LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087683.D
Acq On : 5 Jun 2016 2:08
Operator : UM/SJ
Sample : H3383-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-WALL-4BGL

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.770	12	16	19	rBV	4458185	7861054	100.00%	18.404%
2	1.907	26	28	49	rVB	1855195	4039521	51.39%	9.457%
3	2.170	49	51	78	rVB	93326	339610	4.32%	0.795%
4	5.050	301	303	309	rBV	208698	319702	4.07%	0.748%
5	5.462	335	339	341	rBV	2659779	3285221	41.79%	7.691%
6	6.490	425	429	431	rBV	2679006	3478935	44.26%	8.145%
7	6.627	438	441	443	rBV	2987595	3303667	42.03%	7.735%
8	6.856	459	461	464	rBV	885023	725478	9.23%	1.699%
9	7.016	472	475	477	rBV	2763256	2531505	32.20%	5.927%
10	7.427	507	511	513	rBV	1449311	2180061	27.73%	5.104%
11	8.148	571	574	576	rBV	687542	943709	12.00%	2.209%
12	9.222	665	668	671	rBV	3228972	3546895	45.12%	8.304%
13	9.611	700	702	705	rVB	198953	210190	2.67%	0.492%
14	9.896	724	727	730	rVB	1167350	1075716	13.68%	2.518%
15	10.685	793	796	798	rBV	2127568	2246294	28.57%	5.259%
16	11.382	854	857	859	rVB	1045082	1105596	14.06%	2.588%
17	11.919	901	904	906	rBV	144745	184474	2.35%	0.432%
18	12.971	993	996	998	rBV	3278476	3431864	43.66%	8.035%
19	14.011	1084	1087	1089	rBV	1098728	1020083	12.98%	2.388%
20	14.868	1160	1162	1165	rBV	139400	131890	1.68%	0.309%
21	15.440	1209	1212	1215	rBV	594553	751362	9.56%	1.759%

Sum of corrected areas: 42712827

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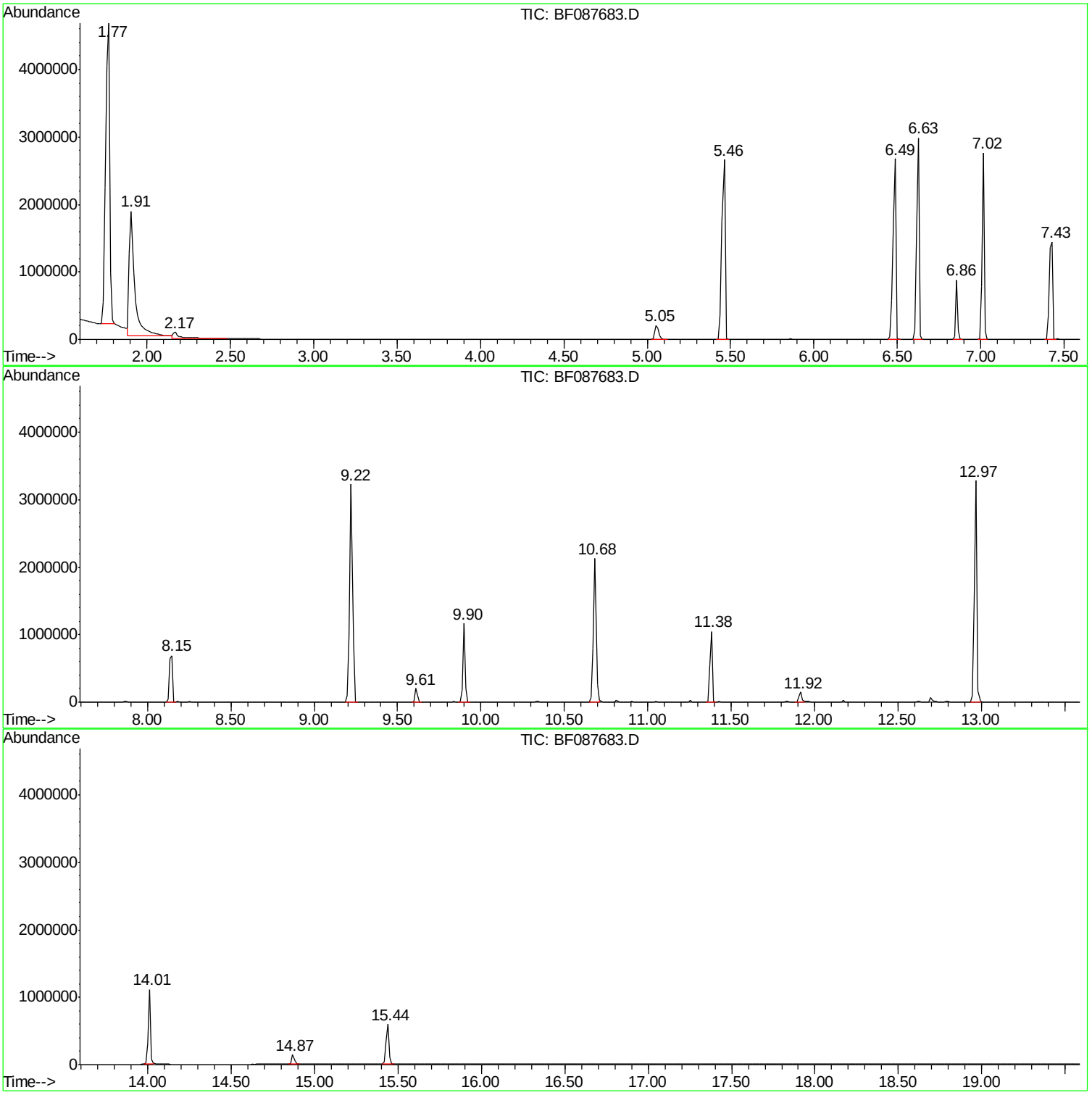
Instrument :
BNA_F
ClientSampleId :
WEST-WALL-4BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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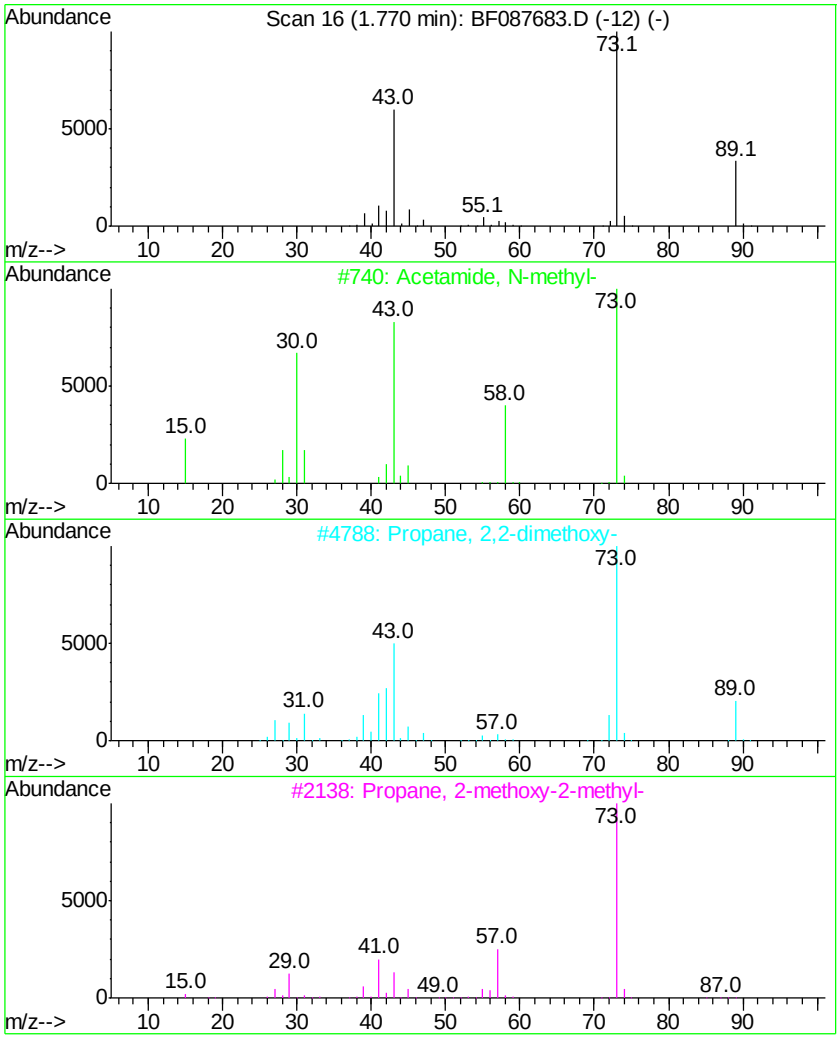
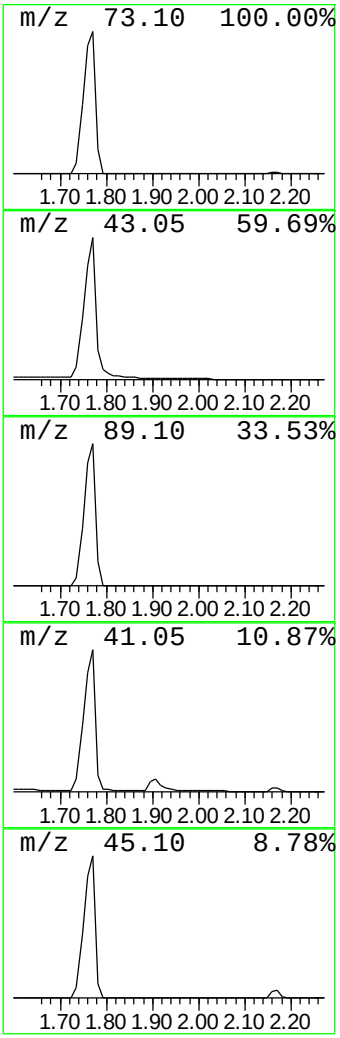
Peak Number 1 unknown1.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.77	216.71 ng	7861050	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	43
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9





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Sample : H3383-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-WALL-4BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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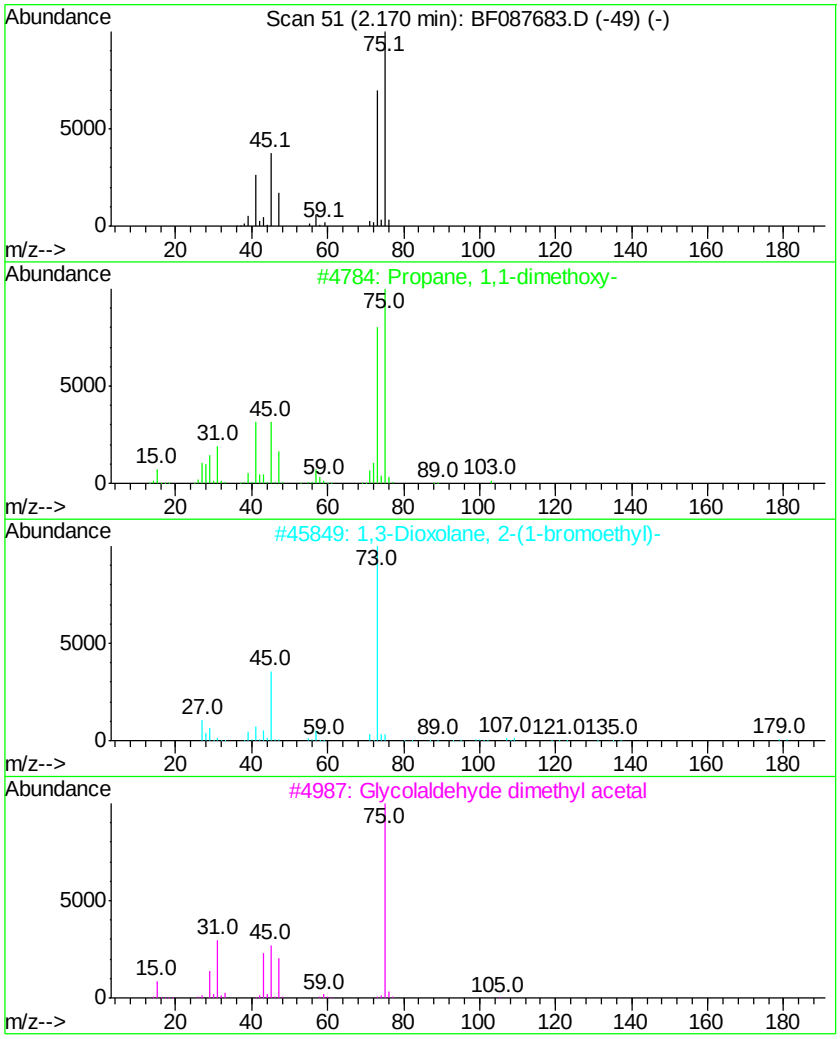
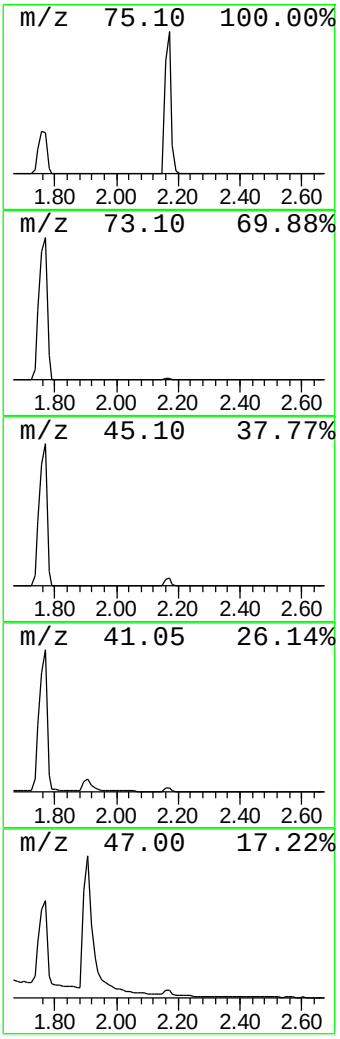
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	9.36 ng	339610	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
3	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	Glycine	75	C2H5NO2	000056-40-6	7





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Instrument : BNA_F
ClientSampleId : WEST-WALL-4BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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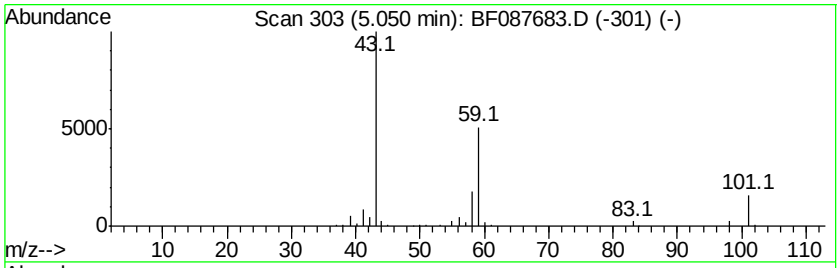
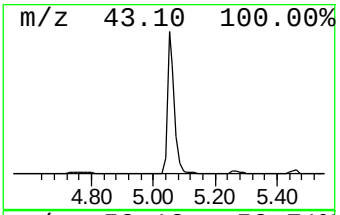
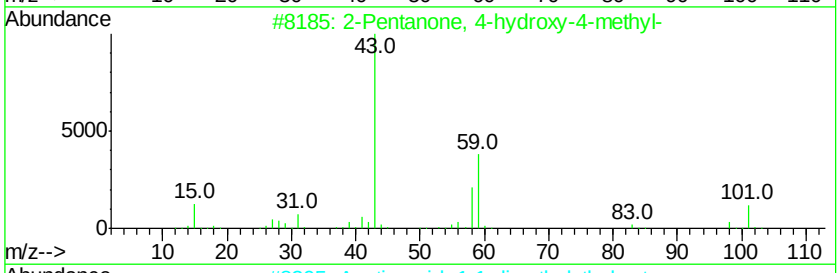
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

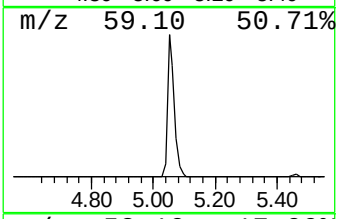
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	8.81 ng	319702	1,4-Dichlorobenzene-d4	6.86

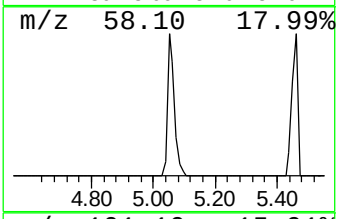
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9

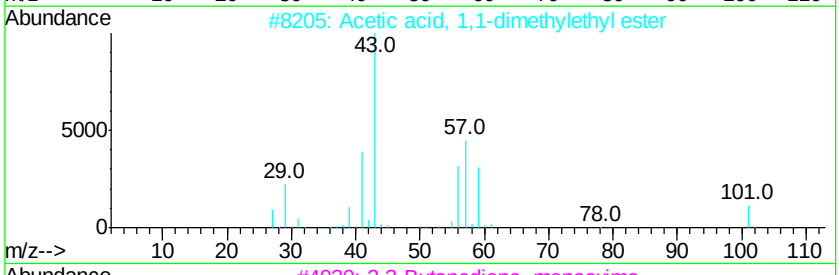


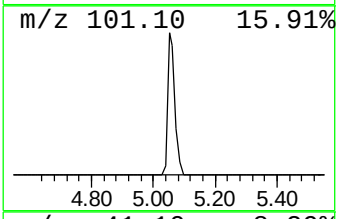


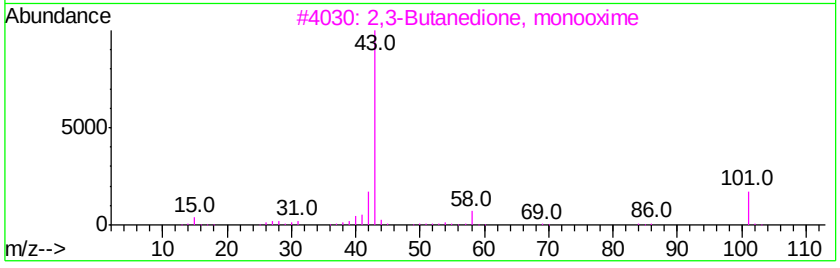


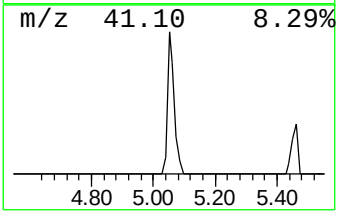












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TIC Library : C:\Database\NIST11.L
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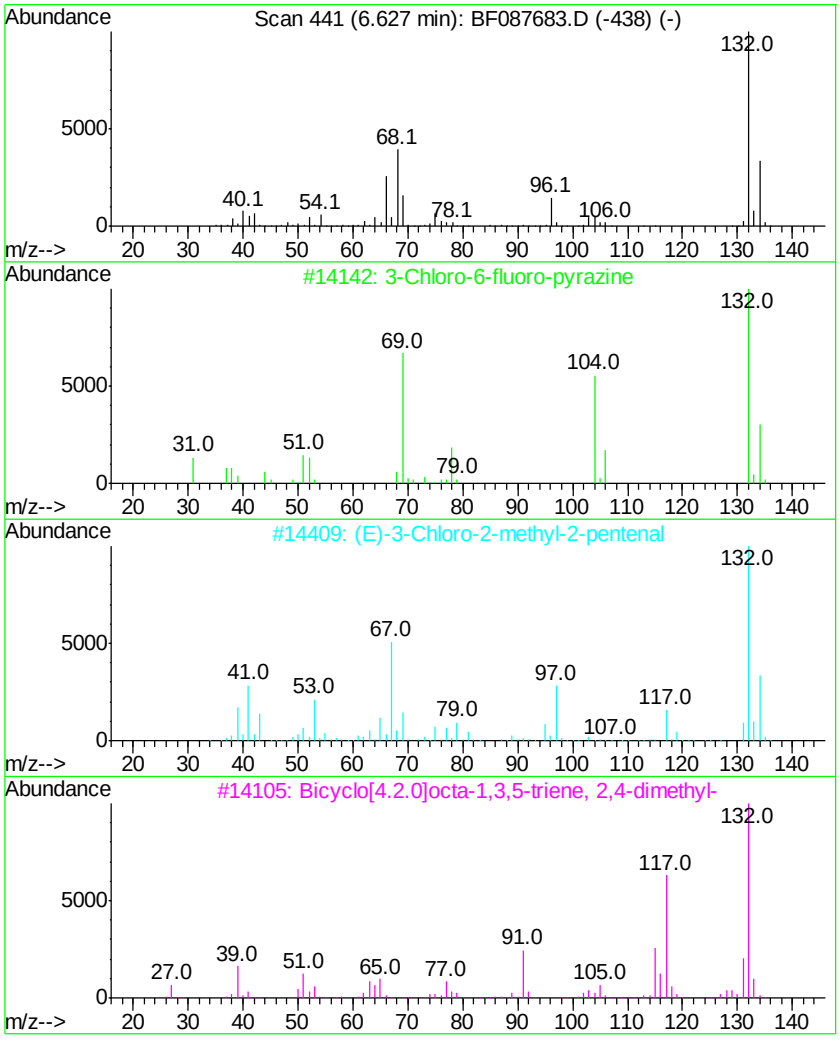
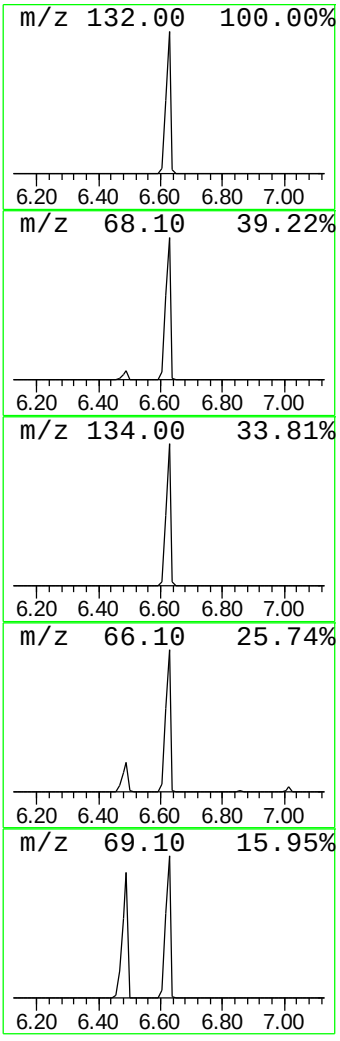
****

Peak Number 5 unknown6.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	91.08 ng	3303670	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

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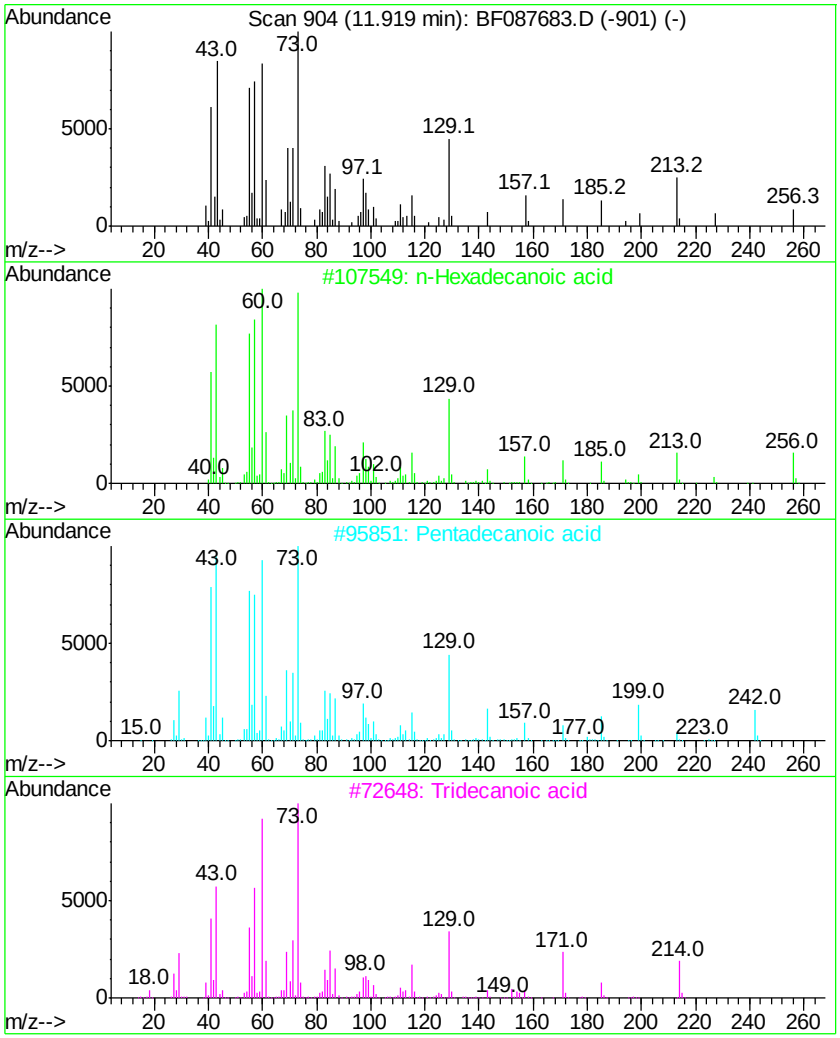
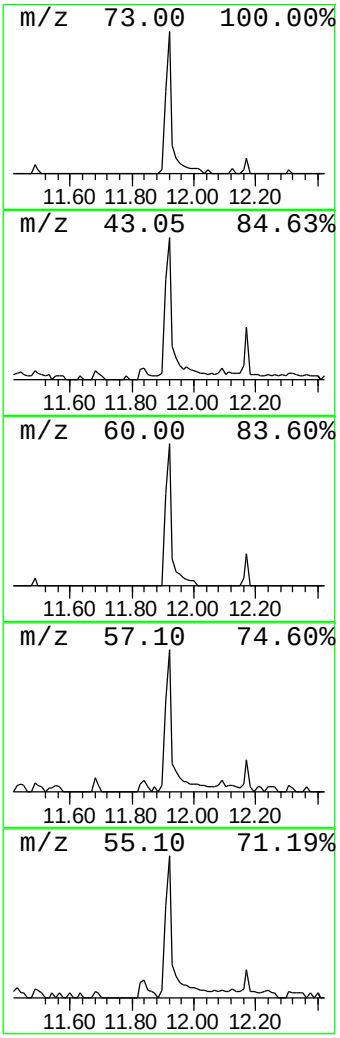
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.34 ng	184474	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	18





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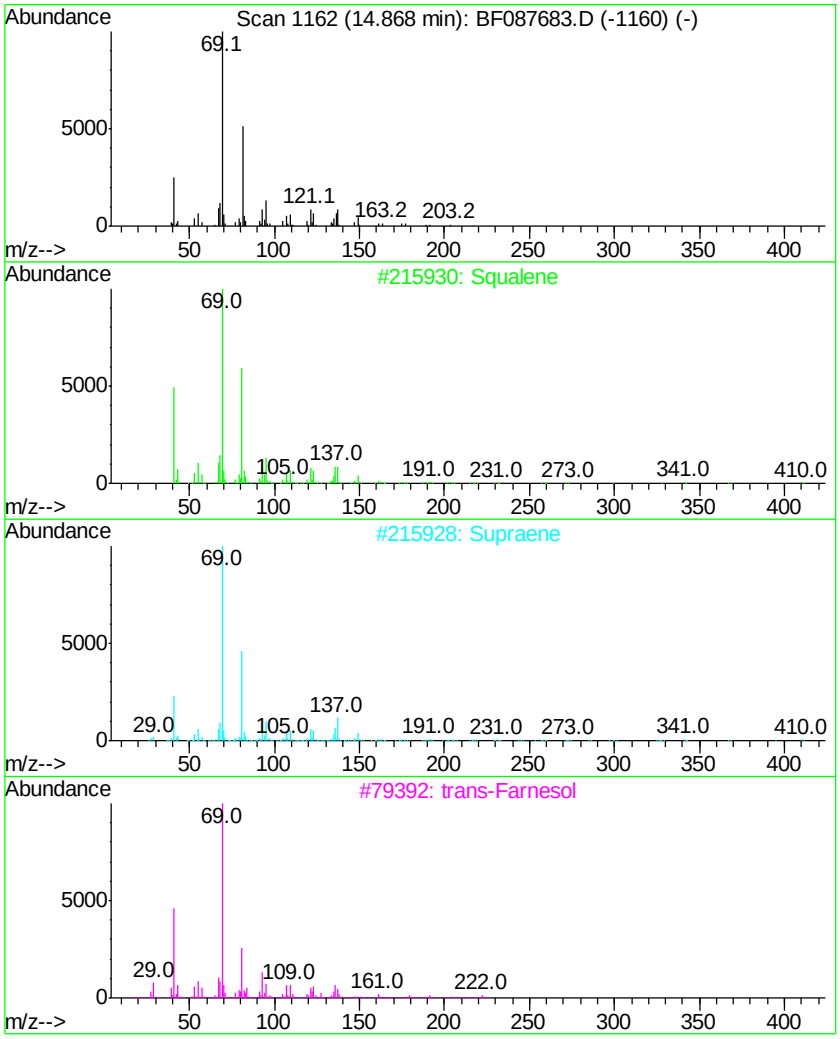
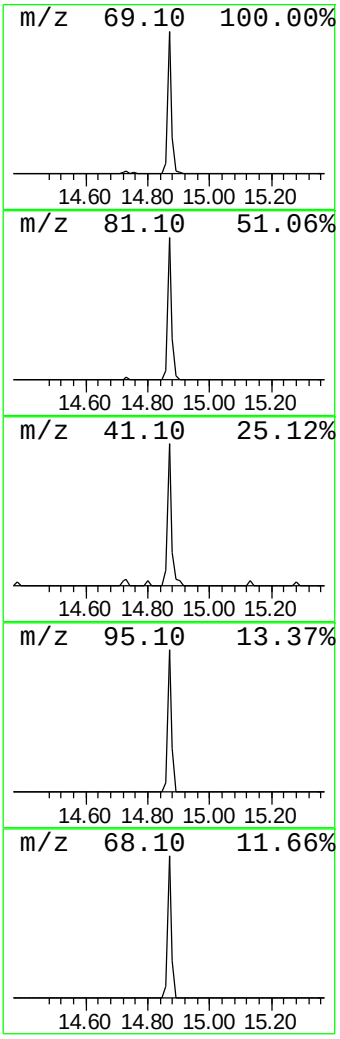
Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.51 ng	131890	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	trans-Farnesol	222	C15H26O	000106-28-5	83
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown1.77	1.77	216.7	ng	7861050	1	6.86	725478	20.0
Propane, 1,1-dime...	2.17	9.4	ng	339610	1	6.86	725478	20.0
2-Pentanone, 4-hy...	5.05	8.8	ng	319702	1	6.86	725478	20.0
unknown6.63	6.63	91.1	ng	3303670	1	6.86	725478	20.0
n-Hexadecanoic acid	11.92	3.3	ng	184474	4	11.38	1105600	20.0
Squalene	14.87	3.5	ng	131890	6	15.44	751362	20.0