LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112778.D
Acq On : 28 Feb 2019 23:05
Operator : JU/SJ
Sample : K1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-1(17-18)

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	5.351	550	555	559	rBV	3147786	3234013	88.69%	9.793%
2	6.375	724	729	732	rBV	3480707	3400806	93.26%	10.298%
3	6.510	748	752	755	rBV	3742009	3444108	94.45%	10.429%
4	6.745	788	792	795	rBV	1232537	1102465	30.23%	3.338%
5	6.898	814	818	822	rBV	3040289	2697433	73.97%	8.168%
6	7.298	881	886	889	rBV	2255798	2139146	58.66%	6.477%
7	8.022	1005	1009	1013	rBV	1587342	1342394	36.81%	4.065%
8	9.098	1188	1192	1195	rBV	4289583	3646466	100.00%	11.041%
9	9.374	1235	1239	1243	rBV	47984	43779	1.20%	0.133%
10	9.486	1255	1258	1262	rBV	208181	184017	5.05%	0.557%
11	9.663	1285	1288	1295	rVB2	30459	55775	1.53%	0.169%
12	9.769	1302	1306	1315	rBV	1400737	1373380	37.66%	4.159%
13	10.551	1435	1439	1443	rBV	2074877	1921439	52.69%	5.818%
14	11.245	1554	1557	1561	rBV	1227495	1153042	31.62%	3.491%
15	11.786	1645	1649	1659	rBV2	322372	345836	9.48%	1.047%
16	12.568	1778	1782	1791	rBV	116250	139154	3.82%	0.421%
17	12.710	1801	1806	1810	rBV	102567	133984	3.67%	0.406%
18	12.827	1822	1826	1830	rBV	2963144	2726018	74.76%	8.254%
19	13.733	1976	1980	1986	rBV3	150535	203230	5.57%	0.615%
20	13.874	1999	2004	2007	rBV	1257335	1190225	32.64%	3.604%
21	14.057	2032	2035	2039	rBV	102057	96796	2.65%	0.293%
22	14.362	2084	2087	2093	rBV	170970	150378	4.12%	0.455%
23	14.656	2134	2137	2141	rVB	204250	198626	5.45%	0.601%
24	14.980	2188	2192	2197	rBV	221747	240973	6.61%	0.730%
25	15.280	2238	2243	2248	rVV2	1069277	1276292	35.00%	3.865%
26	15.333	2248	2252	2257	rVB	177542	241885	6.63%	0.732%
27	15.745	2317	2322	2326	rBV	149584	206532	5.66%	0.625%
28	16.215	2399	2402	2411	rVB	81595	137122	3.76%	0.415%

Sum of corrected areas: 33025314

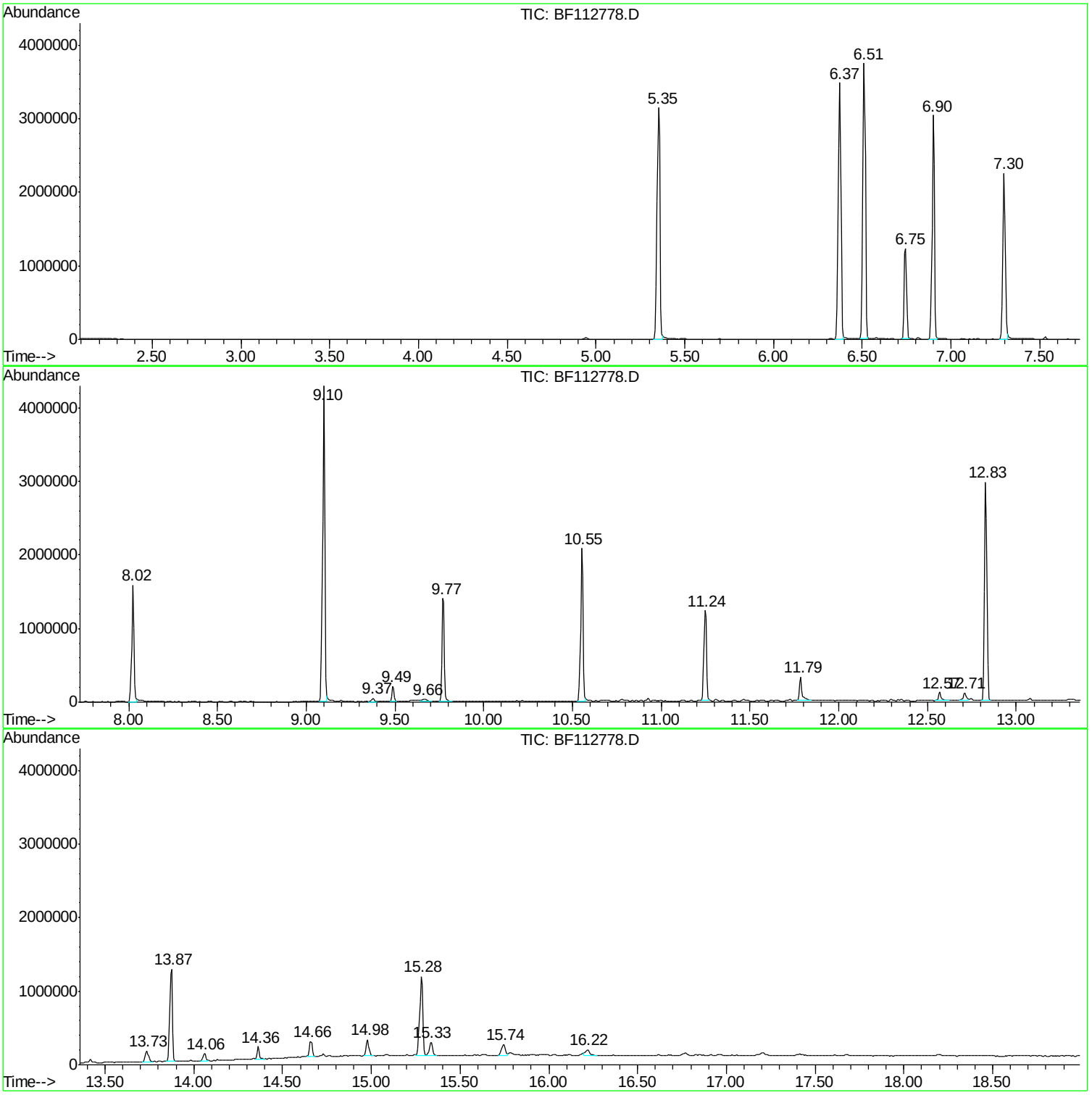
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112778.D
Acq On : 28 Feb 2019 23:05
Operator : JU/SJ
Sample : K1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-1(17-18)

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112778.D
Acq On : 28 Feb 2019 23:05
Operator : JU/SJ
Sample : K1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-1(17-18)

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

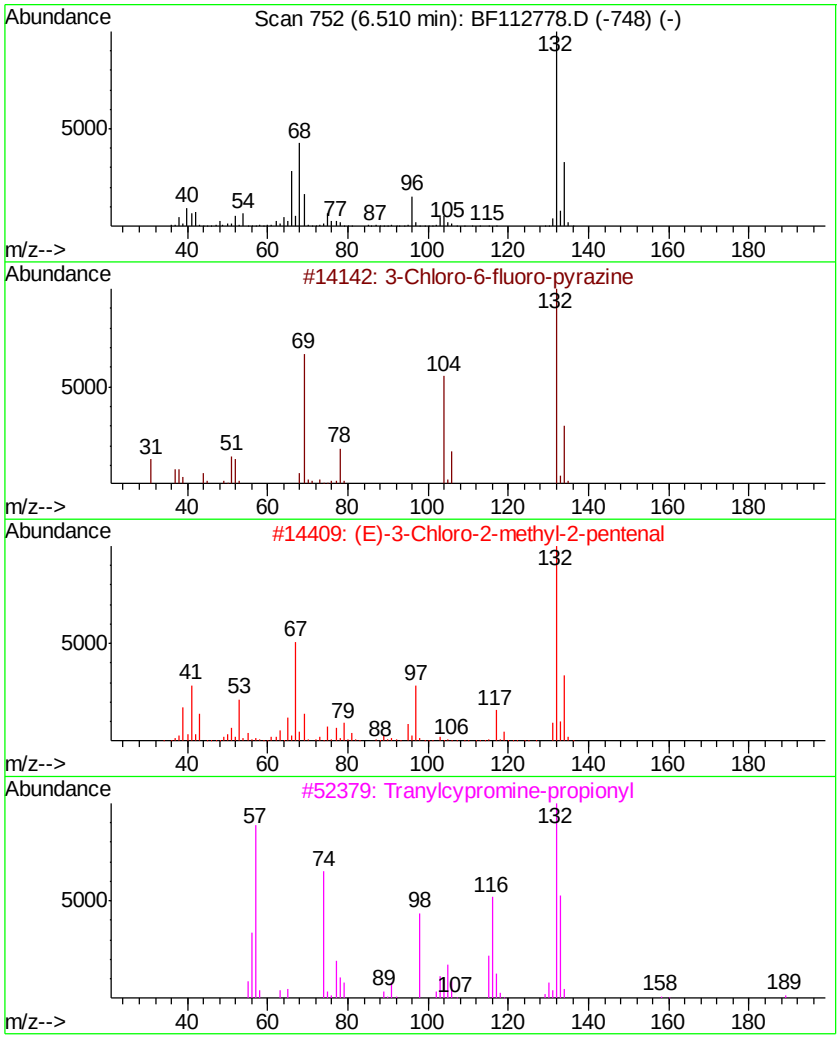
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

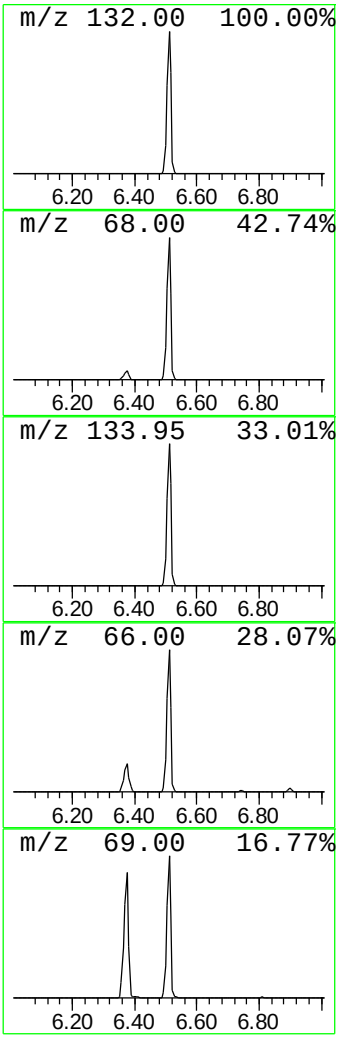
****

Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	62.48 ng	3444110	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Data File : BF112778.D
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Operator : JU/SJ
Sample : K1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-1(17-18)

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

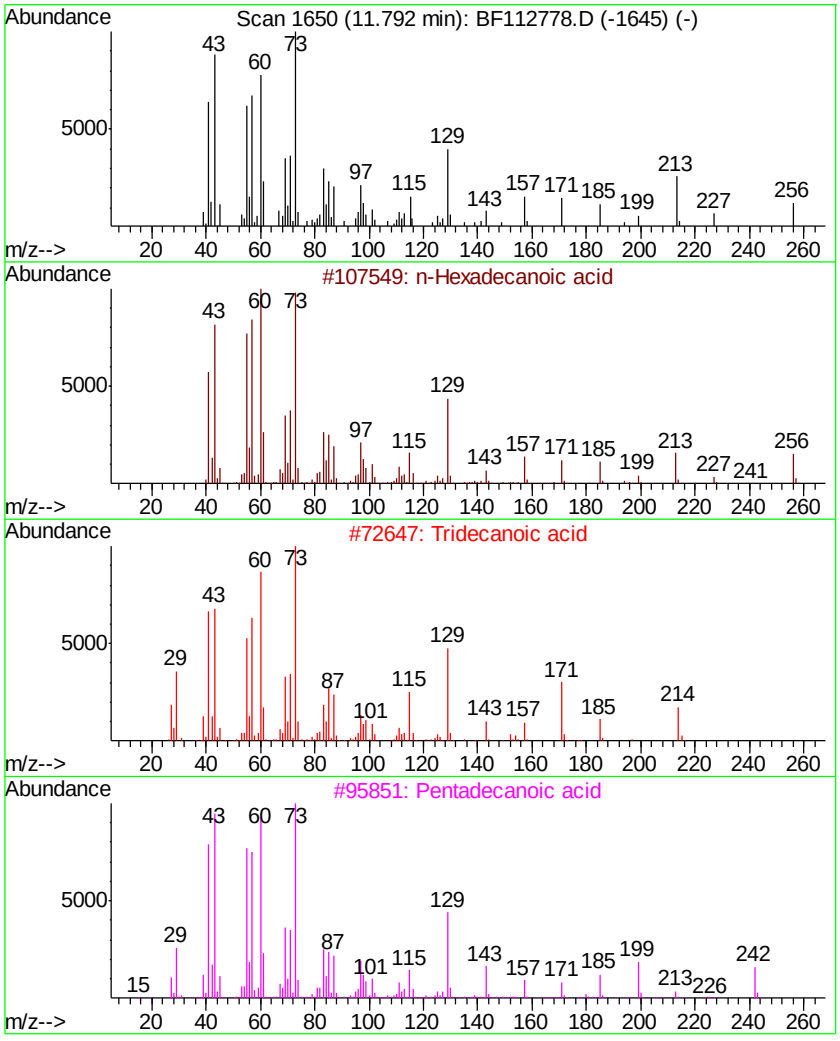
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

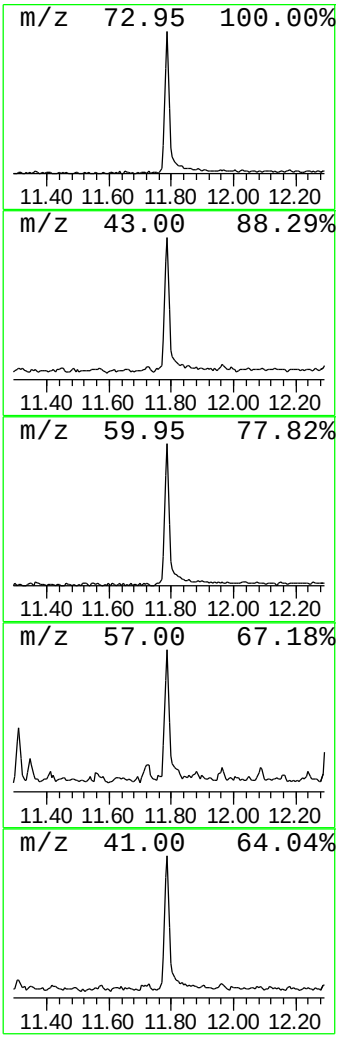
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	6.00 ng	345836	Phenanthrene-d10	11.24

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	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Library Search Compound Report

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Data File : BF112778.D
Acq On : 28 Feb 2019 23:05
Operator : JU/SJ
Sample : K1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-1(17-18)

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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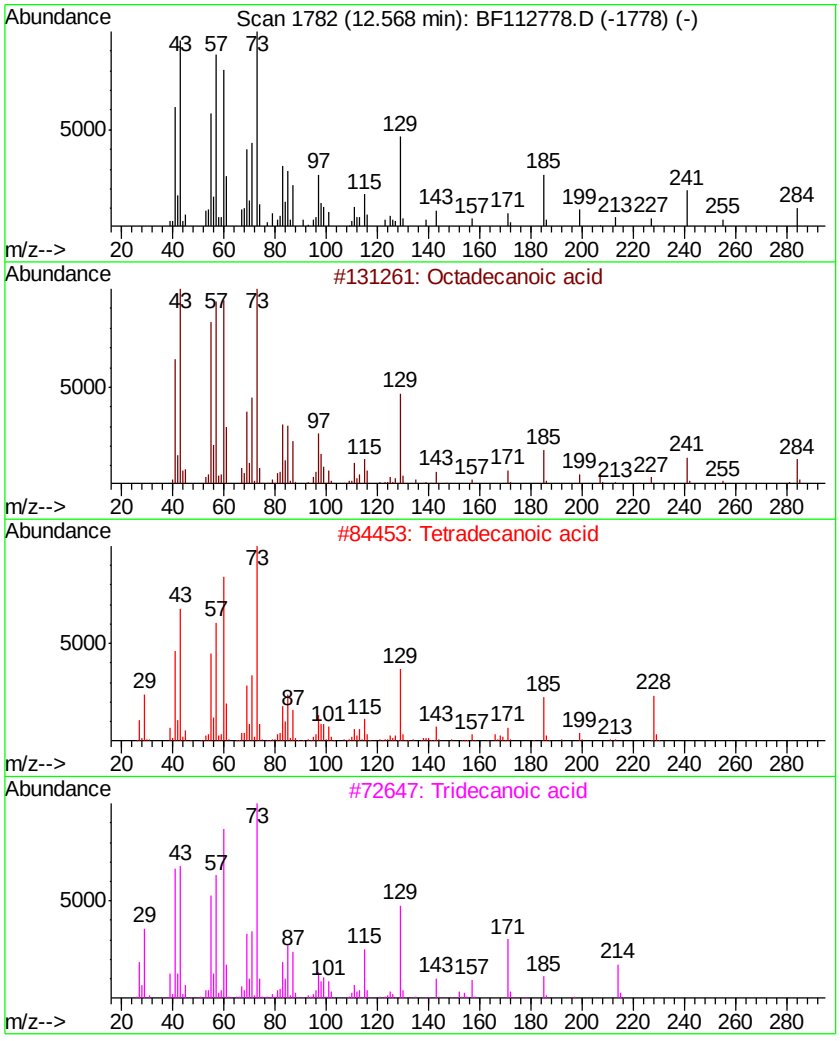
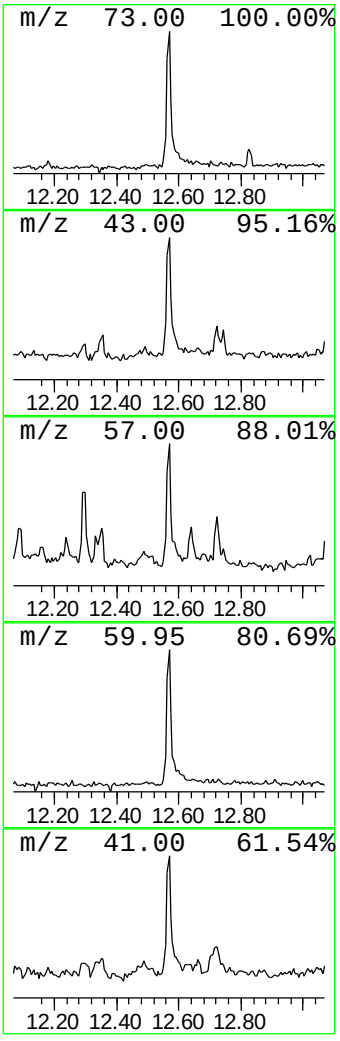
Peak Number 4 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	2.34 ng	139154	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





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Operator : JU/SJ
Sample : K1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-1(17-18)

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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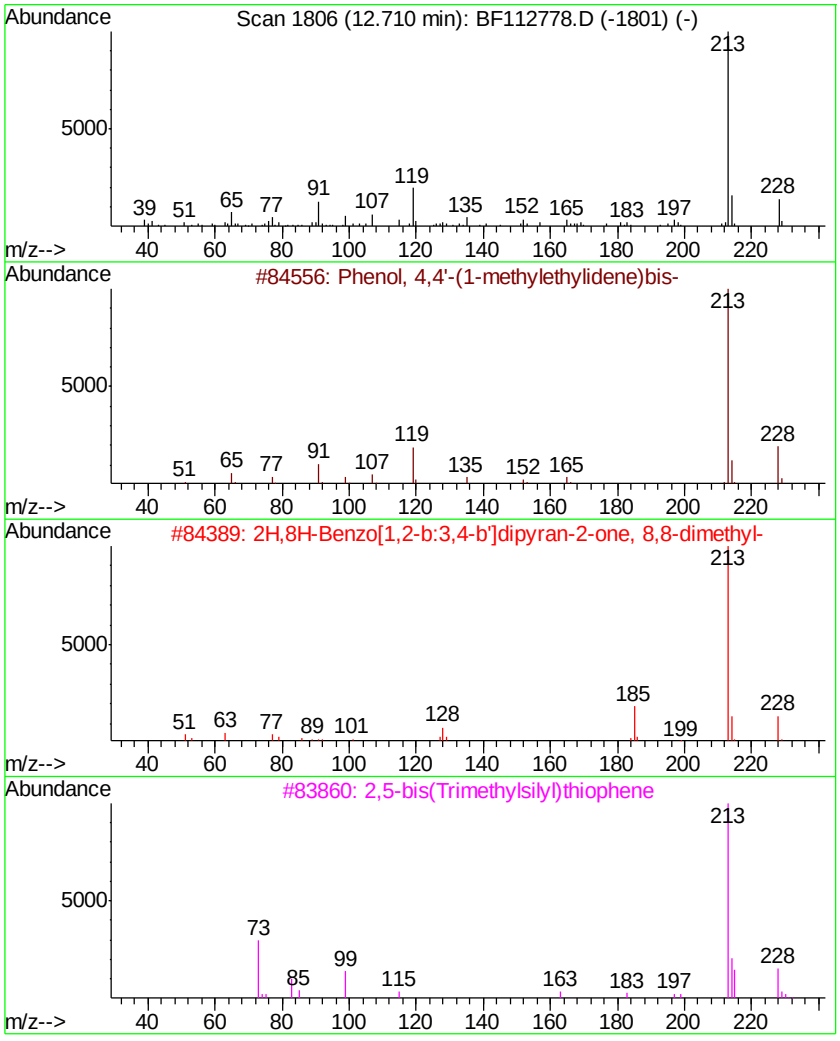
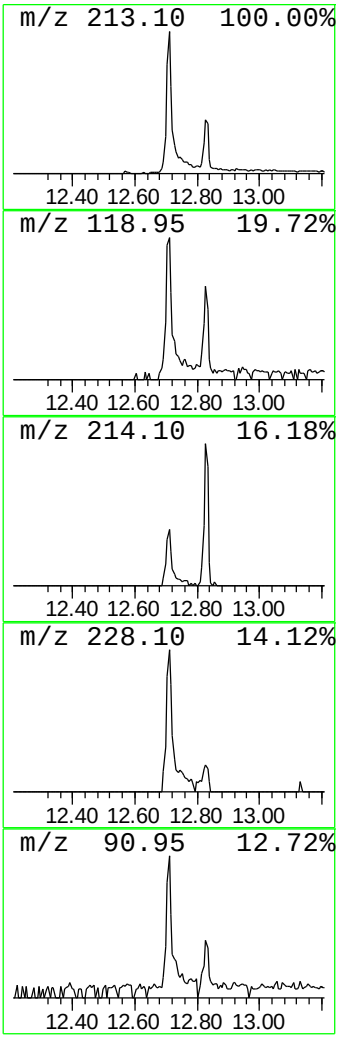
Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	2.25 ng	133984	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	53
3	2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	53
4	6-Methyl-2-(methylthio)-4-pyrimi...	270	C12H22N2OSSi	1000332-17-1	50
5	4-Bromo-2-(methylamino)tropone	213	C8H8BrNO	1000241-45-0	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
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Operator : JU/SJ
Sample : K1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-1(17-18)

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

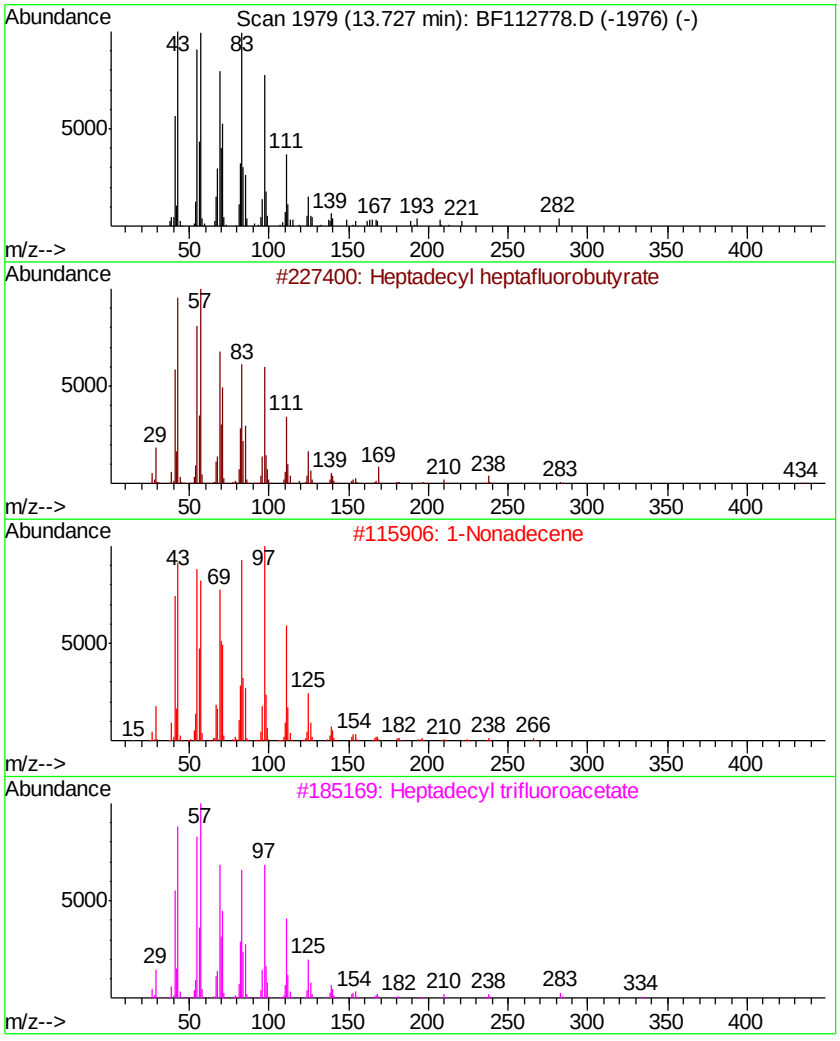
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

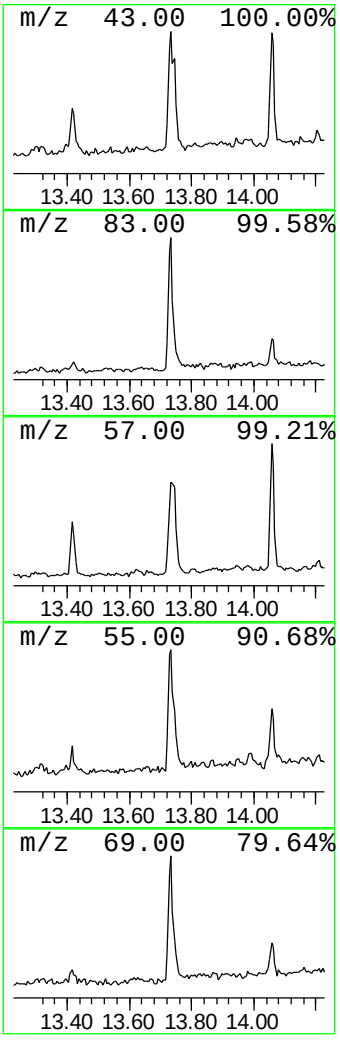
****

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	3.41 ng	203230	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5	1-Docosene	308	C22H44	001599-67-3	87





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Sample : K1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-1(17-18)

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

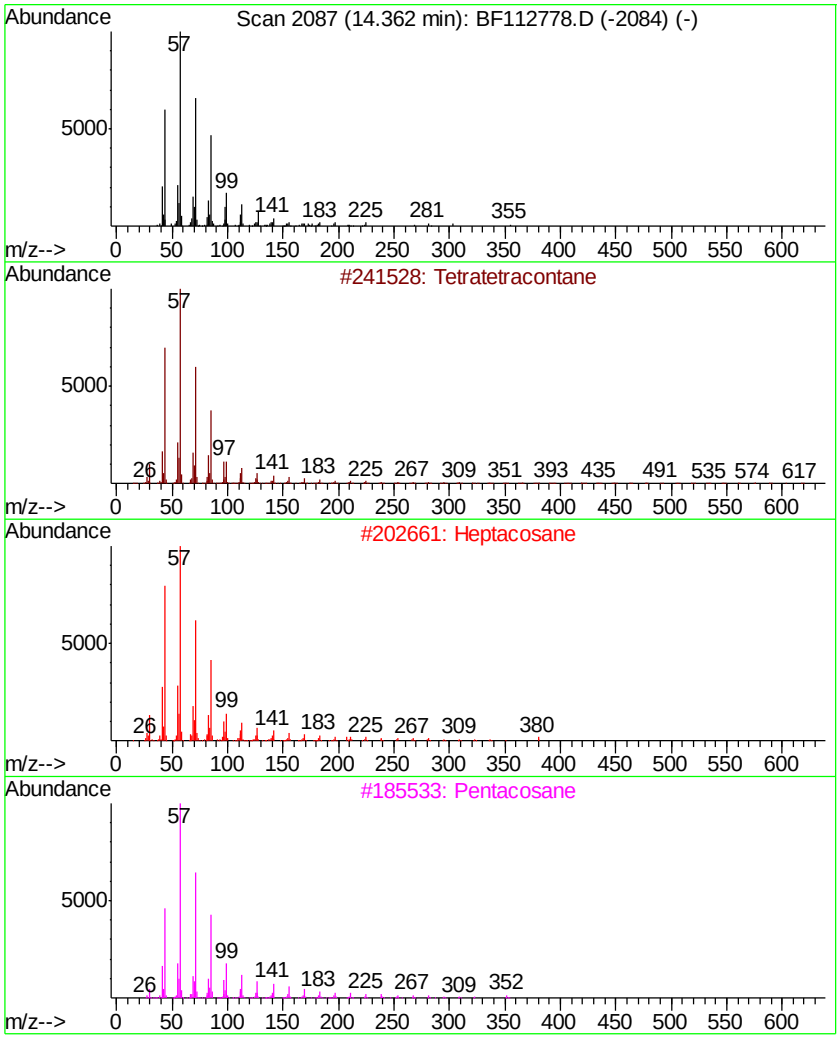
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

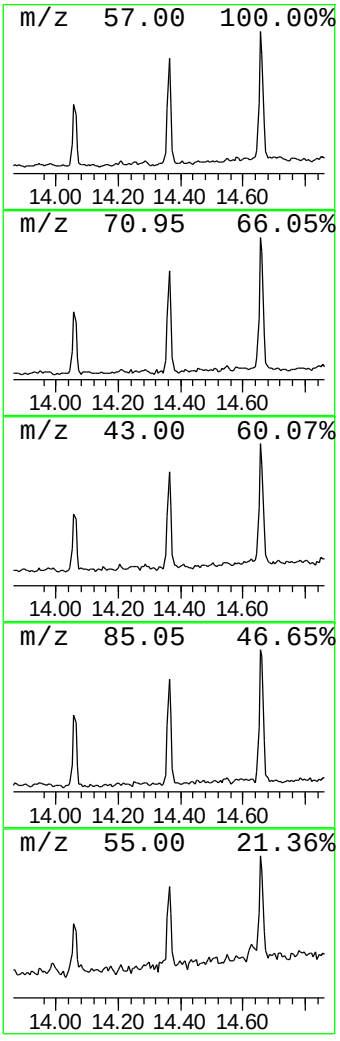
****

Peak Number 7 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	2.53 ng	150378	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Heptacosane	380	C27H56	000593-49-7	90
3	Pentacosane	352	C25H52	000629-99-2	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : B-1(17-18)

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

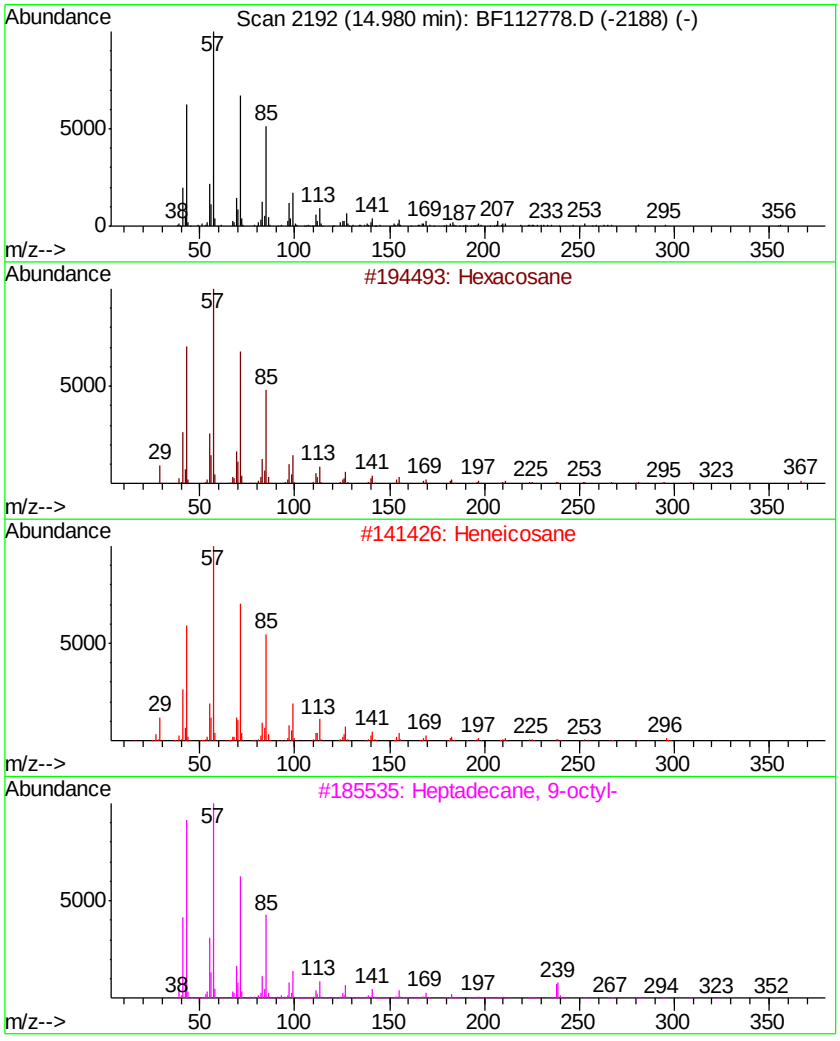
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

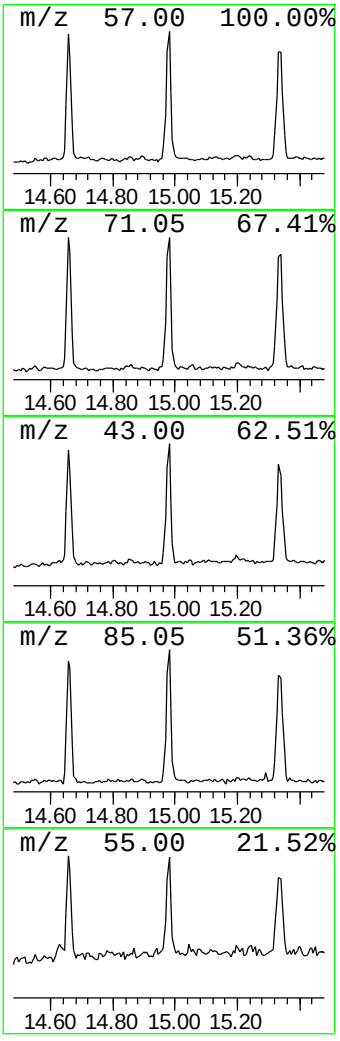
****

Peak Number 9 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	3.78 ng	240973	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5	Octadecane	254	C18H38	000593-45-3	87





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TIC Library : C:\DATABASE\NIST11.L
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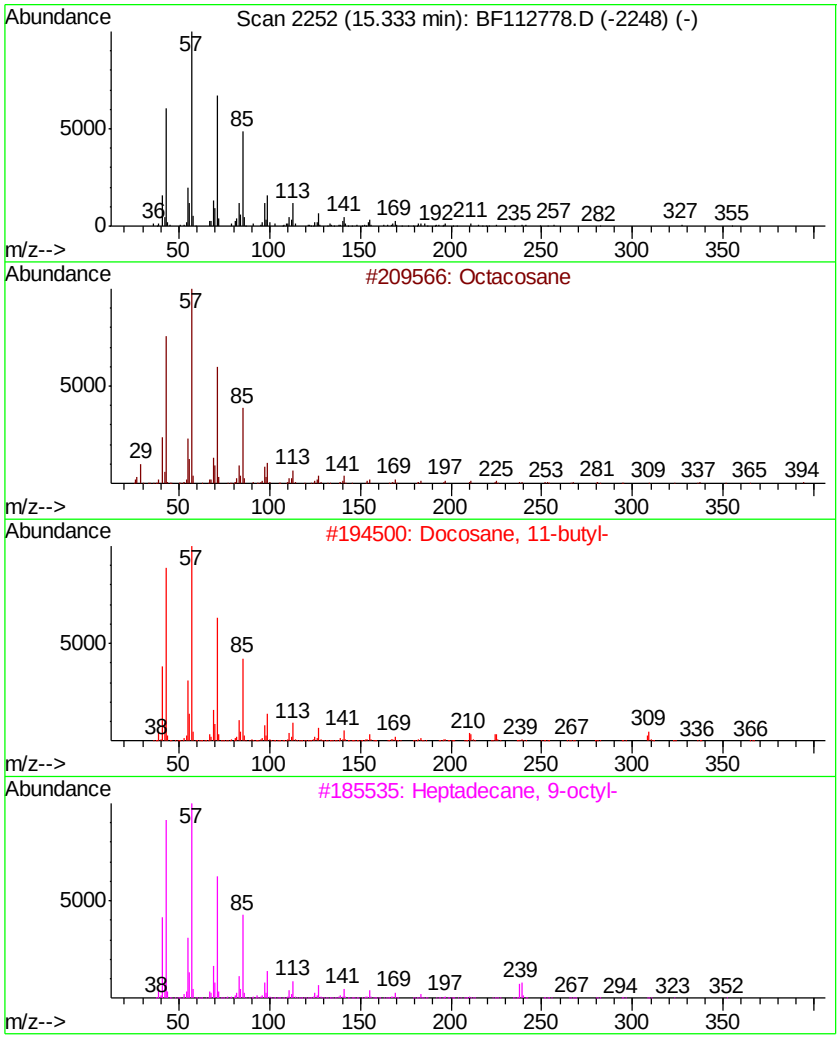
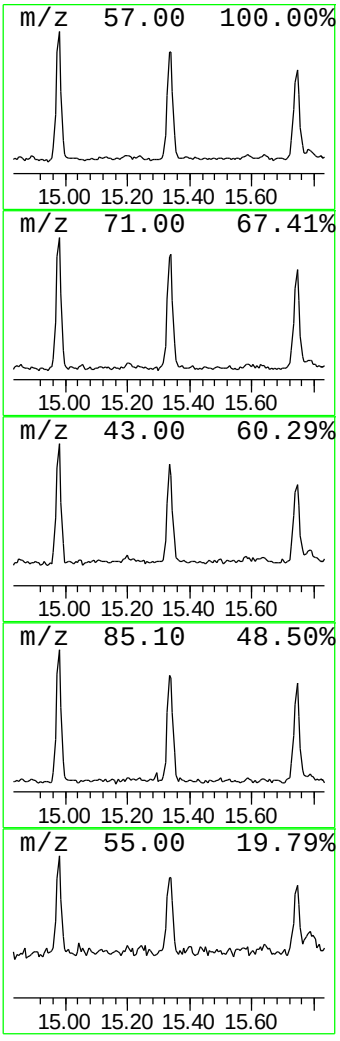
Peak Number 10 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	3.79 ng	241885	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Library Search Compound Report

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Acq On : 28 Feb 2019 23:05
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Sample : K1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-1(17-18)

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

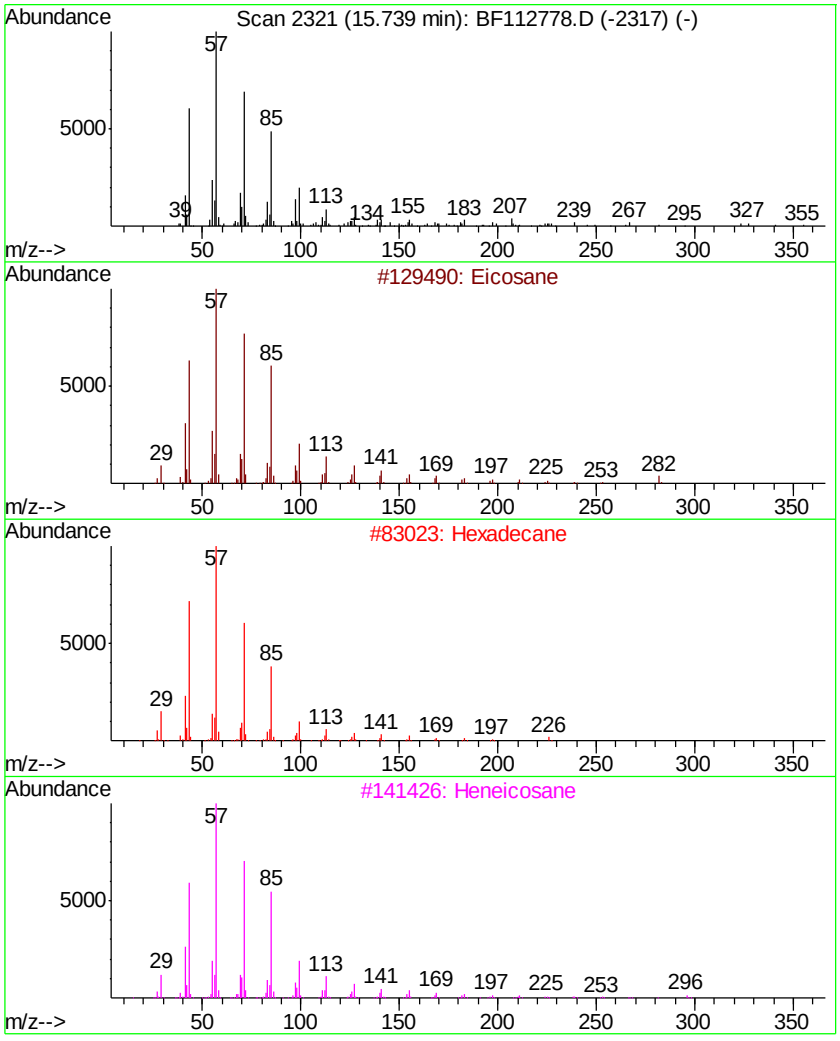
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

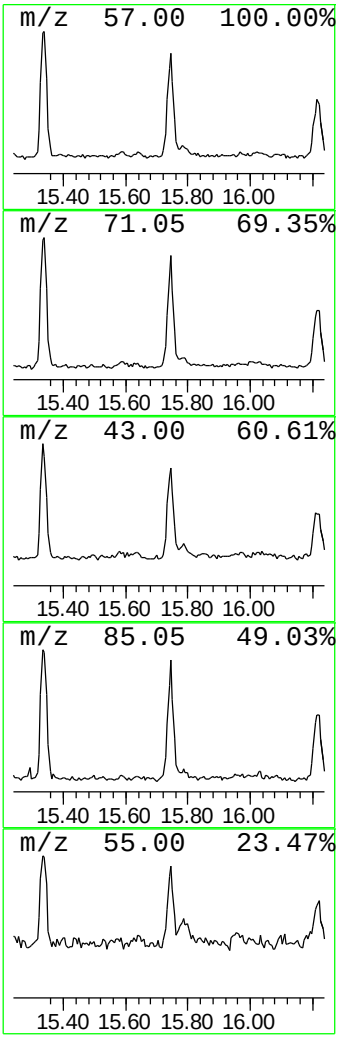
****

Peak Number 11 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	3.24 ng	206532	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Hexadecane	226	C16H34	000544-76-3	94
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Octacosane	394	C28H58	000630-02-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022819\
Data File : BF112778.D
Acq On : 28 Feb 2019 23:05
Operator : JU/SJ
Sample : K1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-1(17-18)

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	62.5	ng	3444110	1	6.75	1102470	20.0
n-Hexadecanoic acid	11.79	6.0	ng	345836	4	11.24	1153040	20.0
Octadecanoic acid	12.57	2.3	ng	139154	5	13.87	1190230	20.0
Phenol, 4,4'-(1-m...	12.71	2.3	ng	133984	5	13.87	1190230	20.0
Heptadecyl heptaf...	13.73	3.4	ng	203230	5	13.87	1190230	20.0
Tetratetracontane	14.36	2.5	ng	150378	5	13.87	1190230	20.0
Hexacosane	14.98	3.8	ng	240973	6	15.28	1276290	20.0
Octacosane	15.33	3.8	ng	241885	6	15.28	1276290	20.0
Eicosane	15.74	3.2	ng	206532	6	15.28	1276290	20.0