LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112850.D
Acq On : 5 Mar 2019 12:44
Operator : JU/SJ
Sample : K1704-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B106-022719

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-BF022719.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	5.357	551	556	559	rBV	3704592	3843252	86.39%	9.275%
2	6.381	725	730	733	rBV	3571918	4115984	92.52%	9.933%
3	6.516	748	753	756	rBV	4292269	4115714	92.52%	9.933%
4	6.745	788	792	795	rBV	1240821	1015725	22.83%	2.451%
5	6.904	814	819	822	rBV	3517948	3209851	72.16%	7.747%
6	7.304	882	887	890	rBV	2615907	2559172	57.53%	6.176%
7	8.027	1006	1010	1024	rBV	1239325	1270892	28.57%	3.067%
8	9.104	1188	1193	1196	rBV	4718840	4448549	100.00%	10.736%
9	9.492	1255	1259	1271	rVB	263691	254074	5.71%	0.613%
10	9.774	1303	1307	1321	rVB	1551670	1388323	31.21%	3.351%
11	10.557	1436	1440	1452	rBV	2644660	2798888	62.92%	6.755%
12	11.004	1512	1516	1522	rVB	142625	185170	4.16%	0.447%
13	11.251	1555	1558	1566	rBV	1357123	1359997	30.57%	3.282%
14	11.792	1646	1650	1658	rBV	588393	811952	18.25%	1.960%
15	11.851	1658	1660	1665	rVB3	73952	97232	2.19%	0.235%
16	12.574	1780	1783	1797	rVB	589298	1043456	23.46%	2.518%
17	12.839	1823	1828	1831	rBV	3873030	3718061	83.58%	8.973%
18	13.739	1977	1981	1987	rBV	595888	723418	16.26%	1.746%
19	13.880	2001	2005	2012	rVB	1260360	1244308	27.97%	3.003%
20	14.062	2034	2036	2047	rVB	117907	222025	4.99%	0.536%
21	14.368	2085	2088	2094	rBV2	181312	244867	5.50%	0.591%
22	14.662	2135	2138	2145	rVB	171903	225839	5.08%	0.545%
23	14.733	2147	2150	2152	rBV	93647	115223	2.59%	0.278%
24	14.986	2189	2193	2195	rBV	173730	226591	5.09%	0.547%
25	15.292	2240	2245	2250	rBV	973865	1165095	26.19%	2.812%
26	15.339	2250	2253	2267	rVB	212801	385130	8.66%	0.929%
27	15.745	2319	2322	2327	rVB	189293	266096	5.98%	0.642%
28	15.798	2327	2331	2338	rVB2	134805	230650	5.18%	0.557%
29	16.221	2399	2403	2407	rBV	90258	150556	3.38%	0.363%

Sum of corrected areas: 41436090

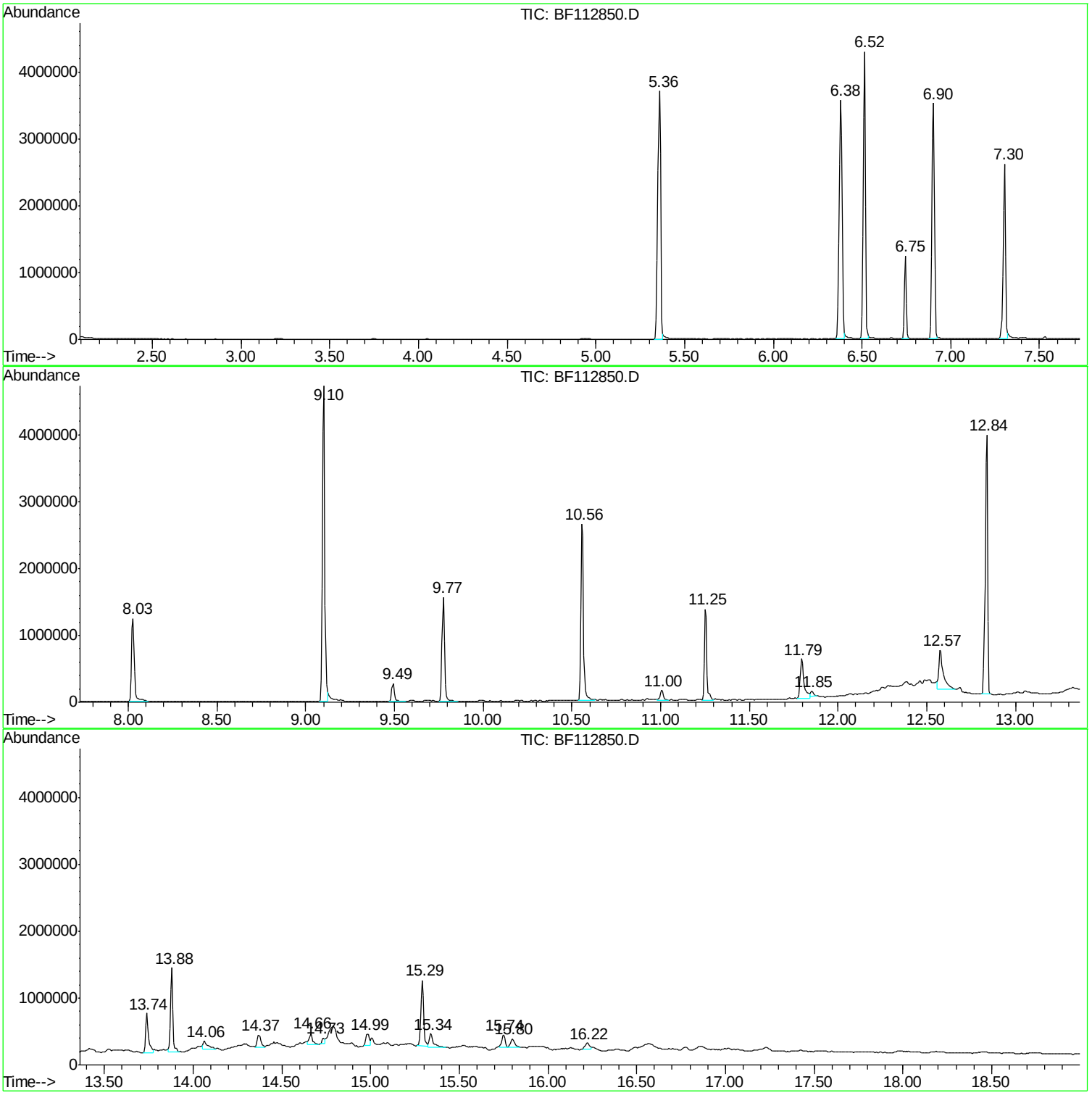
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112850.D
Acq On : 5 Mar 2019 12:44
Operator : JU/SJ
Sample : K1704-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-028-B106-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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

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ClientSampleId : PST-028-B106-022719

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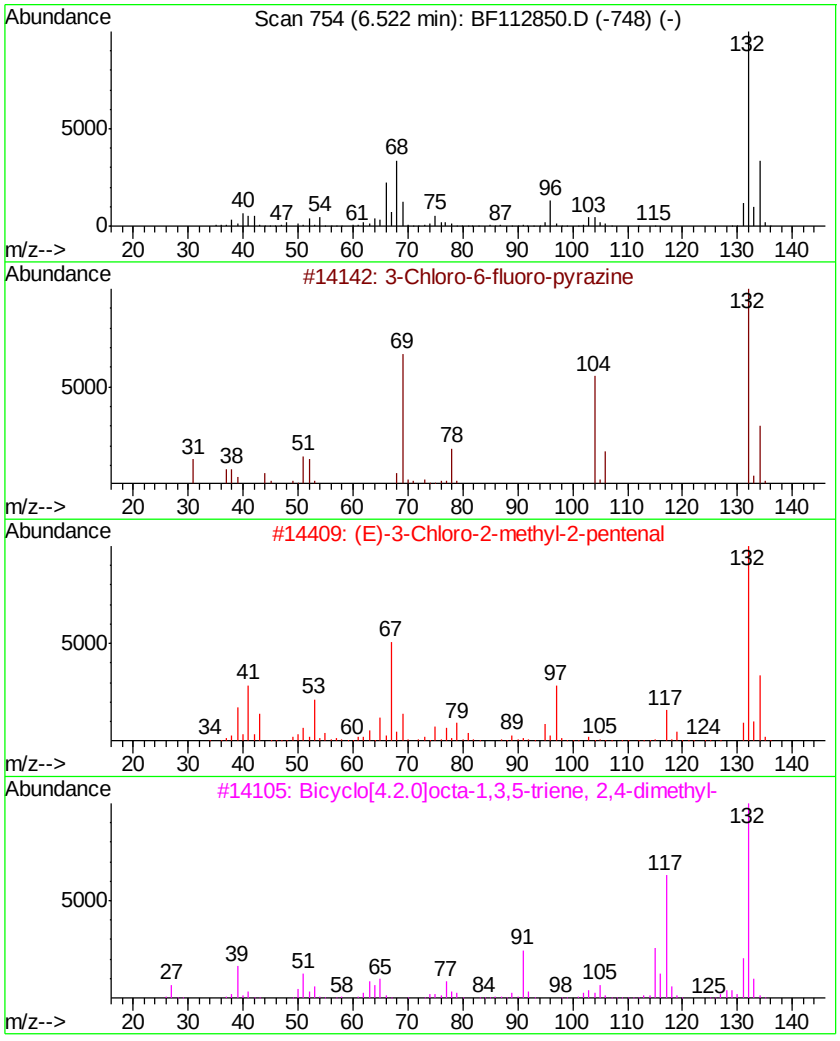
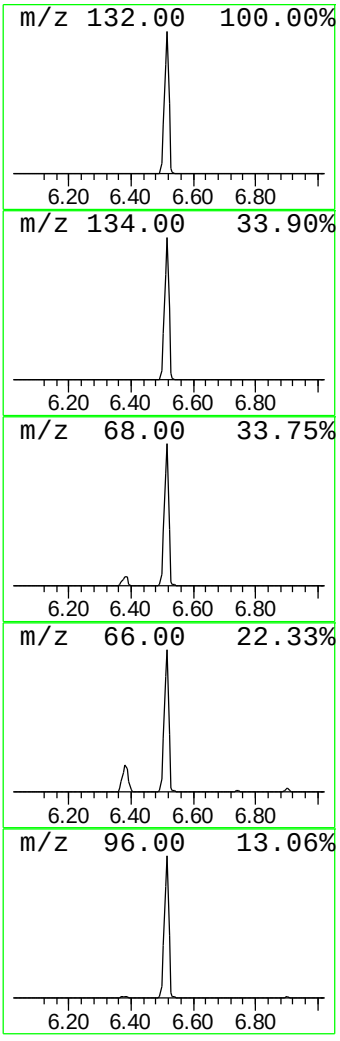
Peak Number 1 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	81.04 ng	4115710	1,4-Dichlorobenzene-d4	6.75

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	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument : BNA_F
ClientSampleId : PST-028-B106-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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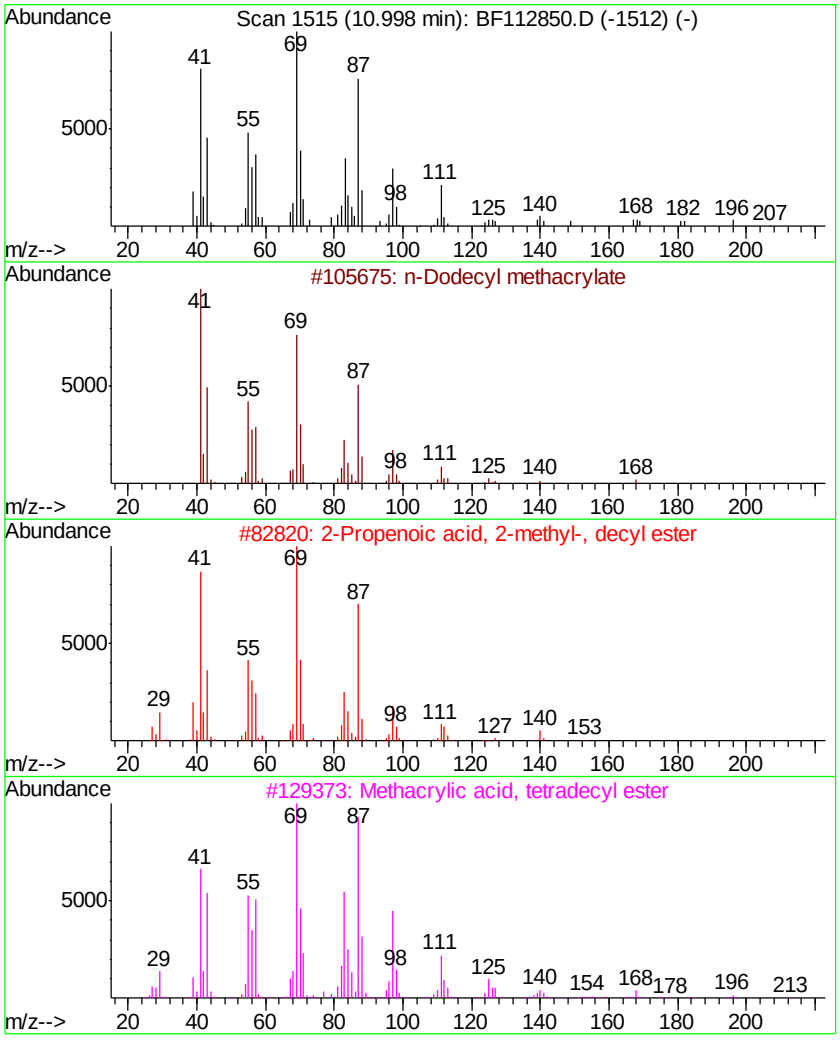
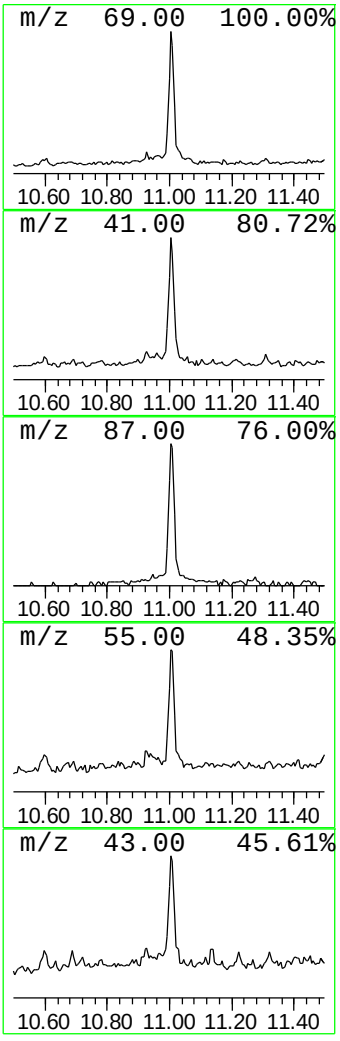
Peak Number 3 n-Dodecyl methacrylate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	2.72 ng	185170	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	91
2	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	86
3	Methacrylic acid, tetradecyl ester	282	C18H34O2	1000340-29-0	58
4	Cyclopentane, 1-butyl-2-propyl-	168	C12H24	062199-50-2	52
5	Cyclopentane, (3-methylbutyl)-	140	C10H20	001005-68-1	52





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Sample : K1704-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B106-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

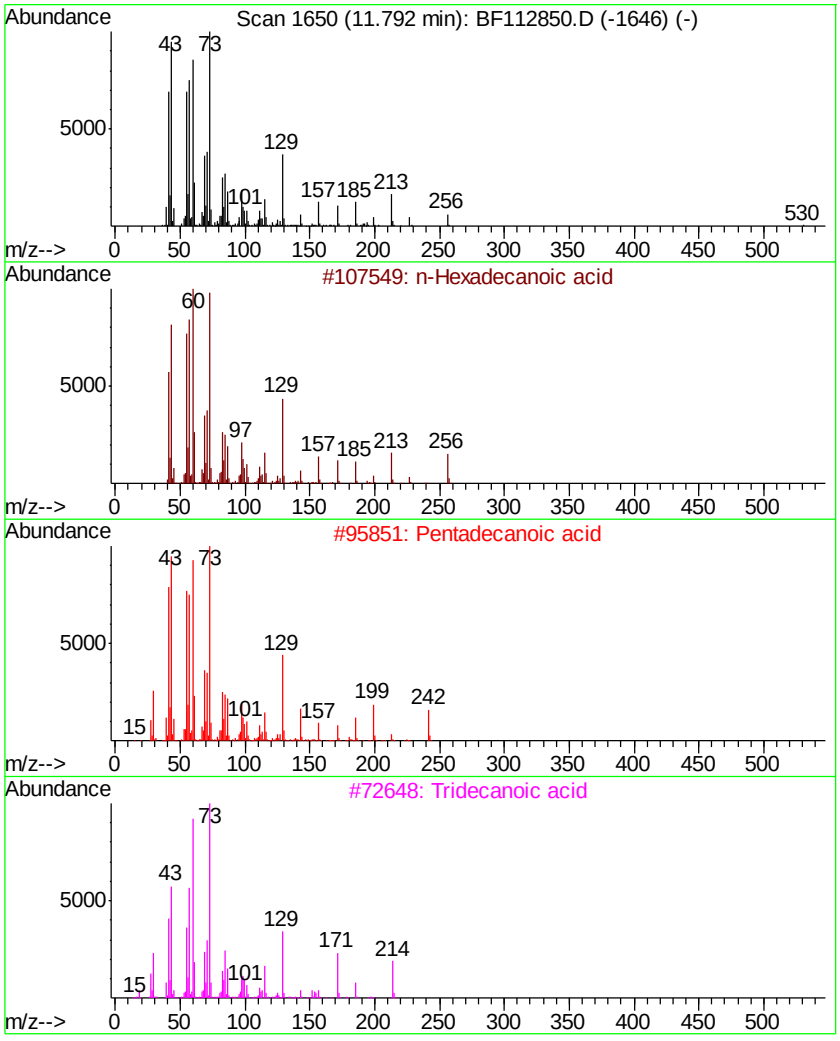
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

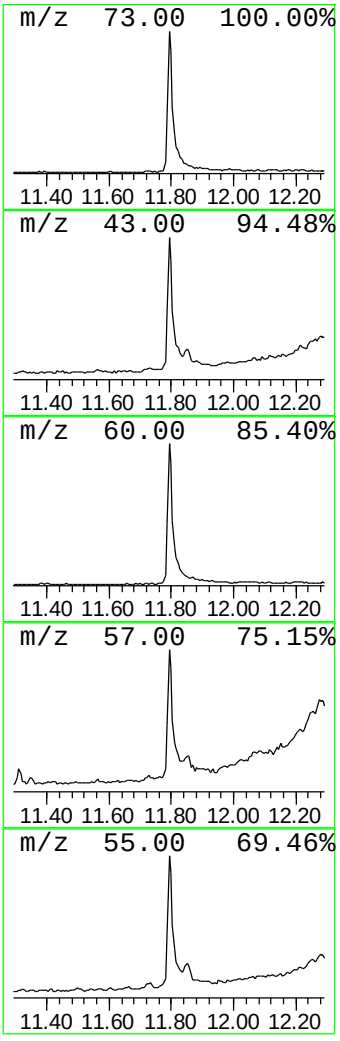
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	11.94 ng	811952	Phenanthrene-d10	11.25

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	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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Operator : JU/SJ
Sample : K1704-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B106-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

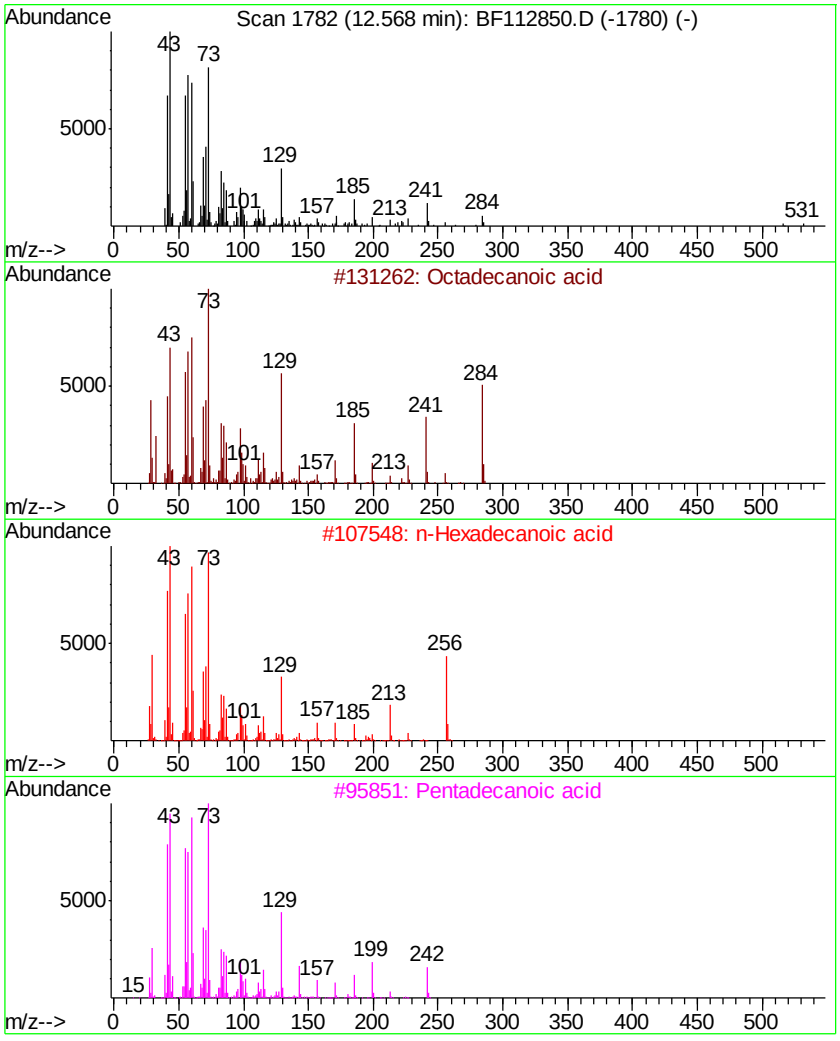
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

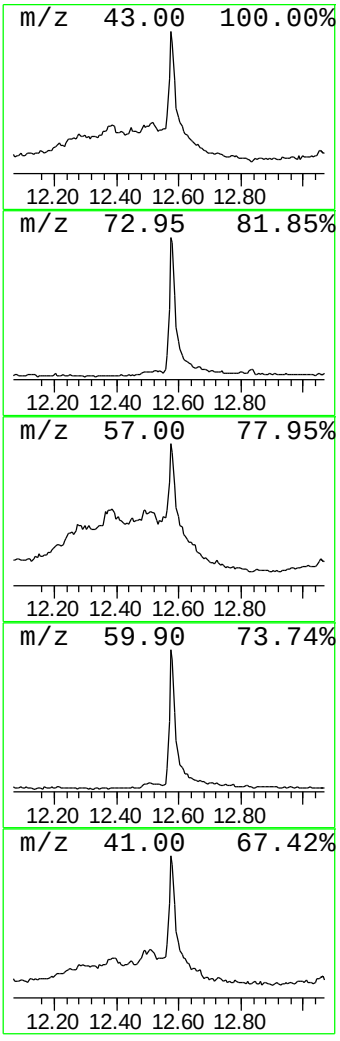
****

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	16.77 ng	1043460	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	81





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Misc :
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Instrument : BNA_F
ClientSampleId : PST-028-B106-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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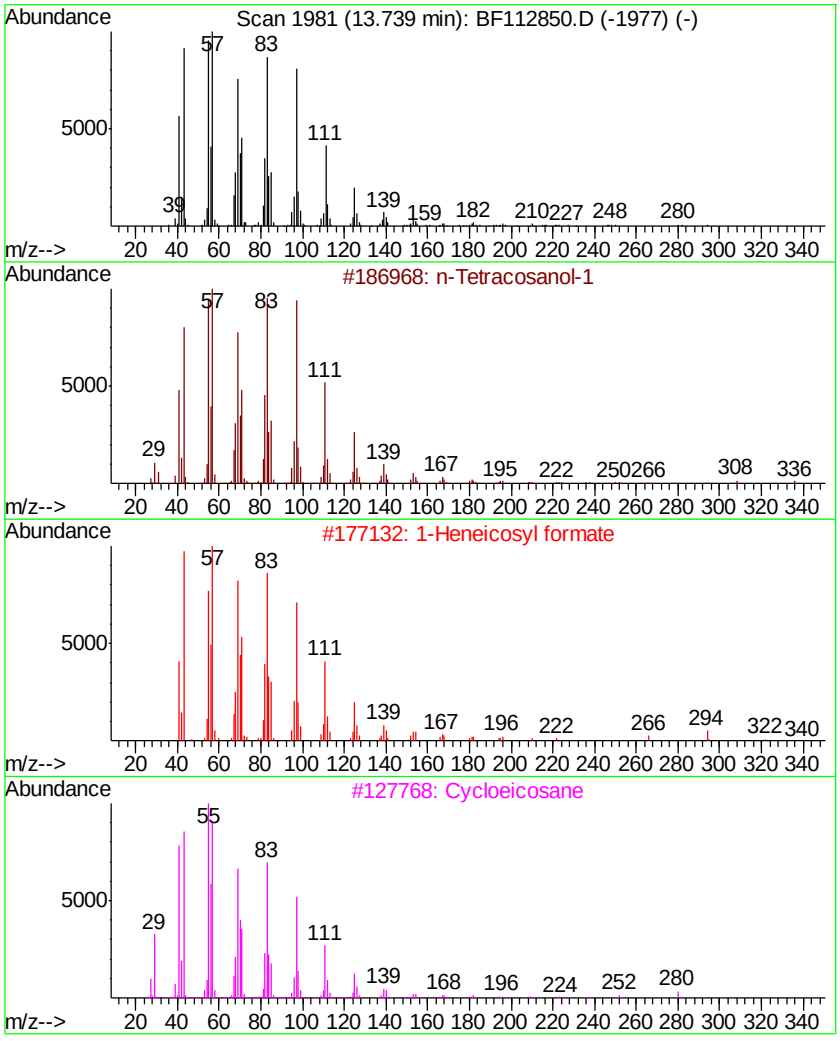
TIC Integration Parameters: LSCINT.P

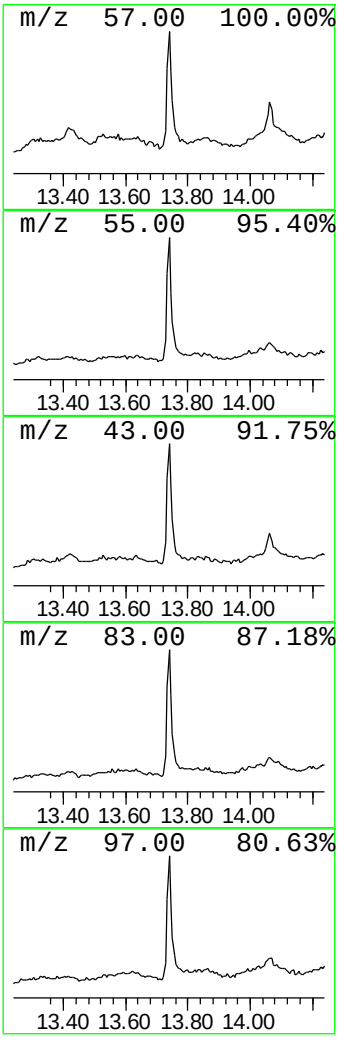
****

Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	11.63 ng	723418	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Cycloeicosane	280	C20H40	000296-56-0	93
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





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Misc :
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Instrument : BNA_F
ClientSampleId : PST-028-B106-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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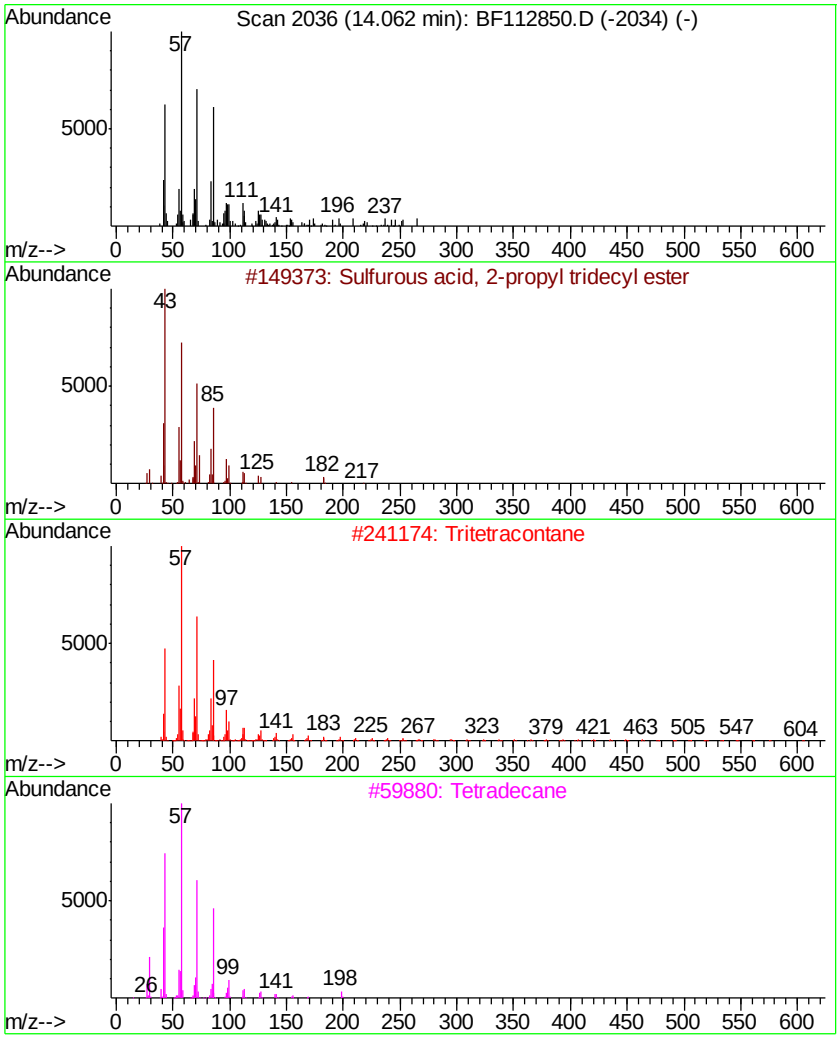
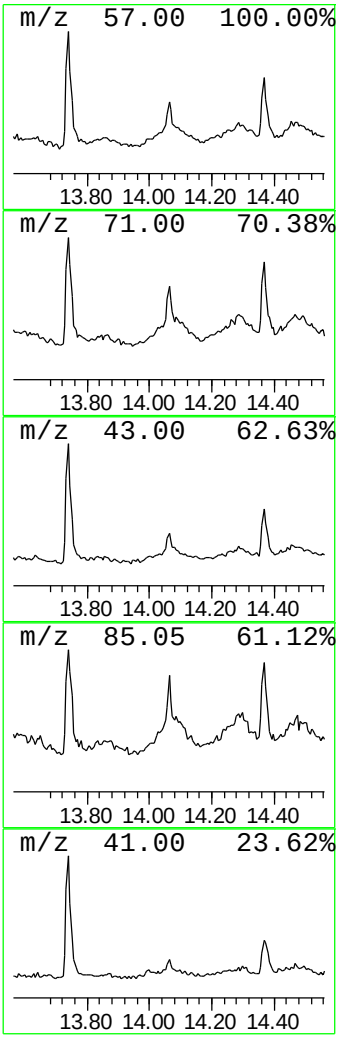
****

Peak Number 7 Sulfurous acid, 2-propyl tr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.06	3.57 ng	222025	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	64
2	Tritetracontane	605	C43H88	007098-21-7	53
3	Tetradecane	198	C14H30	000629-59-4	52
4	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	38
5	Sulfurous acid, pentyl tetradecy...	348	C19H40O3S	1000309-14-7	35





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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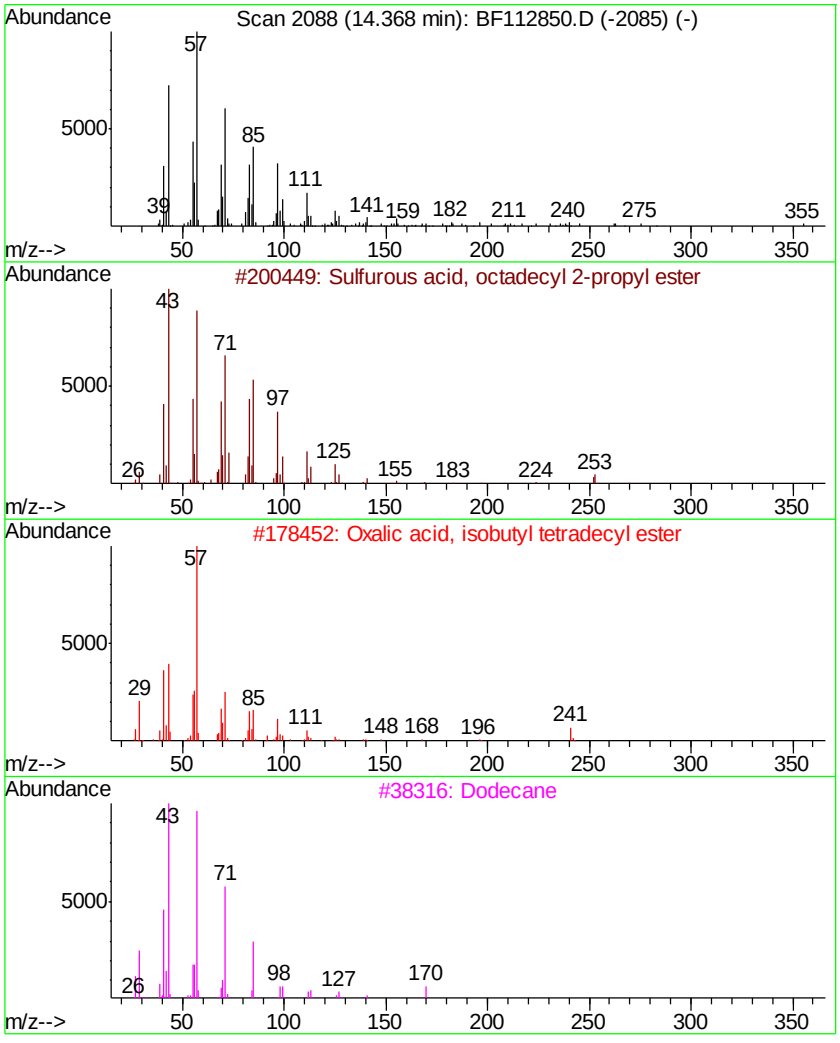
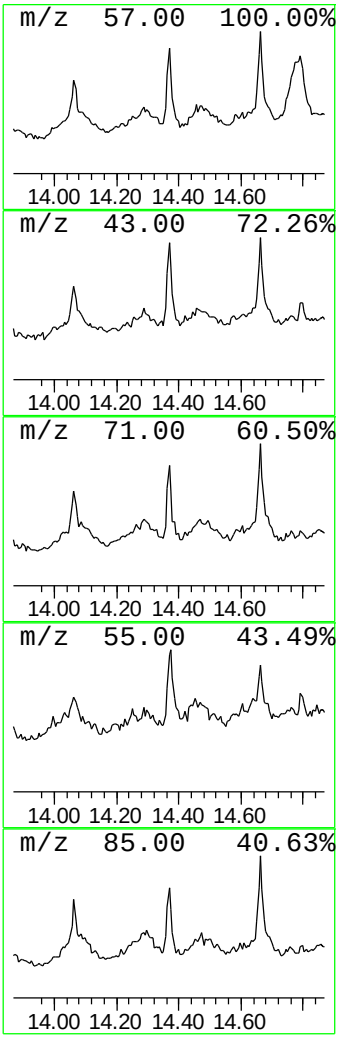
Peak Number 8 Sulfurous acid, octadecyl 2... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	3.94 ng	244867	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	83
2	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	83
3	Dodecane	170	C12H26	000112-40-3	70
4	Heptadecane	240	C17H36	000629-78-7	70
5	Undecane	156	C11H24	001120-21-4	70





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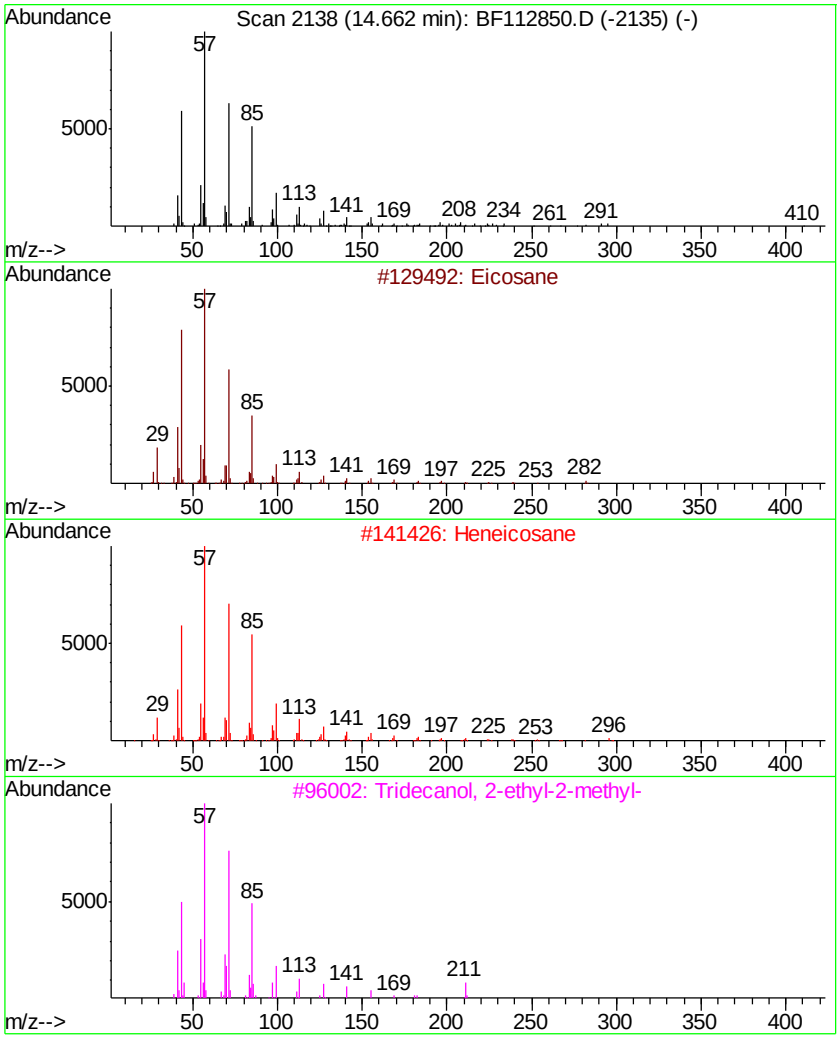
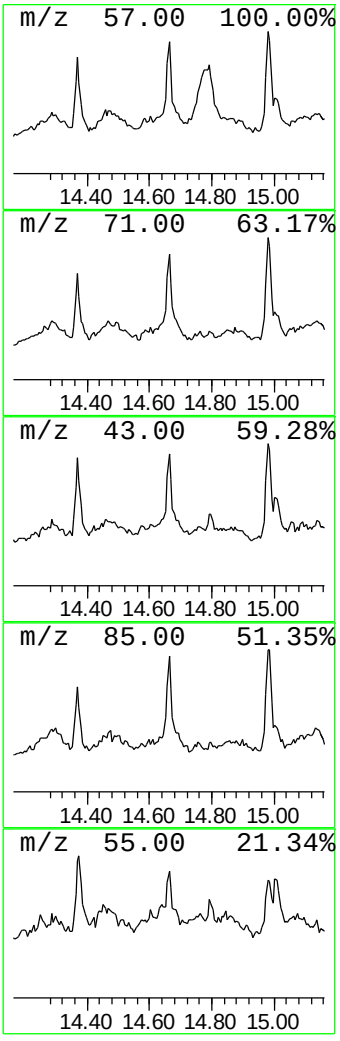
Peak Number 9 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.88 ng	225839	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86
4	Docosane	310	C22H46	000629-97-0	78
5	Octadecane	254	C18H38	000593-45-3	78





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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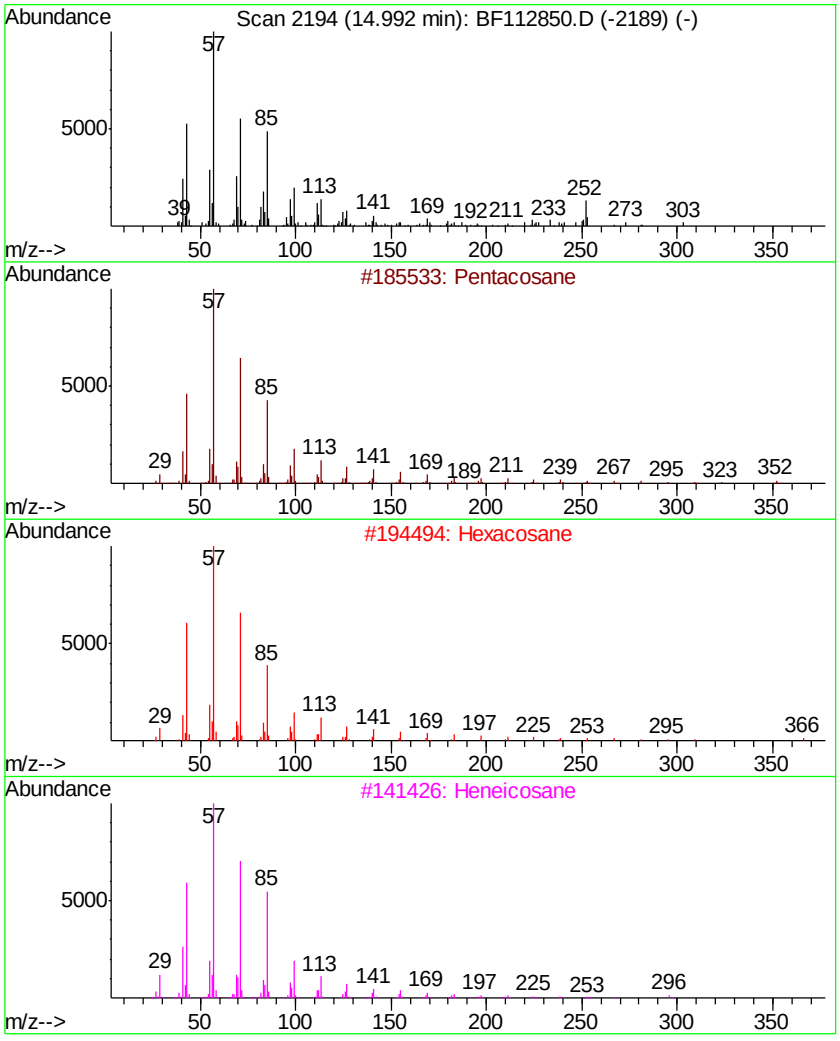
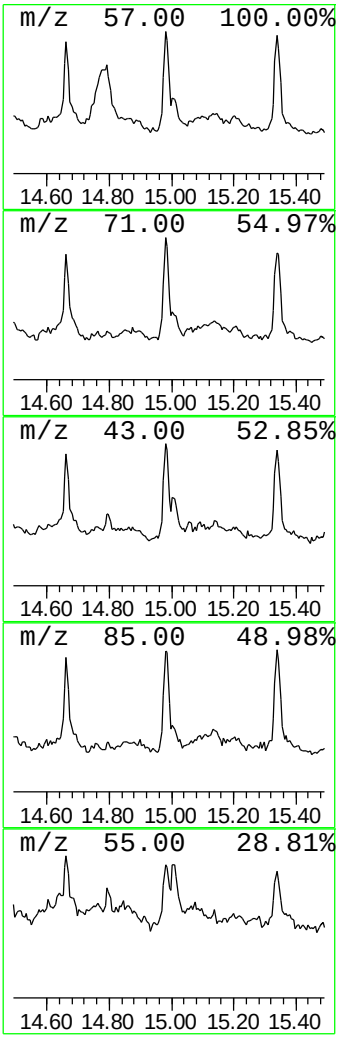
Peak Number 10 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	3.89 ng	226591	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





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Instrument : BNA_F
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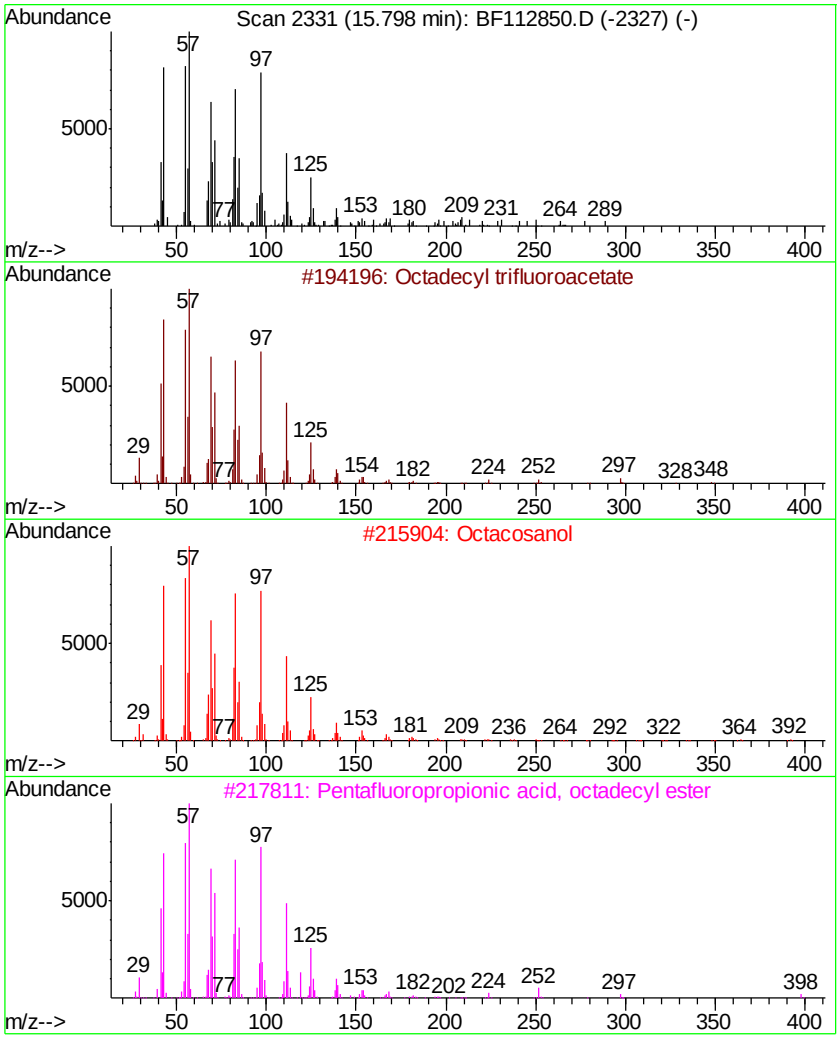
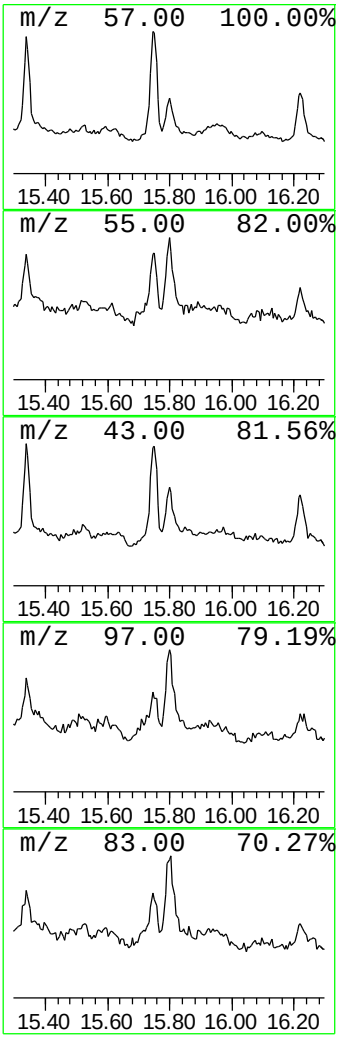
Peak Number 12 Octadecyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	3.96 ng	230650	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	95
2	Octacosanol	410	C28H58O	000557-61-9	95
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	95
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	95
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	95





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112850.D
Acq On : 5 Mar 2019 12:44
Operator : JU/SJ
Sample : K1704-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B106-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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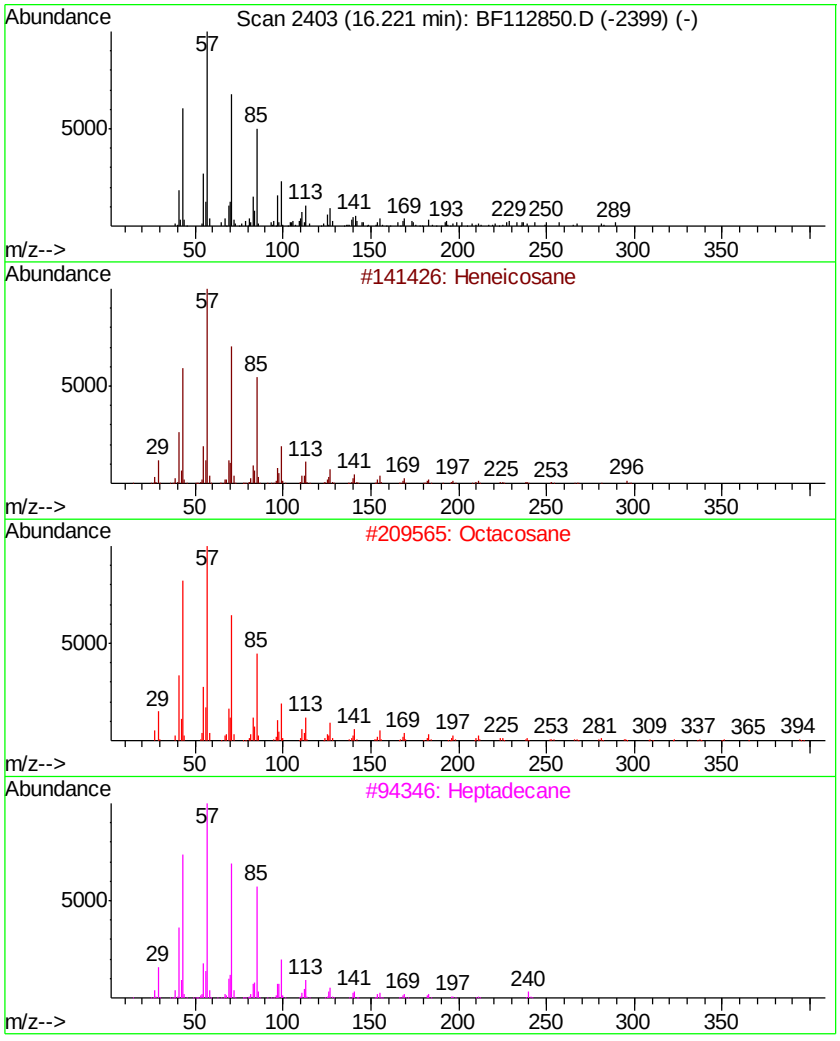
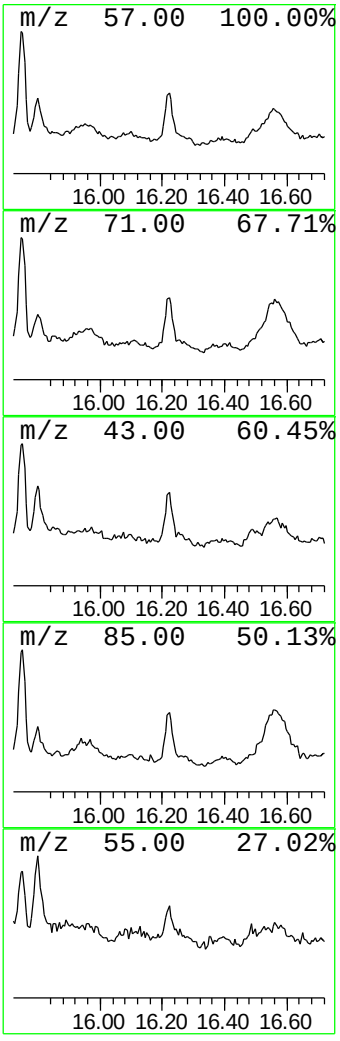
Peak Number 13 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	2.58 ng	150556	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane	240	C17H36	000629-78-7	86
4	Hexacosane	366	C26H54	000630-01-3	83
5	2-methyloctacosane	408	C29H60	1000376-72-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
Data File : BF112850.D
Acq On : 5 Mar 2019 12:44
Operator : JU/SJ
Sample : K1704-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B106-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.52	6.52	81.0	ng	4115710	1	6.75	1015730	20.0
n-Dodecyl methacr...	11.00	2.7	ng	185170	4	11.25	1360000	20.0
n-Hexadecanoic acid	11.79	11.9	ng	811952	4	11.25	1360000	20.0
Octadecanoic acid	12.57	16.8	ng	1043460	5	13.88	1244310	20.0
n-Tetracosanol-1	13.74	11.6	ng	723418	5	13.88	1244310	20.0
Sulfurous acid, 2...	14.06	3.6	ng	222025	5	13.88	1244310	20.0
Sulfurous acid, o...	14.37	3.9	ng	244867	5	13.88	1244310	20.0
Eicosane	14.66	3.9	ng	225839	6	15.29	1165100	20.0
Pentacosane	14.99	3.9	ng	226591	6	15.29	1165100	20.0
Octadecyl trifluo...	15.80	4.0	ng	230650	6	15.29	1165100	20.0
Heneicosane	16.22	2.6	ng	150556	6	15.29	1165100	20.0