LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020119\
Data File : BF112359.D
Acq On : 1 Feb 2019 18:46
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	507	rBV	23183	27094	2.33%	0.173%
2	5.469	572	575	593	rBV	540367	632977	54.41%	4.034%
3	6.481	744	747	766	rBV	568746	698954	60.09%	4.455%
4	6.610	766	769	778	rBV	784732	732563	62.98%	4.669%
5	6.834	804	807	815	rBV	844490	793593	68.22%	5.058%
6	6.992	830	834	844	rBV	670883	593706	51.04%	3.784%
7	7.398	900	903	913	rBV	359624	398257	34.24%	2.538%
8	8.116	1020	1025	1033	rBV	946565	996782	85.69%	6.353%
9	8.710	1122	1126	1129	rBV2	29101	27313	2.35%	0.174%
10	8.834	1144	1147	1152	rBV	25914	27410	2.36%	0.175%
11	8.934	1160	1164	1171	rVB2	27463	32234	2.77%	0.205%
12	9.192	1204	1208	1217	rBV	760008	764404	65.71%	4.872%
13	9.269	1218	1221	1224	rVV	28943	27172	2.34%	0.173%
14	9.457	1250	1253	1258	rBV2	16228	24291	2.09%	0.155%
15	9.534	1261	1266	1268	rBV2	26369	30055	2.58%	0.192%
16	9.586	1272	1275	1278	rVV	52339	51477	4.43%	0.328%
17	9.651	1283	1286	1288	rBV	17259	15825	1.36%	0.101%
18	9.733	1297	1300	1304	rVB	18462	17441	1.50%	0.111%
19	9.798	1307	1311	1316	rVB	33663	34031	2.93%	0.217%
20	9.875	1320	1324	1327	rVV	999114	948340	81.53%	6.044%
21	9.904	1327	1329	1333	rVB	67469	62704	5.39%	0.400%
22	10.033	1345	1351	1354	rBV5	7992	14920	1.28%	0.095%
23	10.081	1356	1359	1363	rVV2	32395	33700	2.90%	0.215%
24	10.116	1363	1365	1369	rVV3	15056	16197	1.39%	0.103%
25	10.298	1394	1396	1399	rVB	42704	31409	2.70%	0.200%
26	10.422	1413	1417	1423	rVB	61791	61655	5.30%	0.393%
27	10.516	1429	1433	1438	rVB4	11861	19448	1.67%	0.124%
28	10.663	1455	1458	1469	rVB	360429	373996	32.15%	2.384%
29	10.769	1473	1476	1485	rVB2	36609	49339	4.24%	0.314%
30	10.969	1505	1510	1513	rBV3	13601	21307	1.83%	0.136%
31	11.216	1548	1552	1555	rBV2	30612	29258	2.52%	0.186%
32	11.251	1555	1558	1564	rVB3	22053	30593	2.63%	0.195%
33	11.357	1573	1576	1579	rBV	875452	809310	69.57%	5.158%
34	11.380	1579	1580	1587	rVV	267231	219912	18.91%	1.402%

LSC Area Percent Report

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Acq On : 1 Feb 2019 18:46
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	11.433	1587	1589	1593	rVB	49020	47572	4.09%	0.303%
36	11.598	1613	1617	1622	rBV	17372	25324	2.18%	0.161%
37	11.645	1622	1625	1627	rBV2	25190	20871	1.79%	0.133%
38	11.745	1638	1642	1645	rBV	370057	314257	27.02%	2.003%
39	11.863	1658	1662	1663	rBV	27909	27412	2.36%	0.175%
40	11.892	1663	1667	1673	rVB3	46257	71068	6.11%	0.453%
41	11.975	1678	1681	1683	rVV	51762	55364	4.76%	0.353%
42	11.998	1683	1685	1690	rVV	23077	22437	1.93%	0.143%
43	12.051	1691	1694	1700	rVB3	22368	25080	2.16%	0.160%
44	12.157	1708	1712	1714	rBV3	19727	20930	1.80%	0.133%
45	12.339	1740	1743	1744	rBV2	14212	13114	1.13%	0.084%
46	12.427	1752	1758	1760	rBV	1335150	1163247	100.00%	7.414%
47	12.451	1760	1762	1768	rVV	898133	796406	68.46%	5.076%
48	12.498	1768	1770	1773	rVB3	13682	14907	1.28%	0.095%
49	12.533	1773	1776	1780	rVB	150990	117583	10.11%	0.749%
50	12.574	1780	1783	1787	rBV	263305	238454	20.50%	1.520%
51	12.669	1796	1799	1802	rBV5	18675	24831	2.13%	0.158%
52	12.804	1816	1822	1828	rBV	211638	255074	21.93%	1.626%
53	12.857	1828	1831	1834	rVB3	15760	20874	1.79%	0.133%
54	12.939	1839	1845	1853	rBV	604693	618427	53.16%	3.942%
55	13.027	1855	1860	1862	rBV5	15816	29072	2.50%	0.185%
56	13.133	1870	1878	1882	rBV	44425	84270	7.24%	0.537%
57	13.163	1882	1883	1887	rVV3	18462	26423	2.27%	0.168%
58	13.198	1887	1889	1891	rVV2	35236	29556	2.54%	0.188%
59	13.233	1892	1895	1897	rVV4	24146	32333	2.78%	0.206%
60	13.257	1897	1899	1902	rVB4	21319	20076	1.73%	0.128%
61	13.363	1914	1917	1919	rBV2	17534	21555	1.85%	0.137%
62	13.833	1994	1997	2003	rVB5	45983	55145	4.74%	0.351%
63	13.921	2010	2012	2017	rBV6	26748	38907	3.34%	0.248%
64	13.998	2021	2025	2028	rVV	938515	996222	85.64%	6.350%
65	14.027	2028	2030	2033	rVB	98895	88936	7.65%	0.567%
66	14.151	2049	2051	2053	rBV2	46192	32854	2.82%	0.209%
67	14.457	2100	2103	2108	rBV2	74734	90795	7.81%	0.579%
68	14.757	2152	2154	2157	rVB	107208	86558	7.44%	0.552%
69	15.039	2200	2202	2208	rBV2	80236	131609	11.31%	0.839%
70	15.092	2208	2211	2214	rVB	139610	160028	13.76%	1.020%
71	15.410	2262	2265	2270	rVB	92624	106225	9.13%	0.677%

LSC Area Percent Report

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Data File : BF112359.D
Acq On : 1 Feb 2019 18:46
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

72	15.468	2271	2275	2280	rBV	792286	1005338	86.43%	6.408%
73	15.892	2345	2347	2352	rVB	90295	112556	9.68%	0.717%

Sum of corrected areas: 15689357

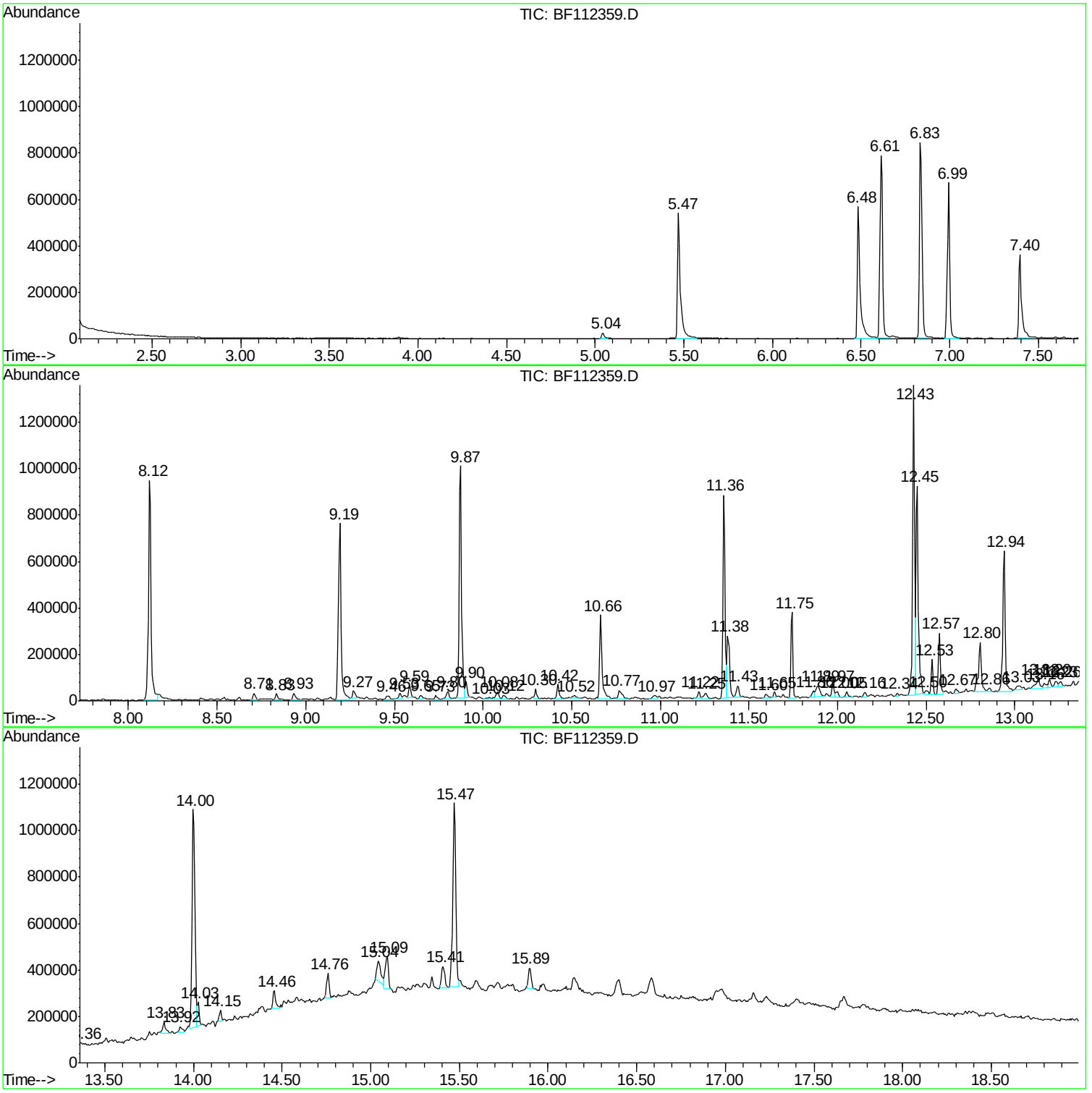
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020119\
Data File : BF112359.D
Acq On : 1 Feb 2019 18:46
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 : BF112359.D
Acq On : 1 Feb 2019 18:46
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

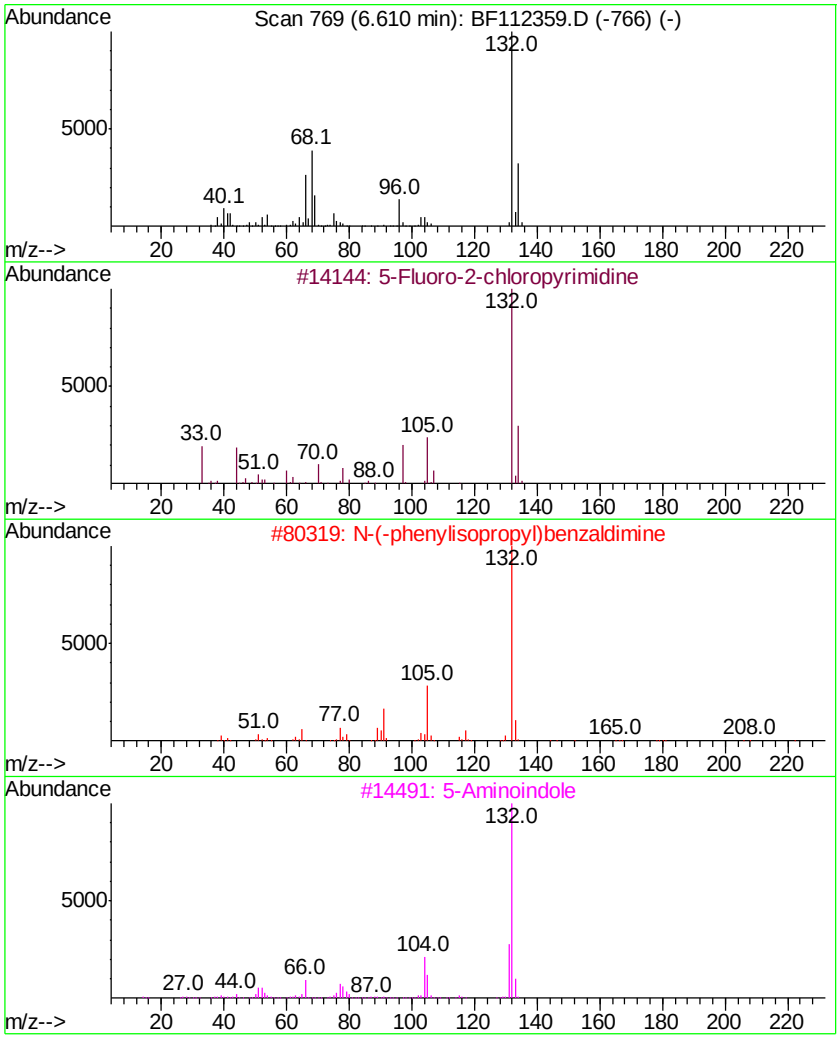
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

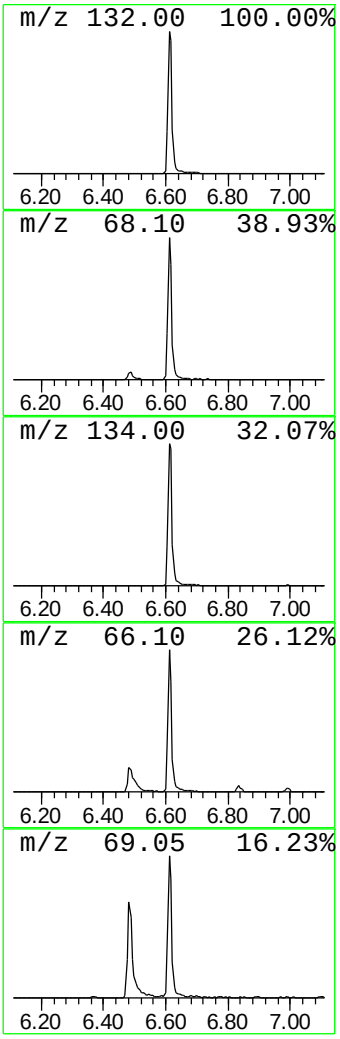
****

Peak Number 1 unknown6.61 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	18.46 ng	732563	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	10
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020119\
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Misc :
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Instrument : BNA_F
ClientSampleId : OR-02-013119-A

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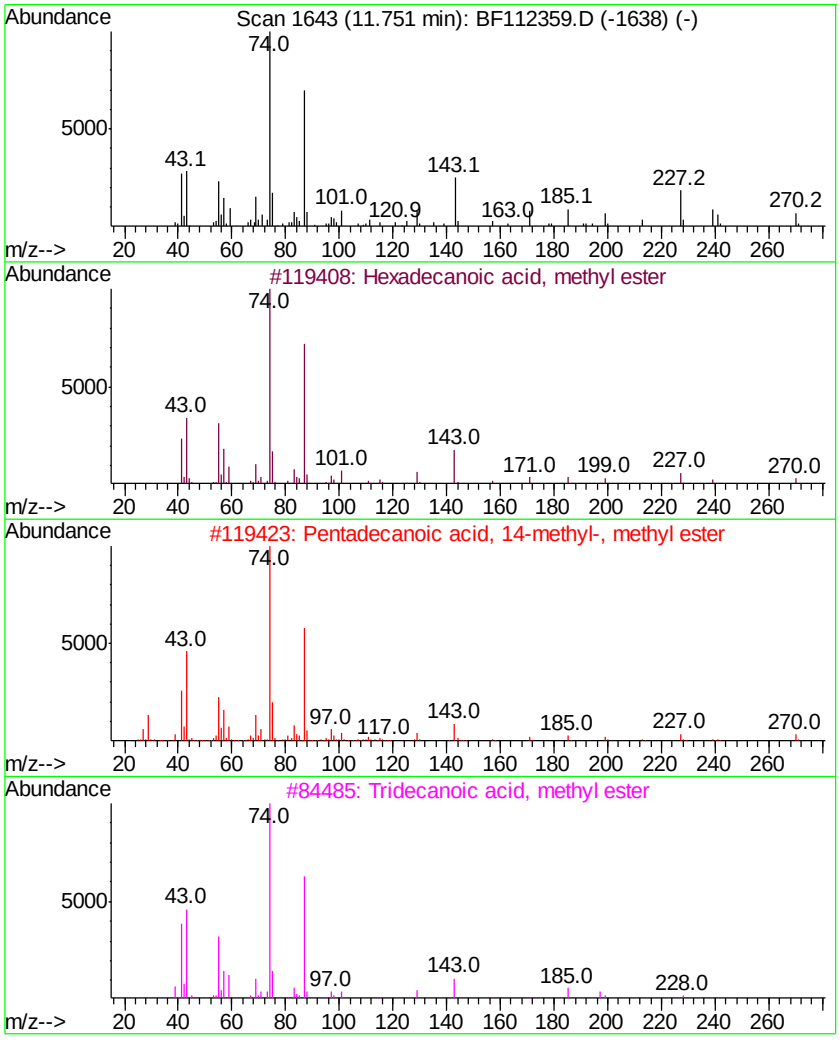
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

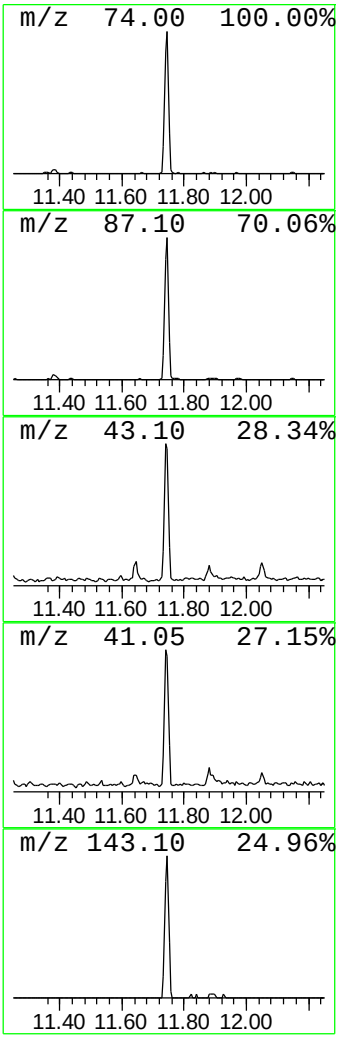
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	7.77 ng	314257	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	91
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020119\
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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

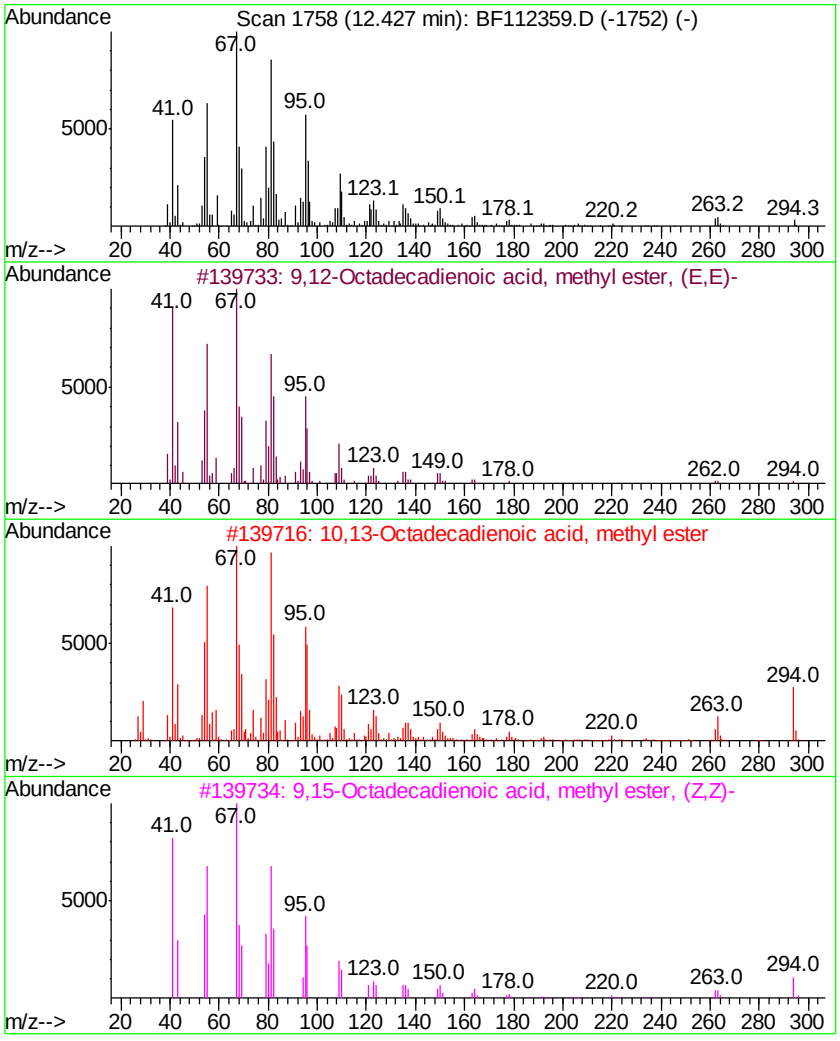
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

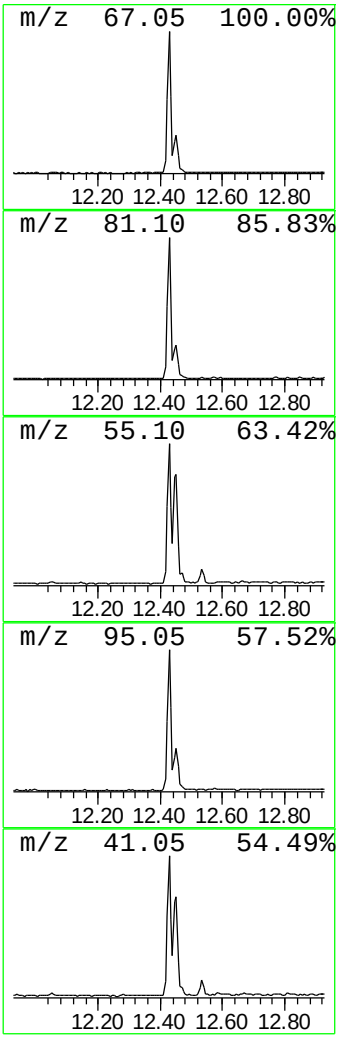
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	28.75 ng	1163250	Phenanthrene-d10	11.36

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	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





Library Search Compound Report

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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

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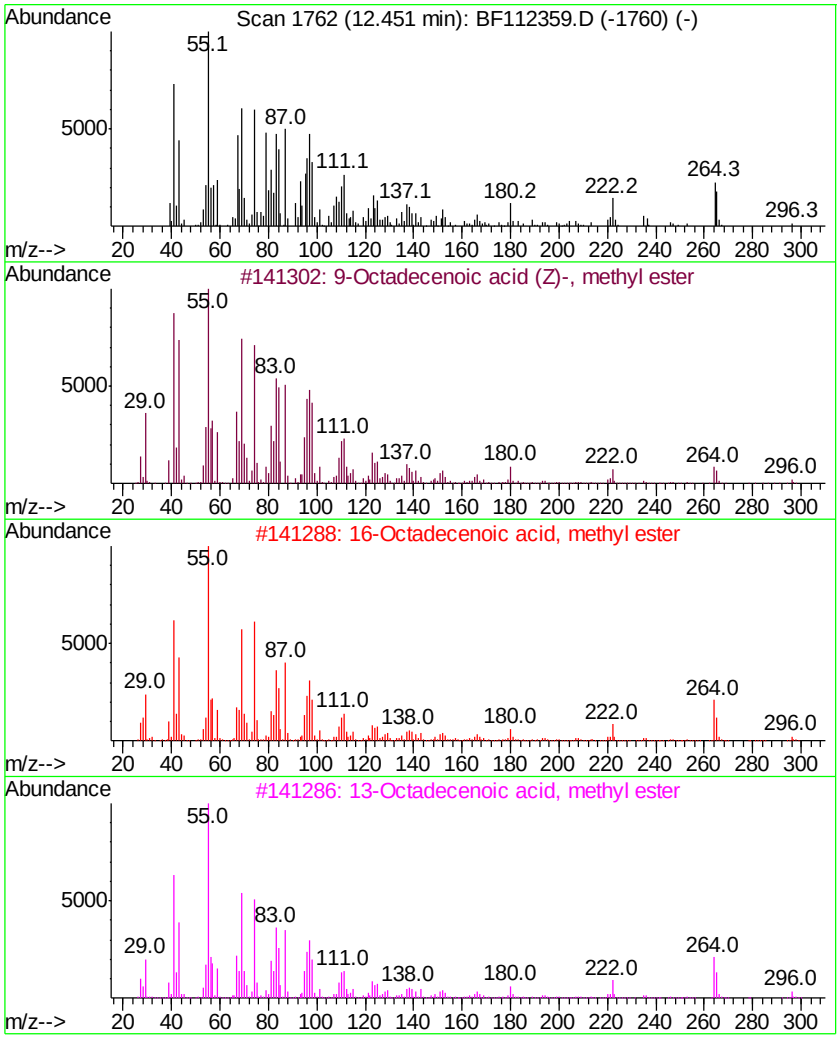
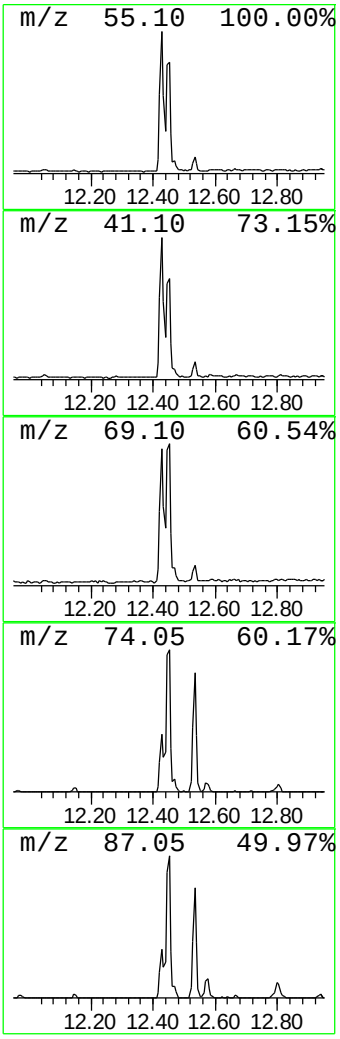
Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	19.68 ng	796406	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	98
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	97
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	96
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	96





Library Search Compound Report

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Misc :
ALS Vial : 13 Sample Multiplier: 1

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

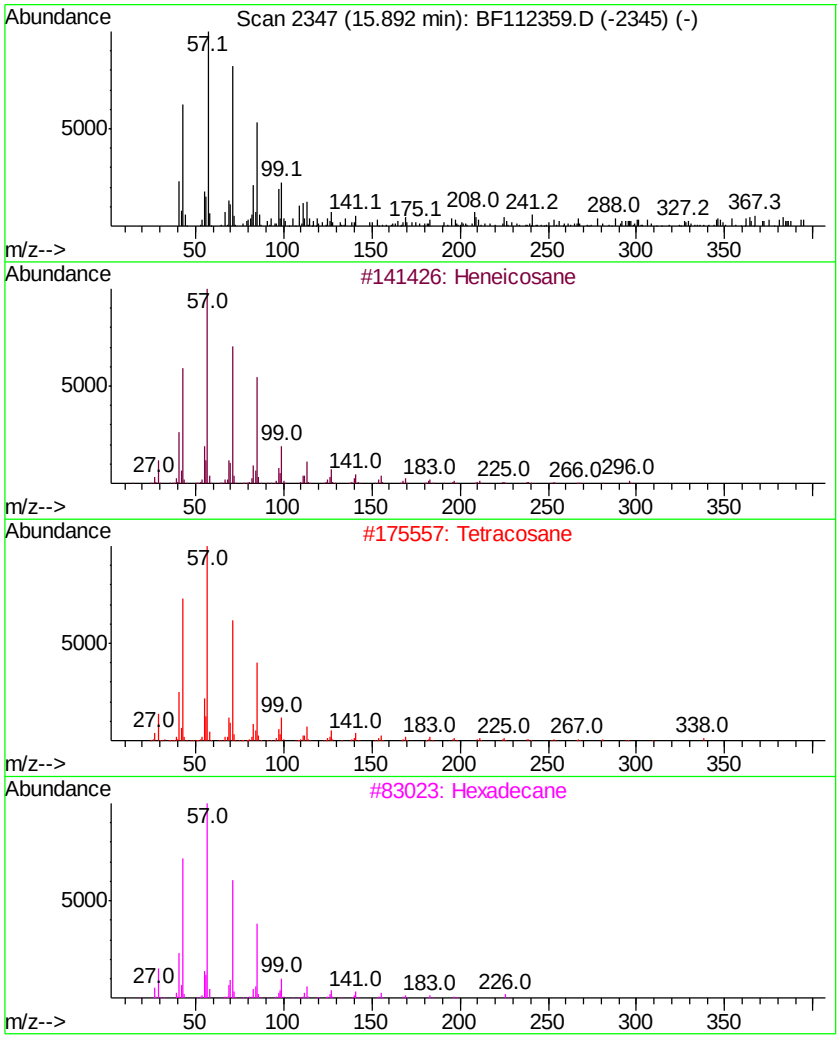
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

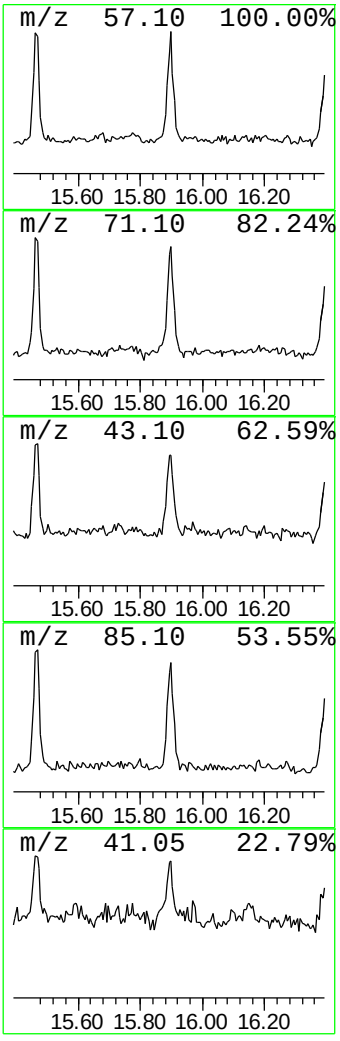
****

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	2.24 ng	112556	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Tetracosane	338	C24H50	000646-31-1	94
3	Hexadecane	226	C16H34	000544-76-3	93
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	76
5	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020119\
Data File : BF112359.D
Acq On : 1 Feb 2019 18:46
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	18.5	ng	732563	1	6.83	793593	20.0
Hexadecanoic acid...	11.75	7.8	ng	314257	4	11.36	809310	20.0
9,12-Octadecadien...	12.43	28.8	ng	1163250	4	11.36	809310	20.0
9-Octadecenoic ac...	12.45	19.7	ng	796406	4	11.36	809310	20.0
Heneicosane	15.89	2.2	ng	112556	6	15.47	1005340	20.0