LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112017\
Data File : BF100752.D
Acq On : 21 Nov 2017 1:14
Operator : SJ/JU
Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	5.098	508	512	522	rBV	114703	139724	7.94%	0.784%
2	5.492	574	579	582	rBV	1588836	1465725	83.30%	8.219%
3	6.498	744	750	759	rBV	1543359	1511925	85.93%	8.478%
4	6.639	770	774	777	rBV	1669906	1545295	87.83%	8.665%
5	6.875	810	814	817	rBB	569623	504716	28.69%	2.830%
6	7.028	836	840	843	rBV	1462352	1230980	69.96%	6.903%
7	7.433	904	909	912	rBV	1036542	922215	52.41%	5.171%
8	8.151	1027	1031	1035	rBV	741467	646019	36.72%	3.623%
9	9.227	1209	1214	1217	rBV	2051021	1759510	100.00%	9.867%
10	9.616	1277	1280	1284	rBV	141819	122226	6.95%	0.685%
11	9.833	1313	1317	1319	rVB	45573	33880	1.93%	0.190%
12	9.910	1326	1330	1333	rBV	758024	645174	36.67%	3.618%
13	9.939	1333	1335	1338	rVB	27416	20265	1.15%	0.114%
14	10.110	1359	1364	1368	rVB3	15618	21132	1.20%	0.118%
15	10.333	1399	1402	1404	rVB	58893	47071	2.68%	0.264%
16	10.457	1419	1423	1426	rVB	28716	28562	1.62%	0.160%
17	10.698	1460	1464	1467	rBV	861087	770846	43.81%	4.323%
18	10.804	1479	1482	1491	rVB	59016	62860	3.57%	0.352%
19	11.251	1553	1558	1560	rBV2	34720	31296	1.78%	0.175%
20	11.286	1560	1564	1570	rVB2	15736	23021	1.31%	0.129%
21	11.392	1579	1582	1585	rBV	584253	557694	31.70%	3.127%
22	11.416	1585	1586	1590	rVV	207405	141456	8.04%	0.793%
23	11.468	1592	1595	1598	rVB	69000	53843	3.06%	0.302%
24	11.610	1614	1619	1624	rBV3	26450	34488	1.96%	0.193%
25	11.780	1644	1648	1651	rBV	31598	24883	1.41%	0.140%
26	11.898	1665	1668	1669	rBV	24054	25588	1.45%	0.143%
27	11.921	1669	1672	1675	rVB2	42705	51004	2.90%	0.286%
28	12.010	1683	1687	1689	rBV2	44587	47173	2.68%	0.265%
29	12.439	1756	1760	1762	rBV2	25470	35562	2.02%	0.199%
30	12.463	1762	1764	1766	rVV	108101	97020	5.51%	0.544%
31	12.486	1766	1768	1773	rVB3	91457	78619	4.47%	0.441%
32	12.610	1785	1789	1792	rBV	340791	303167	17.23%	1.700%
33	12.774	1812	1817	1822	rVB	252053	229851	13.06%	1.289%
34	12.839	1822	1828	1833	rBV	290786	332022	18.87%	1.862%

LSC Area Percent Report

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Data File : BF100752.D
Acq On : 21 Nov 2017 1:14
Operator : SJ/JU
Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.886	1833	1836	1841	rVB2	16054	22640	1.29%	0.127%
36	12.980	1844	1852	1855	rBV	1381853	1253845	71.26%	7.031%
37	13.057	1859	1865	1869	rBV3	21953	39293	2.23%	0.220%
38	13.162	1880	1883	1887	rVB	40944	39421	2.24%	0.221%
39	13.268	1897	1901	1903	rBV2	33357	33163	1.88%	0.186%
40	13.668	1966	1969	1975	rVB	35769	34964	1.99%	0.196%
41	13.780	1981	1988	1991	rBV3	31300	50767	2.89%	0.285%
42	13.809	1991	1993	1995	rVB	27343	20897	1.19%	0.117%
43	13.833	1995	1997	1999	rBV	26137	28652	1.63%	0.161%
44	13.862	1999	2002	2009	rVB2	145273	176330	10.02%	0.989%
45	14.033	2023	2031	2034	rBV2	667658	792451	45.04%	4.444%
46	14.057	2034	2035	2043	rVB	173023	130910	7.44%	0.734%
47	14.251	2065	2068	2072	rBV4	15560	21881	1.24%	0.123%
48	14.292	2072	2075	2080	rVB7	14113	21122	1.20%	0.118%
49	14.415	2093	2096	2099	rVB	31033	30649	1.74%	0.172%
50	14.451	2100	2102	2106	rBV	21877	22491	1.28%	0.126%
51	14.504	2106	2111	2114	rBV6	25344	48971	2.78%	0.275%
52	14.545	2115	2118	2120	rBV3	18948	20353	1.16%	0.114%
53	14.651	2133	2136	2140	rBV	278958	233106	13.25%	1.307%
54	14.874	2171	2174	2177	rBV	41969	41622	2.37%	0.233%
55	15.074	2204	2208	2211	rBV	129949	196358	11.16%	1.101%
56	15.180	2224	2226	2230	rVB	25704	25322	1.44%	0.142%
57	15.380	2257	2260	2266	rVB	76342	121977	6.93%	0.684%
58	15.445	2266	2271	2276	rBV	95439	144168	8.19%	0.808%
59	15.509	2277	2282	2293	rVB	355153	512903	29.15%	2.876%
60	16.986	2529	2533	2539	rVB3	31681	57823	3.29%	0.324%
61	17.433	2605	2609	2618	rVB	30440	63806	3.63%	0.358%
62	17.592	2629	2636	2643	rBV3	41017	102361	5.82%	0.574%

Sum of corrected areas: 17833058

LSC Report - Integrated Chromatogram

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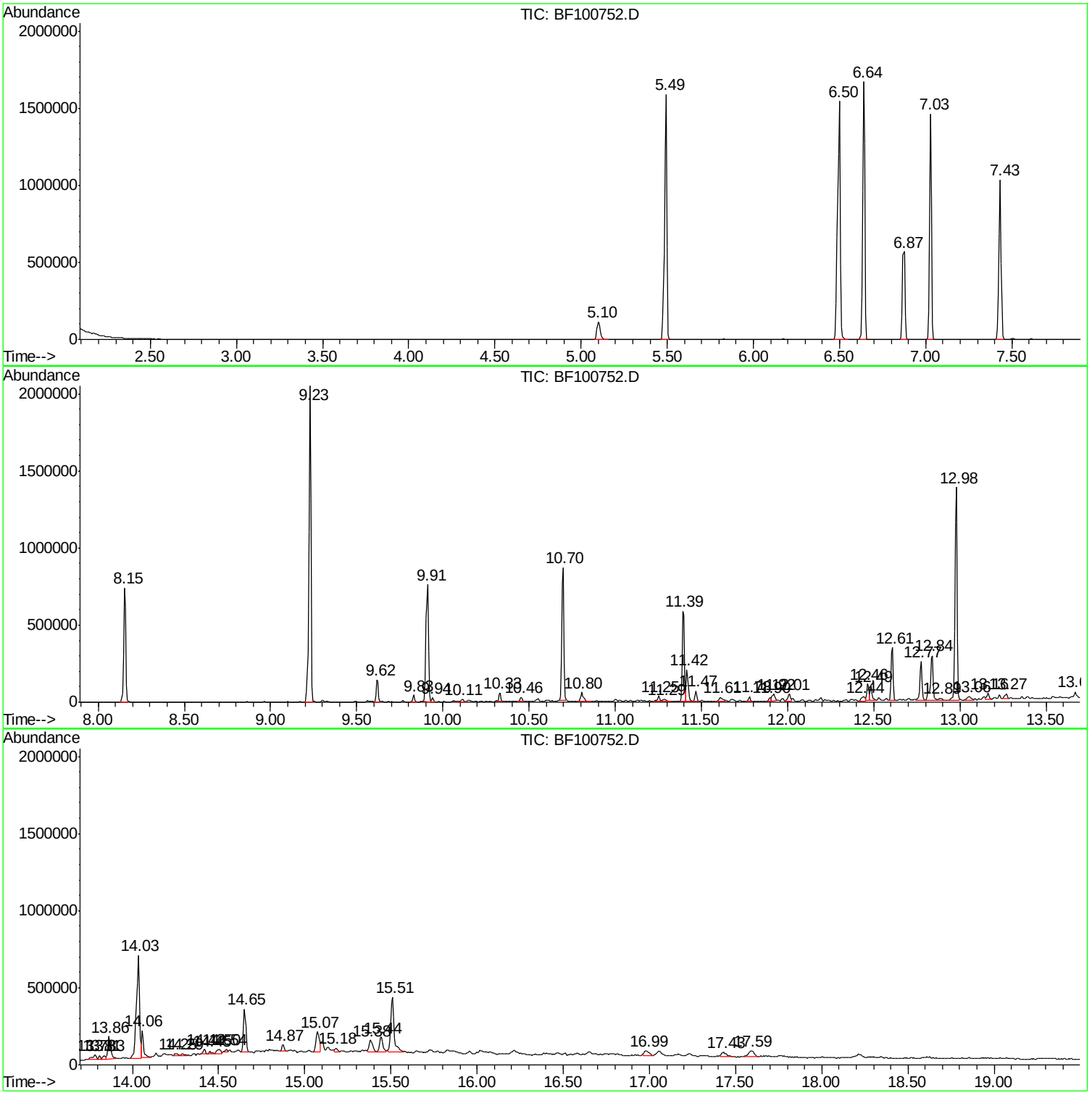
Operator : SJ/JU
Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112017\
Data File : BF100752.D
Acq On : 21 Nov 2017 1:14
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Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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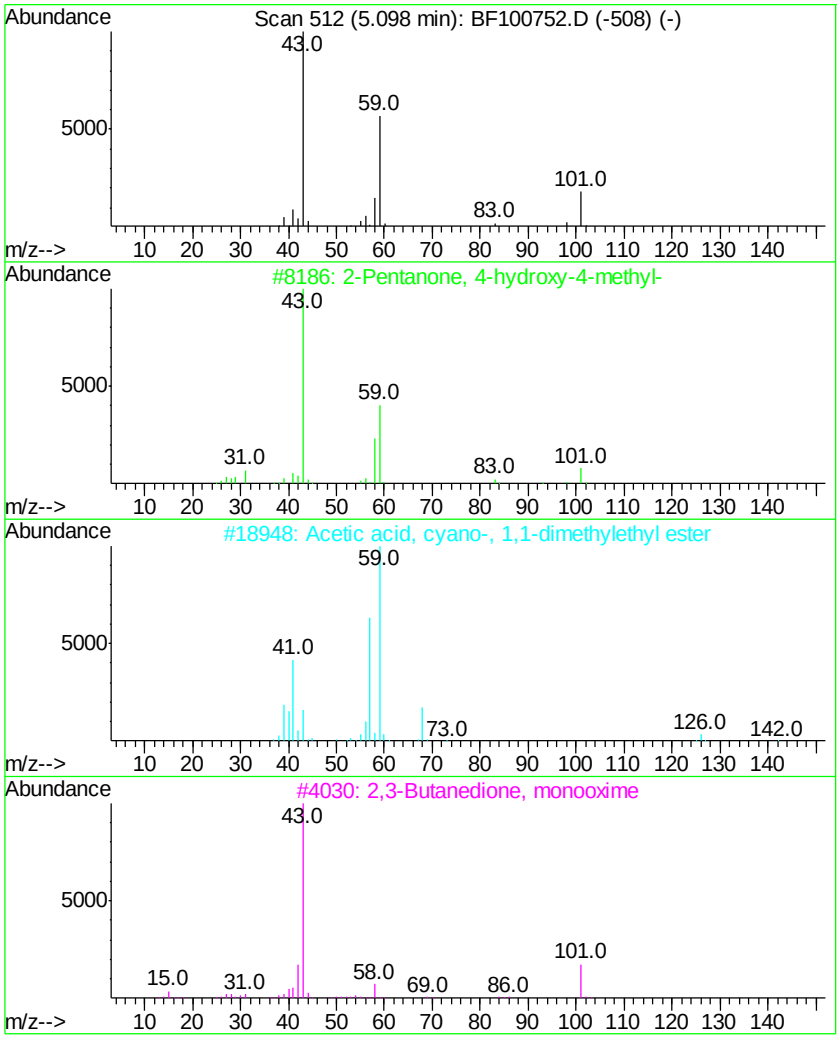
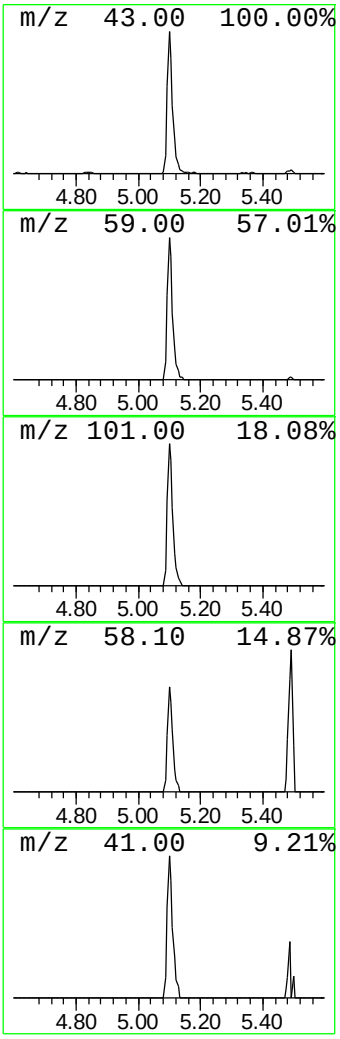
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	5.54 ng	139724	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Acq On : 21 Nov 2017 1:14
Operator : SJ/JU
Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

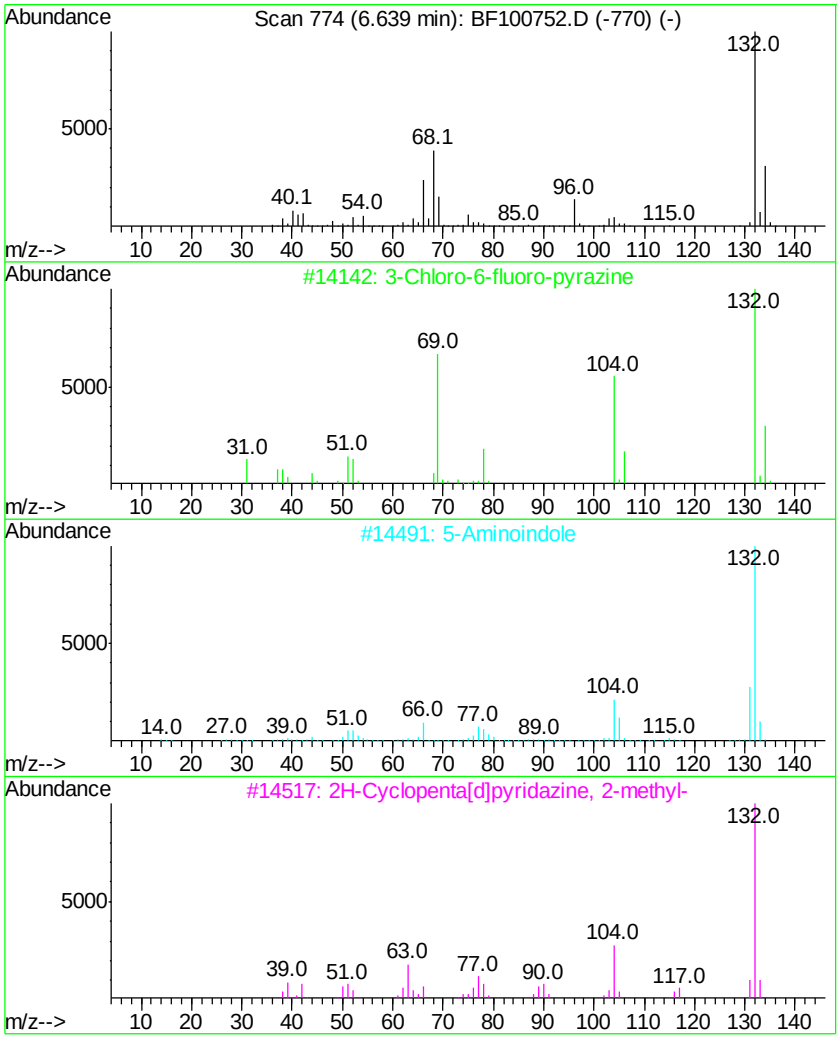
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

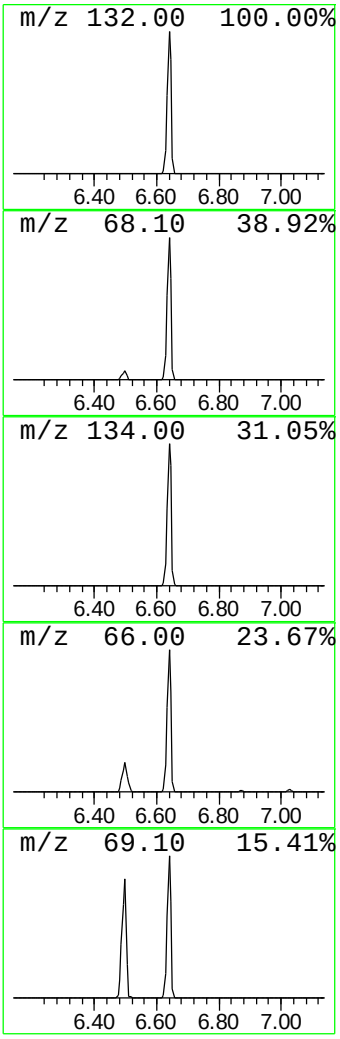
****

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	61.23 ng	1545300	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Sample : I6300-05
Misc :
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Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
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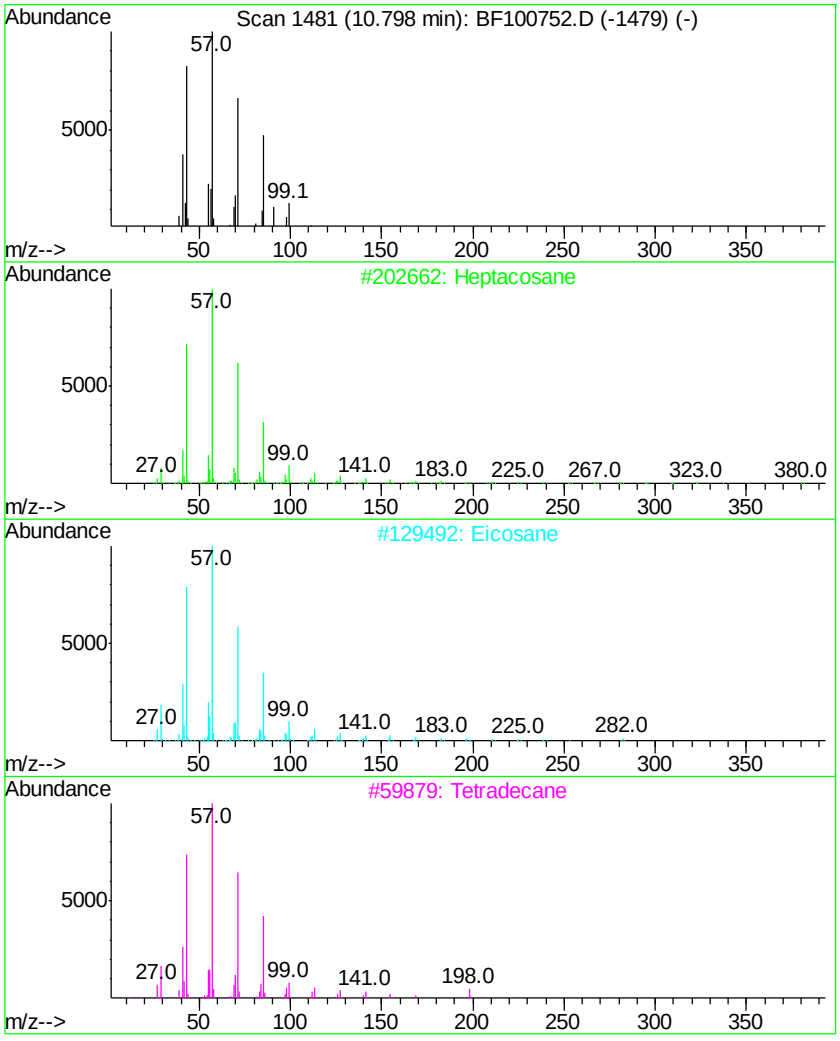
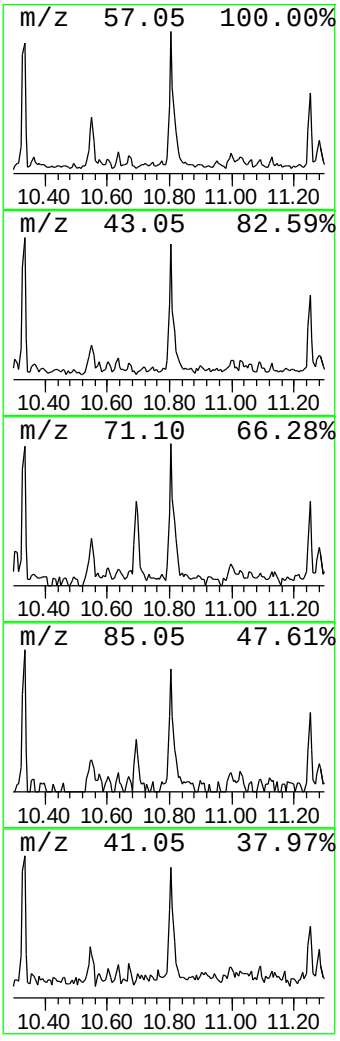
****

Peak Number 4 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.25 ng	62860	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	86
2	Eicosane	282	C20H42	000112-95-8	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	86
5	Hexadecane	226	C16H34	000544-76-3	86





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Acq On : 21 Nov 2017 1:14
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Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

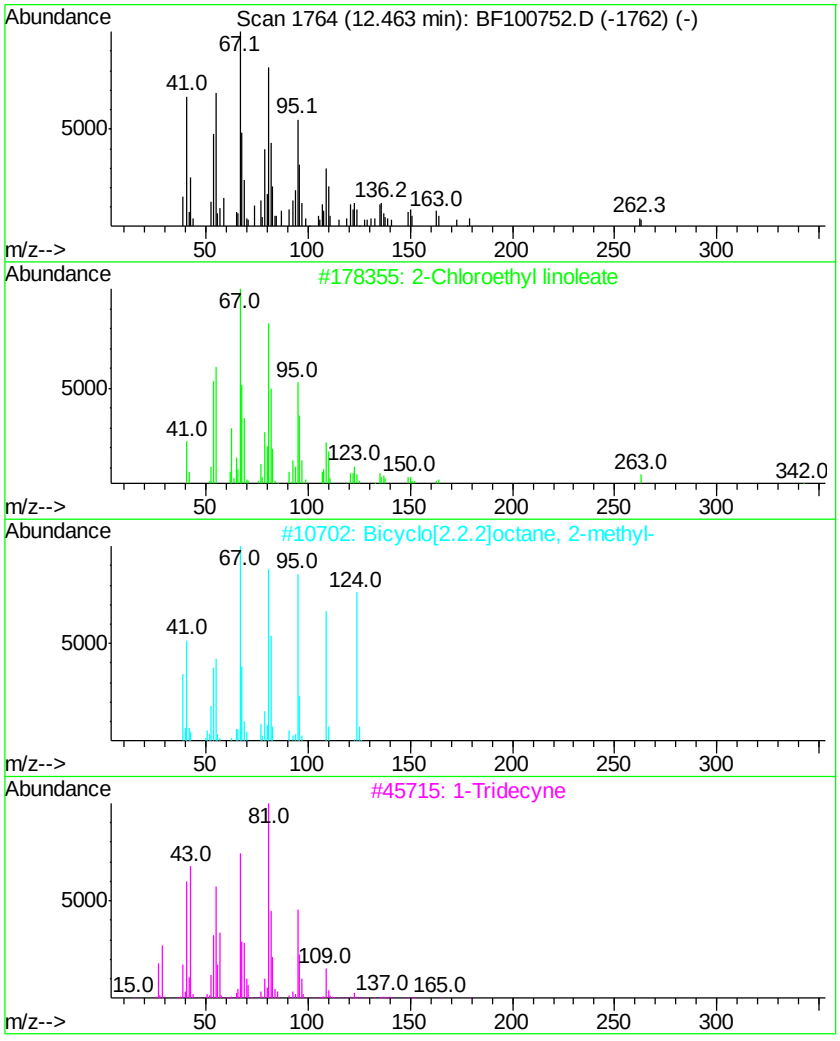
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

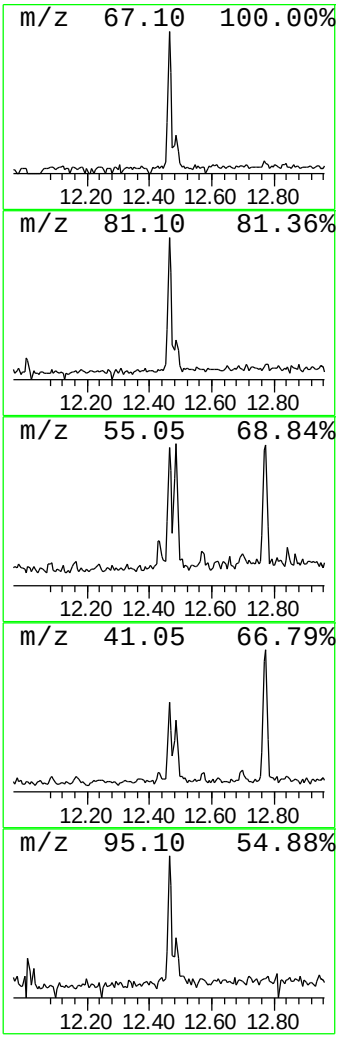
****

Peak Number 5 2-Chloroethyl linoleate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	3.48 ng	97020	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	87
2	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	87
3	1-Tridecyne	180	C13H24	026186-02-7	72
4	11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	70
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	70





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Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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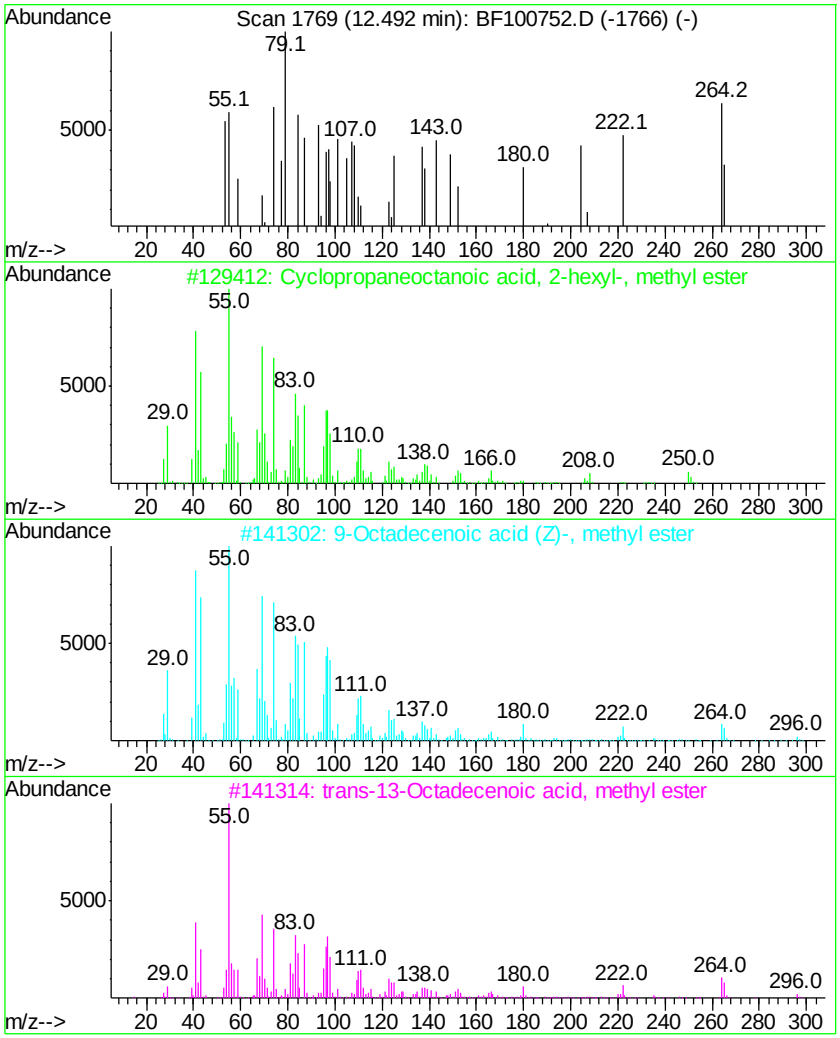
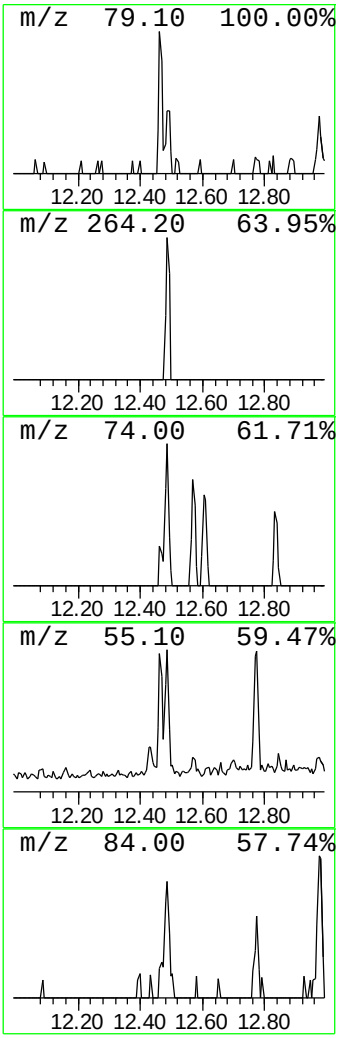
Peak Number 6 Cyclopropaneoctanoic acid, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	2.82 ng	78619	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	76
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	76
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	72
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	72
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	64





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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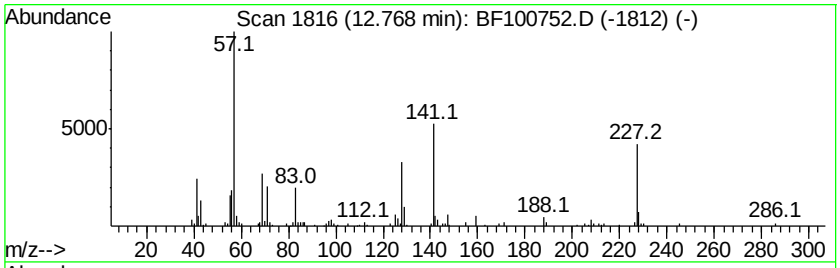
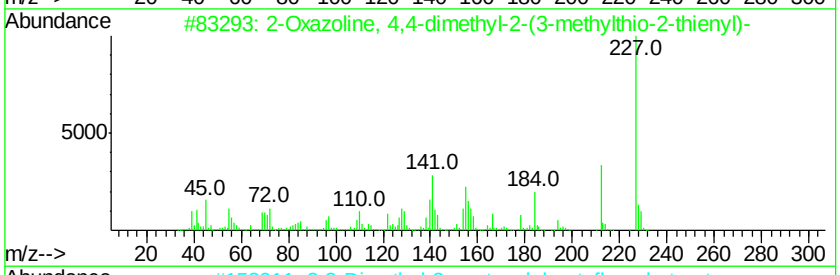
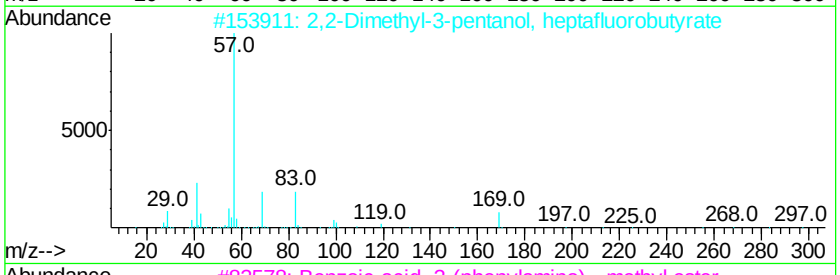
Peak Number 7 unknown12.77 Concentration Rank 4

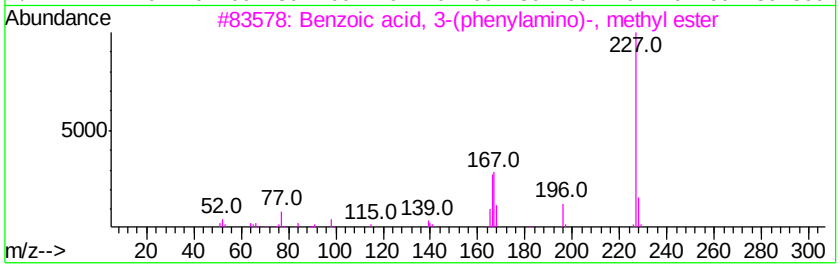
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	5.80 ng	229851	Chrysene-d12	14.03

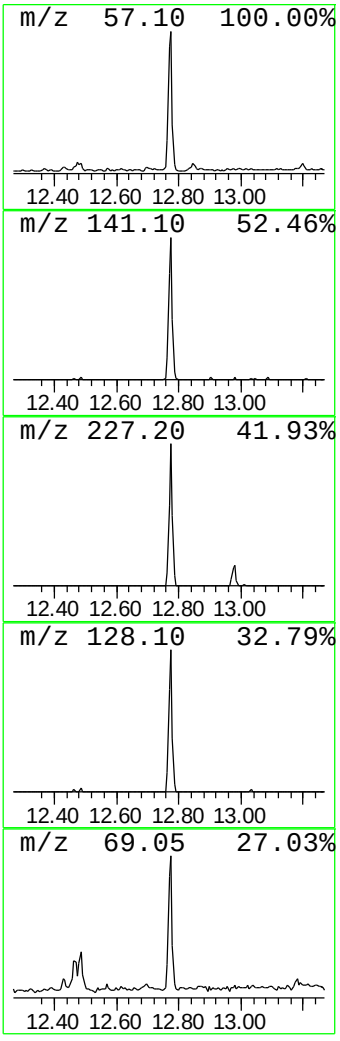
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Oxazoline, 4,4-dimethyl-2-(3-m...	227	C10H13NOS2	256425-32-8	22
2	2,2-Dimethyl-3-pentanol, heptafl...	312	C11H15F7O2	1000364-14-4	10
3	Benzoic acid, 3-(phenylamino)-, ...	227	C14H13NO2	055622-43-0	10
4	2,4-Difluorobenzoic acid, 4-dode...	326	C19H28F2O2	1000338-56-4	10
5	3-Methyl-thiophene-2-carboxamide	141	C6H7NOS	076655-99-7	10











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Data File : BF100752.D
Acq On : 21 Nov 2017 1:14
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Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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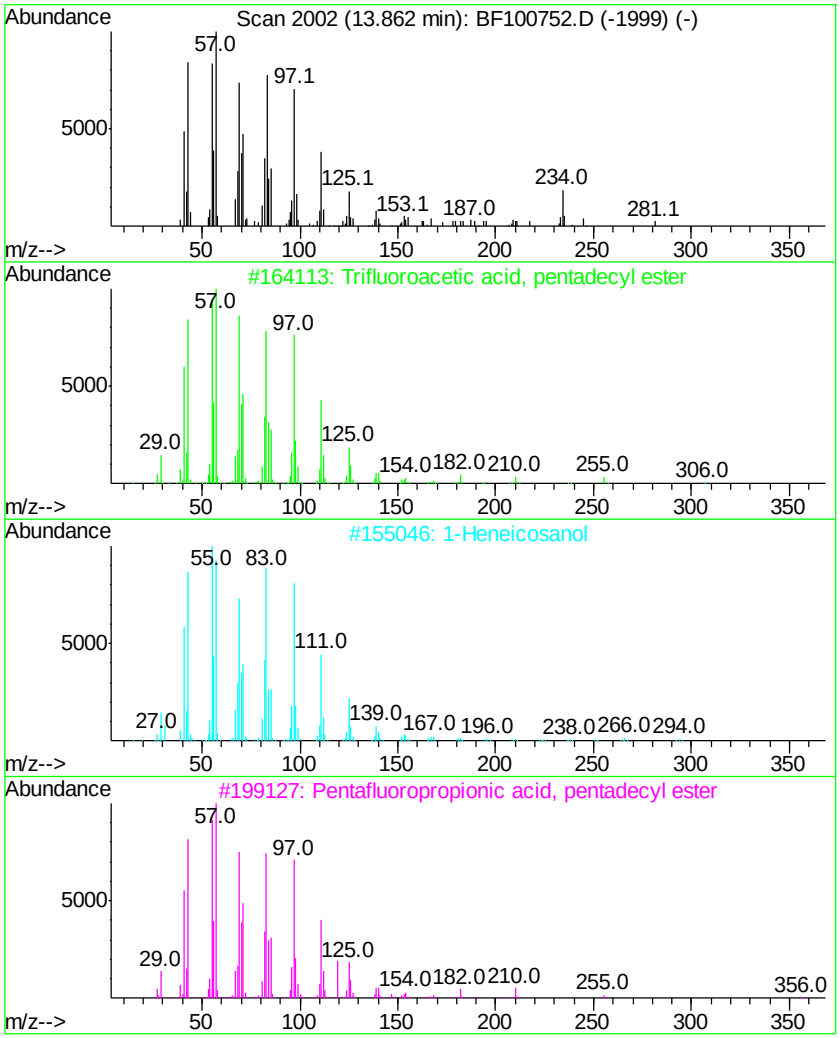
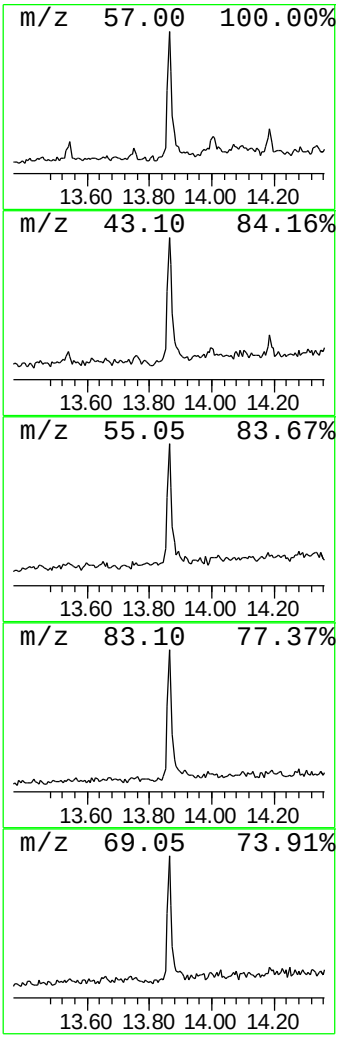
Peak Number 8 Trifluoroacetic acid, penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.45 ng	176330	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112017\
Data File : BF100752.D
Acq On : 21 Nov 2017 1:14
Operator : SJ/JU
Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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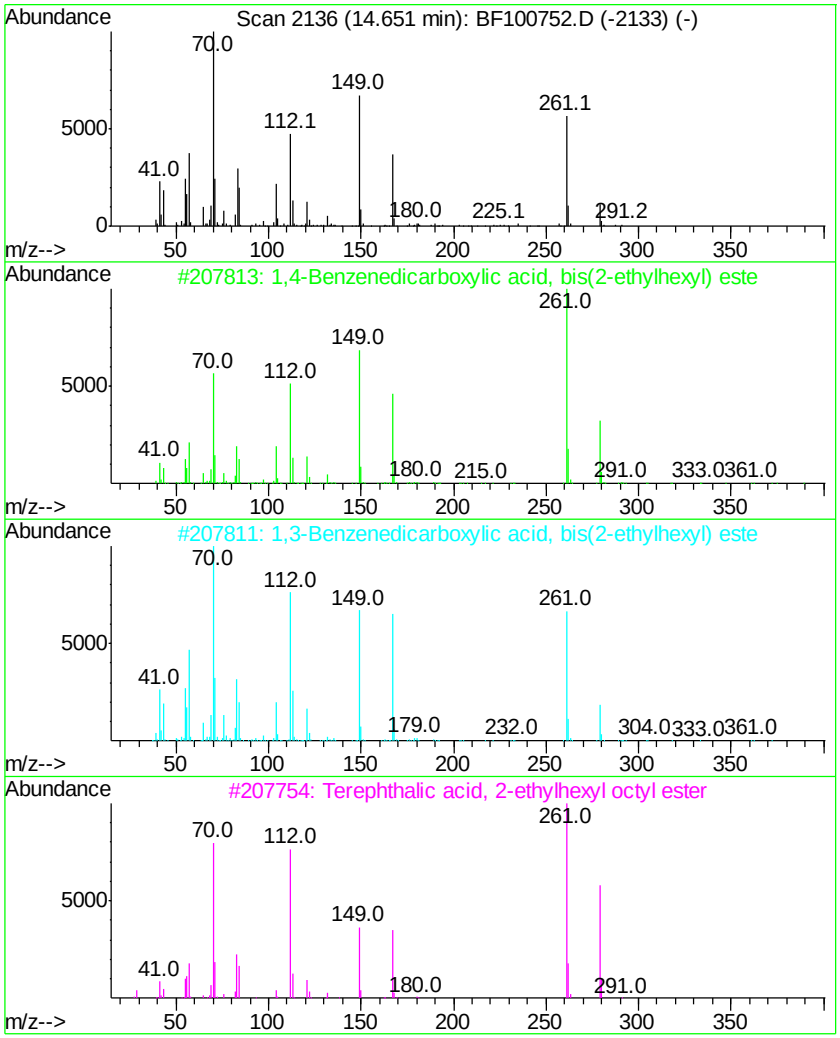
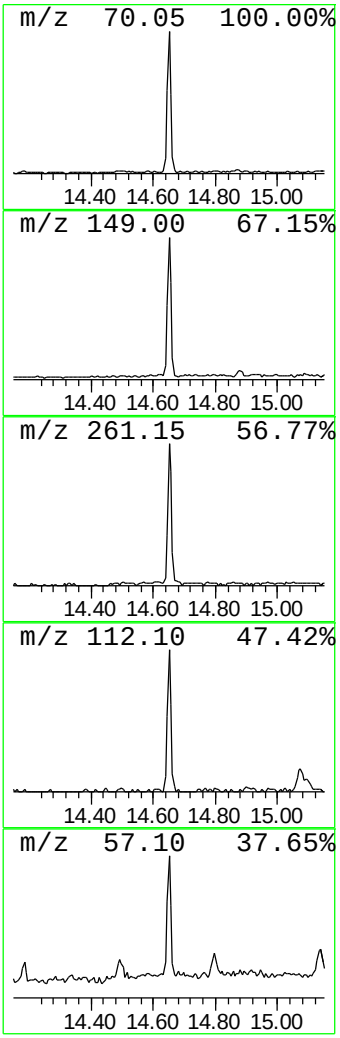
Peak Number 9 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	5.88 ng	233106	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
3	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	53
4	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	49
5	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43





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Data File : BF100752.D
Acq On : 21 Nov 2017 1:14
Operator : SJ/JU
Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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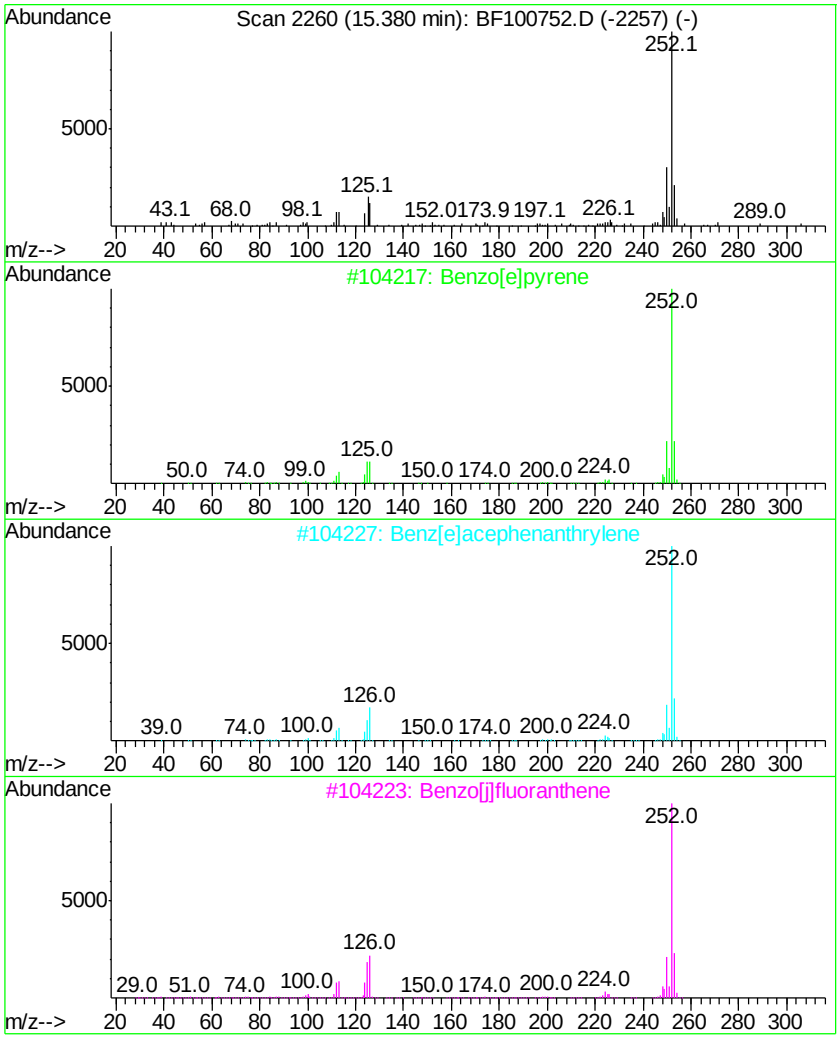
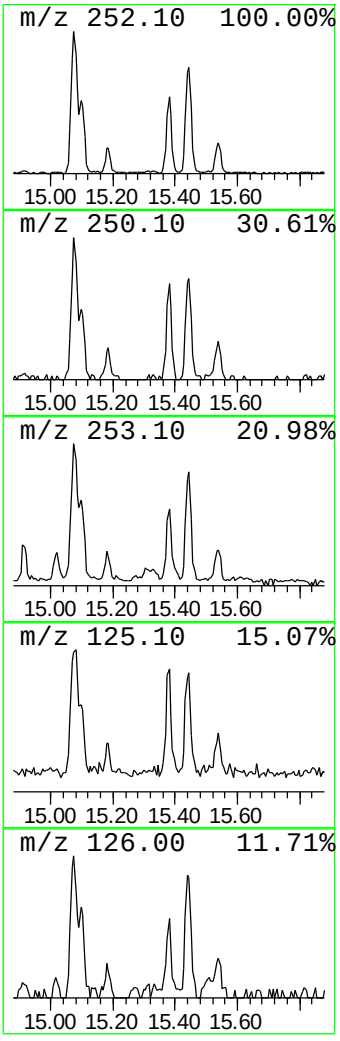
Peak Number 10 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.38	4.76 ng	121977	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Perylene	252	C20H12	000198-55-0	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112017\
Data File : BF100752.D
Acq On : 21 Nov 2017 1:14
Operator : SJ/JU
Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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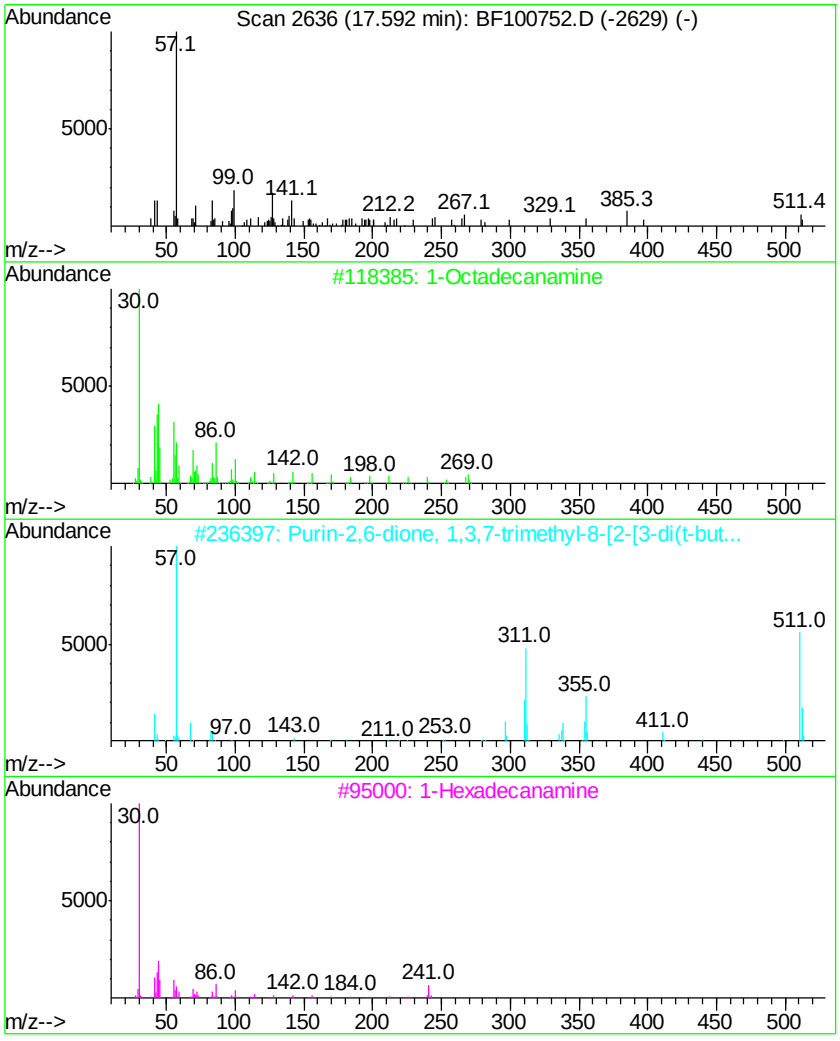
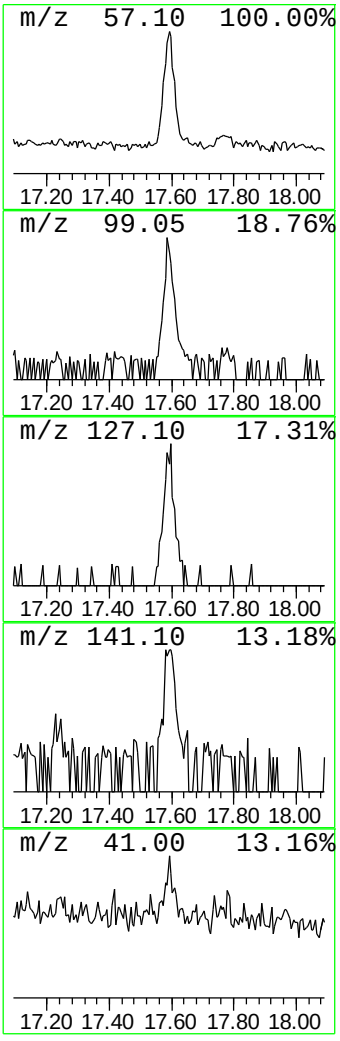
Peak Number 11 unknown17.59 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.59	3.99 ng	102361	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanamine	269	C18H39N	000124-30-1	9
2	Purin-2,6-dione, 1,3,7-trimethyl...	511	C26H33N5O6	1000128-16-7	5
3	1-Hexadecanamine	241	C16H35N	000143-27-1	4
4	1-Tetradecanamine	213	C14H31N	002016-42-4	2
5	1,3-Dioxolane, 2,2-dimethyl-4-[[...	412	C25H48O4	056256-32-7	1





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112017\
Data File : BF100752.D
Acq On : 21 Nov 2017 1:14
Operator : SJ/JU
Sample : I6300-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-111717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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
2-Pentanone, 4-hy...	5.10	5.5	ng	139724	1	6.87	504716	20.0
unknown6.64	6.64	61.2	ng	1545300	1	6.87	504716	20.0
Heptacosane	10.80	2.3	ng	62860	4	11.39	557694	20.0
2-Chloroethyl lin...	12.46	3.5	ng	97020	4	11.39	557694	20.0
Cyclopropaneoctan...	12.49	2.8	ng	78619	4	11.39	557694	20.0
unknown12.77	12.77	5.8	ng	229851	5	14.03	792451	20.0
Trifluoroacetic a...	13.86	4.5	ng	176330	5	14.03	792451	20.0
1,4-Benzenedicarb...	14.65	5.9	ng	233106	5	14.03	792451	20.0
Benzo[e]pyrene	15.38	4.8	ng	121977	6	15.51	512903	20.0
unknown17.59	17.59	4.0	ng	102361	6	15.51	512903	20.0