LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020119\
Data File : BF112370.D
Acq On : 2 Feb 2019 1:06
Operator : JU/SJ
Sample : K1011-13 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-013119-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-BF012519.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	5.040	499	502	514	rBV	23630	31351	2.36%	0.177%
2	5.469	572	575	594	rBV	569434	683066	51.32%	3.848%
3	6.481	744	747	763	rBV	640170	764699	57.45%	4.308%
4	6.610	766	769	777	rBV	875359	785080	58.98%	4.423%
5	6.834	804	807	817	rBV	896341	851201	63.95%	4.796%
6	6.992	830	834	844	rBV	718152	627016	47.11%	3.533%
7	7.398	900	903	914	rBV	397643	434629	32.65%	2.449%
8	8.116	1019	1025	1039	rBV	1070428	1123942	84.44%	6.332%
9	8.710	1122	1126	1130	rBV2	32567	26925	2.02%	0.152%
10	8.834	1145	1147	1151	rBV	29538	26522	1.99%	0.149%
11	8.934	1160	1164	1171	rBV2	32794	40791	3.06%	0.230%
12	9.192	1204	1208	1218	rBV	907189	870071	65.37%	4.902%
13	9.275	1218	1222	1224	rBV	35218	33843	2.54%	0.191%
14	9.463	1250	1254	1259	rBV	18467	25330	1.90%	0.143%
15	9.534	1263	1266	1268	rBV	30499	31478	2.36%	0.177%
16	9.586	1272	1275	1278	rVV	59054	59748	4.49%	0.337%
17	9.651	1283	1286	1288	rBV3	22675	20439	1.54%	0.115%
18	9.733	1297	1300	1304	rBV	19209	22143	1.66%	0.125%
19	9.798	1304	1311	1316	rVV2	51181	80918	6.08%	0.456%
20	9.875	1320	1324	1327	rVV	1223244	1115739	83.82%	6.286%
21	9.904	1327	1329	1338	rVV	84899	101016	7.59%	0.569%
22	9.981	1338	1342	1346	rVB7	9210	15502	1.16%	0.087%
23	10.081	1353	1359	1362	rVV2	35890	40851	3.07%	0.230%
24	10.116	1362	1365	1370	rVB5	18246	21178	1.59%	0.119%
25	10.192	1375	1378	1381	rBV2	14379	16628	1.25%	0.094%
26	10.298	1389	1396	1399	rBV2	47634	49502	3.72%	0.279%
27	10.375	1403	1409	1411	rBV5	8216	14158	1.06%	0.080%
28	10.422	1414	1417	1422	rVV	70506	68681	5.16%	0.387%
29	10.516	1429	1433	1439	rVB5	13229	23280	1.75%	0.131%
30	10.663	1455	1458	1469	rBV	399976	413720	31.08%	2.331%
31	10.769	1474	1476	1486	rVB	42391	59620	4.48%	0.336%
32	10.969	1504	1510	1513	rBV5	19584	31683	2.38%	0.178%
33	11.216	1548	1552	1555	rBV2	33760	35272	2.65%	0.199%
34	11.257	1555	1559	1564	rVB3	32102	40507	3.04%	0.228%

LSC Area Percent Report

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Data File : BF112370.D
Acq On : 2 Feb 2019 1:06
Operator : JU/SJ
Sample : K1011-13 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-013119-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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.298	1564	1566	1570	rVB2	16849	18403	1.38%	0.104%
36	11.357	1573	1576	1579	rBV	950954	936356	70.35%	5.275%
37	11.380	1579	1580	1586	rVV	300284	258343	19.41%	1.455%
38	11.439	1586	1590	1593	rVB	61127	61575	4.63%	0.347%
39	11.598	1612	1617	1621	rBV	23266	27932	2.10%	0.157%
40	11.645	1622	1625	1627	rVV2	28863	24752	1.86%	0.139%
41	11.692	1631	1633	1638	rVB4	18147	21278	1.60%	0.120%
42	11.745	1638	1642	1645	rBV	474874	379951	28.55%	2.141%
43	11.863	1658	1662	1664	rBV	36546	44281	3.33%	0.249%
44	11.892	1664	1667	1673	rVB3	55425	73713	5.54%	0.415%
45	11.975	1678	1681	1684	rVV2	58187	70852	5.32%	0.399%
46	11.998	1684	1685	1688	rVV	27557	16352	1.23%	0.092%
47	12.051	1691	1694	1700	rVB3	25711	28443	2.14%	0.160%
48	12.157	1708	1712	1716	rBV2	19911	23598	1.77%	0.133%
49	12.427	1751	1758	1760	rBV	1477728	1331054	100.00%	7.499%
50	12.451	1760	1762	1768	rVV	1179060	1003019	75.36%	5.651%
51	12.504	1768	1771	1773	rVV4	17486	23402	1.76%	0.132%
52	12.533	1773	1776	1780	rVB	173487	135558	10.18%	0.764%
53	12.574	1780	1783	1788	rBV	274194	243609	18.30%	1.372%
54	12.674	1796	1800	1804	rBV6	15689	23507	1.77%	0.132%
55	12.757	1811	1814	1817	rBV5	17038	19750	1.48%	0.111%
56	12.804	1817	1822	1828	rVV	250307	276025	20.74%	1.555%
57	12.857	1828	1831	1835	rVB4	18969	23055	1.73%	0.130%
58	12.939	1841	1845	1849	rBV	686051	604484	45.41%	3.406%
59	13.016	1856	1858	1862	rBV4	17772	25050	1.88%	0.141%
60	13.133	1871	1878	1881	rBV2	39421	63215	4.75%	0.356%
61	13.163	1881	1883	1885	rBV2	15108	14615	1.10%	0.082%
62	13.198	1887	1889	1892	rVB	29199	25289	1.90%	0.142%
63	13.239	1892	1896	1898	rBV3	24277	33128	2.49%	0.187%
64	13.363	1914	1917	1919	rBV	20507	18962	1.42%	0.107%
65	13.510	1939	1942	1944	rBV2	20928	20939	1.57%	0.118%
66	13.751	1981	1983	1986	rBV	21128	20461	1.54%	0.115%
67	13.774	1986	1987	1991	rBV3	13101	15957	1.20%	0.090%
68	13.833	1994	1997	1999	rBV4	44378	39450	2.96%	0.222%
69	13.969	2018	2020	2021	rBV	21768	17888	1.34%	0.101%
70	14.004	2021	2026	2029	rVV	932826	1057606	79.46%	5.958%
71	14.027	2029	2030	2036	rVB	107715	83950	6.31%	0.473%

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Misc :
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Instrument : BNA_F
ClientSampleId : OR-02-013119-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
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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.151	2048	2051	2057	rBV4	49859	65914	4.95%	0.371%
73	14.451	2100	2102	2107	rVB2	67771	70373	5.29%	0.396%
74	14.757	2151	2154	2157	rVB	95550	87495	6.57%	0.493%
75	15.045	2199	2203	2206	rBV	97802	155207	11.66%	0.874%
76	15.092	2208	2211	2214	rVB	143476	156649	11.77%	0.883%
77	15.345	2252	2254	2261	rVB	64004	84474	6.35%	0.476%
78	15.410	2262	2265	2270	rVV	115851	141721	10.65%	0.798%
79	15.474	2271	2276	2288	rVB	801651	1141535	85.76%	6.431%
80	15.898	2344	2348	2354	rVB	111877	154151	11.58%	0.868%

Sum of corrected areas: 17749850

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020119\
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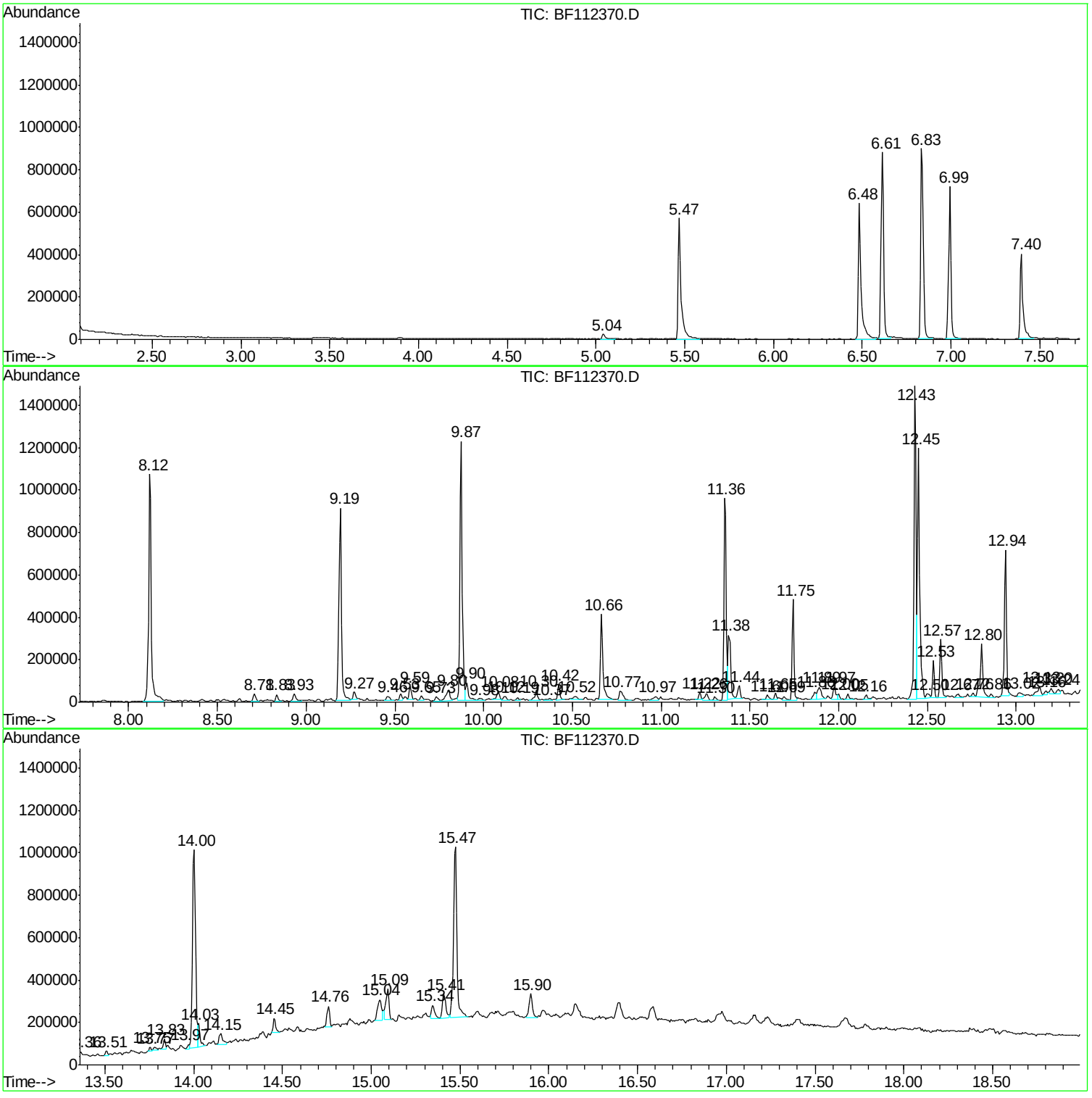
Operator : JU/SJ
Sample : K1011-13 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-02-013119-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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\BF020119\
Data File : BF112370.D
Acq On : 2 Feb 2019 1:06
Operator : JU/SJ
Sample : K1011-13 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-013119-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

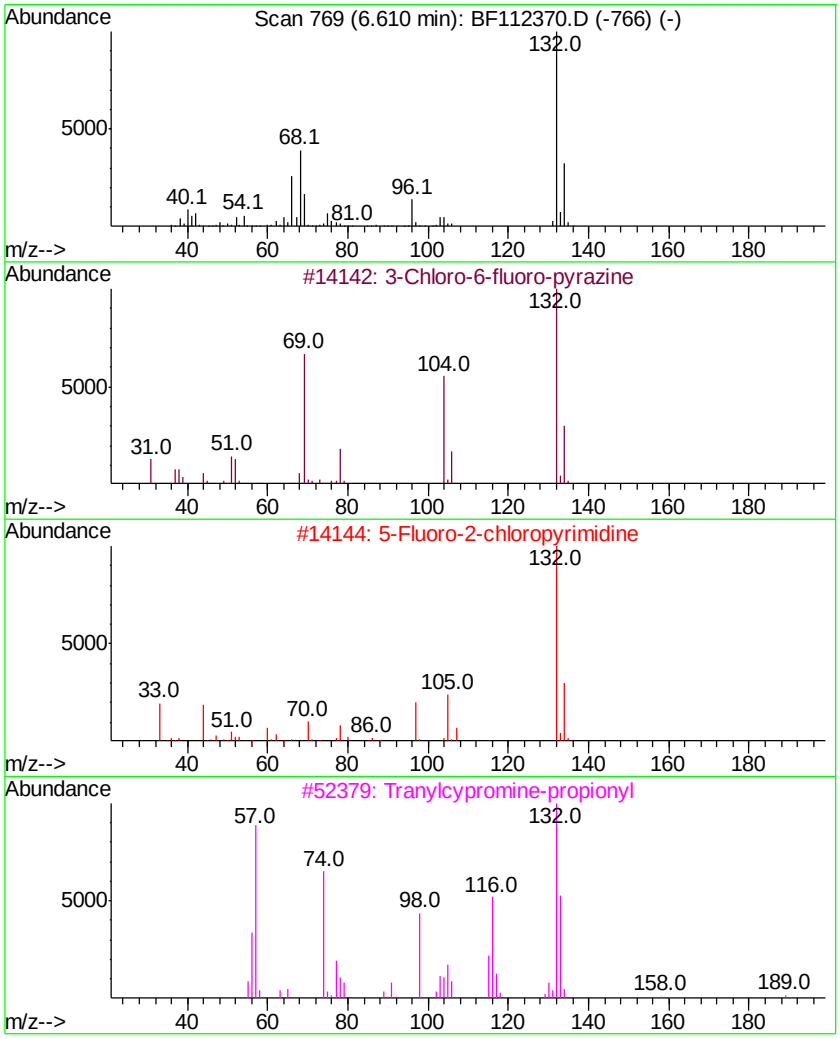
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

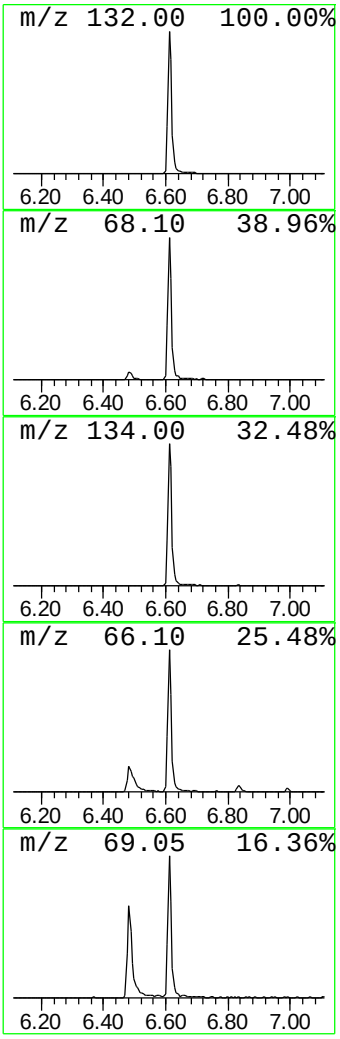
****

Peak Number 1 unknown6.61 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	18.45 ng	785080	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

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Data File : BF112370.D
Acq On : 2 Feb 2019 1:06
Operator : JU/SJ
Sample : K1011-13 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-013119-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

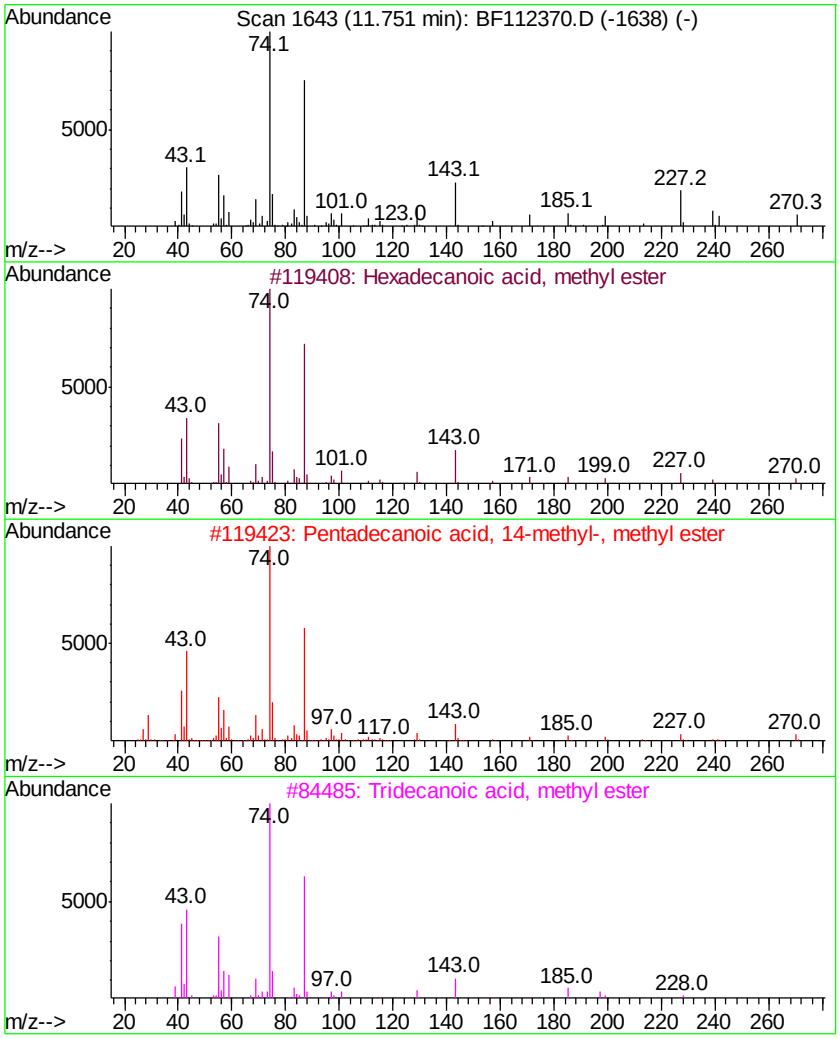
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

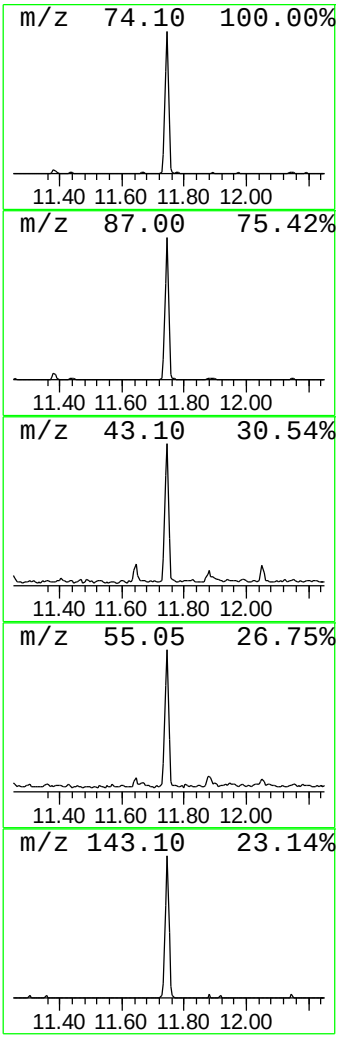
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	8.12 ng	379951	Phenanthrene-d10	11.36

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	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020119\
Data File : BF112370.D
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

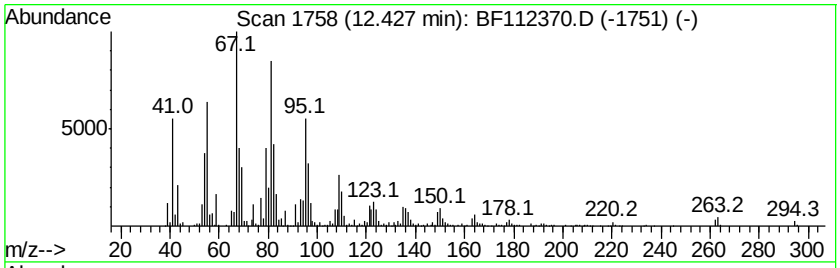
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

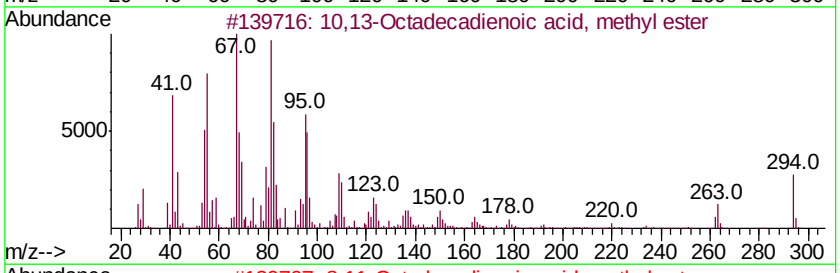
****

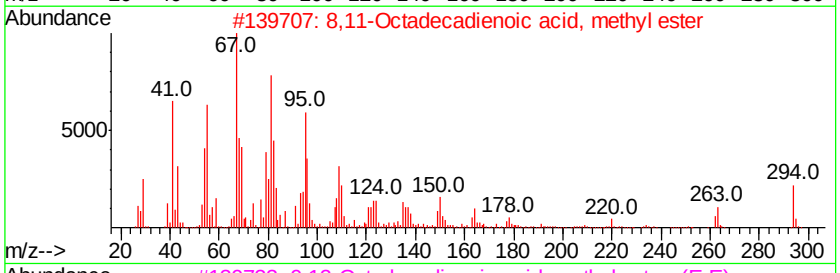
Peak Number 4 10,13-Octadecadienoic acid,... Concentration Rank 1

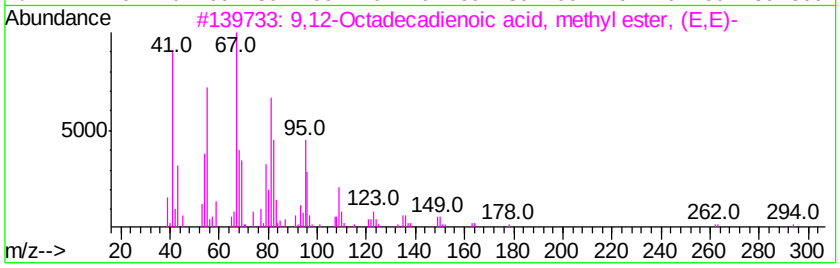
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	28.43 ng	1331050	Phenanthrene-d10	11.36

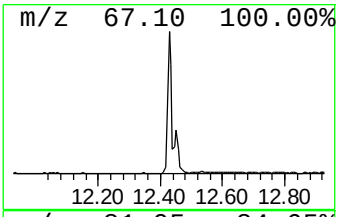
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
2	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99

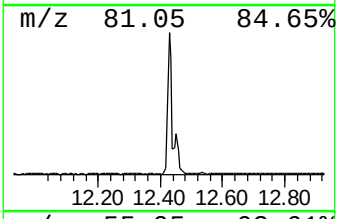


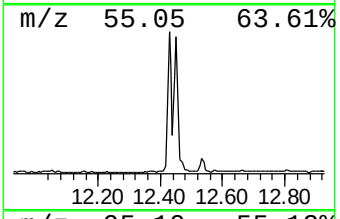


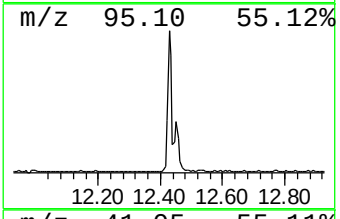


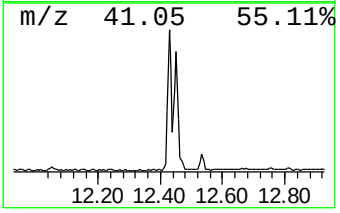












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020119\
Data File : BF112370.D
Acq On : 2 Feb 2019 1:06
Operator : JU/SJ
Sample : K1011-13 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-013119-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

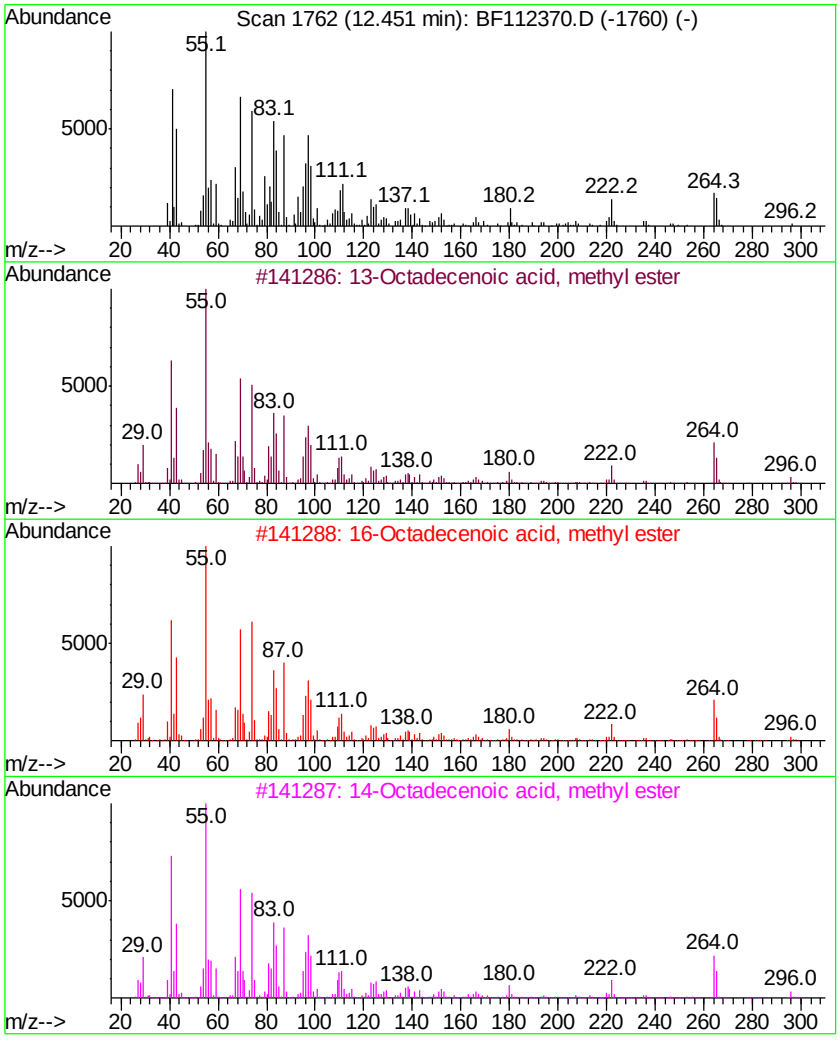
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

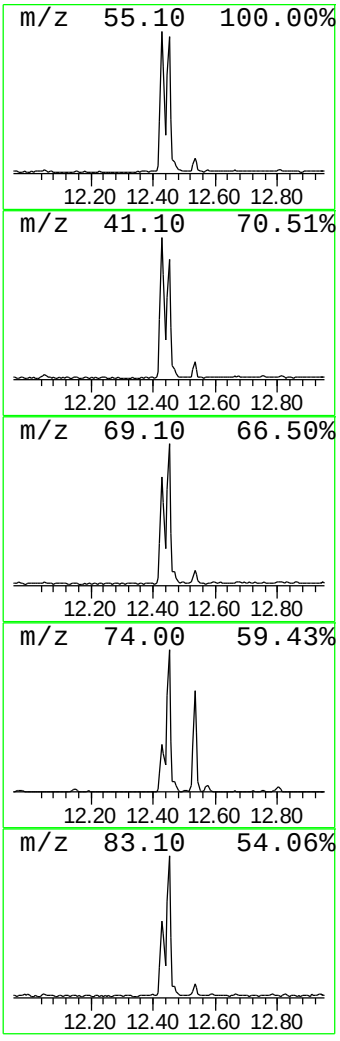
****

Peak Number 5 13-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	21.42 ng	1003020	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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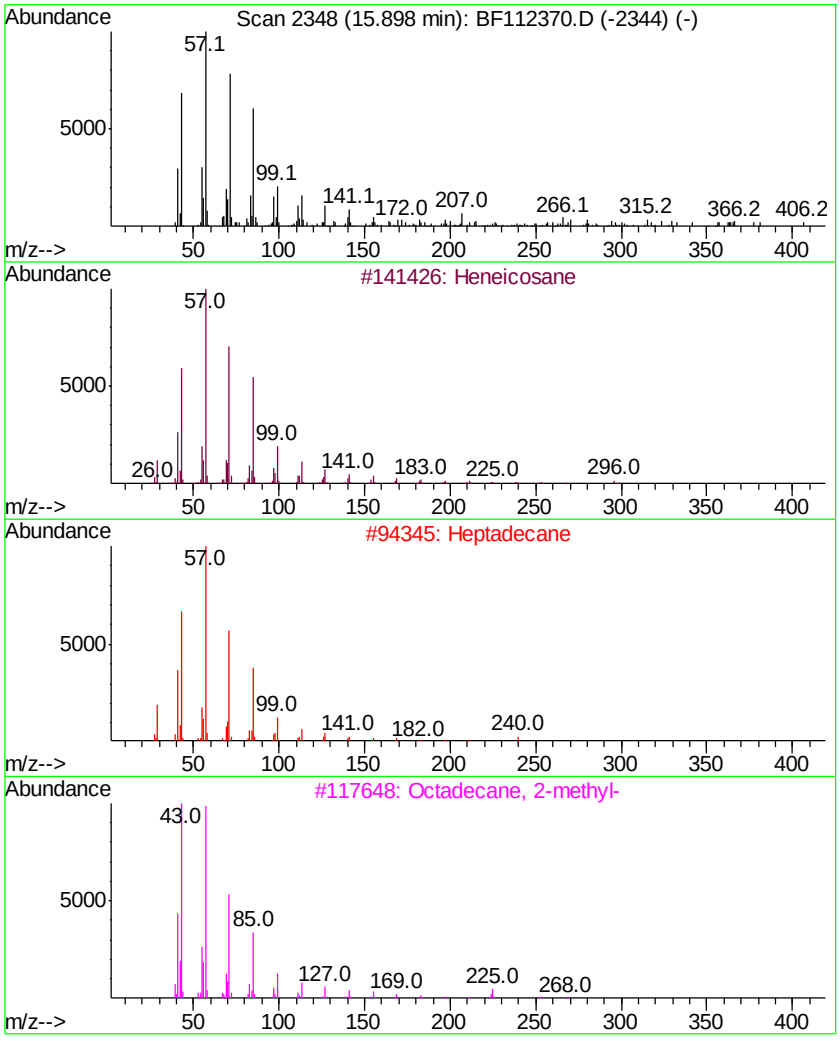
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

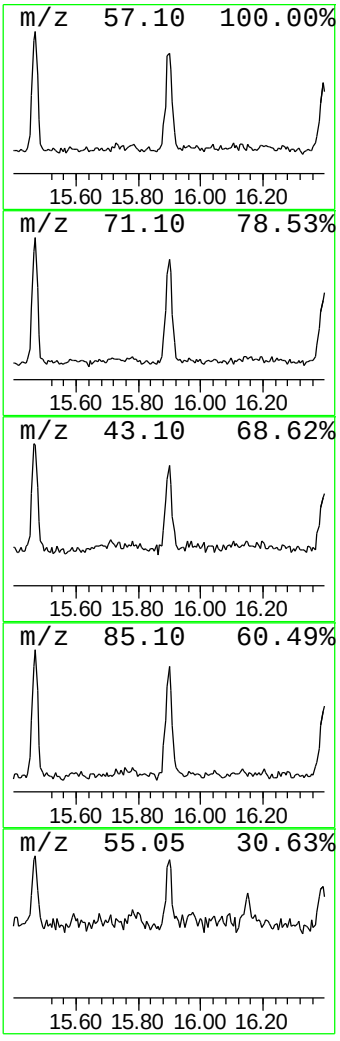
****

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	2.70 ng	154151	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Heptadecane	240	C17H36	000629-78-7	91
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
4	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	91
5	Octacosane	394	C28H58	000630-02-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020119\
Data File : BF112370.D
Acq On : 2 Feb 2019 1:06
Operator : JU/SJ
Sample : K1011-13 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-013119-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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
unknown6.61	6.61	18.4	ng	785080	1	6.83	851201	20.0
Hexadecanoic acid...	11.75	8.1	ng	379951	4	11.36	936356	20.0
10,13-Octadecadie...	12.43	28.4	ng	1331050	4	11.36	936356	20.0
13-Octadecenoic a...	12.45	21.4	ng	1003020	4	11.36	936356	20.0
Heneicosane	15.90	2.7	ng	154151	6	15.47	1141540	20.0