LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109011.D
Acq On : 14 Sep 2018 22:41
Operator : JU/SJ
Sample : J4883-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SV30518L

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-BF091418.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	4.878	428	432	434	rBV	82587	82104	2.01%	0.250%
2	4.901	434	436	445	rVB	51191	63007	1.55%	0.192%
3	5.319	503	507	511	rBV	1589867	1532904	37.61%	4.676%
4	6.343	677	681	689	rBV	1119339	1099045	26.96%	3.352%
5	6.484	701	705	709	rBV	2898419	2862520	70.23%	8.731%
6	6.719	741	745	748	rBV	1236222	967365	23.73%	2.951%
7	6.878	767	772	775	rVB	3091993	2660973	65.28%	8.117%
8	7.278	835	840	843	rBV	2281463	2325490	57.05%	7.093%
9	8.001	959	963	966	rBV	1441163	1248713	30.63%	3.809%
10	9.078	1141	1146	1149	rBV	4490637	4071175	99.88%	12.418%
11	9.466	1209	1212	1215	rVB	198508	150945	3.70%	0.460%
12	9.748	1256	1260	1264	rBV2	1695888	1504541	36.91%	4.589%
13	10.536	1389	1394	1397	rBV	2686875	2633186	64.60%	8.032%
14	11.225	1507	1511	1515	rBV	1734733	1502310	36.86%	4.582%
15	11.772	1600	1604	1606	rBV	359003	364165	8.93%	1.111%
16	11.801	1606	1609	1612	rVB	2018001	1711300	41.98%	5.220%
17	12.548	1733	1736	1745	rVB	172435	185299	4.55%	0.565%
18	12.813	1776	1781	1784	rBV	4085043	4076171	100.00%	12.433%
19	13.719	1932	1935	1945	rVB	117763	153987	3.78%	0.470%
20	13.848	1953	1957	1961	rBV	1376152	1255824	30.81%	3.831%
21	14.342	2038	2041	2044	rBV	76894	66188	1.62%	0.202%
22	14.636	2087	2091	2095	rVB	131851	123192	3.02%	0.376%
23	14.954	2141	2145	2151	rBV	163837	173589	4.26%	0.529%
24	15.254	2190	2196	2201	rBV	1024459	1107098	27.16%	3.377%
25	15.307	2201	2205	2212	rVB	168079	208446	5.11%	0.636%
26	15.713	2269	2274	2280	rVB2	128614	182909	4.49%	0.558%
27	16.177	2348	2353	2365	rVB2	85292	151415	3.71%	0.462%
28	16.724	2441	2446	2452	rBV3	36077	61627	1.51%	0.188%
29	16.795	2452	2458	2467	rBV3	82691	195518	4.80%	0.596%
30	17.359	2551	2554	2565	rVB4	27291	63472	1.56%	0.194%

Sum of corrected areas: 32784478

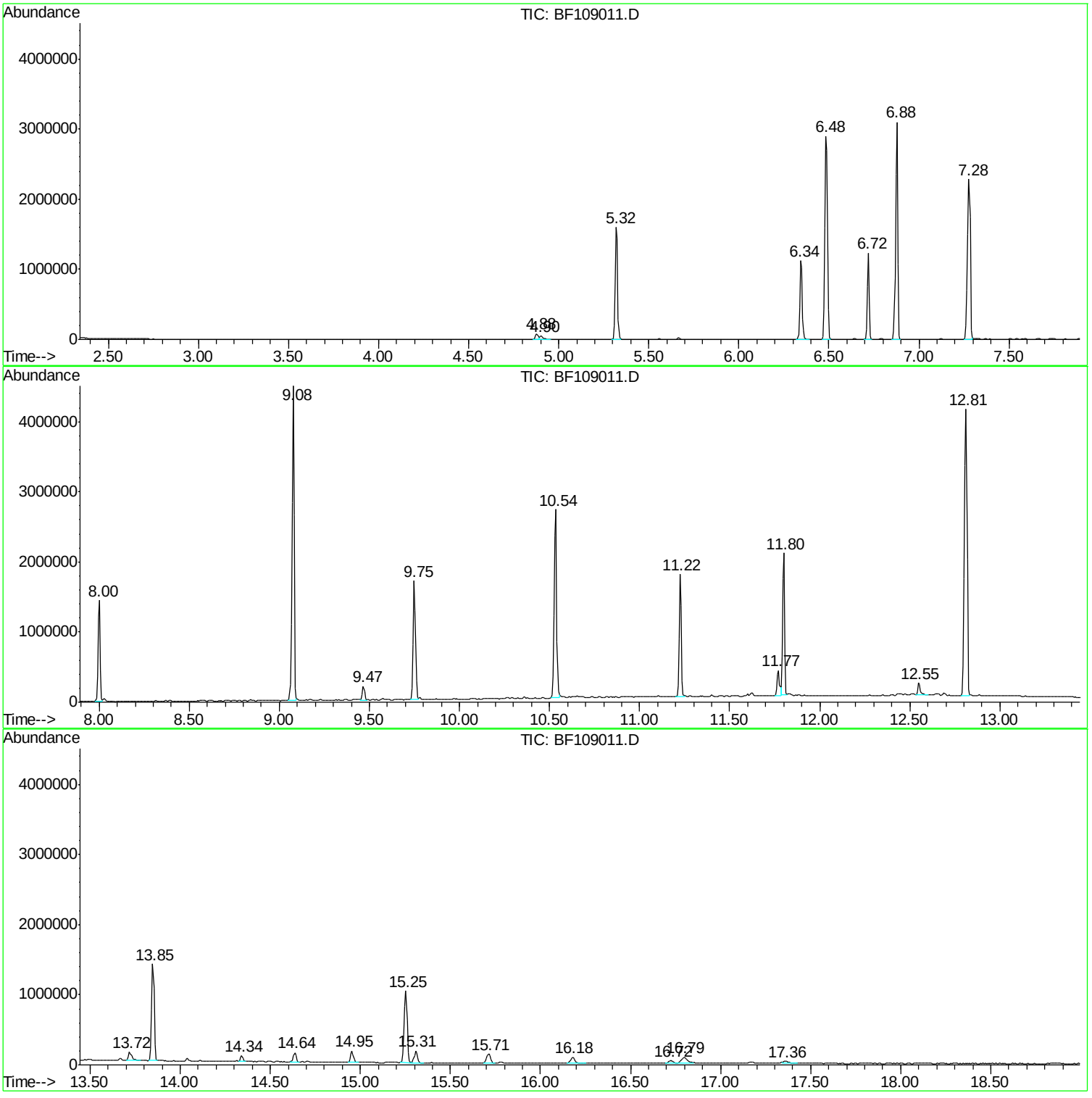
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109011.D
Acq On : 14 Sep 2018 22:41
Operator : JU/SJ
Sample : J4883-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SV30518L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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\BF091418\
Data File : BF109011.D
Acq On : 14 Sep 2018 22:41
Operator : JU/SJ
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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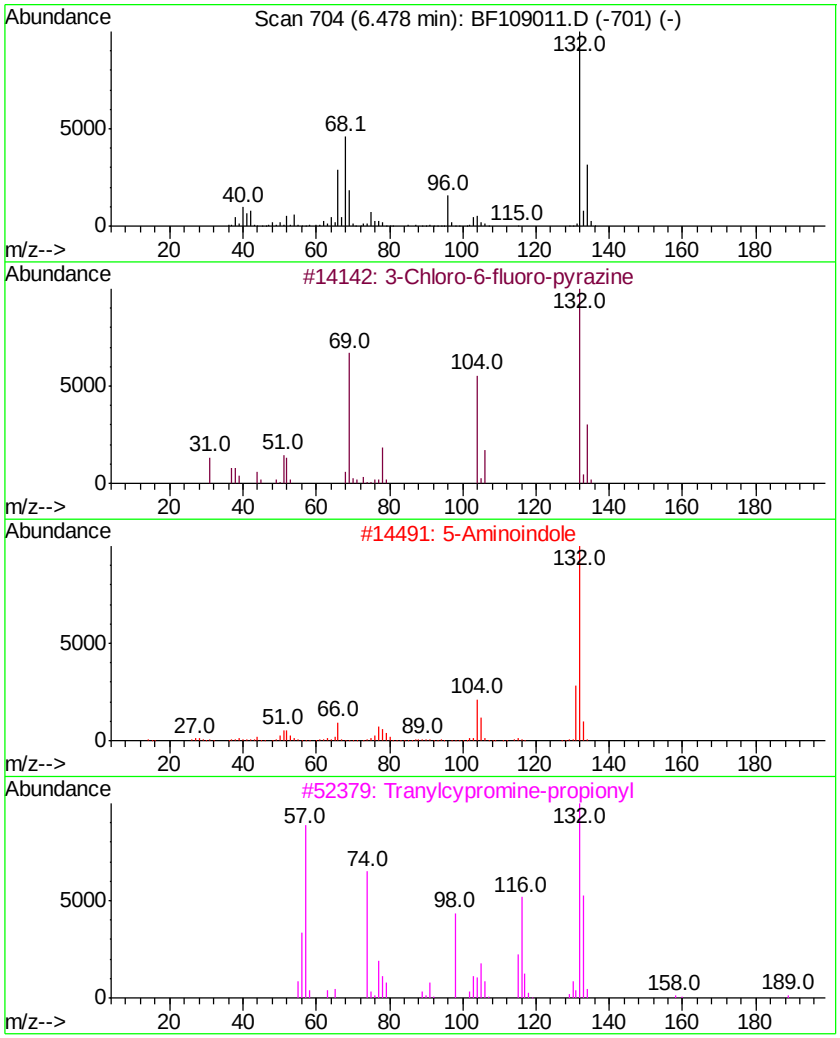
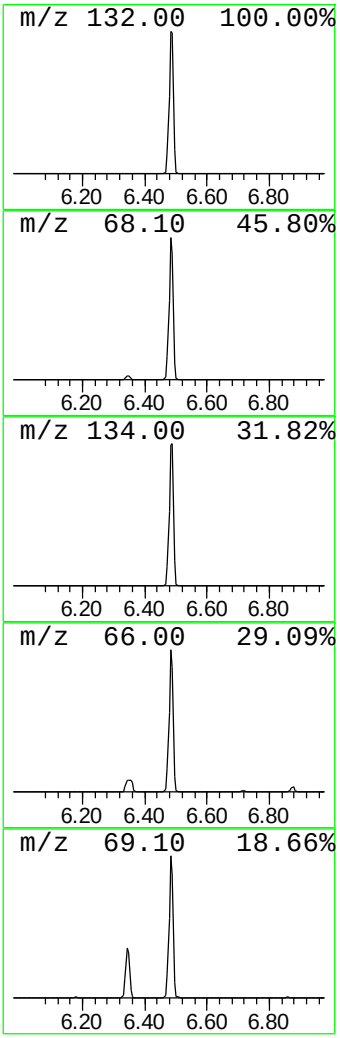
Peak Number 1 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	59.18 ng	2862520	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Misc :
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Instrument : BNA_F
ClientSampleId : SV30518L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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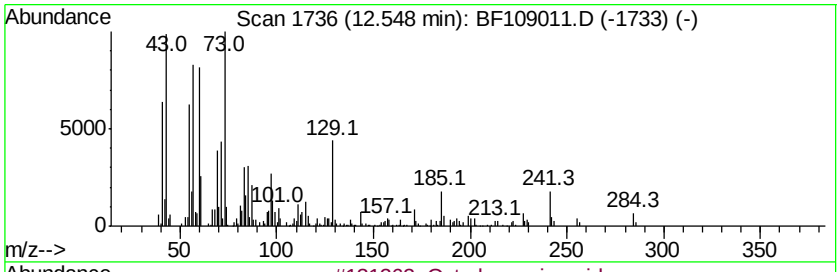
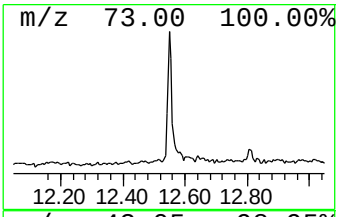
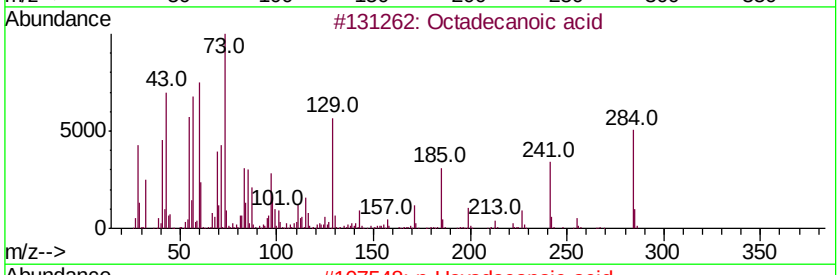
Peak Number 3 Octadecanoic acid Concentration Rank 7

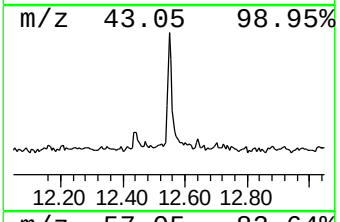
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	2.95 ng	185299	Chrysene-d12	13.85

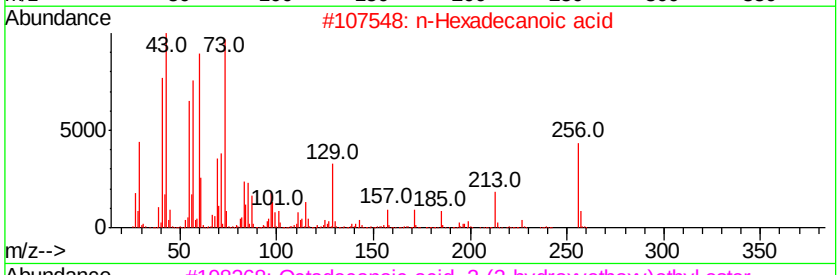
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81

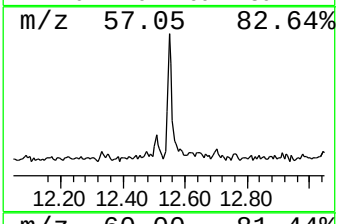


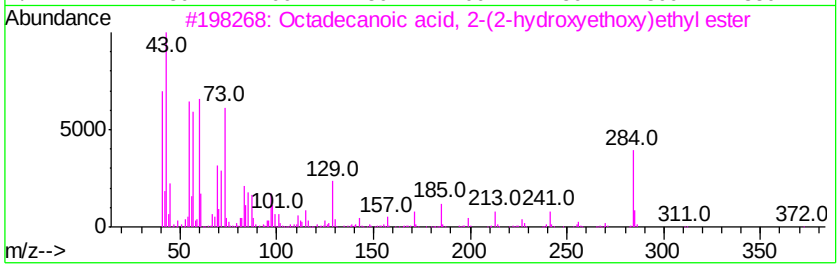


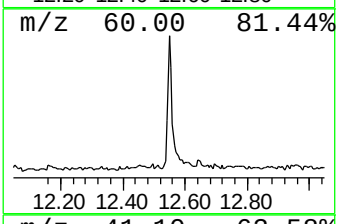


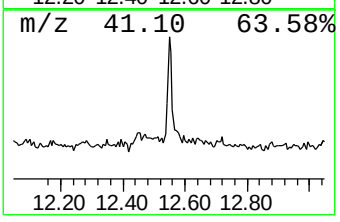












Library Search Compound Report

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Data File : BF109011.D
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Operator : JU/SJ
Sample : J4883-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SV30518L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

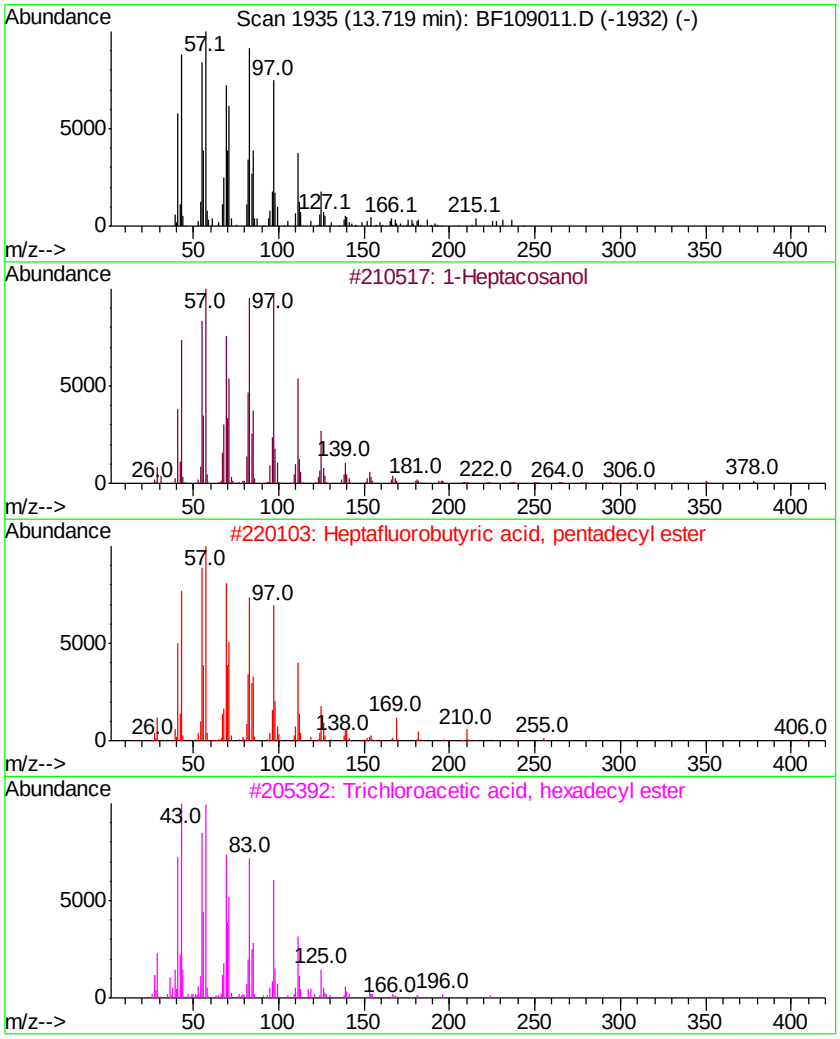
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

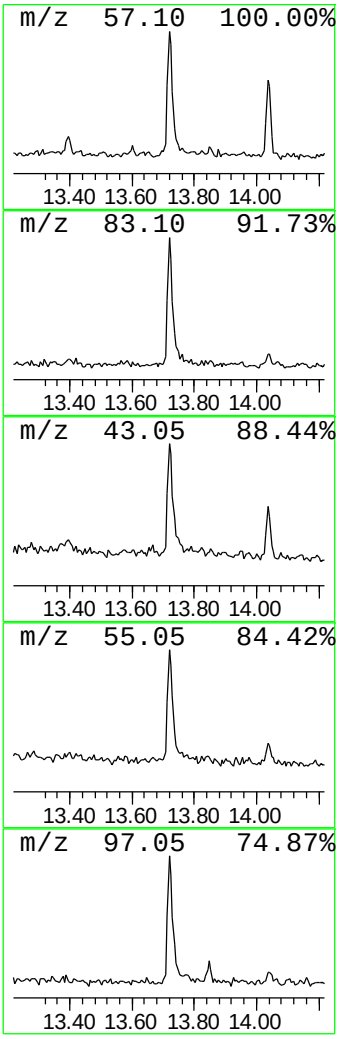
****

Peak Number 4 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.45 ng	153987	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	1-Docosene	308	C22H44	001599-67-3	91
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SV30518L

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

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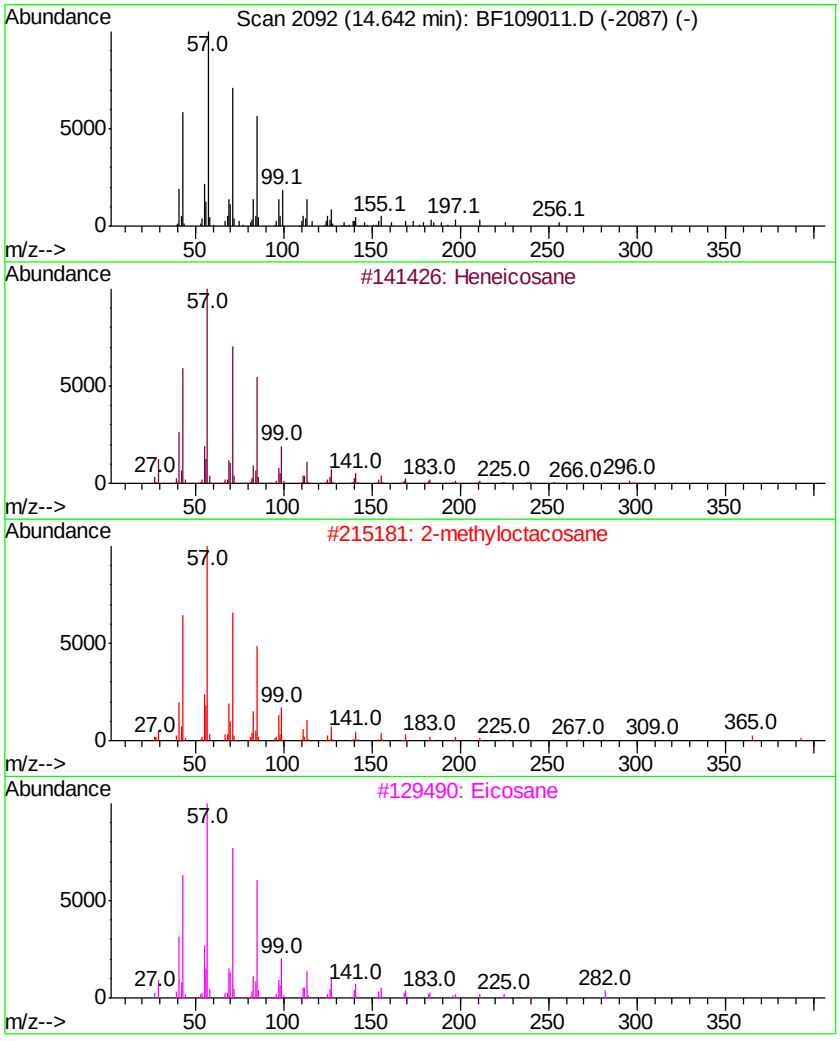
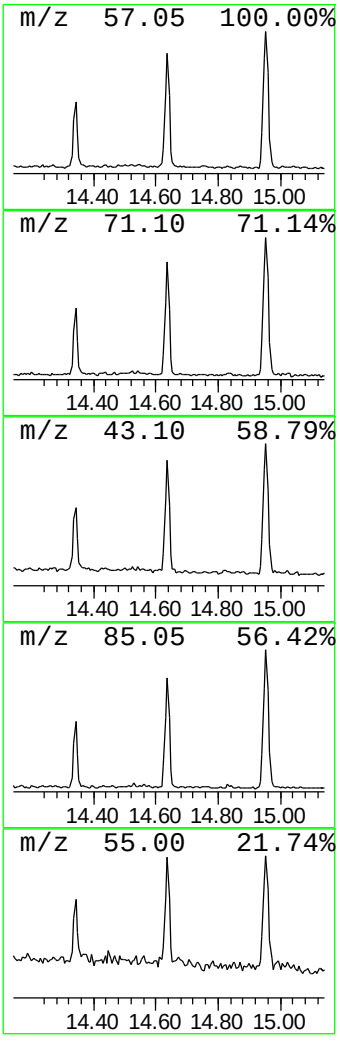
Peak Number 5 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.23 ng	123192	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Eicosane	282	C20H42	000112-95-8	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87





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Sample : J4883-03
Misc :
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Instrument : BNA_F
ClientSampleId : SV30518L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
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TIC Library : C:\DATABASE\NIST11.L
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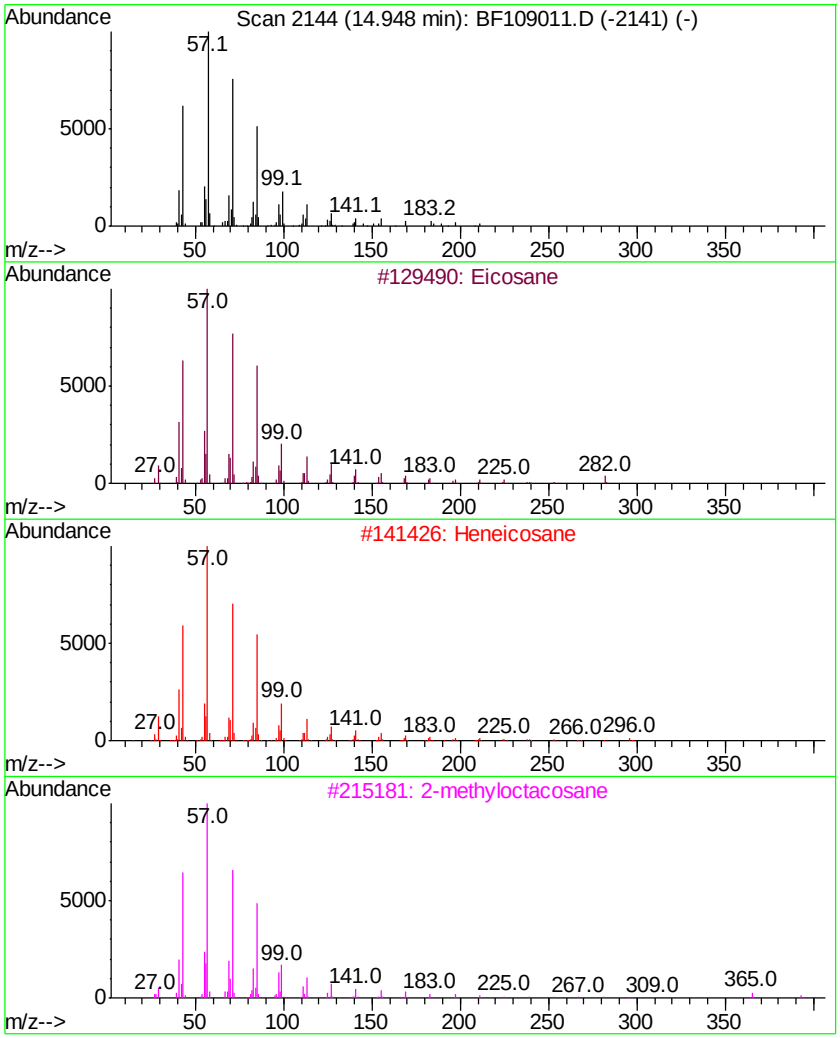
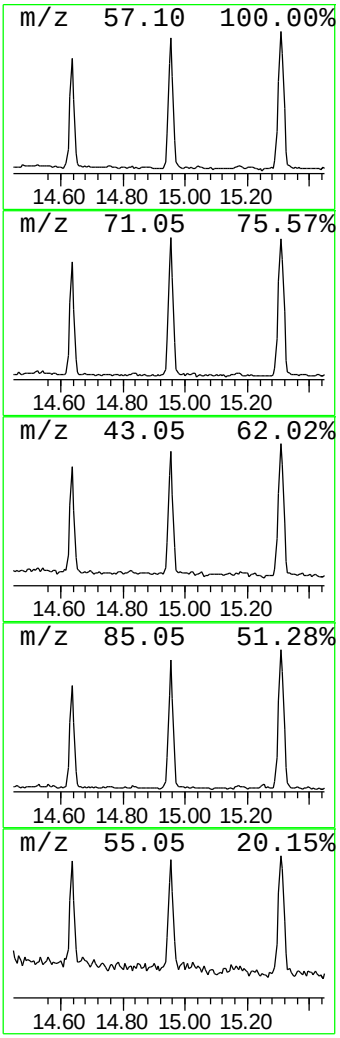
Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.14 ng	173589	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SV30518L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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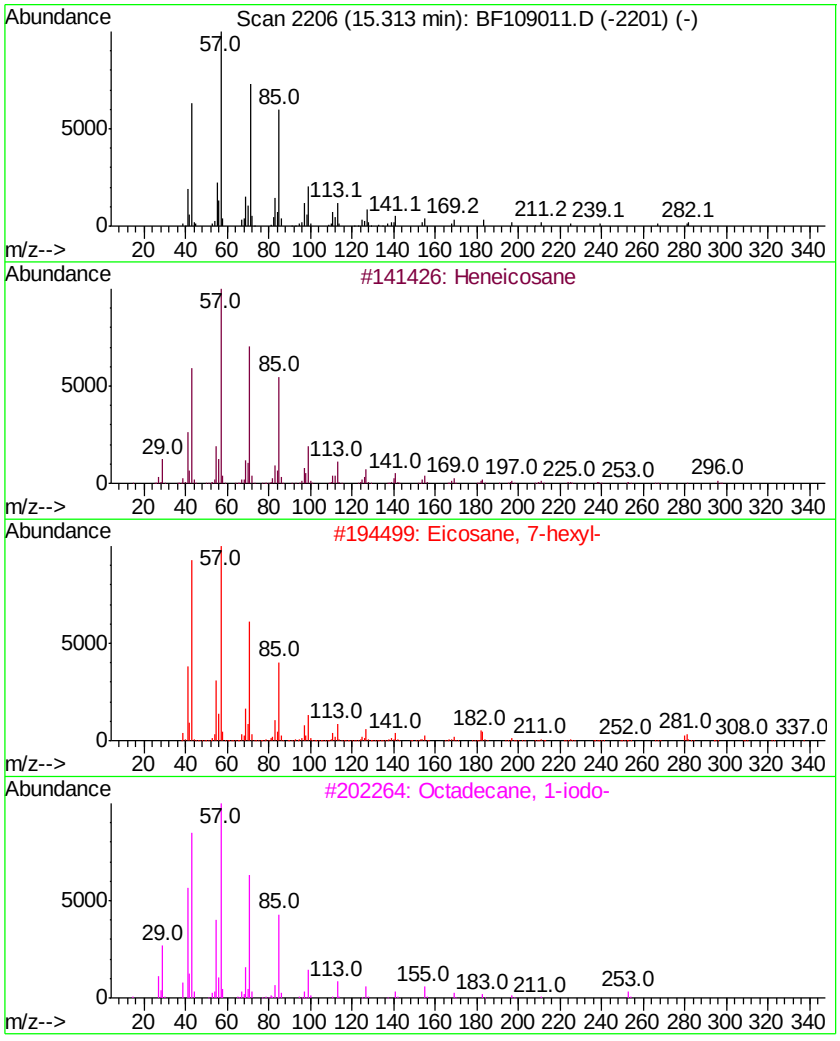
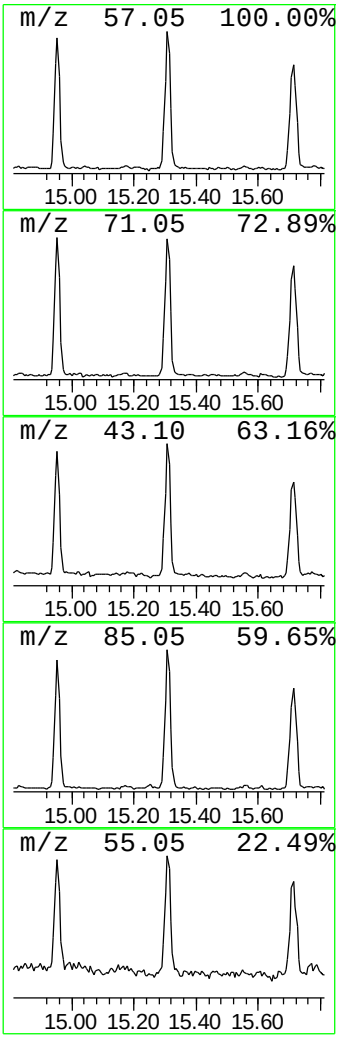
Peak Number 7 Eicosane, 7-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	3.77 ng	208446	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Octadecane	254	C18H38	000593-45-3	83





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TIC Library : C:\DATABASE\NIST11.L
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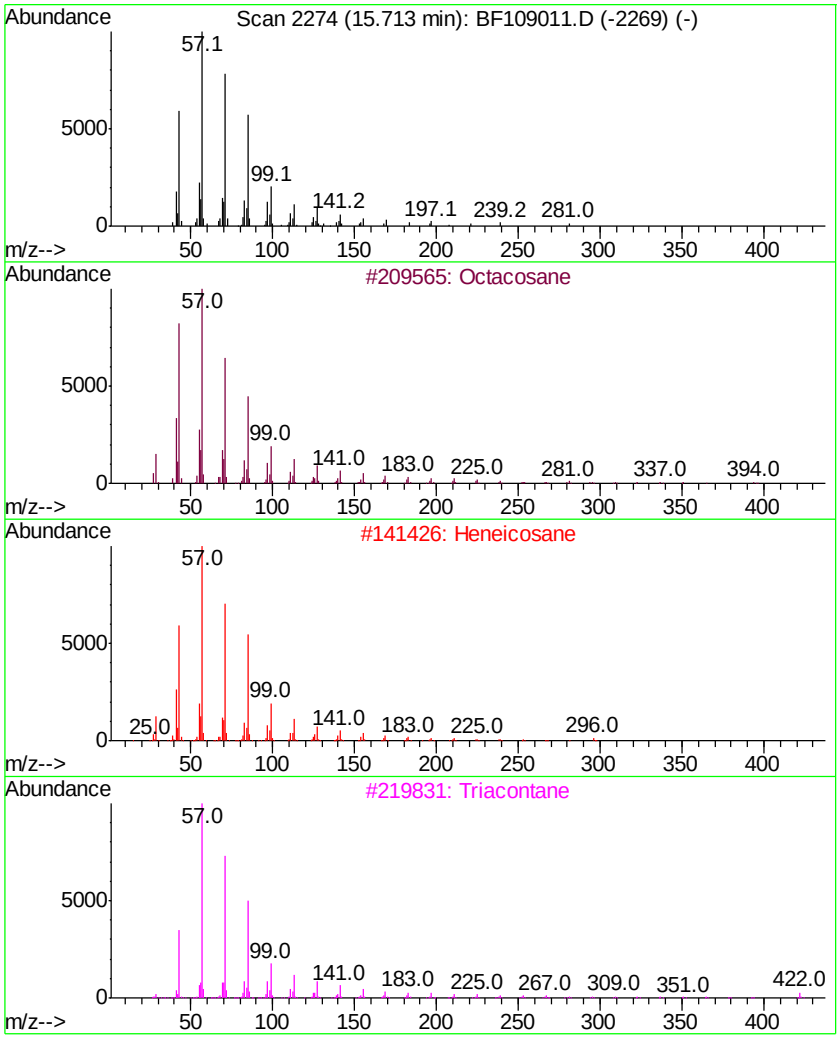
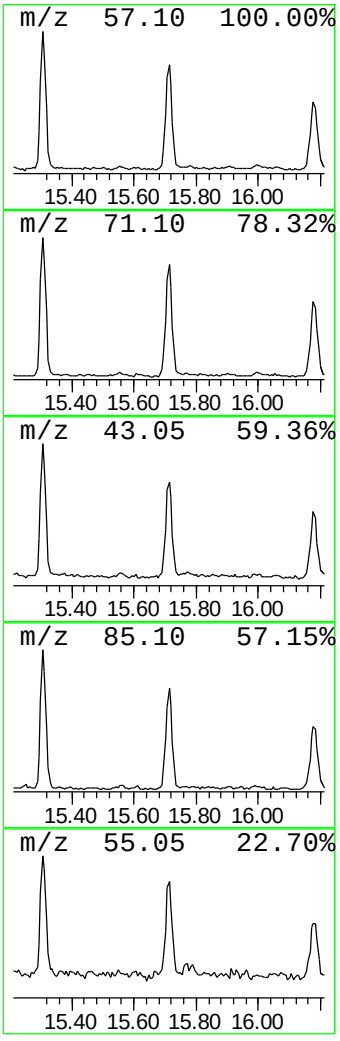
****

Peak Number 8 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.30 ng	182909	Perylene-d12	15.25

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	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Octadecane	254	C18H38	000593-45-3	91





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ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SV30518L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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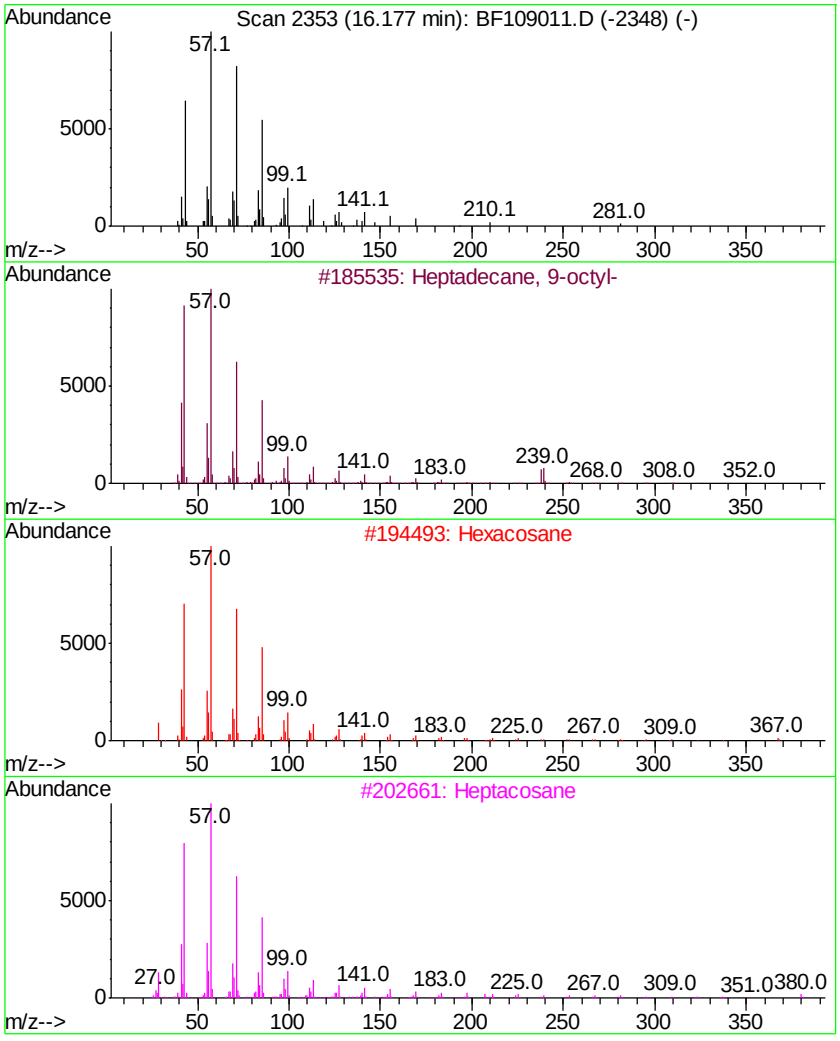
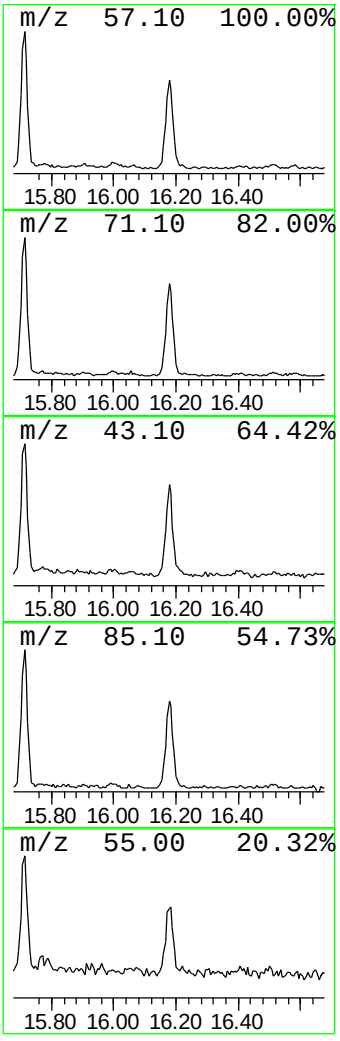
Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.74 ng	151415	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	2-methyltetracosane	352	C25H52	1000376-72-6	91
5	Hentriacontane	437	C31H64	000630-04-6	91





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Misc :
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Instrument : BNA_F
ClientSampleId : SV30518L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

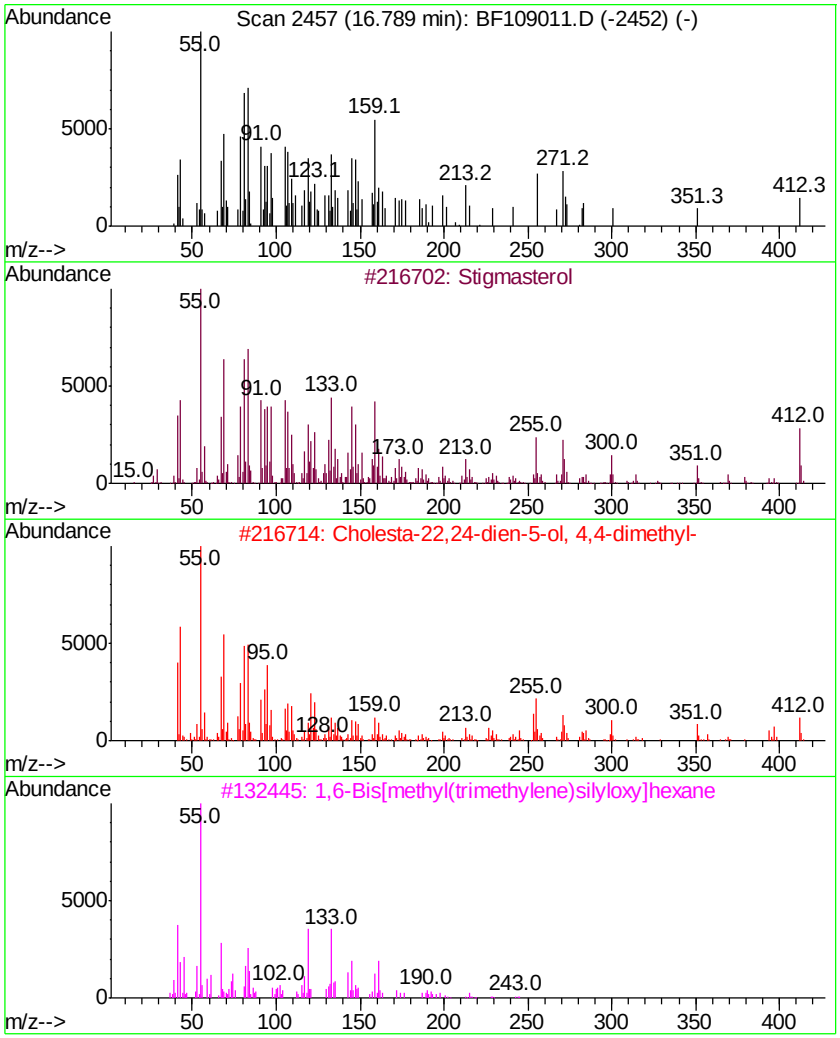
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

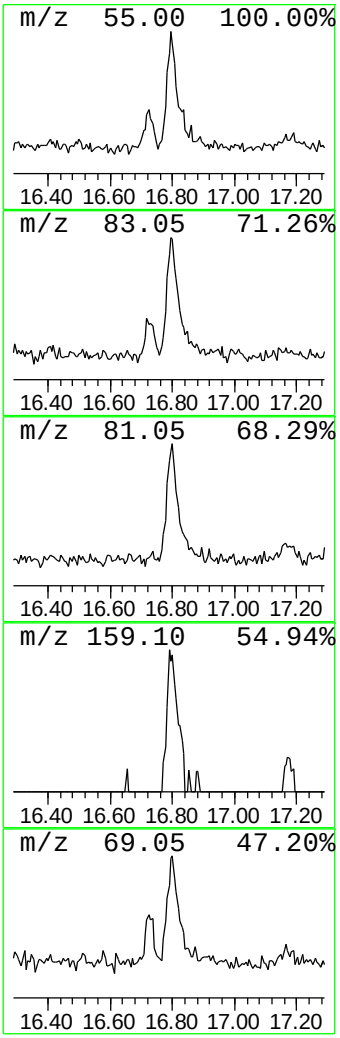
****

Peak Number 10 Stigmasterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.79	3.53 ng	195518	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmasterol	412	C29H48O	000083-48-7	99
2	Cholesta-22,24-dien-5-ol, 4,4-di...	412	C29H48O	1000128-66-1	41
3	1,6-Bis[methyl(trimethylene)silv...	286	C14H30O2Si2	1000217-00-5	35
4	Silane, dimethyl(but-2-enyloxy)i...	230	C12H26O2Si	1000348-05-6	12
5	22-Stigmasten-3-one	412	C29H48O	004736-95-2	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091418\
Data File : BF109011.D
Acq On : 14 Sep 2018 22:41
Operator : JU/SJ
Sample : J4883-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SV30518L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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
unknown6.48	6.48	59.2	ng	2862520	1	6.72	967365	20.0
Octadecanoic acid	12.55	3.0	ng	185299	5	13.85	1255820	20.0
1-Heptacosanol	13.72	2.5	ng	153987	5	13.85	1255820	20.0
Heneicosane	14.64	2.2	ng	123192	6	15.25	1107100	20.0
Eicosane	14.95	3.1	ng	173589	6	15.25	1107100	20.0
Eicosane, 7-hexyl-	15.31	3.8	ng	208446	6	15.25	1107100	20.0
Octacosane	15.71	3.3	ng	182909	6	15.25	1107100	20.0
Heptadecane, 9-oc...	16.18	2.7	ng	151415	6	15.25	1107100	20.0
Stigmasterol	16.79	3.5	ng	195518	6	15.25	1107100	20.0