K6



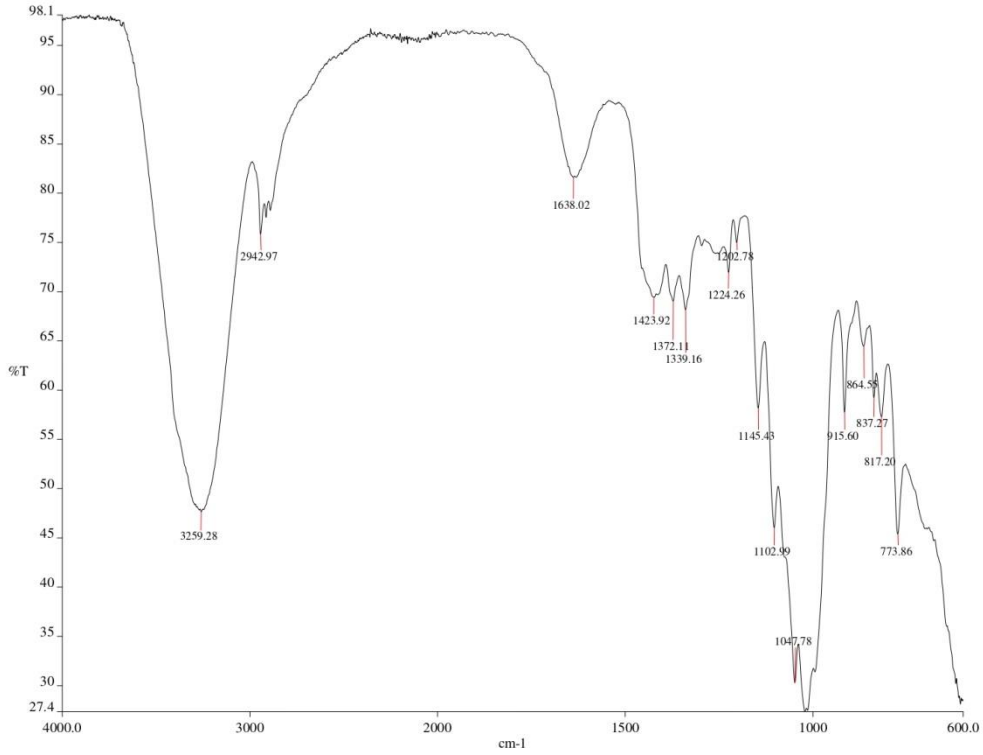
Appendix 19 g): FTIR Spectrum of K7



Appendix 19 h): FTIR Spectrum of K8

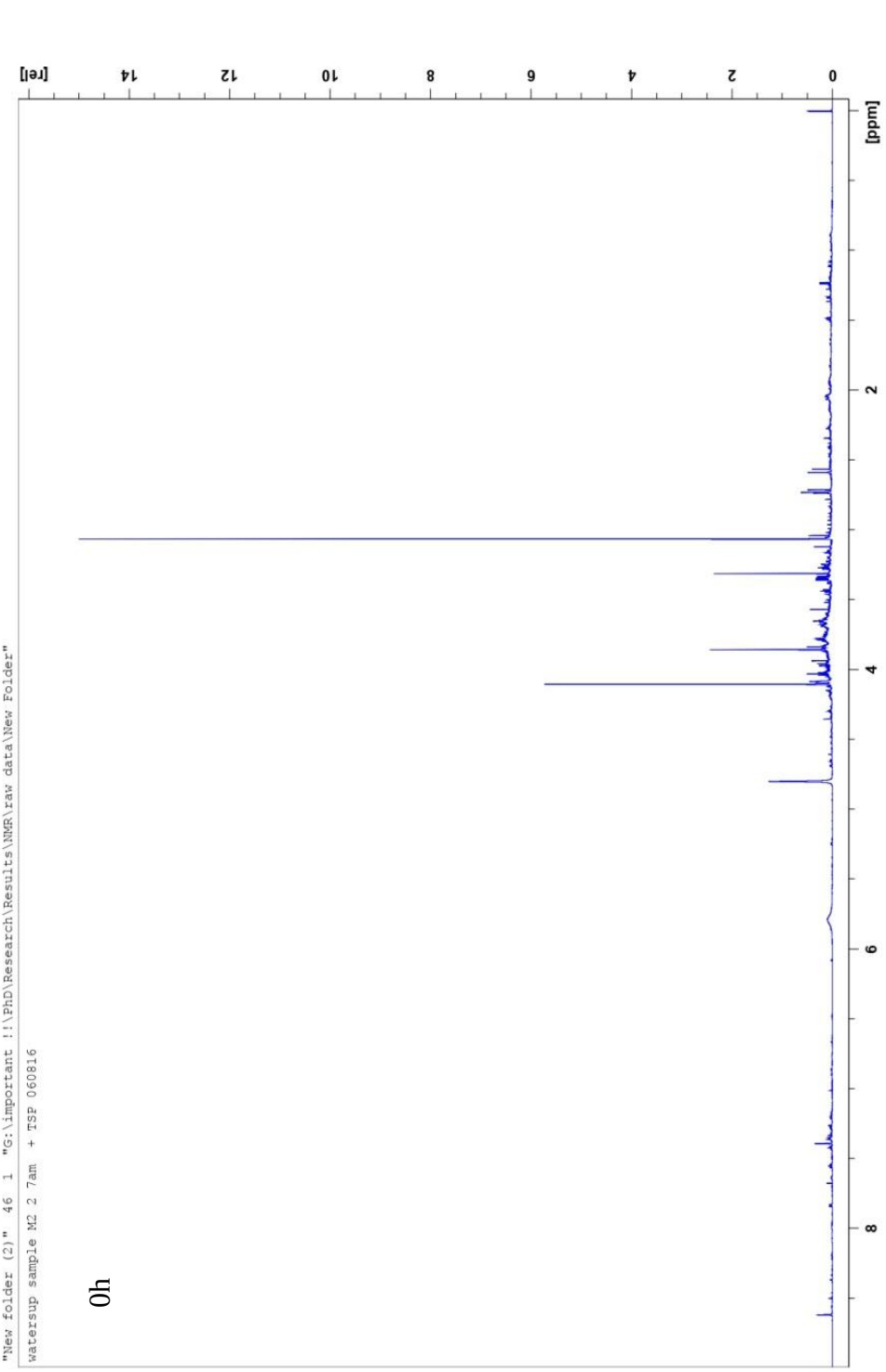


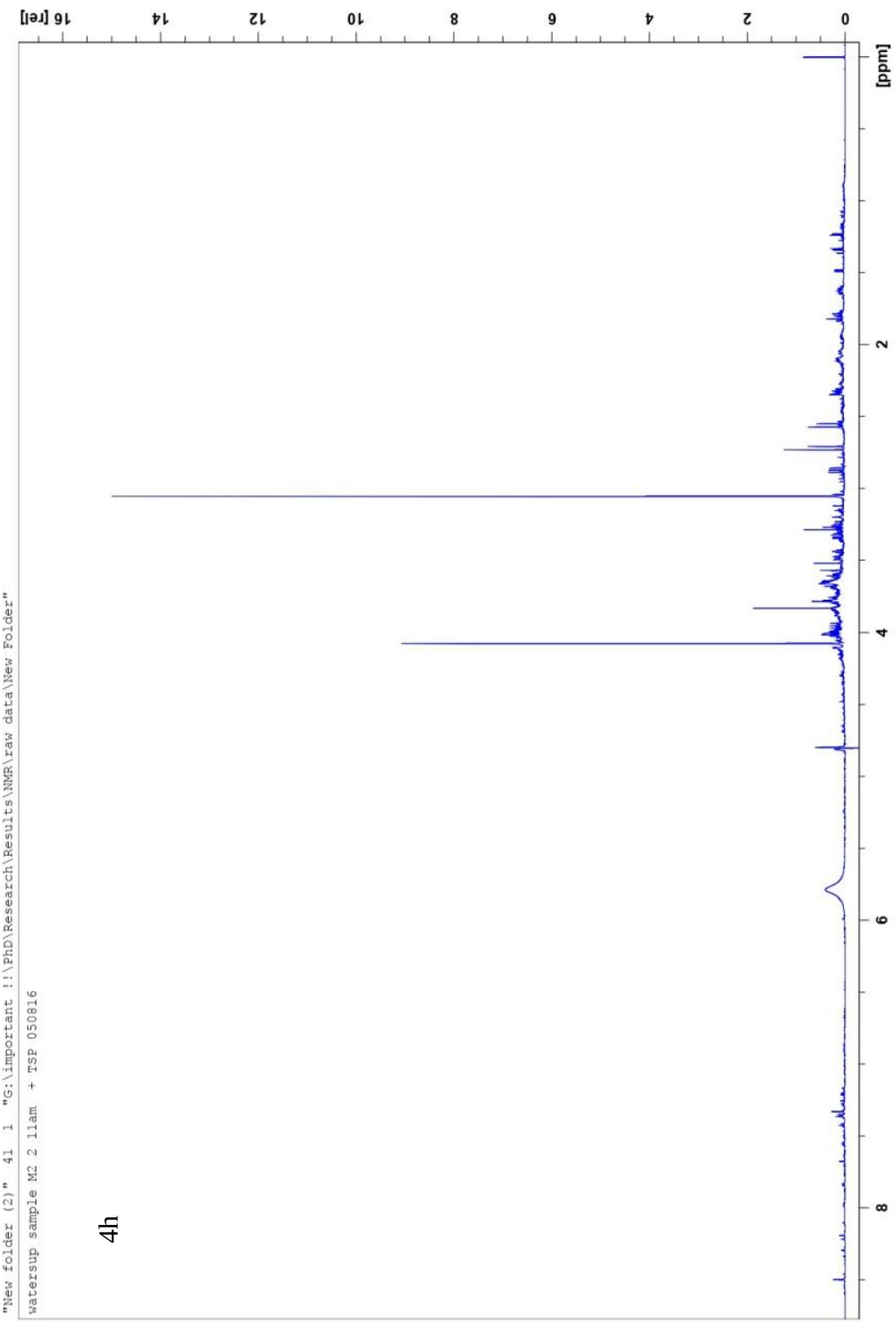
Appendix 19 i): FTIR Spectrum of K9

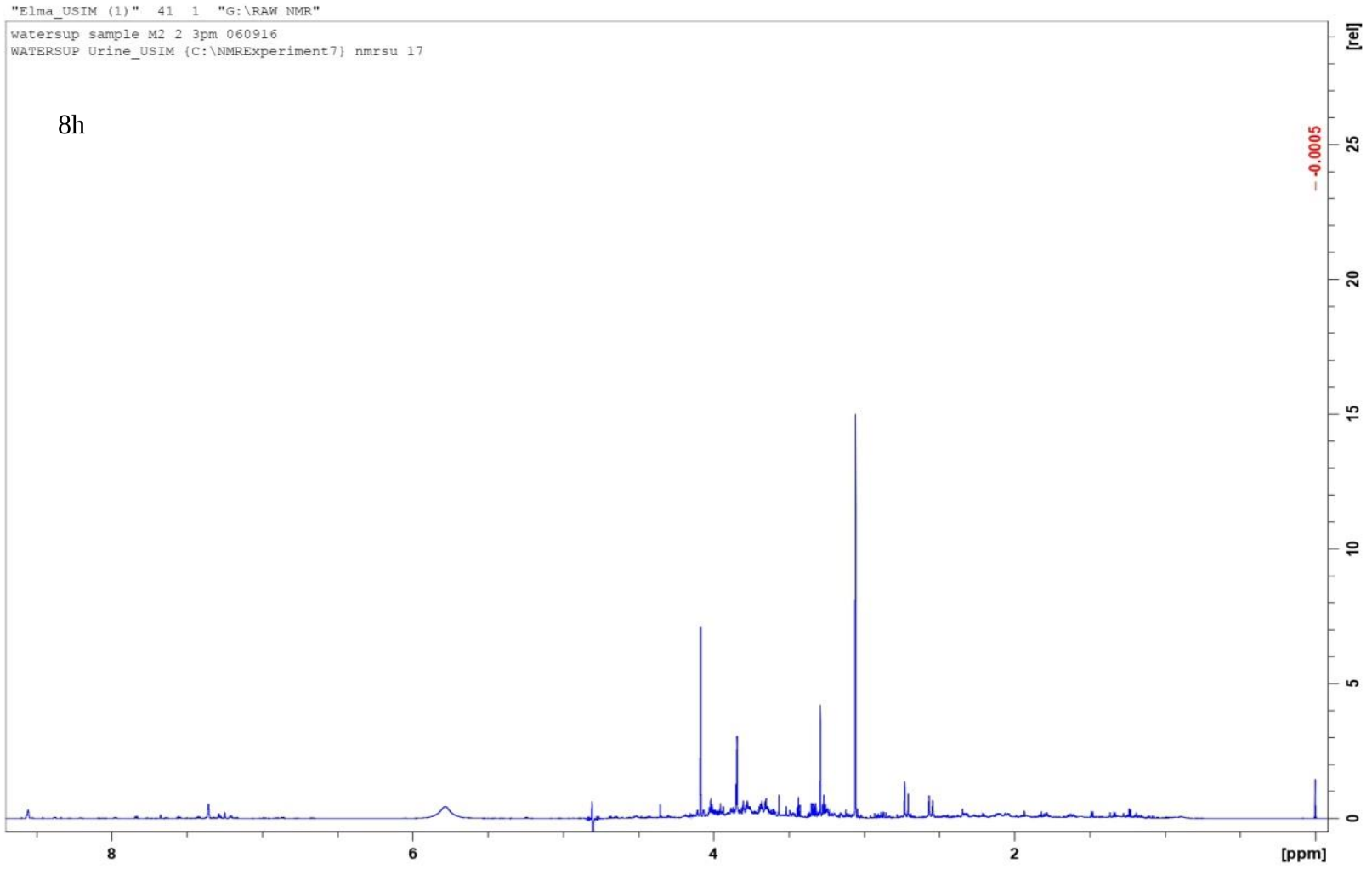


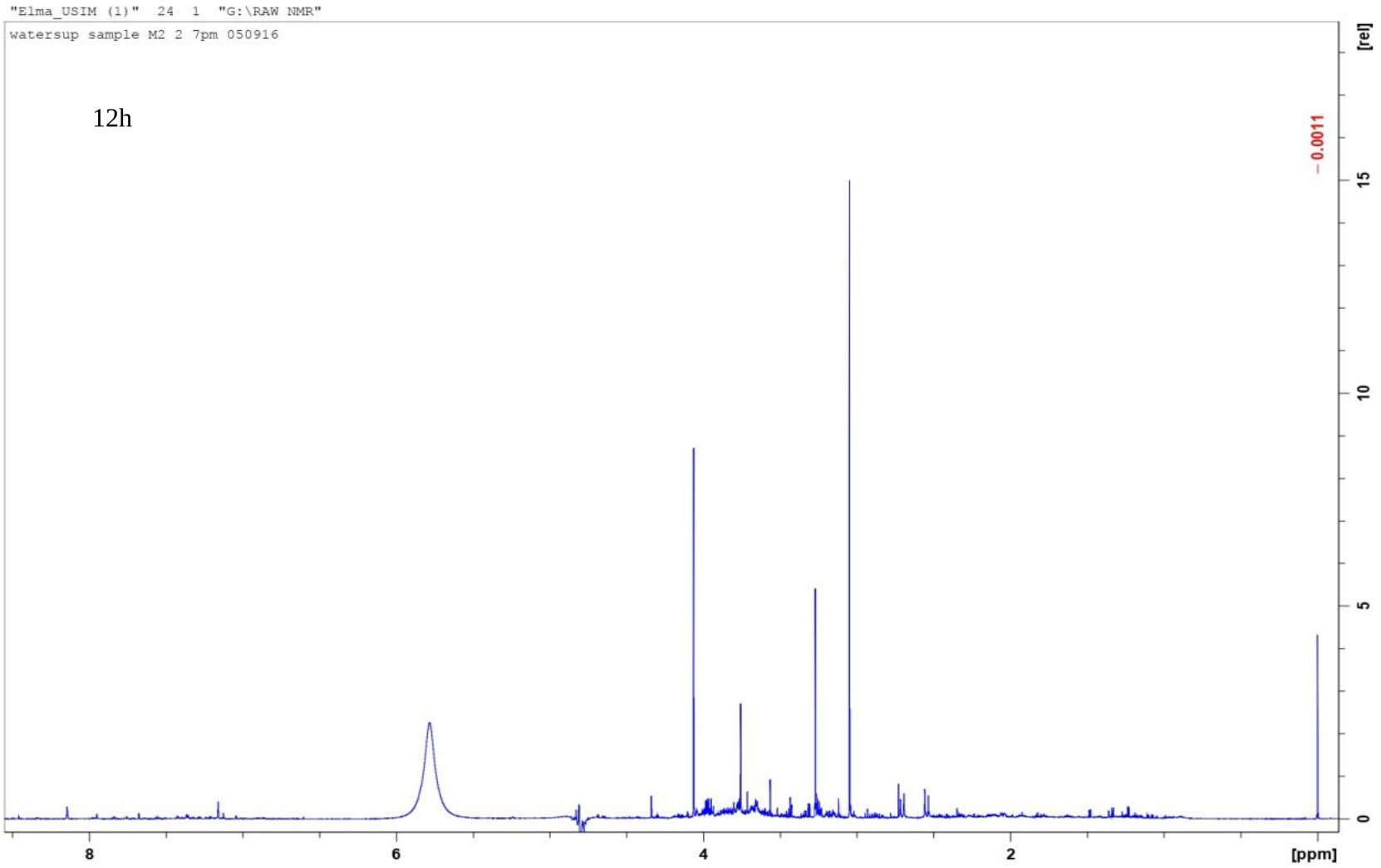
Appendix 19 j): FTIR Spectrum of K10

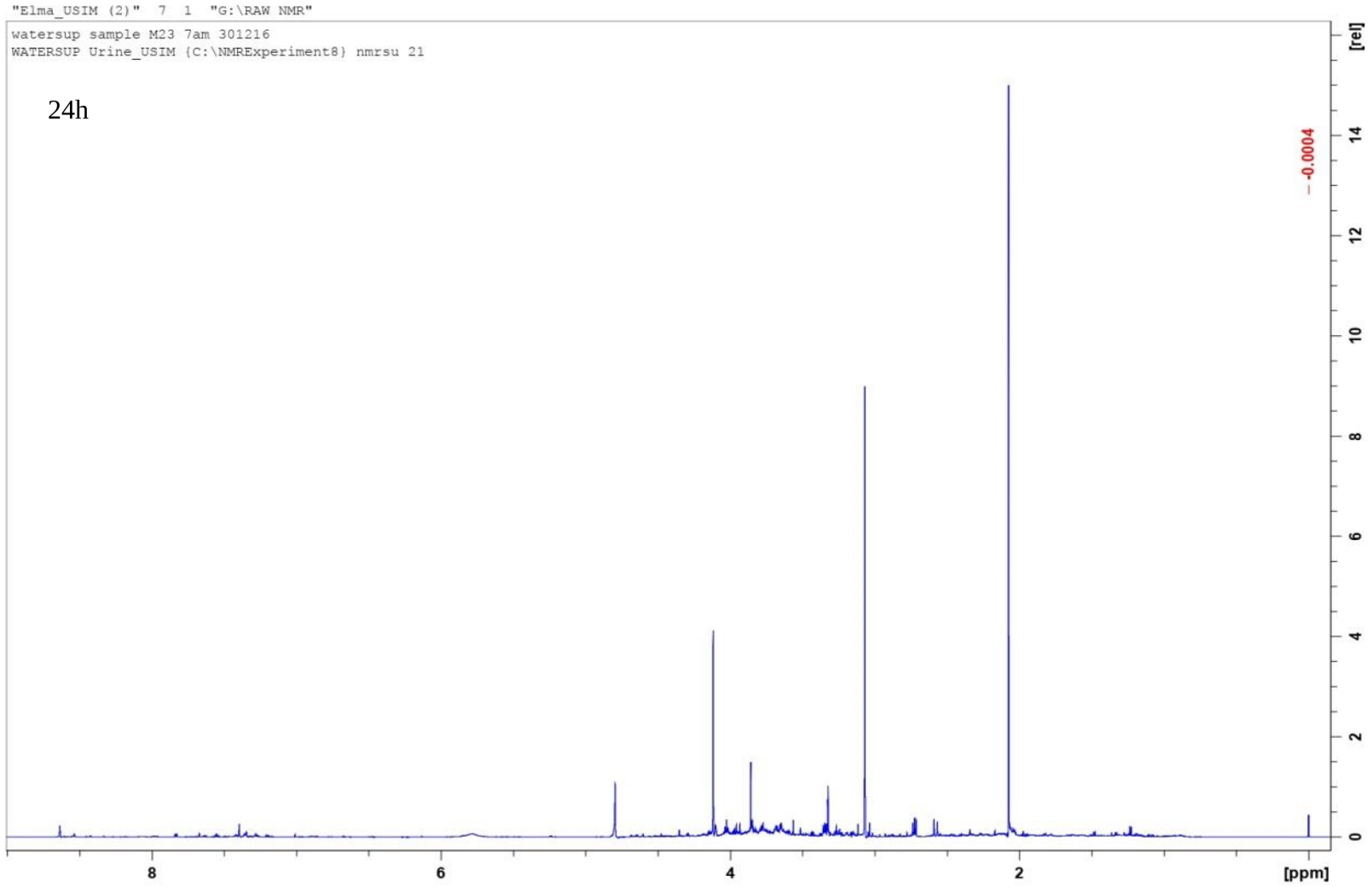
Appendix 20: ^{1}H-NMR Spectra from 0h to 60h

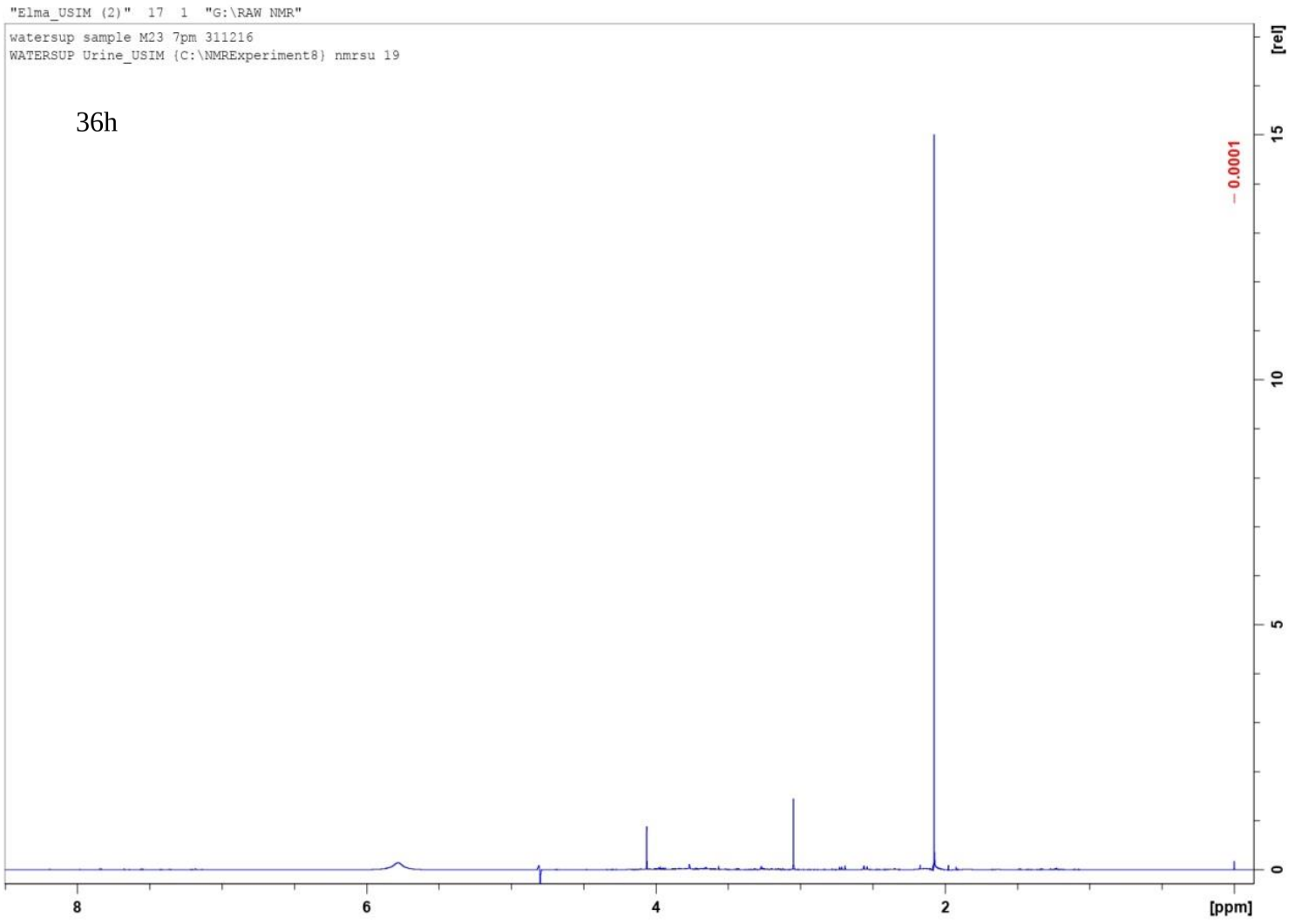



"New folder (2)" 41 1 "G:\important !!\PhD\Research\Results\NMR\raw data\New Folder"
watersup sample M2 2 11am + TSP 050816
4h
[rel]
16
14
12
10
8
6
4
2
0
[ppm]
8
6
4
2


"Elma_USIM (1)" 41 1 "G:\RAW NMR"
watersup sample M2 2 3pm 060916
WATERSUP Urine_USIM {C:\NMRExperiment7} nmrsu 17
8h
-0.0005
[rel]
25
20
15
10
5
0
8
6
4
2
[ppm]


"Elma_USIM (1)" 24 1 "G:\RAW NMR"
watersup sample M2 2 7pm 050916
12h
0.0011
[rel]
15
10
5
0
8
6
4
2
[ppm]


"Elma_USIM (2)" 7 1 "G:\RAW NMR"
watersup sample M23 7am 301216
WATERSUP Urine_USIM {C:\NMRExperiment8} nmrsu 21
24h
-0.0004
[rel]
14
12
10
8
6
4
2
0
8
6
4
2
[ppm]


"Elma_USIM (2)" 17 1 "G:\RAW NMR"
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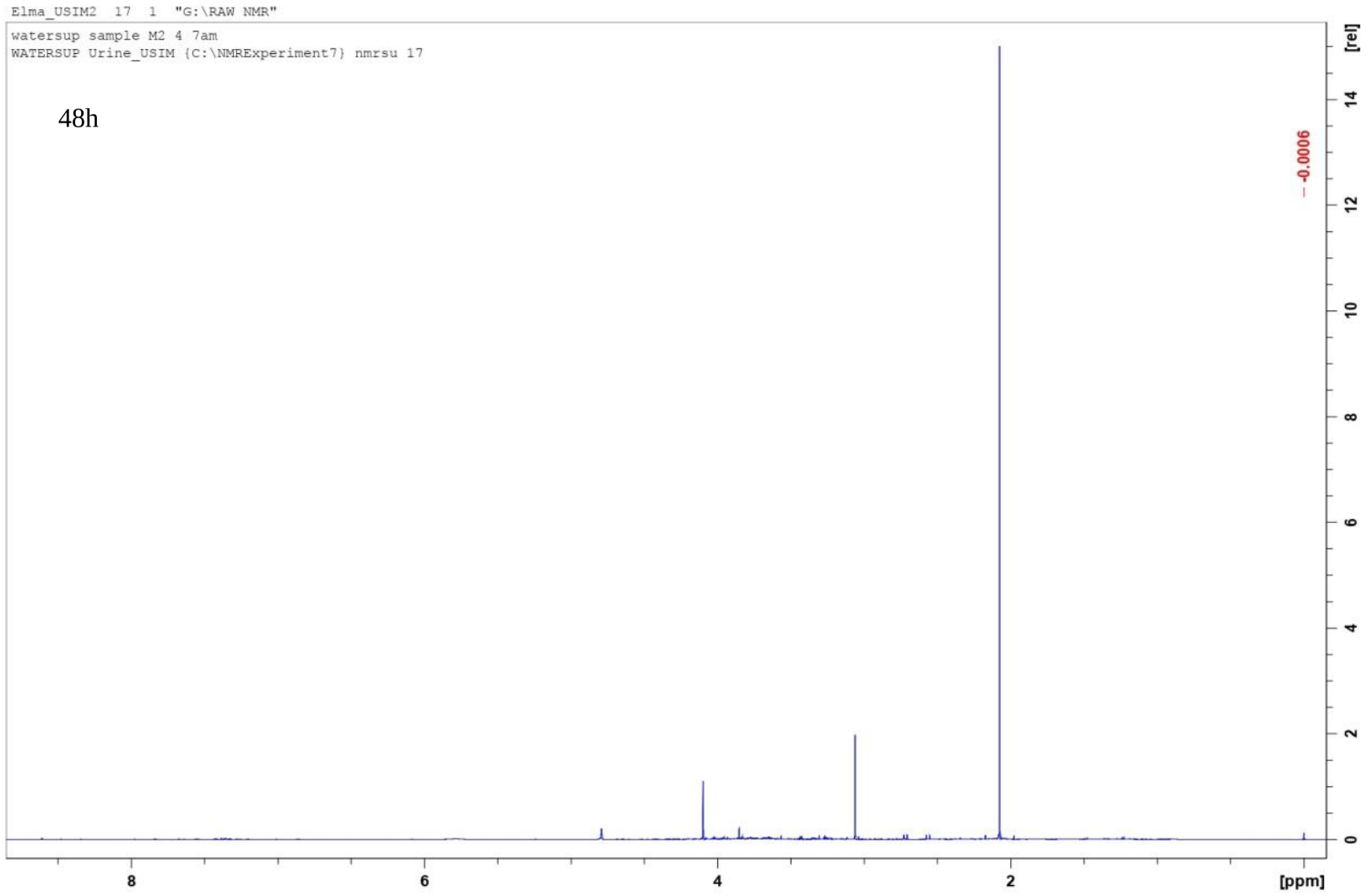
WATERSUP Urine_USIM {C:\NMRExperiment8} nmrsu 19
36h
0.0001
[rel]
15
10
5
0
8
6
4
2
[ppm]


Elma_USIM2 17 1 "G:\RAW NMR"
watersup sample M2 4 7am
WATERSUP Urine_USIM {C:\NMRExperiment7} nmrsu 17
48h
-0.0006
[rel]
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2
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6
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10
12
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4
2
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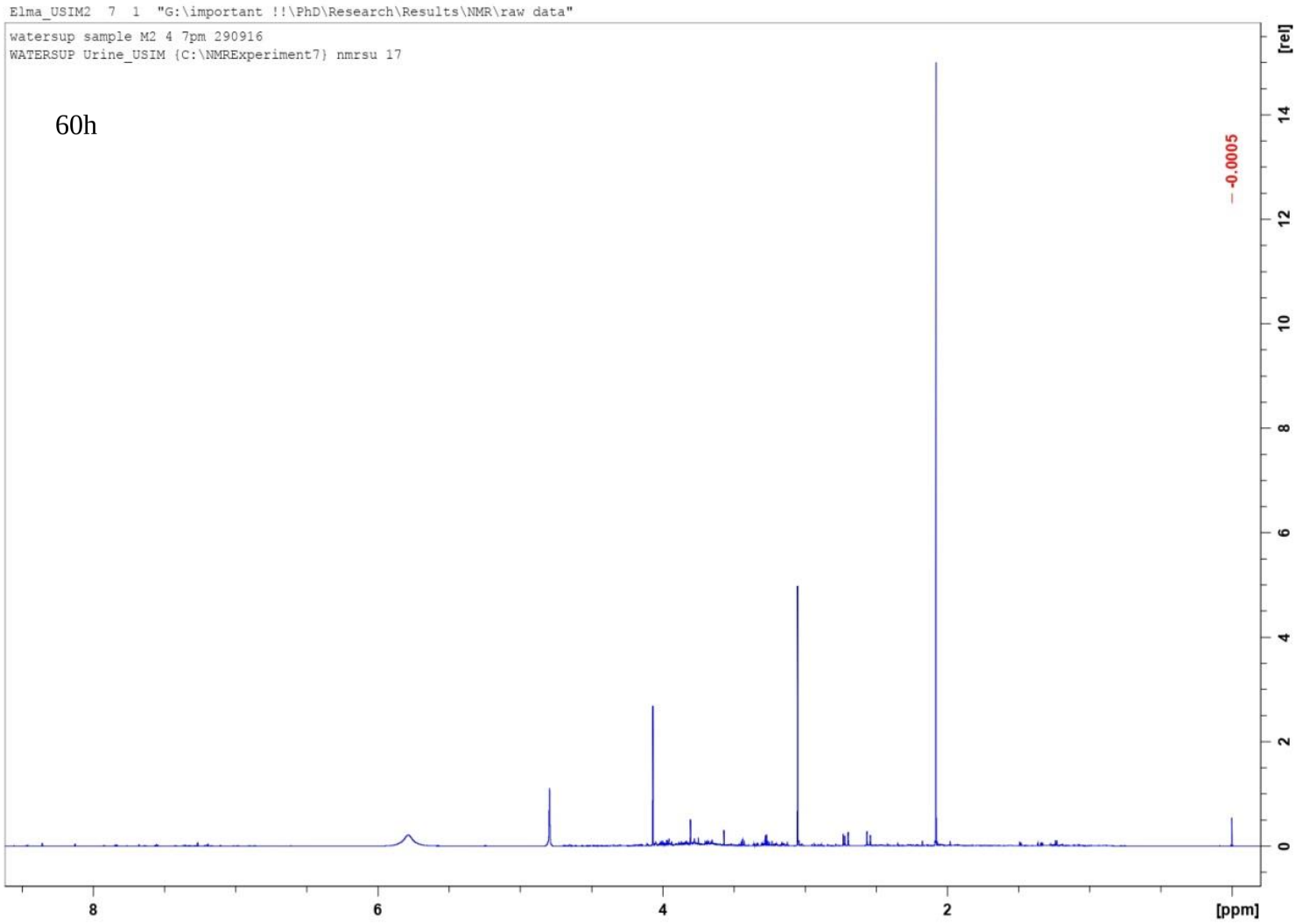
Elma_USIM2 7 1 "G:\important !!\PhD\Research\Results\NMR\raw data"
watersup sample M2 4 7pm 290916
WATERSUP Urine_USIM {C:\NMRExperiment7} nmrsu 17
60h
-0.0005
[rel]
14
12
10
8
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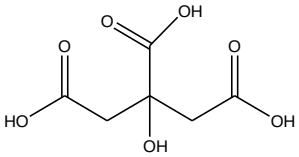
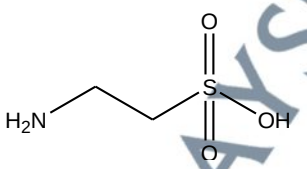
4
2
0
8
6
4
2
[ppm]

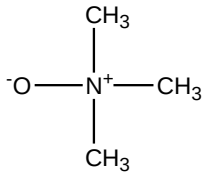
Appendix 21: Chemical Structures of Metabolites Identified in Urine using ^{1}H-NMR



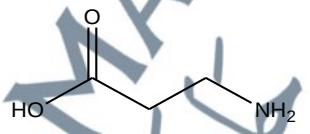
Citrate



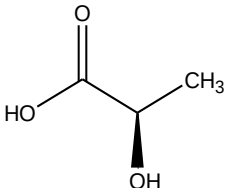
Taurine



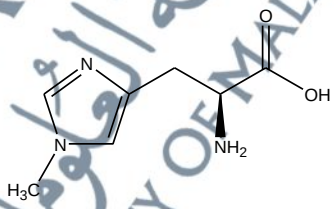
Trimethylamine-N-Oxide



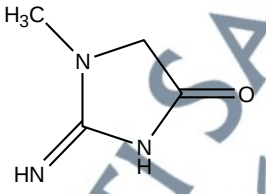
Alanine



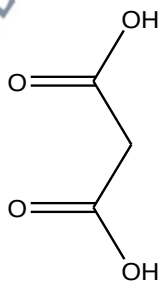
Lactate



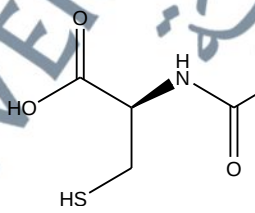
π-methylhistidine



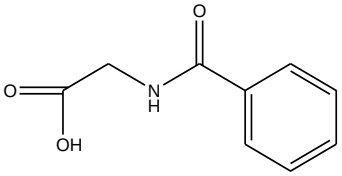
Creatinine



Malonic acid



N- acetylcysteine



Hippurate

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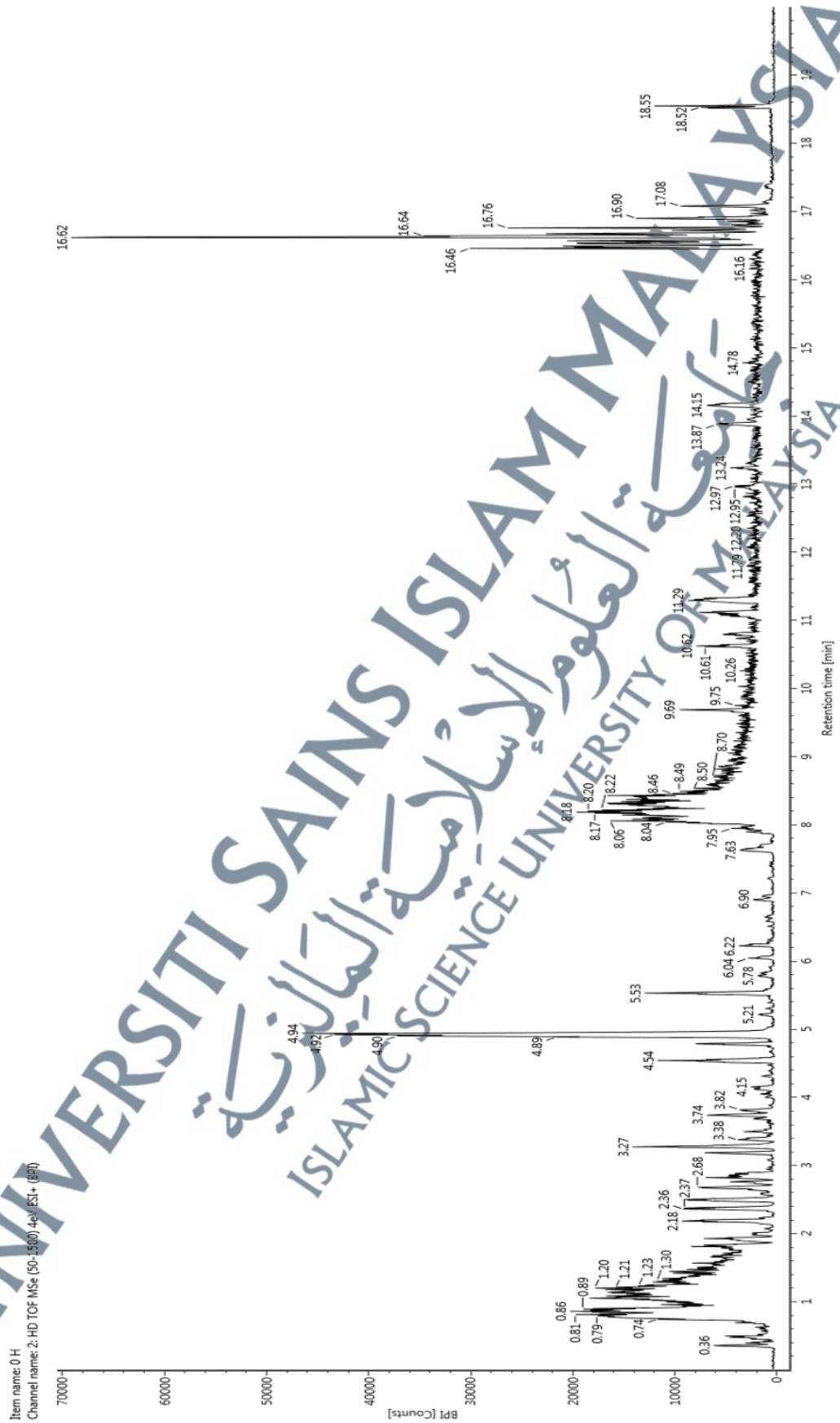
Appendix 22: LC-QToF-MS Spectrum of Metabolites Identified in Urine



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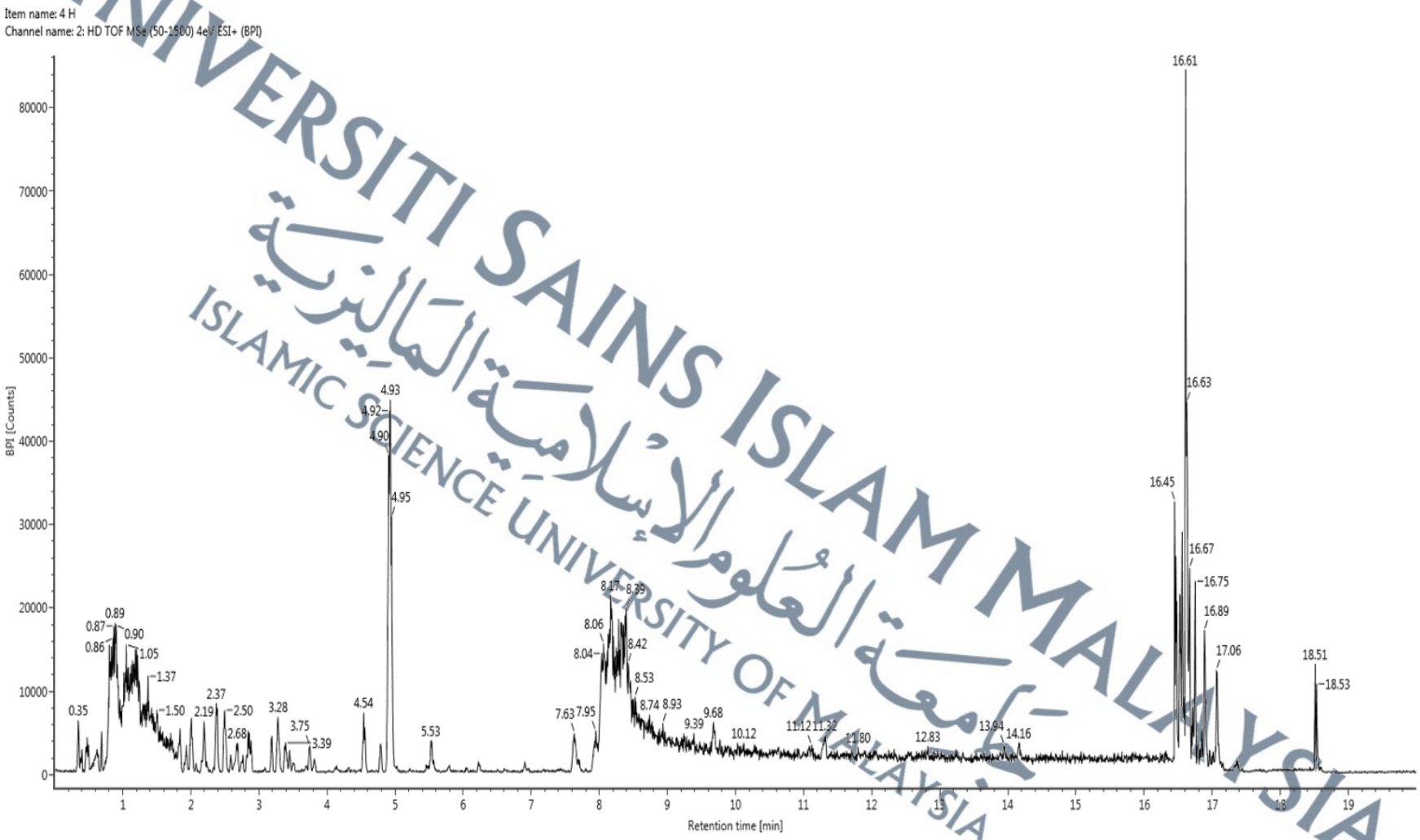

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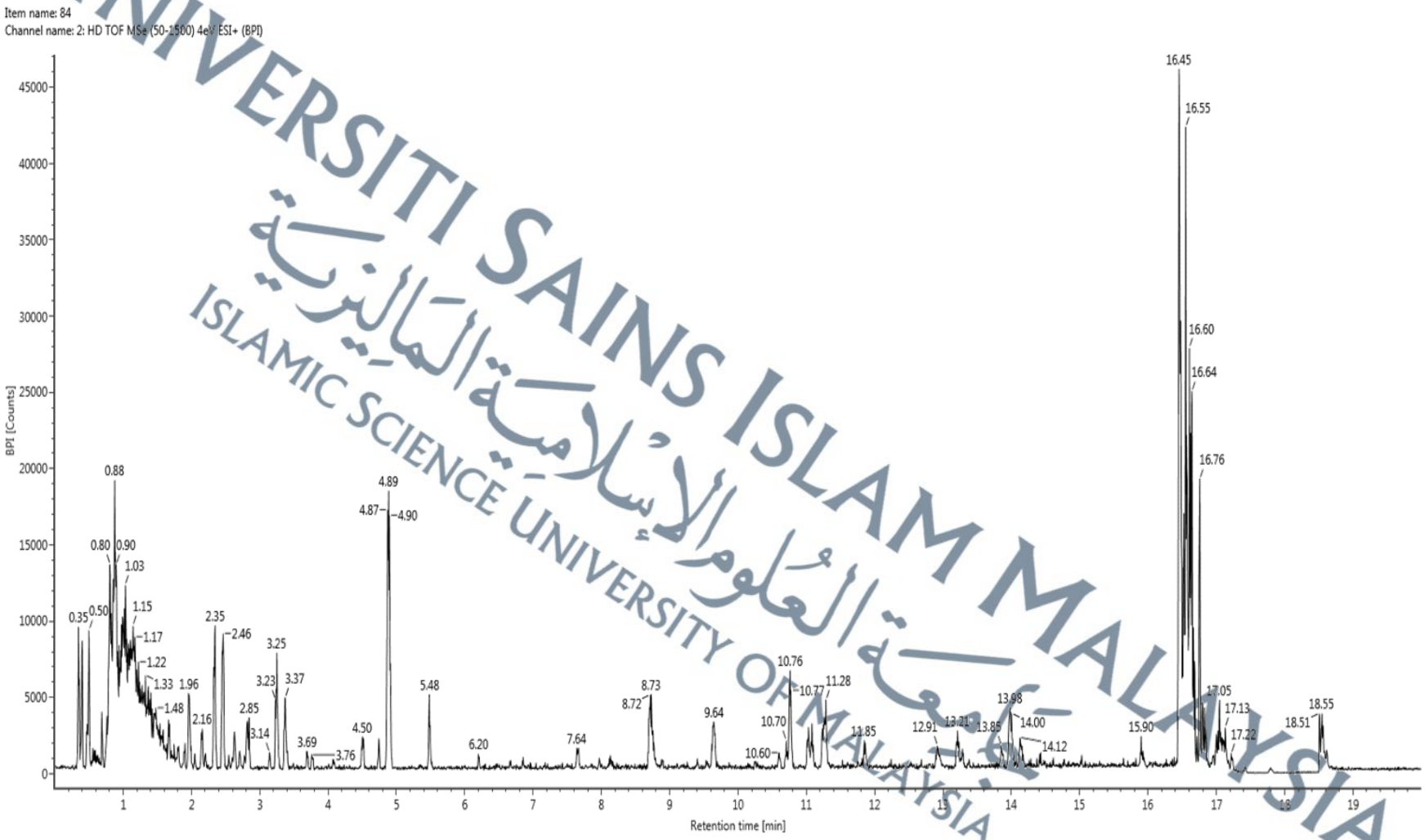

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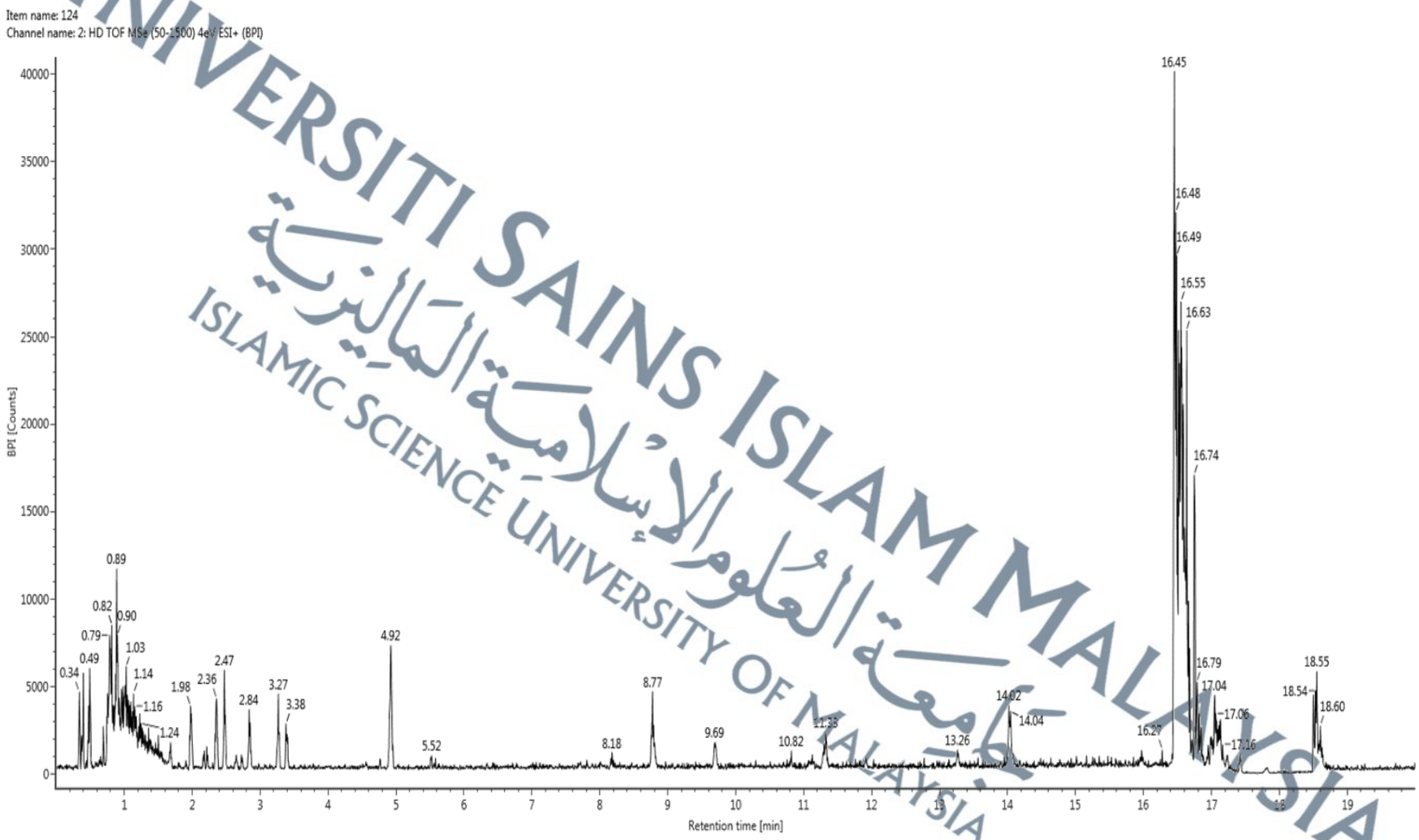

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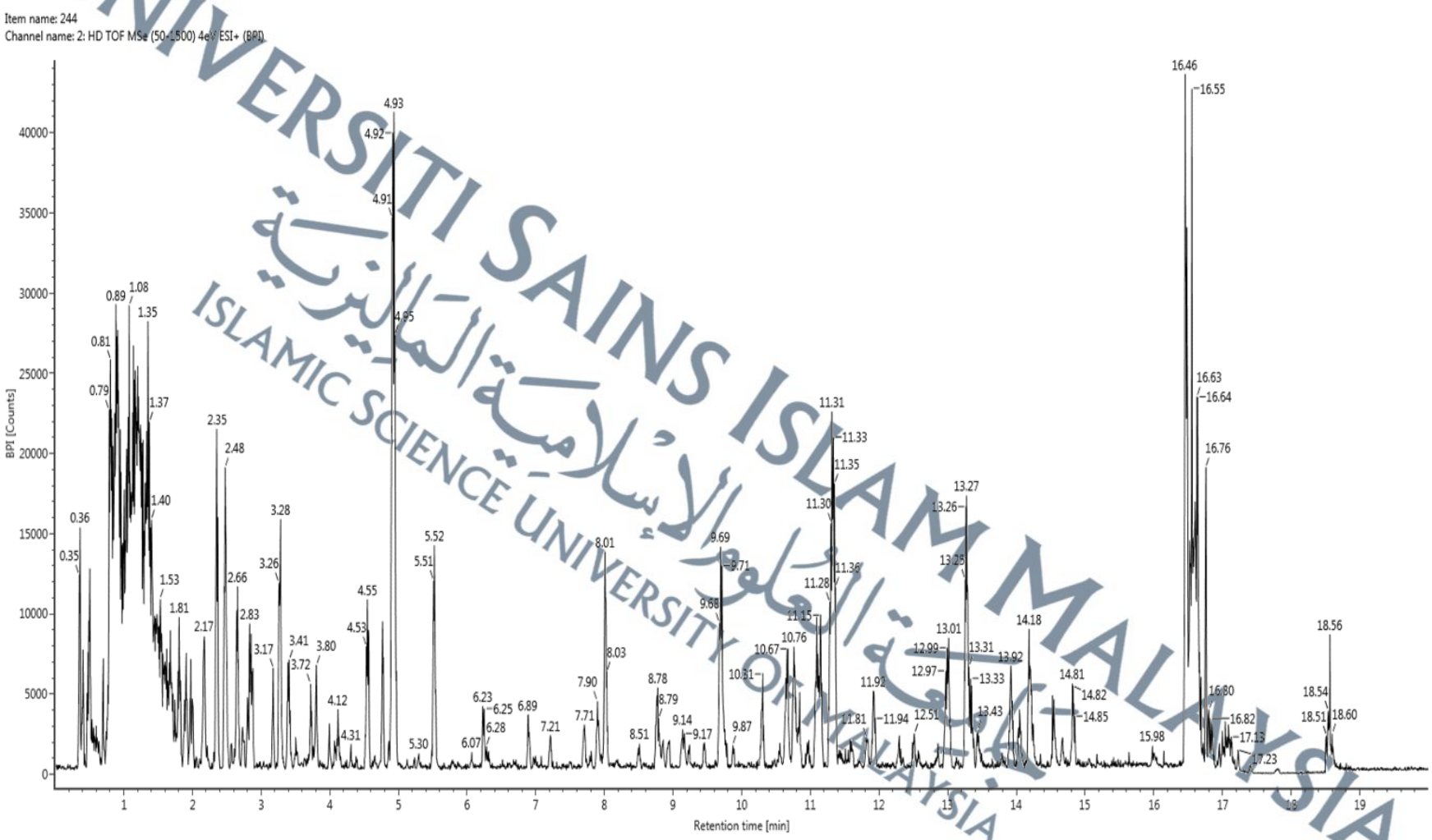

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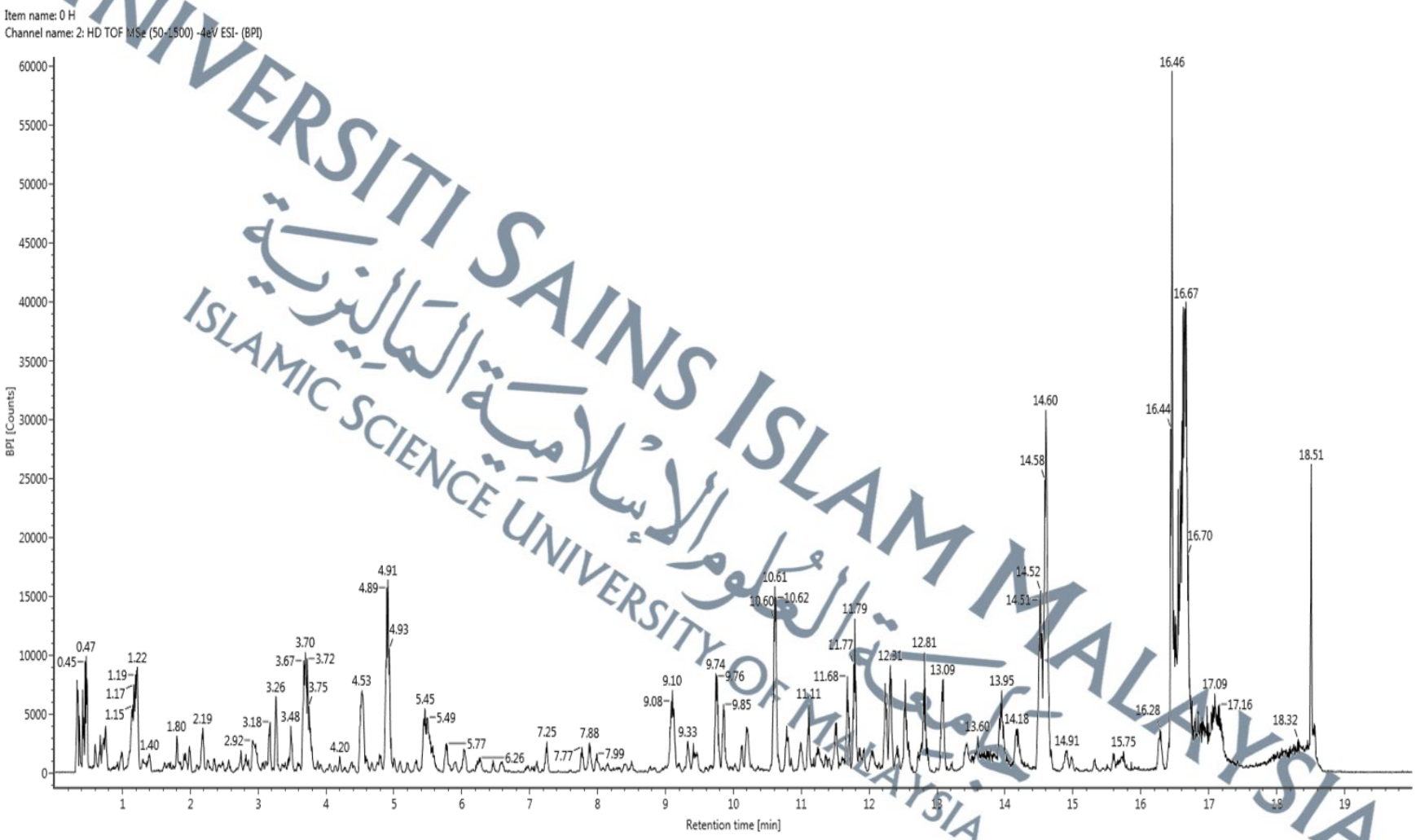

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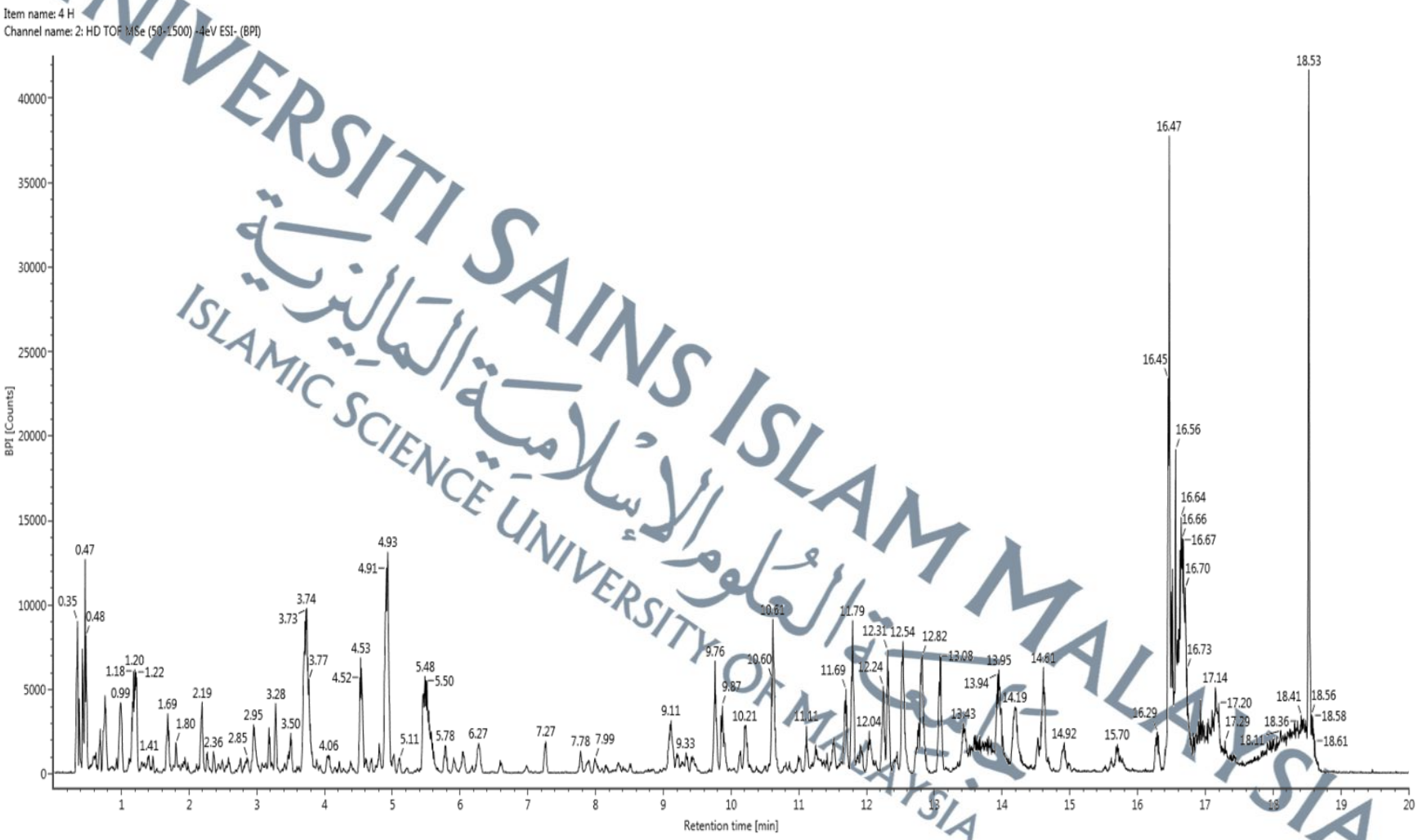

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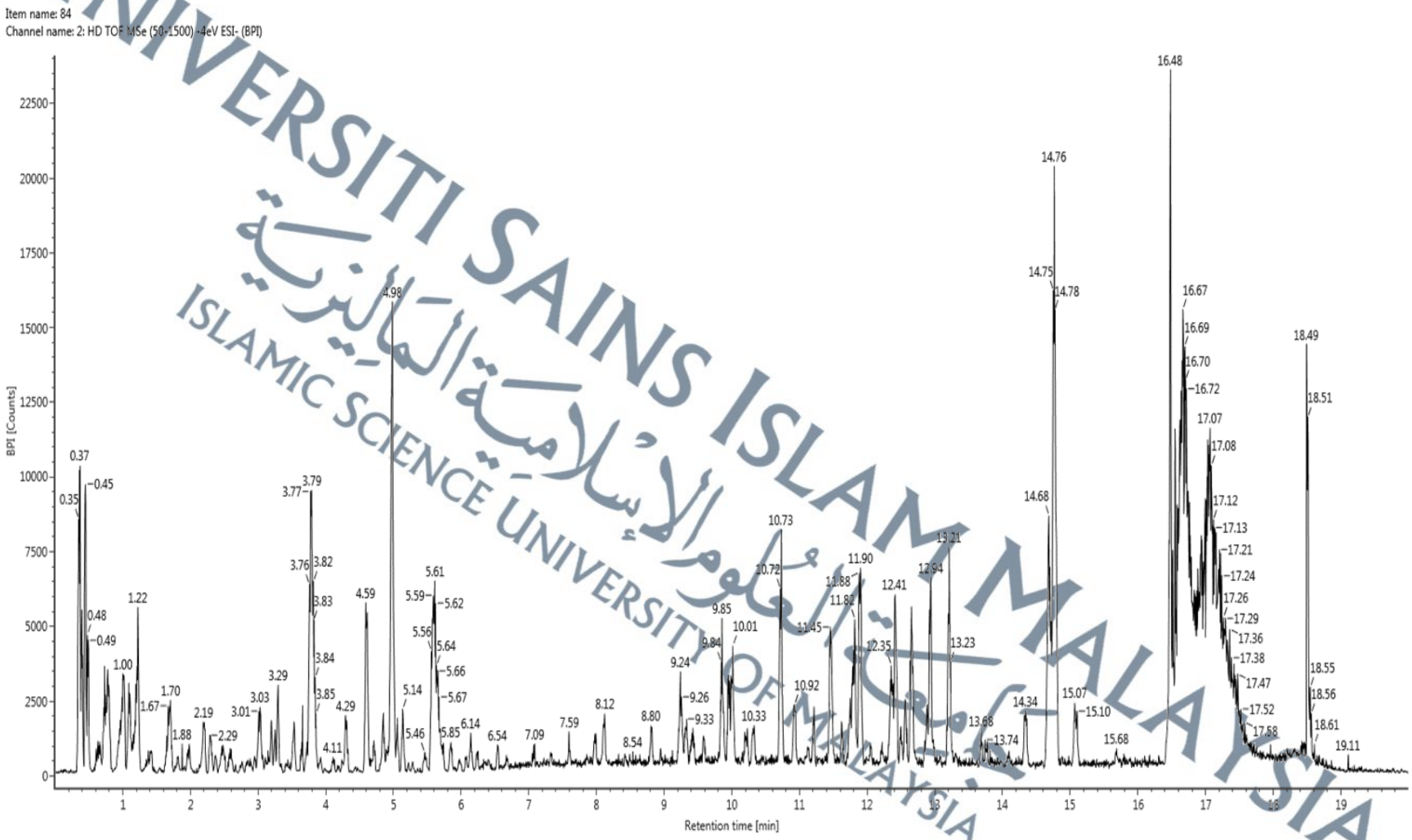

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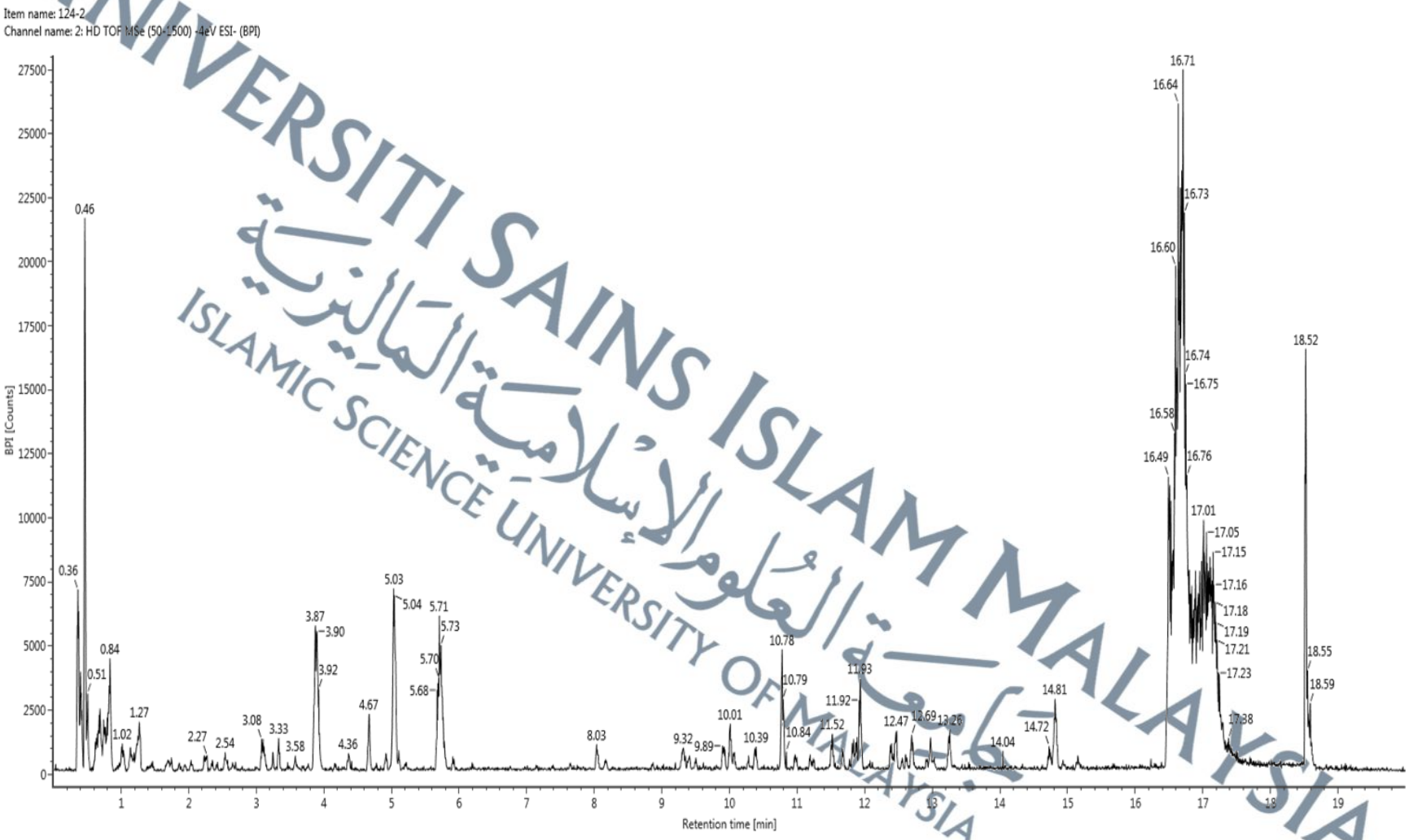

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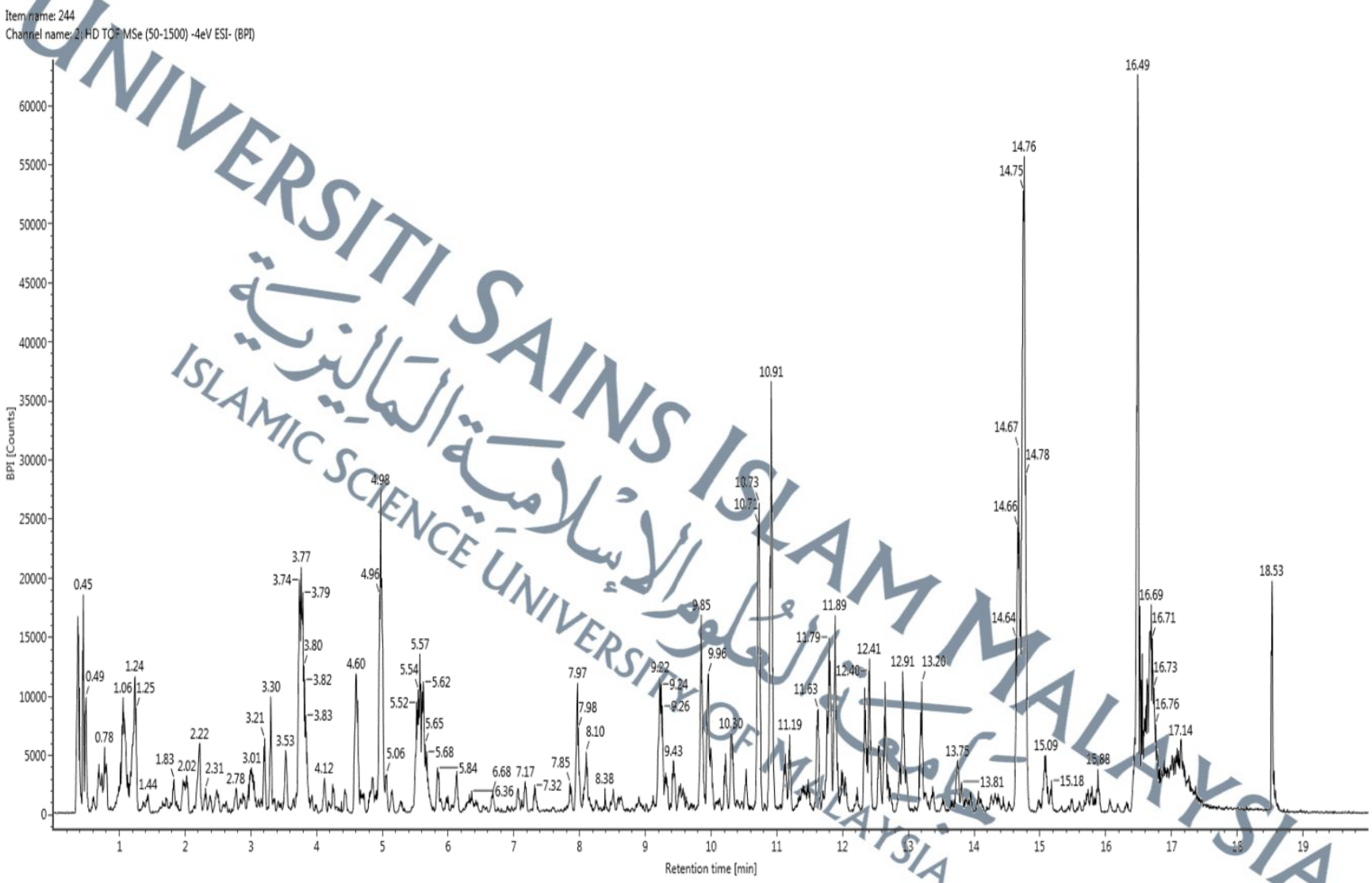

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