LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113213.D
Acq On : 21 Mar 2019 17:26
Operator : JU/SJ
Sample : K1694-05 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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	566	rBV	207453	241745	19.69%	2.034%
2	6.363	724	727	740	rBV	297438	334265	27.23%	2.813%
3	6.492	746	749	760	rBV	401559	353325	28.78%	2.973%
4	6.722	784	788	805	rBV	1099178	962033	78.37%	8.096%
5	6.875	811	814	827	rBV	292235	282074	22.98%	2.374%
6	7.280	879	883	891	rBV	149243	176110	14.35%	1.482%
7	8.004	1002	1006	1014	rBV	1100954	1033619	84.20%	8.698%
8	9.080	1185	1189	1201	rBV	319467	364218	29.67%	3.065%
9	9.169	1201	1204	1209	rVB3	16448	16548	1.35%	0.139%
10	9.474	1253	1256	1260	rBV2	21337	30442	2.48%	0.256%
11	9.698	1291	1294	1298	rBV	19783	17093	1.39%	0.144%
12	9.757	1300	1304	1320	rVB	1248312	1227520	100.00%	10.330%
13	10.192	1375	1378	1381	rBV2	23968	22118	1.80%	0.186%
14	10.304	1394	1397	1403	rVB	18338	21319	1.74%	0.179%
15	10.539	1433	1437	1449	rBV	180194	212581	17.32%	1.789%
16	10.668	1456	1459	1464	rBV3	31816	42314	3.45%	0.356%
17	11.116	1531	1535	1537	rBV	28955	28920	2.36%	0.243%
18	11.233	1551	1555	1558	rBV	1187416	1095262	89.23%	9.217%
19	11.310	1566	1568	1572	rVB	32040	31276	2.55%	0.263%
20	11.539	1603	1607	1609	rBV2	29640	28251	2.30%	0.238%
21	11.633	1620	1623	1629	rVB	352452	301302	24.55%	2.535%
22	11.739	1637	1641	1643	rBV	25005	26620	2.17%	0.224%
23	11.768	1643	1646	1652	rVV2	71199	73826	6.01%	0.621%
24	11.845	1656	1659	1662	rBV	41425	45439	3.70%	0.382%
25	11.945	1673	1676	1678	rBV	24894	21430	1.75%	0.180%
26	12.033	1688	1691	1694	rBV2	17809	23083	1.88%	0.194%
27	12.210	1719	1721	1724	rBV3	12326	16287	1.33%	0.137%
28	12.286	1730	1734	1736	rBV	29060	34464	2.81%	0.290%
29	12.315	1736	1739	1741	rBV	1215760	1054288	85.89%	8.872%
30	12.339	1741	1743	1746	rVB	1013423	767312	62.51%	6.457%
31	12.427	1754	1758	1759	rBV	150889	146553	11.94%	1.233%
32	12.445	1759	1761	1764	rVV	153791	142757	11.63%	1.201%
33	12.474	1764	1766	1771	rVB5	23397	36305	2.96%	0.306%
34	12.557	1778	1780	1785	rVB5	13539	13043	1.06%	0.110%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113213.D
Acq On : 21 Mar 2019 17:26
Operator : JU/SJ
Sample : K1694-05 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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	12.598	1785	1787	1794	rVB7	12318	18440	1.50%	0.155%
36	12.668	1794	1799	1802	rBV	162403	176811	14.40%	1.488%
37	12.698	1802	1804	1806	rVB2	25327	20784	1.69%	0.175%
38	12.810	1820	1823	1833	rVB	315928	318641	25.96%	2.681%
39	12.892	1833	1837	1841	rBV6	17709	30050	2.45%	0.253%
40	12.998	1849	1855	1860	rBV2	42831	67605	5.51%	0.569%
41	13.068	1862	1867	1870	rBV2	44178	60825	4.96%	0.512%
42	13.104	1870	1873	1875	rBV	30146	30157	2.46%	0.254%
43	13.227	1891	1894	1896	rBV2	16999	17203	1.40%	0.145%
44	13.398	1921	1923	1926	rBV2	20386	19489	1.59%	0.164%
45	13.862	1998	2002	2005	rBV	1020334	1042770	84.95%	8.775%
46	15.280	2238	2243	2246	rBV	595106	760278	61.94%	6.398%
47	18.556	2797	2800	2805	rBV6	43082	96654	7.87%	0.813%

Sum of corrected areas: 11883449

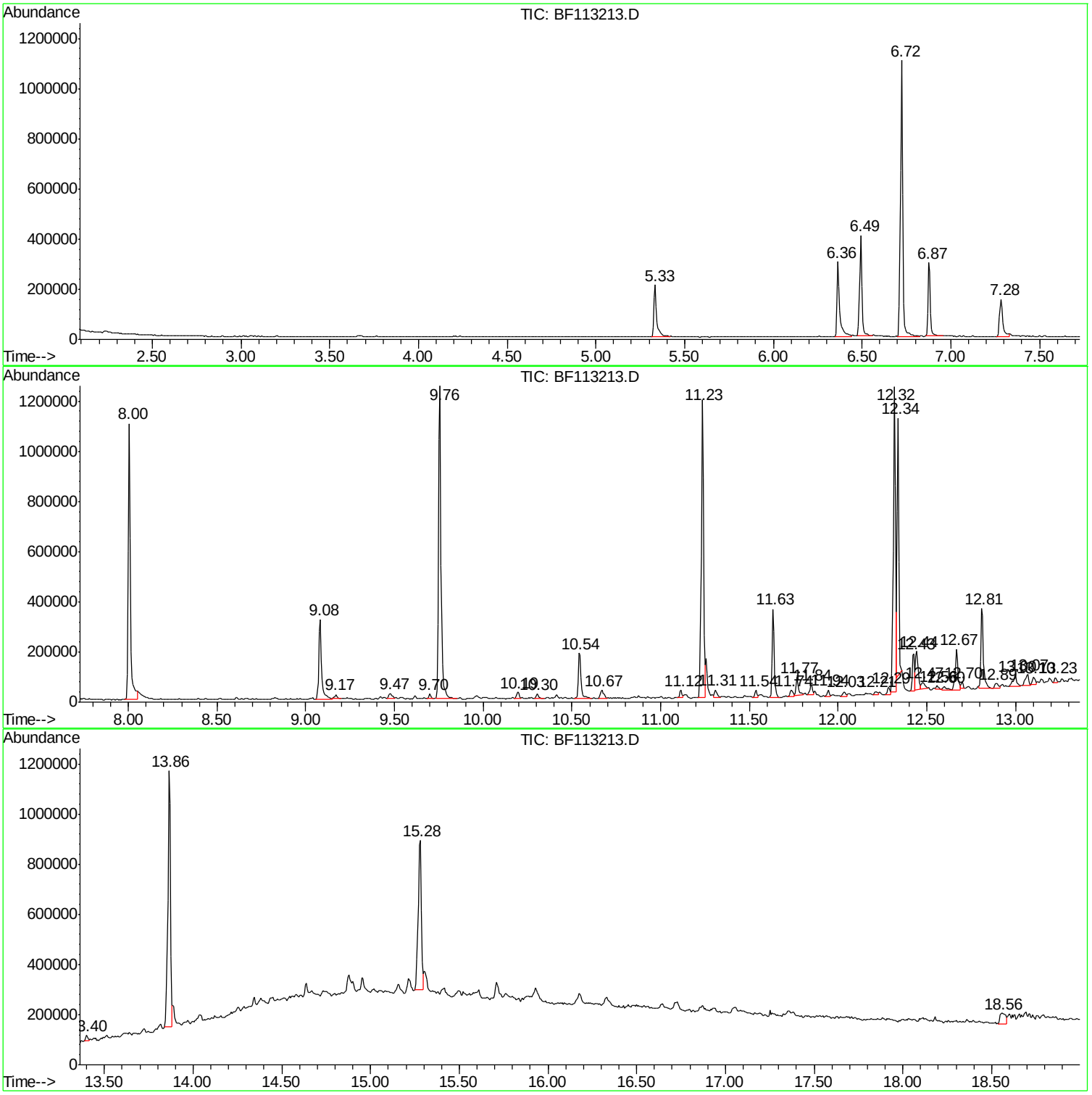
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113213.D
Acq On : 21 Mar 2019 17:26
Operator : JU/SJ
Sample : K1694-05 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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 : BF113213.D
Acq On : 21 Mar 2019 17:26
Operator : JU/SJ
Sample : K1694-05 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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

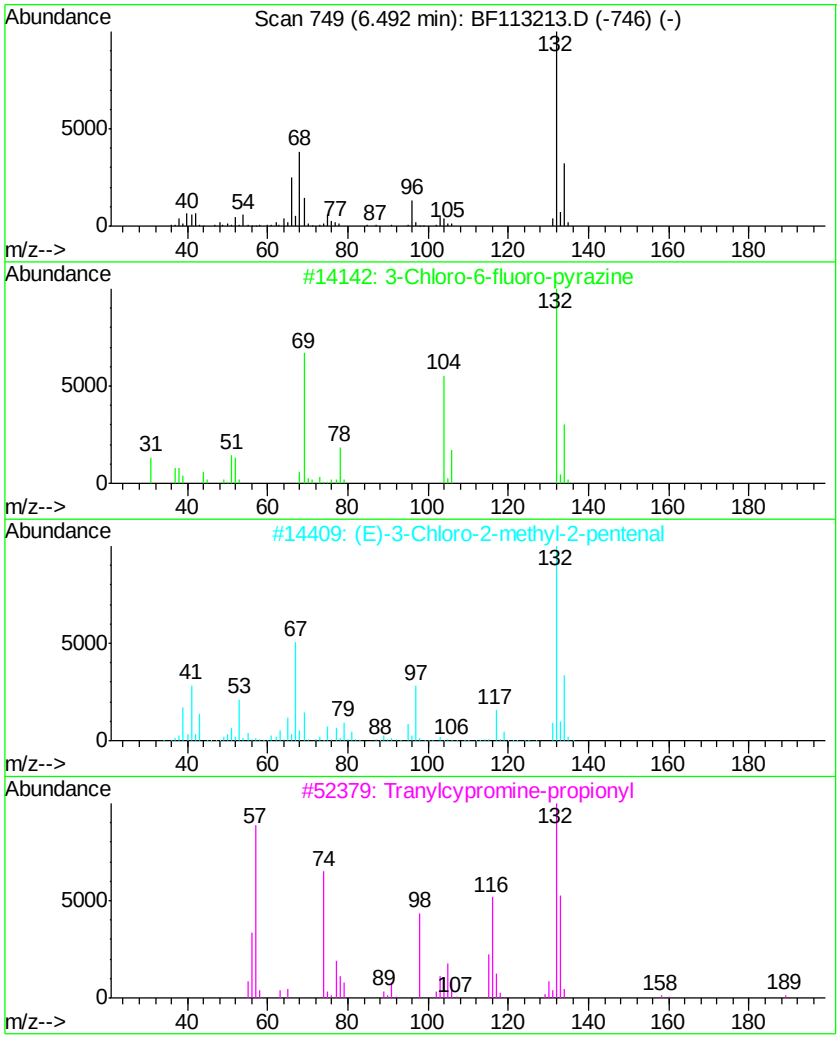
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

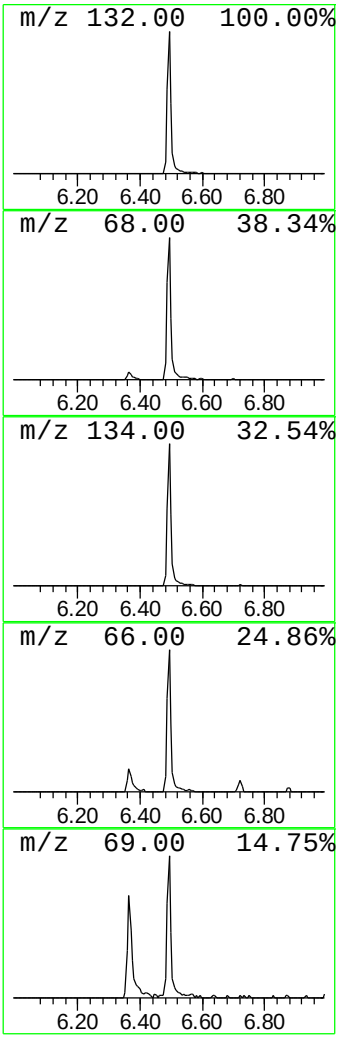
****

Peak Number 1 unknown6.49 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	7.35 ng	353325	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113213.D
Acq On : 21 Mar 2019 17:26
Operator : JU/SJ
Sample : K1694-05 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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

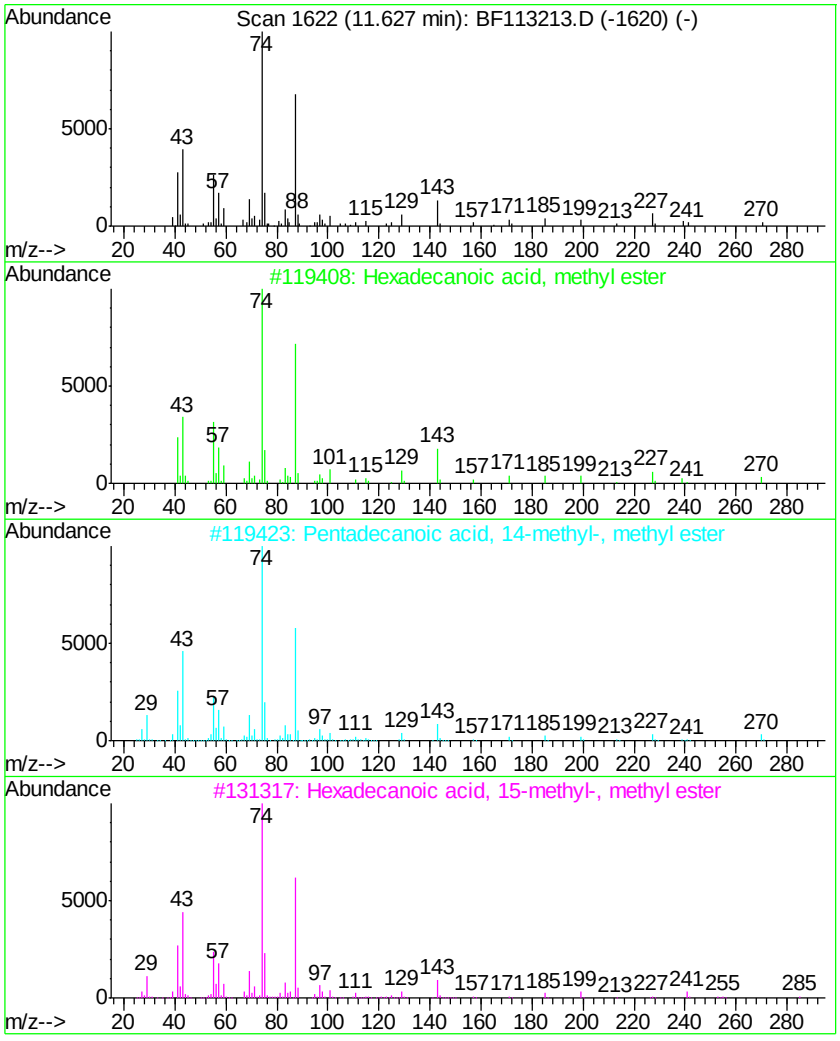
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

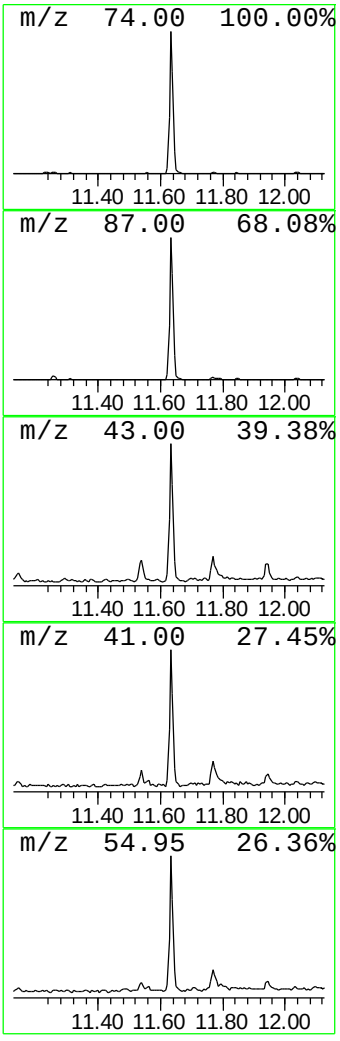
****

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	5.50 ng	301302	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	87
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113213.D
Acq On : 21 Mar 2019 17:26
Operator : JU/SJ
Sample : K1694-05 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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

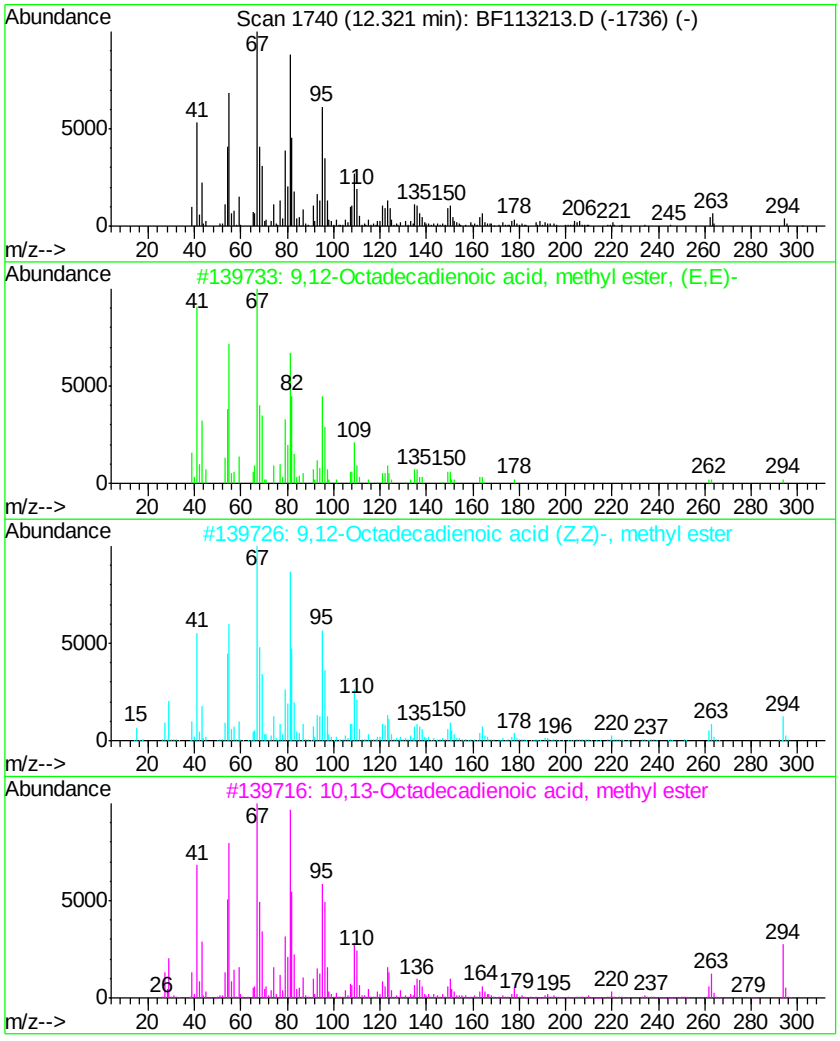
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

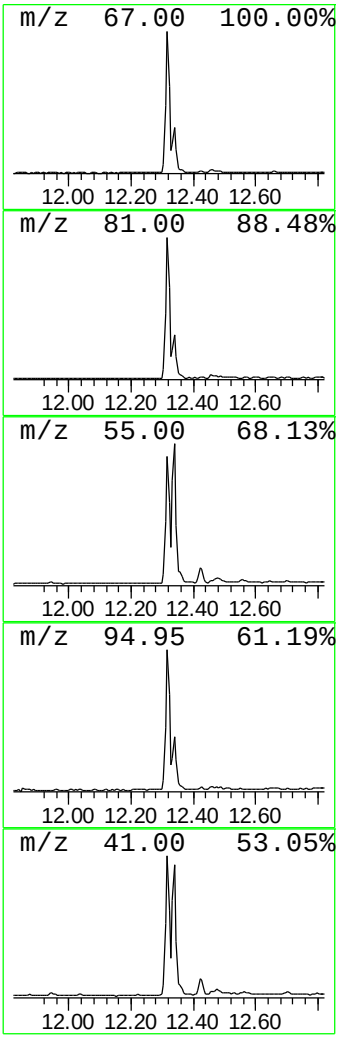
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	19.25 ng	1054290	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	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113213.D
Acq On : 21 Mar 2019 17:26
Operator : JU/SJ
Sample : K1694-05 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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

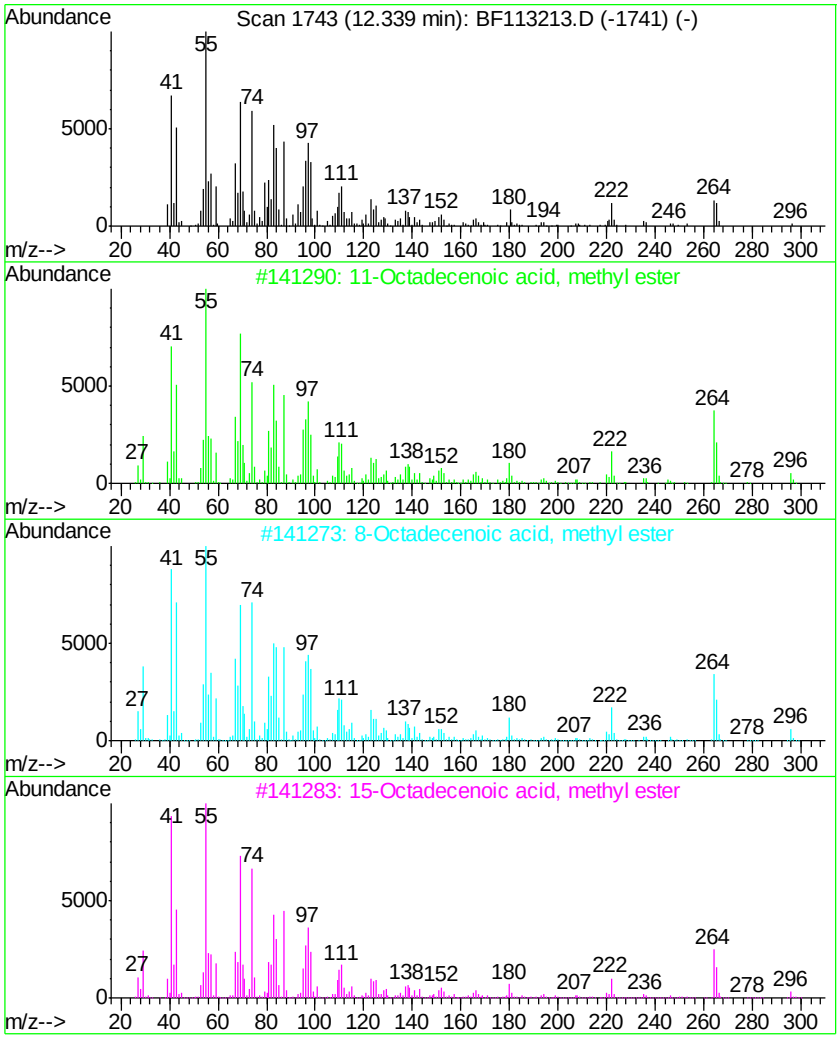
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

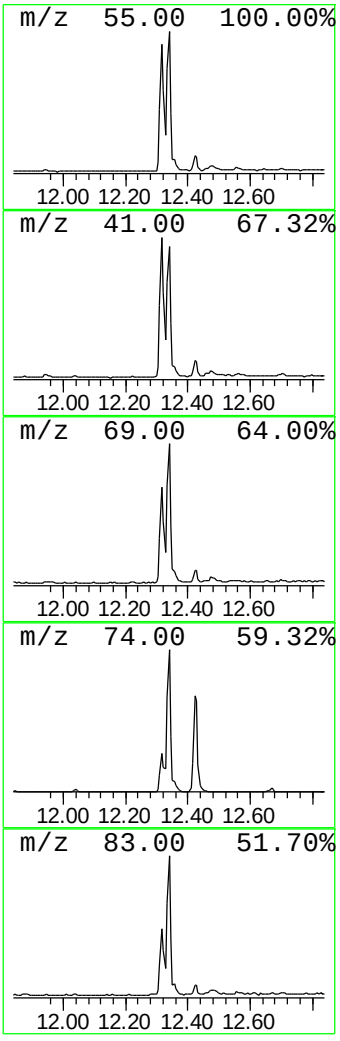
****

Peak Number 5 11-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	14.01 ng	767312	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113213.D
Acq On : 21 Mar 2019 17:26
Operator : JU/SJ
Sample : K1694-05 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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

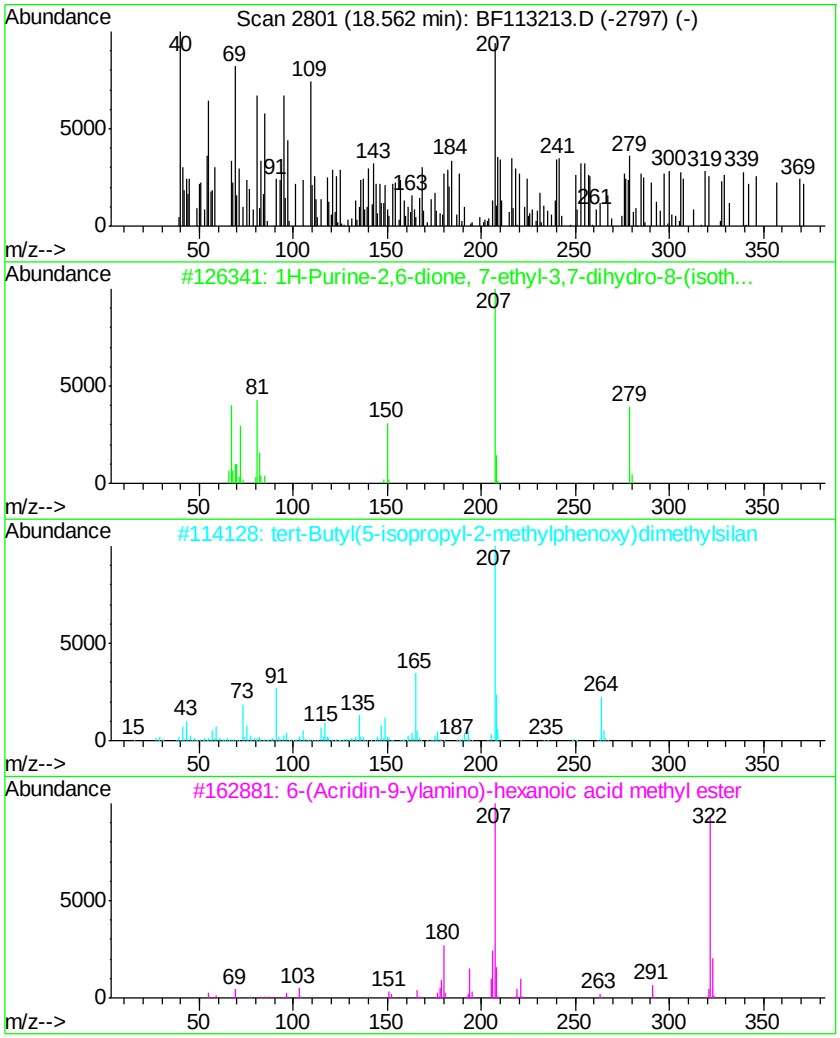
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

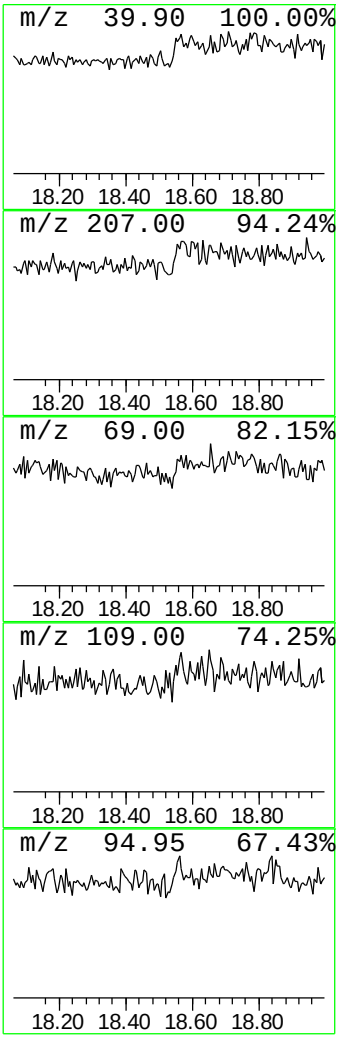
****

Peak Number 6 unknown18.56 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.56	2.54 ng	96654	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Purine-2,6-dione, 7-ethyl-3,7...	279	C11H13N5O2S	027042-75-7	27
2	tert-Butyl(5-isopropyl-2-methylp...	264	C16H28OSi	1000367-02-3	25
3	6-(Acridin-9-ylamino)-hexanoic a...	322	C20H22N2O2	194363-01-4	22
4	1(3H)-Isobenzofuranone, 6,7-dime...	342	C19H18O6	1000350-76-1	22
5	Spiro-3-(2-butyl-2,4-diazabicycl...	250	C15H26N2O	1000194-74-4	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113213.D
Acq On : 21 Mar 2019 17:26
Operator : JU/SJ
Sample : K1694-05 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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	7.3	ng	353325	1	6.72	962033	20.0
Hexadecanoic acid...	11.63	5.5	ng	301302	4	11.23	1095260	20.0
9,12-Octadecadien...	12.32	19.3	ng	1054290	4	11.23	1095260	20.0
11-Octadecenoic a...	12.34	14.0	ng	767312	4	11.23	1095260	20.0
unknown18.56	18.56	2.5	ng	96654	6	15.28	760278	20.0