LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087686.D
Acq On : 5 Jun 2016 3:39
Operator : UM/SJ
Sample : H3383-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-12BGL

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	4433135	7825523	100.00%	18.663%
2	1.907	26	28	49	rVB	1748355	3960927	50.62%	9.446%
3	2.170	49	51	85	rVB	100818	411670	5.26%	0.982%
4	5.050	301	303	308	rBV	205786	313295	4.00%	0.747%
5	5.462	335	339	341	rBV	2674767	3282049	41.94%	7.827%
6	6.490	425	429	431	rBV	2552752	3433799	43.88%	8.189%
7	6.627	438	441	443	rBV	2936808	3261083	41.67%	7.777%
8	6.856	459	461	464	rBV	843344	701508	8.96%	1.673%
9	7.016	472	475	477	rBV	2708380	2503728	31.99%	5.971%
10	7.416	507	510	513	rBV	1426103	2105496	26.91%	5.021%
11	8.148	571	574	576	rBV	745956	936616	11.97%	2.234%
12	9.222	665	668	671	rBV	3051648	3245786	41.48%	7.741%
13	9.611	700	702	705	rVB	217536	212190	2.71%	0.506%
14	9.896	724	727	730	rVB	1210986	1065615	13.62%	2.541%
15	10.685	793	796	798	rBV	2121482	2222000	28.39%	5.299%
16	11.382	854	857	859	rVB	978574	1066247	13.63%	2.543%
17	11.919	901	904	906	rBV	150390	216582	2.77%	0.517%
18	12.971	993	996	998	rBV	3004658	3119992	39.87%	7.441%
19	13.965	1078	1083	1085	rBV2	29178	105531	1.35%	0.252%
20	14.011	1085	1087	1089	rVB	1108106	988596	12.63%	2.358%
21	14.868	1160	1162	1165	rBV	237871	230951	2.95%	0.551%
22	15.440	1209	1212	1214	rBV	582043	722461	9.23%	1.723%

Sum of corrected areas: 41931645

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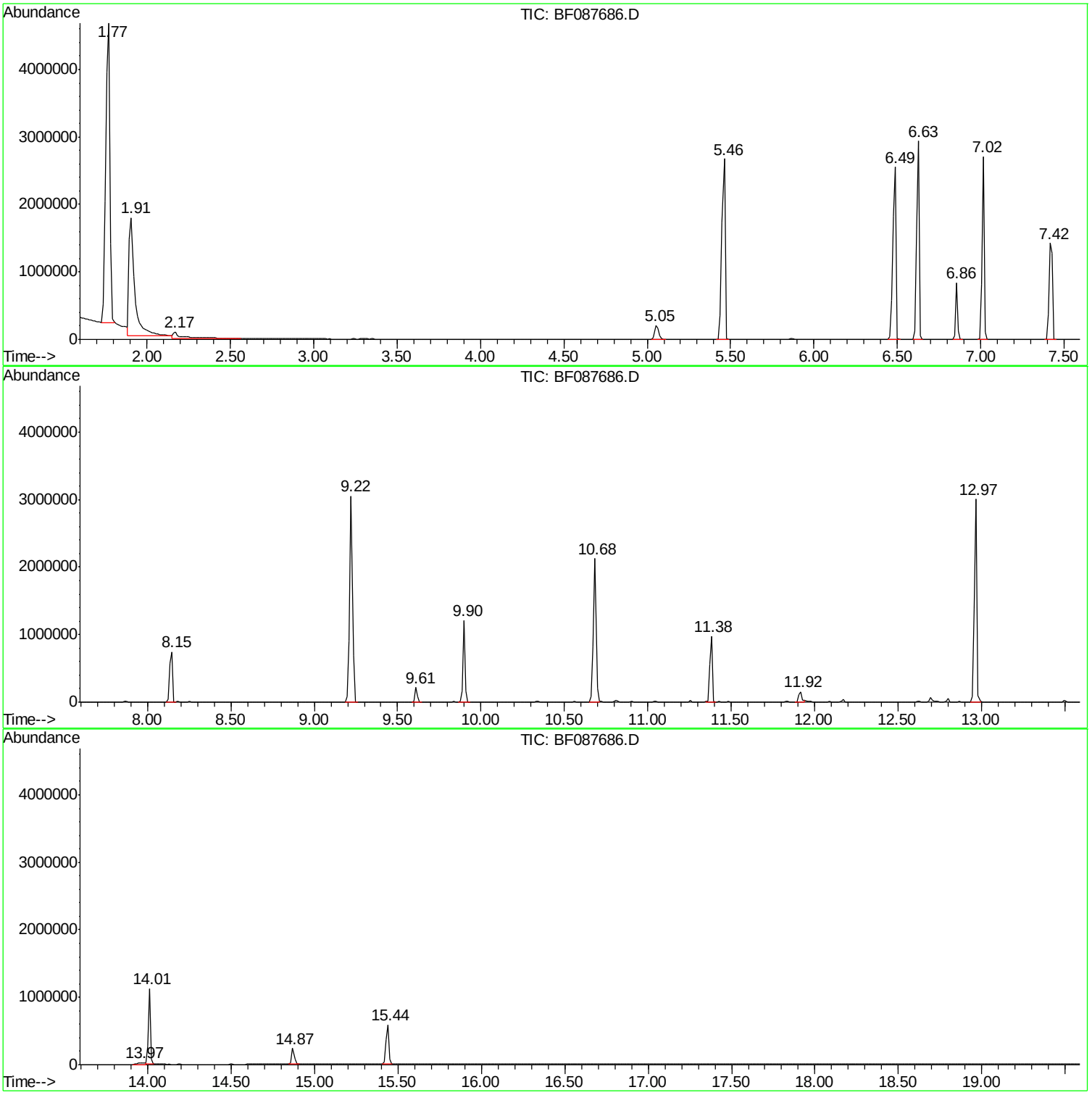
Instrument :
BNA_F
ClientSampleId :
BOTTOM-12BGL

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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Acq On : 5 Jun 2016 3:39
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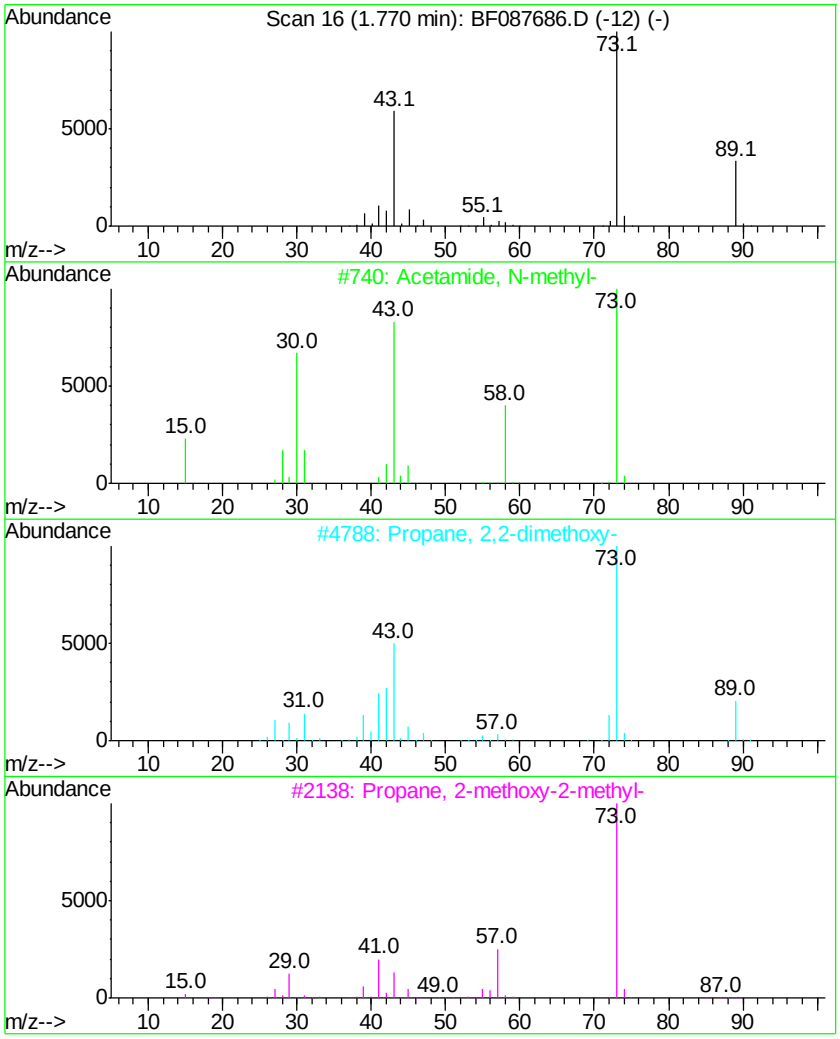
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

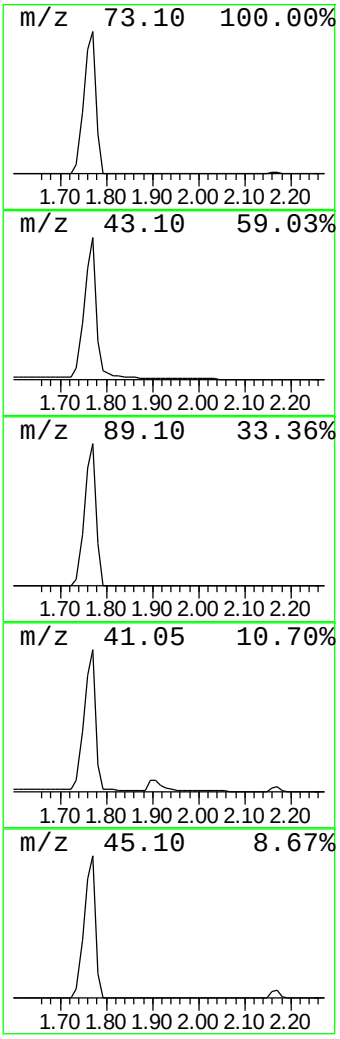
****

Peak Number 1 unknown1.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.77	223.11 ng	7825520	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	36
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9





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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-12BGL

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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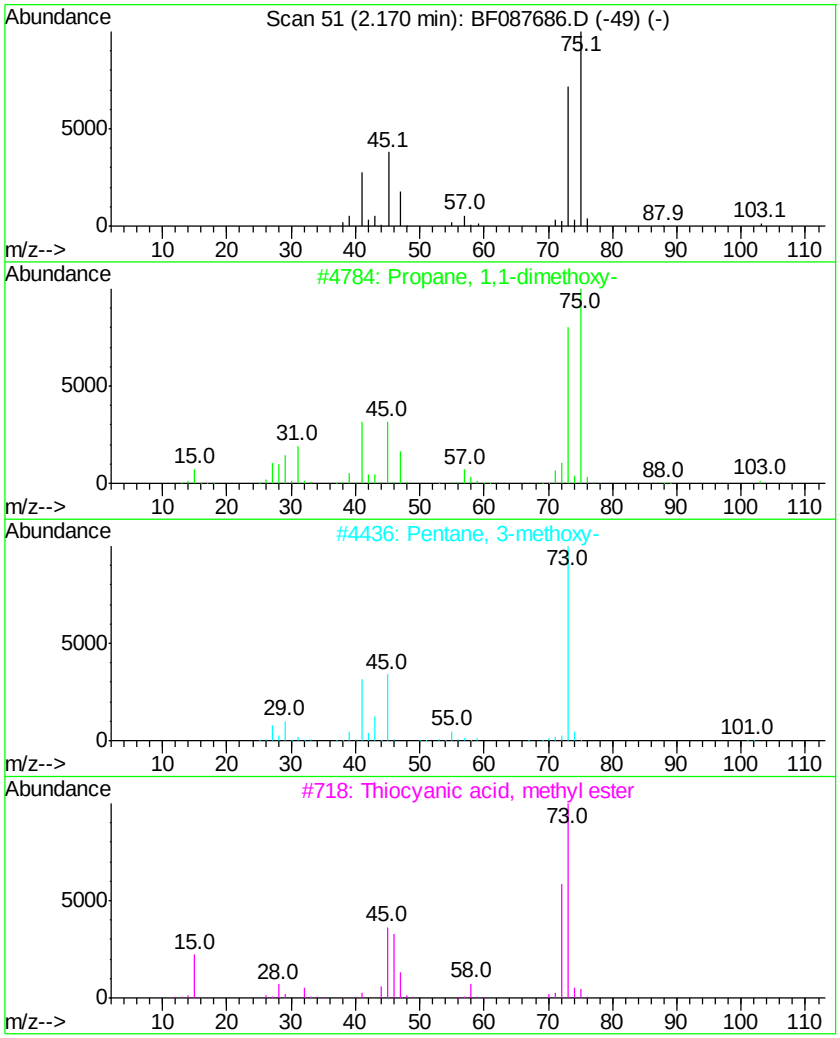
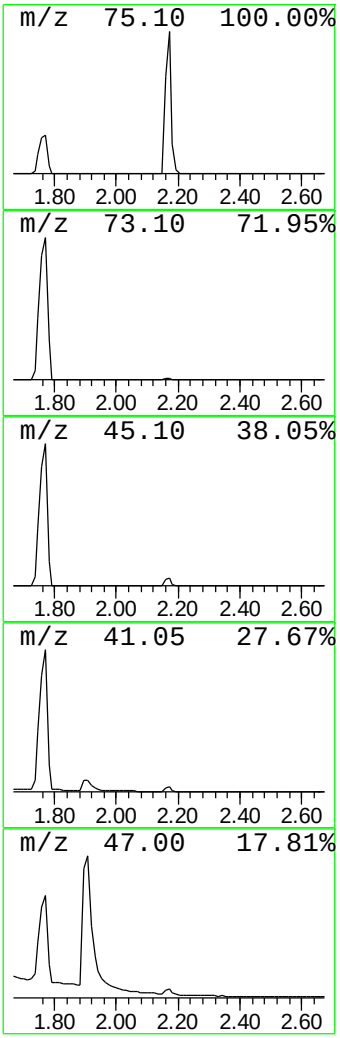
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	11.74 ng	411670	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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
4	Hydrazine, 1-methyl-1-(1-methyle...	88	C4H12N2	033668-54-1	9
5	.beta.-D-Glucopyranoside, methyl...	176	C7H12O5	003056-46-0	9





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Misc :
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Instrument : BNA_F
ClientSampleId : BOTTOM-12BGL

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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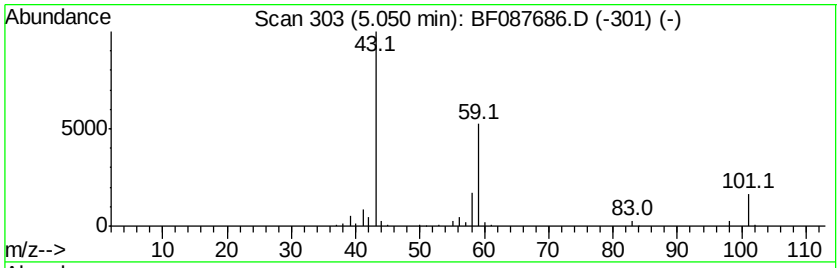
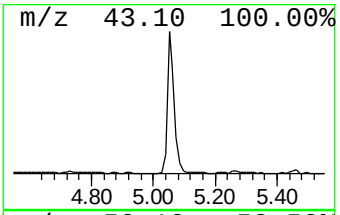
****

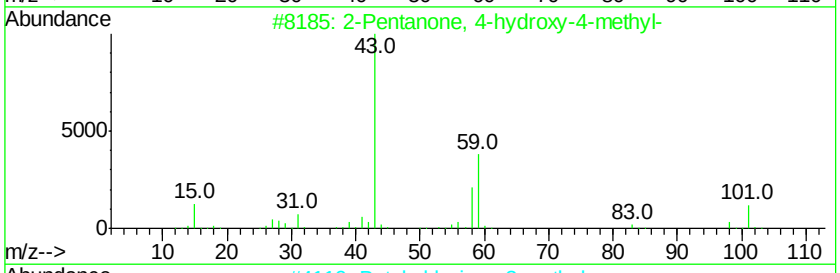
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

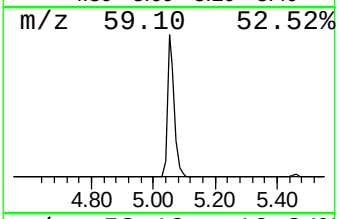
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	8.93 ng	313295	1,4-Dichlorobenzene-d4	6.86

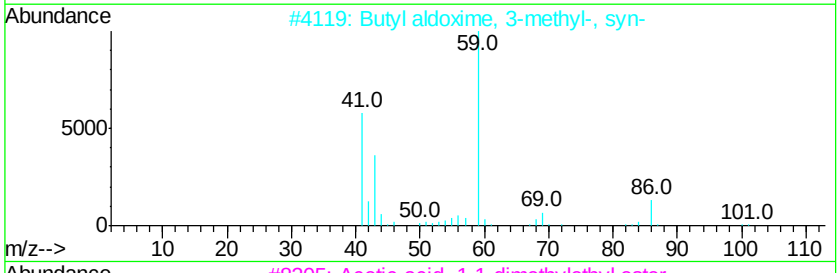
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10

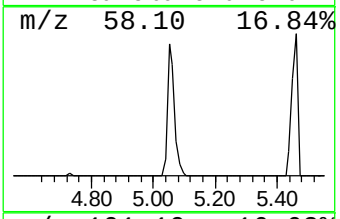


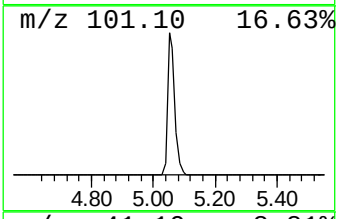


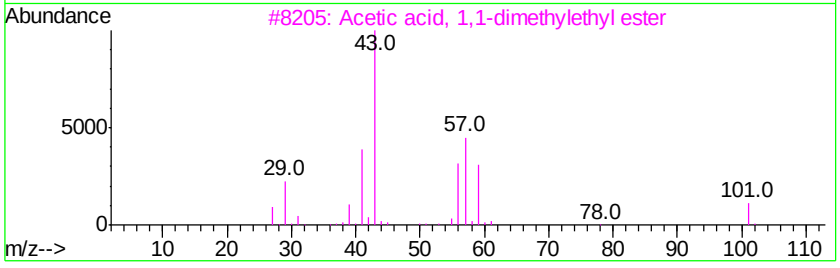


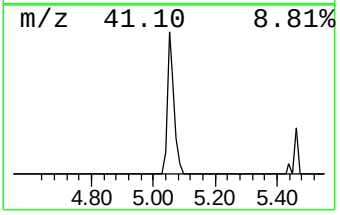












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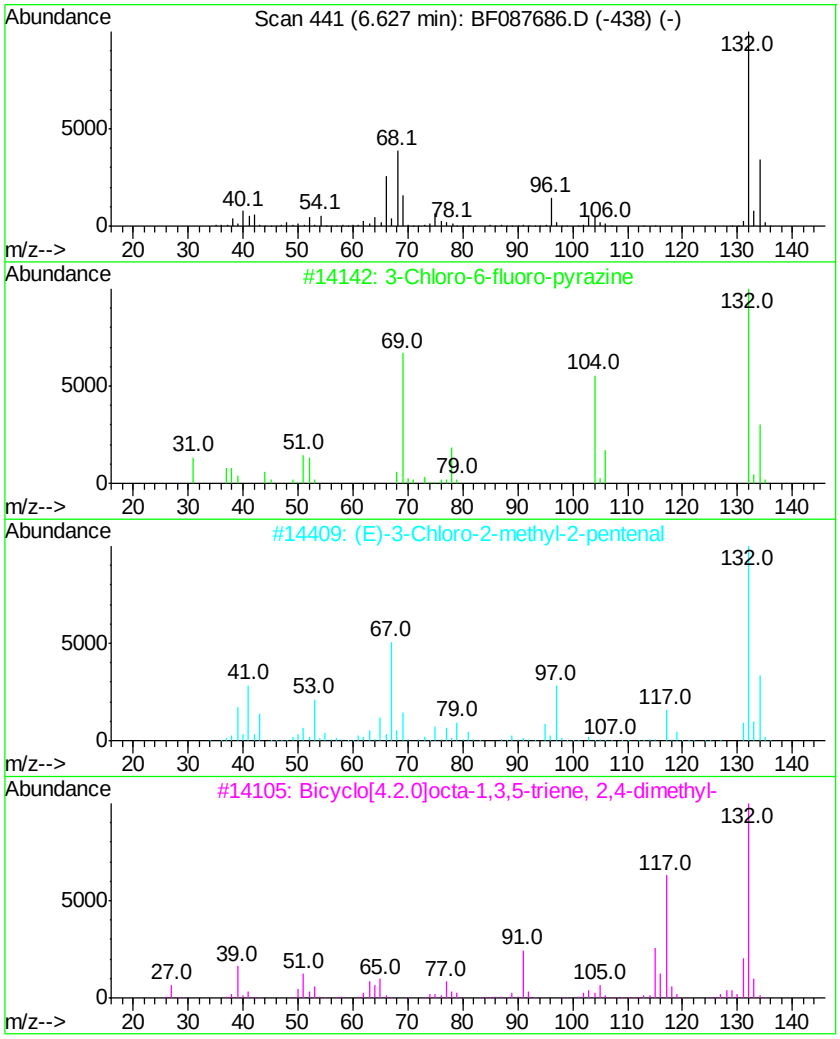
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

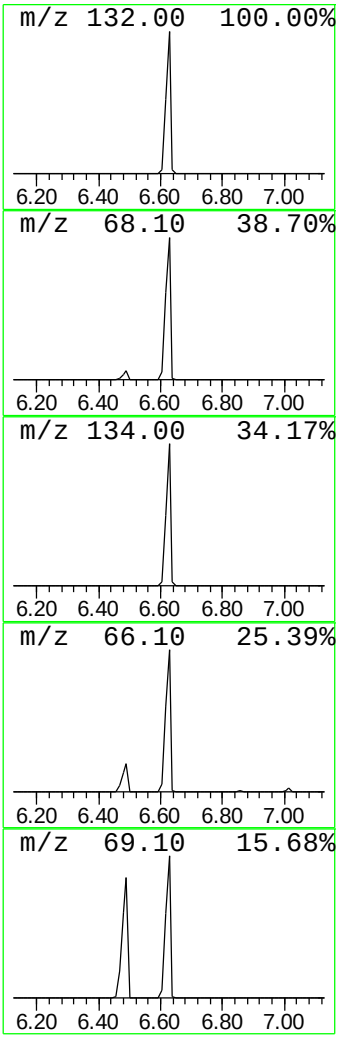
****

Peak Number 5 unknown6.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	92.97 ng	3261080	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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

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TIC Library : C:\Database\NIST11.L
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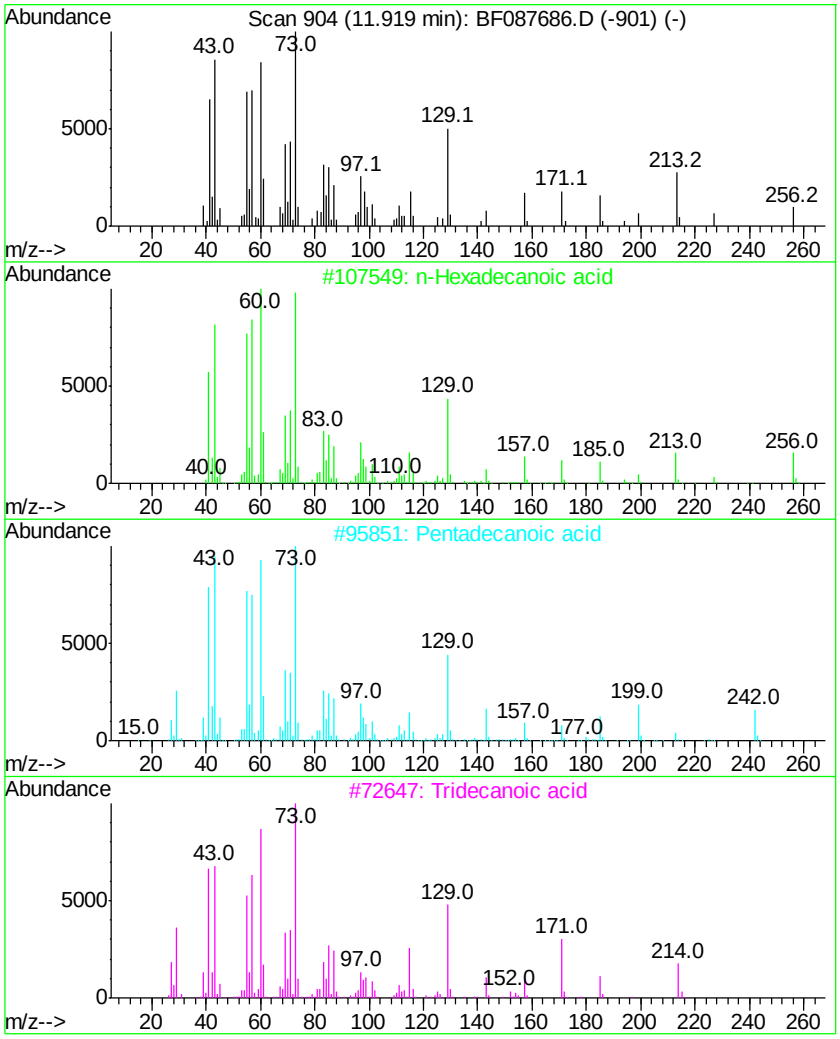
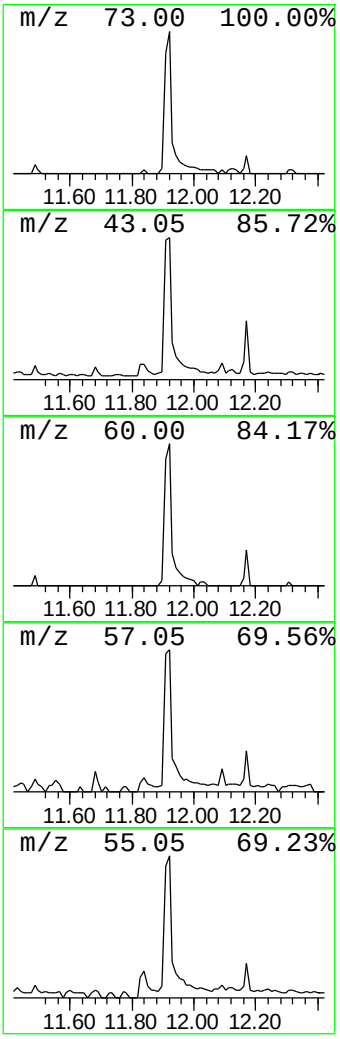
Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.06 ng	216582	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	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	46
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





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TIC Library : C:\Database\NIST11.L
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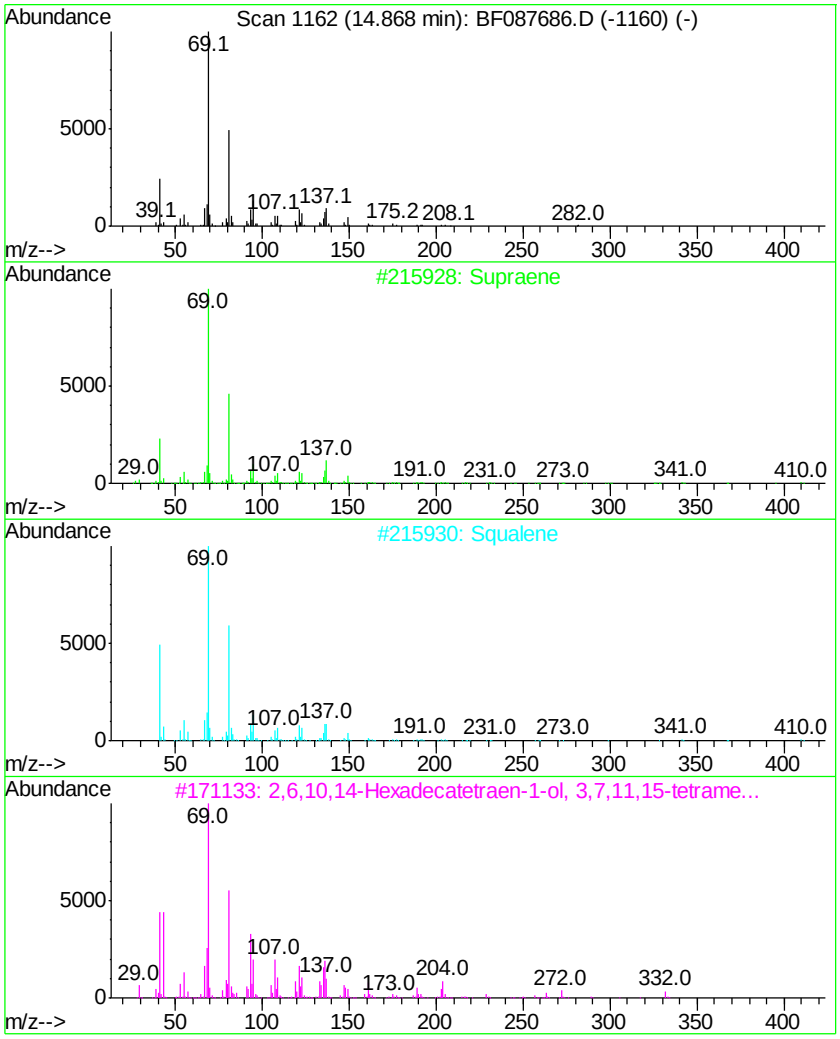
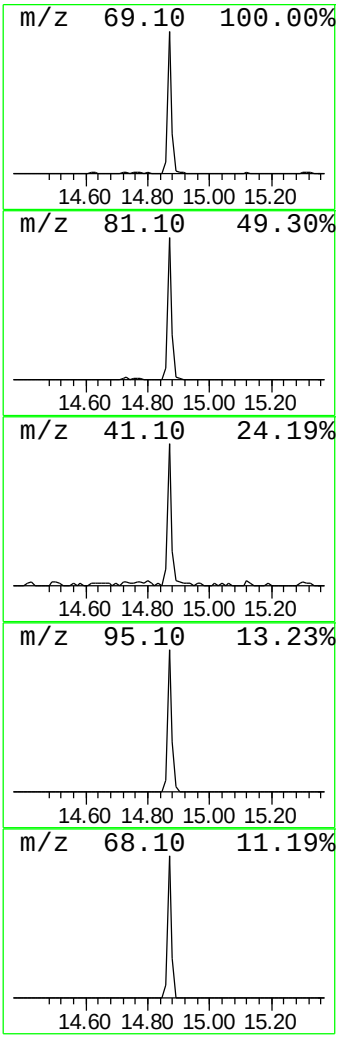
Peak Number 8 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	6.39 ng	230951	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





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	223.1	ng	7825520	1	6.86	701508	20.0
Propane, 1,1-dime...	2.17	11.7	ng	411670	1	6.86	701508	20.0
2-Pentanone, 4-hy...	5.05	8.9	ng	313295	1	6.86	701508	20.0
unknown6.63	6.63	93.0	ng	3261080	1	6.86	701508	20.0
n-Hexadecanoic acid	11.92	4.1	ng	216582	4	11.38	1066250	20.0
Supraene	14.87	6.4	ng	230951	6	15.44	722461	20.0