LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113211.D
Acq On : 21 Mar 2019 16:30
Operator : JU/SJ
Sample : K1694-01 10X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-032019-A

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	5.334	548	552	562	rBV	219222	258868	6.48%	1.343%
2	6.363	724	727	742	rBV	259133	318364	7.97%	1.651%
3	6.493	746	749	757	rVB	338584	309888	7.76%	1.607%
4	6.722	784	788	796	rBV	991513	882298	22.10%	4.576%
5	6.875	811	814	823	rVB	279486	269143	6.74%	1.396%
6	7.281	874	883	890	rBV	151856	218263	5.47%	1.132%
7	7.534	921	926	930	rVB3	31919	43501	1.09%	0.226%
8	7.645	937	945	950	rBV7	19717	43462	1.09%	0.225%
9	8.004	1002	1006	1013	rBV	1312518	1184793	29.67%	6.146%
10	8.304	1049	1057	1060	rBV7	30834	46992	1.18%	0.244%
11	8.439	1077	1080	1084	rBV	54247	54246	1.36%	0.281%
12	8.610	1105	1109	1113	rBV3	69636	85004	2.13%	0.441%
13	9.034	1178	1181	1185	rVB2	58249	52176	1.31%	0.271%
14	9.081	1185	1189	1194	rBV	345411	350871	8.79%	1.820%
15	9.169	1200	1204	1208	rBV	81287	79093	1.98%	0.410%
16	9.351	1230	1235	1239	rBV3	27626	45539	1.14%	0.236%
17	9.416	1243	1246	1249	rVV2	49228	52028	1.30%	0.270%
18	9.469	1253	1255	1257	rBV2	50999	51959	1.30%	0.270%
19	9.492	1257	1259	1261	rVB	55824	41688	1.04%	0.216%
20	9.698	1291	1294	1298	rBV	66340	56513	1.42%	0.293%
21	9.757	1298	1304	1308	rBV	1368446	1344323	33.67%	6.973%
22	9.957	1336	1338	1342	rVB3	40411	42634	1.07%	0.221%
23	10.192	1375	1378	1381	rVB	63238	56572	1.42%	0.293%
24	10.416	1413	1416	1420	rVB	60647	52459	1.31%	0.272%
25	10.539	1433	1437	1442	rBV	210642	228212	5.72%	1.184%
26	10.669	1455	1459	1460	rBV	82733	87784	2.20%	0.455%
27	11.116	1532	1535	1537	rBV	59274	59171	1.48%	0.307%
28	11.145	1537	1540	1544	rVB2	56348	65179	1.63%	0.338%
29	11.233	1551	1555	1558	rBV	1413846	1322094	33.11%	6.858%
30	11.257	1558	1559	1565	rVV	221309	161739	4.05%	0.839%
31	11.310	1565	1568	1572	rVB	36671	41624	1.04%	0.216%
32	11.539	1604	1607	1609	rBV	51645	45635	1.14%	0.237%
33	11.633	1620	1623	1630	rVB	1202716	1002475	25.11%	5.200%
34	11.769	1643	1646	1651	rBV	90522	92613	2.32%	0.480%

LSC Area Percent Report

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Data File : BF113211.D
Acq On : 21 Mar 2019 16:30
Operator : JU/SJ
Sample : K1694-01 10X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-032019-A

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	11.845	1656	1659	1662	rBV	53237	51772	1.30%	0.269%
36	11.945	1673	1676	1679	rBV	48671	48757	1.22%	0.253%
37	12.322	1736	1740	1742	rBV	3751174	3992634	100.00%	20.710%
38	12.339	1742	1743	1754	rVB2	2710817	2035479	50.98%	10.558%
39	12.422	1754	1757	1759	rBV	462458	433463	10.86%	2.248%
40	12.445	1759	1761	1764	rVV	237697	216864	5.43%	1.125%
41	12.474	1764	1766	1771	rVB4	31078	41172	1.03%	0.214%
42	12.669	1794	1799	1802	rBV	235383	249543	6.25%	1.294%
43	12.816	1820	1824	1832	rVB	341749	333601	8.36%	1.730%
44	12.998	1853	1855	1862	rVB	41755	48122	1.21%	0.250%
45	13.069	1862	1867	1870	rBV2	56981	82582	2.07%	0.428%
46	13.863	1997	2002	2005	rBV	1156919	1193946	29.90%	6.193%
47	14.345	2081	2084	2086	rBV3	39651	40854	1.02%	0.212%
48	14.639	2131	2134	2137	rBV2	44010	50992	1.28%	0.264%
49	14.739	2148	2151	2158	rVB	87841	127331	3.19%	0.660%
50	14.874	2171	2174	2181	rBV	99012	203288	5.09%	1.054%
51	15.215	2229	2232	2237	rBV	82101	109884	2.75%	0.570%
52	15.274	2238	2242	2246	rBV	790901	971427	24.33%	5.039%

Sum of corrected areas: 19278914

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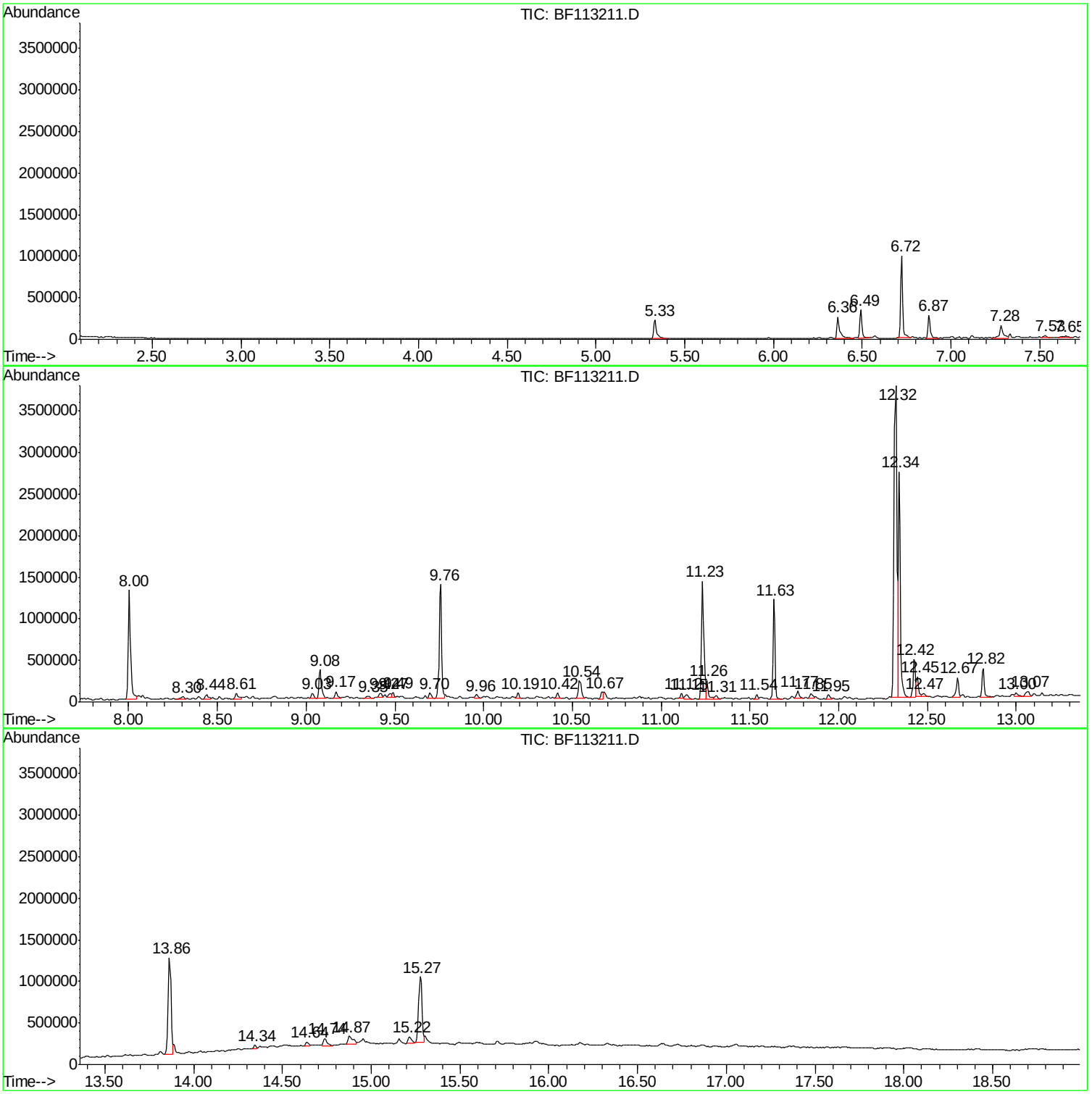
Instrument :
BNA_F
ClientSampleId :
EO-02-032019-A

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\BF032119\
Data File : BF113211.D
Acq On : 21 Mar 2019 16:30
Operator : JU/SJ
Sample : K1694-01 10X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-032019-A

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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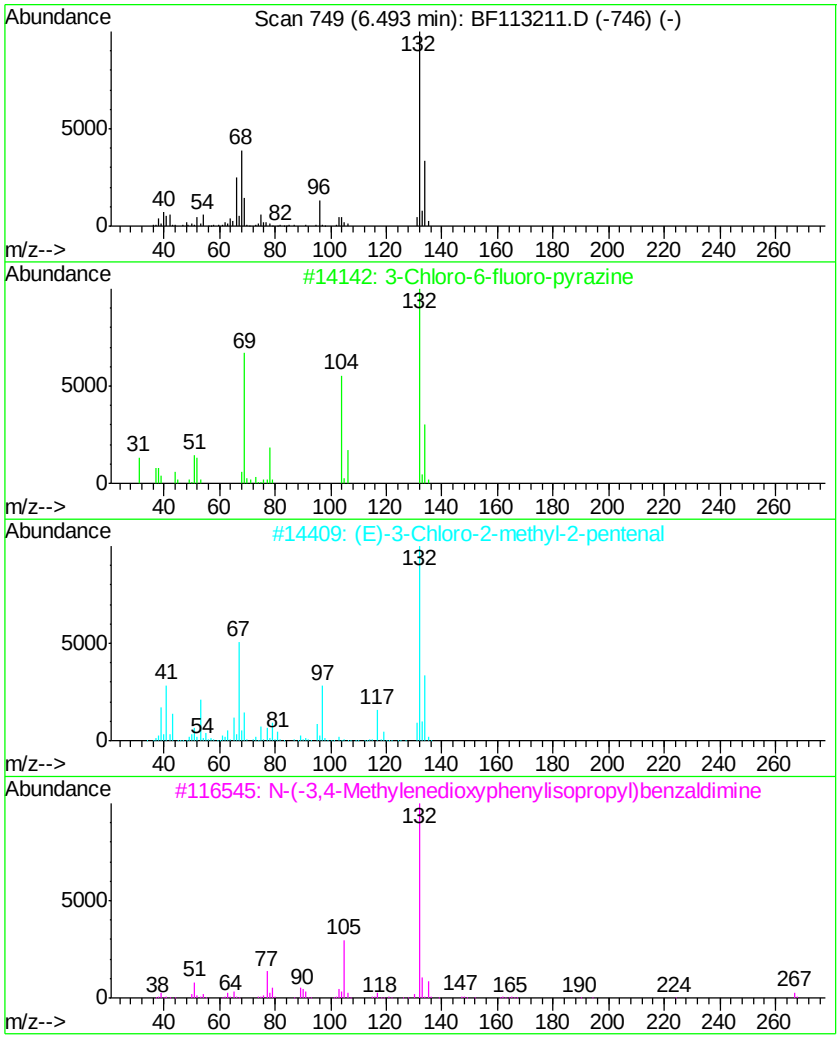
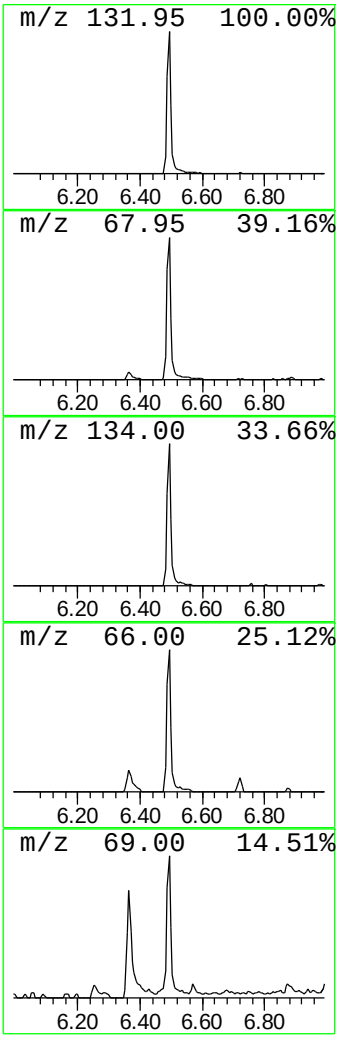
Peak Number 1 unknown6.49 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	7.02 ng	309888	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113211.D
Acq On : 21 Mar 2019 16:30
Operator : JU/SJ
Sample : K1694-01 10X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-032019-A

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

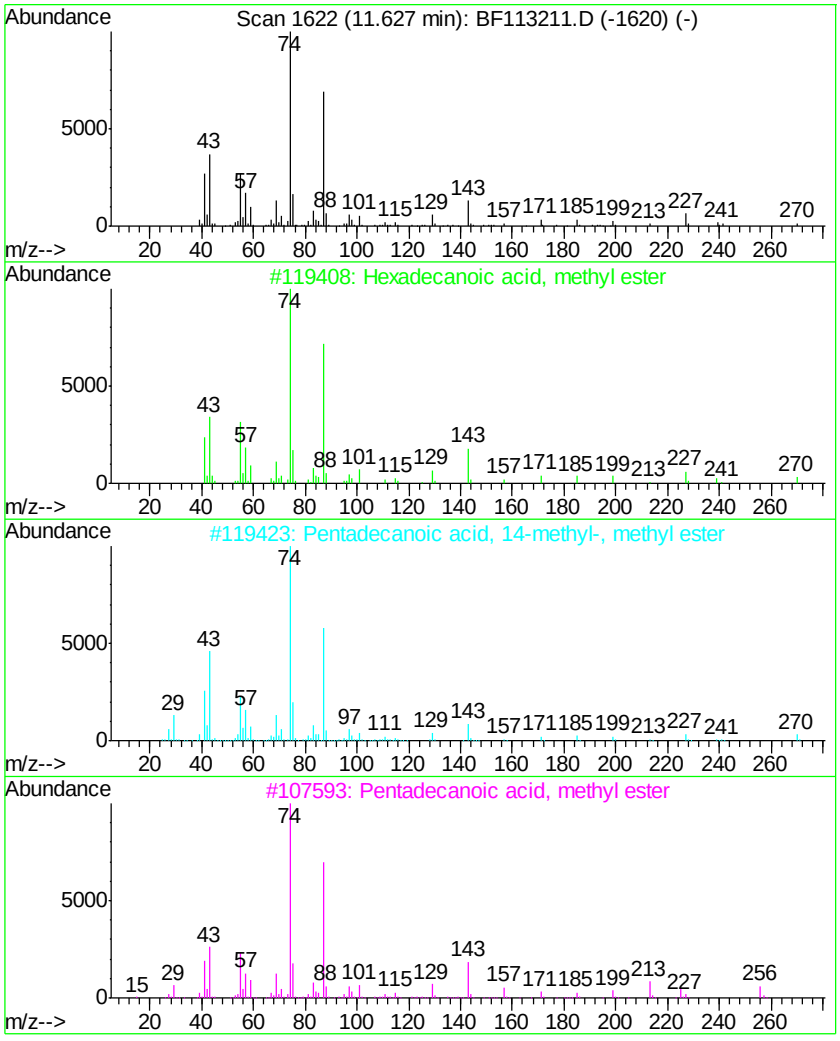
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

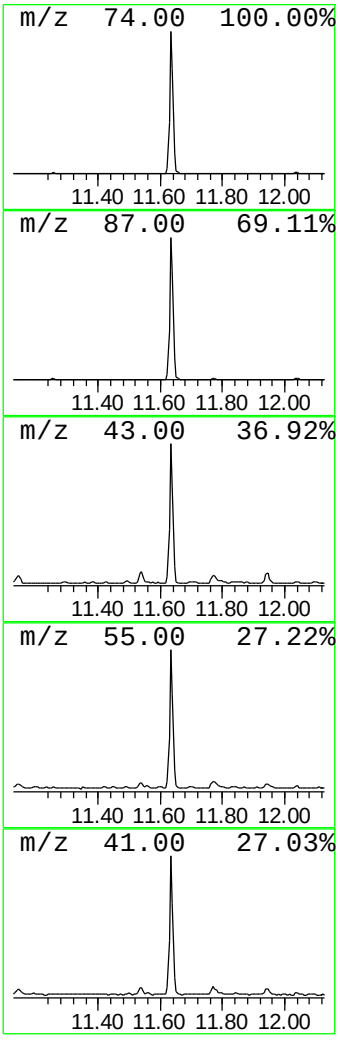
****

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	15.17 ng	1002480	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113211.D
Acq On : 21 Mar 2019 16:30
Operator : JU/SJ
Sample : K1694-01 10X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-032019-A

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

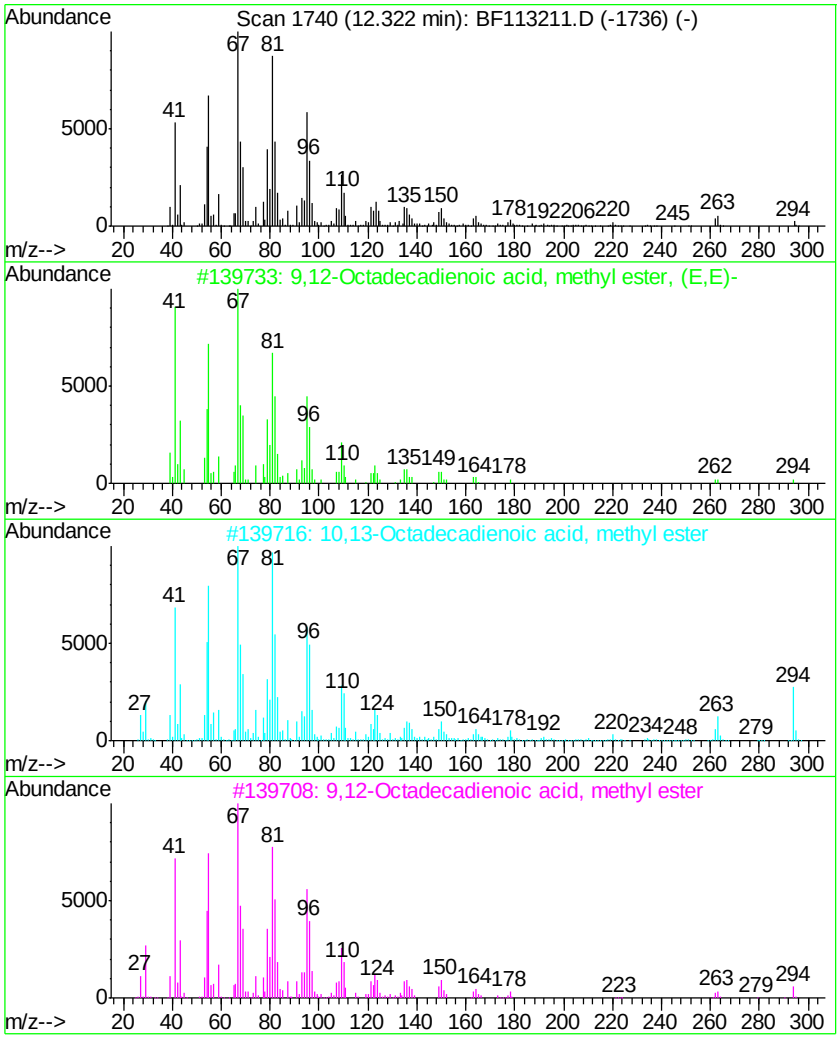
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

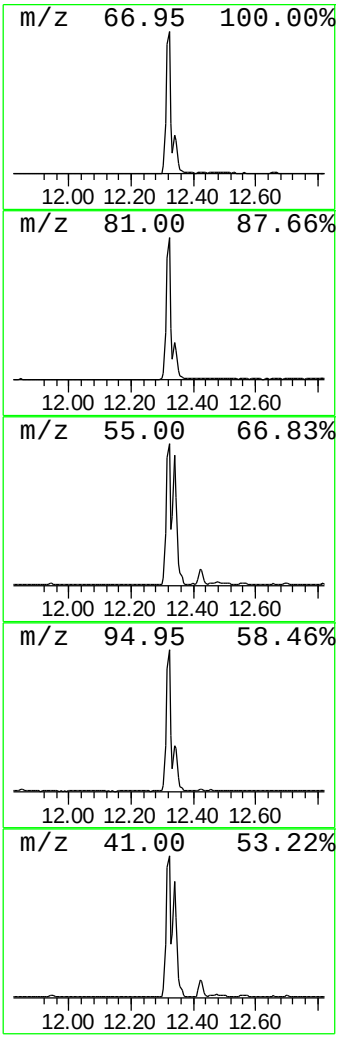
****

Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	60.40 ng	3992630	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





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Instrument : BNA_F
ClientSampleId : EO-02-032019-A

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

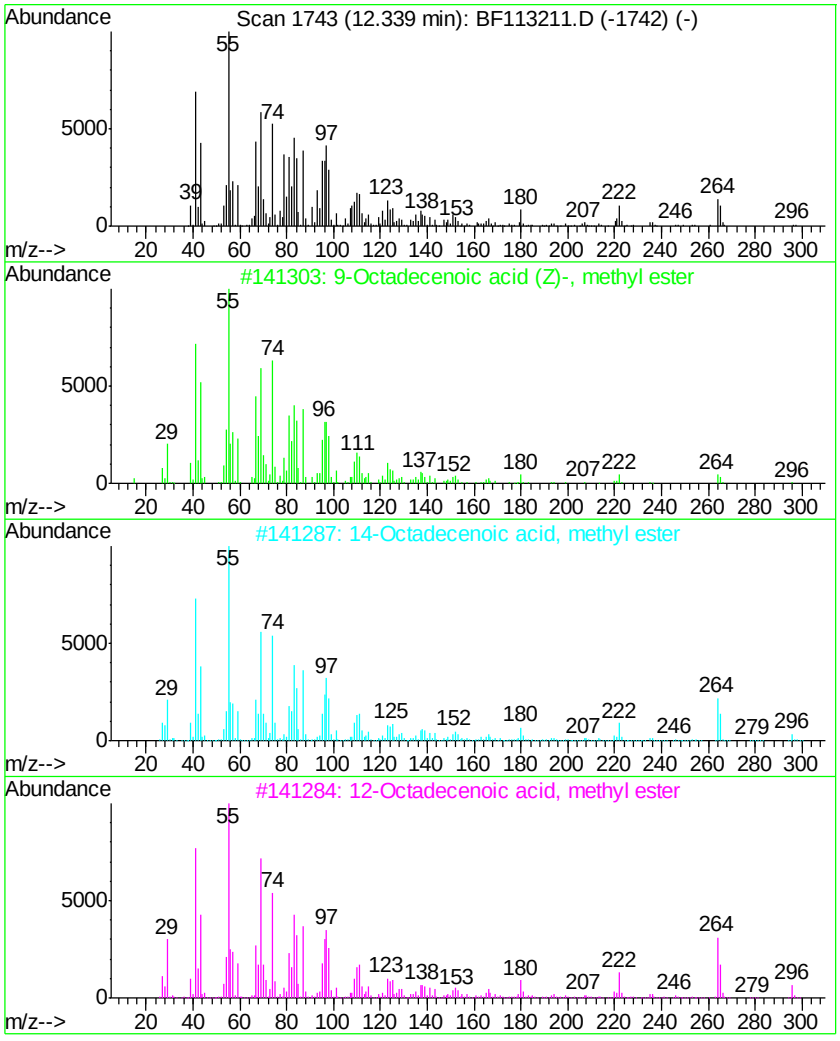
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

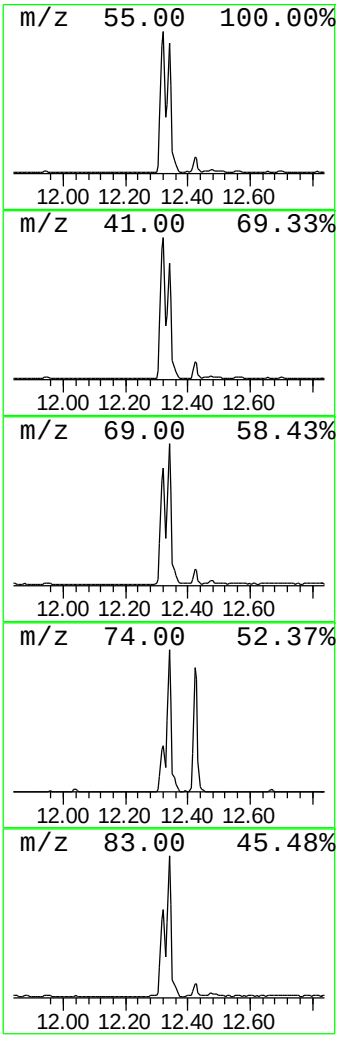
****

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	30.79 ng	2035480	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
3	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99





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Instrument : BNA_F
ClientSampleId : EO-02-032019-A

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

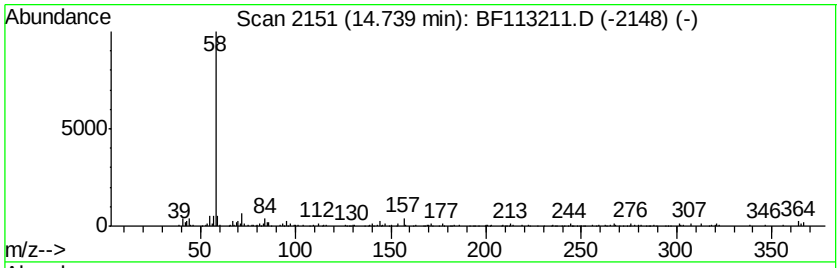
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

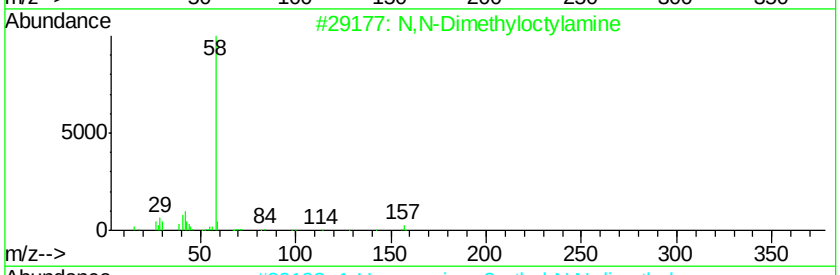
****

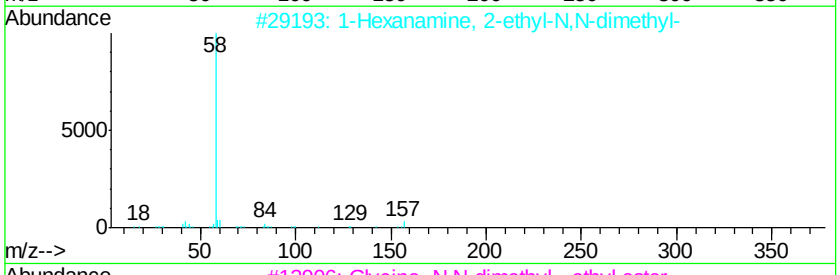
Peak Number 6 N,N-Dimethyloctylamine Concentration Rank 6

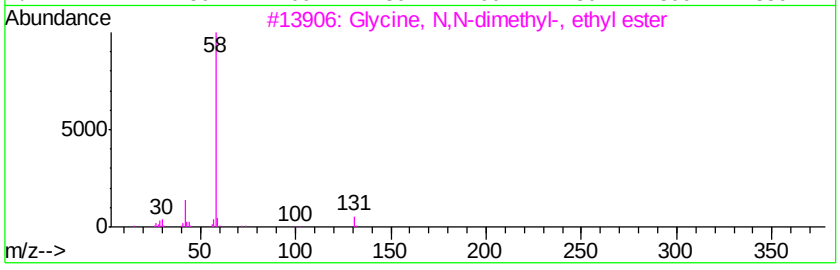
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.62 ng	127331	Perylene-d12	15.27

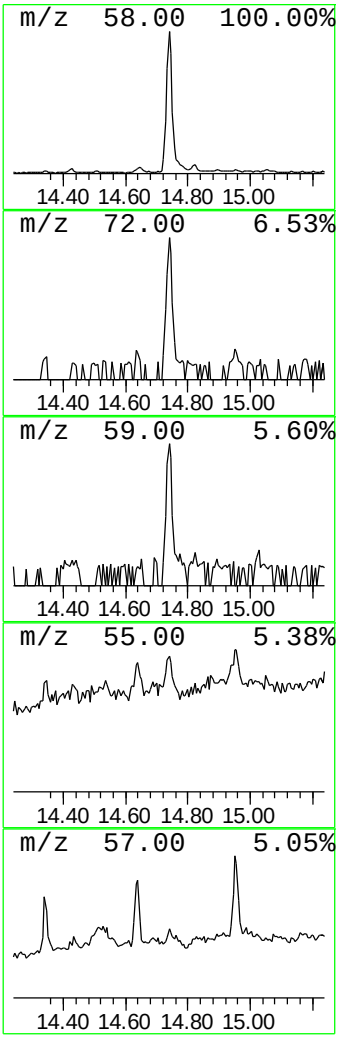
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,N-Dimethyloctylamine	157	C10H23N	007378-99-6	64
2	1-Hexanamine, 2-ethyl-N,N-dimethyl-	157	C10H23N	028056-87-3	64
3	Glycine, N,N-dimethyl-, ethyl ester	131	C6H13NO2	033229-89-9	64
4	Decane,-1,10-diamino,-N,N,N',N'-...	228	C14H32N2	001938-62-1	59
5	Cetrimonium Bromide	363	C19H42BrN	000057-09-0	59











Library Search Compound Report

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

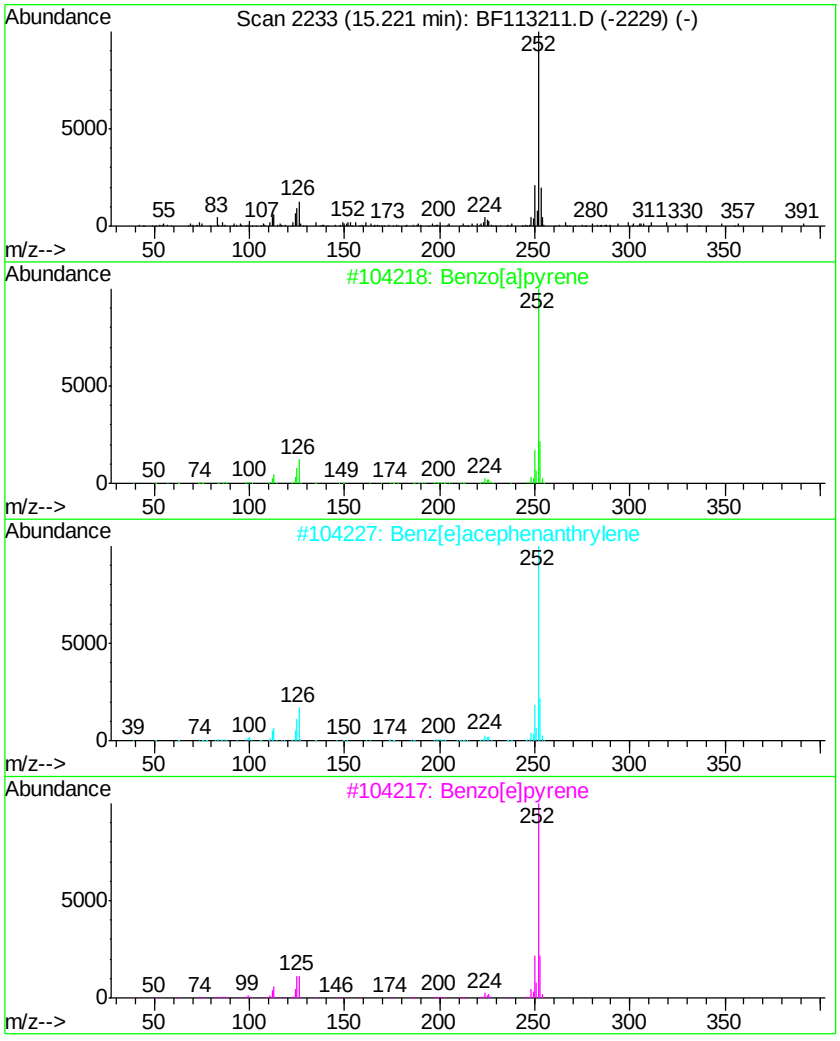
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

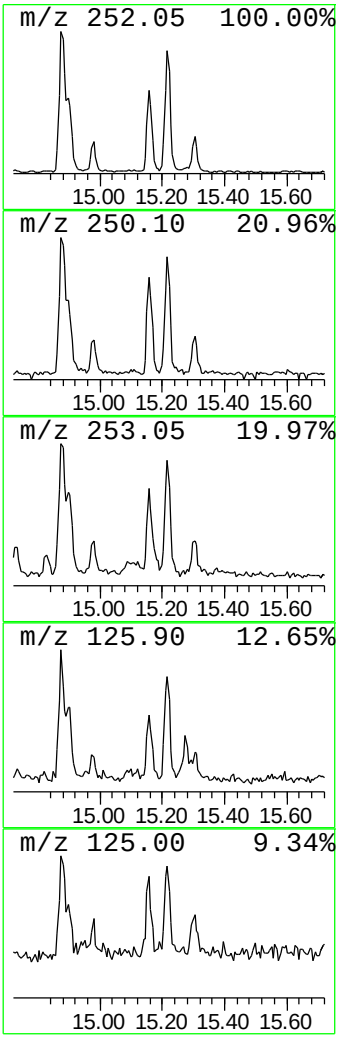
****

Peak Number 7 Benzo[a]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	2.26 ng	109884	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	97
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	97
3	Benzo[e]pyrene	252	C20H12	000192-97-2	97
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5	Perylene	252	C20H12	000198-55-0	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113211.D
Acq On : 21 Mar 2019 16:30
Operator : JU/SJ
Sample : K1694-01 10X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-032019-A

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
unknown6.49	6.49	7.0	ng	309888	1	6.72	882298	20.0
Hexadecanoic acid...	11.63	15.2	ng	1002480	4	11.23	1322090	20.0
9,12-Octadecadien...	12.32	60.4	ng	3992630	4	11.23	1322090	20.0
9-Octadecenoic ac...	12.34	30.8	ng	2035480	4	11.23	1322090	20.0
N,N-Dimethyloctyl...	14.74	2.6	ng	127331	6	15.27	971427	20.0
Benzo[a]pyrene	15.22	2.3	ng	109884	6	15.27	971427	20.0