LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108719.D
Acq On : 1 Sep 2018 5:34
Operator : JU/SJ
Sample : J4729-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-D-B

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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	5.231	489	492	500	rBV	25147	34375	1.35%	0.249%
2	5.666	559	566	582	rBV4	40703	242482	9.55%	1.756%
3	6.660	729	735	740	rBV	65799	148996	5.87%	1.079%
4	6.772	751	754	783	rBV	465240	1020825	40.22%	7.394%
5	7.007	790	794	815	rVB	133572	382404	15.07%	2.770%
6	7.154	815	819	854	rVB	1244027	1887074	74.36%	13.668%
7	7.566	885	889	910	rBV	507019	1273138	50.16%	9.221%
8	8.284	1007	1011	1034	rBV	172717	439362	17.31%	3.182%
9	9.354	1189	1193	1224	rBV	1682203	2537903	100.00%	18.382%
10	9.742	1256	1259	1270	rBV	62989	89776	3.54%	0.650%
11	10.036	1306	1309	1326	rBV	316766	452656	17.84%	3.279%
12	10.695	1418	1421	1428	rBV	51660	51487	2.03%	0.373%
13	10.836	1441	1445	1472	rBV	409434	867352	34.18%	6.282%
14	11.542	1561	1565	1583	rBV	267556	508301	20.03%	3.682%
15	13.118	1829	1833	1862	rBV	2119728	2534184	99.85%	18.355%
16	14.089	1988	1998	2009	rBV8	26242	104812	4.13%	0.759%
17	14.195	2012	2016	2025	rBV	405505	564026	22.22%	4.085%
18	15.018	2152	2156	2161	rBV	50386	53474	2.11%	0.387%
19	15.295	2200	2203	2207	rBV	30209	36245	1.43%	0.263%
20	15.707	2268	2273	2276	rBV	36143	51603	2.03%	0.374%
21	15.754	2276	2281	2299	rVB	201577	396344	15.62%	2.871%
22	16.171	2348	2352	2359	rVB2	34132	55408	2.18%	0.401%
23	16.718	2441	2445	2452	rVB3	25693	41522	1.64%	0.301%
24	17.359	2550	2554	2566	rVB8	13657	32582	1.28%	0.236%

Sum of corrected areas: 13806331

LSC Report - Integrated Chromatogram

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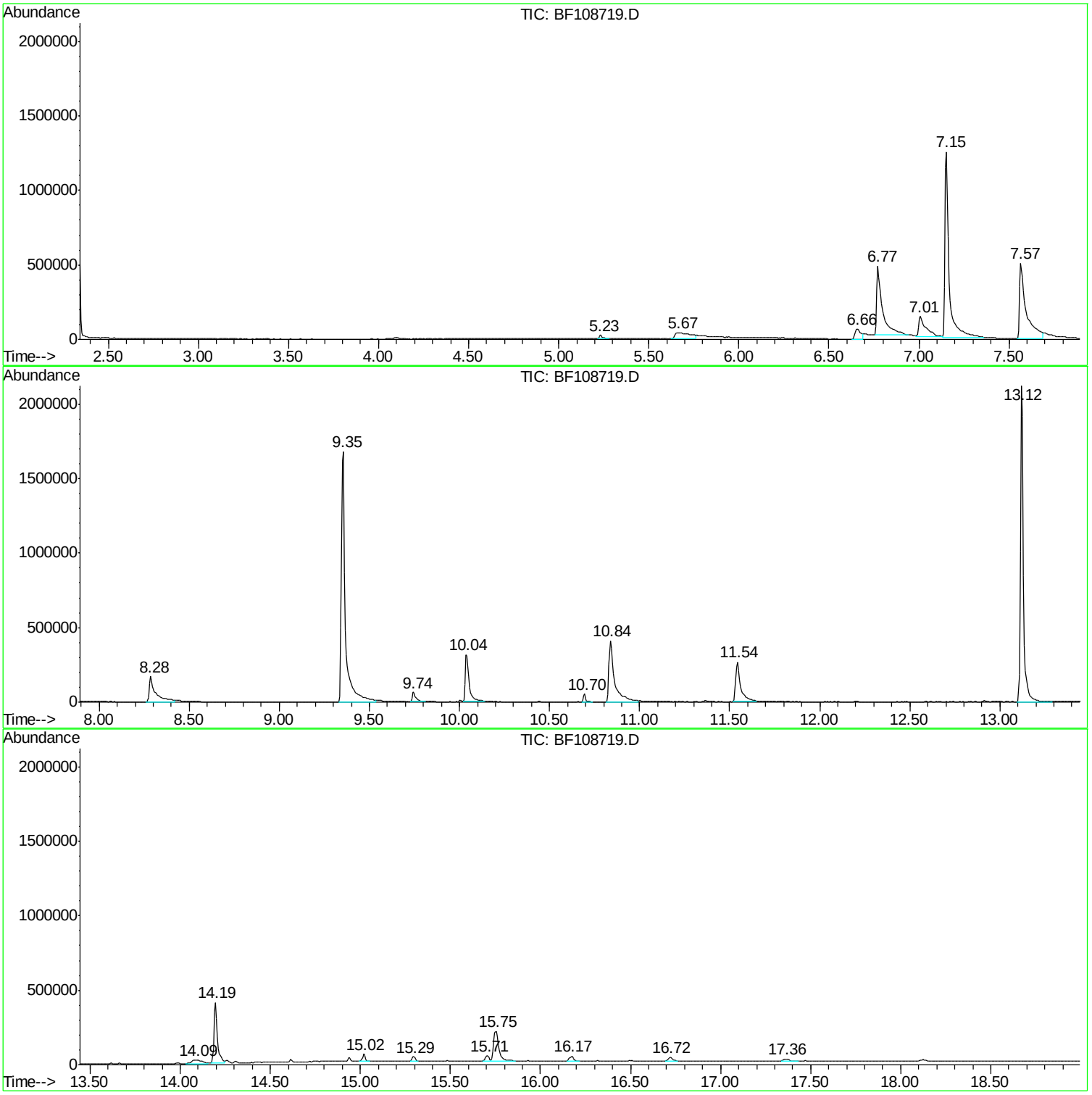
Sample : J4729-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108719.D
Acq On : 1 Sep 2018 5:34
Operator : JU/SJ
Sample : J4729-05
Misc :
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Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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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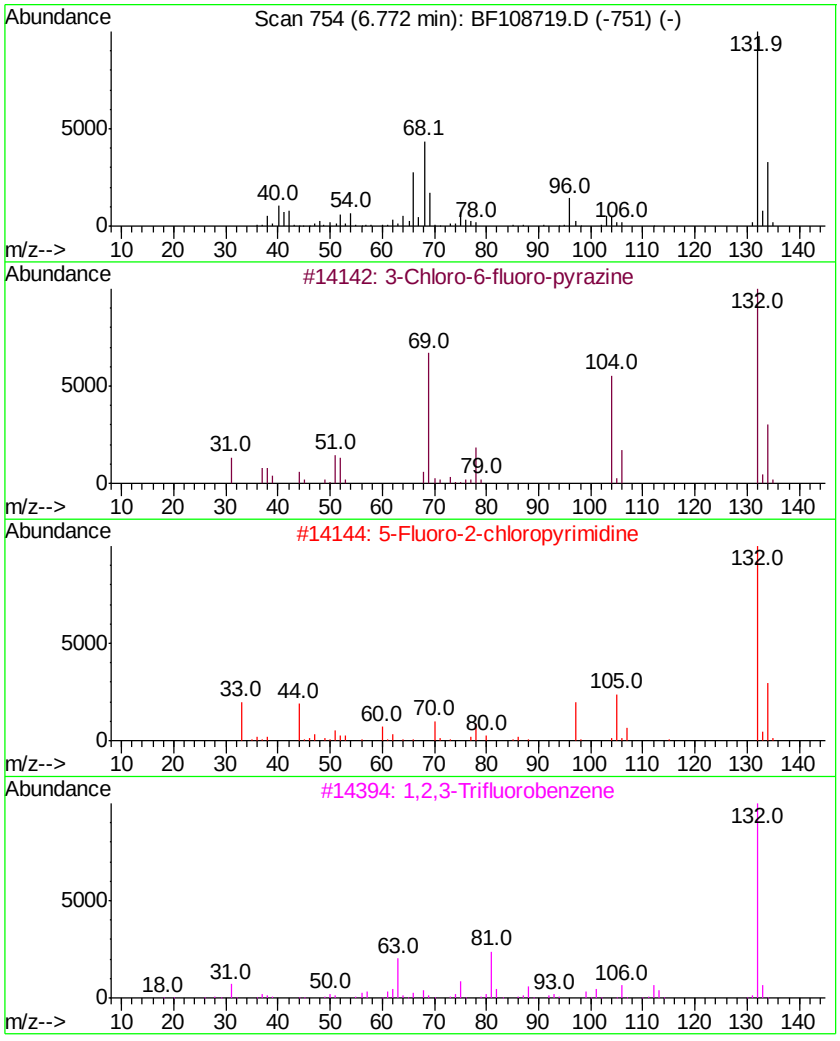
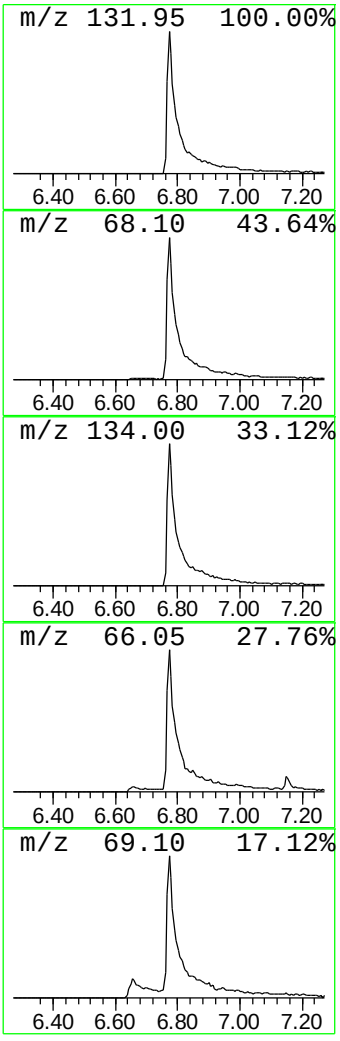
Peak Number 1 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	53.39 ng	1020830	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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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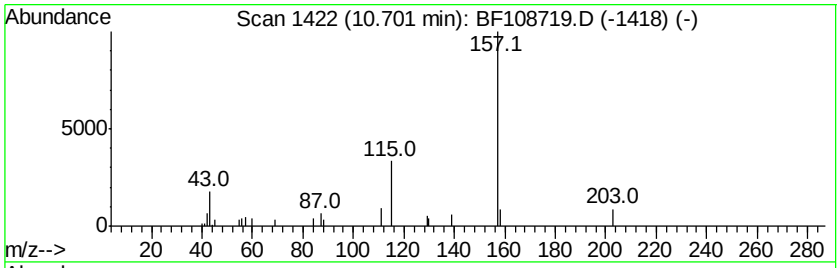
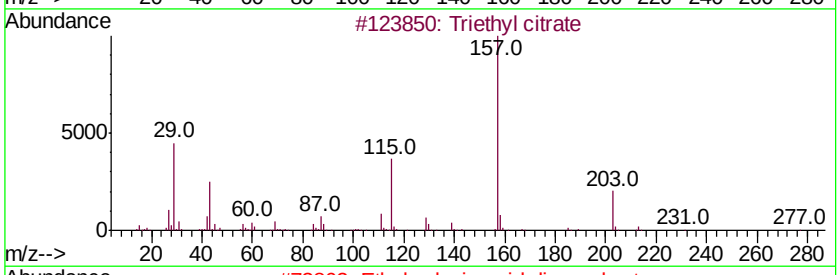
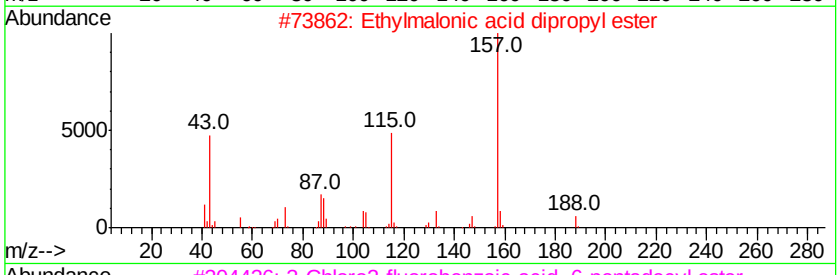
Peak Number 3 Triethyl citrate Concentration Rank 6

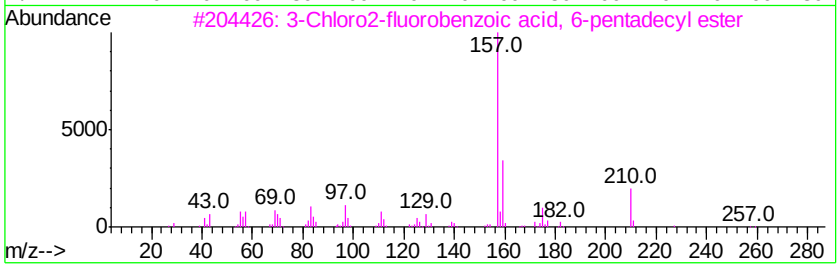
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.27 ng	51487	Acenaphthene-d10	10.04

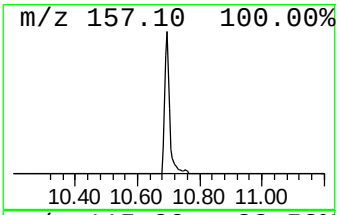
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	86
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	50
3	3-Chloro2-fluorobenzoic acid, 6-...	384	C22H34ClFO2	1000338-65-3	42
4	2-Chlorobenzoic acid, hexadecyl ...	380	C23H37ClO2	070152-86-2	40
5	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	38

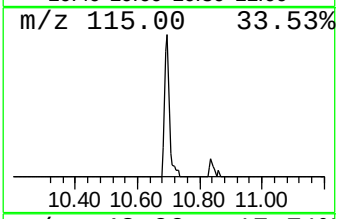


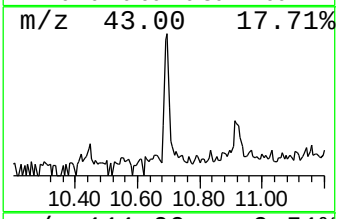


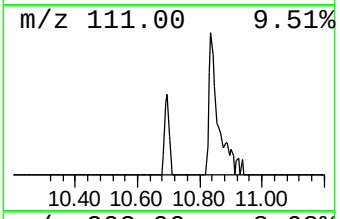


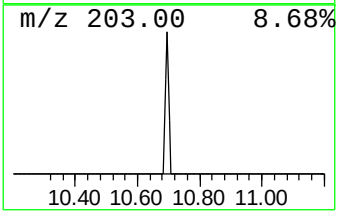












Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

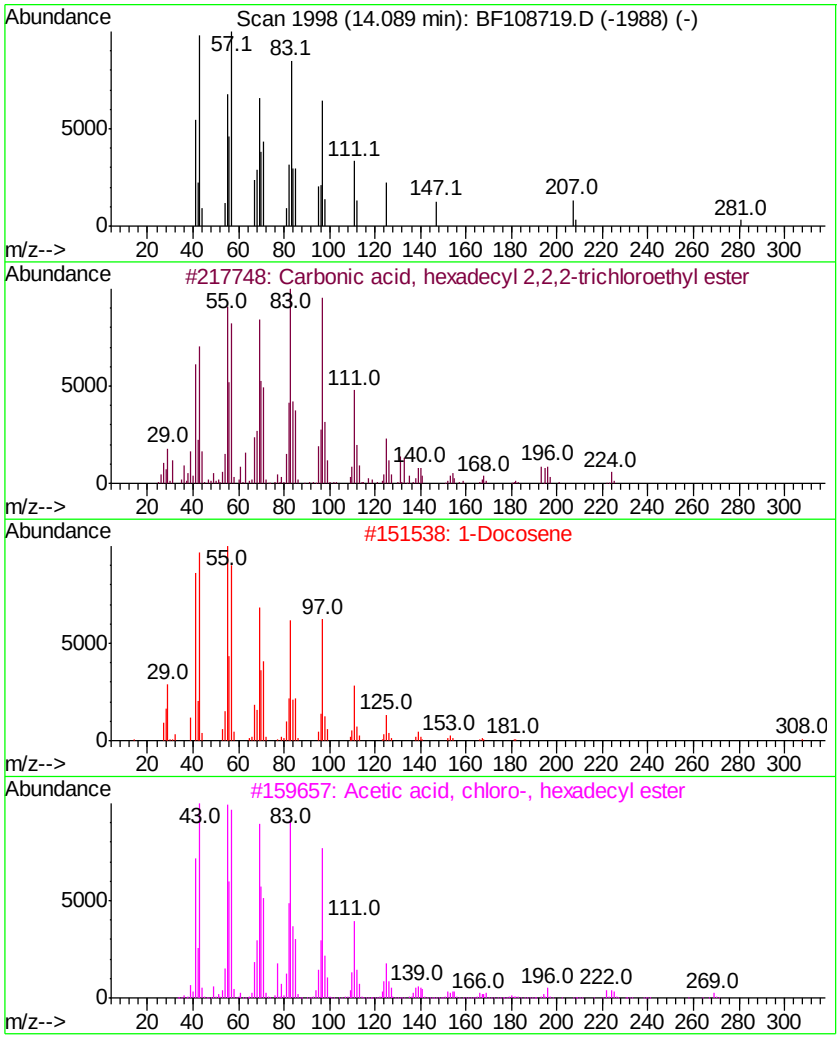
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

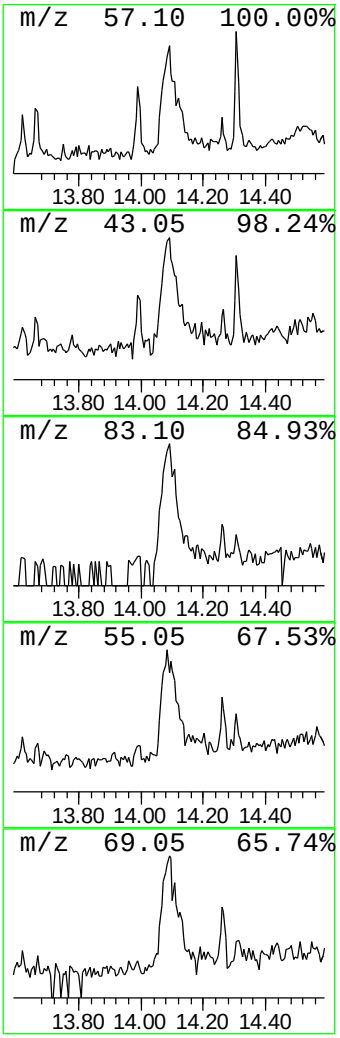
****

Peak Number 4 Carbonic acid, hexadecyl 2,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	3.72 ng	104812	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	91
2	1-Docosene	308	C22H44	001599-67-3	90
3	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	87





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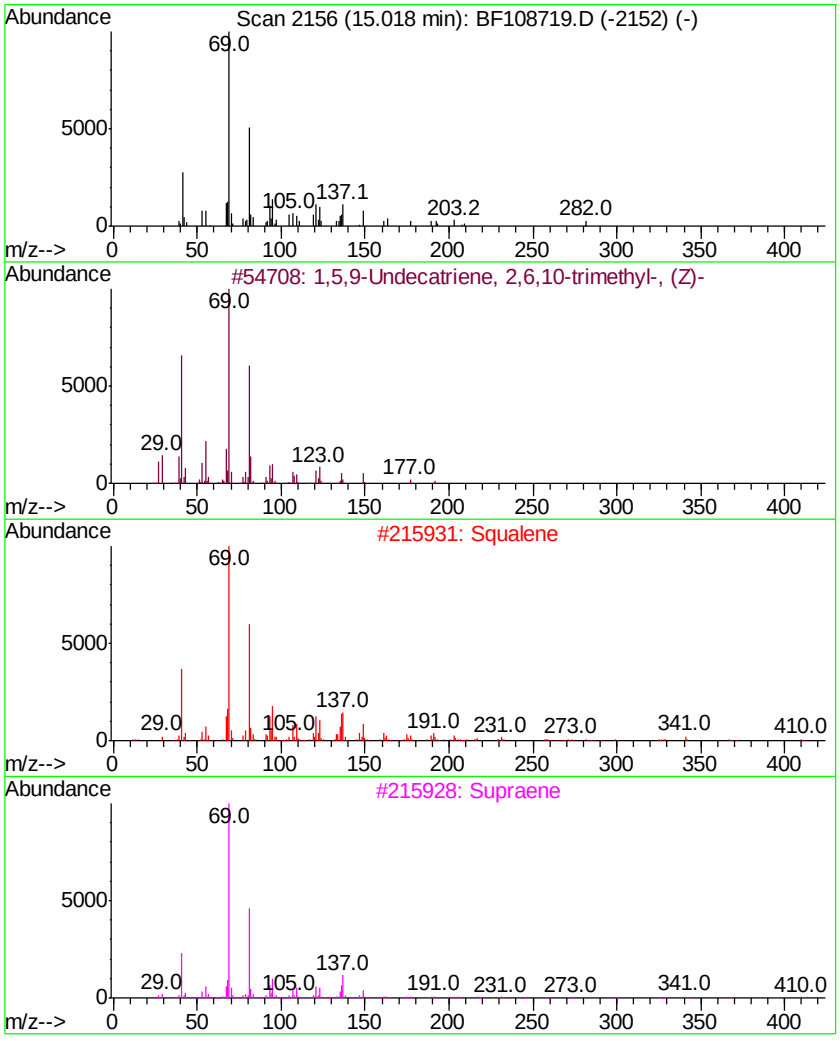
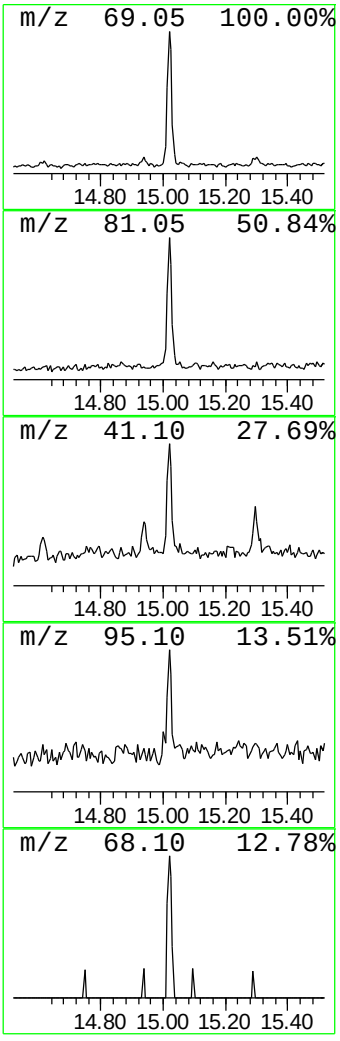
****

Peak Number 5 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.70 ng	53474	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
2	Squalene	410	C30H50	000111-02-4	87
3	Supraene	410	C30H50	007683-64-9	87
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





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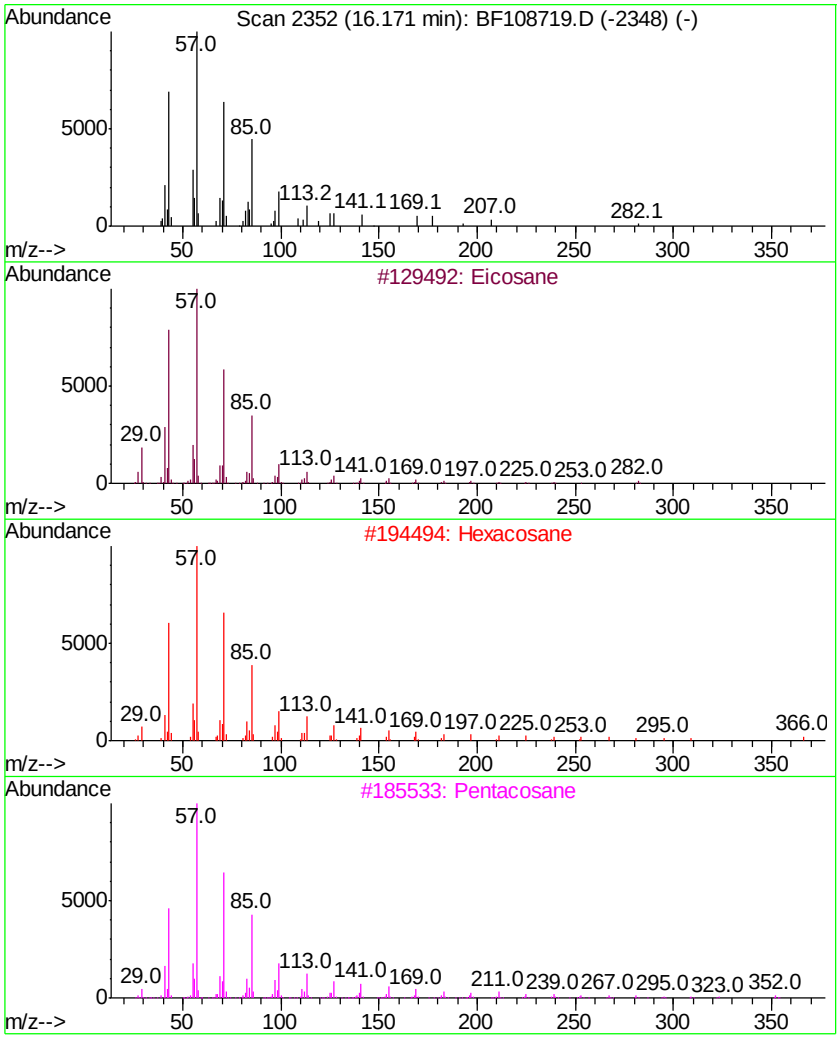
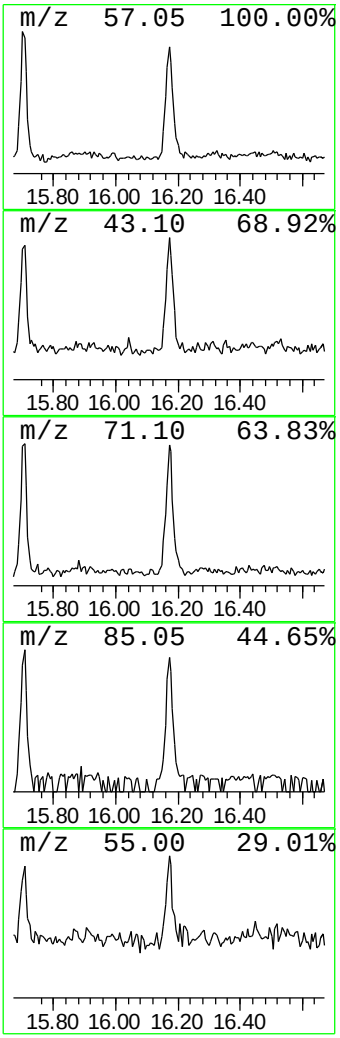
****

Peak Number 6 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.80 ng	55408	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Octadecane	254	C18H38	000593-45-3	90





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

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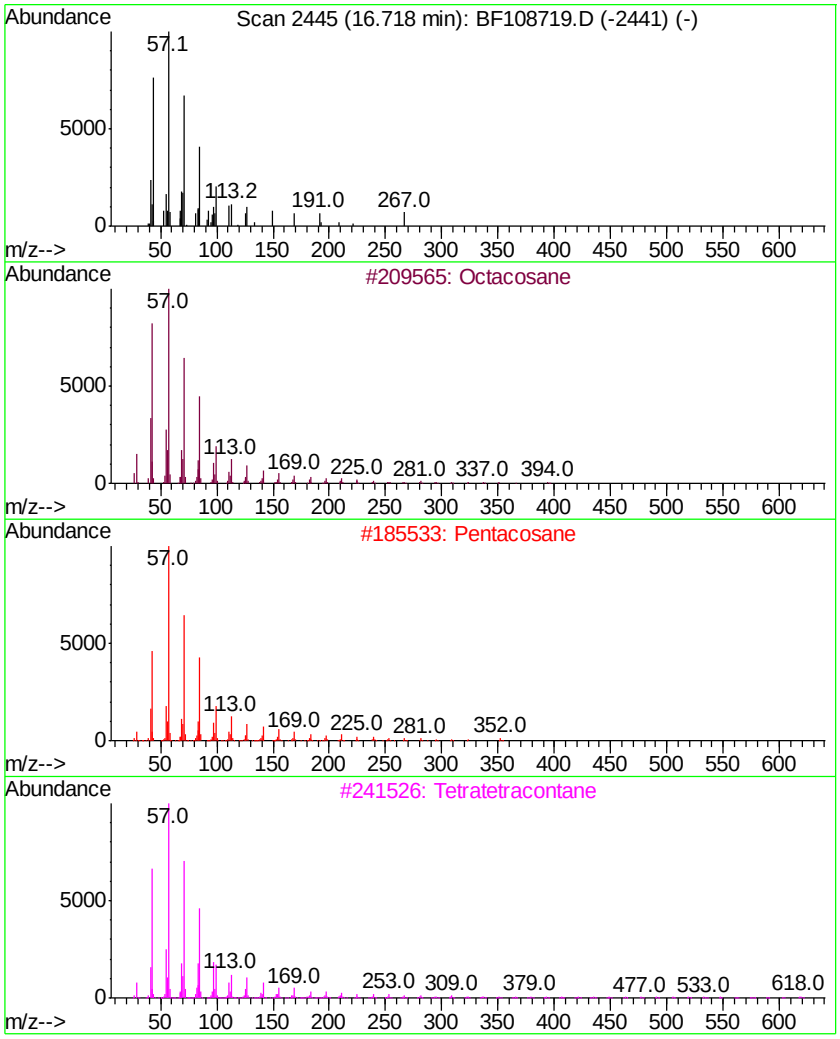
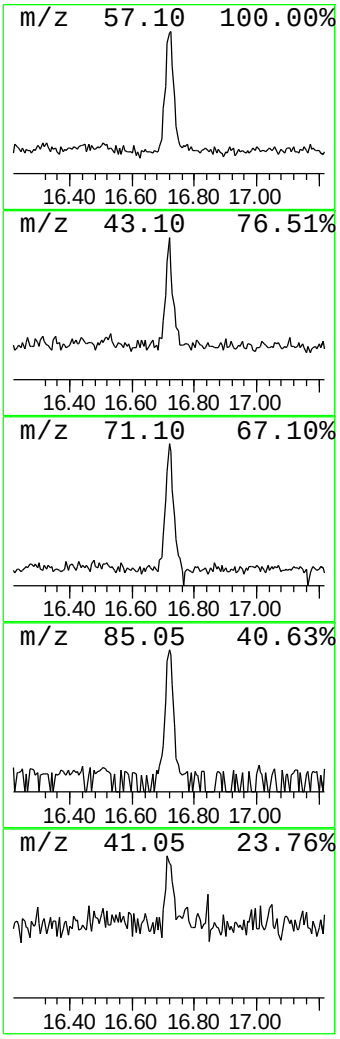
Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	2.10 ng	41522	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Pentacosane	352	C25H52	000629-99-2	90
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Heptacosane	380	C27H56	000593-49-7	78
5	Hexadecane	226	C16H34	000544-76-3	78





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
unknown6.77	6.77	53.4	ng	1020830	1	7.01	382404	20.0
Triethyl citrate	10.70	2.3	ng	51487	3	10.04	452656	20.0
Carbonic acid, he...	14.09	3.7	ng	104812	5	14.19	564026	20.0
1,5,9-Undecatrien...	15.02	2.7	ng	53474	6	15.75	396344	20.0
Eicosane	16.17	2.8	ng	55408	6	15.75	396344	20.0
Octacosane	16.72	2.1	ng	41522	6	15.75	396344	20.0