LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121418\
Data File : BF111441.D
Acq On : 15 Dec 2018 1:35
Operator : JU/SJ
Sample : J6322-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-6-C-2-120718

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-BF121418.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	4.369	384	388	395	rBV	87745	109494	2.33%	0.267%
2	5.004	492	496	506	rVB	201057	254518	5.42%	0.620%
3	5.428	563	568	571	rBV	4002103	4010918	85.39%	9.776%
4	6.439	735	740	758	rBV	4575567	4696989	100.00%	11.448%
5	6.569	758	762	765	rBV	4627725	4395646	93.58%	10.714%
6	6.792	797	800	804	rBV	1324154	1223910	26.06%	2.983%
7	6.951	823	827	831	rBV	4290184	3915915	83.37%	9.544%
8	7.357	891	896	899	rBV	3348213	3086444	65.71%	7.523%
9	8.075	1014	1018	1034	rBV	1561863	1493557	31.80%	3.640%
10	9.151	1197	1201	1215	rBV	4545300	4479103	95.36%	10.917%
11	9.545	1264	1268	1277	rBV	289052	258504	5.50%	0.630%
12	9.833	1313	1317	1321	rBV	1419779	1289598	27.46%	3.143%
13	10.621	1446	1451	1465	rBV	2295006	2331956	49.65%	5.684%
14	11.316	1565	1569	1571	rBV	1321125	1152667	24.54%	2.809%
15	11.339	1571	1573	1577	rVV	278461	237357	5.05%	0.579%
16	11.386	1577	1581	1585	rVB2	72301	81982	1.75%	0.200%
17	11.545	1603	1608	1617	rBV2	39674	80251	1.71%	0.196%
18	11.845	1656	1659	1670	rBV	564267	664464	14.15%	1.620%
19	12.368	1745	1748	1753	rBV5	52531	70588	1.50%	0.172%
20	12.527	1772	1775	1778	rBV	365895	323224	6.88%	0.788%
21	12.633	1789	1793	1799	rBV2	273440	359986	7.66%	0.877%
22	12.757	1809	1814	1816	rBV	243199	269676	5.74%	0.657%
23	12.804	1820	1822	1827	rVB4	50724	50713	1.08%	0.124%
24	12.904	1834	1839	1842	rBV	3510224	3406151	72.52%	8.302%
25	13.804	1990	1992	2002	rVB4	137130	181068	3.85%	0.441%
26	13.951	2013	2017	2020	rBV2	1133570	1120195	23.85%	2.730%
27	14.804	2159	2162	2168	rVB	302982	296552	6.31%	0.723%
28	15.056	2203	2205	2208	rVB	119248	114168	2.43%	0.278%
29	15.392	2258	2262	2266	rBV	579519	733936	15.63%	1.789%
30	15.851	2337	2340	2345	rVB	230032	339137	7.22%	0.827%

Sum of corrected areas: 41028667

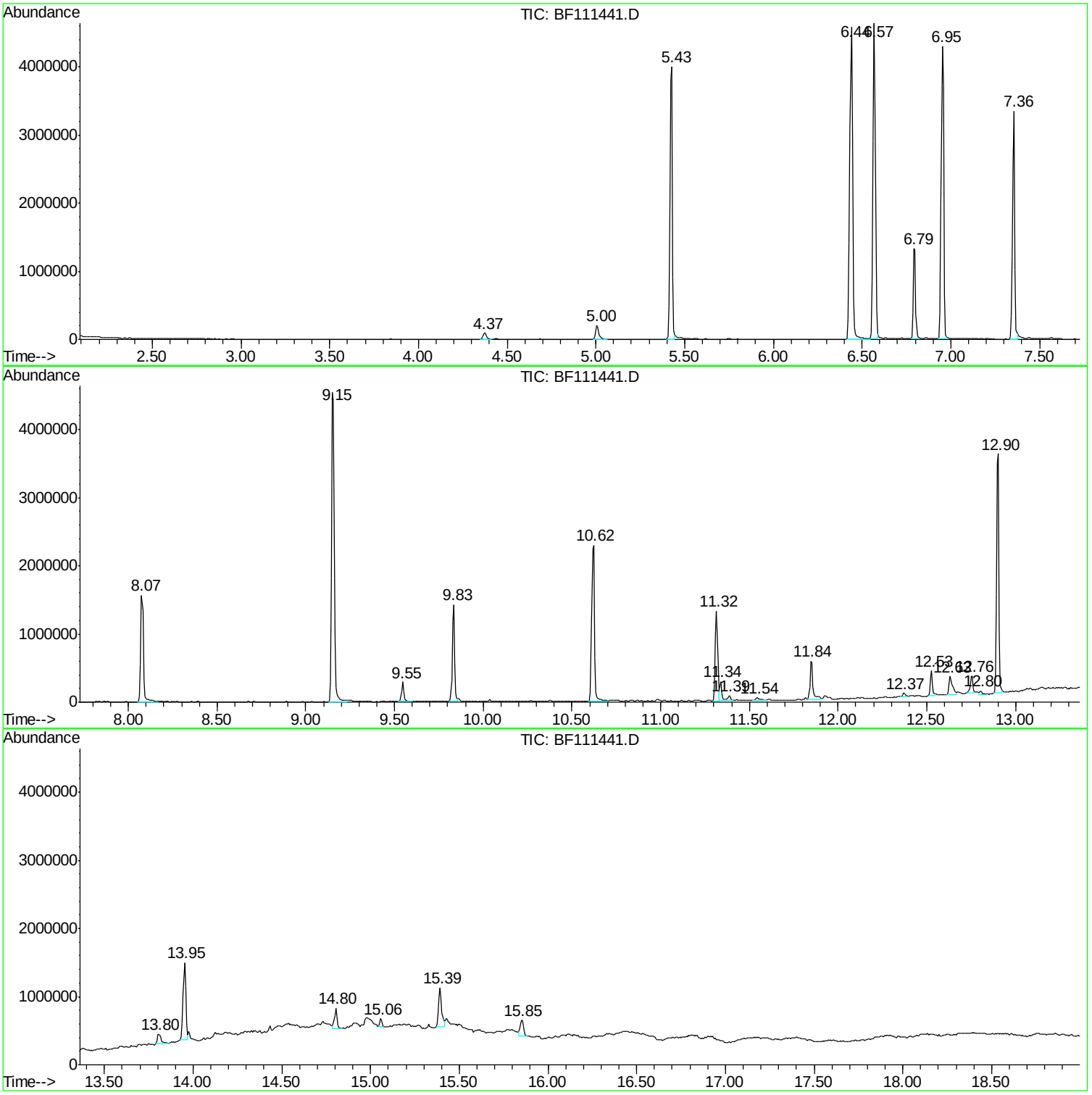
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121418\
Data File : BF111441.D
Acq On : 15 Dec 2018 1:35
Operator : JU/SJ
Sample : J6322-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-6-C-2-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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\BF121418\
Data File : BF111441.D
Acq On : 15 Dec 2018 1:35
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : SUP-6-C-2-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

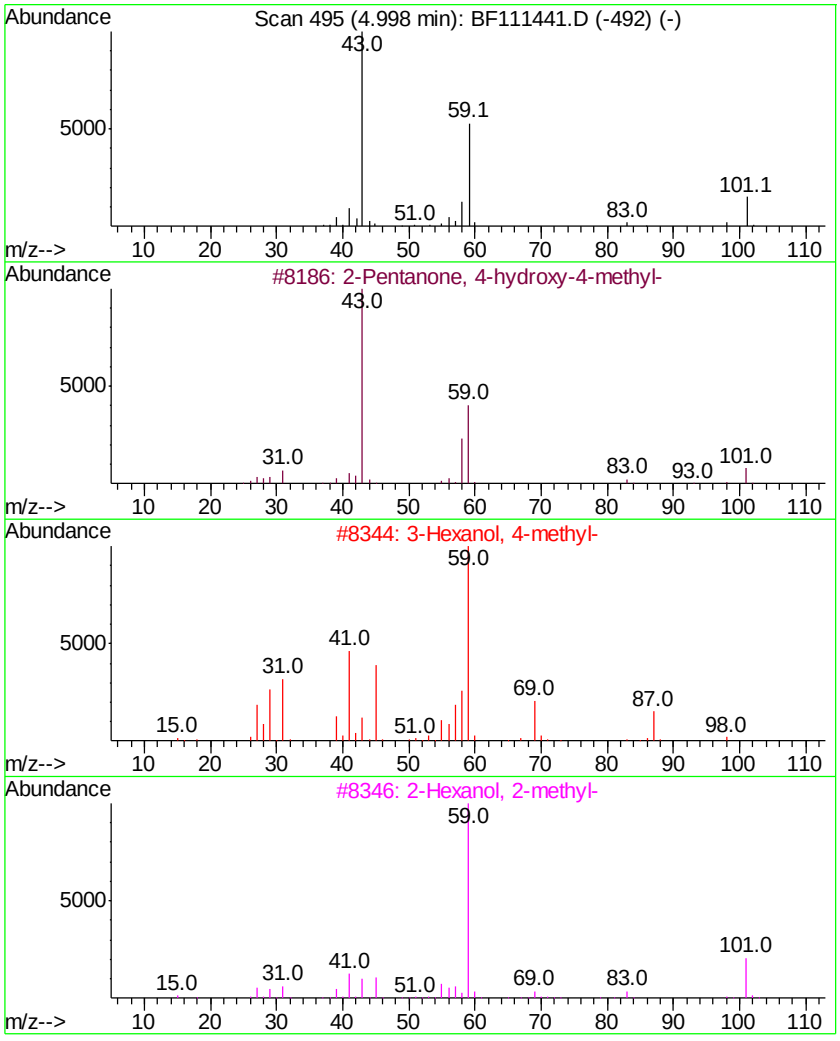
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

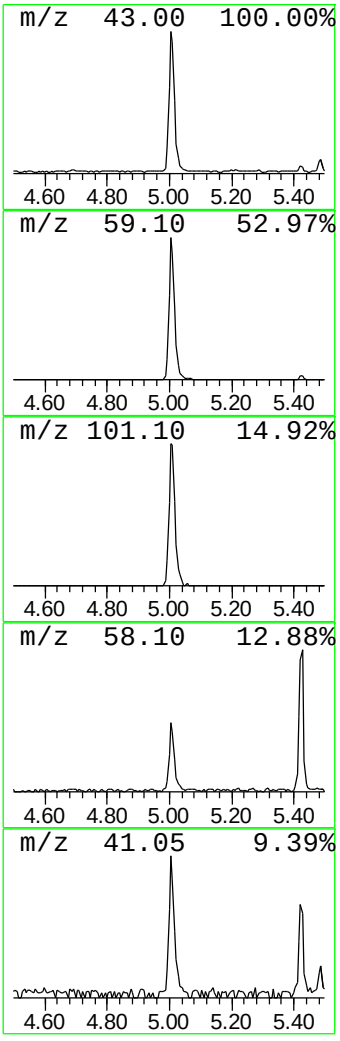
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.16 ng	254518	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Library Search Compound Report

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Data File : BF111441.D
Acq On : 15 Dec 2018 1:35
Operator : JU/SJ
Sample : J6322-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-6-C-2-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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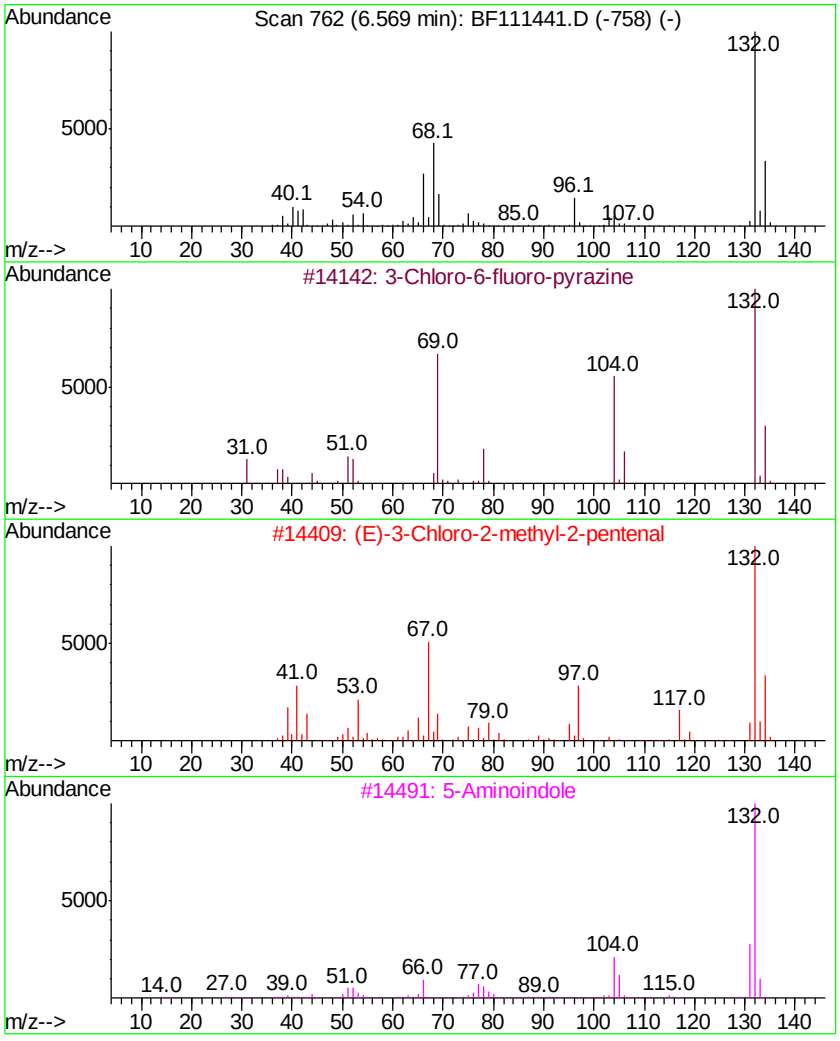
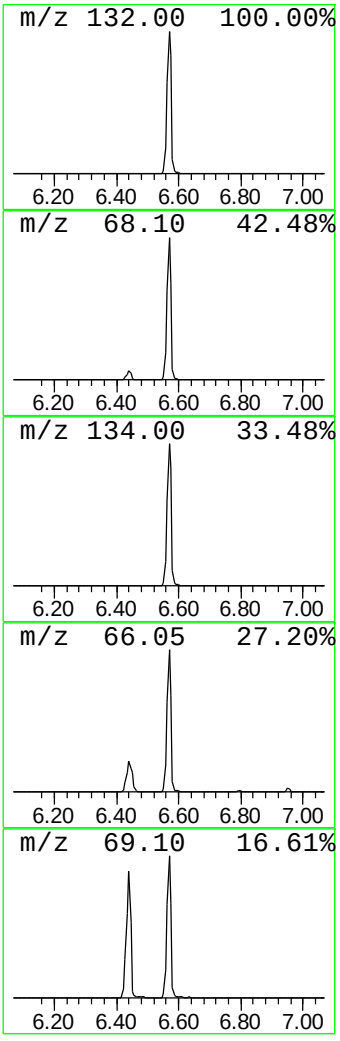
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	71.83 ng	4395650	1,4-Dichlorobenzene-d4	6.80

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

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Data File : BF111441.D
Acq On : 15 Dec 2018 1:35
Operator : JU/SJ
Sample : J6322-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-6-C-2-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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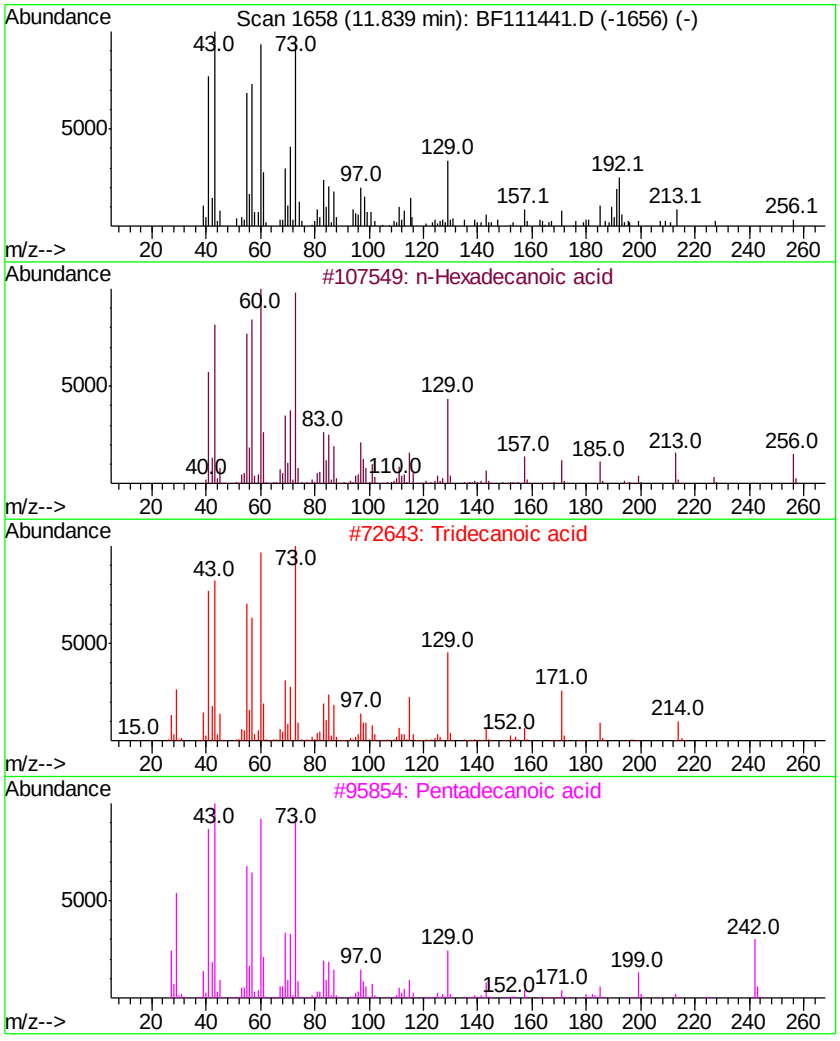
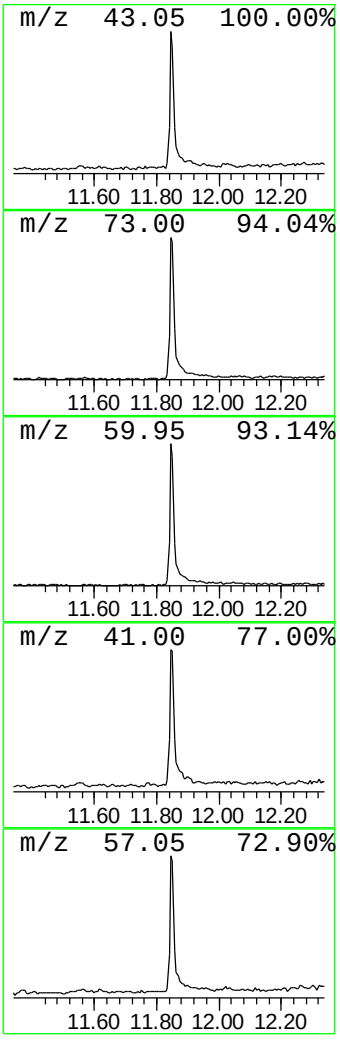
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	11.53 ng	664464	Phenanthrene-d10	11.32

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121418\
Data File : BF111441.D
Acq On : 15 Dec 2018 1:35
Operator : JU/SJ
Sample : J6322-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-6-C-2-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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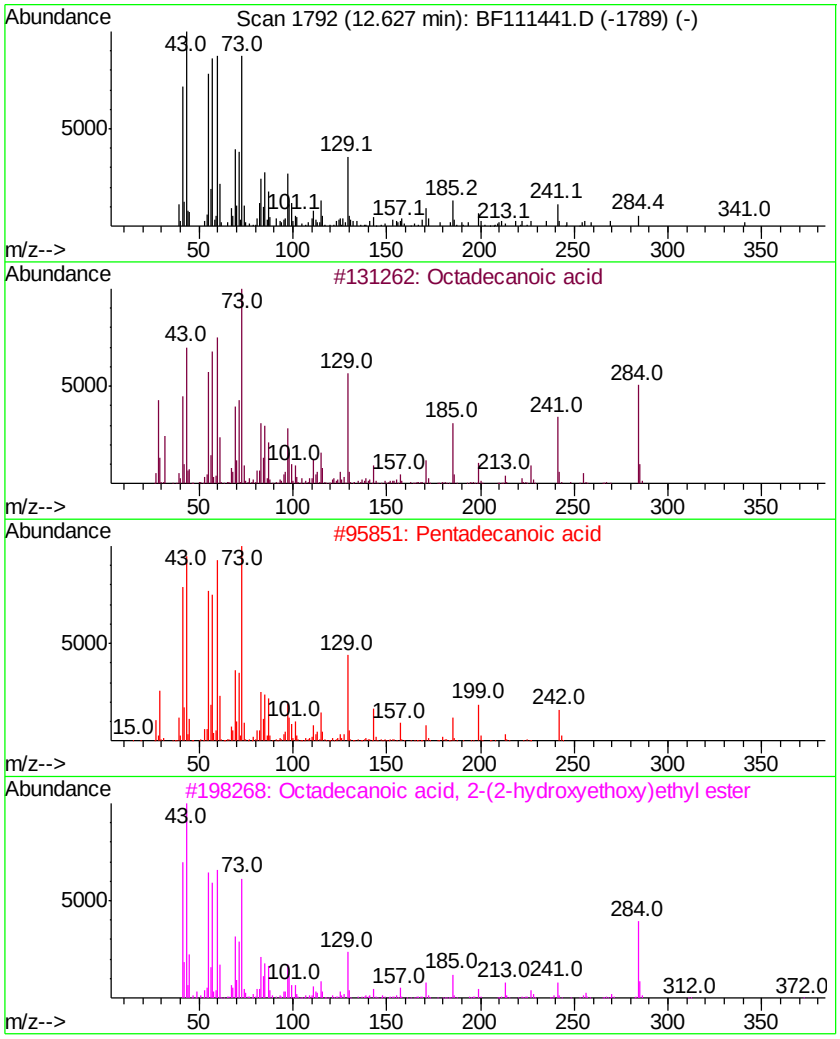
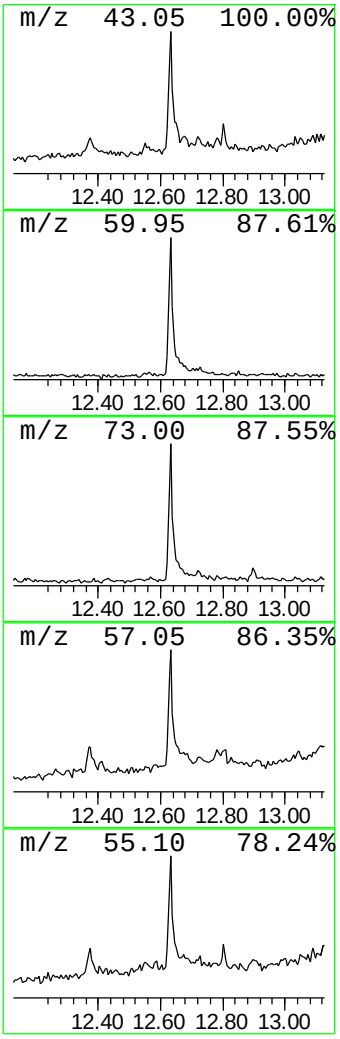
Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	6.43 ng	359986	Chrysene-d12	13.95

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	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121418\
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Operator : JU/SJ
Sample : J6322-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-6-C-2-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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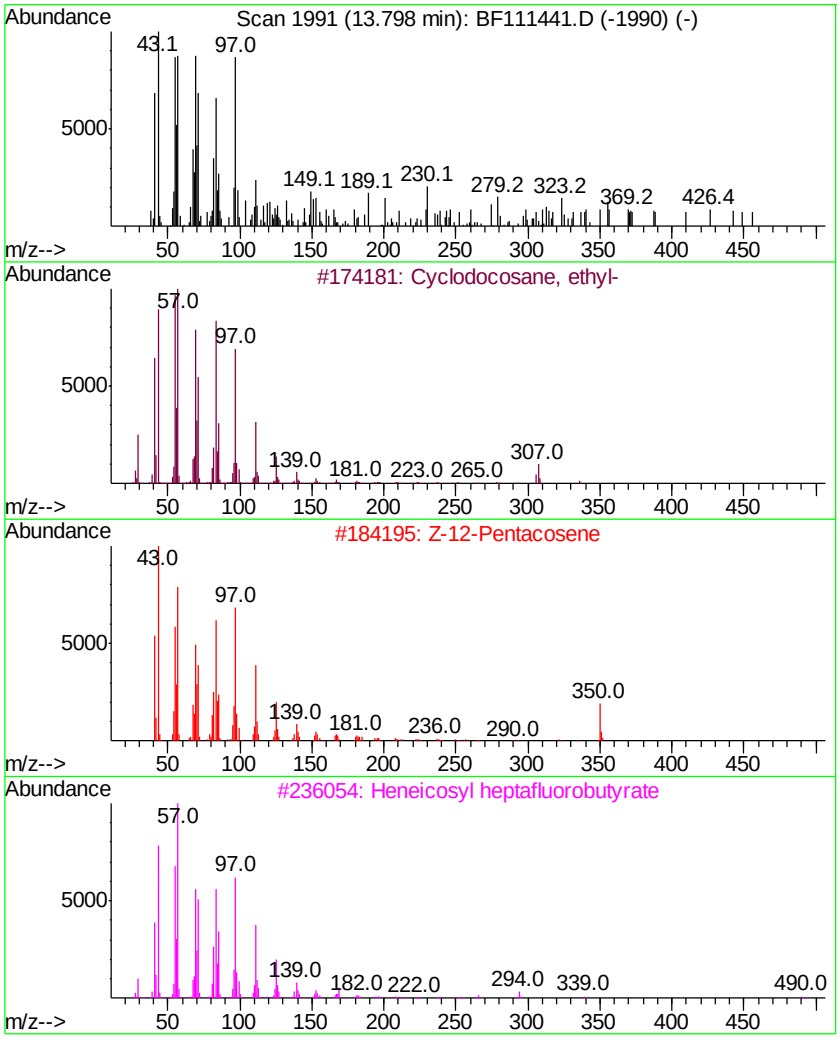
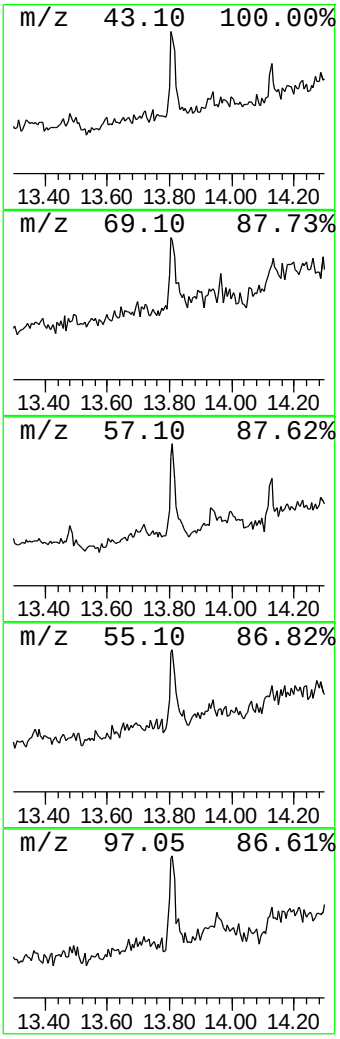
Peak Number 6 Cyclodocosane, ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.23 ng	181068	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	90
2	Z-12-Pentacosene	350	C25H50	1000131-09-4	90
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	83
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121418\
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Acq On : 15 Dec 2018 1:35
Operator : JU/SJ
Sample : J6322-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-6-C-2-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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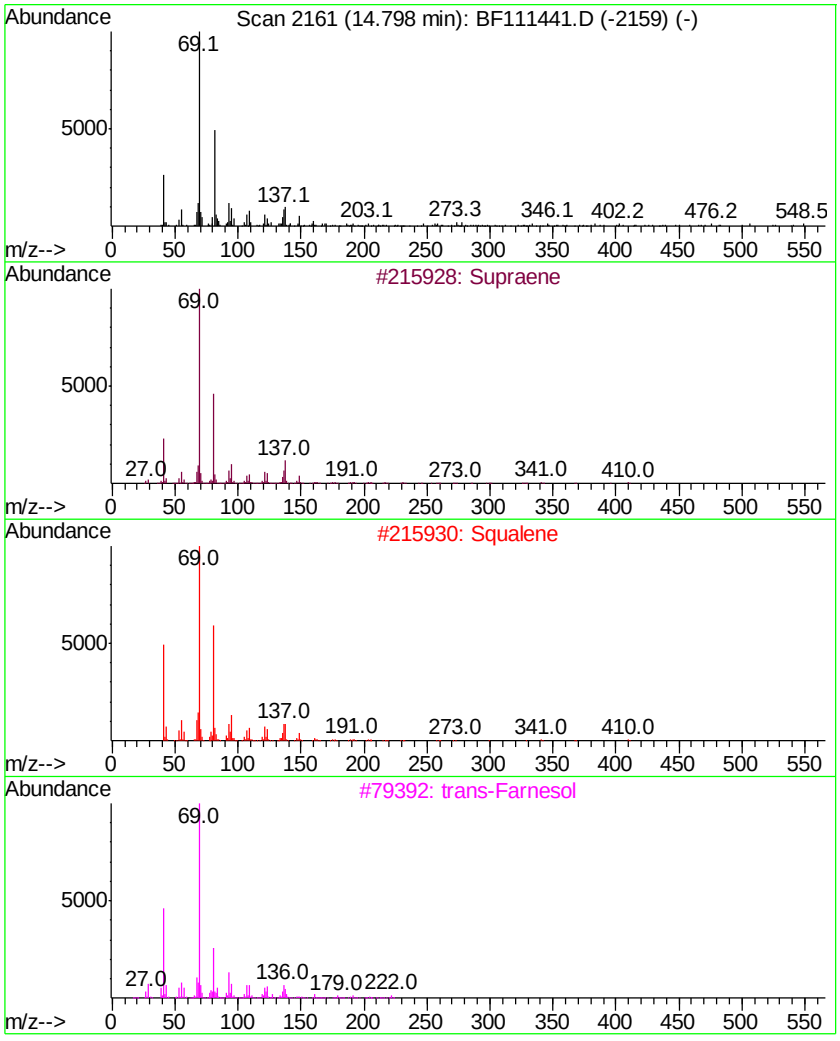
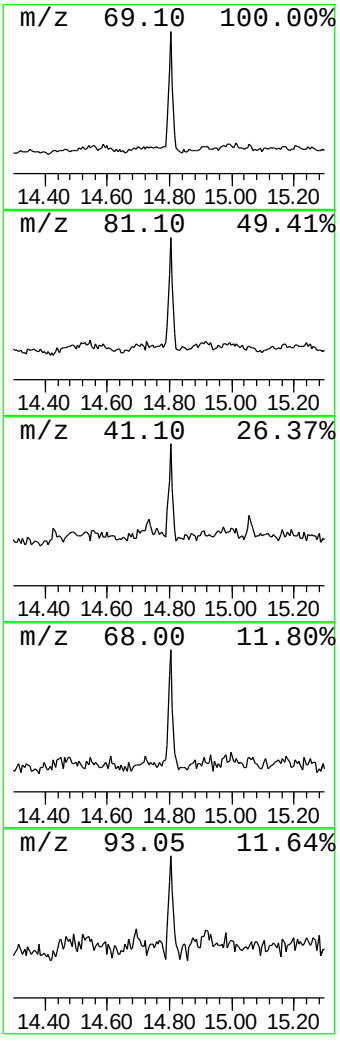
Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	8.08 ng	296552	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	99
2	Squalene	410	C30H50	000111-02-4	98
3	trans-Farnesol	222	C15H26O	000106-28-5	72
4	11-Dodecen-2-one, 7,7-dimethyl-	210	C14H26O	035194-22-0	59
5	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59





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Sample : J6322-21
Misc :
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Instrument : BNA_F
ClientSampleId : SUP-6-C-2-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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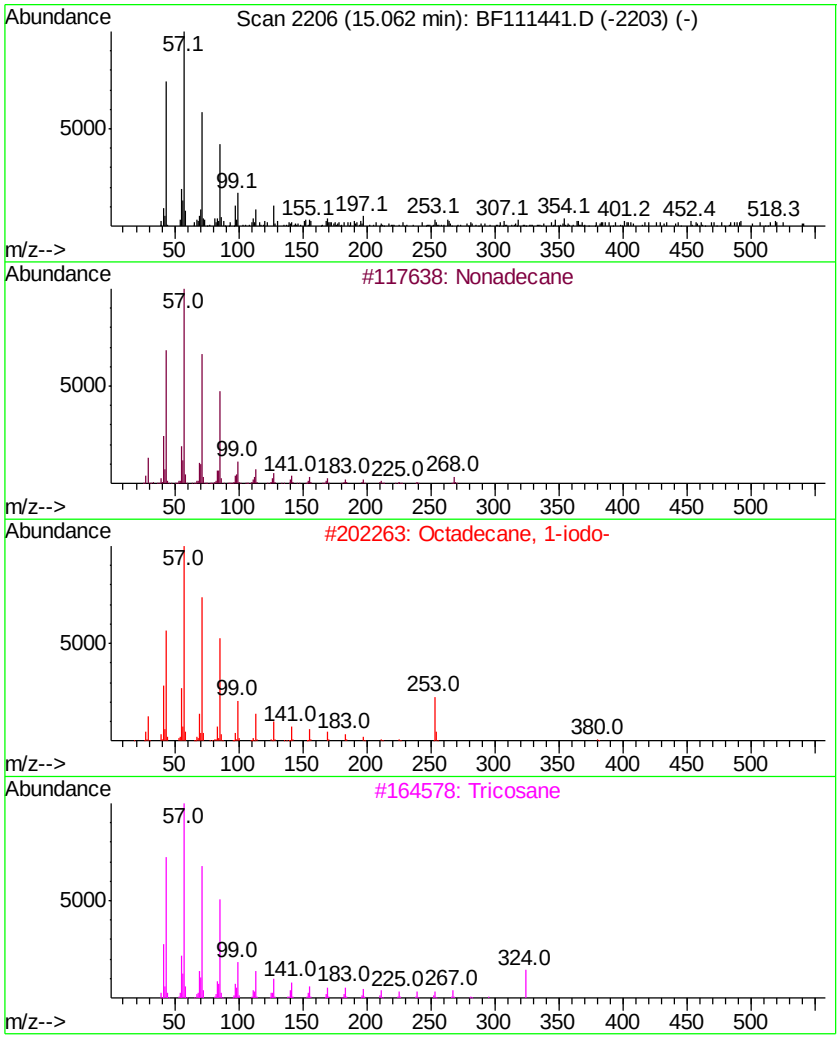
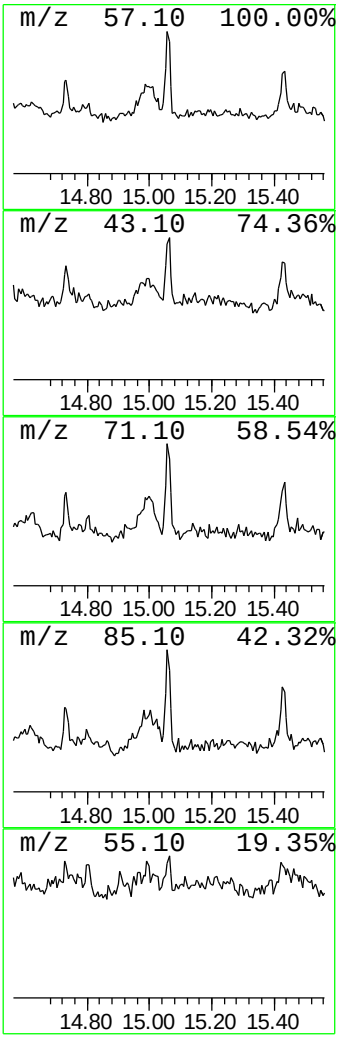
Peak Number 8 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	3.11 ng	114168	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	78
3	Tricosane	324	C23H48	000638-67-5	60
4	Eicosane	282	C20H42	000112-95-8	60
5	Octadecane	254	C18H38	000593-45-3	60





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Instrument : BNA_F
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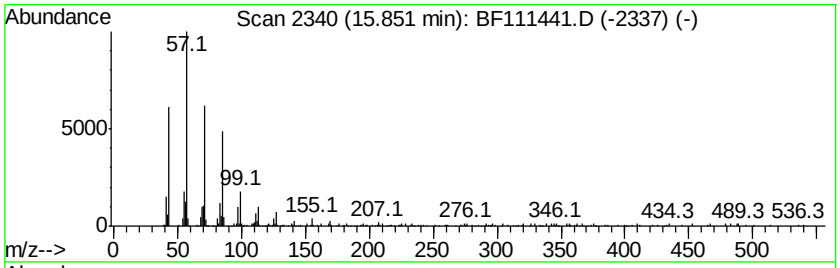
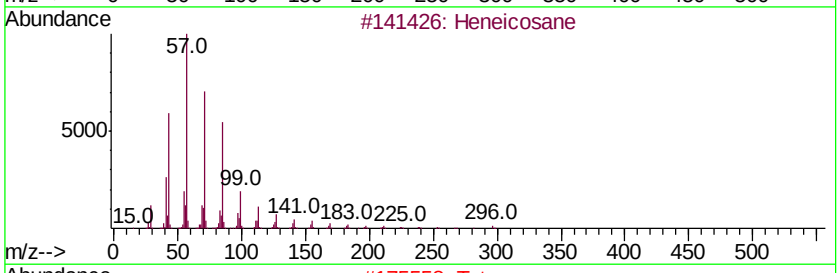
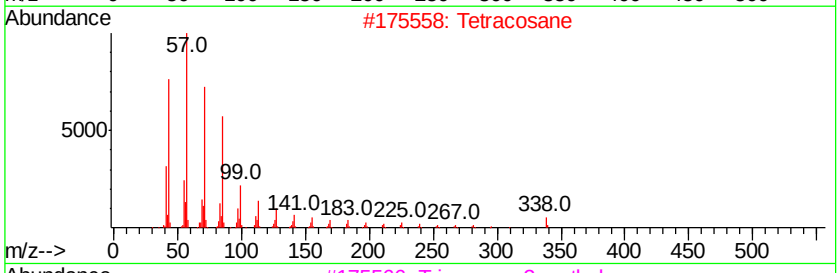
Peak Number 9 Heneicosane Concentration Rank 4

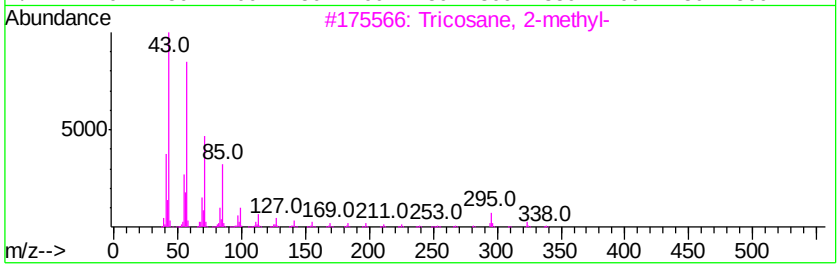
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	9.24 ng	339137	Perylene-d12	15.39

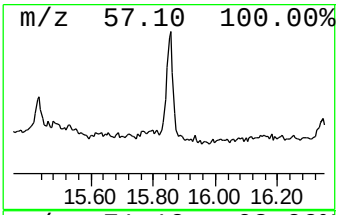
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Tetracosane	338	C24H50	000646-31-1	81
3	Tricosane, 2-methyl-	338	C24H50	001928-30-9	81
4	Hentriacontane	437	C31H64	000630-04-6	74
5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	72

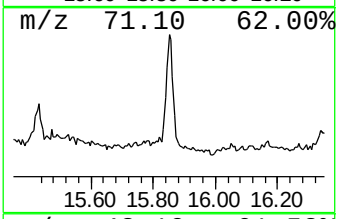


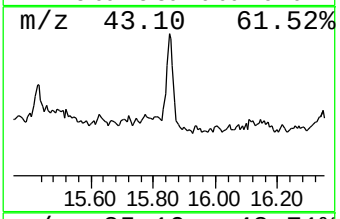


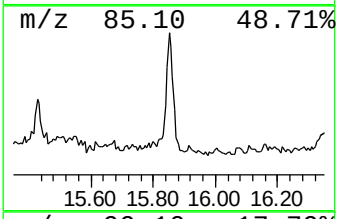


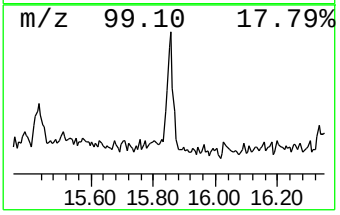












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121418\
Data File : BF111441.D
Acq On : 15 Dec 2018 1:35
Operator : JU/SJ
Sample : J6322-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-6-C-2-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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
2-Pentanone, 4-hy...	5.00	4.2	ng	254518	1	6.80	1223910	20.0
unknown6.57	6.57	71.8	ng	4395650	1	6.80	1223910	20.0
n-Hexadecanoic acid	11.84	11.5	ng	664464	4	11.32	1152670	20.0
Octadecanoic acid	12.63	6.4	ng	359986	5	13.95	1120200	20.0
Cyclodocosane, et...	13.80	3.2	ng	181068	5	13.95	1120200	20.0
Supraene	14.80	8.1	ng	296552	6	15.39	733936	20.0
Nonadecane	15.06	3.1	ng	114168	6	15.39	733936	20.0
Heneicosane	15.85	9.2	ng	339137	6	15.39	733936	20.0