LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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	4.916	478	481	489	rVB	45383	58225	1.23%	0.142%
2	5.339	548	553	556	rBV	3067847	3176506	66.92%	7.730%
3	6.369	722	728	745	rBV	3306005	3554190	74.88%	8.649%
4	6.498	746	750	753	rBV	3809368	3436467	72.40%	8.363%
5	6.728	786	789	793	rBV	980510	766526	16.15%	1.865%
6	6.886	812	816	819	rBV	3097263	2541222	53.54%	6.184%
7	7.286	879	884	896	rBV	2161317	2184172	46.02%	5.315%
8	8.010	1003	1007	1014	rBV	940213	911439	19.20%	2.218%
9	9.086	1186	1190	1206	rBV	3833812	3626826	76.41%	8.826%
10	9.480	1253	1257	1267	rVB	194484	190627	4.02%	0.464%
11	9.763	1301	1305	1316	rBV	1148749	1128978	23.79%	2.747%
12	10.545	1434	1438	1454	rBV	2916549	2893450	60.96%	7.041%
13	11.239	1552	1556	1566	rBV	1366675	1353512	28.52%	3.294%
14	11.780	1644	1648	1658	rBV	777963	855516	18.02%	2.082%
15	12.445	1757	1761	1763	rBV	99944	89756	1.89%	0.218%
16	12.480	1763	1767	1777	rVV4	42103	93722	1.97%	0.228%
17	12.557	1777	1780	1793	rVV	491342	644009	13.57%	1.567%
18	12.668	1793	1799	1803	rVB	89661	125849	2.65%	0.306%
19	12.821	1820	1825	1828	rBV	4964515	4746408	100.00%	11.551%
20	13.062	1859	1866	1869	rBV	58028	67458	1.42%	0.164%
21	13.304	1902	1907	1911	rVB4	40976	49099	1.03%	0.119%
22	13.404	1921	1924	1926	rVB	75134	58906	1.24%	0.143%
23	13.727	1974	1979	1987	rBV	310628	441938	9.31%	1.075%
24	13.862	1997	2002	2011	rBV	1803335	1854193	39.07%	4.512%
25	14.045	2029	2033	2043	rBV	246444	245011	5.16%	0.596%
26	14.345	2081	2084	2090	rBV	410572	385135	8.11%	0.937%
27	14.615	2126	2130	2132	rBV	171472	186078	3.92%	0.453%
28	14.639	2132	2134	2143	rVV	595179	673581	14.19%	1.639%
29	14.709	2143	2146	2150	rVB	125811	127529	2.69%	0.310%
30	14.874	2170	2174	2181	rVB	47764	83997	1.77%	0.204%
31	14.956	2184	2188	2199	rBV	675181	764153	16.10%	1.860%
32	15.209	2228	2231	2236	rVB2	36535	57188	1.20%	0.139%
33	15.268	2236	2241	2245	rBV	1256485	1580876	33.31%	3.847%
34	15.315	2245	2249	2257	rVB	616427	823479	17.35%	2.004%

LSC Area Percent Report

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Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-MH-07-COMP

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

35	15.715	2312	2317	2323	rBV	475754	718037	15.13%	1.747%
36	16.186	2391	2397	2404	rBV	241545	418263	8.81%	1.018%
37	16.733	2484	2490	2496	rVB3	89896	179255	3.78%	0.436%

Sum of corrected areas: 41091576

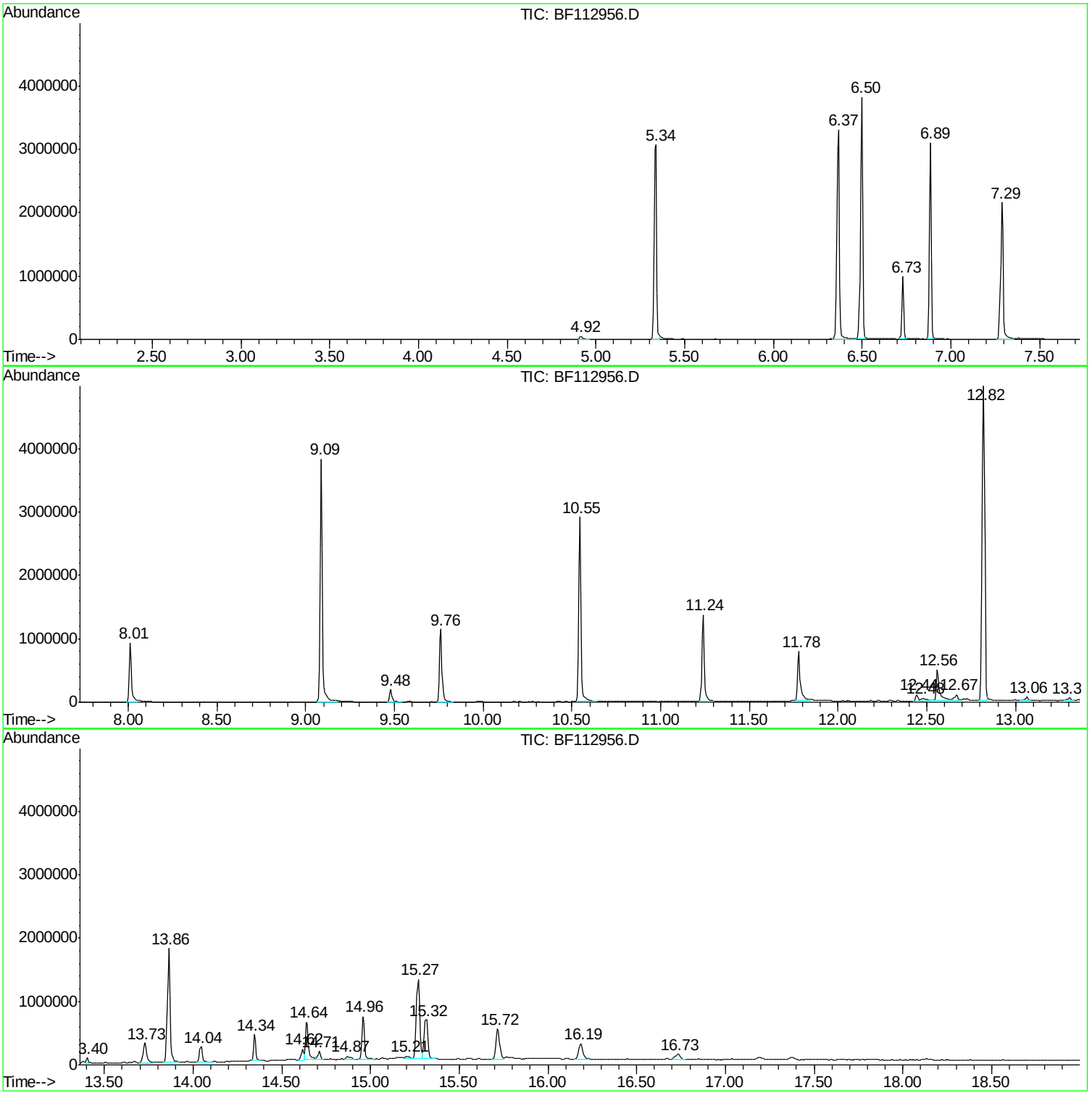
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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

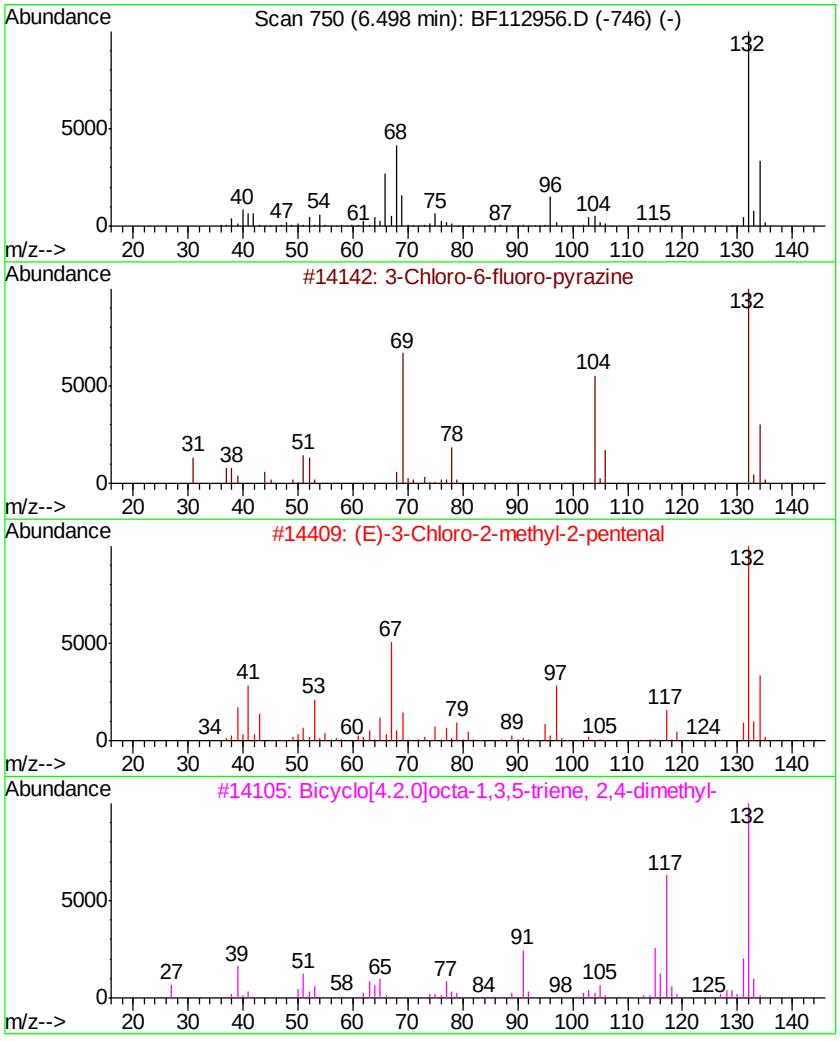
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

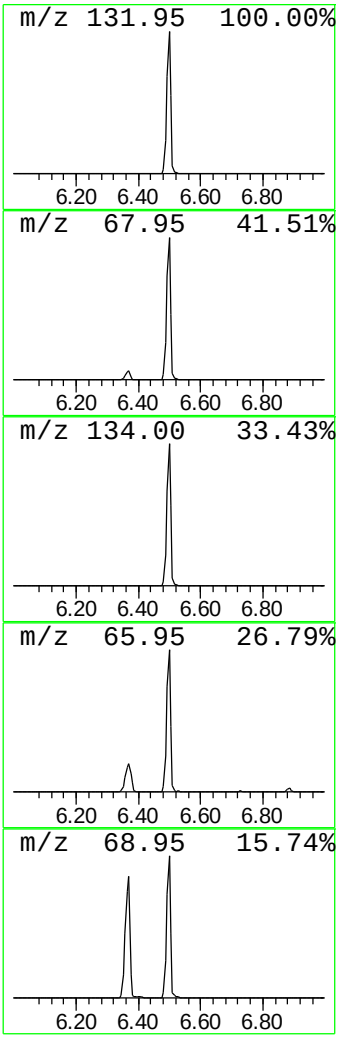
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	89.66 ng	3436470	1,4-Dichlorobenzene-d4	6.73

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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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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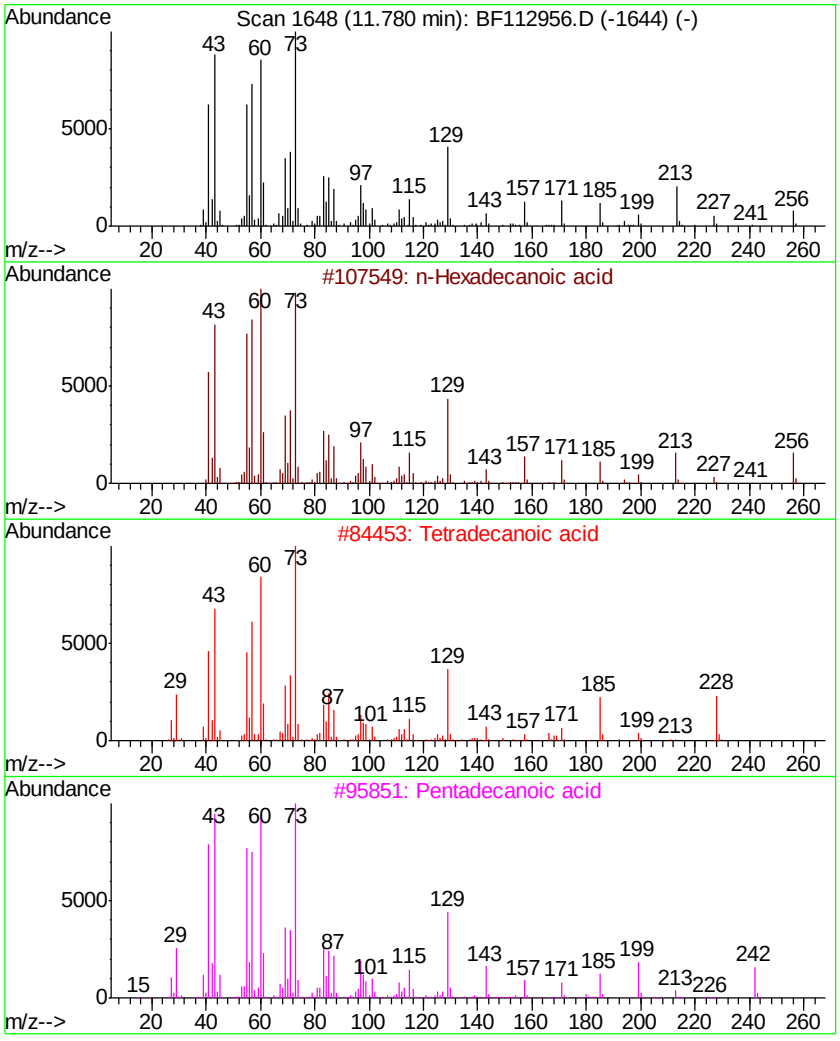
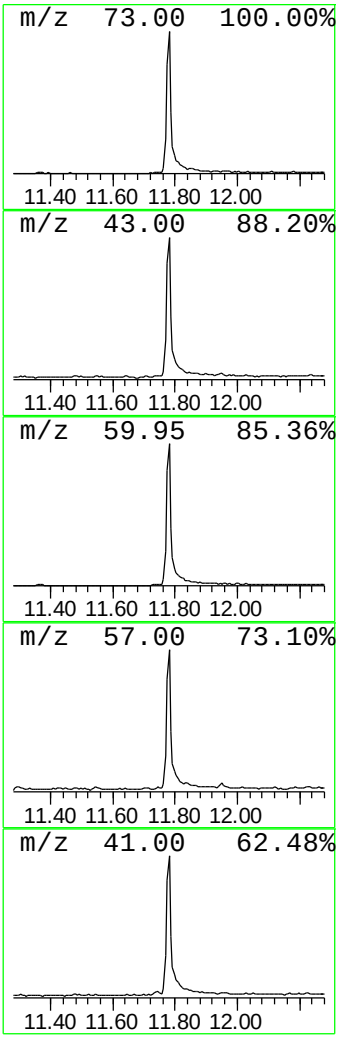
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	12.64 ng	855516	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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

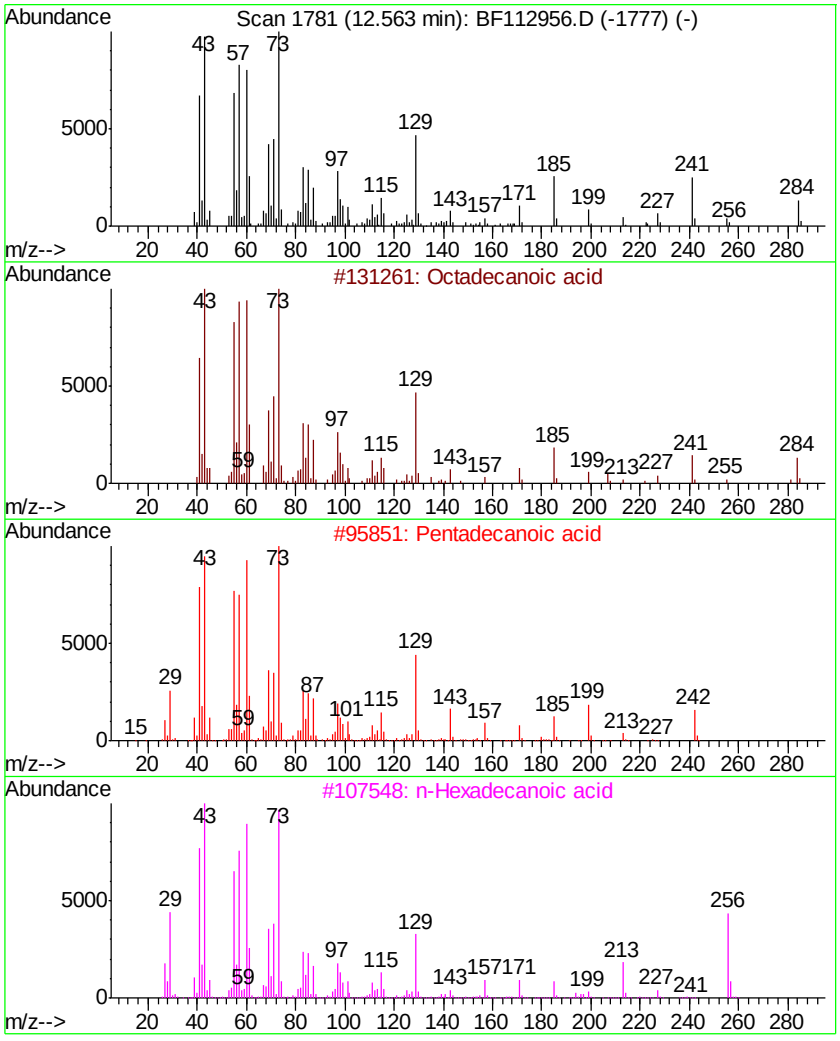
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

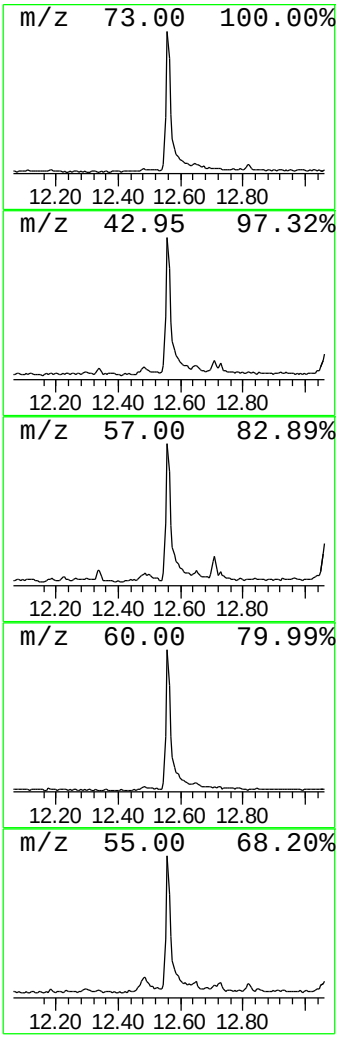
****

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	6.95 ng	644009	Chrysene-d12	13.86

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	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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

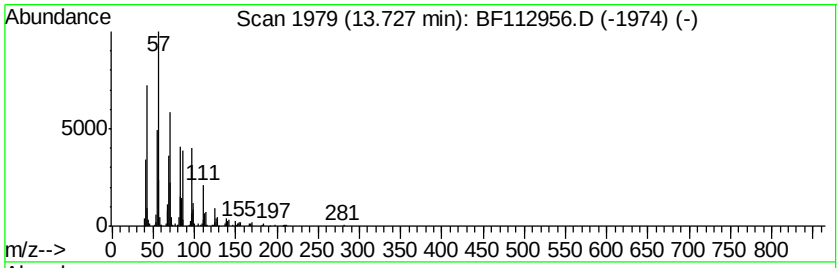
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

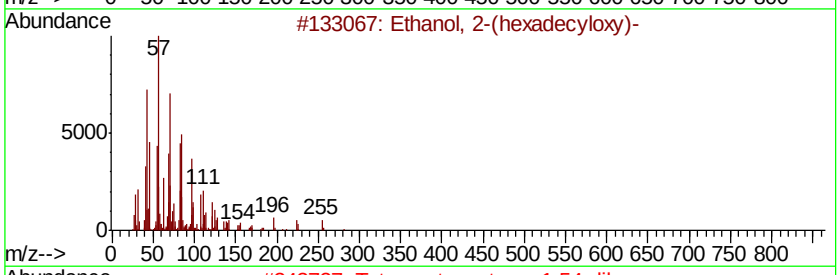
****

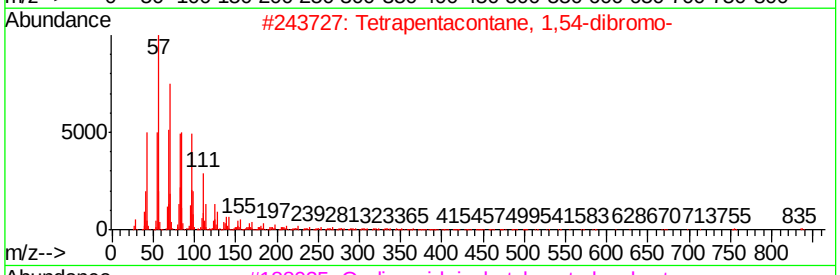
Peak Number 5 Ethanol, 2-(hexadecyloxy)- Concentration Rank 9

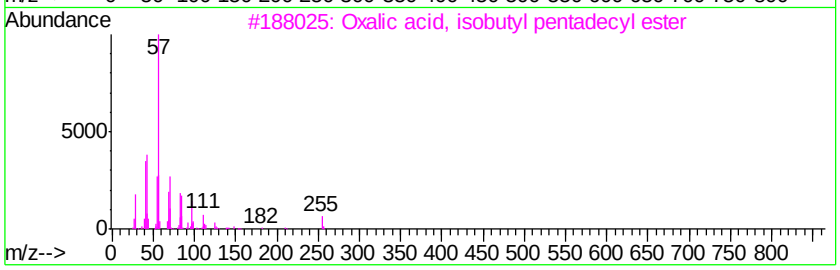
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.77 ng	441938	Chrysene-d12	13.86

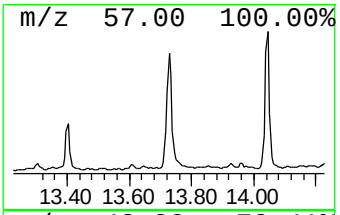
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91
2	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	87
3	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87

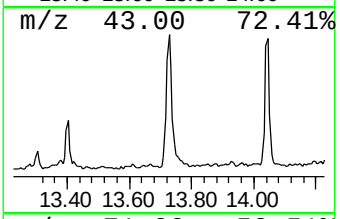


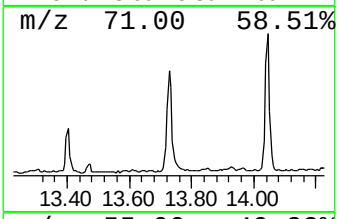


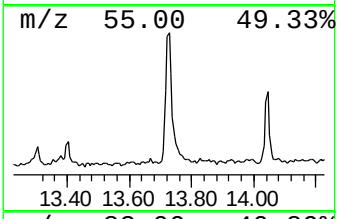


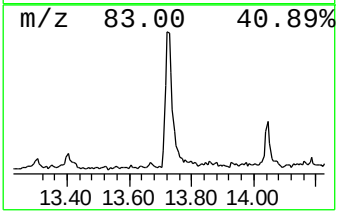












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Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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

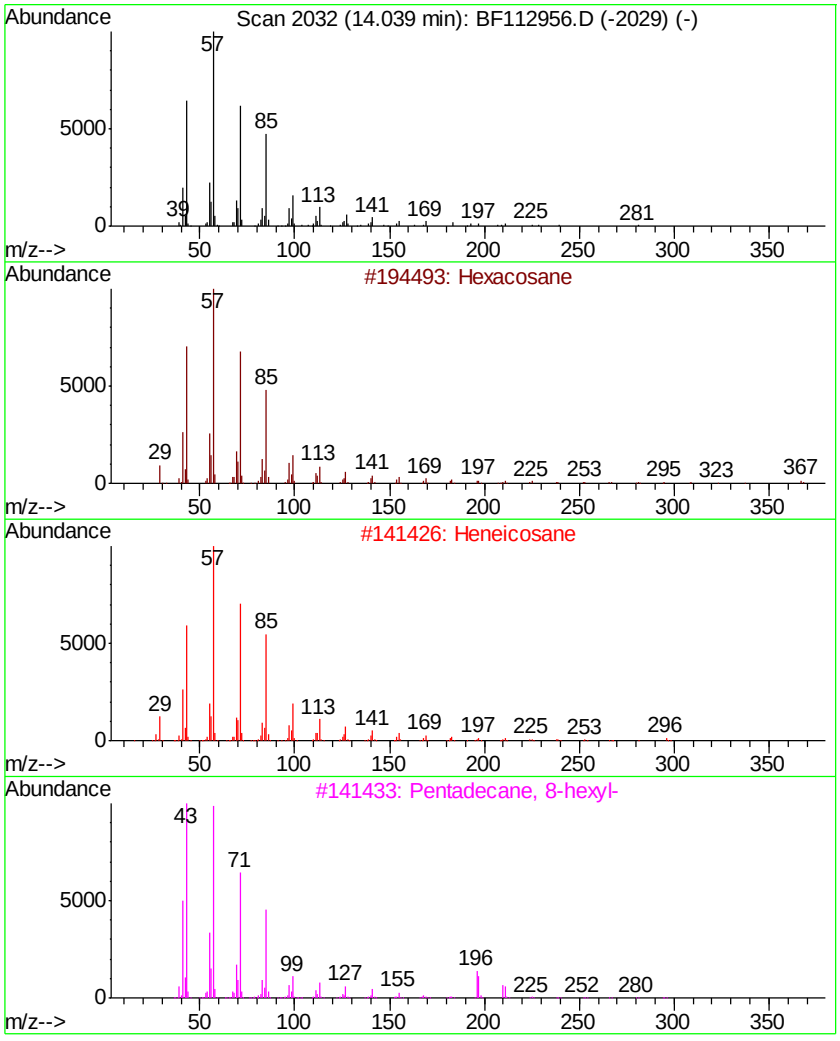
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

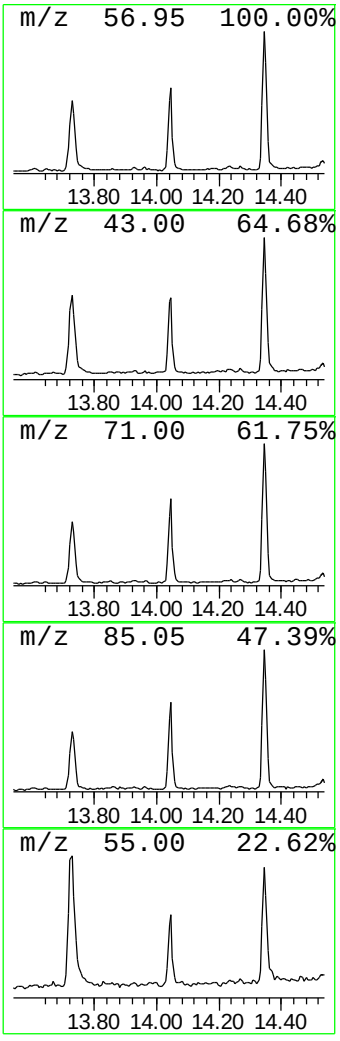
****

Peak Number 6 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.64 ng	245011	Chrysene-d12	13.86

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	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
5	Tetratetracontane	619	C44H90	007098-22-8	87





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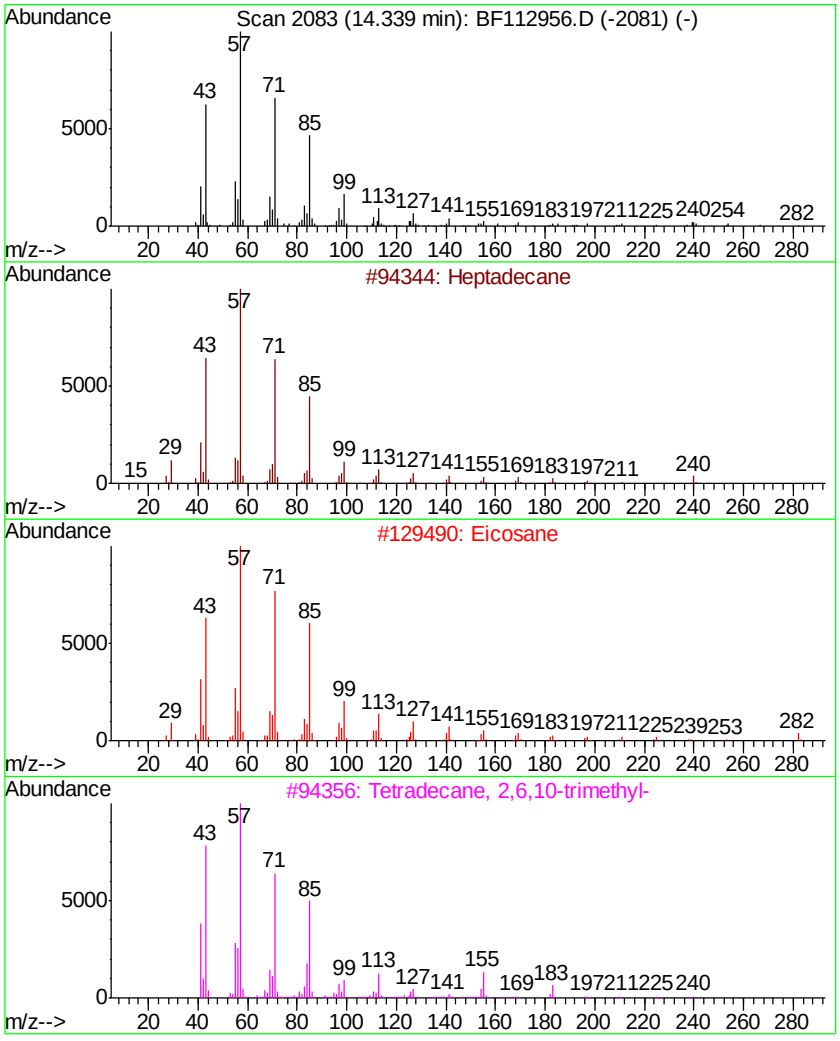
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

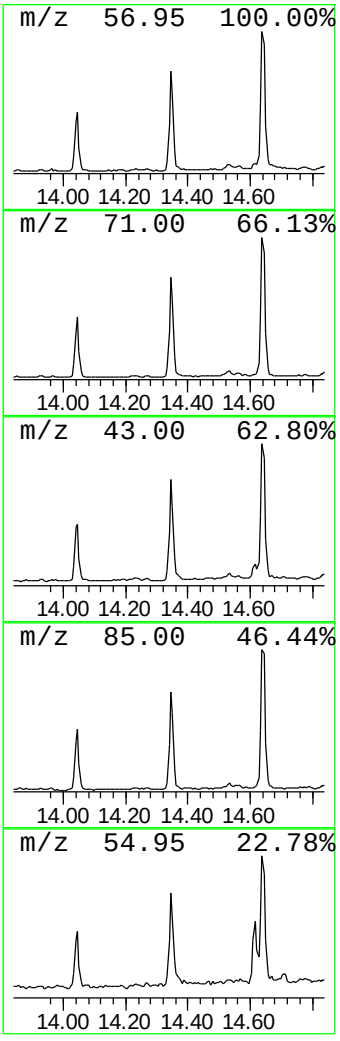
****

Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	4.15 ng	385135	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	95
2	Eicosane	282	C20H42	000112-95-8	94
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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

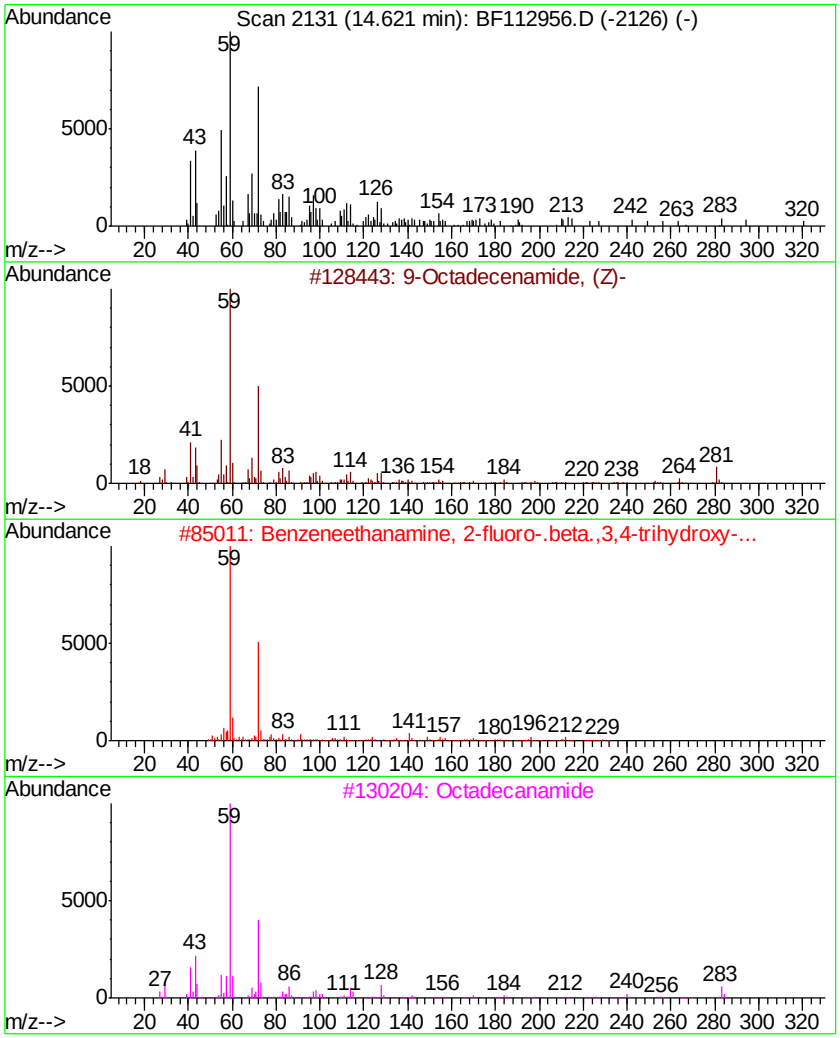
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

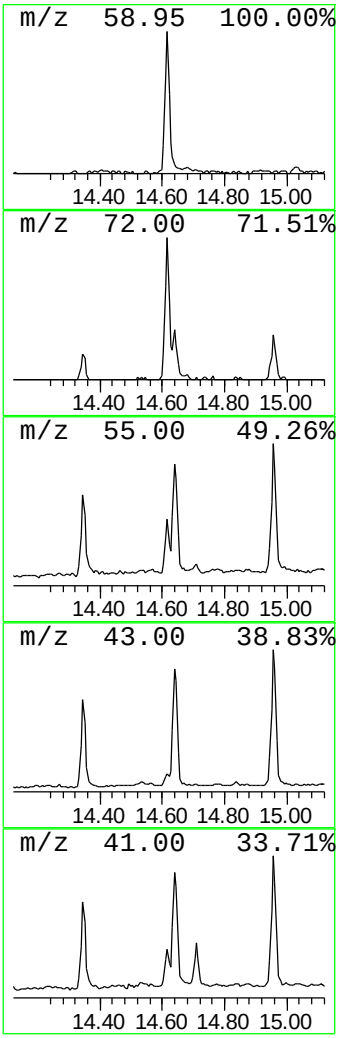
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.35 ng	186078	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
3	Octadecanamide	283	C18H37NO	000124-26-5	50
4	Dodecanamide	199	C12H25NO	001120-16-7	43
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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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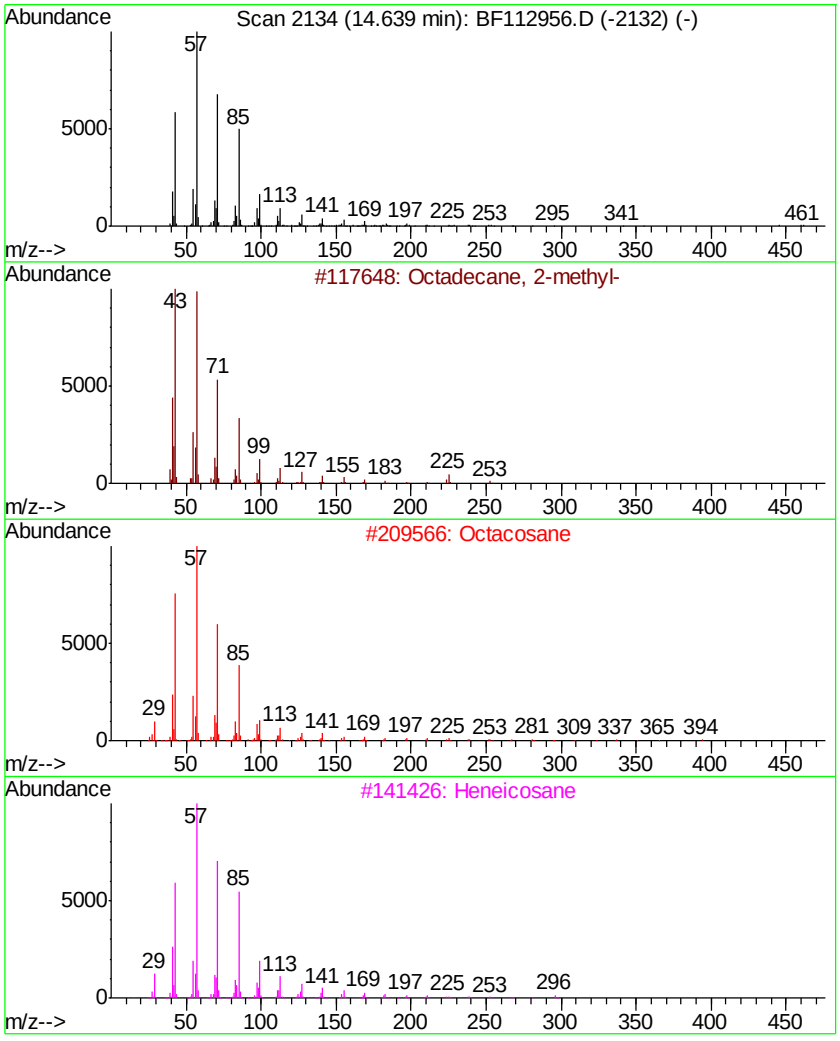
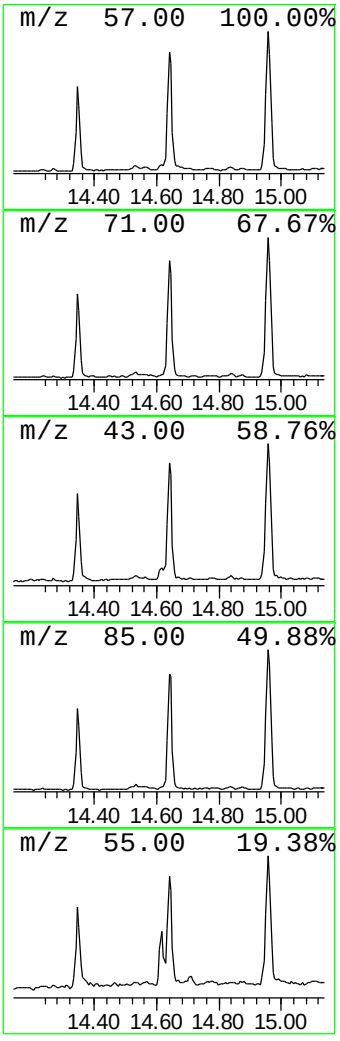
Peak Number 9 Octadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	8.52 ng	673581	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Triacontane	422	C30H62	000638-68-6	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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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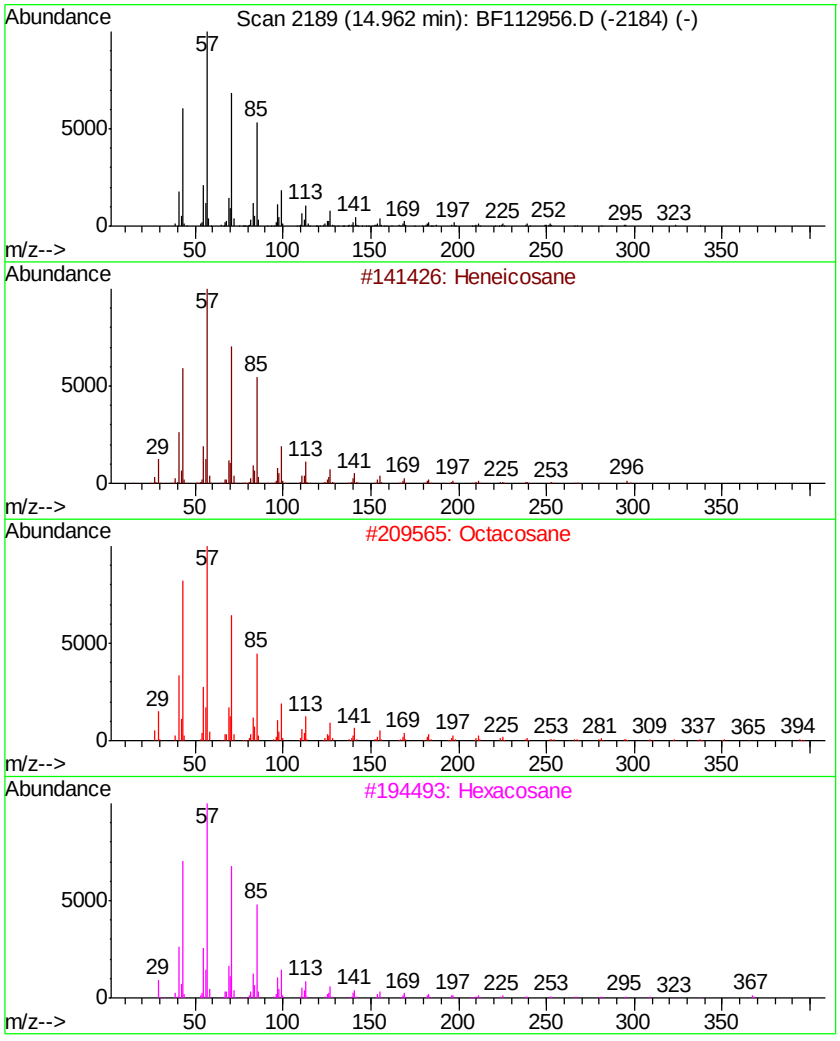
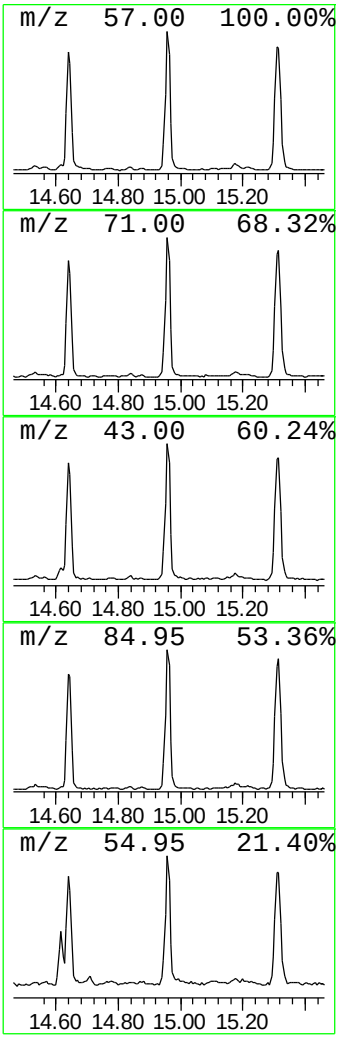
Peak Number 10 unknown14.96 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	9.67 ng	764153	Perylene-d12	15.27

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	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Octadecane	254	C18H38	000593-45-3	90





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Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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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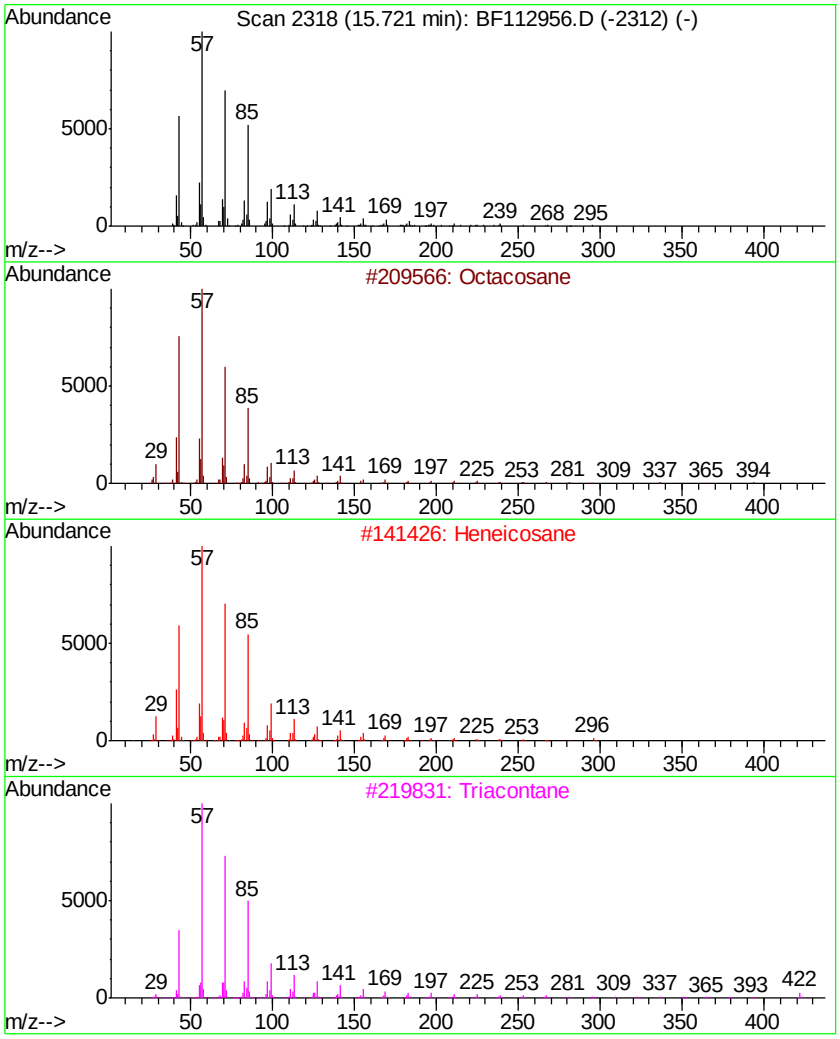
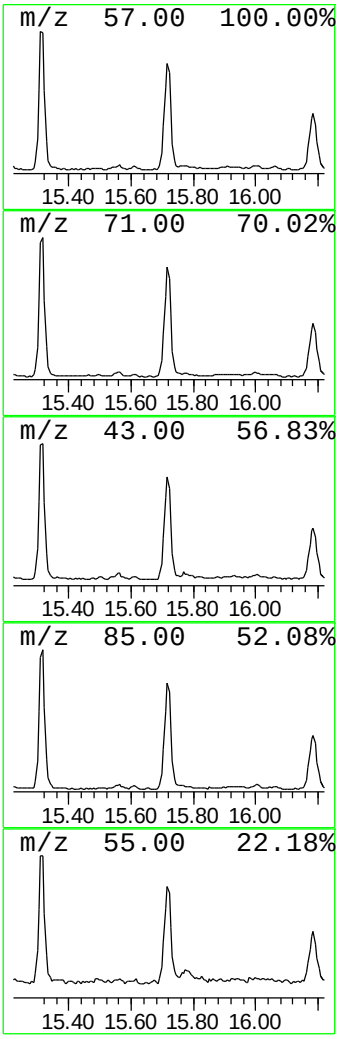
Peak Number 11 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	9.08 ng	718037	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Triacontane	422	C30H62	000638-68-6	90
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90





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Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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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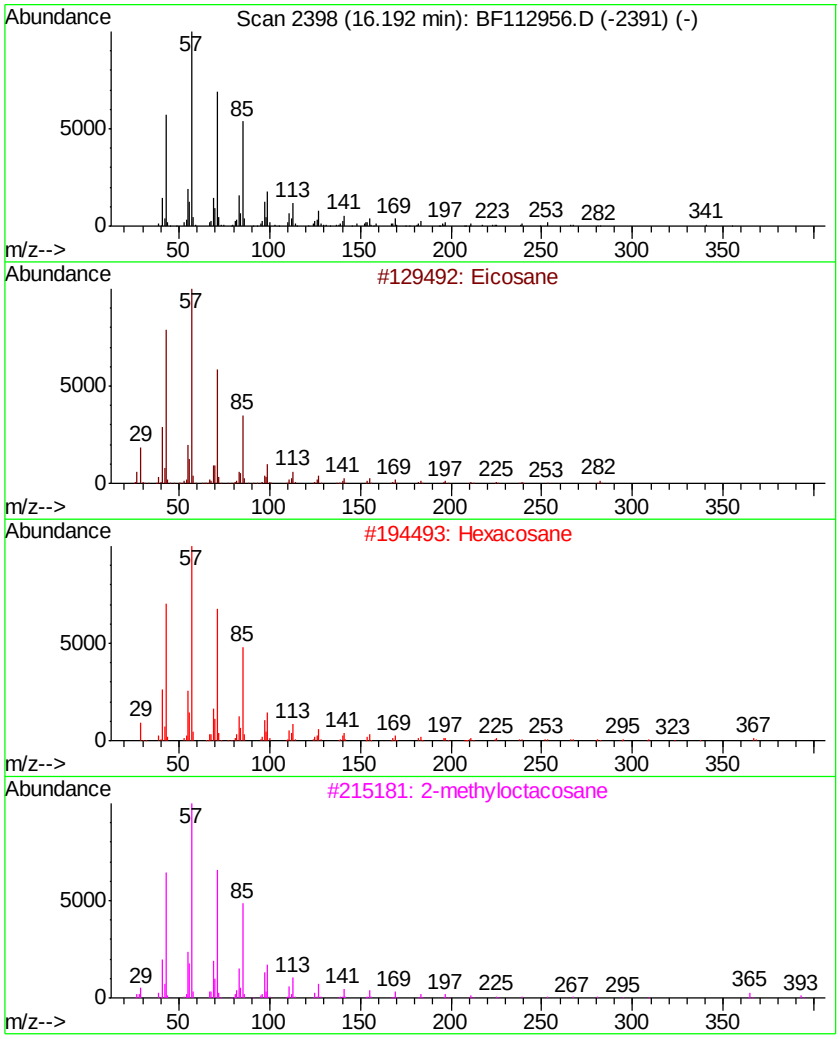
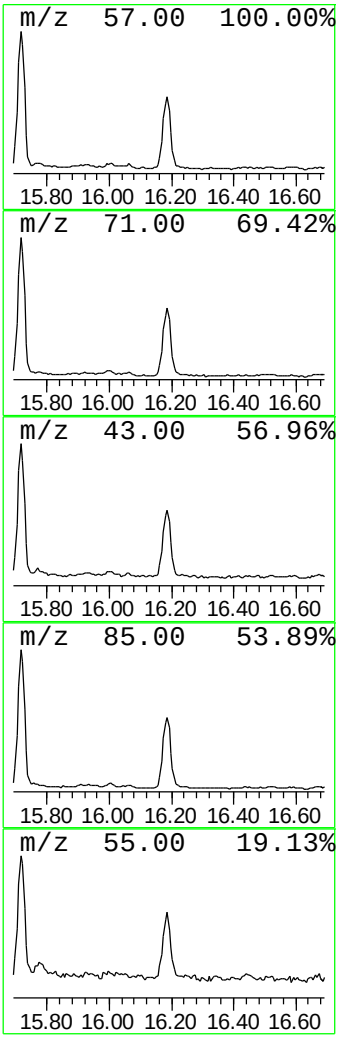
Peak Number 12 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	5.29 ng	418263	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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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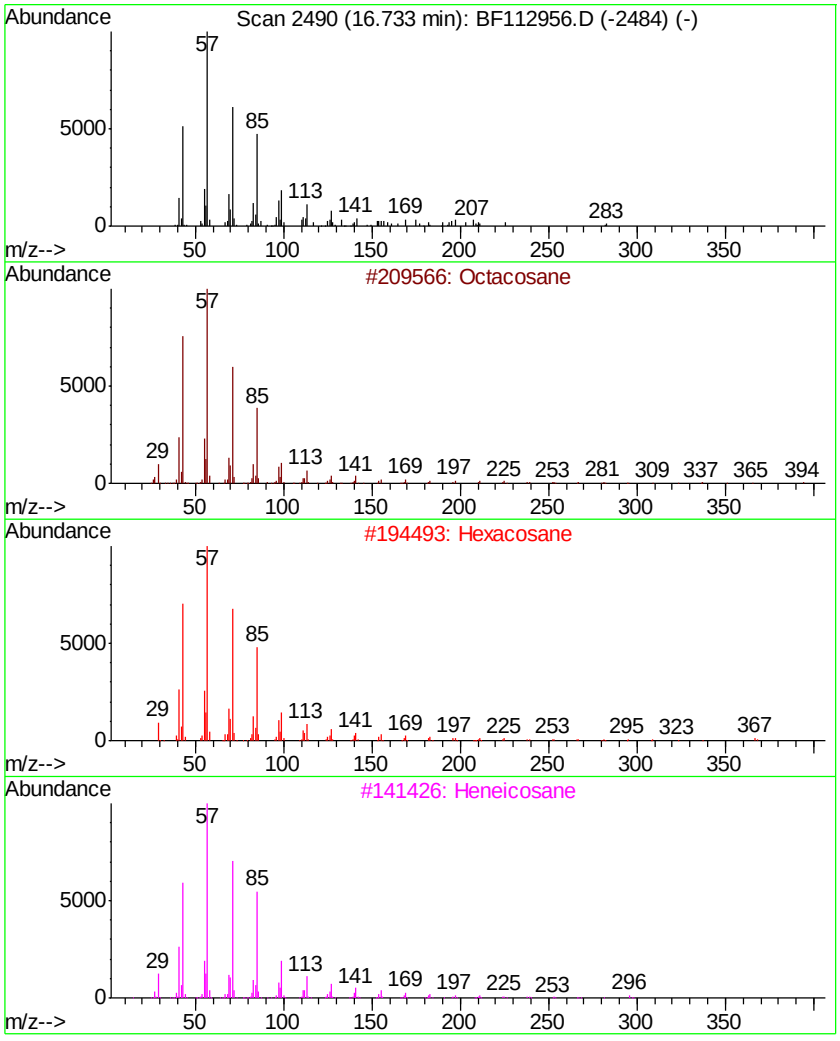
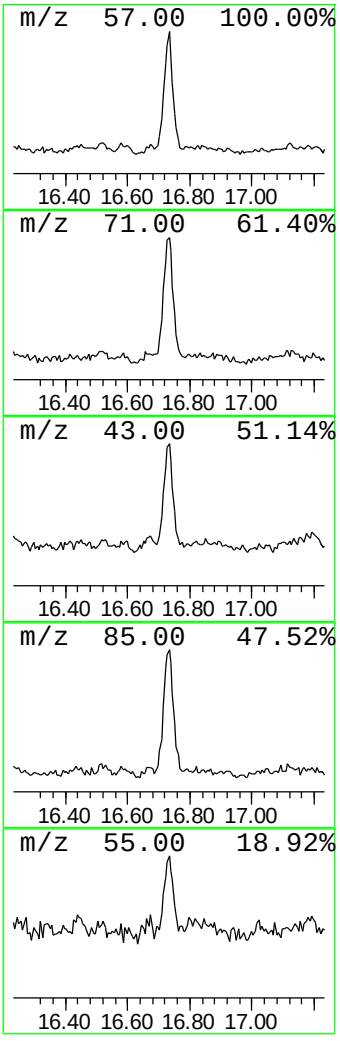
Peak Number 13 unknown16.73 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	2.27 ng	179255	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
Data File : BF112956.D
Acq On : 11 Mar 2019 15:58
Operator : JU/SJ
Sample : K1837-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-07-COMP

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
unknown6.50	6.50	89.7	ng	3436470	1	6.73	766526	20.0
n-Hexadecanoic acid	11.78	12.6	ng	855516	4	11.24	1353510	20.0
Octadecanoic acid	12.56	7.0	ng	644009	5	13.86	1854190	20.0
Ethanol, 2-(hexad...	13.73	4.8	ng	441938	5	13.86	1854190	20.0
Hexacosane	14.04	2.6	ng	245011	5	13.86	1854190	20.0
Heptadecane	14.34	4.2	ng	385135	5	13.86	1854190	20.0
9-Octadecenamide,...	14.62	2.4	ng	186078	6	15.27	1580880	20.0
Octadecane, 2-met...	14.64	8.5	ng	673581	6	15.27	1580880	20.0
unknown14.96	14.96	9.7	ng	764153	6	15.27	1580880	20.0
Octacosane	15.72	9.1	ng	718037	6	15.27	1580880	20.0
Eicosane	16.19	5.3	ng	418263	6	15.27	1580880	20.0
unknown16.73	16.73	2.3	ng	179255	6	15.27	1580880	20.0