LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112770.D
Acq On : 28 Feb 2019 19:29
Operator : JU/SJ
Sample : K1650-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5(9-10)

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	550	556	559	rBV	3105036	3186553	83.93%	9.206%
2	6.375	724	729	732	rBV	3471680	3385494	89.17%	9.781%
3	6.510	748	752	756	rBV	3584327	3435388	90.48%	9.925%
4	6.745	788	792	795	rBV	1352011	1136084	29.92%	3.282%
5	6.810	800	803	810	rVB	78901	74195	1.95%	0.214%
6	6.898	814	818	822	rBV	2976371	2643923	69.64%	7.638%
7	7.298	881	886	889	rBV	2259533	2133210	56.18%	6.163%
8	8.022	1005	1009	1013	rBV	1541874	1437246	37.85%	4.152%
9	9.098	1188	1192	1203	rBV	4211229	3796805	100.00%	10.969%
10	9.374	1236	1239	1249	rBV	186076	161522	4.25%	0.467%
11	9.492	1255	1259	1262	rBV	238286	214449	5.65%	0.620%
12	9.669	1286	1289	1296	rVB3	25115	42991	1.13%	0.124%
13	9.774	1303	1307	1314	rVB	1791989	1596044	42.04%	4.611%
14	10.557	1435	1440	1443	rBV	2400468	2222238	58.53%	6.420%
15	11.251	1554	1558	1561	rBV	1796924	1537712	40.50%	4.442%
16	11.786	1645	1649	1658	rBV2	348518	363765	9.58%	1.051%
17	12.568	1777	1782	1790	rBV	164403	199026	5.24%	0.575%
18	12.710	1802	1806	1810	rVB	60221	64946	1.71%	0.188%
19	12.833	1822	1827	1830	rBV	3378764	3122350	82.24%	9.020%
20	13.733	1977	1980	1988	rBV2	163637	205789	5.42%	0.595%
21	13.874	2000	2004	2008	rBV	1356670	1173340	30.90%	3.390%
22	14.062	2032	2036	2039	rBV	102788	97669	2.57%	0.282%
23	14.362	2084	2087	2091	rBV	162098	144726	3.81%	0.418%
24	14.662	2135	2138	2142	rVB	208693	199712	5.26%	0.577%
25	14.980	2188	2192	2197	rBV	211603	242535	6.39%	0.701%
26	15.286	2239	2244	2248	rVB	986625	1172343	30.88%	3.387%
27	15.339	2249	2253	2258	rVB	211475	248903	6.56%	0.719%
28	15.745	2318	2322	2327	rBV	158097	228962	6.03%	0.661%
29	16.221	2399	2403	2407	rVB2	96754	146438	3.86%	0.423%

Sum of corrected areas: 34614358

LSC Report - Integrated Chromatogram

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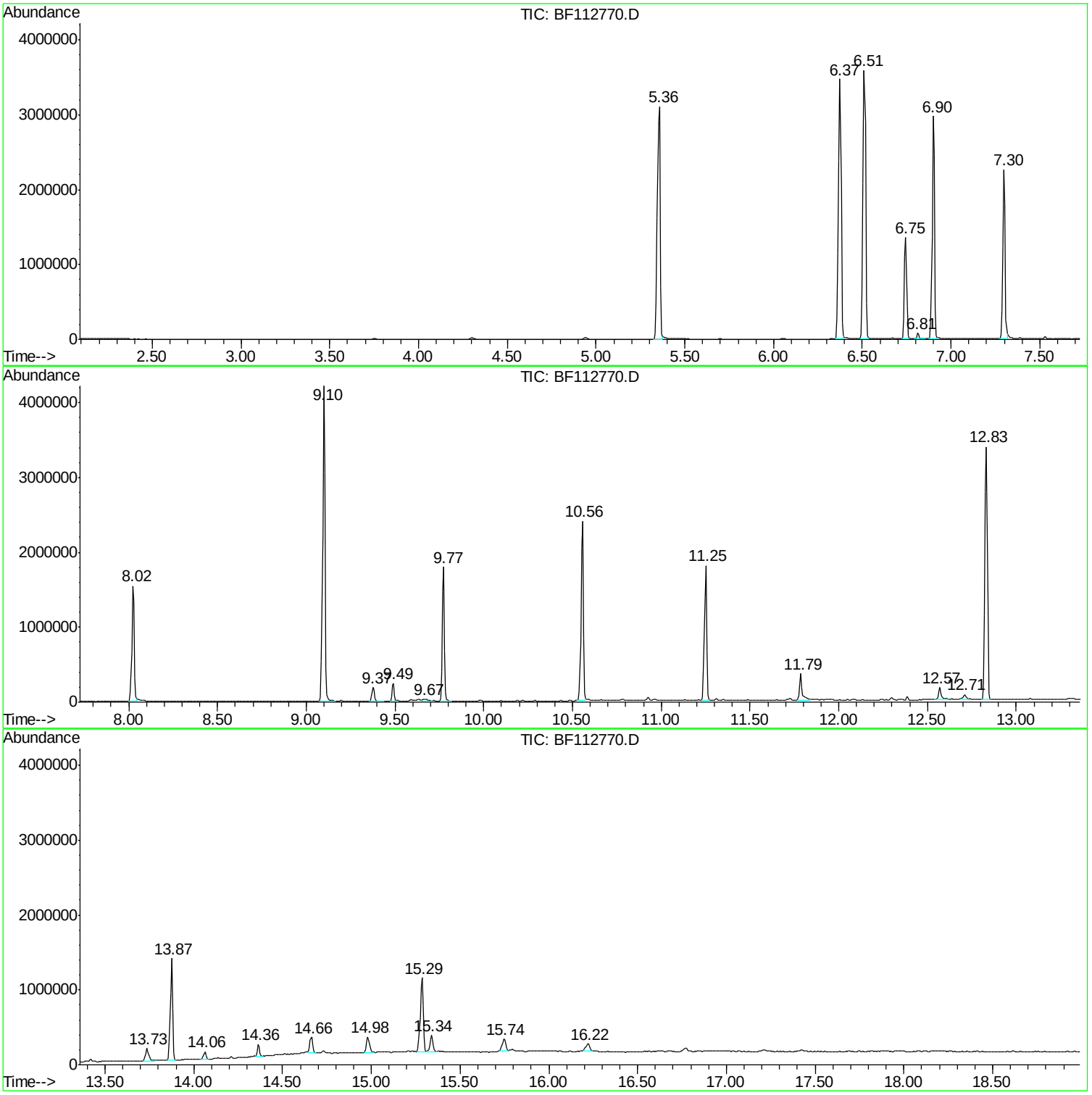
Data File : BF112770.D
Acq On : 28 Feb 2019 19:29
Operator : JU/SJ
Sample : K1650-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5(9-10)

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

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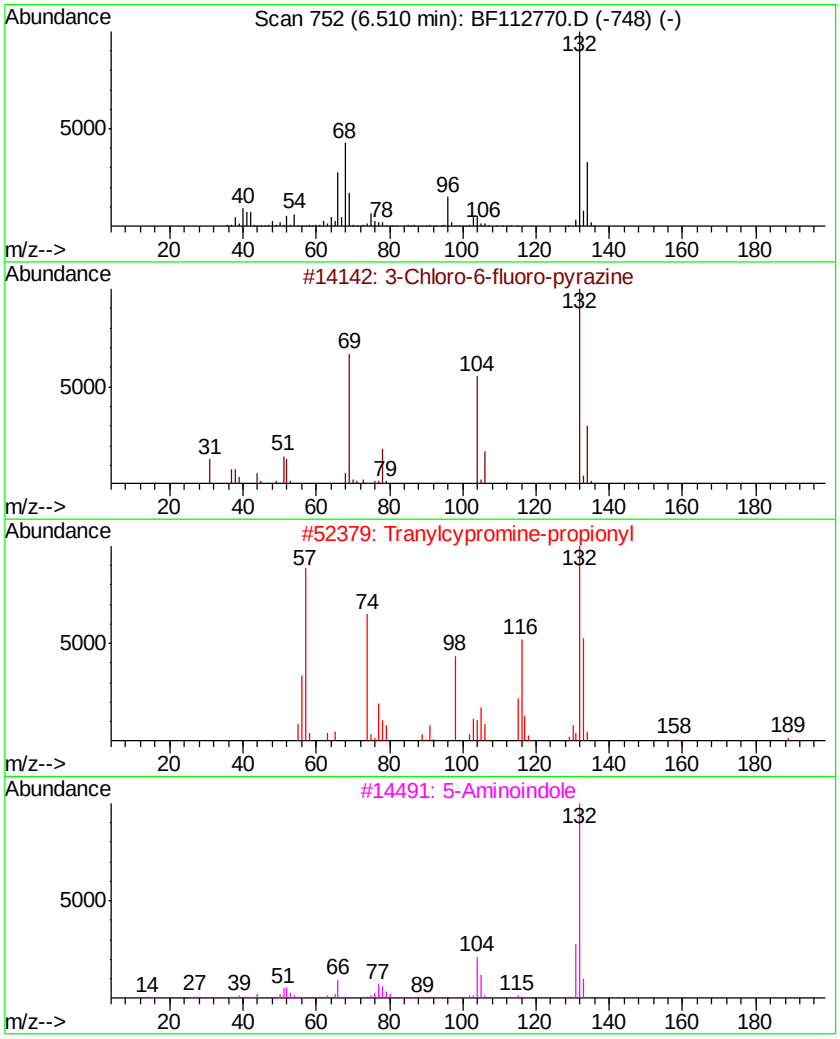
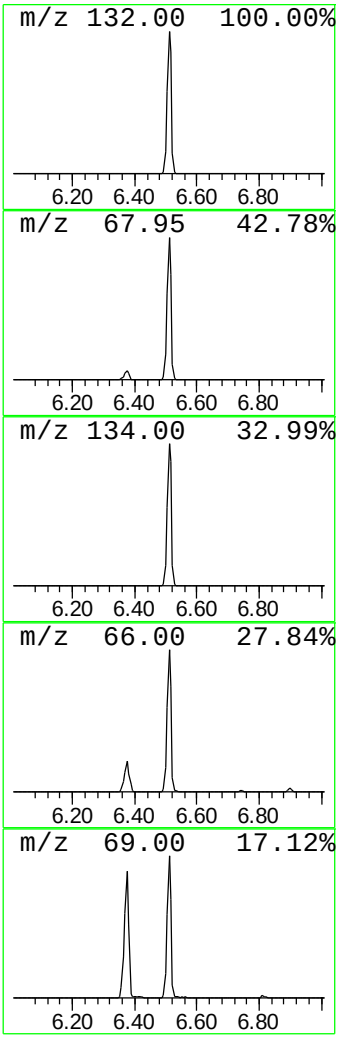
Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	60.48 ng	3435390	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Operator : JU/SJ
Sample : K1650-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5(9-10)

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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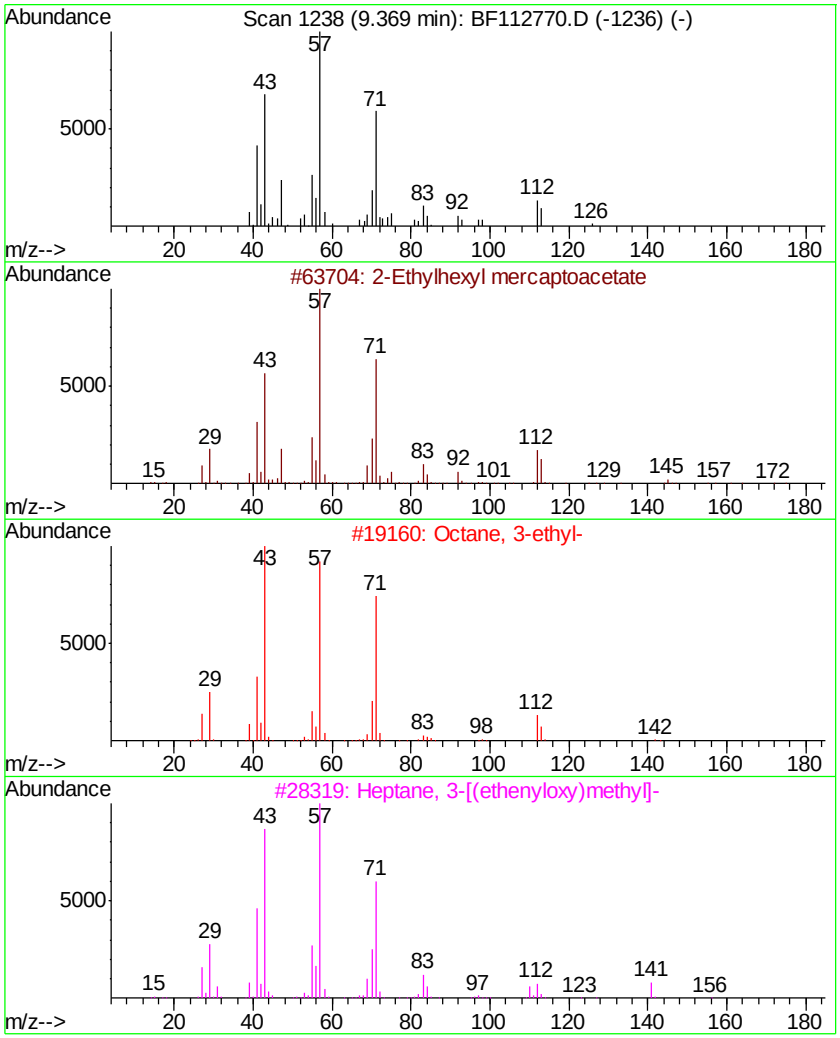
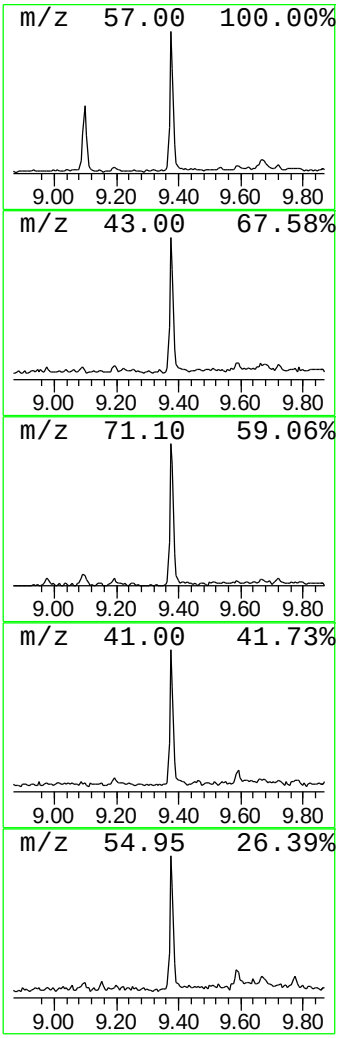
Peak Number 3 2-Ethylhexyl mercaptoacetate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.37	2.02 ng	161522	Acenaphthene-d10	9.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	87
2	Octane, 3-ethyl-	142	C10H22	005881-17-4	53
3	Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	50
4	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	47
5	Decane, 4-methyl-	156	C11H24	002847-72-5	47





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5(9-10)

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

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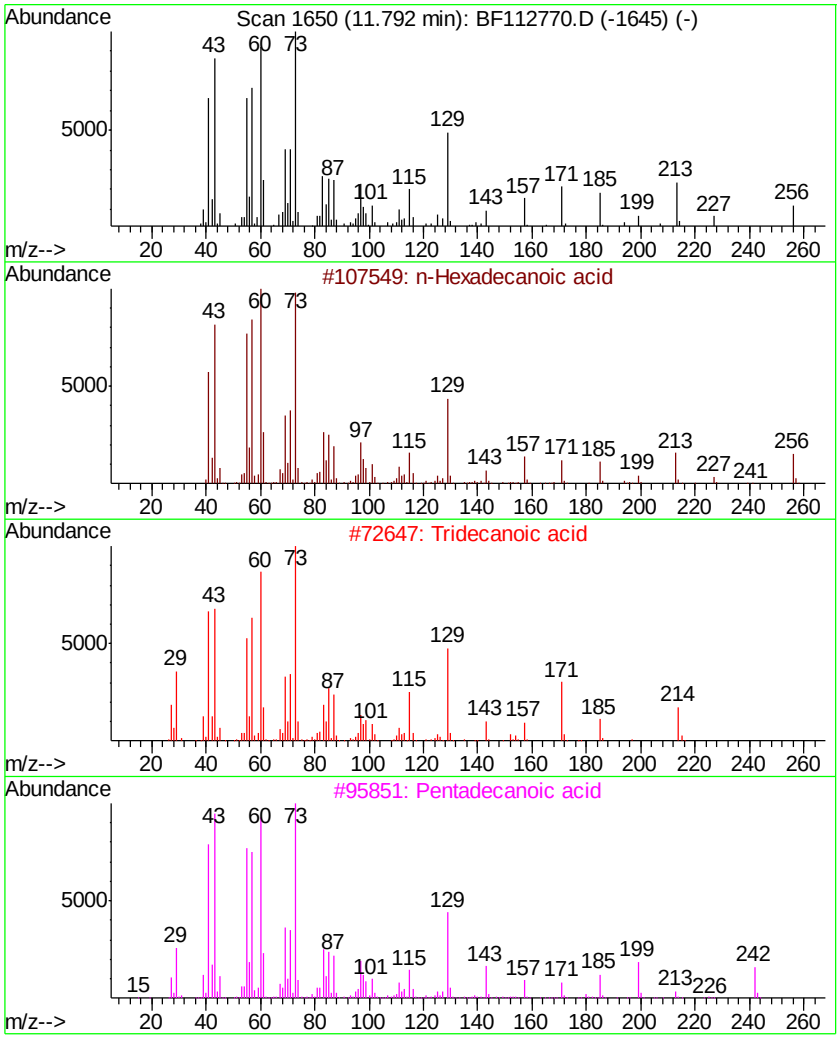
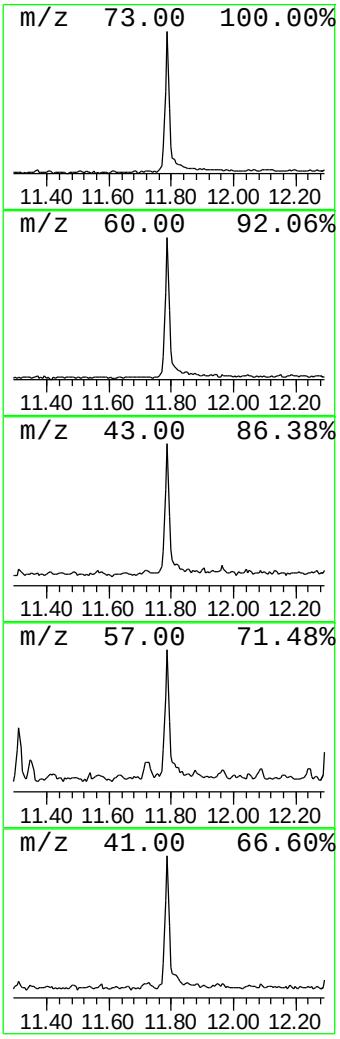
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	4.73 ng	363765	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	30





Library Search Compound Report

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Data File : BF112770.D
Acq On : 28 Feb 2019 19:29
Operator : JU/SJ
Sample : K1650-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5(9-10)

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

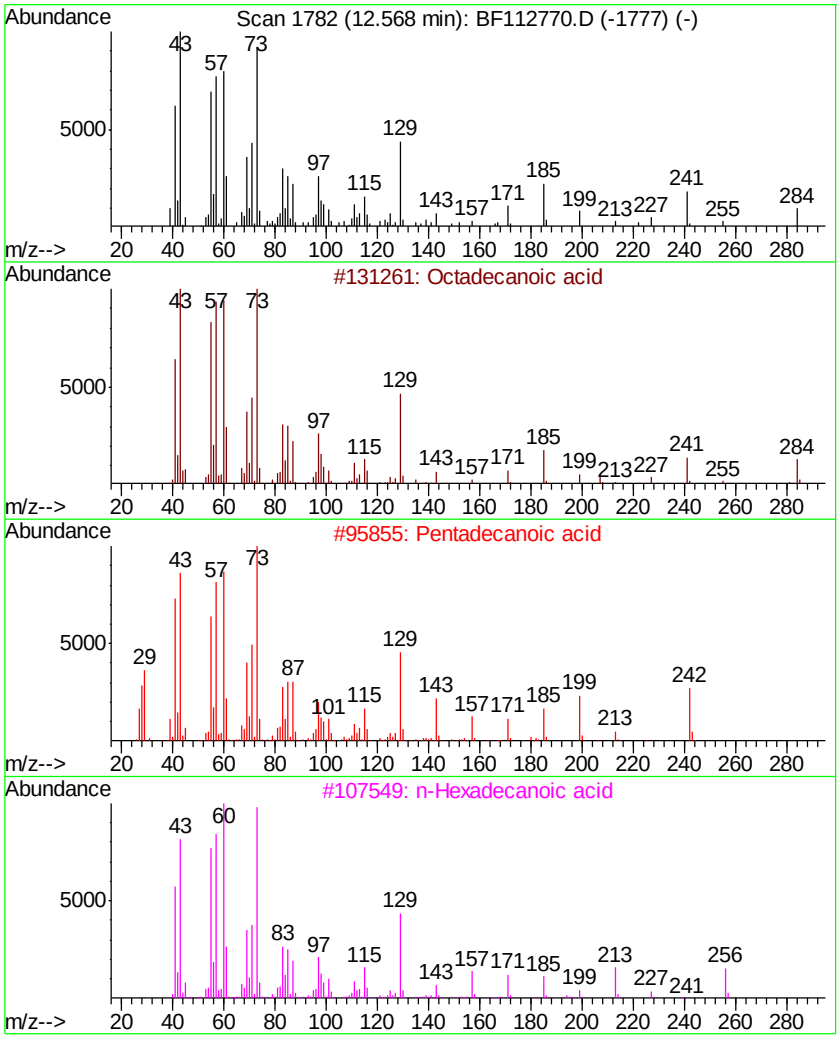
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

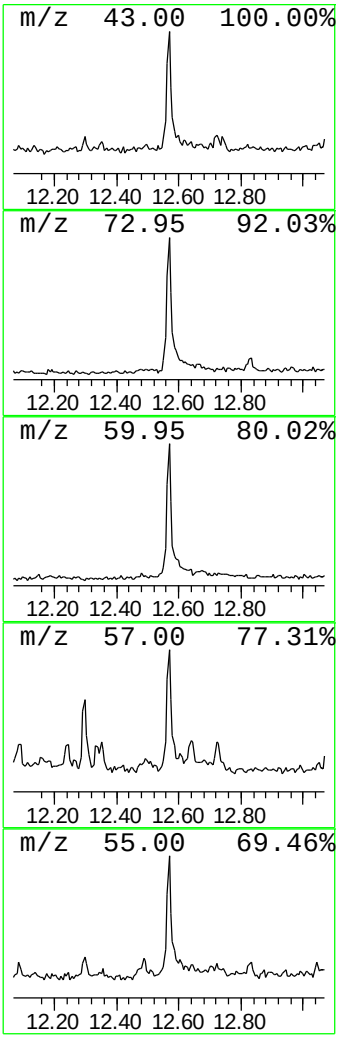
****

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.39 ng	199026	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Library Search Compound Report

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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : B-5(9-10)

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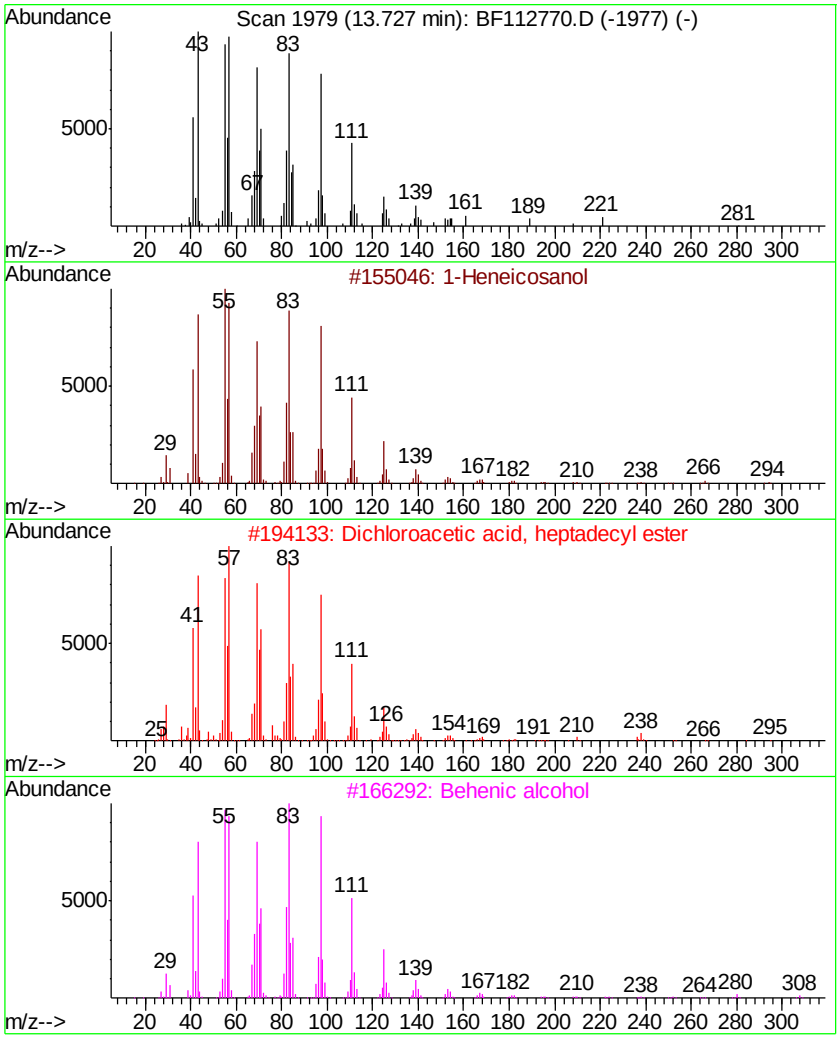
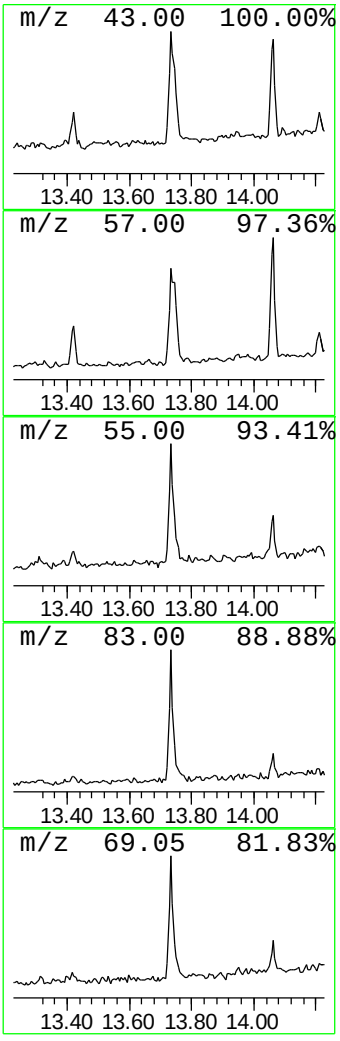
****

Peak Number 6 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	3.51 ng	205789	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





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Instrument : BNA_F
ClientSampleId : B-5(9-10)

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

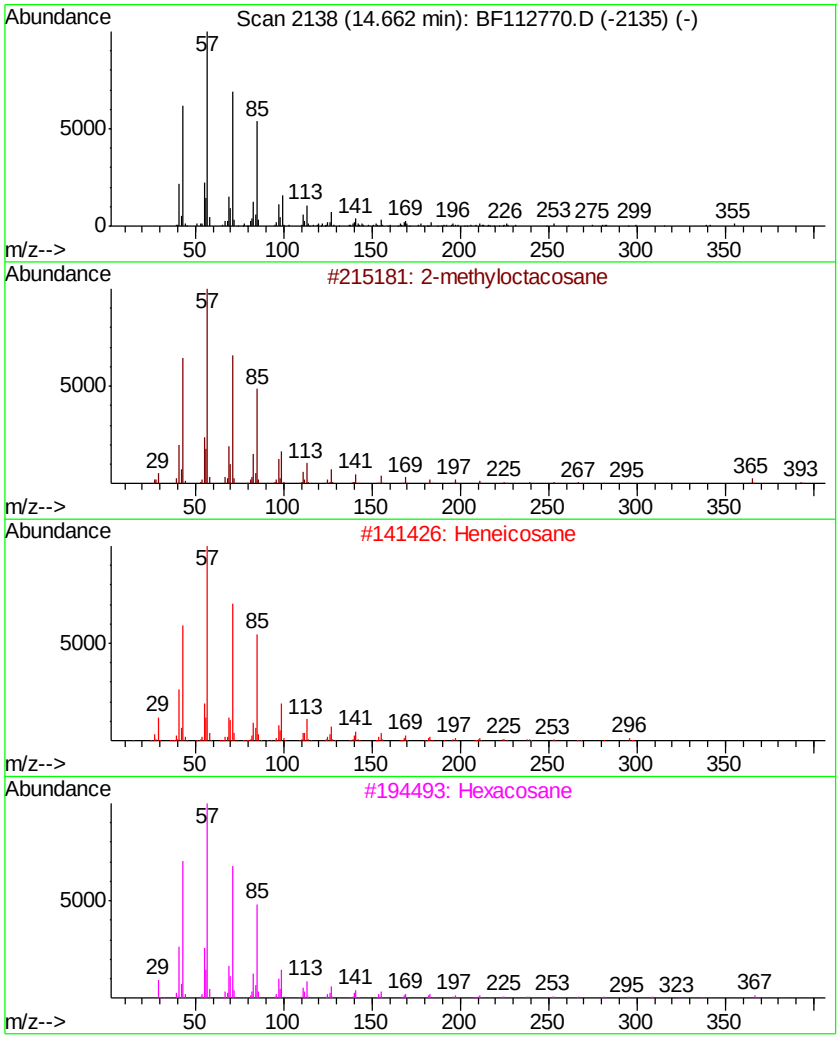
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

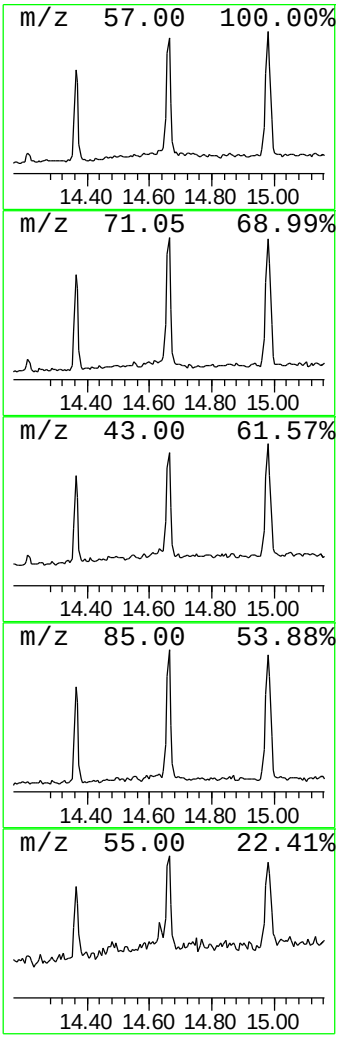
****

Peak Number 8 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.41 ng	199712	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





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Operator : JU/SJ
Sample : K1650-11
Misc :
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Instrument : BNA_F
ClientSampleId : B-5(9-10)

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

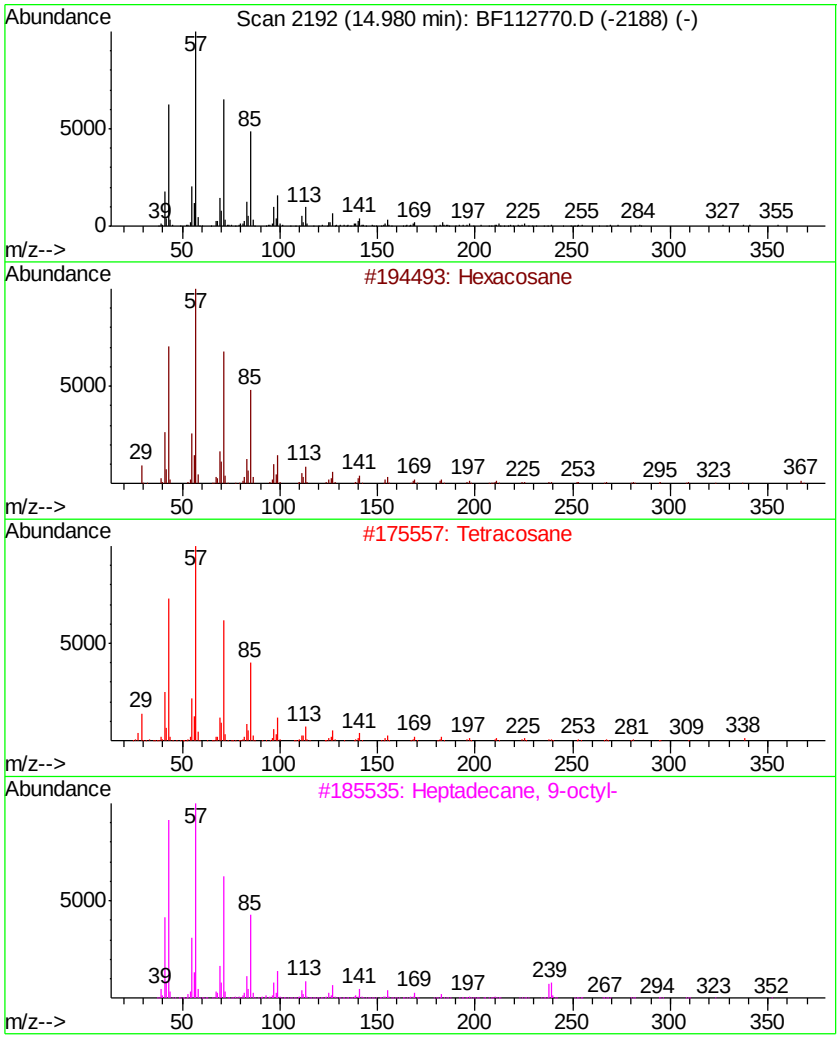
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

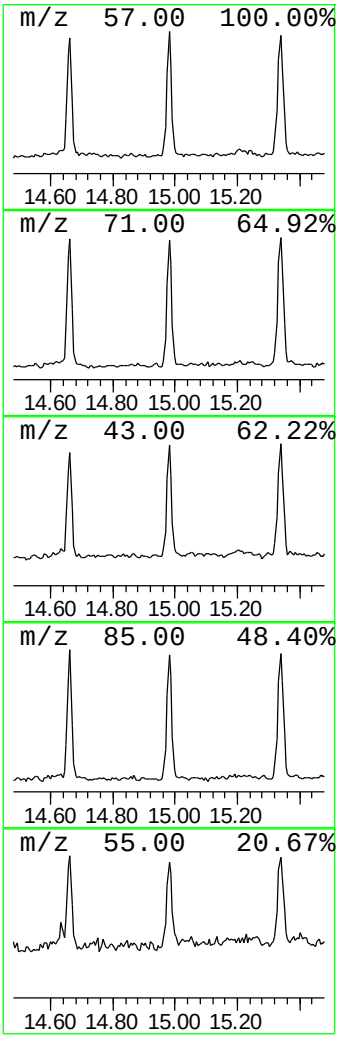
****

Peak Number 9 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	4.14 ng	242535	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5	Heneicosane	296	C21H44	000629-94-7	90





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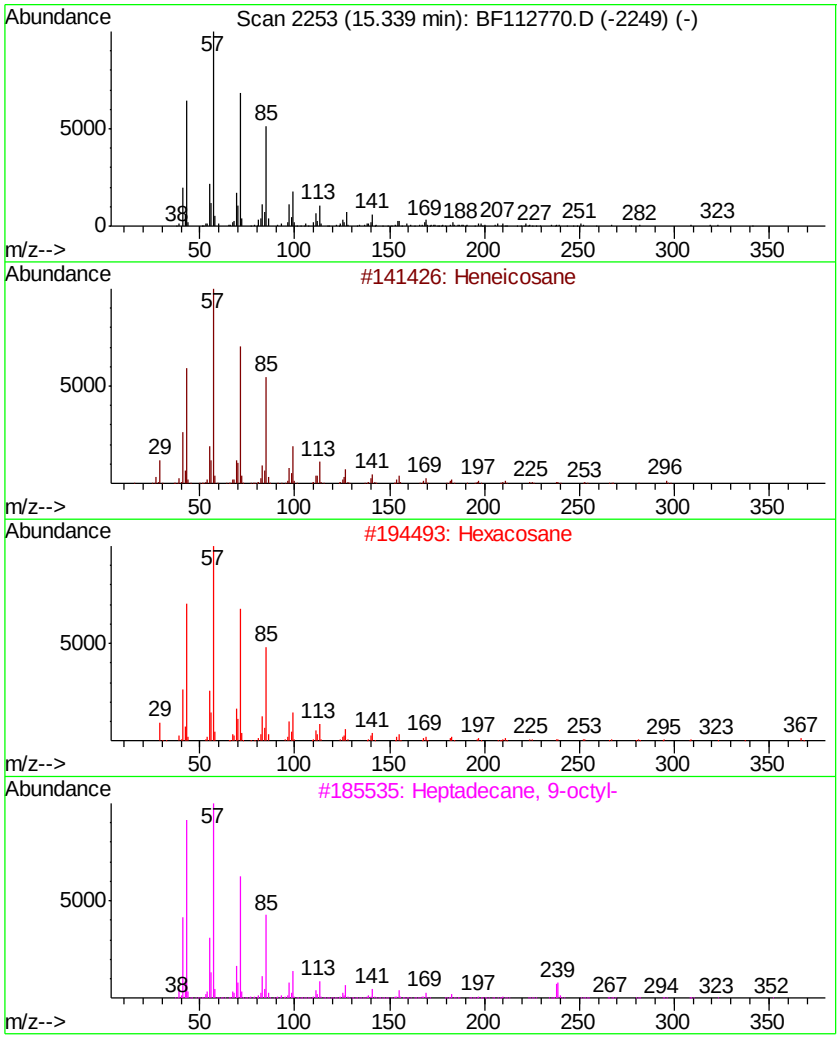
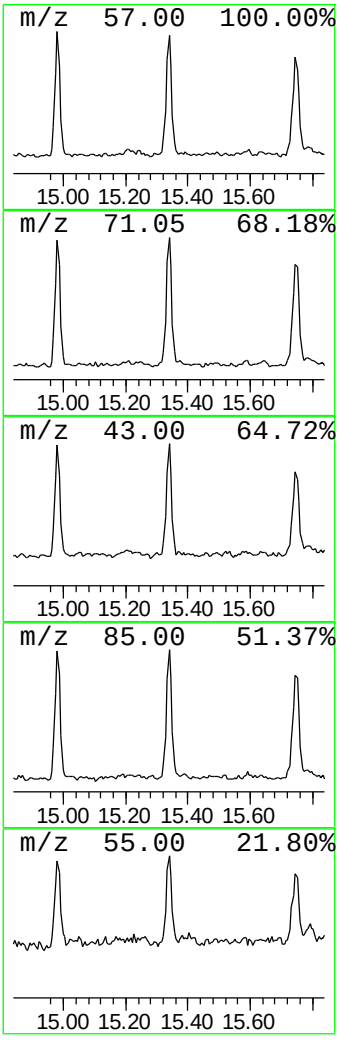
****

Peak Number 10 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	4.25 ng	248903	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Pentacosane	352	C25H52	000629-99-2	87
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87





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Instrument : BNA_F
ClientSampleId : B-5(9-10)

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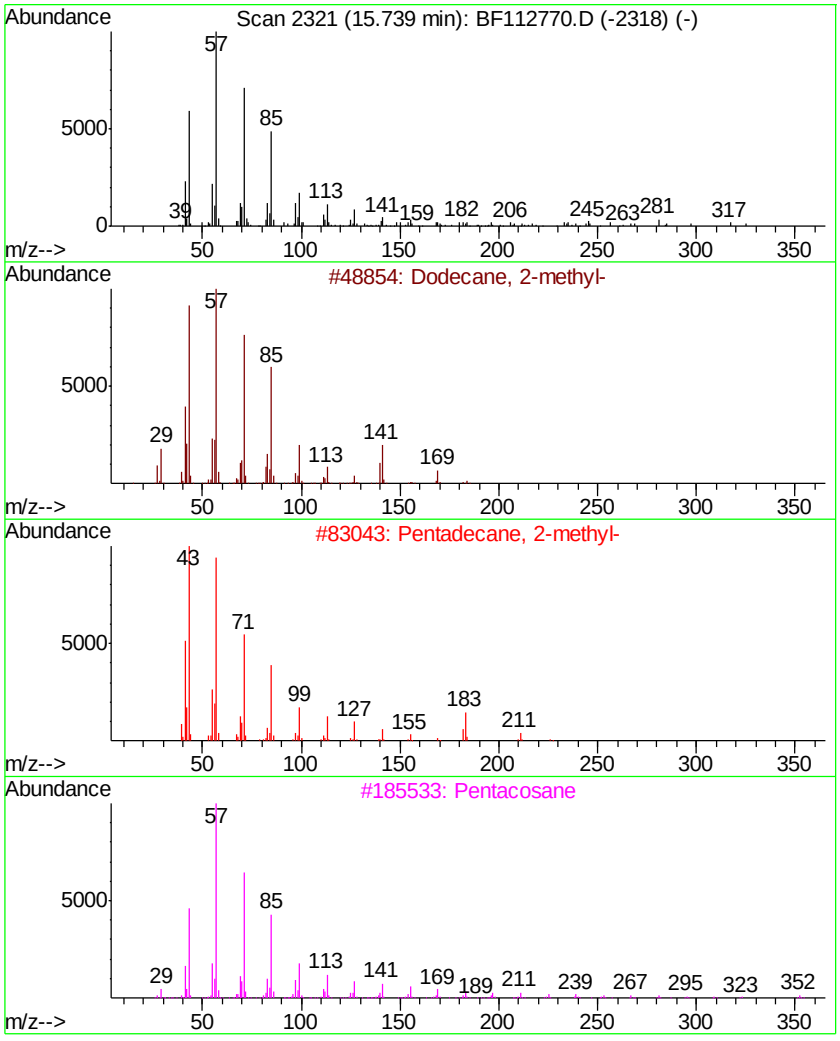
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

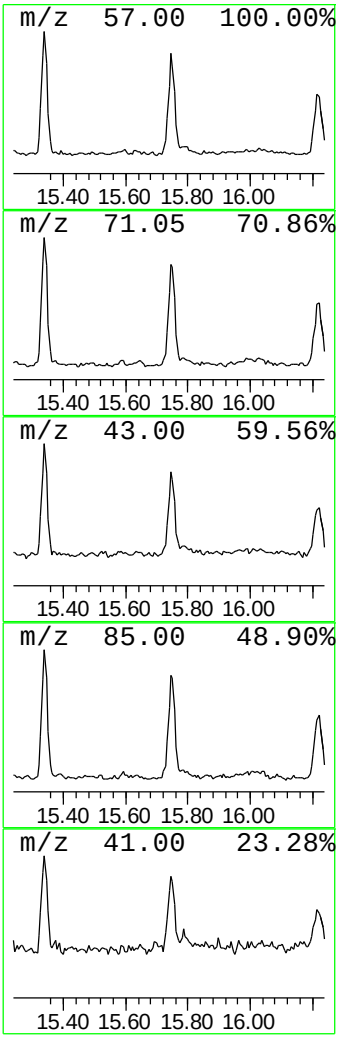
****

Peak Number 11 Dodecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	3.91 ng	228962	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	90
3	Pentacosane	352	C25H52	000629-99-2	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Triacontane	422	C30H62	000638-68-6	86





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Data File : BF112770.D
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Operator : JU/SJ
Sample : K1650-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
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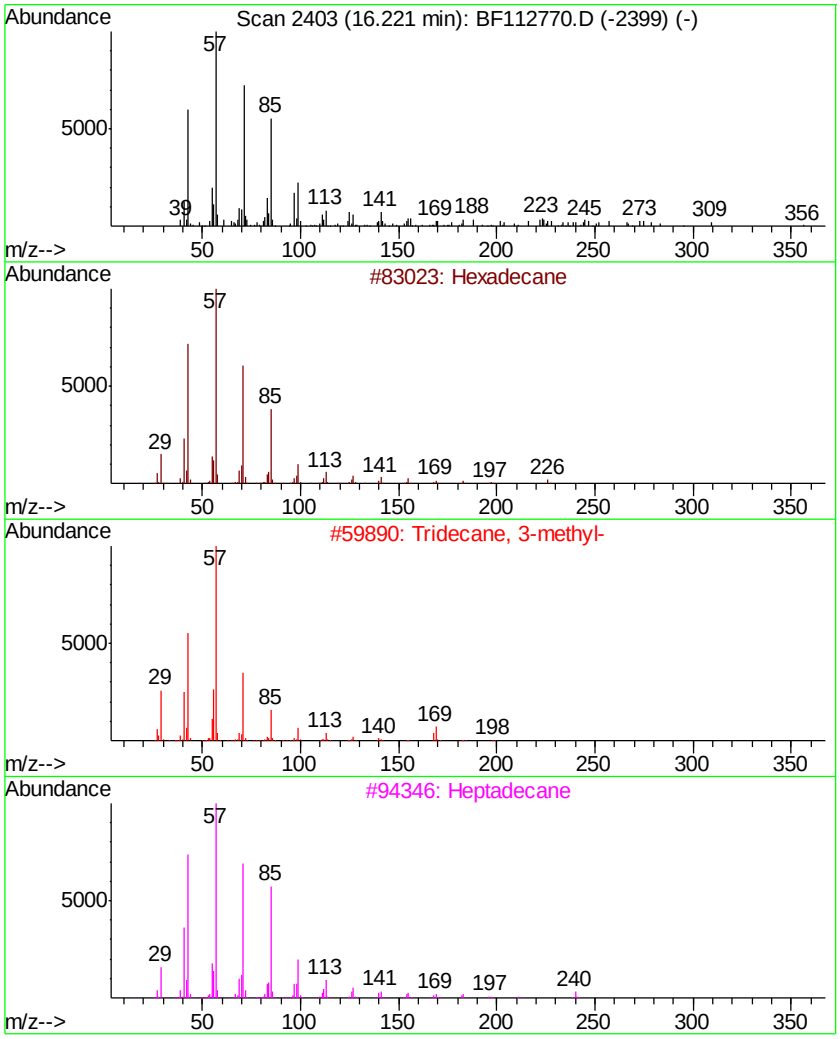
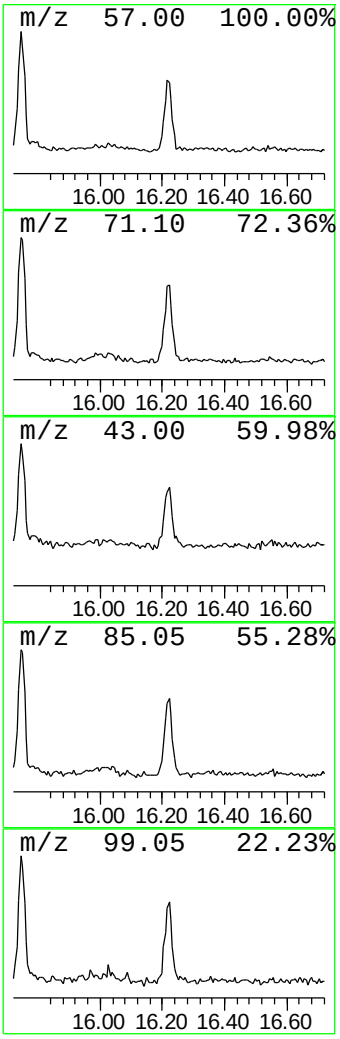
****

Peak Number 12 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	2.50 ng	146438	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
3	Heptadecane	240	C17H36	000629-78-7	76
4	Heneicosane	296	C21H44	000629-94-7	68
5	Nonadecane	268	C19H40	000629-92-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022819\
Data File : BF112770.D
Acq On : 28 Feb 2019 19:29
Operator : JU/SJ
Sample : K1650-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5(9-10)

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
unknown6.51	6.51	60.5	ng	3435390	1	6.75	1136080	20.0
2-Ethylhexyl merc...	9.37	2.0	ng	161522	3	9.77	1596040	20.0
n-Hexadecanoic acid	11.79	4.7	ng	363765	4	11.25	1537710	20.0
Octadecanoic acid	12.57	3.4	ng	199026	5	13.87	1173340	20.0
1-Heneicosanol	13.73	3.5	ng	205789	5	13.87	1173340	20.0
2-methyloctacosane	14.66	3.4	ng	199712	6	15.29	1172340	20.0
Hexacosane	14.98	4.1	ng	242535	6	15.29	1172340	20.0
Heneicosane	15.34	4.3	ng	248903	6	15.29	1172340	20.0
Dodecane, 2-methyl-	15.74	3.9	ng	228962	6	15.29	1172340	20.0
Hexadecane	16.22	2.5	ng	146438	6	15.29	1172340	20.0