LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111219\
Data File : BF117764.D
Acq On : 12 Nov 2019 17:22
Operator : JU
Sample : K5788-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

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-BF110619.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	2.216	17	22	55	rVB	1177731	2068001	36.21%	3.570%
2	5.139	511	519	526	rBV	933704	1087353	19.04%	1.877%
3	5.539	582	587	590	rBV	4999506	4703616	82.36%	8.120%
4	6.545	752	758	762	rBV	4832172	5040096	88.25%	8.701%
5	6.692	778	783	786	rBV	5670052	5084102	89.02%	8.776%
6	6.922	819	822	826	rVB	1824911	1642684	28.76%	2.836%
7	6.981	829	832	838	rBV	89533	76343	1.34%	0.132%
8	7.080	845	849	853	rBV	4853680	4083811	71.51%	7.050%
9	7.486	913	918	921	rBV	3277738	3130507	54.81%	5.404%
10	8.210	1035	1041	1044	rBV	2499662	2097938	36.73%	3.622%
11	9.286	1220	1224	1228	rBV	6080935	5711071	100.00%	9.859%
12	9.369	1235	1238	1240	rBV	83431	71658	1.25%	0.124%
13	9.404	1240	1244	1248	rVB2	199433	208832	3.66%	0.360%
14	9.563	1265	1271	1274	rBV2	121190	112129	1.96%	0.194%
15	9.680	1288	1291	1295	rVB	669516	533036	9.33%	0.920%
16	9.898	1324	1328	1333	rVB	64048	68842	1.21%	0.119%
17	9.974	1336	1341	1344	rVV	2454505	2213371	38.76%	3.821%
18	10.763	1470	1475	1478	rBV	3252263	3179501	55.67%	5.489%
19	10.880	1492	1495	1503	rVB3	68833	100719	1.76%	0.174%
20	11.463	1590	1594	1597	rBV	2368374	2053468	35.96%	3.545%
21	11.486	1597	1598	1601	rVV	266603	156048	2.73%	0.269%
22	11.533	1601	1606	1609	rVB3	138738	158939	2.78%	0.274%
23	11.692	1628	1633	1641	rBV5	45775	91496	1.60%	0.158%
24	11.986	1677	1683	1688	rBV2	652092	658365	11.53%	1.137%
25	12.080	1695	1699	1701	rBV2	80324	81587	1.43%	0.141%
26	12.163	1710	1713	1717	rBV2	69310	69225	1.21%	0.120%
27	12.515	1770	1773	1777	rBV	117660	152666	2.67%	0.264%
28	12.557	1777	1780	1785	rVB2	103842	128005	2.24%	0.221%
29	12.680	1798	1801	1805	rBV	742874	624079	10.93%	1.077%
30	12.774	1814	1817	1825	rBV	300741	363045	6.36%	0.627%
31	12.910	1835	1840	1843	rBV	620075	624514	10.94%	1.078%
32	13.057	1861	1865	1868	rBV	5295606	4704270	82.37%	8.121%
33	13.239	1894	1896	1899	rVB2	97798	79168	1.39%	0.137%
34	13.286	1902	1904	1906	rBV	89447	77476	1.36%	0.134%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : WC-1

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

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.633	1960	1963	1966	rBV	103545	104746	1.83%	0.181%
36	13.745	1980	1982	1986	rVB	88149	82499	1.44%	0.142%
37	13.962	2015	2019	2029	rVB2	408293	599552	10.50%	1.035%
38	14.109	2039	2044	2047	rBV2	1941414	2256317	39.51%	3.895%
39	14.139	2047	2049	2051	rVB	326876	253756	4.44%	0.438%
40	14.274	2070	2072	2075	rBV	156631	156403	2.74%	0.270%
41	14.586	2122	2125	2129	rBV2	183786	161854	2.83%	0.279%
42	14.904	2177	2179	2182	rVB	186773	163786	2.87%	0.283%
43	15.174	2222	2225	2229	rBV	323358	532053	9.32%	0.918%
44	15.262	2237	2240	2242	rBV	161811	159479	2.79%	0.275%
45	15.556	2287	2290	2294	rBV	262615	307927	5.39%	0.532%
46	15.627	2297	2302	2305	rBV	1503360	1914304	33.52%	3.305%

Sum of corrected areas: 57928637

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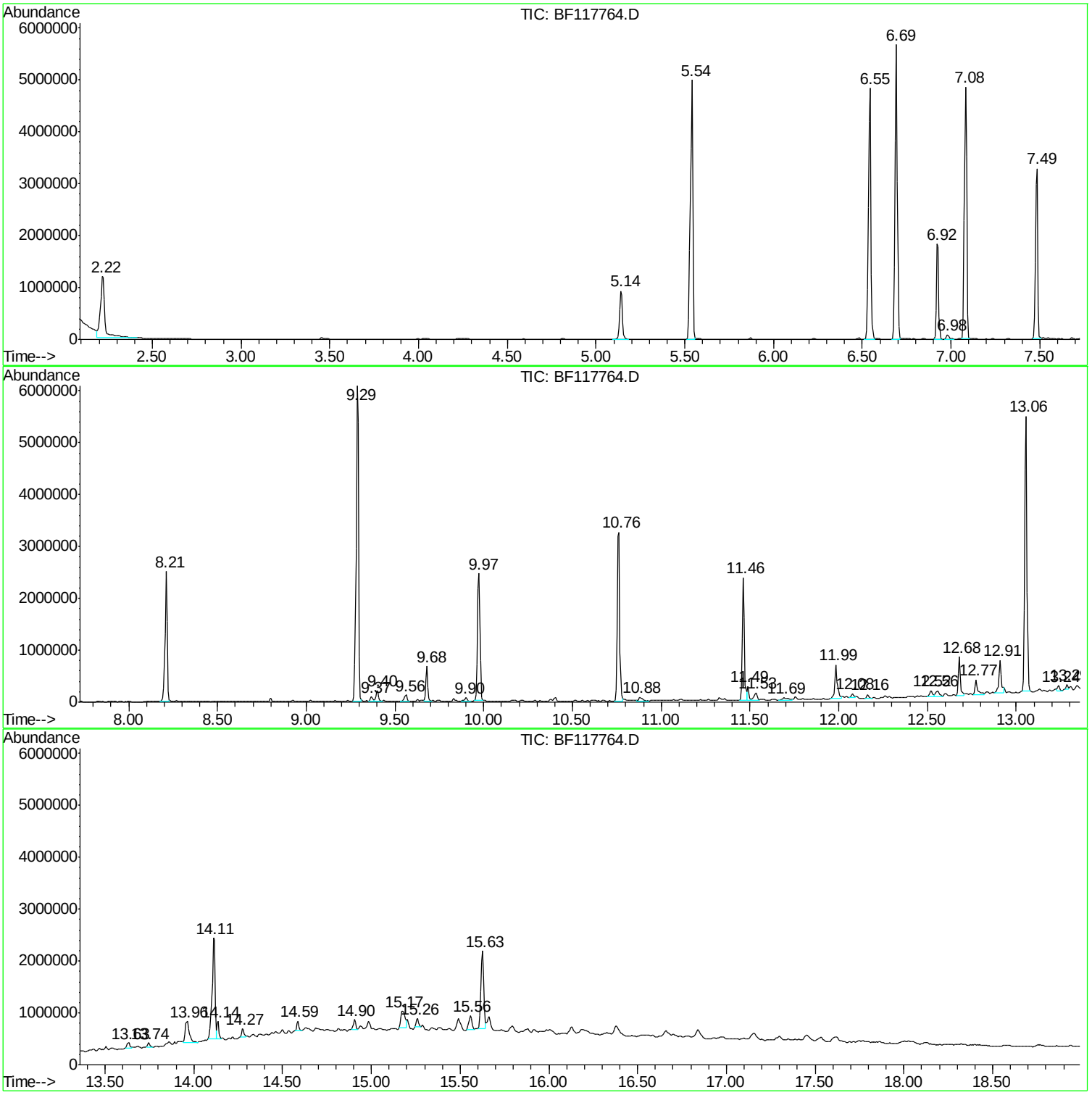
Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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

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Data File : BF117764.D
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Operator : JU
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

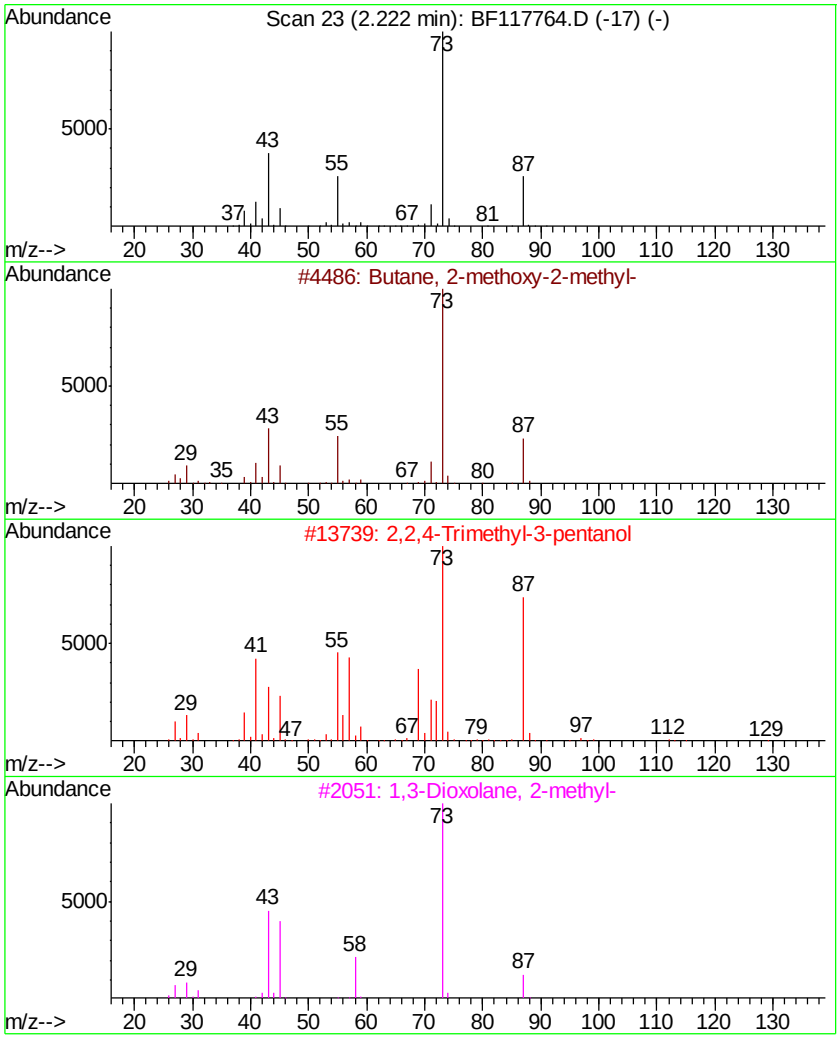
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

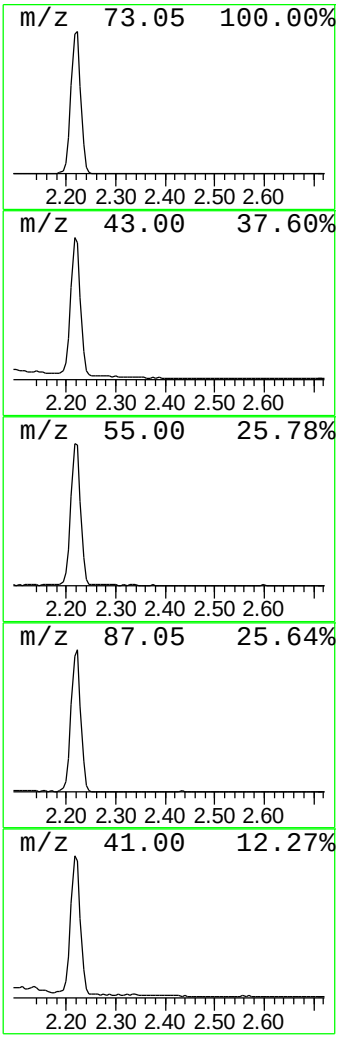
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	25.18 ng	2068000	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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Data File : BF117764.D
Acq On : 12 Nov 2019 17:22
Operator : JU
Sample : K5788-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

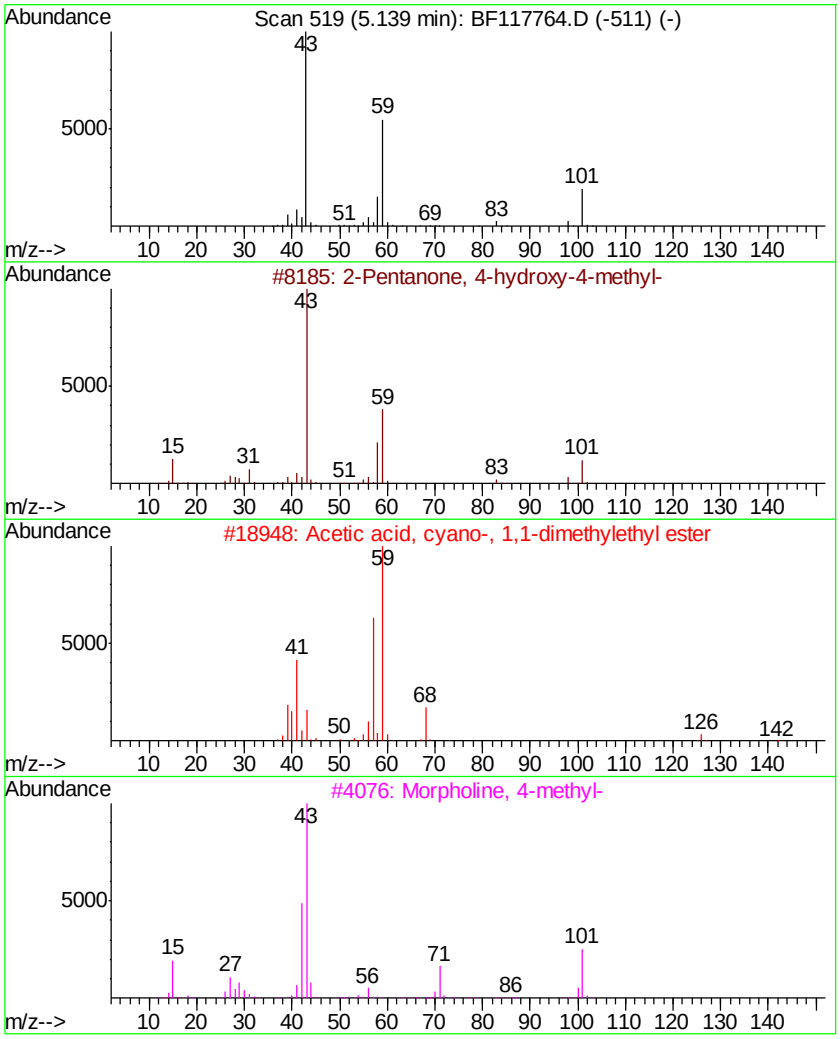
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

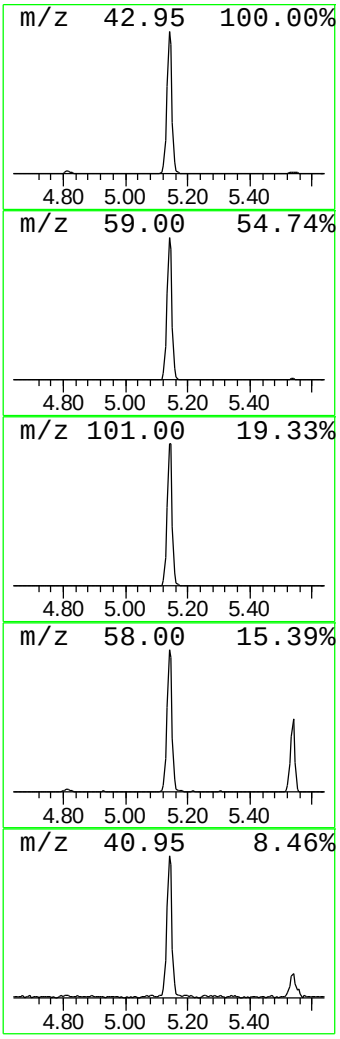
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	13.24 ng	1087350	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Data File : BF117764.D
Acq On : 12 Nov 2019 17:22
Operator : JU
Sample : K5788-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

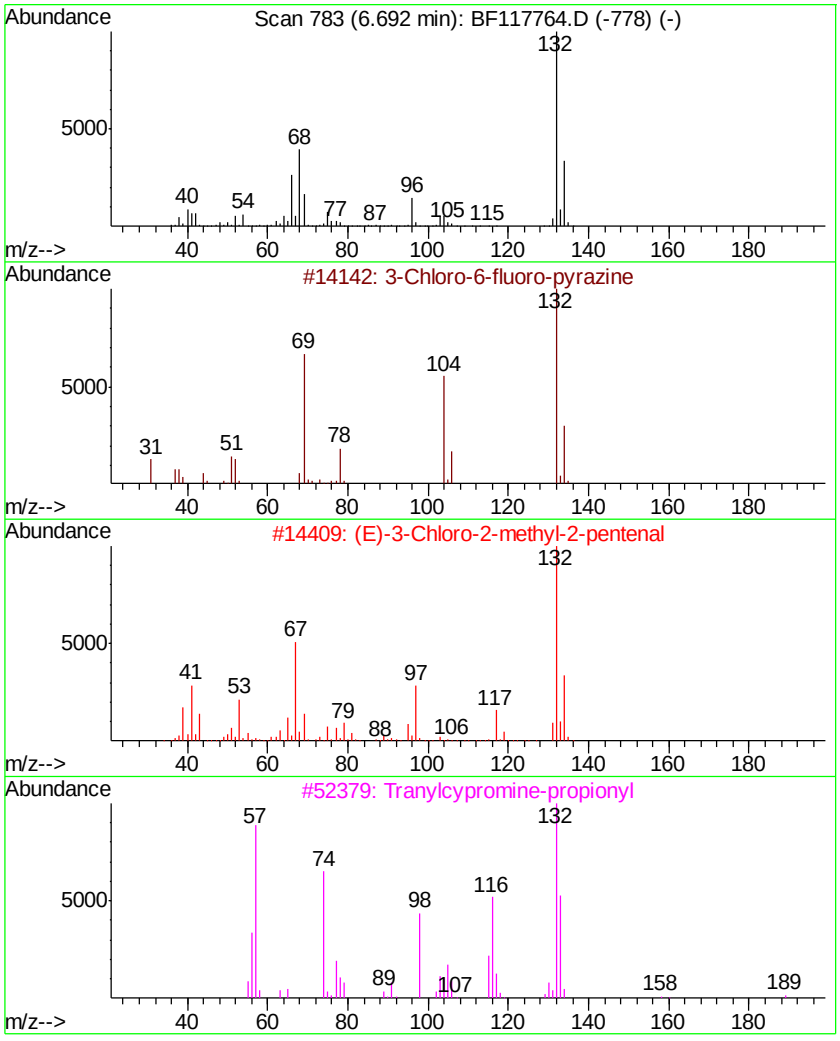
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

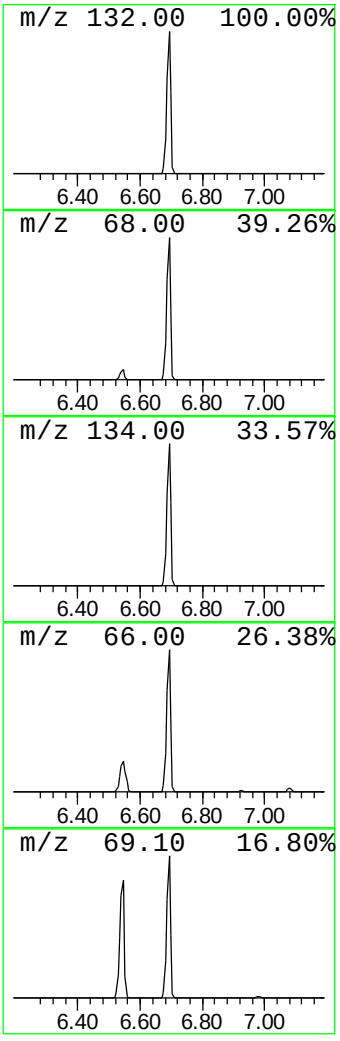
****

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	61.90 ng	5084100	1,4-Dichlorobenzene-d4	6.93

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Instrument : BNA_F
ClientSampleId : WC-1

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

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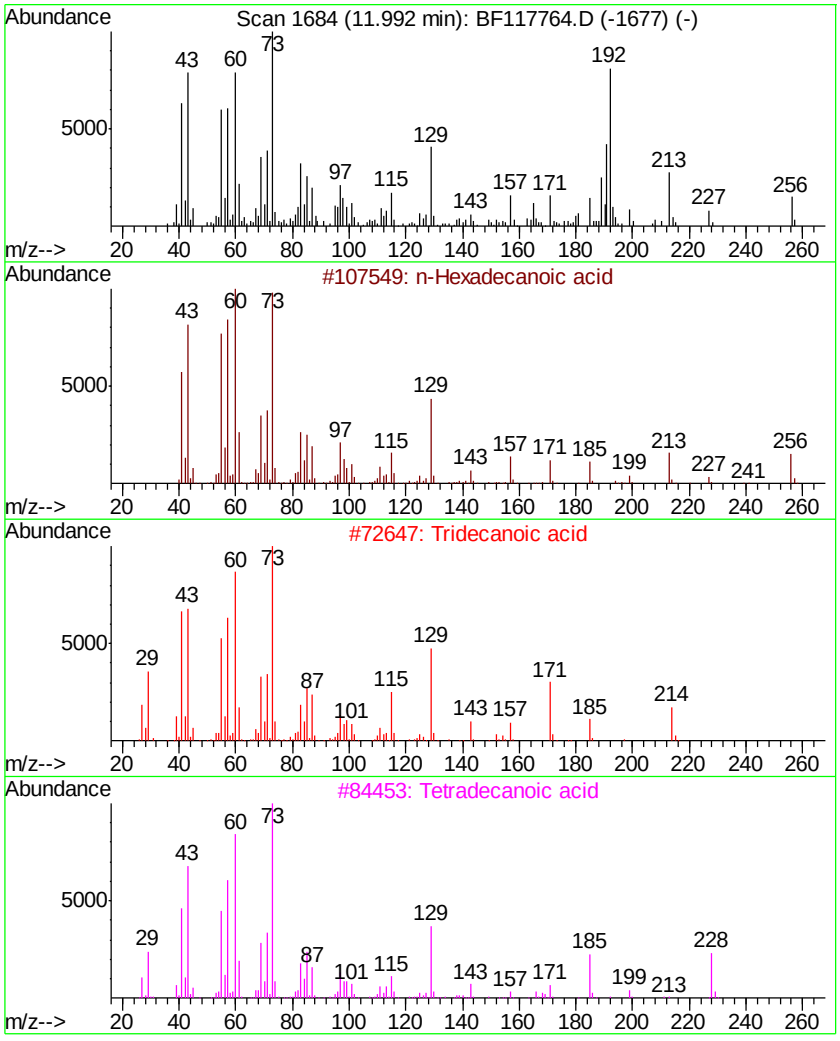
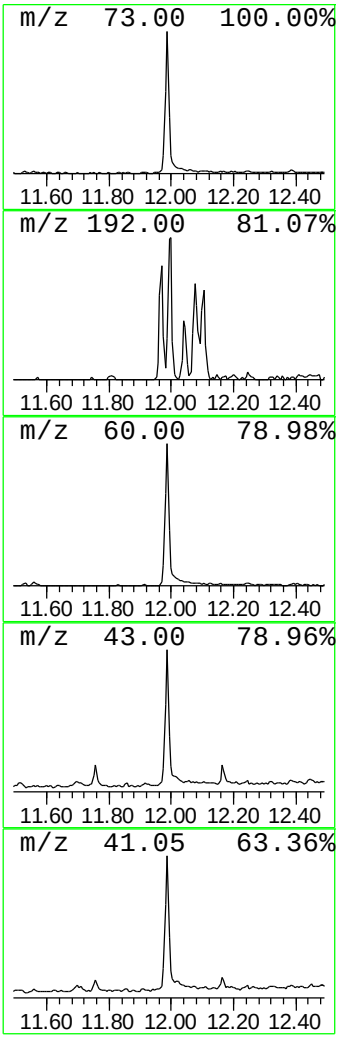
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	6.41 ng	658365	Phenanthrene-d10	11.46

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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





Library Search Compound Report

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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
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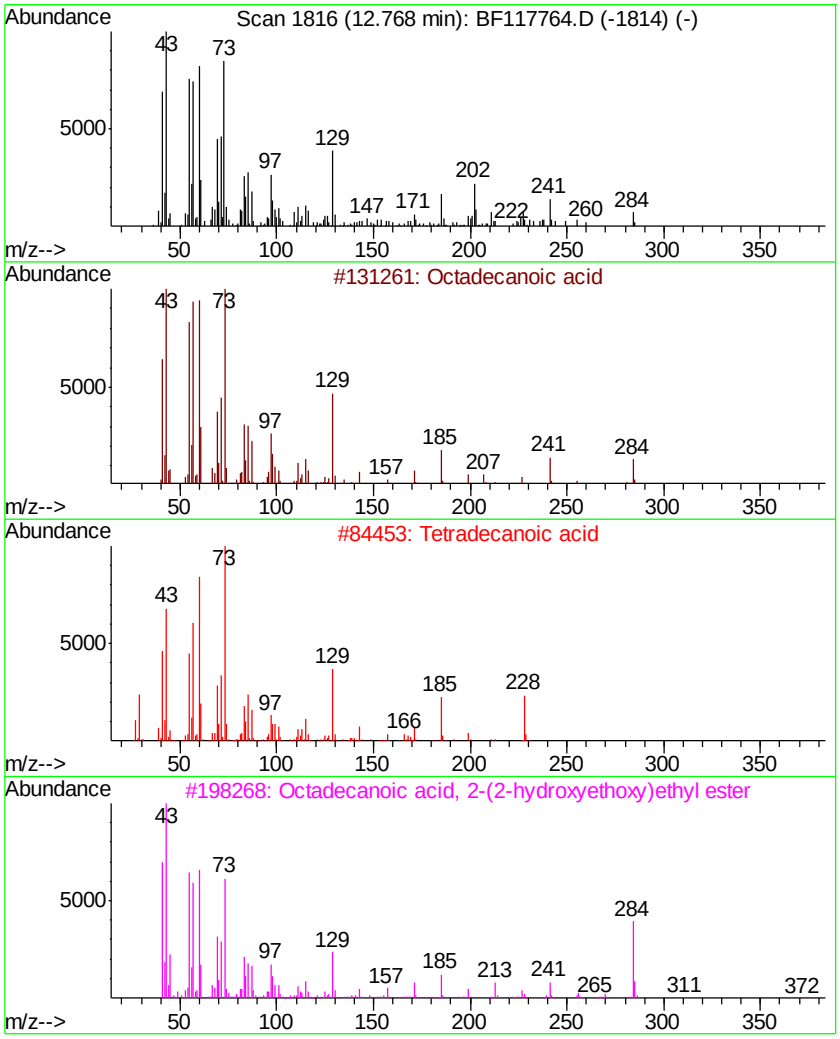
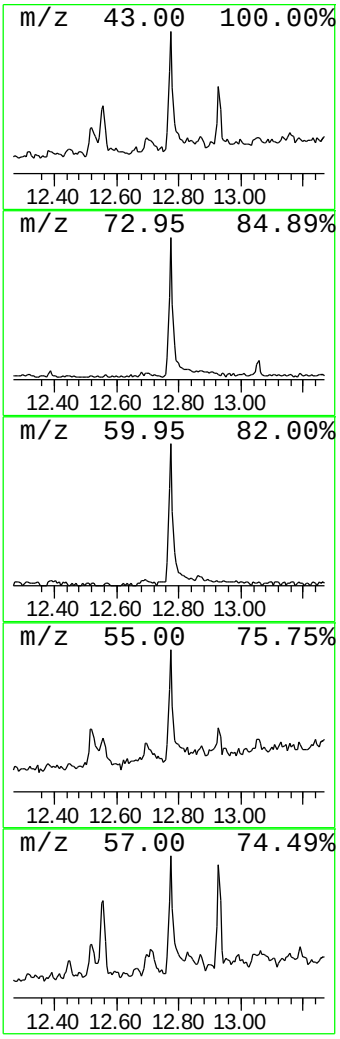
Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	3.54 ng	363045	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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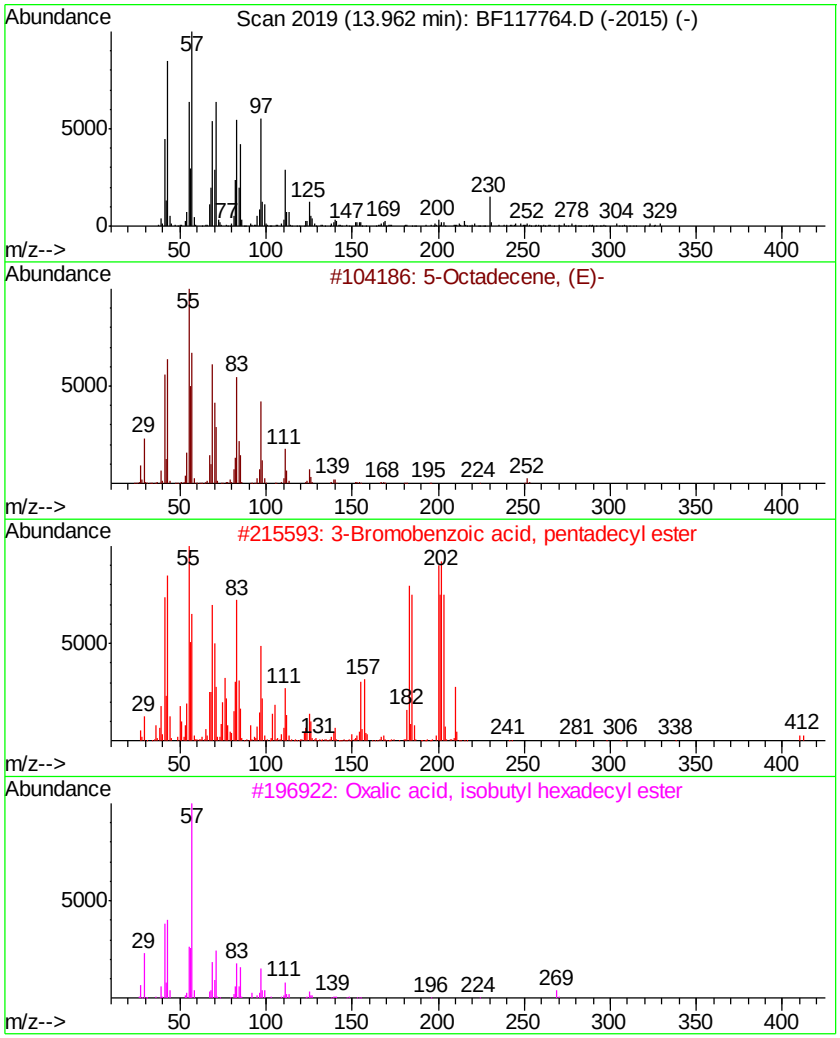
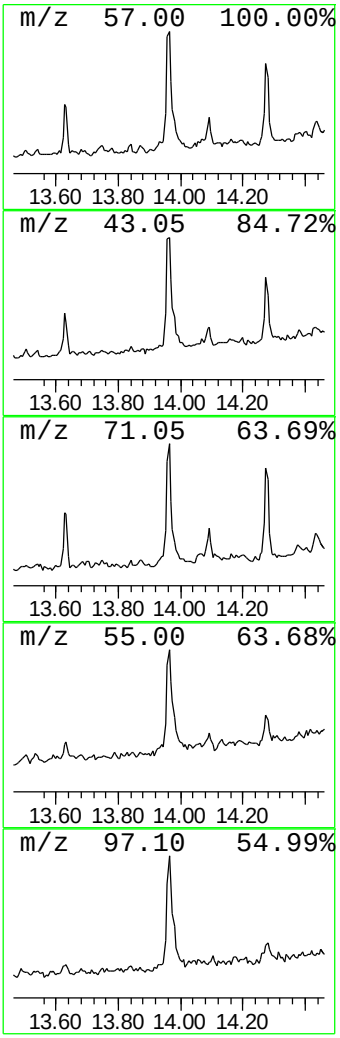
Peak Number 7 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	5.31 ng	599552	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
2	3-Bromobenzoic acid, pentadecyl ...	410	C22H35BrO2	1000281-95-1	93
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-methoxy...	2.22	25.2	ng	2068000	1	6.93	1642680	20.0
2-Pentanone, 4-hy...	5.14	13.2	ng	1087350	1	6.93	1642680	20.0
unknown6.69	6.69	61.9	ng	5084100	1	6.93	1642680	20.0
n-Hexadecanoic acid	11.99	6.4	ng	658365	4	11.46	2053470	20.0
Octadecanoic acid	12.77	3.5	ng	363045	4	11.46	2053470	20.0
5-Octadecene, (E)-	13.96	5.3	ng	599552	5	14.12	2256320	20.0