

Research Database

GC-MS DATA BASE

NIST Mass Spectral Library 2014

(Upgraded to NIST 17)





PERIYAR UNIVERSITY

SALEM - 636011, TAMIL NADU, INDIA
NAAC A Grade - State University - NIRF Rank 90

ANNEXURE

GAS CHROMATOGRAPHY-MASS SPECTROMETER (GC-MS).

SR.	DESCRIPTION	QTY.
I.	GCMS System:-	
1.	225-35010-44 Shimadzu Gas Chromatograph Mass Spectrometer, Model GCMS-QP2020 EI - GC-2010Plus main frame with Split / Splitless Injection port with Advanced Flow Technology with Fast GC-MS capability - Carrier gas head pressure setting up to 970 kPa (141 psi) - Injection Port heating up to 450°C - High power column oven heating up to 450°C from Ambient - Capable of installing 3 injectors and 4 detectors on single GC - Rapid column oven heating with rates from -250°C to +250°C 20 ramp / 21 plateau column oven heating steps - Split / Splitless capillary injector with temperature range of ambient +5°C to 450°C - Mass Range 1.5m/z to 1,090 m/z - Resolution of R=2M (FWHM) (Unit Mass Resolution) - Maximum Scan rate of 20000 μ /sec - Electron Impact Ionization (EI) - EI Scan Sensitivity S/N Ratio ≥ 2000 RMS for 1pg Octafluoronaphthalene m/z 272 - Vacuum System with Turbo Molecular Pump with Dual Inlet 190 L/sec / 170 L/sec (He) Turbomolecular pump differentialexhaust system in differential pumping modes - Auxiliary pumping with 30 ltr/min rotary pump (Quoted separately). - Direct interface between GC & MS with independent heating up to 350°C - Direct compatibility of capillary columns with I.D. 50μm to 530μm - Rigid Structure, Repeller type, heated lens stack Ion Source - Mass analyzer : Metal quadrapole mass filter with pre rod - Mass stability : ± 0.1 u/48 hrs - Filaments : Dual - Independent Ion source heating up to 300°C - Variable Ionization voltage from upto 200 eV - Variable Ionization current from 5 to 250 μA - Rock Solid Inert Metal Quadrupole Analyzer with rotateable pre-rods - High sensitive off-Axis Conversion Dynode Electron Multiplier Tube Detector with over drive noise suppression lens - Automatic Adjustment of Retention Time (AART) - Advance Scanning Speed Protocol (ASSP) - Full Scan and Selected Ion Monitoring (SIM) Mode with Fast Automated Simultaneous SCAN/SIM (FASST) - Ecology Mode saves power and carrier gas in analysis stand by mode	1 No.

2.	225-31912-92 GCMS Insight software package Instrument control through MS WINDOWS based 64-Bit GCMS Solutions Software for control of GC temp., interface temp.; AFC pressure and flow rates; split ratio; all MS parameters in SCAN and SIM modes; Start up and Shut down of vacuum system; User, Manual and Auto tuning; Setting of Data Acquisition, Data Handling Parameters, Report Formats; Real Time Data Acquisition, display of chromatograms and mass spectra of data under acquisition, Snapshot Function; automatic analysis through Sample Schedule; Post Run analysis, Quantitation, Private and Public Library Search software; GLP / GMP, System Suitability, Audit Trail functions and GC detection signal acquisition capability with Automatic Adjustment of Retention Time (AART), Fast Automated SIM/SCAN (FASST) & compound finder function. GCMS Insight software package is an automatic method creation function and multi data processing.	1 No.
3.	APAEDW-KIT001394 Edwards E2M1.5 Pump Kit	1 No.
II.	Database:-	1 No.
4.	978-1-118-98089-7 NIST Mass Spectral Library 2014 for GCMS	1 No.
IV.	Liquid Auto Injector:-	
5.	221-72315-58 Auto Injector AOC-20i for GC-2010 includes installation attachment	1 No.
6.	221-72300-58AOC-20S (added to AOC-20i for 150 vials capacity)	1 No.
7.	226-54120-51 1.5ml Crimp Vial clear kit	1 No.
8.	225-10681-91 Installation Kit for AOC-20s	1 No.
VI.	Set of Essential Consumables Consisting of:-	
9.	225-10340-91 Filament	2 Nos.
10.	221-76650-01 Low Bleed Septum Set, LB-2 (50 /pkt)	1 No.
11.	201-35584 Injection Port Rubber Septa (20 pcs/Pkt)	5 Nos.
12.	036-11203-84 O Ring, 4D P5 (5 pcs/pkt)	1 No.
13.	221-41444-01 Glass Insert for split	2 Nos.
14.	221-48335-01 Glass Insert for splitless/WBI	2 Nos.
15.	221-34121-93 Molecular Sieve Filter	2 Nos.
16.	221-42559-92 Filter Assy.	2 Nos.
17.	221-48441-91 Buffer Tube Assy.	1 No.
18.	221-49065-91 AU Gaskets (5pcs/pkt)	1 No.
19.	221-32126-05 Capillary column Ferrule set 0.5mm(10/pkt)	1 No.
20.	670-15003-03 Vespel Ferrule, GVF/004 (10 pcs/pkt)	2 Nos.
21.	670-15003-04 Vespel Ferrule, GVF/005 (10 pcs/pkt)	2 Nos.
22.	670-15003-07 Vespel Ferrule, GVF/007 (10 pcs/pkt)	2 Nos.
23.	670-11009 Nut, SS NE 16/012, (5 pcs/pkt)	2 Nos.
24.	036-11251 O Ring, 4D P50	5 Nos.
25.	225-10167-91 Capillary Adapter (MS)	1 No.
26.	221-42998 Nipple for Gasket (Injector)	1 No.
27.	225-20051-91 Toolkit	1 No.
28.	221-48600 Silica Wool, 2gm	1 No.
29.	226-59203-01 GCMS GS Kit*	1 No.

	*This GCMS GS Kit includes the following items:	
i)	221-75954-30 SH-Rxi-5Sil MS, 30m, 0.25mm, 0.25um	1 No.
ii)	226-50712-00 "Shimadzu 1 Triple Oxygen/Moisture/ Hydrocarbon) Helium-specific Filter Kit - 1/8" SS"	1 No.
iii)	226-54110-31 1.5mL Clear, Screw top Vials with caps and septa	1 No.
iv)	227-35001-01 GC Consumables trial kit*	1 No.
	*This GC Consumables trial kit includes the following items:	
i)	221-34618 Microliter Syringe 10ul, AOC-20i Syringe	1 No.
ii)	221-75181 Ceramic Column Cutter	1 No.
iii)	670-15003-03 Graphite Ferrules (4 pcs/pkt)	1 No.
iv)	221-75180 Injection Port Rubber Septa (5 pc/pkt)	1 No.
v)	221-75193 Glass Insert, Split	1 No.
vi)	221-75197 Glass Insert, Splitless	1 No.
vii)	036-11203-84 Viton O-rings (2 pcs/pkt)	1 No.
30.	221-41532-91 Spl Jig	1 No.
31.	221-47159 Column Hanger	1 No.
	Additional Injector	
32.	221-71042-44 OCI/PTV-2010	1 No.
33.	221-49381-01 Insert for OCI/PTV-2010	1 No.
34.	221-37282-02 Micro Syringe for OCI/PTV	1 No.
35.	221-44548-93 AOC-20i Standing Pole Kit	1 No.
	Additional Detector	
36.	221-77550-42 Electron Capture Detector ECD-2010 Exceed	1 No.
37.	221-77510-48 ECD-2010 Exceed Detector with cell	1 No.
38.	221-49664-42 By Pass Kit for ECD Exceed	1 No.
39.	221-48458-48 Auxillary Control Unit	1 No.
40.	221-73345-48 FID-2010Plus	1 No.
VII.	Local supply from India:-	
41.	Helium Gas Cylinder	1 No.
42.	Regulator for Helium Gas Cylinder	1 No.
43.	Nitrogen Gas Cylinder	1 No.
44.	Regulator for Nitrogen Gas Cylinder	1 No.
45.	Hydrogen Gas Cylinder	1 No.
46.	Regulator for Hydrogen Gas Cylinder	1 No.
47.	Zero Air Gas Cylinder	1 No.
48.	Regulator for Zero Air Gas Cylinder	1 No.
49.	Gas purification panel four stage (He, N2, H2 & Zero Air)	1 Set.
50.	1.5 Ton split Air conditioner	1 No.
51.	Numeric 7.5 KVA Online UPS 60 minutes backup	1 No.
52.	Brander Computer as per your tender specification	1 No.
53.	LaserJet Colour Printer	1 No.
54.	Capillary Column Plus GCMS GS Kit	4 Nos.
55.	Oxygen Filter	1 No.

1.	225-21900-58 Shimadzu Static Head Space Sampler, HS-20 ▪ Loop & Valve based Static HS with direct interface with GC ▪ 90 Vial carousal, 12 Vial incubator with 5 Stage Vial mixer / shaker ▪ Vial Temp. up to 300°C, Transfer line / Interface Temp. 350°C ▪ Electronic carrier gas Control & Vial pressurization with leak check ▪ Fully PC Controlled thro' Shimadzu LabSolution GC Software ▪ Complete inert sample flow line with Sulfinert Sample Loop (1ml) ▪ USB interface	1 No.
2.	223-07736-92 HS-20 Support Kit	
3.	221-73335-41 Advance Flow Controller, AFC-2010 (for HS-20)	1 No.
4.	225-21913-41 AFC Installation Kit	1 No.
5.	221-73340-43 AUX-APC (for Vial Pressurization)	1 No.
6.	225-21914-41 APC Installation Kit 1	1 No.
7.	225-21914-45 APC Installation Kit, Vent	1 No.
8.	226-84520-01 Vial HS-20, 20ml (100PC)	1 No.
9.	226-84524-11 Cap, Sili/PTFE, Crimp (100PC)	1 No.
10.	225-04424-01 Joint Split G 0.5/0.8	1 No.
11.	226-84002-00 Hand Crimper for 20mm top headspace vials	1 No.
12.	226-84012-00 Decapper for 20mm Top Headspace vials	1 No.

27
13.8.18
REGISTRAR

13/8/18

Document1 - Microsoft Word

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Peak#	R.Time	Area	Area%	Height	Height%	Name
22	26.561	649747	1.71	174964	0.99	1-Naphthalenopropanol, alpha-ethenyldcahydro-5-(h
23	27.132	355439	0.94	176471	1.00	1-Hexacosanol
24	27.278	2518340	6.63	585784	3.31	OLEAN-12-EN-3-OL, (3.BETA.)-
25	27.325	1727408	4.55	460547	2.60	METHYL COMMATE C
		37999511	100.00	17695359	100.00	

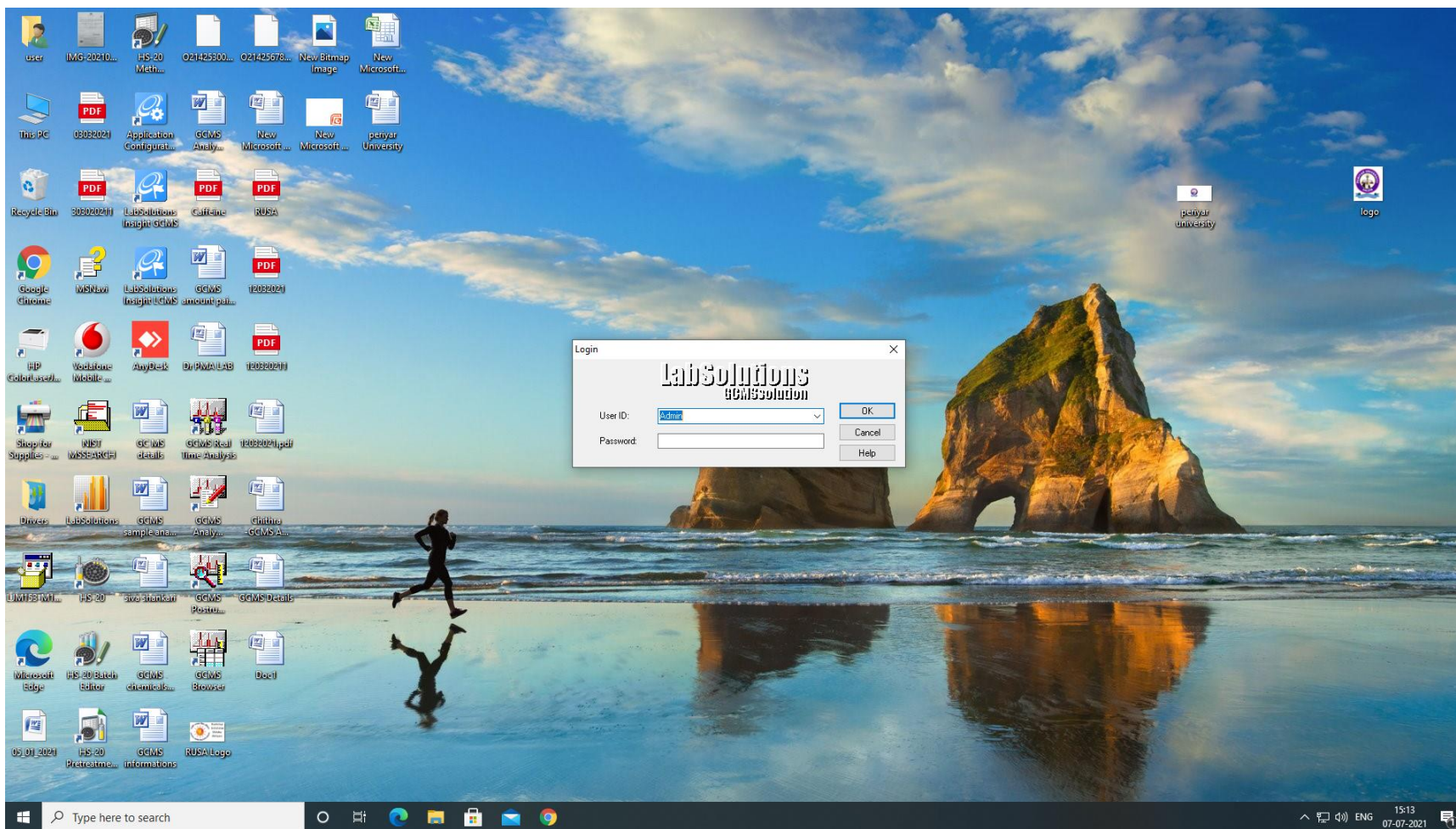
Library
<< Target >>
Line#:1 R.Time:3.095(Scan#:20) MassPeaks:244
RawMode:Averaged 3.090-3.100(19-21) BasePeak:91.00(387136)
BG Mode:Averaged 3.155-3.165(32-34) Group 1 - Event 1 Scan

Hit#:1 Entry:2640 Library:NIST17lib
SI:83 Formula:CHSN3S CAS:79-19-6 MolWeight:91 RetIndex:0
CompName:Hydrazinecarbothioamide

Hit#:2 Entry:2638 Library:NIST17lib
SI:82 Formula:CHSN3S CAS:79-19-6 MolWeight:91 RetIndex:0
CompName:Hydrazinecarbothioamide

Page: 1 of 1 Words: 0 English (United States)

10:30 14-07-2021



Folder: D:\GCMS BATCH														
Real Time	Val#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	Level#	Inj. Volume	ISTD Amt.	Report Output	Report File	Tuning File	Data Description
 Data Acquisition	1	1 BLANK E	E	0:Unknown	IT QT	-03-2020.qgm	NY'e.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
	2	1 E	E 1	0:Unknown	IT QT	-03-2020.qgm	ick\E1.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
	3	2 Ter	Ter	0:Unknown	IT QT	-03-2020.qgm	k\Ter.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
	4	4 C2	C2	0:Unknown	IT QT	-03-2020.qgm	D\C2.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
	5	5 S1	S1	0:Unknown	IT QT	-03-2020.qgm	D\S1.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
	6	6 S2	S2	0:Unknown	IT QT	-03-2020.qgm	D\S2.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
	7	7 T4	T4	0:Unknown	IT QT	-03-2020.qgm	D\T4.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
	8	8 Sample4	Sample 4	0:Unknown	IT QT	-03-2020.qgm	mple 4.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
	9	9 Sample 5	Sample5	0:Unknown	IT QT	-03-2020.qgm	mple5.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	

Vacuum Control

Auto Startup

Auto Shutdown

Not Ready

Close

Cancel

Option

Advanced >>

After Starting up Vacuum

Vacuum Leak Check

Stabilization Waiting

Cancel

GC Not Ready

MS Vac. Not Ready

Flow

0 0

Press TotalF:

Split(Valve:Open)

Temperature

32 32 32

SPL1 Oven I/F

31

IonSrc

Vacuum

L.Vac. H.Vac.

Ionization Mode

E1

GC Consumables

MS Consumables

Detail...

GOO

Message	SubMessage	Date	Time	Code	User Name	Application Name	Instrument Name	PC Name
Message (LogFile /								



Folder: D:\GCMS BATCH

Real Time	Val#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	Level#	Inj. Volume	ISTD Amt.	Report Output	Report File	Tuning File	Data Description
1	1	BLANK E	E	0:Unknown	IT QT	-03-2020.qgm	NY'e.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
2	1	E	E 1	0:Unknown	IT QT	-03-2020.qgm	ick'E1.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
3	2	Ter	Ter	0:Unknown	IT QT	-03-2020.qgm	k\Ter.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
4	4	C2	C2	0:Unknown	IT QT	-03-2020.qgm	D\C2.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
5	5	S1	S1	0:Unknown	IT QT	-03-2020.qgm	D\S1.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
6	6	S2	S2	0:Unknown	IT QT	-03-2020.qgm	D\S2.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
7	7	T4	T4	0:Unknown	IT QT	-03-2020.qgm	D\T4.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
8	8	Sample4	Sample 4	0:Unknown	IT QT	-03-2020.qgm	mple 4.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	
9	9	Sample 5	Sample5	0:Unknown	IT QT	-03-2020.qgm	mple5.qgd	1	1	(Level1 Con	☐ Print		19_N_F1.qgt	

GC Not Ready

MS Vac. Not Ready

Flow

0 0

Press TotalF:

Split(Valve:Open)

Temperature

32 32 32

SPL1 Oven I/F

31

IonSrc

Vacuum

L.Vac. H.Vac.

Ionization Mode

E1

GC Consumables

MS Consumables

Detail...

NUM

15:15

07-07-2021

Ready

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NUM

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Ready

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NUM

15:15

07-07-2021

Ready

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Ready

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NUM

15:15

07-07-2021

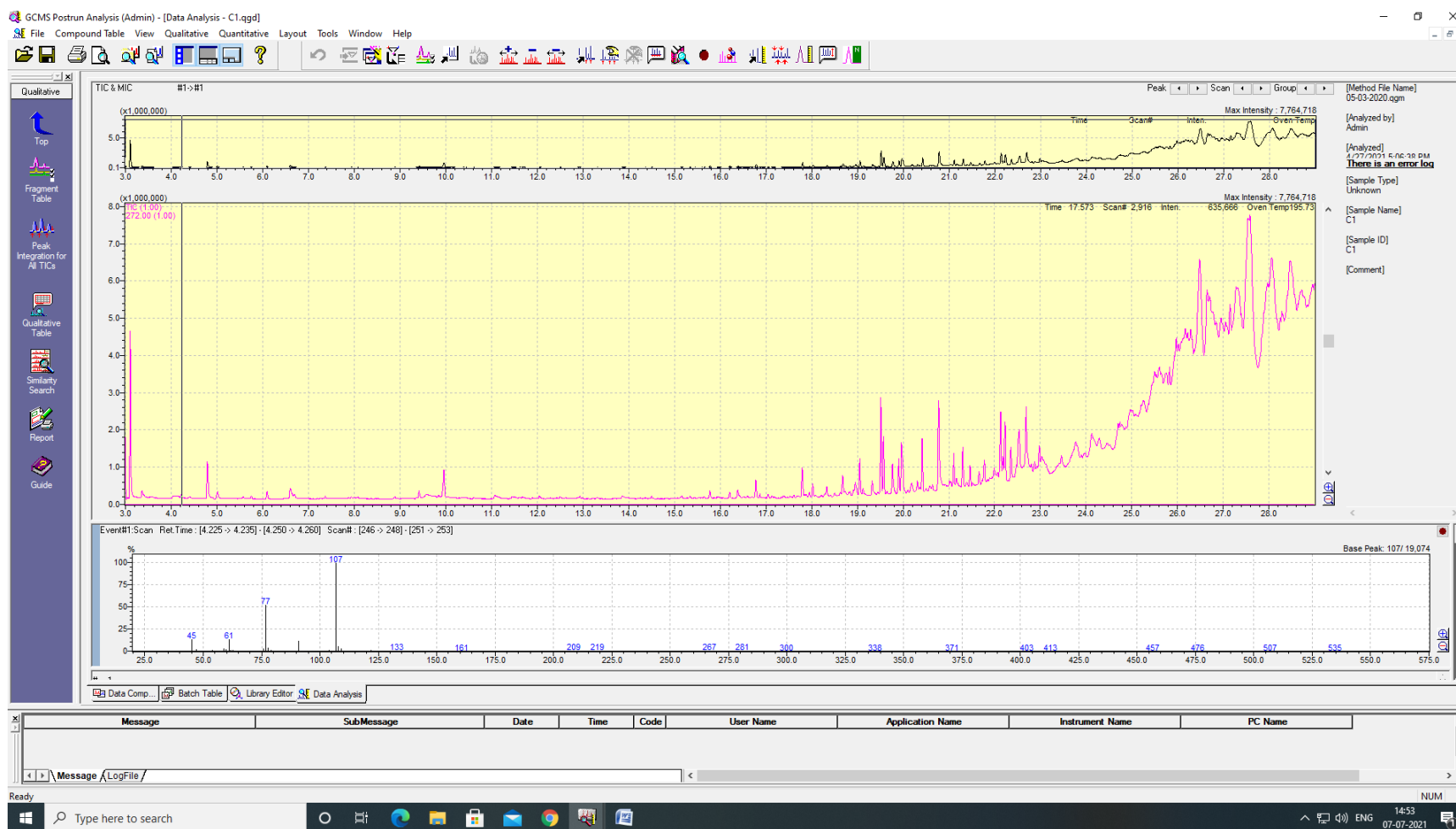
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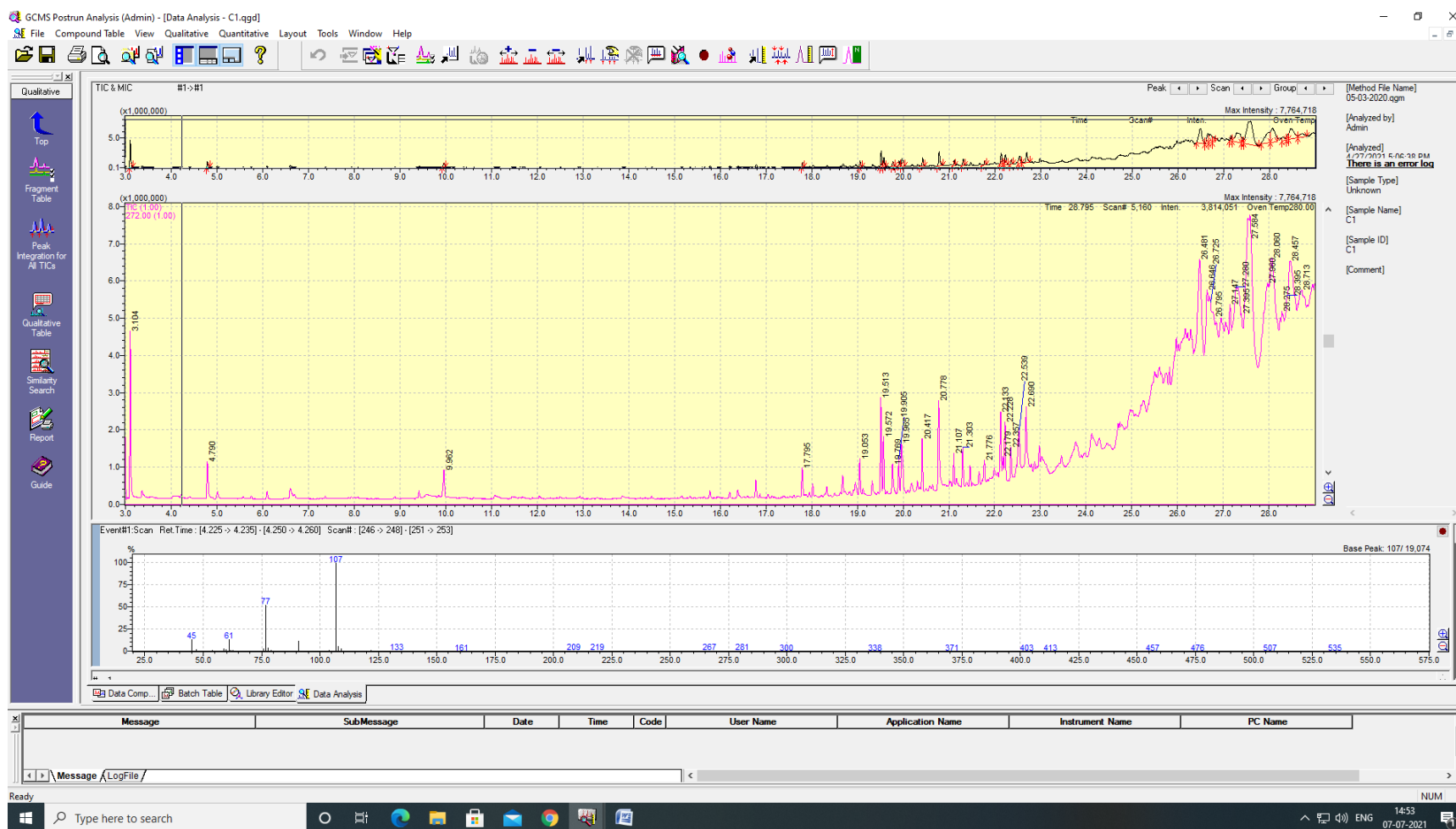
Type here to search

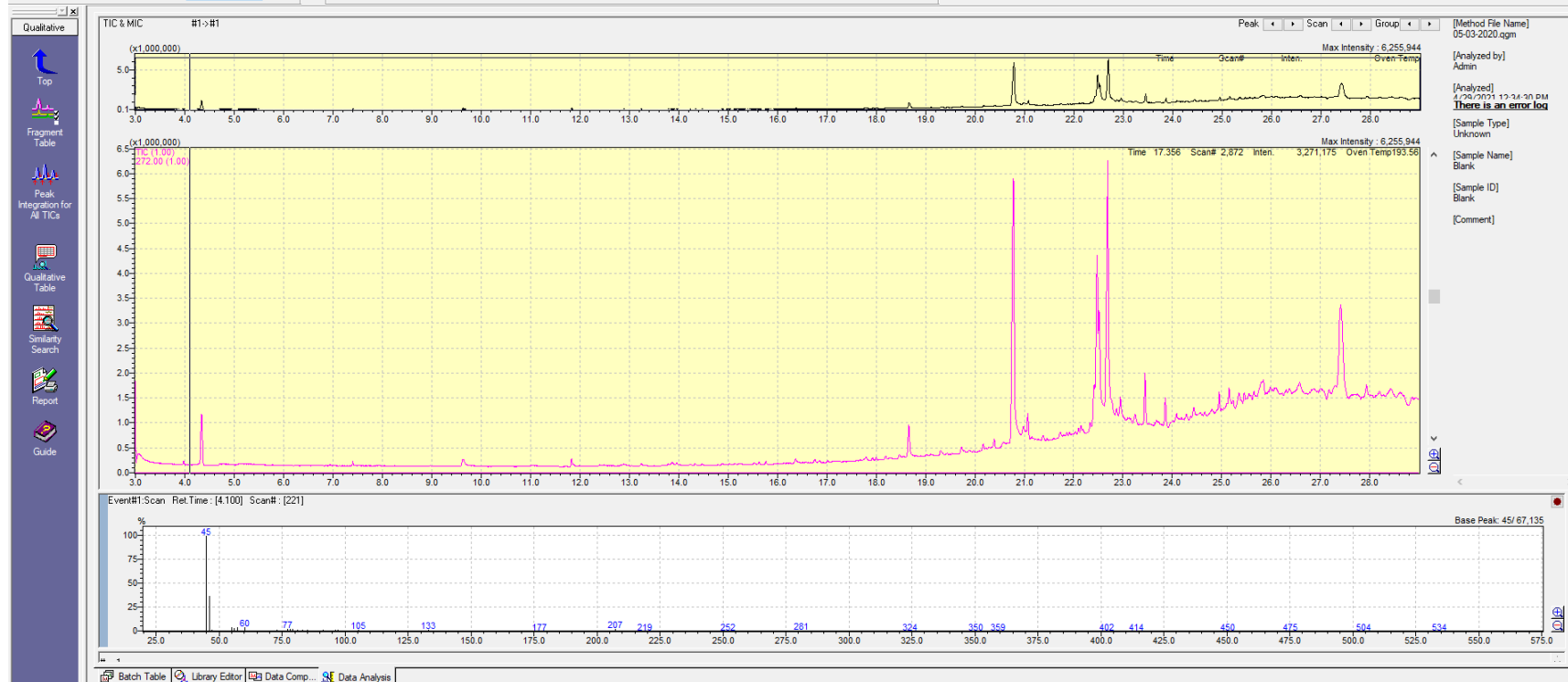
NUM

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07-07-2021







Message	SubMessage	Date	Time	Code	User Name	Application Name	Instrument Name	PC Name
Message /LogFile/								

Qualitative Table											
Print Edit View Similarity Search											
Peak#	Ret. Time	Start Tm	End Tm	m/z	Area	Area%	Height	Height%	A/H	Mark	Name
1	3.105	3.080	3.165	TIC	5716359	3.10	4452790	8.92	1.28		
2	4.790	4.765	4.845	TIC	1678227	0.91	963946	1.93	1.74		
3	9.962	9.915	10.000	TIC	1521846	0.83	712933	1.43	2.14		
4	17.795	17.760	17.835	TIC	1231749	0.67	752914	1.51	1.64		
5	19.053	19.025	19.095	TIC	1477947	0.80	941072	1.88	1.57		
6	19.513	19.480	19.545	TIC	4007753	2.17	2568940	5.15	1.56		
7	19.572	19.545	19.615	TIC	2408974	1.31	1519143	3.04	1.59	V	
8	19.769	19.735	19.820	TIC	1419929	0.77	765977	1.53	1.85		
9	19.905	19.820	19.935	TIC	1290717	0.70	863472	1.77	1.46	V	
10	19.966	19.935	20.035	TIC	3288944	1.78	1309230	2.62	2.51	V	
11	20.417	20.340	20.455	TIC	2468842	1.34	1419849	2.84	1.74	V	
12	20.778	20.735	20.860	TIC	4802258	2.60	2332914	4.67	2.06		
13	21.107	21.070	21.135	TIC	1261058	0.68	899765	1.72	1.47		
14	21.303	21.265	21.345	TIC	1829037	0.99	1051614	2.11	1.74		
15	21.776	21.695	21.815	TIC	1285904	0.70	604103	1.21	2.13		
16	22.133	22.095	22.160	TIC	3471716	1.88	1809002	3.62	1.92	V	
17	22.179	22.160	22.200	TIC	1073332	0.58	617897	1.24	1.74	V	
18	22.228	22.200	22.275	TIC	3007071	1.63	1575416	3.16	1.91	V	
19	22.357	22.320	22.400	TIC	1554881	0.84	877537	1.76	1.77		
20	22.539	22.495	22.585	TIC	3687304	2.00	1196906	2.40	3.08	V	
21	22.690	22.585	22.770	TIC	4354421	2.36	1668320	3.34	2.61	V	
22	26.481	26.395	26.575	TIC	12298618	6.67	2460568	4.93	5.00		
23	26.646	26.580	26.670	TIC	5144559	2.79	1657839	3.32	3.10		
24	26.725	26.670	26.750	TIC	5860077	3.18	1219737	2.44	4.80	V	
25	26.795	26.750	26.820	TIC	3099188	1.68	727321	1.46	4.26	V	
26	27.147	27.115	27.180	TIC	1704235	0.92	852465	1.71	2.00		
27	27.280	27.180	27.385	TIC	13151828	7.13	1504083	3.01	8.74	V	
28	27.395	27.385	27.425	TIC	1845473	1.00	948903	1.90	1.95	V	
29	27.584	27.425	27.755	TIC	36979975	20.06	3852862	7.72	9.60	V	
30	27.960	27.805	28.005	TIC	13467752	7.30	1760993	3.53	7.65		
31	28.060	28.005	28.170	TIC	15990426	8.67	2317608	4.64	6.90	V	
32	28.275	28.260	28.355	TIC	2345357	1.27	568771	1.14	4.12	V	
33	28.395	28.355	28.410	TIC	2240991	1.22	861000	1.72	2.60	V	
34	28.457	28.410	28.605	TIC	12614242	6.84	1713163	3.43	7.36	V	
35	28.713	28.605	28.810	TIC	4795815	2.60	598074	1.20	8.02	V	

Spectrum Process \ TIC

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Qualitative Table										
Print Edit View Similarity Search										
	Spectrum			Background			Search	Report	Event	Name
	Ret. Time	Start Tm	End Tm	Ret. Time	StartRT	EndRT				
1	---	3.100	3.110	---	3.165	3.175	Done	☒	1	Acetic acid, [(phenylmethoxy)imino]-, trimethylsilyl ester
2	---	4.785	4.795	---	4.845	4.855	Done	☒	1	3-PENTEN-2-ONE, 4-METHYL-
3	---	9.955	9.965	---	10.000	10.010	Done	☒	1	UNDECANE
4	---	17.790	17.800	---	17.835	17.845	Done	☒	1	1-OCTADECANOL
5	---	19.050	19.060	---	19.095	19.105	Done	☒	1	1-OCTADECENE
6	---	19.510	19.520	---	19.545	19.555		☒	1	
7	---	19.565	19.575	---	19.615	19.625		☒	1	
8	---	19.765	19.775	---	19.820	19.830		☒	1	
9	---	19.900	19.910	---	19.935	19.945		☒	1	
10	---	19.960	19.970	---	20.035	20.045		☒	1	
11	---	20.410	20.420	---	20.455	20.465		☒	1	
12	---	20.775	20.785	---	20.850	20.870		☒	1	
13	---	21.100	21.110	---	21.135	21.145		☒	1	
14	---	21.300	21.310	---	21.345	21.355		☒	1	
15	---	21.770	21.780	---	21.815	21.825		☒	1	
16	---	22.125	22.135	---	22.160	22.170		☒	1	
17	---	22.175	22.185	---	22.200	22.210		☒	1	
18	---	22.225	22.235	---	22.275	22.285		☒	1	
19	---	22.350	22.360	---	22.400	22.410		☒	1	
20	---	22.535	22.545	---	22.585	22.595		☒	1	
21	---	22.685	22.695	---	22.770	22.780		☒	1	
22	---	26.475	26.485	---	26.575	26.585		☒	1	
23	---	26.640	26.650	---	26.670	26.680		☒	1	
24	---	26.720	26.730	---	26.750	26.760		☒	1	
25	---	26.790	26.800	---	26.820	26.830		☒	1	
26	---	27.140	27.150	---	27.180	27.190		☒	1	
27	---	27.275	27.285	---	27.385	27.395		☒	1	
28	---	27.390	27.400	---	27.425	27.435		☒	1	
29	---	27.580	27.590	---	27.755	27.765		☒	1	
30	---	27.955	27.965	---	28.005	28.015		☒	1	
31	---	28.055	28.065	---	28.170	28.180		☒	1	
32	---	28.270	28.280	---	28.355	28.365		☒	1	
33	---	28.390	28.400	---	28.410	28.420		☒	1	
34	---	28.450	28.460	---	28.605	28.615		☒	1	
35	---	28.710	28.720	---	28.810	28.820		☒	1	

Qualitative Table										
Print Edit View Similarity Search										
	Spectrum			Background			Search	Report	Event	Name
	Ret. Time	Start Tm	End Tm	Ret. Time	Start RT	End RT				
1	---	3.100	3.110	---	3.165	3.175	Done	✓	1	Acetic acid, [(phenylmethoxy)imino]-, trimethylsilyl ester
2	---	4.765	4.795	---	4.845	4.855	Done	✓	1	3-PENTEN-2-ONE, 4-METHYL-
3	---	9.955	9.965	---	10.000	10.010	Done	✓	1	UNDECANE
4	---	17.790	17.800	---	17.835	17.845	Done	✓	1	1-OCTADECANOL
5	---	19.050	19.060	---	19.095	19.105	Done	✓	1	1-OCTADECENE
6	---	19.510	19.520	---	19.545	19.555	Done	✓	1	2,6,10-TRIMETHYL-14-ETHYLENE-14-PENTADECNE
7	---	19.565	19.575	---	19.615	19.625	Done	✓	1	2-Pentadecanone, 6,10,14-trimethyl-
8	---	19.765	19.775	---	19.820	19.830	Done	✓	1	Neophytadiene
9	---	19.900	19.910	---	19.935	19.945	Done	✓	1	9-Heptadecanone
10	---	19.960	19.970	---	20.035	20.045	Done	✓	1	Neophytadiene
11	---	20.410	20.420	---	20.455	20.465	Done	✓	1	HEXADECANOIC ACID, METHYL ESTER
12	---	20.775	20.785	---	20.860	20.870	Done	✓	1	n-Hexadecanoic acid
13	---	21.100	21.110	---	21.135	21.145	Done	✓	1	1-OCTADECENE
14	---	21.300	21.310	---	21.345	21.355	Done	✓	1	BICYCLOHEXYL-4-PHENYL-
15	---	21.770	21.780	---	21.815	21.825	Done	✓	1	BICYCLOHEXYL-4-PHENYL-
16	---	22.125	22.135	---	22.160	22.170	Done	✓	1	cyclohexane, [1,1'-biphenyl]-4-yl-
17	---	22.175	22.185	---	22.200	22.210	Done	✓	1	9-Octadecenoic acid (Z)-, methyl ester
18	---	22.225	22.235	---	22.275	22.285	Done	✓	1	2-HEXADECEN-1-OL, 3,7,11,15-TETRAMETHYL-, [R-(R'), R''-(E)]-
19	---	22.350	22.360	---	22.400	22.410	Done	✓	1	OCTADECANOIC ACID, METHYL ESTER
20	---	22.535	22.545	---	22.585	22.595	Done	✓	1	cyclohexane, [1,1'-biphenyl]-4-yl-
21	---	22.695	22.695	---	22.770	22.780	Done	✓	1	Octadecanoic acid
22	---	26.475	26.485	---	26.575	26.585	Done	✓	1	9-Octadecenoic acid (Z)-, 2-hydroxyethyl ester
23	---	26.640	26.650	---	26.670	26.680	Done	✓	1	1,1':2,1':3,1'-Quaterphenyl-
24	---	26.720	26.730	---	26.750	26.760	Done	✓	1	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester
25	---	26.790	26.800	---	26.820	26.830	Done	✓	1	Decyl oleate
26	---	27.140	27.150	---	27.180	27.190	Done	✓	1	1-Hexacosanol
27	---	27.275	27.285	---	27.385	27.395	Done	✓	1	5-ALPHA-CHOLEST-3-EN-3-ONE, 14-METHYL-
28	---	27.390	27.400	---	27.425	27.435	Done	✓	1	Palmitic acid vinyl ester
29	---	27.580	27.590	---	27.755	27.765	Done	✓	1	5-Octadecenoic acid (Z)-, 2-hydroxyethyl ester
30	---	27.955	27.965	---	28.005	28.015	Done	✓	1	Oleic acid, butyl ester
31	---	28.055	28.065	---	28.170	28.180	Done	✓	1	Hexadecanoic acid, 2-hydroxy-1,3-propanediyl ester
32	---	28.270	28.280	---	28.355	28.365	Done	✓	1	4-Bromo-4-cholesten-3-one
33	---	28.390	28.400	---	28.410	28.420	Done	✓	1	2,5-Cyclohexadiene-1,4-dione, 2-ethyl-
34	---	28.450	28.460	---	28.605	28.615	Done	✓	1	Hexadecanoic acid, 2-hydroxy-1,3-propanediyl ester
35	---	28.710	28.720	---	28.910	28.920	Done	✓	1	Glycerol 2-acetate 1,3-dipalmitate

